



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:40 AM UTC

PDB ID : 4AAS / pdb_00004aas
EMDB ID : EMD-2000
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 : 2011-12-05
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:

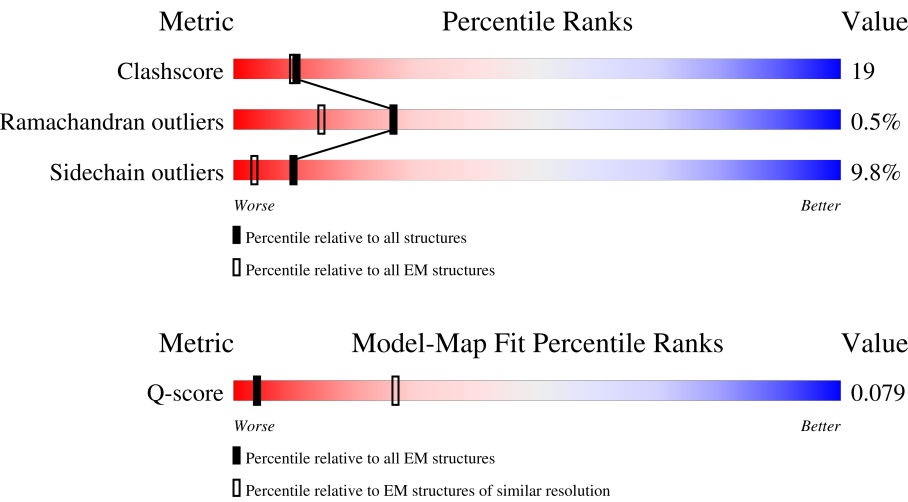
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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.



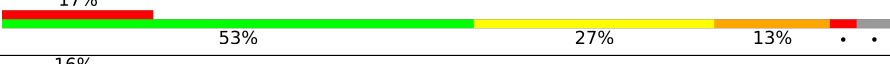
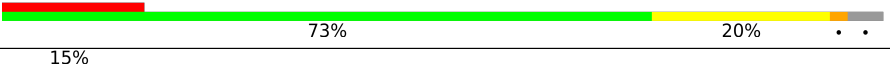
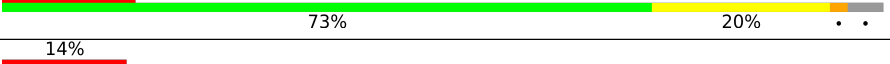
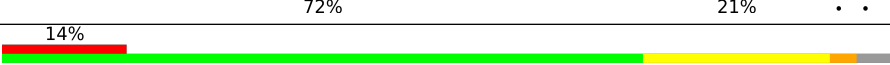
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	328 (8.00 - 9.00)

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	
1	B	548	
1	C	548	
1	D	548	

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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 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 54062 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:

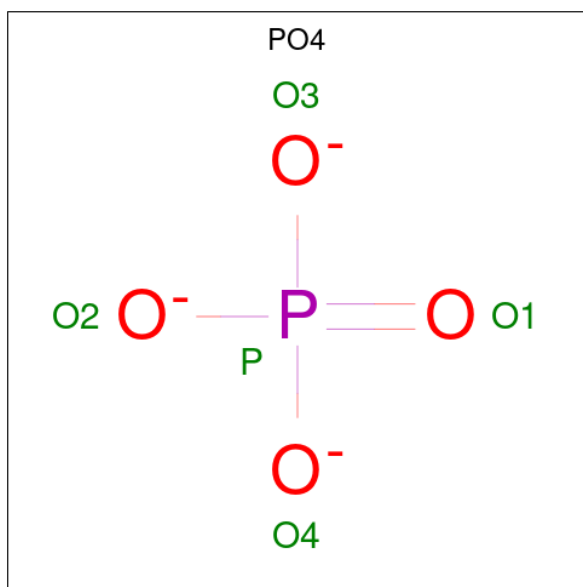
Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	engineered mutation	UNP P0A6F5
B	398	ALA	ASP	engineered mutation	UNP P0A6F5

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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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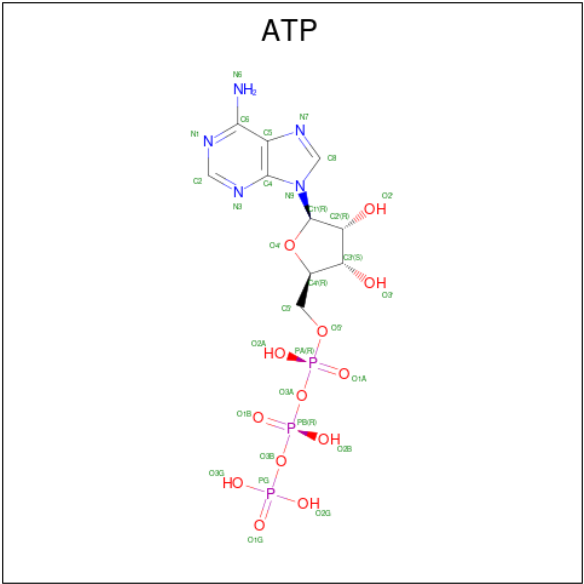
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Mol	Chain	Residues	Atoms		AltConf
2	F	1	Total	P	0
			1	1	
2	G	1	Total	P	0
			1	1	

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

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

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

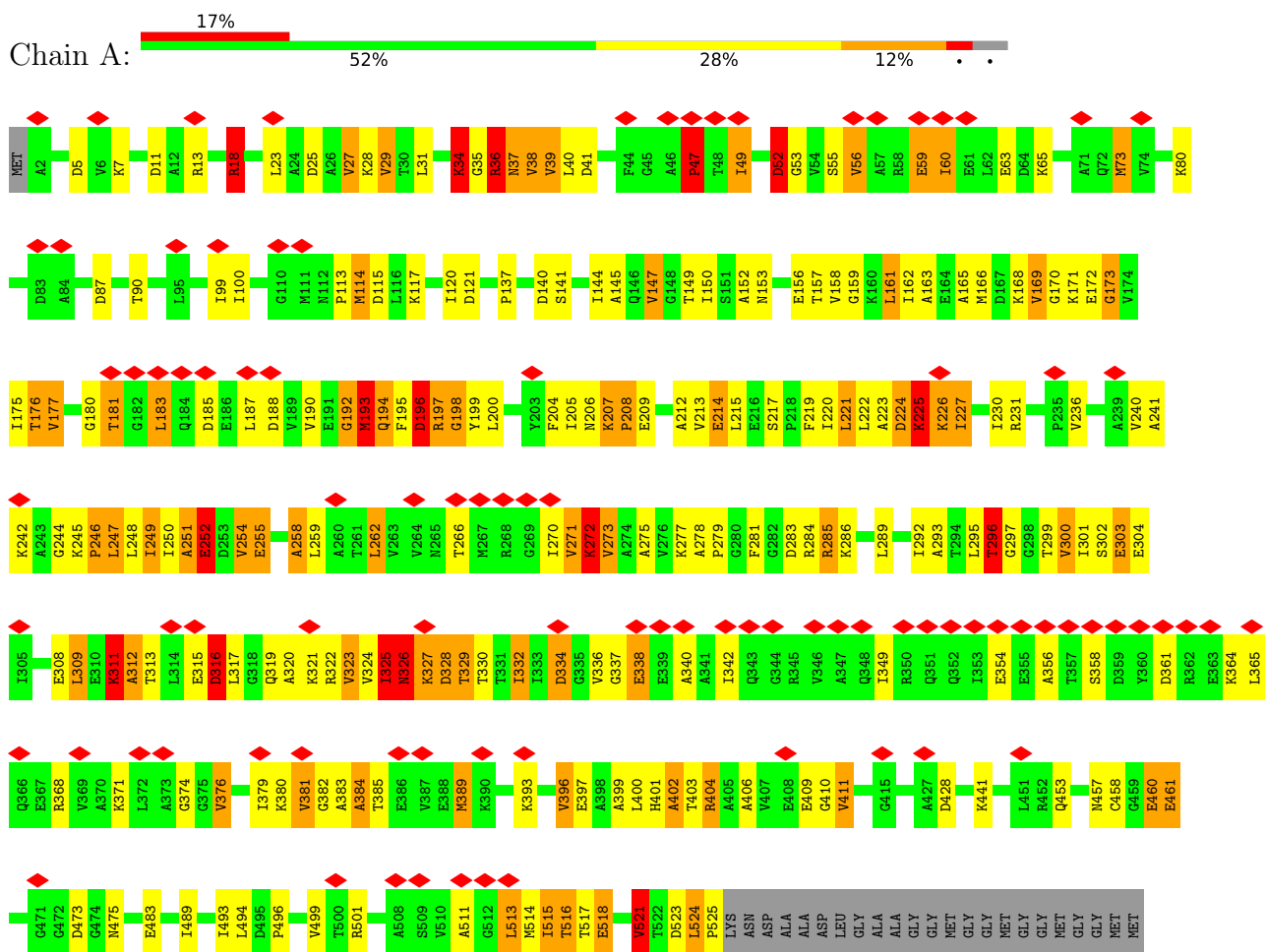


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0
4	E	1	Total 31	C 10	N 5	O 13	P 3	0
4	F	1	Total 31	C 10	N 5	O 13	P 3	0
4	G	1	Total 31	C 10	N 5	O 13	P 3	0

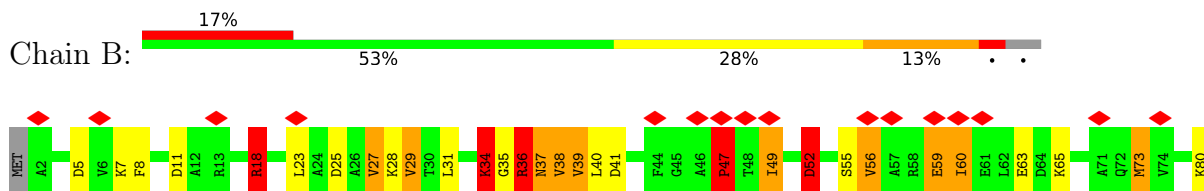
3 Residue-property plots

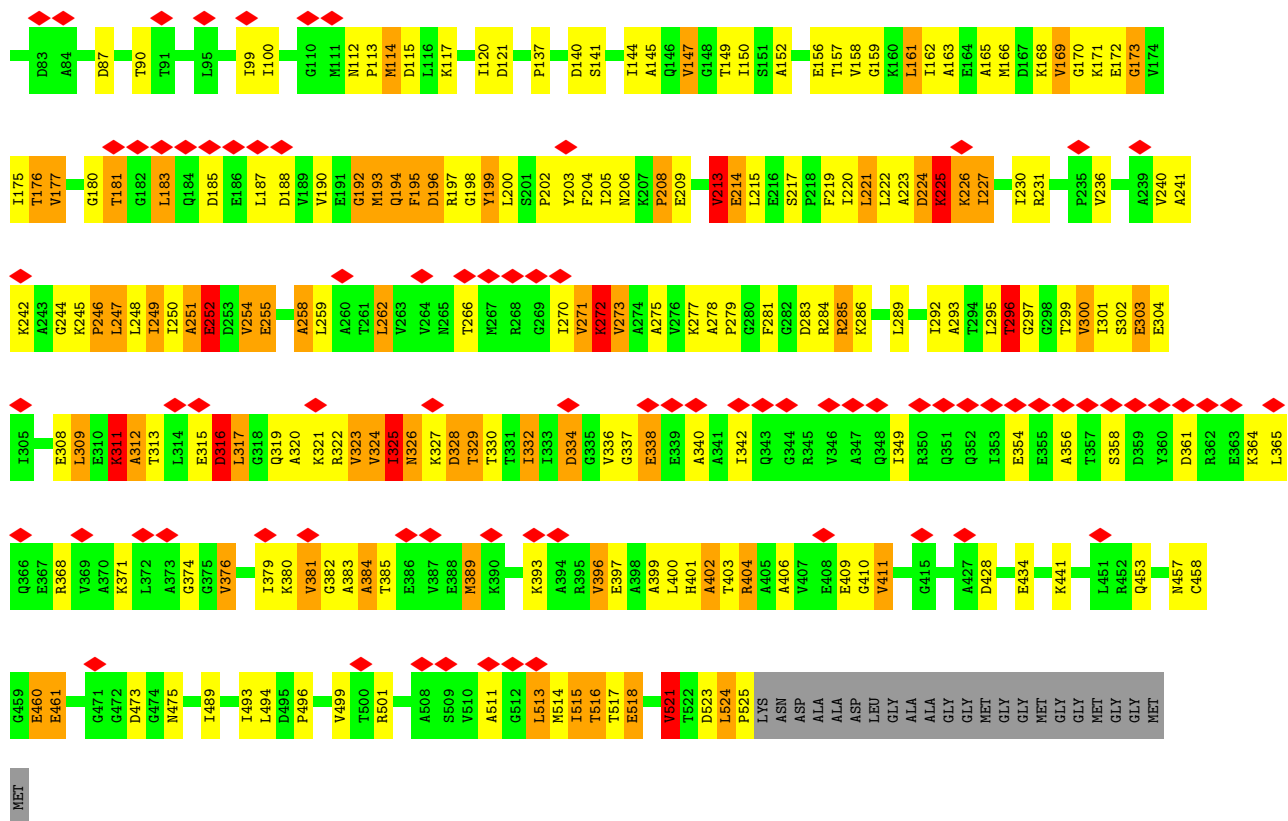
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 60 KDA CHAPERONIN

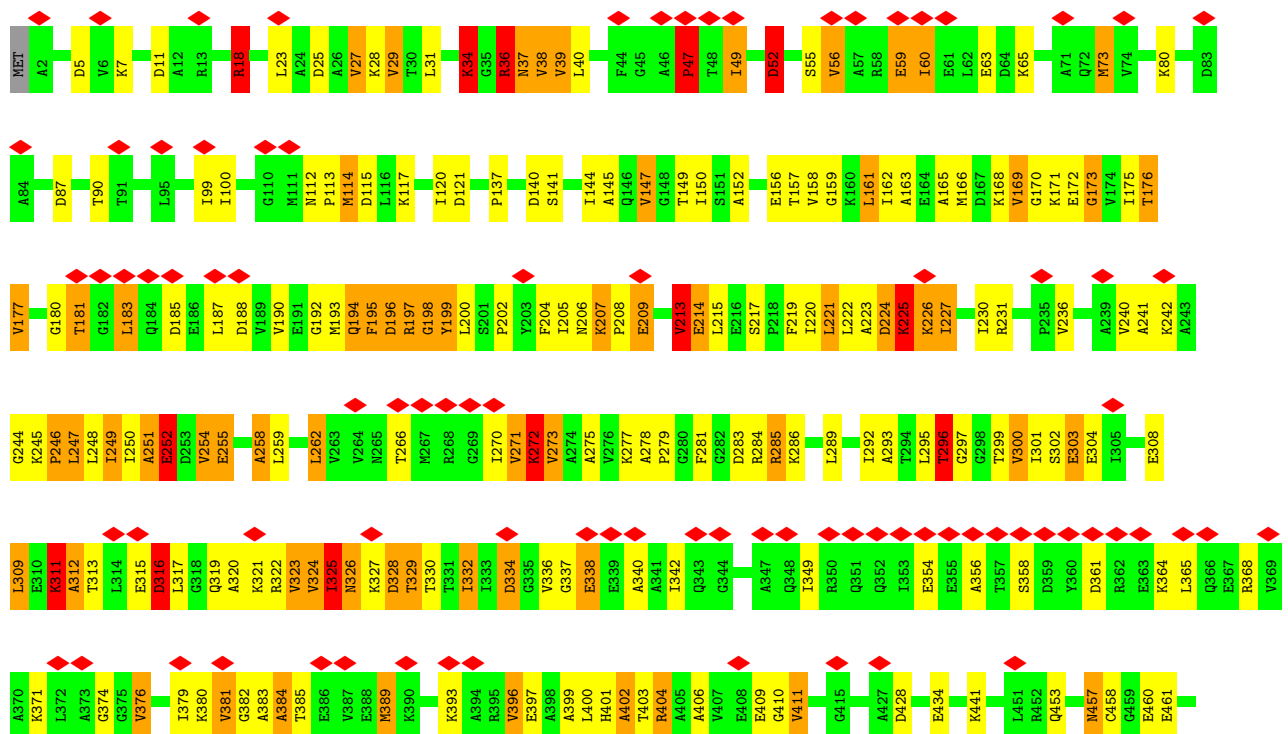


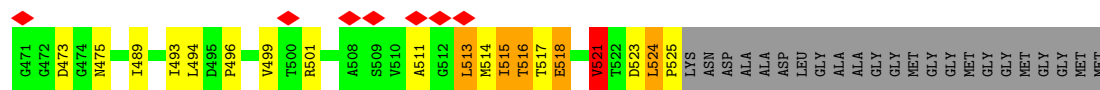
• Molecule 1: 60 KDA CHAPERONIN



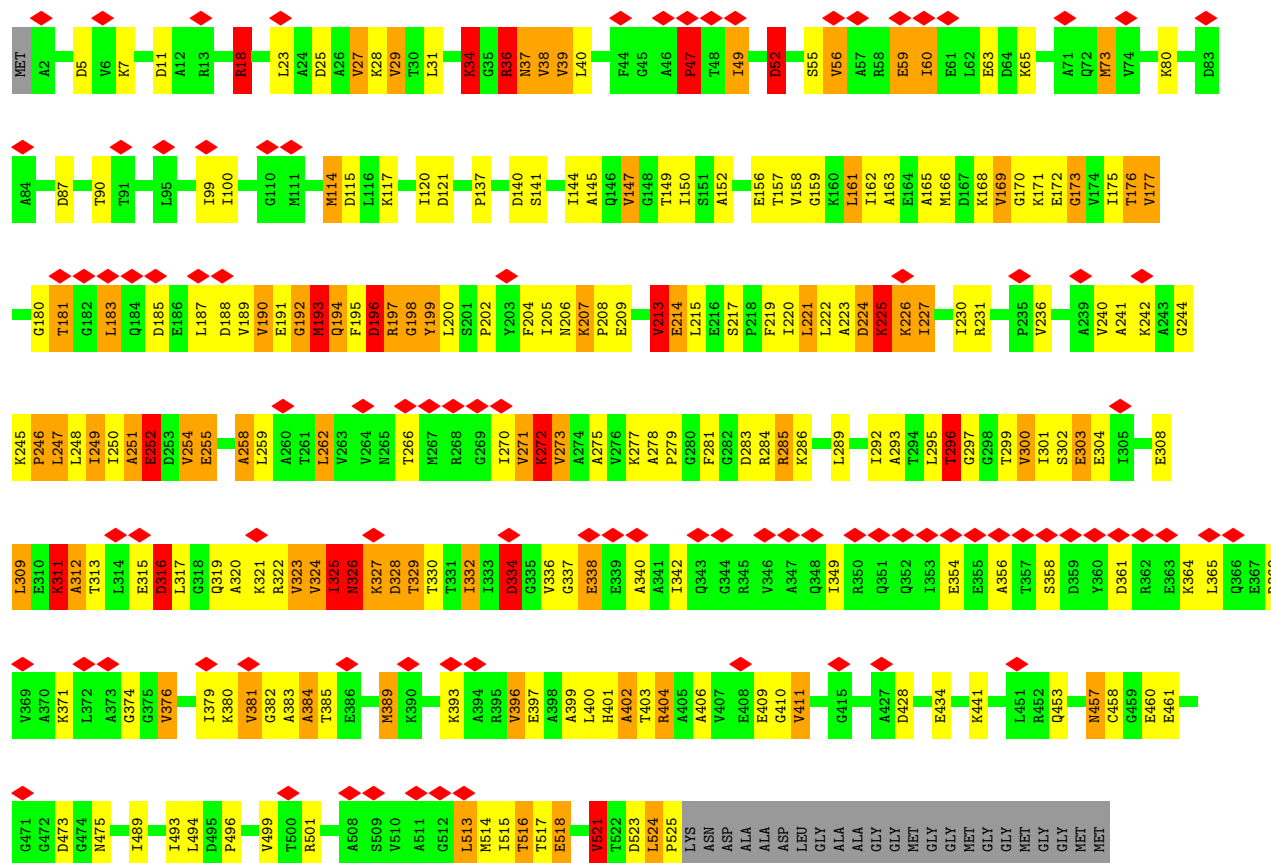


• Molecule 1: 60 KDA CHAPERONIN

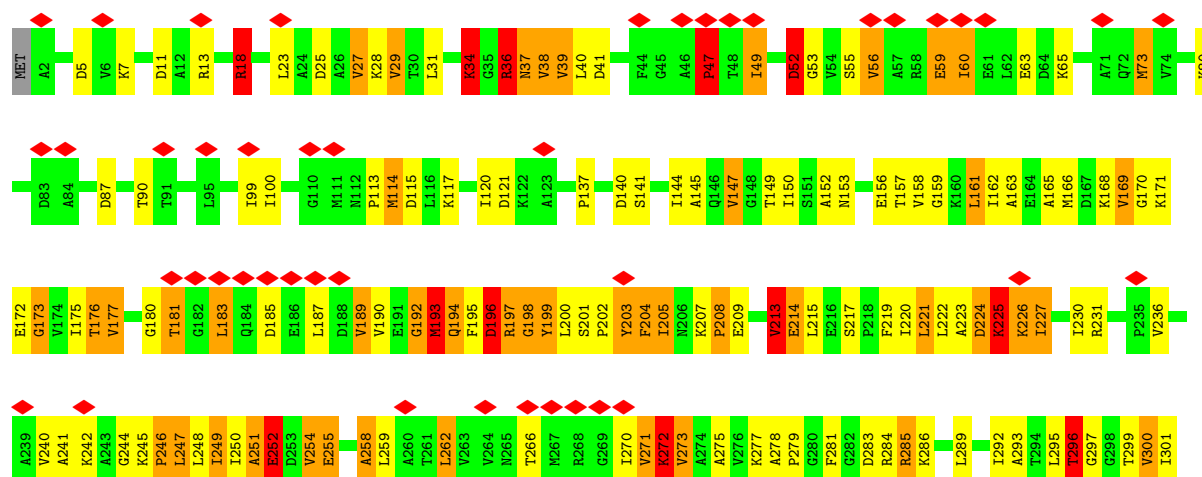


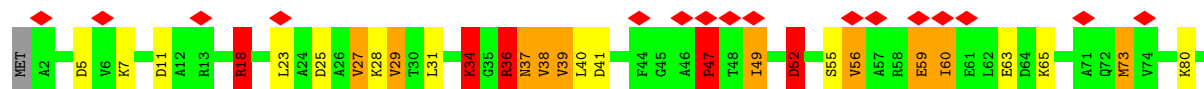


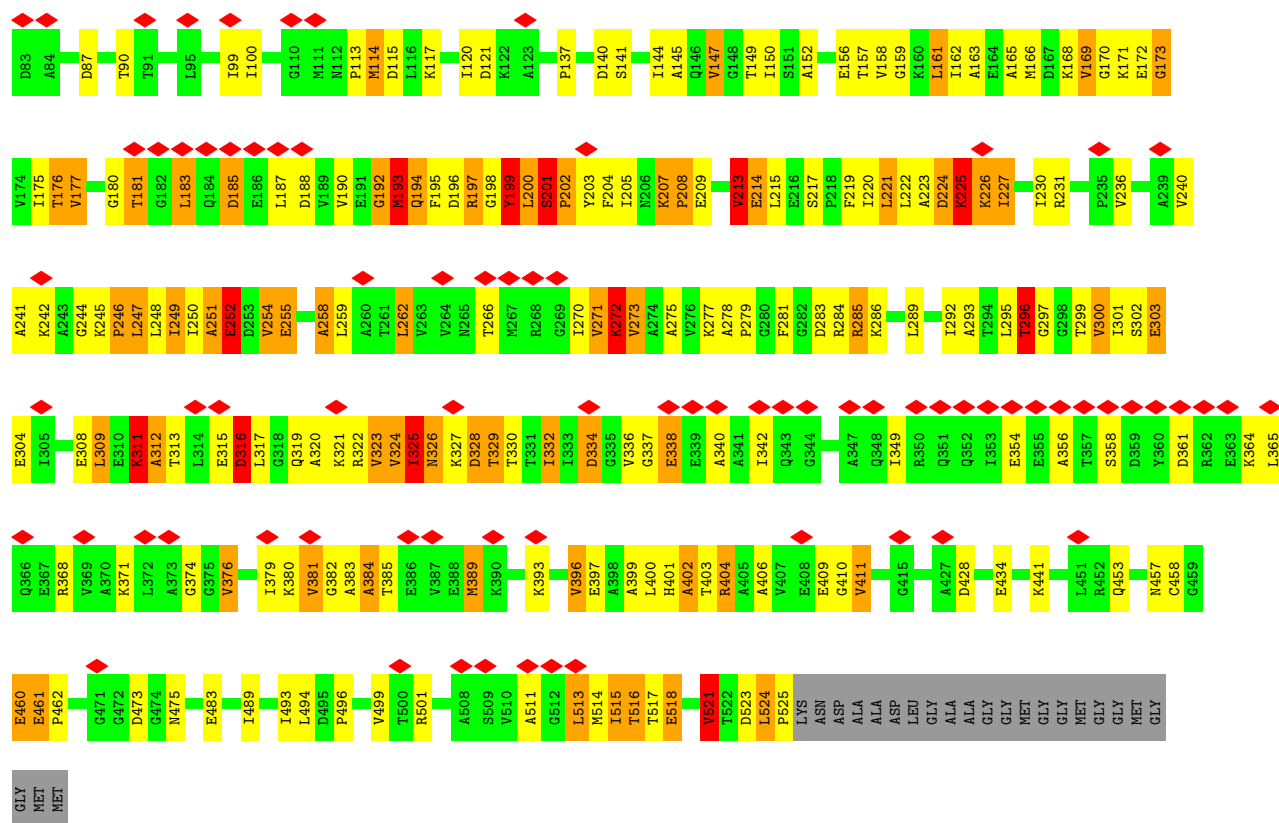
• Molecule 1: 60 KDA CHAPERONIN



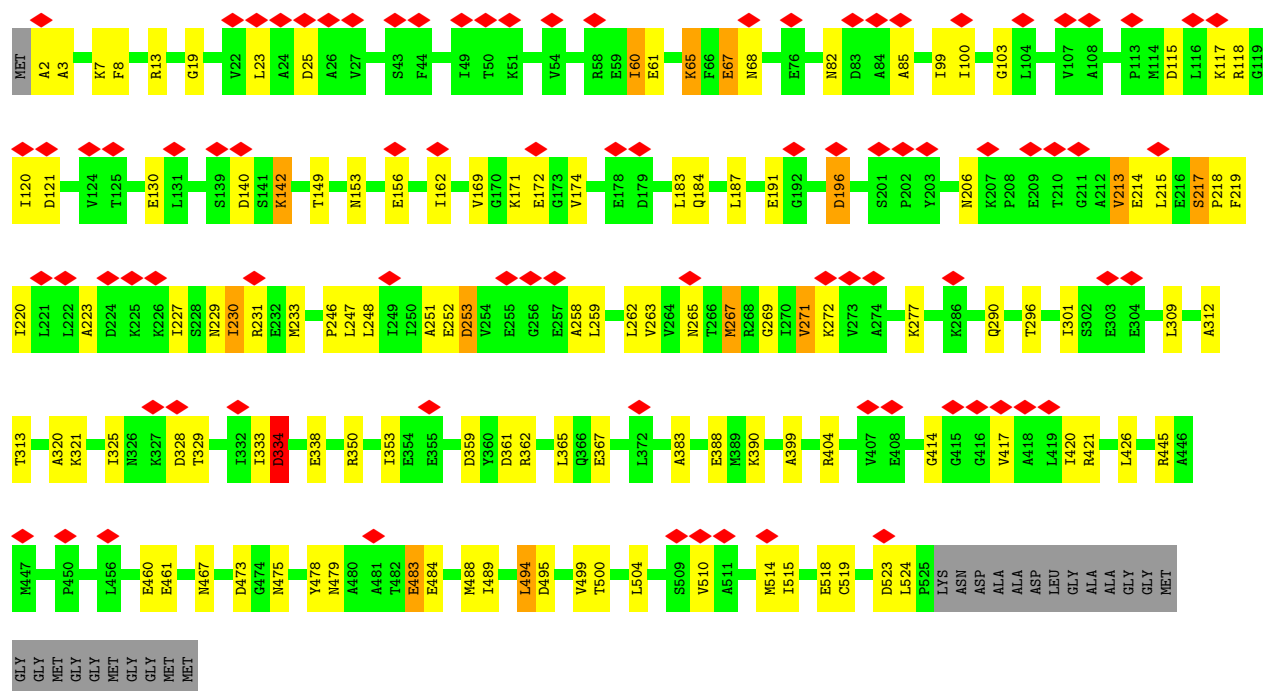
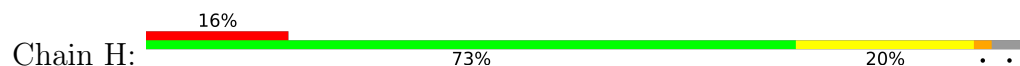
• Molecule 1: 60 KDA CHAPERONIN



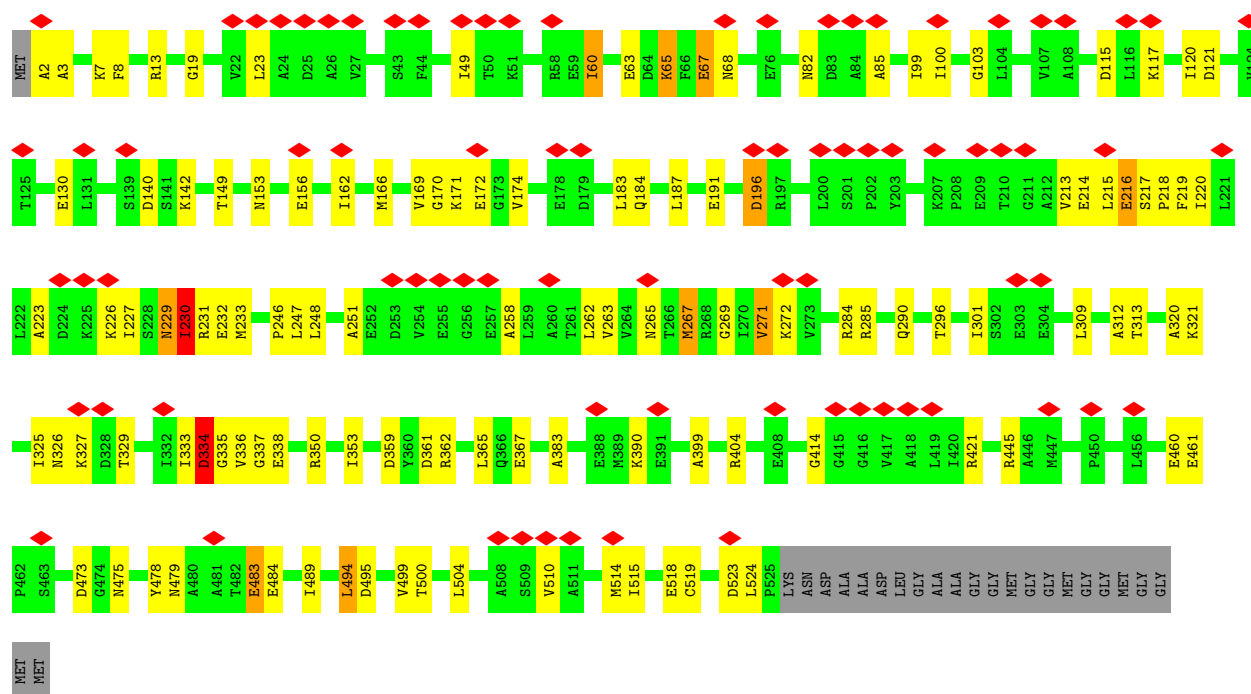
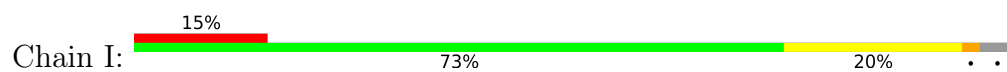




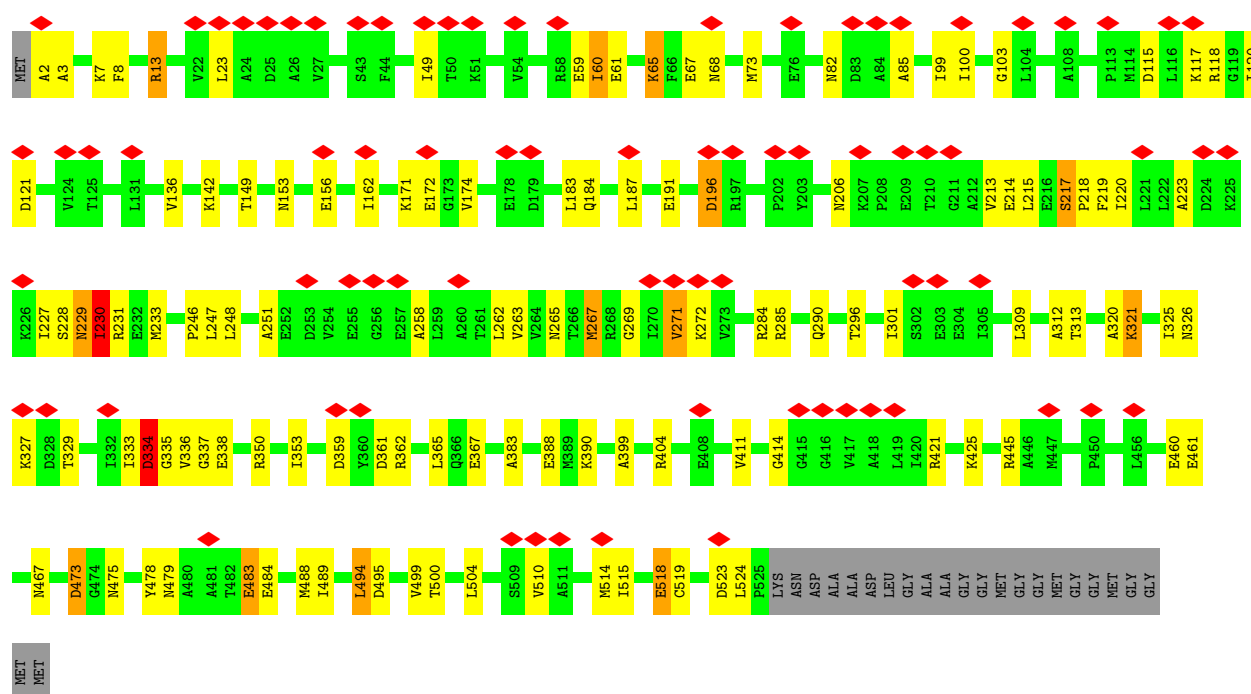
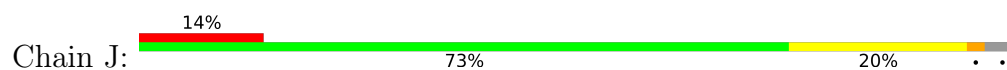
• Molecule 1: 60 KDA CHAPERONIN



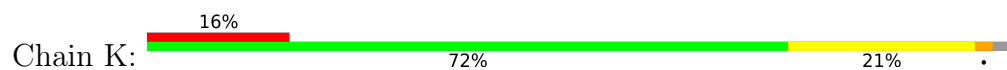
• Molecule 1: 60 KDA CHAPERONIN

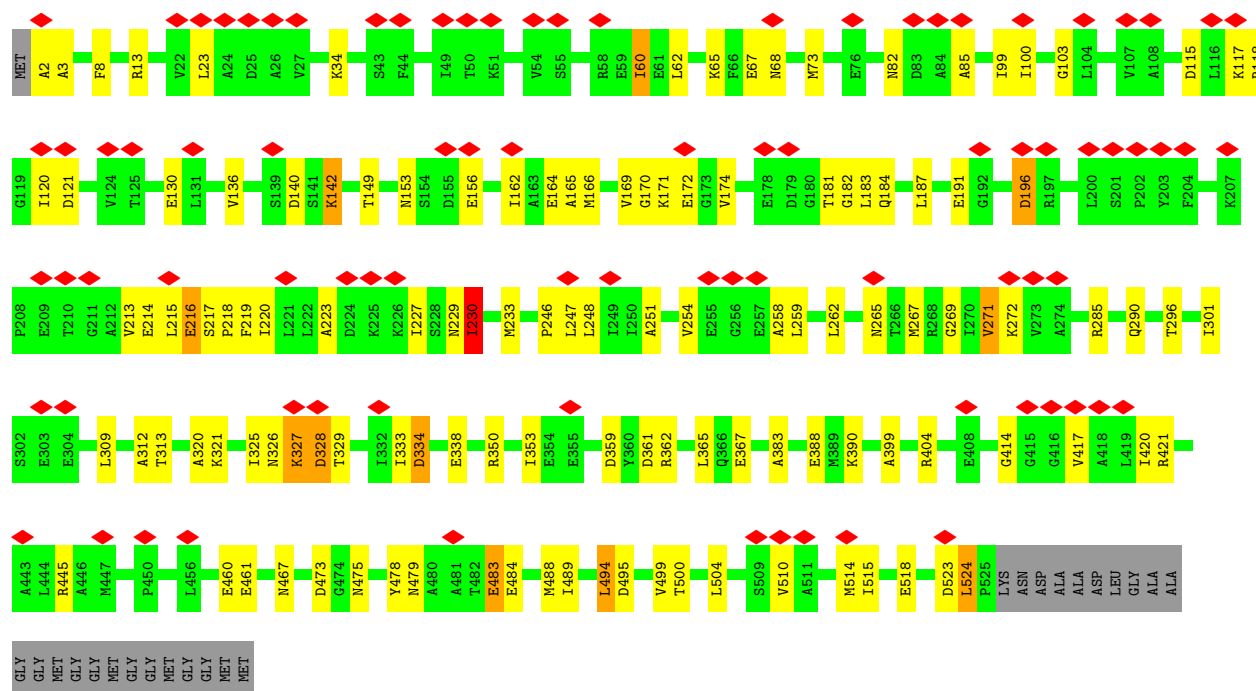


• Molecule 1: 60 KDA CHAPERONIN

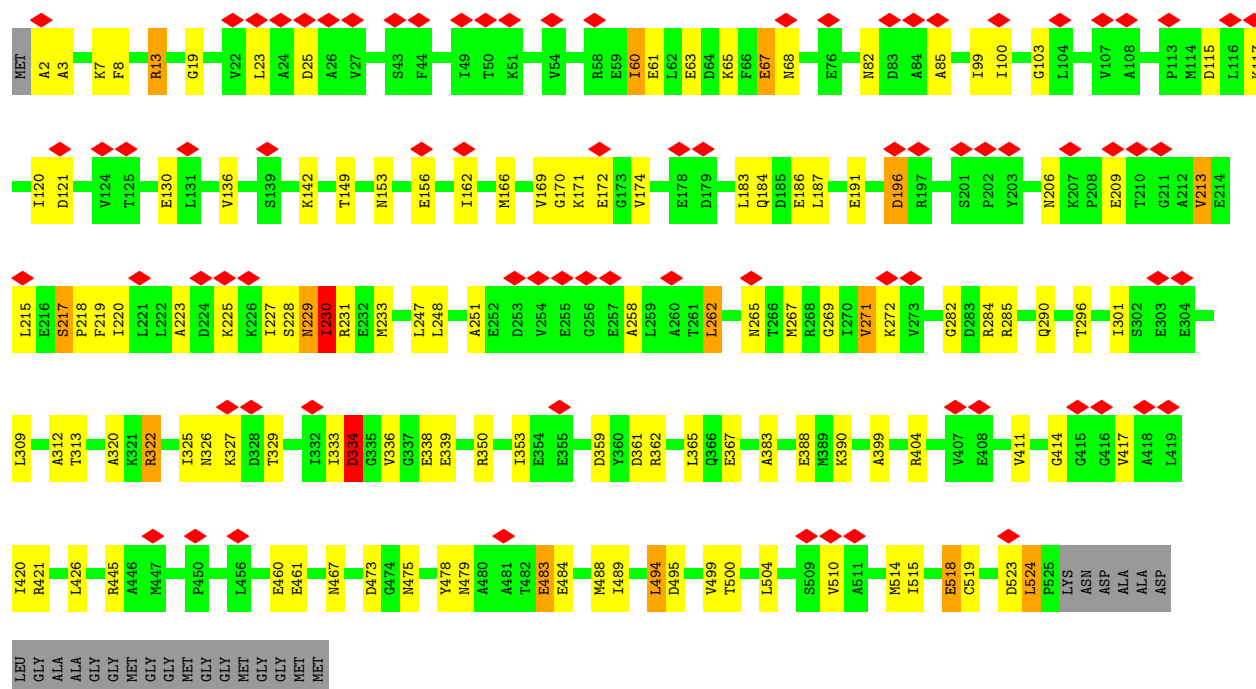


• Molecule 1: 60 KDA CHAPERONIN



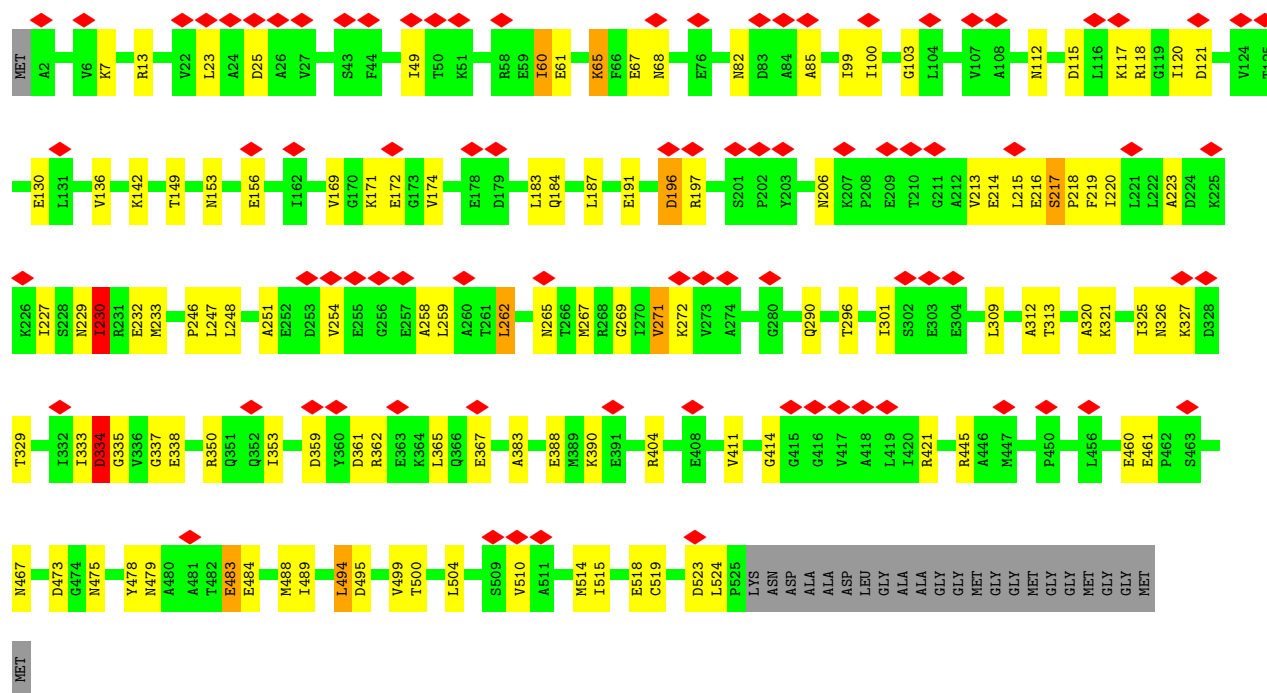


• Molecule 1: 60 KDA CHAPERONIN

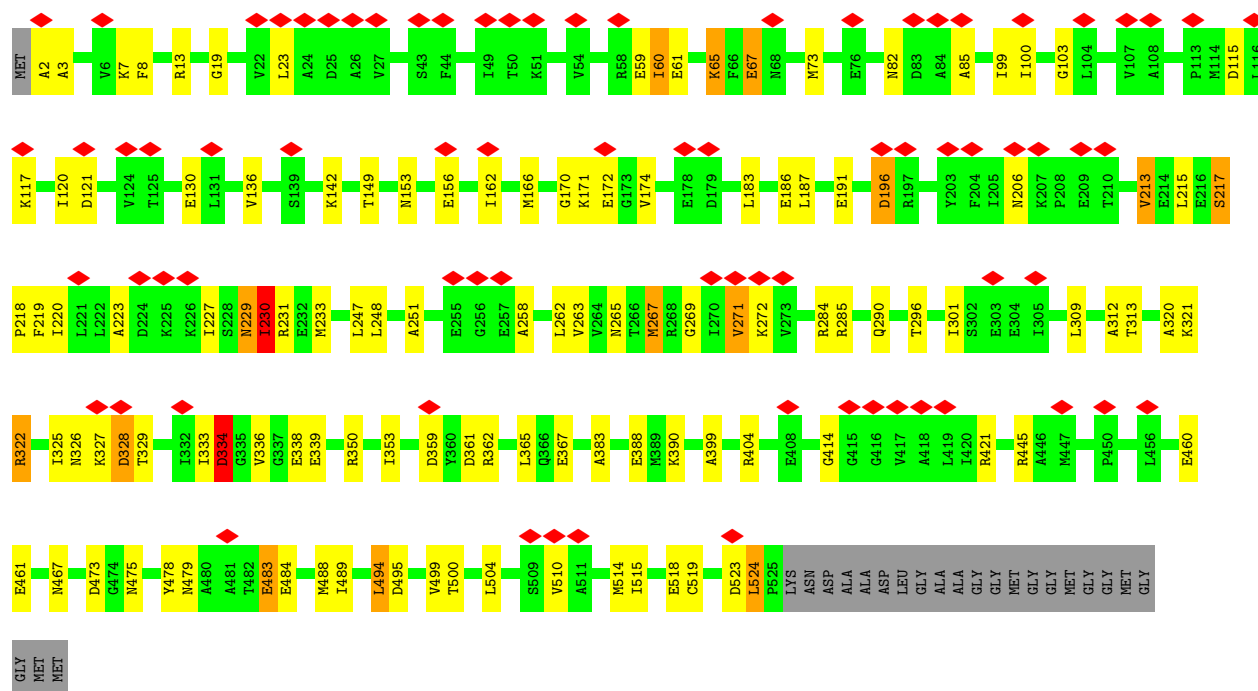
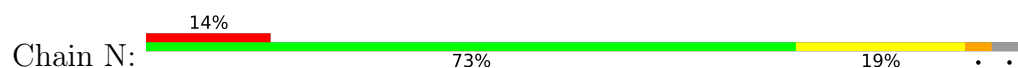


• Molecule 1: 60 KDA CHAPERONIN





• Molecule 1: 60 KDA CHAPERONIN



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	5500	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	2.618	Depositor
Minimum map value	-1.717	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.105	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: ATP, PO4, 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	11/3873 (0.3%)	1.90	137/5229 (2.6%)
1	B	1.18	13/3872 (0.3%)	1.91	140/5227 (2.7%)
1	C	1.17	12/3872 (0.3%)	1.91	137/5227 (2.6%)
1	D	1.18	12/3872 (0.3%)	1.92	138/5227 (2.6%)
1	E	1.19	13/3872 (0.3%)	1.93	142/5227 (2.7%)
1	F	1.18	12/3872 (0.3%)	1.93	140/5227 (2.7%)
1	G	1.18	12/3872 (0.3%)	1.93	143/5227 (2.7%)
1	H	0.77	1/3872 (0.0%)	1.29	29/5227 (0.6%)
1	I	0.78	1/3872 (0.0%)	1.27	22/5227 (0.4%)
1	J	0.77	1/3872 (0.0%)	1.29	29/5227 (0.6%)
1	K	0.77	1/3872 (0.0%)	1.28	23/5227 (0.4%)
1	L	0.76	1/3872 (0.0%)	1.30	29/5227 (0.6%)
1	M	0.78	1/3872 (0.0%)	1.29	31/5227 (0.6%)
1	N	0.77	1/3872 (0.0%)	1.29	26/5227 (0.5%)
All	All	0.99	92/54209 (0.2%)	1.63	1166/73180 (1.6%)

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	18
1	B	0	16
1	C	0	15
1	D	0	17
1	E	0	18
1	F	0	17
1	G	0	16
1	H	0	5
1	I	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	8
1	K	0	6
1	L	0	6
1	M	0	6
1	N	0	9
All	All	0	164

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	LYS	C-N	-19.76	1.07	1.33
1	C	7	LYS	C-N	-19.76	1.07	1.33
1	A	7	LYS	C-N	-19.76	1.07	1.33
1	G	7	LYS	C-N	-19.75	1.07	1.33
1	E	7	LYS	C-N	-19.74	1.07	1.33
1	F	7	LYS	C-N	-19.68	1.07	1.33
1	D	7	LYS	C-N	-19.67	1.07	1.33
1	G	213	VAL	C-N	-19.14	1.08	1.33
1	E	213	VAL	C-N	-19.12	1.08	1.33
1	B	213	VAL	C-N	-19.11	1.08	1.33
1	D	213	VAL	C-N	-19.10	1.08	1.33
1	F	213	VAL	C-N	-19.02	1.08	1.33
1	C	213	VAL	C-N	-19.00	1.08	1.33
1	C	11	ASP	C-N	13.52	1.52	1.33
1	A	11	ASP	C-N	13.47	1.52	1.33
1	D	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	13.43	1.52	1.33
1	B	11	ASP	C-N	13.40	1.52	1.33
1	G	11	ASP	C-N	13.37	1.52	1.33
1	C	230	ILE	C-N	13.31	1.50	1.33
1	E	230	ILE	C-N	13.30	1.50	1.33
1	G	230	ILE	C-N	13.29	1.50	1.33
1	B	230	ILE	C-N	13.29	1.50	1.33
1	A	230	ILE	C-N	13.28	1.50	1.33
1	D	230	ILE	C-N	13.28	1.50	1.33
1	F	230	ILE	C-N	13.27	1.50	1.33
1	A	513	LEU	C-N	-11.53	1.18	1.33
1	D	513	LEU	C-N	-11.51	1.18	1.33
1	G	513	LEU	C-N	-11.50	1.18	1.33
1	C	513	LEU	C-N	-11.47	1.19	1.33
1	F	513	LEU	C-N	-11.47	1.19	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	513	LEU	C-N	-11.46	1.19	1.33
1	B	513	LEU	C-N	-11.40	1.19	1.33
1	D	518	GLU	C-N	-10.16	1.19	1.33
1	F	518	GLU	C-N	-10.16	1.19	1.33
1	C	518	GLU	C-N	-10.10	1.19	1.33
1	E	518	GLU	C-N	-10.09	1.19	1.33
1	A	518	GLU	C-N	-10.08	1.19	1.33
1	B	518	GLU	C-N	-10.04	1.19	1.33
1	G	518	GLU	C-N	-10.03	1.19	1.33
1	F	52	ASP	C-N	-9.24	1.20	1.33
1	G	52	ASP	C-N	-9.22	1.20	1.33
1	E	52	ASP	C-N	-9.21	1.20	1.33
1	A	52	ASP	C-N	-9.20	1.20	1.33
1	B	52	ASP	C-N	-9.20	1.20	1.33
1	C	52	ASP	C-N	-9.18	1.20	1.33
1	D	52	ASP	C-N	-9.14	1.20	1.33
1	D	381	VAL	CA-CB	-7.16	1.46	1.54
1	E	381	VAL	CA-CB	-7.15	1.46	1.54
1	G	200	LEU	CA-C	-7.15	1.43	1.52
1	G	381	VAL	CA-CB	-7.13	1.46	1.54
1	F	381	VAL	CA-CB	-7.13	1.46	1.54
1	A	381	VAL	CA-CB	-7.12	1.46	1.54
1	C	381	VAL	CA-CB	-7.09	1.46	1.54
1	B	381	VAL	CA-CB	-7.08	1.46	1.54
1	D	193	MET	C-N	6.37	1.42	1.33
1	E	193	MET	C-N	6.33	1.42	1.33
1	A	193	MET	C-N	6.32	1.42	1.33
1	F	193	MET	C-N	5.88	1.42	1.33
1	C	198	GLY	CA-C	5.71	1.56	1.52
1	G	29	VAL	C-N	5.34	1.40	1.33
1	E	29	VAL	C-N	5.33	1.40	1.33
1	B	29	VAL	C-N	5.31	1.40	1.33
1	D	29	VAL	C-N	5.31	1.40	1.33
1	A	29	VAL	C-N	5.30	1.40	1.33
1	F	29	VAL	C-N	5.30	1.40	1.33
1	E	198	GLY	CA-C	5.29	1.56	1.52
1	B	198	GLY	C-N	5.23	1.41	1.33
1	C	29	VAL	C-N	5.23	1.40	1.33
1	B	304	GLU	CA-CB	5.22	1.61	1.53
1	F	304	GLU	CA-CB	5.22	1.61	1.53
1	G	304	GLU	CA-CB	5.21	1.61	1.53
1	C	304	GLU	CA-CB	5.20	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	GLU	CA-CB	5.19	1.61	1.53
1	D	304	GLU	CA-CB	5.19	1.61	1.53
1	E	304	GLU	CA-CB	5.18	1.61	1.53
1	B	198	GLY	CA-C	5.15	1.56	1.52
1	C	524	LEU	C-N	-5.09	1.26	1.34
1	B	524	LEU	C-N	-5.08	1.26	1.34
1	N	524	LEU	C-N	-5.08	1.26	1.34
1	H	524	LEU	C-N	-5.08	1.26	1.34
1	A	524	LEU	C-N	-5.07	1.26	1.34
1	M	524	LEU	C-N	-5.06	1.26	1.34
1	E	524	LEU	C-N	-5.06	1.26	1.34
1	F	524	LEU	C-N	-5.05	1.26	1.34
1	G	524	LEU	C-N	-5.05	1.26	1.34
1	L	524	LEU	C-N	-5.05	1.26	1.34
1	D	524	LEU	C-N	-5.05	1.26	1.34
1	J	524	LEU	C-N	-5.04	1.26	1.34
1	K	524	LEU	C-N	-5.04	1.26	1.34
1	I	524	LEU	C-N	-5.04	1.26	1.34

All (1166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	518	GLU	CA-C-N	16.85	150.10	122.29
1	F	518	GLU	C-N-CA	16.85	150.10	122.29
1	B	518	GLU	CA-C-N	16.85	150.09	122.29
1	B	518	GLU	C-N-CA	16.85	150.09	122.29
1	A	518	GLU	CA-C-N	16.84	150.07	122.29
1	A	518	GLU	C-N-CA	16.84	150.07	122.29
1	D	518	GLU	CA-C-N	16.83	150.06	122.29
1	D	518	GLU	C-N-CA	16.83	150.06	122.29
1	C	518	GLU	CA-C-N	16.82	150.05	122.29
1	C	518	GLU	C-N-CA	16.82	150.05	122.29
1	G	518	GLU	CA-C-N	16.80	150.02	122.29
1	G	518	GLU	C-N-CA	16.80	150.02	122.29
1	E	518	GLU	CA-C-N	16.80	150.00	122.29
1	E	518	GLU	C-N-CA	16.80	150.00	122.29
1	F	7	LYS	CA-C-N	-16.57	95.85	122.36
1	F	7	LYS	C-N-CA	-16.57	95.85	122.36
1	C	7	LYS	CA-C-N	-16.56	95.87	122.36
1	C	7	LYS	C-N-CA	-16.56	95.87	122.36
1	A	7	LYS	CA-C-N	-16.54	95.89	122.36
1	A	7	LYS	C-N-CA	-16.54	95.89	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	LYS	CA-C-N	-16.54	95.89	122.36
1	B	7	LYS	C-N-CA	-16.54	95.89	122.36
1	G	7	LYS	CA-C-N	-16.52	95.93	122.36
1	G	7	LYS	C-N-CA	-16.52	95.93	122.36
1	D	7	LYS	CA-C-N	-16.51	95.94	122.36
1	D	7	LYS	C-N-CA	-16.51	95.94	122.36
1	A	518	GLU	O-C-N	-16.51	104.26	122.09
1	E	7	LYS	CA-C-N	-16.51	95.95	122.36
1	E	7	LYS	C-N-CA	-16.51	95.95	122.36
1	B	518	GLU	O-C-N	-16.50	104.27	122.09
1	E	518	GLU	O-C-N	-16.46	104.31	122.09
1	C	518	GLU	O-C-N	-16.46	104.31	122.09
1	D	518	GLU	O-C-N	-16.45	104.32	122.09
1	F	518	GLU	O-C-N	-16.43	104.35	122.09
1	G	518	GLU	O-C-N	-16.39	104.39	122.09
1	C	29	VAL	O-C-N	16.37	138.69	121.83
1	B	29	VAL	O-C-N	16.34	138.66	121.83
1	D	29	VAL	O-C-N	16.33	138.65	121.83
1	E	29	VAL	O-C-N	16.32	138.64	121.83
1	G	29	VAL	O-C-N	16.31	138.63	121.83
1	A	29	VAL	O-C-N	16.29	138.60	121.83
1	F	29	VAL	O-C-N	16.29	138.60	121.83
1	C	34	LYS	CB-CA-C	15.60	135.37	110.88
1	D	34	LYS	CB-CA-C	15.59	135.36	110.88
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	B	29	VAL	CA-C-N	-14.05	101.13	120.38
1	B	29	VAL	C-N-CA	-14.05	101.13	120.38
1	E	29	VAL	CA-C-N	-14.05	101.13	120.38
1	E	29	VAL	C-N-CA	-14.05	101.13	120.38
1	C	29	VAL	CA-C-N	-14.04	101.14	120.38
1	C	29	VAL	C-N-CA	-14.04	101.14	120.38
1	F	29	VAL	CA-C-N	-14.04	101.14	120.38
1	F	29	VAL	C-N-CA	-14.04	101.14	120.38
1	G	29	VAL	CA-C-N	-14.03	101.16	120.38
1	G	29	VAL	C-N-CA	-14.03	101.16	120.38
1	A	29	VAL	CA-C-N	-14.02	101.17	120.38
1	A	29	VAL	C-N-CA	-14.02	101.17	120.38
1	D	56	VAL	CB-CA-C	-12.20	96.04	112.02
1	F	56	VAL	CB-CA-C	-12.20	96.04	112.02
1	E	56	VAL	CB-CA-C	-12.18	96.07	112.02
1	A	56	VAL	CB-CA-C	-12.17	96.08	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	VAL	CB-CA-C	-12.16	96.09	112.02
1	G	56	VAL	CB-CA-C	-12.16	96.09	112.02
1	C	56	VAL	CB-CA-C	-12.13	96.13	112.02
1	G	230	ILE	O-C-N	12.05	133.56	121.87
1	A	7	LYS	O-C-N	12.02	139.22	123.11
1	E	230	ILE	O-C-N	12.02	133.53	121.87
1	C	7	LYS	O-C-N	12.00	139.20	123.11
1	G	7	LYS	O-C-N	11.99	139.18	123.11
1	C	230	ILE	O-C-N	11.98	133.49	121.87
1	F	7	LYS	O-C-N	11.98	139.16	123.11
1	B	230	ILE	O-C-N	11.96	133.47	121.87
1	E	7	LYS	O-C-N	11.96	139.13	123.11
1	A	230	ILE	O-C-N	11.94	133.45	121.87
1	B	7	LYS	O-C-N	11.93	139.09	123.11
1	D	230	ILE	O-C-N	11.93	133.44	121.87
1	D	7	LYS	O-C-N	11.91	139.07	123.11
1	F	230	ILE	O-C-N	11.90	133.42	121.87
1	D	213	VAL	O-C-N	11.53	136.15	123.00
1	B	213	VAL	O-C-N	11.53	136.14	123.00
1	C	213	VAL	O-C-N	11.52	136.13	123.00
1	G	213	VAL	O-C-N	11.51	136.12	123.00
1	E	213	VAL	O-C-N	11.50	136.12	123.00
1	F	213	VAL	O-C-N	11.48	136.08	123.00
1	A	39	VAL	O-C-N	11.46	134.83	123.14
1	F	39	VAL	O-C-N	11.41	134.78	123.14
1	B	39	VAL	O-C-N	11.40	134.77	123.14
1	E	39	VAL	O-C-N	11.40	134.77	123.14
1	G	39	VAL	O-C-N	11.38	134.75	123.14
1	D	39	VAL	O-C-N	11.36	134.72	123.14
1	C	39	VAL	O-C-N	11.28	134.64	123.14
1	D	225	LYS	N-CA-CB	10.98	125.97	110.26
1	F	225	LYS	N-CA-CB	10.96	125.93	110.26
1	G	225	LYS	N-CA-CB	10.95	125.92	110.26
1	C	225	LYS	N-CA-CB	10.94	125.91	110.26
1	A	225	LYS	N-CA-CB	10.94	125.90	110.26
1	B	225	LYS	N-CA-CB	10.91	125.87	110.26
1	E	225	LYS	N-CA-CB	10.90	125.84	110.26
1	A	214	GLU	CB-CA-C	-10.79	90.76	109.65
1	B	214	GLU	CB-CA-C	-10.79	90.77	109.65
1	C	214	GLU	CB-CA-C	-10.78	90.78	109.65
1	E	214	GLU	CB-CA-C	-10.78	90.78	109.65
1	F	214	GLU	CB-CA-C	-10.78	90.79	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	214	GLU	CB-CA-C	-10.77	90.80	109.65
1	D	214	GLU	CB-CA-C	-10.75	90.83	109.65
1	G	199	TYR	CA-C-N	-10.47	101.55	121.54
1	G	199	TYR	C-N-CA	-10.47	101.55	121.54
1	E	213	VAL	CA-C-N	-10.13	105.31	122.33
1	E	213	VAL	C-N-CA	-10.13	105.31	122.33
1	C	213	VAL	CA-C-N	-10.12	105.34	122.33
1	C	213	VAL	C-N-CA	-10.12	105.34	122.33
1	D	213	VAL	CA-C-N	-10.12	105.34	122.33
1	D	213	VAL	C-N-CA	-10.12	105.34	122.33
1	F	213	VAL	CA-C-N	-10.11	105.35	122.33
1	F	213	VAL	C-N-CA	-10.11	105.35	122.33
1	B	213	VAL	CA-C-N	-10.10	105.36	122.33
1	B	213	VAL	C-N-CA	-10.10	105.36	122.33
1	G	213	VAL	CA-C-N	-10.10	105.36	122.33
1	G	213	VAL	C-N-CA	-10.10	105.36	122.33
1	F	195	PHE	CA-CB-CG	-10.01	103.79	113.80
1	E	203	TYR	CA-C-N	-9.46	105.89	122.26
1	E	203	TYR	C-N-CA	-9.46	105.89	122.26
1	D	114	MET	N-CA-CB	9.46	124.03	110.12
1	B	401	HIS	CA-CB-CG	9.41	123.21	113.80
1	A	401	HIS	CA-CB-CG	9.38	123.18	113.80
1	D	316	ASP	N-CA-CB	9.38	124.04	110.16
1	E	401	HIS	CA-CB-CG	9.38	123.18	113.80
1	A	316	ASP	N-CA-CB	9.37	124.03	110.16
1	C	401	HIS	CA-CB-CG	9.37	123.17	113.80
1	F	316	ASP	N-CA-CB	9.37	124.03	110.16
1	B	316	ASP	N-CA-CB	9.37	124.03	110.16
1	D	401	HIS	CA-CB-CG	9.36	123.16	113.80
1	G	401	HIS	CA-CB-CG	9.36	123.16	113.80
1	G	316	ASP	N-CA-CB	9.35	124.00	110.16
1	C	316	ASP	N-CA-CB	9.34	123.98	110.16
1	E	316	ASP	N-CA-CB	9.34	123.97	110.16
1	F	401	HIS	CA-CB-CG	9.30	123.11	113.80
1	E	192	GLY	CA-C-N	-9.29	109.91	122.72
1	E	192	GLY	C-N-CA	-9.29	109.91	122.72
1	B	52	ASP	CA-C-N	-9.27	103.23	121.41
1	B	52	ASP	C-N-CA	-9.27	103.23	121.41
1	F	192	GLY	CA-C-N	-9.27	109.93	122.72
1	F	192	GLY	C-N-CA	-9.27	109.93	122.72
1	G	221	LEU	CA-C-N	-9.27	109.97	122.85
1	G	221	LEU	C-N-CA	-9.27	109.97	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	GLY	CA-C-N	-9.26	109.94	122.72
1	A	192	GLY	C-N-CA	-9.26	109.94	122.72
1	D	221	LEU	CA-C-N	-9.26	109.98	122.85
1	D	221	LEU	C-N-CA	-9.26	109.98	122.85
1	B	221	LEU	CA-C-N	-9.26	109.98	122.85
1	B	221	LEU	C-N-CA	-9.26	109.98	122.85
1	F	221	LEU	CA-C-N	-9.25	109.99	122.85
1	F	221	LEU	C-N-CA	-9.25	109.99	122.85
1	E	52	ASP	CA-C-N	-9.25	103.28	121.41
1	E	52	ASP	C-N-CA	-9.25	103.28	121.41
1	D	52	ASP	CA-C-N	-9.24	103.30	121.41
1	D	52	ASP	C-N-CA	-9.24	103.30	121.41
1	F	52	ASP	CA-C-N	-9.23	103.31	121.41
1	F	52	ASP	C-N-CA	-9.23	103.31	121.41
1	A	52	ASP	CA-C-N	-9.23	103.32	121.41
1	A	52	ASP	C-N-CA	-9.23	103.32	121.41
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	G	52	ASP	CA-C-N	-9.23	103.33	121.41
1	G	52	ASP	C-N-CA	-9.23	103.33	121.41
1	D	192	GLY	CA-C-N	-9.22	110.00	122.72
1	D	192	GLY	C-N-CA	-9.22	110.00	122.72
1	A	221	LEU	CA-C-N	-9.21	110.04	122.85
1	A	221	LEU	C-N-CA	-9.21	110.04	122.85
1	C	52	ASP	CA-C-N	-9.21	103.36	121.41
1	C	52	ASP	C-N-CA	-9.21	103.36	121.41
1	C	221	LEU	CA-C-N	-9.20	110.06	122.85
1	C	221	LEU	C-N-CA	-9.20	110.06	122.85
1	M	267	MET	CG-SD-CE	9.04	120.79	100.90
1	I	267	MET	CG-SD-CE	9.00	120.70	100.90
1	N	267	MET	CG-SD-CE	8.99	120.68	100.90
1	L	267	MET	CG-SD-CE	8.98	120.65	100.90
1	H	267	MET	CG-SD-CE	8.95	120.59	100.90
1	J	267	MET	CG-SD-CE	8.94	120.57	100.90
1	M	359	ASP	CA-CB-CG	-8.90	103.70	112.60
1	K	267	MET	CG-SD-CE	8.87	120.42	100.90
1	K	359	ASP	CA-CB-CG	-8.79	103.81	112.60
1	I	359	ASP	CA-CB-CG	-8.77	103.83	112.60
1	J	359	ASP	CA-CB-CG	-8.76	103.84	112.60
1	L	359	ASP	CA-CB-CG	-8.74	103.86	112.60
1	H	359	ASP	CA-CB-CG	-8.73	103.87	112.60
1	N	359	ASP	CA-CB-CG	-8.72	103.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	73	MET	CB-CA-C	-8.42	97.60	110.90
1	G	252	GLU	N-CA-CB	8.42	122.22	110.01
1	D	73	MET	CB-CA-C	-8.41	97.61	110.90
1	F	73	MET	CB-CA-C	-8.41	97.61	110.90
1	B	73	MET	CB-CA-C	-8.41	97.62	110.90
1	E	252	GLU	N-CA-CB	8.40	122.19	110.01
1	C	252	GLU	N-CA-CB	8.40	122.19	110.01
1	A	73	MET	CB-CA-C	-8.40	97.63	110.90
1	D	252	GLU	N-CA-CB	8.40	122.18	110.01
1	C	73	MET	CB-CA-C	-8.39	97.65	110.90
1	E	73	MET	CB-CA-C	-8.39	97.65	110.90
1	A	252	GLU	N-CA-CB	8.38	122.17	110.01
1	A	326	ASN	CA-CB-CG	8.38	120.98	112.60
1	B	252	GLU	N-CA-CB	8.38	122.17	110.01
1	B	326	ASN	CA-CB-CG	8.38	120.98	112.60
1	F	252	GLU	N-CA-CB	8.38	122.16	110.01
1	F	326	ASN	CA-CB-CG	8.38	120.98	112.60
1	G	326	ASN	CA-CB-CG	8.38	120.98	112.60
1	D	326	ASN	CA-CB-CG	8.37	120.97	112.60
1	C	326	ASN	CA-CB-CG	8.36	120.96	112.60
1	E	326	ASN	CA-CB-CG	8.36	120.95	112.60
1	H	196	ASP	N-CA-CB	-8.29	98.65	110.58
1	C	371	LYS	CB-CA-C	8.28	123.98	110.90
1	E	371	LYS	CB-CA-C	8.27	123.96	110.90
1	B	371	LYS	CB-CA-C	8.27	123.96	110.90
1	A	371	LYS	CB-CA-C	8.26	123.95	110.90
1	G	371	LYS	CB-CA-C	8.25	123.93	110.90
1	D	371	LYS	CB-CA-C	8.25	123.93	110.90
1	F	114	MET	N-CA-CB	8.25	122.24	110.12
1	A	114	MET	N-CA-CB	8.24	122.24	110.12
1	F	371	LYS	CB-CA-C	8.24	123.92	110.90
1	C	411	VAL	CB-CA-C	-8.14	100.63	111.70
1	F	411	VAL	CB-CA-C	-8.13	100.65	111.70
1	B	411	VAL	CB-CA-C	-8.12	100.66	111.70
1	G	411	VAL	CB-CA-C	-8.11	100.67	111.70
1	N	328	ASP	N-CA-CB	-8.12	100.29	111.65
1	E	411	VAL	CB-CA-C	-8.11	100.67	111.70
1	D	411	VAL	CB-CA-C	-8.10	100.69	111.70
1	A	411	VAL	CB-CA-C	-8.10	100.69	111.70
1	A	518	GLU	CB-CA-C	8.06	123.64	110.90
1	D	321	LYS	N-CA-C	-8.06	102.44	111.71
1	E	518	GLU	CB-CA-C	8.05	123.62	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	LYS	N-CA-C	-8.03	102.48	111.71
1	C	321	LYS	N-CA-C	-8.03	102.48	111.71
1	B	321	LYS	N-CA-C	-8.02	102.49	111.71
1	E	321	LYS	N-CA-C	-8.02	102.49	111.71
1	C	311	LYS	N-CA-CB	8.00	121.88	110.12
1	G	311	LYS	N-CA-CB	7.99	121.86	110.12
1	F	311	LYS	N-CA-CB	7.99	121.86	110.12
1	B	311	LYS	N-CA-CB	7.98	121.85	110.12
1	E	311	LYS	N-CA-CB	7.97	121.84	110.12
1	G	518	GLU	CB-CA-C	7.96	123.48	110.90
1	F	321	LYS	N-CA-C	-7.96	102.56	111.71
1	F	518	GLU	CB-CA-C	7.96	123.47	110.90
1	G	321	LYS	N-CA-C	-7.96	102.56	111.71
1	B	518	GLU	CB-CA-C	7.95	123.47	110.90
1	A	311	LYS	N-CA-CB	7.94	121.79	110.12
1	C	518	GLU	CB-CA-C	7.93	123.44	110.90
1	D	311	LYS	N-CA-CB	7.93	121.78	110.12
1	D	518	GLU	CB-CA-C	7.90	123.38	110.90
1	G	201	SER	CA-C-N	7.80	129.59	119.84
1	G	201	SER	C-N-CA	7.80	129.59	119.84
1	C	114	MET	N-CA-CB	7.74	121.50	110.12
1	A	34	LYS	N-CA-CB	7.73	121.21	110.01
1	F	34	LYS	N-CA-CB	7.71	121.19	110.01
1	E	34	LYS	N-CA-CB	7.71	121.19	110.01
1	G	34	LYS	N-CA-CB	7.70	121.18	110.01
1	B	34	LYS	N-CA-CB	7.70	121.18	110.01
1	M	367	GLU	CB-CA-C	-7.70	95.89	110.67
1	M	333	ILE	N-CA-C	7.66	118.46	110.72
1	L	461	GLU	CB-CA-C	-7.59	101.35	110.08
1	A	193	MET	O-C-N	-7.57	114.72	123.27
1	L	367	GLU	CB-CA-C	-7.57	96.13	110.67
1	D	11	ASP	O-C-N	-7.56	113.37	122.22
1	E	193	MET	O-C-N	-7.56	114.73	123.27
1	L	225	LYS	N-CA-CB	-7.56	98.93	110.42
1	K	196	ASP	N-CA-CB	-7.55	99.71	110.58
1	A	11	ASP	O-C-N	-7.54	113.39	122.22
1	N	367	GLU	CB-CA-C	-7.54	96.19	110.67
1	D	193	MET	O-C-N	-7.54	114.75	123.27
1	I	367	GLU	CB-CA-C	-7.54	96.20	110.67
1	B	11	ASP	O-C-N	-7.53	113.41	122.22
1	E	11	ASP	O-C-N	-7.53	113.41	122.22
1	L	333	ILE	N-CA-C	7.53	118.32	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	ASP	O-C-N	-7.53	113.41	122.22
1	F	11	ASP	O-C-N	-7.52	113.42	122.22
1	N	333	ILE	N-CA-C	7.52	118.31	110.72
1	G	11	ASP	O-C-N	-7.50	113.44	122.22
1	F	193	MET	O-C-N	-7.49	114.81	123.27
1	J	367	GLU	CB-CA-C	-7.48	96.30	110.67
1	H	333	ILE	N-CA-C	7.48	118.28	110.72
1	K	333	ILE	N-CA-C	7.47	118.27	110.72
1	F	258	ALA	N-CA-CB	7.46	120.83	110.01
1	G	258	ALA	N-CA-CB	7.46	120.83	110.01
1	I	333	ILE	N-CA-C	7.46	118.25	110.72
1	B	192	GLY	CA-C-N	-7.45	109.97	122.64
1	B	192	GLY	C-N-CA	-7.45	109.97	122.64
1	B	258	ALA	N-CA-CB	7.45	120.81	110.01
1	D	258	ALA	N-CA-CB	7.45	120.81	110.01
1	E	258	ALA	N-CA-CB	7.45	120.81	110.01
1	K	367	GLU	CB-CA-C	-7.45	96.37	110.67
1	A	258	ALA	N-CA-CB	7.44	120.79	110.01
1	H	367	GLU	CB-CA-C	-7.43	96.40	110.67
1	C	258	ALA	N-CA-CB	7.43	120.78	110.01
1	G	114	MET	N-CA-CB	7.38	120.97	110.12
1	B	114	MET	N-CA-CB	7.33	120.90	110.12
1	A	87	ASP	N-CA-CB	7.33	122.69	111.56
1	E	87	ASP	N-CA-CB	7.29	122.64	111.56
1	J	333	ILE	N-CA-C	7.26	118.05	110.72
1	E	114	MET	N-CA-CB	7.26	120.79	110.12
1	N	461	GLU	CB-CA-C	-7.25	101.74	110.08
1	A	39	VAL	CA-C-N	-7.24	112.79	123.00
1	A	39	VAL	C-N-CA	-7.24	112.79	123.00
1	B	358	SER	CA-C-N	7.23	129.97	120.28
1	B	358	SER	C-N-CA	7.23	129.97	120.28
1	K	115	ASP	CB-CA-C	7.23	122.33	110.90
1	B	87	ASP	N-CA-CB	7.21	122.53	111.56
1	D	358	SER	CA-C-N	7.21	129.94	120.28
1	D	358	SER	C-N-CA	7.21	129.94	120.28
1	F	358	SER	CA-C-N	7.21	129.94	120.28
1	F	358	SER	C-N-CA	7.21	129.94	120.28
1	M	115	ASP	CB-CA-C	7.21	122.29	110.90
1	D	87	ASP	N-CA-CB	7.21	122.52	111.56
1	C	87	ASP	N-CA-CB	7.20	122.51	111.56
1	G	87	ASP	N-CA-CB	7.20	122.50	111.56
1	F	39	VAL	CA-C-N	-7.20	112.85	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	39	VAL	C-N-CA	-7.20	112.85	123.00
1	A	358	SER	CA-C-N	7.20	129.92	120.28
1	A	358	SER	C-N-CA	7.20	129.92	120.28
1	E	358	SER	CA-C-N	7.19	129.92	120.28
1	E	358	SER	C-N-CA	7.19	129.92	120.28
1	E	39	VAL	CA-C-N	-7.18	112.88	123.00
1	E	39	VAL	C-N-CA	-7.18	112.88	123.00
1	F	87	ASP	N-CA-CB	7.18	122.47	111.56
1	B	39	VAL	CA-C-N	-7.18	112.88	123.00
1	B	39	VAL	C-N-CA	-7.18	112.88	123.00
1	G	39	VAL	CA-C-N	-7.17	112.88	123.00
1	G	39	VAL	C-N-CA	-7.17	112.88	123.00
1	C	358	SER	CA-C-N	7.15	129.86	120.28
1	C	358	SER	C-N-CA	7.15	129.86	120.28
1	D	39	VAL	CA-C-N	-7.14	112.93	123.00
1	D	39	VAL	C-N-CA	-7.14	112.93	123.00
1	E	457	ASN	CA-CB-CG	-7.14	105.45	112.60
1	L	196	ASP	N-CA-CB	-7.14	100.30	110.58
1	A	457	ASN	CA-CB-CG	-7.14	105.46	112.60
1	B	457	ASN	CA-CB-CG	-7.14	105.46	112.60
1	C	457	ASN	CA-CB-CG	-7.14	105.46	112.60
1	H	115	ASP	CB-CA-C	7.13	122.17	110.90
1	D	457	ASN	CA-CB-CG	-7.13	105.47	112.60
1	C	39	VAL	CA-C-N	-7.13	112.95	123.00
1	C	39	VAL	C-N-CA	-7.13	112.95	123.00
1	K	267	MET	N-CA-CB	-7.13	99.84	110.60
1	F	457	ASN	CA-CB-CG	-7.12	105.48	112.60
1	G	457	ASN	CA-CB-CG	-7.12	105.48	112.60
1	G	358	SER	CA-C-N	7.11	129.81	120.28
1	G	358	SER	C-N-CA	7.11	129.81	120.28
1	C	338	GLU	CB-CA-C	7.09	123.87	109.76
1	E	338	GLU	CB-CA-C	7.08	123.85	109.76
1	A	338	GLU	CB-CA-C	7.07	123.83	109.76
1	D	338	GLU	CB-CA-C	7.07	123.83	109.76
1	G	338	GLU	CB-CA-C	7.07	123.83	109.76
1	N	267	MET	N-CA-CB	-7.06	99.94	110.60
1	N	196	ASP	N-CA-CB	-7.06	100.41	110.58
1	F	338	GLU	CB-CA-C	7.06	123.81	109.76
1	B	338	GLU	CB-CA-C	7.05	123.80	109.76
1	H	461	GLU	CB-CA-C	-7.04	101.98	110.08
1	C	149	THR	CB-CA-C	-7.04	99.83	110.88
1	G	34	LYS	CB-CA-C	7.03	121.92	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	34	LYS	CB-CA-C	7.03	121.92	110.88
1	F	401	HIS	CB-CG-CD2	-7.02	122.07	131.20
1	F	149	THR	CB-CA-C	-7.01	99.88	110.88
1	J	115	ASP	CB-CA-C	7.01	121.97	110.90
1	F	34	LYS	CB-CA-C	7.00	121.87	110.88
1	M	196	ASP	N-CA-CB	-7.00	100.50	110.58
1	A	34	LYS	CB-CA-C	7.00	121.86	110.88
1	E	34	LYS	CB-CA-C	6.99	121.86	110.88
1	D	196	ASP	CA-CB-CG	-6.98	105.62	112.60
1	I	196	ASP	N-CA-CB	-6.98	100.52	110.58
1	A	401	HIS	CB-CG-CD2	-6.98	122.13	131.20
1	D	401	HIS	CB-CG-CD2	-6.97	122.14	131.20
1	B	401	HIS	CB-CG-CD2	-6.96	122.15	131.20
1	E	401	HIS	CB-CG-CD2	-6.96	122.15	131.20
1	A	149	THR	CB-CA-C	-6.96	99.96	110.88
1	C	401	HIS	CB-CG-CD2	-6.96	122.16	131.20
1	F	39	VAL	N-CA-CB	6.96	124.08	111.21
1	E	39	VAL	N-CA-CB	6.96	124.08	111.21
1	G	401	HIS	CB-CG-CD2	-6.96	122.16	131.20
1	M	267	MET	N-CA-CB	-6.95	100.10	110.60
1	A	39	VAL	N-CA-CB	6.95	124.06	111.21
1	B	39	VAL	N-CA-CB	6.95	124.06	111.21
1	J	267	MET	N-CA-CB	-6.95	100.11	110.60
1	D	149	THR	CB-CA-C	-6.95	99.97	110.88
1	B	149	THR	CB-CA-C	-6.94	99.98	110.88
1	D	39	VAL	N-CA-CB	6.94	124.04	111.21
1	G	149	THR	CB-CA-C	-6.93	99.99	110.88
1	G	39	VAL	N-CA-CB	6.93	124.03	111.21
1	C	39	VAL	N-CA-CB	6.93	124.03	111.21
1	E	149	THR	CB-CA-C	-6.92	100.01	110.88
1	L	267	MET	N-CA-CB	-6.91	100.16	110.60
1	M	115	ASP	CA-CB-CG	-6.91	105.69	112.60
1	C	173	GLY	CA-C-N	-6.89	109.95	122.43
1	C	173	GLY	C-N-CA	-6.89	109.95	122.43
1	H	267	MET	N-CA-CB	-6.89	100.19	110.60
1	F	173	GLY	CA-C-N	-6.88	109.98	122.43
1	F	173	GLY	C-N-CA	-6.88	109.98	122.43
1	K	115	ASP	CA-CB-CG	-6.88	105.72	112.60
1	I	267	MET	N-CA-CB	-6.87	100.23	110.60
1	J	196	ASP	N-CA-CB	-6.87	100.69	110.58
1	J	523	ASP	CB-CA-C	6.87	122.18	109.54
1	B	173	GLY	CA-C-N	-6.87	110.00	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	GLY	C-N-CA	-6.87	110.00	122.43
1	A	173	GLY	CA-C-N	-6.86	110.01	122.43
1	A	173	GLY	C-N-CA	-6.86	110.01	122.43
1	E	173	GLY	CA-C-N	-6.86	110.01	122.43
1	E	173	GLY	C-N-CA	-6.86	110.01	122.43
1	G	523	ASP	CB-CA-C	6.86	121.89	109.62
1	F	523	ASP	CB-CA-C	6.85	121.88	109.62
1	A	523	ASP	CB-CA-C	6.85	121.88	109.62
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	D	523	ASP	CB-CA-C	6.83	121.84	109.62
1	C	523	ASP	CB-CA-C	6.83	121.84	109.62
1	G	173	GLY	CA-C-N	-6.83	110.07	122.43
1	G	173	GLY	C-N-CA	-6.83	110.07	122.43
1	E	523	ASP	CB-CA-C	6.83	121.84	109.62
1	C	196	ASP	CA-CB-CG	-6.82	105.78	112.60
1	H	115	ASP	CA-CB-CG	-6.80	105.80	112.60
1	F	36	ARG	CA-C-N	6.80	134.53	121.54
1	F	36	ARG	C-N-CA	6.80	134.53	121.54
1	G	36	ARG	CA-C-N	6.79	134.51	121.54
1	G	36	ARG	C-N-CA	6.79	134.51	121.54
1	D	36	ARG	CA-C-N	6.78	134.50	121.54
1	D	36	ARG	C-N-CA	6.78	134.50	121.54
1	B	523	ASP	CB-CA-C	6.78	121.76	109.62
1	A	36	ARG	CA-C-N	6.78	134.48	121.54
1	A	36	ARG	C-N-CA	6.78	134.48	121.54
1	J	115	ASP	CA-CB-CG	-6.77	105.83	112.60
1	A	80	LYS	CB-CA-C	6.76	122.34	110.85
1	C	80	LYS	CB-CA-C	6.75	122.33	110.85
1	E	80	LYS	CB-CA-C	6.75	122.33	110.85
1	B	80	LYS	CB-CA-C	6.75	122.33	110.85
1	C	36	ARG	CA-C-N	6.75	134.44	121.54
1	C	36	ARG	C-N-CA	6.75	134.44	121.54
1	D	80	LYS	CB-CA-C	6.75	122.33	110.85
1	G	80	LYS	CB-CA-C	6.75	122.33	110.85
1	F	80	LYS	CB-CA-C	6.75	122.33	110.85
1	J	473	ASP	N-CA-CB	6.74	124.05	111.52
1	B	36	ARG	CA-C-N	6.73	134.40	121.54
1	B	36	ARG	C-N-CA	6.73	134.40	121.54
1	E	36	ARG	CA-C-N	6.73	134.40	121.54
1	E	36	ARG	C-N-CA	6.73	134.40	121.54
1	B	324	VAL	N-CA-CB	-6.73	100.41	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	185	ASP	CA-CB-CG	-6.73	105.87	112.60
1	B	251	ALA	N-CA-CB	-6.71	100.70	110.70
1	L	523	ASP	CB-CA-C	6.71	121.89	109.54
1	F	324	VAL	N-CA-CB	-6.71	100.44	111.44
1	C	324	VAL	N-CA-CB	-6.71	100.44	111.44
1	D	324	VAL	N-CA-CB	-6.71	100.44	111.44
1	E	252	GLU	CB-CG-CD	6.70	123.99	112.60
1	E	324	VAL	N-CA-CB	-6.70	100.45	111.44
1	G	324	VAL	N-CA-CB	-6.70	100.45	111.44
1	A	324	VAL	N-CA-CB	-6.70	100.46	111.44
1	C	251	ALA	N-CA-CB	-6.70	100.72	110.70
1	D	251	ALA	N-CA-CB	-6.68	100.74	110.70
1	E	251	ALA	N-CA-CB	-6.68	100.74	110.70
1	A	251	ALA	N-CA-CB	-6.68	100.75	110.70
1	F	251	ALA	N-CA-CB	-6.68	100.75	110.70
1	B	252	GLU	CB-CG-CD	6.67	123.94	112.60
1	A	252	GLU	CB-CG-CD	6.67	123.93	112.60
1	B	247	LEU	CB-CA-C	-6.66	97.52	109.71
1	E	196	ASP	CA-CB-CG	-6.66	105.94	112.60
1	G	251	ALA	N-CA-CB	-6.66	100.78	110.70
1	G	252	GLU	CB-CG-CD	6.66	123.92	112.60
1	C	247	LEU	CB-CA-C	-6.66	97.52	109.71
1	F	252	GLU	CB-CG-CD	6.66	123.92	112.60
1	A	247	LEU	CB-CA-C	-6.66	97.53	109.71
1	F	140	ASP	N-CA-CB	-6.66	100.87	110.45
1	D	252	GLU	CB-CG-CD	6.65	123.91	112.60
1	C	252	GLU	CB-CG-CD	6.65	123.90	112.60
1	G	230	ILE	CA-C-N	-6.64	111.57	120.54
1	G	230	ILE	C-N-CA	-6.64	111.57	120.54
1	G	247	LEU	CB-CA-C	-6.64	97.56	109.71
1	B	140	ASP	N-CA-CB	-6.64	100.89	110.45
1	F	247	LEU	CB-CA-C	-6.64	97.56	109.71
1	D	140	ASP	N-CA-CB	-6.64	100.89	110.45
1	D	247	LEU	CB-CA-C	-6.64	97.57	109.71
1	C	140	ASP	N-CA-CB	-6.63	100.90	110.45
1	E	247	LEU	CB-CA-C	-6.63	97.58	109.71
1	E	230	ILE	CA-C-N	-6.62	111.60	120.54
1	E	230	ILE	C-N-CA	-6.62	111.60	120.54
1	K	461	GLU	CB-CA-C	-6.62	102.47	110.08
1	A	140	ASP	N-CA-CB	-6.62	100.92	110.45
1	E	140	ASP	N-CA-CB	-6.62	100.92	110.45
1	B	230	ILE	CA-C-N	-6.61	111.61	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	ILE	C-N-CA	-6.61	111.61	120.54
1	G	140	ASP	N-CA-CB	-6.60	100.94	110.45
1	E	304	GLU	CB-CA-C	-6.60	100.52	110.88
1	B	304	GLU	CB-CA-C	-6.59	100.53	110.88
1	F	304	GLU	CB-CA-C	-6.59	100.53	110.88
1	C	230	ILE	CA-C-N	-6.58	111.65	120.54
1	C	230	ILE	C-N-CA	-6.58	111.65	120.54
1	F	59	GLU	CB-CA-C	6.58	122.36	109.72
1	D	230	ILE	CA-C-N	-6.58	111.65	120.54
1	D	230	ILE	C-N-CA	-6.58	111.65	120.54
1	H	328	ASP	N-CA-CB	-6.58	101.39	111.66
1	A	230	ILE	CA-C-N	-6.57	111.67	120.54
1	A	230	ILE	C-N-CA	-6.57	111.67	120.54
1	A	304	GLU	CB-CA-C	-6.57	100.56	110.88
1	D	304	GLU	CB-CA-C	-6.57	100.57	110.88
1	G	304	GLU	CB-CA-C	-6.57	100.57	110.88
1	C	195	PHE	CA-C-N	-6.56	113.17	122.41
1	C	195	PHE	C-N-CA	-6.56	113.17	122.41
1	F	230	ILE	CA-C-N	-6.56	111.69	120.54
1	F	230	ILE	C-N-CA	-6.56	111.69	120.54
1	C	304	GLU	CB-CA-C	-6.55	100.60	110.88
1	B	315	GLU	CA-C-N	6.50	129.52	120.29
1	B	315	GLU	C-N-CA	6.50	129.52	120.29
1	C	194	GLN	N-CA-CB	-6.46	100.43	110.57
1	D	315	GLU	CA-C-N	6.43	129.43	120.29
1	D	315	GLU	C-N-CA	6.43	129.43	120.29
1	F	198	GLY	CA-C-N	6.43	130.89	121.31
1	F	198	GLY	C-N-CA	6.43	130.89	121.31
1	C	315	GLU	CA-C-N	6.42	129.41	120.29
1	C	315	GLU	C-N-CA	6.42	129.41	120.29
1	A	315	GLU	CA-C-N	6.42	129.40	120.29
1	A	315	GLU	C-N-CA	6.42	129.40	120.29
1	F	315	GLU	CA-C-N	6.41	129.40	120.29
1	F	315	GLU	C-N-CA	6.41	129.40	120.29
1	N	217	SER	CB-CA-C	-6.41	104.68	110.71
1	B	27	VAL	N-CA-C	6.40	116.55	110.53
1	G	315	GLU	CA-C-N	6.40	129.38	120.29
1	G	315	GLU	C-N-CA	6.40	129.38	120.29
1	D	27	VAL	N-CA-C	6.40	116.55	110.53
1	J	467	ASN	CA-CB-CG	-6.40	106.20	112.60
1	E	315	GLU	CA-C-N	6.38	129.34	120.29
1	E	315	GLU	C-N-CA	6.38	129.34	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	27	VAL	N-CA-C	6.36	116.51	110.53
1	B	272	LYS	N-CA-CB	-6.35	100.47	110.06
1	E	27	VAL	N-CA-C	6.35	116.50	110.53
1	J	217	SER	CB-CA-C	-6.35	104.74	110.71
1	F	27	VAL	N-CA-C	6.35	116.50	110.53
1	A	198	GLY	CA-C-N	6.34	130.76	121.31
1	A	198	GLY	C-N-CA	6.34	130.76	121.31
1	G	272	LYS	N-CA-CB	-6.34	100.48	110.06
1	C	272	LYS	N-CA-CB	-6.34	100.49	110.06
1	F	40	LEU	CB-CA-C	-6.34	99.64	110.16
1	A	27	VAL	N-CA-C	6.34	116.49	110.53
1	G	27	VAL	N-CA-C	6.34	116.49	110.53
1	A	40	LEU	CB-CA-C	-6.33	99.65	110.16
1	D	272	LYS	N-CA-CB	-6.33	100.50	110.06
1	F	272	LYS	N-CA-CB	-6.33	100.50	110.06
1	A	272	LYS	N-CA-CB	-6.33	100.50	110.06
1	M	467	ASN	CA-CB-CG	-6.33	106.27	112.60
1	B	40	LEU	CB-CA-C	-6.33	99.66	110.16
1	G	40	LEU	CB-CA-C	-6.32	99.66	110.16
1	C	40	LEU	CB-CA-C	-6.32	99.67	110.16
1	E	272	LYS	N-CA-CB	-6.31	100.53	110.06
1	D	40	LEU	CB-CA-C	-6.31	99.69	110.16
1	E	40	LEU	CB-CA-C	-6.30	99.69	110.16
1	F	244	GLY	N-CA-C	-6.30	107.02	115.21
1	M	67	GLU	CB-CG-CD	6.28	123.28	112.60
1	E	244	GLY	N-CA-C	-6.28	107.05	115.21
1	D	168	LYS	CB-CA-C	6.27	120.67	110.95
1	E	168	LYS	CB-CA-C	6.26	120.66	110.95
1	E	461	GLU	CB-CA-C	6.26	116.37	110.17
1	B	168	LYS	CB-CA-C	6.26	120.65	110.95
1	A	168	LYS	CB-CA-C	6.25	120.64	110.95
1	I	473	ASP	N-CA-CB	6.25	122.10	111.66
1	D	244	GLY	N-CA-C	-6.25	107.09	115.21
1	G	168	LYS	CB-CA-C	6.25	120.64	110.95
1	M	473	ASP	N-CA-CB	6.25	122.09	111.66
1	C	244	GLY	N-CA-C	-6.24	107.10	115.21
1	G	244	GLY	N-CA-C	-6.24	107.10	115.21
1	C	168	LYS	CB-CA-C	6.24	120.61	110.95
1	L	217	SER	CB-CA-C	-6.23	104.85	110.71
1	I	67	GLU	CB-CG-CD	6.23	123.19	112.60
1	B	244	GLY	N-CA-C	-6.23	107.11	115.21
1	F	168	LYS	CB-CA-C	6.23	120.60	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	59	GLU	CB-CA-C	6.22	122.34	109.95
1	N	67	GLU	CB-CG-CD	6.22	123.18	112.60
1	H	67	GLU	CB-CG-CD	6.22	123.17	112.60
1	M	112	ASN	CA-C-N	6.22	125.70	119.24
1	M	112	ASN	C-N-CA	6.22	125.70	119.24
1	A	59	GLU	CB-CA-C	6.21	122.31	109.95
1	B	59	GLU	CB-CA-C	6.20	122.29	109.95
1	C	59	GLU	CB-CA-C	6.20	122.29	109.95
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	G	59	GLU	CB-CA-C	6.20	122.28	109.95
1	J	67	GLU	CB-CG-CD	6.19	123.13	112.60
1	E	59	GLU	CB-CA-C	6.19	122.27	109.95
1	F	49	ILE	CA-C-N	-6.19	112.08	122.29
1	F	49	ILE	C-N-CA	-6.19	112.08	122.29
1	A	49	ILE	CA-C-N	-6.18	112.09	122.29
1	A	49	ILE	C-N-CA	-6.18	112.09	122.29
1	B	49	ILE	CA-C-N	-6.17	112.10	122.29
1	B	49	ILE	C-N-CA	-6.17	112.10	122.29
1	A	244	GLY	N-CA-C	-6.17	107.19	115.21
1	E	254	VAL	CB-CA-C	-6.17	101.26	111.32
1	D	254	VAL	CB-CA-C	-6.17	101.27	111.32
1	A	254	VAL	CB-CA-C	-6.16	101.27	111.32
1	C	49	ILE	CA-C-N	-6.16	112.13	122.29
1	C	49	ILE	C-N-CA	-6.16	112.13	122.29
1	G	49	ILE	CA-C-N	-6.16	112.13	122.29
1	G	49	ILE	C-N-CA	-6.16	112.13	122.29
1	F	254	VAL	CB-CA-C	-6.15	101.29	111.32
1	F	332	ILE	CB-CA-C	6.15	119.41	110.98
1	G	254	VAL	CB-CA-C	-6.15	101.30	111.32
1	B	254	VAL	CB-CA-C	-6.14	101.31	111.32
1	L	61	GLU	N-CA-CB	-6.14	100.49	110.81
1	D	332	ILE	CB-CA-C	6.14	119.39	110.98
1	C	332	ILE	CB-CA-C	6.14	119.39	110.98
1	G	332	ILE	CB-CA-C	6.14	119.39	110.98
1	E	49	ILE	CA-C-N	-6.13	112.17	122.29
1	E	49	ILE	C-N-CA	-6.13	112.17	122.29
1	C	254	VAL	CB-CA-C	-6.13	101.33	111.32
1	A	332	ILE	CB-CA-C	6.13	119.37	110.98
1	E	332	ILE	CB-CA-C	6.12	119.37	110.98
1	B	332	ILE	CB-CA-C	6.12	119.36	110.98
1	D	194	GLN	N-CA-CB	-6.07	100.48	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	ILE	N-CA-C	6.07	117.52	108.54
1	G	60	ILE	N-CA-C	6.06	117.51	108.54
1	A	194	GLN	N-CA-CB	-6.06	100.50	110.68
1	B	193	MET	CA-C-N	-6.05	111.13	121.85
1	B	193	MET	C-N-CA	-6.05	111.13	121.85
1	N	59	GLU	CB-CA-C	6.05	121.34	109.72
1	F	206	ASN	CB-CA-C	-6.05	106.83	114.40
1	L	67	GLU	CB-CG-CD	6.05	122.89	112.60
1	E	194	GLN	N-CA-CB	-6.04	100.52	110.68
1	L	473	ASP	N-CA-CB	6.04	121.75	111.66
1	C	60	ILE	N-CA-C	6.04	117.48	108.54
1	A	60	ILE	N-CA-C	6.03	117.47	108.54
1	G	194	GLN	N-CA-CB	-6.03	100.55	110.68
1	D	60	ILE	N-CA-C	6.02	117.46	108.54
1	K	473	ASP	N-CA-CB	6.01	122.70	111.52
1	G	193	MET	CA-C-N	-6.01	114.52	122.99
1	G	193	MET	C-N-CA	-6.01	114.52	122.99
1	G	192	GLY	CA-C-N	-6.00	114.43	122.72
1	G	192	GLY	C-N-CA	-6.00	114.43	122.72
1	E	60	ILE	N-CA-C	6.00	117.42	108.54
1	G	200	LEU	N-CA-CB	6.00	120.63	110.49
1	F	60	ILE	N-CA-C	5.99	117.40	108.54
1	H	361	ASP	CA-CB-CG	-5.98	106.62	112.60
1	D	516	THR	CA-CB-OG1	5.97	118.56	109.60
1	N	361	ASP	CA-CB-CG	-5.97	106.63	112.60
1	J	361	ASP	CA-CB-CG	-5.96	106.64	112.60
1	I	361	ASP	CA-CB-CG	-5.96	106.64	112.60
1	F	194	GLN	N-CA-CB	-5.94	100.49	110.83
1	G	273	VAL	CB-CA-C	-5.94	102.65	111.80
1	F	5	ASP	N-CA-C	-5.93	99.52	109.07
1	B	5	ASP	N-CA-C	-5.93	99.52	109.07
1	A	5	ASP	N-CA-C	-5.93	99.53	109.07
1	D	5	ASP	N-CA-C	-5.93	99.53	109.07
1	E	273	VAL	CB-CA-C	-5.92	102.68	111.80
1	E	5	ASP	N-CA-C	-5.92	99.54	109.07
1	F	273	VAL	CB-CA-C	-5.92	102.68	111.80
1	N	467	ASN	CA-CB-CG	-5.92	106.68	112.60
1	C	273	VAL	CB-CA-C	-5.92	102.69	111.80
1	A	273	VAL	CB-CA-C	-5.91	102.70	111.80
1	C	5	ASP	N-CA-C	-5.91	99.56	109.07
1	G	5	ASP	N-CA-C	-5.91	99.56	109.07
1	A	196	ASP	CA-CB-CG	-5.90	106.70	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	VAL	CB-CA-C	-5.90	102.71	111.80
1	D	273	VAL	CB-CA-C	-5.90	102.72	111.80
1	K	67	GLU	CB-CG-CD	5.89	122.62	112.60
1	C	311	LYS	N-CA-C	-5.89	104.86	111.28
1	B	311	LYS	N-CA-C	-5.89	104.86	111.28
1	E	311	LYS	N-CA-C	-5.89	104.86	111.28
1	F	311	LYS	N-CA-C	-5.88	104.87	111.28
1	H	265	ASN	CA-CB-CG	-5.87	106.73	112.60
1	F	402	ALA	N-CA-CB	-5.87	101.47	110.16
1	D	402	ALA	N-CA-CB	-5.87	101.48	110.16
1	E	402	ALA	N-CA-CB	-5.87	101.48	110.16
1	A	402	ALA	N-CA-CB	-5.87	101.48	110.16
1	K	265	ASN	CA-CB-CG	-5.87	106.73	112.60
1	M	265	ASN	CA-CB-CG	-5.87	106.73	112.60
1	D	87	ASP	CA-CB-CG	-5.86	106.74	112.60
1	G	87	ASP	CA-CB-CG	-5.86	106.74	112.60
1	C	402	ALA	N-CA-CB	-5.86	101.48	110.16
1	G	311	LYS	N-CA-C	-5.86	104.89	111.28
1	A	311	LYS	N-CA-C	-5.85	104.91	111.28
1	E	461	GLU	CA-C-N	5.85	125.32	119.24
1	E	461	GLU	C-N-CA	5.85	125.32	119.24
1	G	402	ALA	N-CA-CB	-5.85	101.51	110.16
1	K	361	ASP	CA-CB-CG	-5.85	106.75	112.60
1	B	87	ASP	CA-CB-CG	-5.84	106.76	112.60
1	B	402	ALA	N-CA-CB	-5.84	101.52	110.16
1	D	461	GLU	CA-C-N	5.84	125.31	119.24
1	D	461	GLU	C-N-CA	5.84	125.31	119.24
1	I	265	ASN	CA-CB-CG	-5.82	106.78	112.60
1	L	265	ASN	CA-CB-CG	-5.81	106.79	112.60
1	J	518	GLU	CB-CG-CD	5.81	122.47	112.60
1	N	61	GLU	N-CA-CB	-5.80	101.06	110.81
1	A	461	GLU	CA-C-N	5.80	125.27	119.24
1	A	461	GLU	C-N-CA	5.80	125.27	119.24
1	D	311	LYS	N-CA-C	-5.80	104.96	111.28
1	F	87	ASP	CA-CB-CG	-5.80	106.80	112.60
1	L	361	ASP	CA-CB-CG	-5.80	106.80	112.60
1	E	87	ASP	CA-CB-CG	-5.79	106.81	112.60
1	J	265	ASN	CA-CB-CG	-5.79	106.81	112.60
1	M	523	ASP	CB-CA-C	5.79	120.19	109.54
1	C	87	ASP	CA-CB-CG	-5.78	106.82	112.60
1	E	301	ILE	CB-CA-C	5.78	119.95	111.33
1	G	301	ILE	CB-CA-C	5.78	119.94	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	265	ASN	CA-CB-CG	-5.78	106.82	112.60
1	D	301	ILE	CB-CA-C	5.78	119.94	111.33
1	N	473	ASP	N-CA-CB	5.78	122.27	111.52
1	F	461	GLU	CA-C-N	5.77	125.24	119.24
1	F	461	GLU	C-N-CA	5.77	125.24	119.24
1	H	473	ASP	N-CA-CB	5.77	122.26	111.52
1	B	301	ILE	CB-CA-C	5.77	119.93	111.33
1	B	461	GLU	CA-C-N	5.77	125.24	119.24
1	B	461	GLU	C-N-CA	5.77	125.24	119.24
1	C	461	GLU	CA-C-N	5.76	125.23	119.24
1	C	461	GLU	C-N-CA	5.76	125.23	119.24
1	F	301	ILE	CB-CA-C	5.76	119.91	111.33
1	A	87	ASP	CA-CB-CG	-5.75	106.85	112.60
1	A	301	ILE	CB-CA-C	5.75	119.89	111.33
1	E	473	ASP	CA-CB-CG	-5.74	106.86	112.60
1	B	473	ASP	CA-CB-CG	-5.74	106.86	112.60
1	D	473	ASP	CA-CB-CG	-5.74	106.86	112.60
1	J	59	GLU	CB-CA-C	5.74	120.74	109.72
1	K	495	ASP	CB-CA-C	5.74	117.76	108.87
1	M	361	ASP	CA-CB-CG	-5.74	106.86	112.60
1	G	473	ASP	CA-CB-CG	-5.74	106.86	112.60
1	C	301	ILE	CB-CA-C	5.73	119.87	111.33
1	C	473	ASP	CA-CB-CG	-5.73	106.87	112.60
1	H	61	GLU	N-CA-CB	-5.73	101.18	110.81
1	M	495	ASP	CB-CA-C	5.73	117.75	108.87
1	K	267	MET	CB-CA-C	5.73	121.23	112.00
1	B	195	PHE	CA-CB-CG	-5.72	108.08	113.80
1	A	473	ASP	CA-CB-CG	-5.72	106.88	112.60
1	F	473	ASP	CA-CB-CG	-5.71	106.89	112.60
1	N	495	ASP	CB-CA-C	5.70	117.71	108.87
1	G	461	GLU	CA-C-N	5.69	125.16	119.24
1	G	461	GLU	C-N-CA	5.69	125.16	119.24
1	J	230	ILE	CB-CA-C	-5.69	102.89	112.16
1	J	61	GLU	N-CA-CB	-5.68	101.26	110.81
1	L	230	ILE	CB-CA-C	-5.68	102.90	112.16
1	A	153	ASN	CA-CB-CG	-5.68	106.92	112.60
1	E	153	ASN	CA-CB-CG	-5.67	106.92	112.60
1	I	523	ASP	CB-CA-C	5.66	119.95	109.54
1	D	198	GLY	O-C-N	-5.65	116.45	123.12
1	F	461	GLU	CB-CA-C	5.65	116.57	110.08
1	A	272	LYS	CB-CG-CD	5.64	124.28	111.30
1	G	330	THR	CB-CA-C	-5.64	100.44	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	68	ASN	CA-CB-CG	5.64	118.24	112.60
1	I	230	ILE	CB-CA-C	-5.64	102.97	112.16
1	D	330	THR	CB-CA-C	-5.64	100.45	109.75
1	N	230	ILE	CB-CA-C	-5.63	102.98	112.16
1	D	272	LYS	CB-CG-CD	5.63	124.25	111.30
1	G	272	LYS	CB-CG-CD	5.63	124.25	111.30
1	E	272	LYS	CB-CG-CD	5.63	124.25	111.30
1	C	272	LYS	CB-CG-CD	5.63	124.25	111.30
1	C	330	THR	CB-CA-C	-5.63	100.47	109.75
1	B	272	LYS	CB-CG-CD	5.62	124.23	111.30
1	E	330	THR	CB-CA-C	-5.62	100.48	109.75
1	B	330	THR	CB-CA-C	-5.62	100.48	109.75
1	A	330	THR	CB-CA-C	-5.62	100.48	109.75
1	F	272	LYS	CB-CG-CD	5.61	124.21	111.30
1	F	330	THR	CB-CA-C	-5.61	100.49	109.75
1	D	515	ILE	CA-C-N	-5.61	115.55	122.84
1	D	515	ILE	C-N-CA	-5.61	115.55	122.84
1	E	515	ILE	CA-C-N	-5.61	115.55	122.84
1	E	515	ILE	C-N-CA	-5.61	115.55	122.84
1	M	13	ARG	N-CA-CB	5.60	118.08	109.91
1	H	467	ASN	CA-CB-CG	-5.59	107.01	112.60
1	E	147	VAL	CB-CA-C	-5.59	104.60	112.14
1	L	467	ASN	CA-CB-CG	-5.59	107.01	112.60
1	B	181	THR	N-CA-C	-5.58	105.34	111.82
1	B	515	ILE	CA-C-N	-5.58	115.58	122.84
1	B	515	ILE	C-N-CA	-5.58	115.58	122.84
1	D	147	VAL	CB-CA-C	-5.58	104.61	112.14
1	B	147	VAL	CB-CA-C	-5.57	104.62	112.14
1	J	495	ASP	CB-CA-C	5.57	117.51	108.87
1	N	13	ARG	N-CA-CB	5.57	118.05	109.91
1	D	181	THR	N-CA-C	-5.57	105.36	111.82
1	A	181	THR	N-CA-C	-5.57	105.36	111.82
1	C	147	VAL	CB-CA-C	-5.57	104.62	112.14
1	G	147	VAL	CB-CA-C	-5.57	104.62	112.14
1	A	147	VAL	CB-CA-C	-5.56	104.63	112.14
1	F	147	VAL	CB-CA-C	-5.56	104.63	112.14
1	D	246	PRO	N-CA-CB	5.55	109.21	103.38
1	E	181	THR	N-CA-C	-5.54	105.39	111.82
1	A	246	PRO	N-CA-CB	5.54	109.20	103.38
1	G	246	PRO	N-CA-CB	5.54	109.20	103.38
1	G	181	THR	N-CA-C	-5.54	105.39	111.82
1	F	181	THR	N-CA-C	-5.54	105.39	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	13	ARG	N-CA-CB	5.54	118.00	109.91
1	H	495	ASP	CB-CA-C	5.53	117.44	108.87
1	M	518	GLU	CB-CG-CD	5.53	122.00	112.60
1	G	515	ILE	CA-C-N	-5.53	115.66	122.84
1	G	515	ILE	C-N-CA	-5.53	115.66	122.84
1	B	246	PRO	N-CA-CB	5.53	109.18	103.38
1	C	246	PRO	N-CA-CB	5.53	109.18	103.38
1	E	246	PRO	N-CA-CB	5.53	109.18	103.38
1	F	515	ILE	CA-C-N	-5.52	115.66	122.84
1	F	515	ILE	C-N-CA	-5.52	115.66	122.84
1	C	181	THR	N-CA-C	-5.52	105.42	111.82
1	I	495	ASP	CB-CA-C	5.52	117.42	108.87
1	I	334	ASP	CA-CB-CG	5.51	118.11	112.60
1	K	60	ILE	N-CA-C	5.51	116.31	107.98
1	C	515	ILE	CA-C-N	-5.51	115.68	122.84
1	C	515	ILE	C-N-CA	-5.51	115.68	122.84
1	E	328	ASP	CA-CB-CG	-5.51	107.09	112.60
1	J	13	ARG	N-CA-CB	5.51	117.95	109.91
1	F	246	PRO	N-CA-CB	5.51	109.16	103.38
1	D	199	TYR	CA-CB-CG	-5.51	103.99	113.90
1	J	267	MET	CB-CA-C	5.51	120.87	112.00
1	B	63	GLU	CB-CG-CD	5.50	121.96	112.60
1	E	173	GLY	N-CA-C	-5.50	104.09	112.51
1	E	172	GLU	N-CA-CB	5.50	117.99	110.01
1	B	396	VAL	CB-CA-C	-5.50	104.71	112.14
1	C	396	VAL	CB-CA-C	-5.50	104.71	112.14
1	A	63	GLU	CB-CG-CD	5.50	121.95	112.60
1	A	515	ILE	CA-C-N	-5.50	115.69	122.84
1	A	515	ILE	C-N-CA	-5.50	115.69	122.84
1	C	172	GLU	N-CA-CB	5.50	117.98	110.01
1	J	68	ASN	CA-CB-CG	5.50	118.10	112.60
1	D	63	GLU	CB-CG-CD	5.50	121.94	112.60
1	E	63	GLU	CB-CG-CD	5.50	121.95	112.60
1	B	328	ASP	CA-CB-CG	-5.49	107.11	112.60
1	G	63	GLU	CB-CG-CD	5.49	121.93	112.60
1	C	328	ASP	CA-CB-CG	-5.49	107.11	112.60
1	G	173	GLY	N-CA-C	-5.49	104.11	112.51
1	H	60	ILE	N-CA-C	5.49	116.27	107.98
1	L	495	ASP	CB-CA-C	5.49	117.38	108.87
1	L	115	ASP	CA-CB-CG	-5.49	107.11	112.60
1	G	396	VAL	CB-CA-C	-5.48	104.74	112.14
1	A	328	ASP	CA-CB-CG	-5.48	107.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	GLU	CB-CG-CD	5.48	121.92	112.60
1	B	172	GLU	N-CA-CB	5.48	117.96	110.01
1	F	328	ASP	CA-CB-CG	-5.48	107.12	112.60
1	F	172	GLU	N-CA-CB	5.48	117.95	110.01
1	A	173	GLY	N-CA-C	-5.48	104.13	112.51
1	N	523	ASP	CB-CA-C	5.47	119.61	109.54
1	A	457	ASN	CB-CA-C	5.47	121.75	110.31
1	E	249	ILE	CB-CA-C	-5.47	103.65	111.31
1	C	63	GLU	CB-CG-CD	5.47	121.90	112.60
1	E	457	ASN	CB-CA-C	5.47	121.74	110.31
1	F	173	GLY	N-CA-C	-5.47	104.14	112.51
1	A	249	ILE	CB-CA-C	-5.47	103.66	111.31
1	G	172	GLU	N-CA-CB	5.47	117.94	110.01
1	N	60	ILE	N-CA-C	5.47	116.23	107.98
1	A	172	GLU	N-CA-CB	5.46	117.93	110.01
1	A	396	VAL	CB-CA-C	-5.46	104.77	112.14
1	D	396	VAL	CB-CA-C	-5.46	104.77	112.14
1	B	457	ASN	CB-CA-C	5.46	121.72	110.31
1	E	396	VAL	CB-CA-C	-5.46	104.77	112.14
1	N	115	ASP	CA-CB-CG	-5.46	107.14	112.60
1	C	249	ILE	CB-CA-C	-5.46	103.67	111.31
1	F	396	VAL	CB-CA-C	-5.46	104.77	112.14
1	A	286	LYS	N-CA-CB	-5.46	102.10	110.12
1	D	172	GLU	N-CA-CB	5.46	117.92	110.01
1	F	249	ILE	CB-CA-C	-5.46	103.67	111.31
1	B	173	GLY	N-CA-C	-5.45	104.17	112.51
1	F	457	ASN	CB-CA-C	5.45	121.71	110.31
1	G	249	ILE	CB-CA-C	-5.45	103.68	111.31
1	G	283	ASP	CA-CB-CG	-5.45	107.15	112.60
1	B	249	ILE	CB-CA-C	-5.45	103.68	111.31
1	E	156	GLU	CB-CA-C	-5.45	98.92	110.31
1	G	457	ASN	CB-CA-C	5.45	121.70	110.31
1	D	249	ILE	CB-CA-C	-5.45	103.69	111.31
1	E	283	ASP	CA-CB-CG	-5.45	107.15	112.60
1	I	60	ILE	N-CA-C	5.45	116.20	107.98
1	D	156	GLU	CB-CA-C	-5.44	98.94	110.31
1	E	28	LYS	N-CA-C	5.44	119.02	112.38
1	F	283	ASP	CA-CB-CG	-5.44	107.16	112.60
1	L	267	MET	CB-CA-C	5.44	120.76	112.00
1	D	328	ASP	CA-CB-CG	-5.44	107.16	112.60
1	G	286	LYS	N-CA-CB	-5.44	102.12	110.12
1	E	286	LYS	N-CA-CB	-5.44	102.13	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	206	ASN	CA-CB-CG	-5.44	107.16	112.60
1	C	173	GLY	N-CA-C	-5.43	104.19	112.51
1	C	283	ASP	CA-CB-CG	-5.43	107.17	112.60
1	D	286	LYS	N-CA-CB	-5.43	102.13	110.12
1	K	328	ASP	N-CA-CB	-5.43	103.18	111.66
1	G	28	LYS	N-CA-C	5.43	119.01	112.38
1	D	173	GLY	N-CA-C	-5.43	104.20	112.51
1	C	286	LYS	N-CA-CB	-5.42	102.14	110.12
1	F	286	LYS	N-CA-CB	-5.42	102.15	110.12
1	B	283	ASP	CA-CB-CG	-5.42	107.18	112.60
1	D	28	LYS	N-CA-C	5.42	118.99	112.38
1	B	286	LYS	N-CA-CB	-5.42	102.15	110.12
1	C	457	ASN	CB-CA-C	5.42	121.64	110.31
1	B	156	GLU	CB-CA-C	-5.42	98.99	110.31
1	K	467	ASN	CA-CB-CG	-5.42	107.18	112.60
1	H	523	ASP	CB-CA-C	5.42	119.50	109.54
1	G	156	GLU	CB-CA-C	-5.41	99.00	110.31
1	I	267	MET	CB-CA-C	5.41	120.71	112.00
1	N	267	MET	CB-CA-C	5.41	120.72	112.00
1	D	283	ASP	CA-CB-CG	-5.41	107.19	112.60
1	G	328	ASP	CA-CB-CG	-5.41	107.19	112.60
1	C	28	LYS	N-CA-C	5.41	118.98	112.38
1	A	283	ASP	CA-CB-CG	-5.41	107.19	112.60
1	B	28	LYS	N-CA-C	5.40	118.97	112.38
1	D	457	ASN	CB-CA-C	5.40	121.61	110.31
1	N	334	ASP	CA-CB-CG	5.39	118.00	112.60
1	C	374	GLY	N-CA-C	-5.38	106.27	112.73
1	K	13	ARG	N-CA-CB	5.38	117.77	109.91
1	L	60	ILE	N-CA-C	5.38	116.11	107.98
1	I	115	ASP	CA-CB-CG	-5.38	107.22	112.60
1	L	13	ARG	N-CA-CB	5.38	117.76	109.91
1	E	153	ASN	N-CA-CB	5.37	119.57	110.49
1	F	374	GLY	N-CA-C	-5.37	106.28	112.73
1	M	267	MET	CB-CA-C	5.37	120.65	112.00
1	A	28	LYS	N-CA-C	5.37	118.93	112.38
1	G	461	GLU	CB-CA-C	5.36	115.48	110.17
1	A	334	ASP	CB-CA-C	5.36	121.09	110.42
1	E	334	ASP	CB-CA-C	5.36	121.09	110.42
1	F	334	ASP	CB-CA-C	5.36	121.09	110.42
1	G	334	ASP	CB-CA-C	5.36	121.09	110.42
1	D	157	THR	N-CA-CB	5.36	117.73	109.91
1	B	334	ASP	CB-CA-C	5.36	121.08	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	312	ALA	CB-CA-C	5.36	119.39	109.54
1	B	112	ASN	CB-CA-C	-5.35	101.23	109.85
1	C	434	GLU	N-CA-CB	5.35	117.77	110.01
1	A	374	GLY	N-CA-C	-5.35	106.31	112.73
1	C	334	ASP	CB-CA-C	5.35	121.07	110.42
1	D	334	ASP	CB-CA-C	5.35	121.07	110.42
1	D	434	GLU	N-CA-CB	5.35	117.77	110.01
1	F	28	LYS	N-CA-C	5.35	118.90	112.38
1	A	516	THR	CA-C-N	5.34	130.65	122.95
1	A	516	THR	C-N-CA	5.34	130.65	122.95
1	B	434	GLU	N-CA-CB	5.34	117.76	110.01
1	G	312	ALA	CB-CA-C	5.34	119.37	109.54
1	C	115	ASP	CA-CB-CG	-5.34	107.26	112.60
1	F	434	GLU	N-CA-CB	5.34	117.75	110.01
1	I	327	LYS	CB-CA-C	5.34	119.35	110.81
1	B	157	THR	N-CA-CB	5.34	117.70	109.91
1	B	312	ALA	CB-CA-C	5.33	119.36	109.54
1	E	434	GLU	N-CA-CB	5.33	117.75	110.01
1	G	157	THR	N-CA-CB	5.33	117.70	109.91
1	E	157	THR	N-CA-CB	5.33	117.69	109.91
1	A	153	ASN	N-CA-CB	5.33	119.50	110.49
1	A	521	VAL	CB-CA-C	5.33	118.11	110.33
1	H	252	GLU	N-CA-CB	5.33	117.95	110.12
1	C	112	ASN	CB-CA-C	-5.33	101.27	109.85
1	E	516	THR	CA-C-N	5.33	130.62	122.95
1	E	516	THR	C-N-CA	5.33	130.62	122.95
1	F	516	THR	CA-C-N	5.33	130.62	122.95
1	F	516	THR	C-N-CA	5.33	130.62	122.95
1	J	60	ILE	N-CA-C	5.33	116.02	107.98
1	G	516	THR	CA-C-N	5.32	130.62	122.95
1	G	516	THR	C-N-CA	5.32	130.62	122.95
1	D	312	ALA	CB-CA-C	5.32	119.33	109.54
1	G	434	GLU	N-CA-CB	5.32	117.73	110.01
1	E	312	ALA	CB-CA-C	5.32	119.33	109.54
1	G	521	VAL	CB-CA-C	5.32	118.09	110.33
1	C	516	THR	CA-C-N	5.32	130.60	122.95
1	C	516	THR	C-N-CA	5.32	130.60	122.95
1	K	523	ASP	CB-CA-C	5.31	119.32	109.54
1	A	312	ALA	CB-CA-C	5.31	119.31	109.54
1	A	11	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	441	LYS	CB-CA-C	5.31	119.61	110.79
1	F	312	ALA	CB-CA-C	5.31	119.31	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	60	ILE	N-CA-C	5.31	116.00	107.98
1	D	374	GLY	N-CA-C	-5.31	106.36	112.73
1	D	516	THR	CA-C-N	5.31	130.59	122.95
1	D	516	THR	C-N-CA	5.31	130.59	122.95
1	L	518	GLU	CB-CG-CD	5.31	121.62	112.60
1	E	374	GLY	N-CA-C	-5.31	106.36	112.73
1	L	68	ASN	CA-CB-CG	5.30	117.90	112.60
1	E	521	VAL	CB-CA-C	5.30	118.07	110.33
1	F	521	VAL	CB-CA-C	5.30	118.07	110.33
1	B	516	THR	CA-C-N	5.30	130.58	122.95
1	B	516	THR	C-N-CA	5.30	130.58	122.95
1	C	521	VAL	CB-CA-C	5.29	118.06	110.33
1	B	18	ARG	CB-CG-CD	5.29	123.48	111.30
1	H	267	MET	CB-CA-C	5.29	120.52	112.00
1	G	374	GLY	N-CA-C	-5.29	106.39	112.73
1	A	303	GLU	N-CA-CB	5.28	118.47	110.28
1	B	374	GLY	N-CA-C	-5.28	106.39	112.73
1	F	18	ARG	CB-CG-CD	5.28	123.43	111.30
1	D	521	VAL	CB-CA-C	5.27	118.03	110.33
1	E	227	ILE	CA-C-N	5.27	127.61	120.44
1	E	227	ILE	C-N-CA	5.27	127.61	120.44
1	G	18	ARG	CB-CG-CD	5.27	123.42	111.30
1	L	334	ASP	CA-CB-CG	5.27	117.87	112.60
1	C	18	ARG	CB-CG-CD	5.26	123.41	111.30
1	F	161	LEU	CB-CA-C	-5.26	102.55	110.92
1	F	389	MET	CB-CA-C	-5.26	102.05	110.79
1	G	389	MET	CB-CA-C	-5.26	102.05	110.79
1	B	273	VAL	N-CA-CB	5.26	118.29	111.19
1	D	18	ARG	CB-CG-CD	5.26	123.40	111.30
1	E	18	ARG	CB-CG-CD	5.26	123.40	111.30
1	F	303	GLU	N-CA-CB	5.26	118.43	110.28
1	G	227	ILE	CA-C-N	5.26	127.60	120.44
1	G	227	ILE	C-N-CA	5.26	127.60	120.44
1	B	389	MET	CB-CA-C	-5.26	102.06	110.79
1	E	11	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	227	ILE	CA-C-N	5.26	127.59	120.44
1	B	227	ILE	C-N-CA	5.26	127.59	120.44
1	A	157	THR	N-CA-CB	5.26	117.59	109.91
1	A	389	MET	CB-CA-C	-5.25	102.07	110.79
1	A	18	ARG	CB-CG-CD	5.25	123.38	111.30
1	M	217	SER	CB-CA-C	-5.25	105.77	110.71
1	E	273	VAL	N-CA-CB	5.25	118.28	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	273	VAL	N-CA-CB	5.25	118.28	111.19
1	M	68	ASN	CA-CB-CG	5.25	117.85	112.60
1	A	273	VAL	N-CA-CB	5.25	118.27	111.19
1	D	303	GLU	N-CA-CB	5.25	118.41	110.28
1	N	321	LYS	N-CA-CB	5.25	117.83	110.12
1	D	161	LEU	CB-CA-C	-5.25	102.58	110.92
1	C	227	ILE	CA-C-N	5.24	127.57	120.44
1	C	227	ILE	C-N-CA	5.24	127.57	120.44
1	M	495	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	227	ILE	CA-C-N	5.24	127.57	120.44
1	A	227	ILE	C-N-CA	5.24	127.57	120.44
1	E	303	GLU	N-CA-CB	5.24	118.40	110.28
1	E	336	VAL	N-CA-CB	5.24	118.44	110.58
1	C	336	VAL	N-CA-CB	5.24	118.44	110.58
1	B	198	GLY	CA-C-N	5.24	131.54	121.54
1	B	198	GLY	C-N-CA	5.24	131.54	121.54
1	C	303	GLU	N-CA-CB	5.24	118.40	110.28
1	D	389	MET	CB-CA-C	-5.24	102.10	110.79
1	E	389	MET	CB-CA-C	-5.24	102.10	110.79
1	G	161	LEU	CB-CA-C	-5.23	102.60	110.92
1	B	521	VAL	CB-CA-C	5.23	117.97	110.33
1	C	161	LEU	CB-CA-C	-5.23	102.60	110.92
1	C	389	MET	CB-CA-C	-5.23	102.11	110.79
1	F	157	THR	N-CA-CB	5.23	117.55	109.91
1	A	161	LEU	CB-CA-C	-5.23	102.60	110.92
1	B	161	LEU	CB-CA-C	-5.23	102.60	110.92
1	C	272	LYS	CG-CD-CE	5.23	123.33	111.30
1	E	161	LEU	CB-CA-C	-5.23	102.60	110.92
1	B	303	GLU	N-CA-CB	5.23	118.38	110.28
1	C	273	VAL	N-CA-CB	5.23	118.25	111.19
1	D	336	VAL	N-CA-CB	5.23	118.42	110.58
1	G	200	LEU	CA-CB-CG	-5.23	98.01	116.30
1	J	334	ASP	CA-CB-CG	5.23	117.83	112.60
1	D	272	LYS	CG-CD-CE	5.22	123.31	111.30
1	D	227	ILE	CA-C-N	5.22	127.54	120.44
1	D	227	ILE	C-N-CA	5.22	127.54	120.44
1	G	273	VAL	N-CA-CB	5.22	118.24	111.19
1	E	272	LYS	CG-CD-CE	5.22	123.31	111.30
1	G	303	GLU	N-CA-CB	5.22	118.37	110.28
1	C	157	THR	N-CA-CB	5.22	117.53	109.91
1	G	272	LYS	CG-CD-CE	5.22	123.30	111.30
1	F	272	LYS	CG-CD-CE	5.21	123.29	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	LYS	CG-CD-CE	5.21	123.29	111.30
1	F	115	ASP	CA-CB-CG	-5.21	107.39	112.60
1	G	336	VAL	N-CA-CB	5.21	118.40	110.58
1	F	273	VAL	N-CA-CB	5.21	118.23	111.19
1	E	515	ILE	N-CA-CB	5.21	116.64	110.55
1	A	336	VAL	N-CA-CB	5.21	118.39	110.58
1	B	115	ASP	CA-CB-CG	-5.20	107.40	112.60
1	I	13	ARG	N-CA-CB	5.20	117.50	109.91
1	A	115	ASP	CA-CB-CG	-5.20	107.40	112.60
1	D	189	VAL	CA-C-N	-5.20	116.61	122.48
1	D	189	VAL	C-N-CA	-5.20	116.61	122.48
1	F	227	ILE	CA-C-N	5.20	127.51	120.44
1	F	227	ILE	C-N-CA	5.20	127.51	120.44
1	A	272	LYS	CG-CD-CE	5.19	123.24	111.30
1	B	336	VAL	N-CA-CB	5.19	118.37	110.58
1	J	327	LYS	CB-CA-C	5.19	119.12	110.81
1	C	209	GLU	N-CA-C	-5.19	106.90	113.18
1	F	336	VAL	N-CA-CB	5.19	118.36	110.58
1	J	425	LYS	CB-CA-C	5.19	119.10	110.90
1	A	156	GLU	CB-CA-C	-5.18	99.48	110.31
1	C	47	PRO	CA-N-CD	-5.18	104.75	112.00
1	B	303	GLU	CB-CG-CD	5.17	121.39	112.60
1	C	303	GLU	CB-CG-CD	5.17	121.40	112.60
1	G	25	ASP	CA-CB-CG	-5.17	107.42	112.60
1	A	25	ASP	CA-CB-CG	-5.17	107.43	112.60
1	M	334	ASP	CA-CB-CG	5.17	117.77	112.60
1	D	25	ASP	CA-CB-CG	-5.17	107.43	112.60
1	A	47	PRO	CA-N-CD	-5.17	104.77	112.00
1	C	25	ASP	CA-CB-CG	-5.17	107.43	112.60
1	D	303	GLU	CB-CG-CD	5.17	121.38	112.60
1	D	115	ASP	CA-CB-CG	-5.17	107.44	112.60
1	F	47	PRO	CA-N-CD	-5.16	104.77	112.00
1	F	303	GLU	CB-CG-CD	5.16	121.38	112.60
1	G	303	GLU	CB-CG-CD	5.16	121.38	112.60
1	G	47	PRO	CA-N-CD	-5.16	104.78	112.00
1	K	388	GLU	CB-CA-C	-5.16	102.78	110.88
1	G	38	VAL	CA-C-N	-5.16	116.45	123.10
1	G	38	VAL	C-N-CA	-5.16	116.45	123.10
1	D	47	PRO	CA-N-CD	-5.16	104.78	112.00
1	E	25	ASP	CA-CB-CG	-5.15	107.45	112.60
1	M	230	ILE	CB-CA-C	-5.15	103.76	112.16
1	B	25	ASP	CA-CB-CG	-5.15	107.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	47	PRO	CA-N-CD	-5.15	104.79	112.00
1	B	47	PRO	CA-N-CD	-5.15	104.79	112.00
1	E	303	GLU	CB-CG-CD	5.15	121.35	112.60
1	K	495	ASP	CA-CB-CG	5.15	117.75	112.60
1	F	38	VAL	CA-C-N	-5.14	116.46	123.10
1	F	38	VAL	C-N-CA	-5.14	116.46	123.10
1	E	224	ASP	CB-CA-C	5.14	119.97	110.56
1	A	303	GLU	CB-CG-CD	5.14	121.34	112.60
1	B	515	ILE	N-CA-CB	5.14	116.56	110.55
1	E	115	ASP	CA-CB-CG	-5.14	107.46	112.60
1	E	38	VAL	CA-C-N	-5.14	116.47	123.10
1	E	38	VAL	C-N-CA	-5.14	116.47	123.10
1	A	224	ASP	CB-CA-C	5.13	119.96	110.56
1	E	225	LYS	CA-C-N	-5.13	113.30	122.07
1	E	225	LYS	C-N-CA	-5.13	113.30	122.07
1	A	515	ILE	N-CA-CB	5.13	116.55	110.55
1	C	224	ASP	CB-CA-C	5.13	119.95	110.56
1	B	224	ASP	CB-CA-C	5.13	119.94	110.56
1	G	515	ILE	N-CA-CB	5.13	116.55	110.55
1	D	441	LYS	CB-CA-C	5.12	119.30	110.79
1	I	495	ASP	CA-CB-CG	5.12	117.72	112.60
1	F	25	ASP	CA-CB-CG	-5.12	107.48	112.60
1	L	388	GLU	CB-CA-C	-5.12	102.84	110.88
1	E	49	ILE	N-CA-CB	-5.12	105.45	111.90
1	D	224	ASP	CB-CA-C	5.11	119.92	110.56
1	F	156	GLU	CB-CA-C	-5.11	99.63	110.31
1	B	441	LYS	CB-CA-C	5.11	119.27	110.79
1	D	38	VAL	CA-C-N	-5.11	116.51	123.10
1	D	38	VAL	C-N-CA	-5.11	116.51	123.10
1	G	441	LYS	CB-CA-C	5.11	119.27	110.79
1	N	388	GLU	CB-CA-C	-5.11	102.86	110.88
1	J	388	GLU	CB-CA-C	-5.11	102.86	110.88
1	A	49	ILE	N-CA-CB	-5.11	105.47	111.90
1	B	225	LYS	CA-C-N	-5.11	113.34	122.07
1	B	225	LYS	C-N-CA	-5.11	113.34	122.07
1	C	198	GLY	CA-C-N	5.10	131.29	121.54
1	C	198	GLY	C-N-CA	5.10	131.29	121.54
1	C	225	LYS	CA-C-N	-5.10	113.34	122.07
1	C	225	LYS	C-N-CA	-5.10	113.34	122.07
1	F	224	ASP	CB-CA-C	5.10	119.89	110.56
1	D	225	LYS	CA-C-N	-5.10	113.36	122.07
1	D	225	LYS	C-N-CA	-5.10	113.36	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	441	LYS	CB-CA-C	5.10	119.25	110.79
1	F	225	LYS	CA-C-N	-5.10	113.36	122.07
1	F	225	LYS	C-N-CA	-5.10	113.36	122.07
1	G	224	ASP	CB-CA-C	5.10	119.89	110.56
1	H	388	GLU	CB-CA-C	-5.10	102.88	110.88
1	B	49	ILE	N-CA-CB	-5.10	105.48	111.90
1	F	441	LYS	CB-CA-C	5.10	119.25	110.79
1	F	49	ILE	N-CA-CB	-5.09	105.49	111.90
1	C	156	GLU	CB-CA-C	-5.09	99.68	110.31
1	K	230	ILE	CB-CA-C	-5.09	103.87	112.16
1	C	354	GLU	CB-CG-CD	5.09	121.25	112.60
1	F	515	ILE	N-CA-CB	5.09	116.50	110.55
1	B	354	GLU	CB-CG-CD	5.08	121.24	112.60
1	C	441	LYS	CB-CA-C	5.08	119.23	110.79
1	B	38	VAL	CA-C-N	-5.08	116.55	123.10
1	B	38	VAL	C-N-CA	-5.08	116.55	123.10
1	C	49	ILE	N-CA-CB	-5.08	105.50	111.90
1	A	38	VAL	CA-C-N	-5.08	116.55	123.10
1	A	38	VAL	C-N-CA	-5.08	116.55	123.10
1	G	225	LYS	CA-C-N	-5.08	113.39	122.07
1	G	225	LYS	C-N-CA	-5.08	113.39	122.07
1	A	225	LYS	CA-C-N	-5.08	113.39	122.07
1	A	225	LYS	C-N-CA	-5.08	113.39	122.07
1	C	38	VAL	CA-C-N	-5.08	116.55	123.10
1	C	38	VAL	C-N-CA	-5.08	116.55	123.10
1	H	68	ASN	CA-CB-CG	5.07	117.67	112.60
1	J	321	LYS	N-CA-CB	5.07	117.57	110.12
1	G	49	ILE	N-CA-CB	-5.07	105.51	111.90
1	L	327	LYS	CB-CA-C	5.07	118.92	110.81
1	D	49	ILE	N-CA-CB	-5.07	105.52	111.90
1	G	354	GLU	CB-CG-CD	5.07	121.21	112.60
1	E	354	GLU	CB-CG-CD	5.06	121.21	112.60
1	F	354	GLU	CB-CG-CD	5.06	121.21	112.60
1	D	354	GLU	CB-CG-CD	5.06	121.20	112.60
1	A	354	GLU	CB-CG-CD	5.05	121.19	112.60
1	G	115	ASP	CA-CB-CG	-5.05	107.55	112.60
1	C	515	ILE	N-CA-CB	5.05	116.46	110.55
1	H	25	ASP	CA-CB-CG	-5.04	107.56	112.60
1	H	334	ASP	CA-CB-CG	5.04	117.64	112.60
1	H	217	SER	CB-CA-C	-5.03	105.98	110.71
1	M	388	GLU	CB-CA-C	-5.03	102.98	110.88
1	H	253	ASP	CA-CB-CG	5.02	117.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	25	ASP	CA-CB-CG	-5.02	107.58	112.60
1	I	321	LYS	N-CA-CB	5.02	117.50	110.12
1	L	25	ASP	CA-CB-CG	-5.02	107.58	112.60
1	M	61	GLU	N-CA-CB	-5.02	102.38	110.81
1	H	495	ASP	CA-CB-CG	5.02	117.62	112.60
1	L	495	ASP	CA-CB-CG	5.02	117.62	112.60
1	M	518	GLU	N-CA-CB	5.02	117.64	110.67
1	A	35	GLY	N-CA-C	-5.01	105.67	112.14
1	B	35	GLY	N-CA-C	-5.01	105.68	112.14
1	M	327	LYS	CB-CA-C	5.01	118.82	110.81
1	B	317	LEU	N-CA-CB	-5.00	102.97	110.17
1	E	317	LEU	N-CA-CB	-5.00	102.97	110.17

There are no chirality outliers.

All (164) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Sidechain
1	A	18	ARG	Sidechain
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
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	18	ARG	Sidechain
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

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Mol	Chain	Res	Type	Group
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	18	ARG	Sidechain
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	18	ARG	Sidechain
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	193	MET	Mainchain
1	E	196	ASP	Peptide
1	E	197	ARG	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
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	18	ARG	Sidechain
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
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	18	ARG	Sidechain
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

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Mol	Chain	Res	Type	Group
1	G	52	ASP	Mainchain
1	H	118	ARG	Sidechain
1	H	362	ARG	Sidechain
1	H	421	ARG	Sidechain
1	H	445	ARG	Sidechain
1	H	478	TYR	Sidechain
1	I	231	ARG	Sidechain
1	I	284	ARG	Sidechain
1	I	285	ARG	Sidechain
1	I	362	ARG	Sidechain
1	I	421	ARG	Sidechain
1	I	445	ARG	Sidechain
1	I	478	TYR	Sidechain
1	J	118	ARG	Sidechain
1	J	231	ARG	Sidechain
1	J	284	ARG	Sidechain
1	J	285	ARG	Sidechain
1	J	362	ARG	Sidechain
1	J	421	ARG	Sidechain
1	J	445	ARG	Sidechain
1	J	478	TYR	Sidechain
1	K	118	ARG	Sidechain
1	K	285	ARG	Sidechain
1	K	362	ARG	Sidechain
1	K	421	ARG	Sidechain
1	K	445	ARG	Sidechain
1	K	478	TYR	Sidechain
1	L	231	ARG	Sidechain
1	L	285	ARG	Sidechain
1	L	322	ARG	Sidechain
1	L	362	ARG	Sidechain
1	L	445	ARG	Sidechain
1	L	478	TYR	Sidechain
1	M	118	ARG	Sidechain
1	M	197	ARG	Sidechain
1	M	362	ARG	Sidechain
1	M	421	ARG	Sidechain
1	M	445	ARG	Sidechain
1	M	478	TYR	Sidechain
1	N	231	ARG	Sidechain
1	N	284	ARG	Sidechain
1	N	285	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	N	322	ARG	Sidechain
1	N	362	ARG	Sidechain
1	N	421	ARG	Sidechain
1	N	445	ARG	Sidechain
1	N	478	TYR	Sidechain
1	N	524	LEU	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3846	0	3968	236	0
1	B	3845	0	3963	243	0
1	C	3845	0	3963	245	0
1	D	3845	0	3963	240	0
1	E	3845	0	3963	246	0
1	F	3845	0	3963	247	0
1	G	3845	0	3963	249	0
1	H	3845	0	3966	71	0
1	I	3845	0	3966	67	0
1	J	3845	0	3966	62	0
1	K	3845	0	3966	85	0
1	L	3845	0	3966	75	0
1	M	3845	0	3966	72	0
1	N	3845	0	3966	61	0
2	A	1	0	0	3	0
2	B	1	0	0	3	0
2	C	1	0	0	3	0
2	D	1	0	0	3	0
2	E	1	0	0	3	0
2	F	1	0	0	3	0
2	G	1	0	0	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	0	0
4	A	31	0	12	3	0
4	B	31	0	12	3	0
4	C	31	0	12	3	0
4	D	31	0	12	3	0
4	E	31	0	12	3	0
4	F	31	0	12	3	0
4	G	31	0	12	3	0
All	All	54062	0	55592	2080	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 19.

All (2080) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:LEU:CD2	1:E:254:VAL:HG21	1.33	1.39
1:A:200:LEU:CD2	1:A:254:VAL:HG21	1.33	1.39
1:F:200:LEU:CD2	1:F:254:VAL:HG21	1.33	1.38
1:B:200:LEU:CD2	1:B:254:VAL:HG21	1.33	1.38
1:C:200:LEU:CD2	1:C:254:VAL:HG21	1.33	1.37
1:C:200:LEU:HD21	1:C:254:VAL:CG2	1.16	1.36
1:D:200:LEU:CD2	1:D:254:VAL:HG21	1.33	1.36
1:F:200:LEU:HD21	1:F:254:VAL:CG2	1.16	1.35
1:B:200:LEU:HD21	1:B:254:VAL:CG2	1.16	1.34
1:D:200:LEU:HD21	1:D:254:VAL:CG2	1.16	1.33
1:E:200:LEU:HD21	1:E:254:VAL:CG2	1.16	1.33
1:A:200:LEU:HD21	1:A:254:VAL:CG2	1.16	1.30
1:H:230:ILE:CD1	1:H:262:LEU:HD12	1.65	1.25
1:F:200:LEU:CD2	1:F:254:VAL:CG2	1.87	1.24
1:K:230:ILE:CD1	1:K:262:LEU:HD12	1.67	1.24
1:M:230:ILE:CD1	1:M:262:LEU:HD12	1.70	1.22
1:E:200:LEU:CD2	1:E:254:VAL:CG2	1.87	1.19
1:A:200:LEU:CD2	1:A:254:VAL:CG2	1.87	1.19
1:H:230:ILE:CD1	1:H:262:LEU:CD1	2.23	1.16
1:M:227:ILE:HD13	1:M:233:MET:HE1	1.26	1.15
1:D:23:LEU:HG	1:D:60:ILE:HD12	1.29	1.15
1:L:227:ILE:HD13	1:L:233:MET:CE	1.75	1.15
1:M:227:ILE:HD13	1:M:233:MET:CE	1.77	1.15
1:K:230:ILE:CD1	1:K:262:LEU:CD1	2.24	1.15
1:C:23:LEU:HG	1:C:60:ILE:HD12	1.30	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:230:ILE:CD1	1:M:262:LEU:CD1	2.25	1.15
1:M:220:ILE:CD1	1:M:296:THR:HG21	1.77	1.14
1:I:220:ILE:CD1	1:I:296:THR:HG21	1.77	1.14
1:E:23:LEU:HG	1:E:60:ILE:HD12	1.29	1.13
1:H:220:ILE:CD1	1:H:296:THR:HG21	1.77	1.13
1:J:220:ILE:CD1	1:J:296:THR:HG21	1.79	1.13
1:L:230:ILE:CD1	1:L:262:LEU:HD12	1.78	1.13
1:A:150:ILE:CD1	1:A:493:ILE:HA	1.79	1.12
1:D:150:ILE:CD1	1:D:493:ILE:HA	1.79	1.13
1:I:230:ILE:CD1	1:I:262:LEU:HD12	1.78	1.13
1:G:150:ILE:CD1	1:G:493:ILE:HA	1.79	1.12
1:K:220:ILE:CD1	1:K:296:THR:HG21	1.79	1.12
1:B:150:ILE:CD1	1:B:493:ILE:HA	1.79	1.12
1:D:200:LEU:CD2	1:D:254:VAL:CG2	1.87	1.12
1:K:227:ILE:HD13	1:K:233:MET:CE	1.80	1.12
1:L:220:ILE:CD1	1:L:296:THR:HG21	1.80	1.12
1:C:200:LEU:CD2	1:C:254:VAL:CG2	1.87	1.12
1:C:150:ILE:CD1	1:C:493:ILE:HA	1.79	1.12
1:B:23:LEU:HG	1:B:60:ILE:HD12	1.28	1.11
1:F:150:ILE:CD1	1:F:493:ILE:HA	1.79	1.11
1:E:150:ILE:CD1	1:E:493:ILE:HA	1.79	1.11
1:N:220:ILE:CD1	1:N:296:THR:HG21	1.79	1.11
1:M:227:ILE:CD1	1:M:233:MET:HE1	1.80	1.11
1:D:190:VAL:HG11	1:D:334:ASP:HB2	1.31	1.10
1:I:230:ILE:CD1	1:I:262:LEU:CD1	2.28	1.10
1:L:230:ILE:CD1	1:L:262:LEU:CD1	2.28	1.10
1:F:23:LEU:HG	1:F:60:ILE:HD12	1.28	1.10
1:A:23:LEU:HG	1:A:60:ILE:HD12	1.28	1.09
1:B:200:LEU:CD2	1:B:254:VAL:CG2	1.87	1.09
1:C:193:MET:HE2	1:C:295:LEU:HD12	1.32	1.09
1:I:230:ILE:HD13	1:I:262:LEU:HD12	1.33	1.09
1:N:230:ILE:HD13	1:N:262:LEU:HG	1.13	1.09
1:D:199:TYR:HB3	1:D:325:ILE:HD11	1.32	1.09
1:H:227:ILE:CD1	1:H:233:MET:HE1	1.81	1.09
1:G:23:LEU:HG	1:G:60:ILE:HD12	1.28	1.09
1:H:23:LEU:HD12	1:H:60:ILE:HD12	1.35	1.08
1:N:230:ILE:CD1	1:N:262:LEU:HG	1.83	1.08
1:J:230:ILE:CD1	1:J:262:LEU:HG	1.83	1.07
1:I:227:ILE:CD1	1:I:233:MET:HE1	1.82	1.07
1:J:227:ILE:CD1	1:J:233:MET:HE1	1.84	1.07
1:J:230:ILE:HD13	1:J:262:LEU:HG	1.13	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:227:ILE:CD1	1:N:233:MET:HE1	1.84	1.07
1:L:230:ILE:HD13	1:L:262:LEU:HD12	1.33	1.06
1:L:227:ILE:HD13	1:L:233:MET:HE1	1.37	1.06
1:H:227:ILE:HD13	1:H:233:MET:CE	1.85	1.06
1:L:227:ILE:CD1	1:L:233:MET:HE1	1.85	1.06
1:J:227:ILE:HD13	1:J:233:MET:HE1	1.06	1.05
1:L:23:LEU:HD12	1:L:60:ILE:HD12	1.39	1.05
1:I:230:ILE:HD13	1:I:262:LEU:CD1	1.86	1.05
1:J:227:ILE:HD13	1:J:233:MET:CE	1.87	1.04
1:L:230:ILE:HD13	1:L:262:LEU:CD1	1.86	1.04
1:N:23:LEU:HD12	1:N:60:ILE:HD12	1.39	1.04
1:J:23:LEU:HD12	1:J:60:ILE:HD12	1.38	1.04
1:I:227:ILE:HD13	1:I:233:MET:CE	1.86	1.03
1:K:23:LEU:HD12	1:K:60:ILE:HD12	1.40	1.03
1:M:230:ILE:HD13	1:M:262:LEU:HD12	1.39	1.03
1:M:23:LEU:HD12	1:M:60:ILE:HD12	1.39	1.03
1:N:227:ILE:HD13	1:N:233:MET:CE	1.88	1.03
1:C:193:MET:HE1	1:C:296:THR:HG23	1.42	1.02
1:N:227:ILE:HD13	1:N:233:MET:HE1	1.06	1.02
1:C:199:TYR:HB3	1:C:325:ILE:HD11	1.38	1.02
1:G:161:LEU:HD11	1:G:185:ASP:HB3	1.42	1.02
1:H:227:ILE:HD13	1:H:233:MET:HE1	1.04	1.02
1:A:49:ILE:HD11	1:G:513:LEU:O	1.60	1.01
1:I:23:LEU:HD12	1:I:60:ILE:HD12	1.39	1.01
1:A:513:LEU:O	1:B:49:ILE:HD11	1.60	1.01
1:E:199:TYR:HB3	1:E:325:ILE:HD11	1.38	1.01
1:F:513:LEU:O	1:G:49:ILE:HD11	1.60	1.01
1:G:199:TYR:HB3	1:G:325:ILE:HD11	1.38	1.01
1:F:199:TYR:HB3	1:F:325:ILE:HD11	1.38	1.01
1:H:230:ILE:HD13	1:H:262:LEU:HD12	1.43	1.01
1:I:227:ILE:HD13	1:I:233:MET:HE1	1.04	1.01
1:B:199:TYR:HB3	1:B:325:ILE:HD11	1.38	1.00
1:G:200:LEU:HD11	1:G:254:VAL:HG21	1.01	1.00
1:C:513:LEU:O	1:D:49:ILE:HD11	1.60	1.00
1:B:513:LEU:O	1:C:49:ILE:HD11	1.60	1.00
1:K:230:ILE:HD13	1:K:262:LEU:HD12	1.40	1.00
1:A:199:TYR:HB3	1:A:325:ILE:HD11	1.38	0.99
1:B:295:LEU:HD22	1:B:342:ILE:CD1	1.93	0.99
1:D:295:LEU:HD22	1:D:342:ILE:CD1	1.93	0.99
1:D:513:LEU:O	1:E:49:ILE:HD11	1.62	0.99
1:K:227:ILE:HD13	1:K:233:MET:HE3	1.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:HD22	1:A:342:ILE:CD1	1.93	0.99
1:C:295:LEU:HD22	1:C:342:ILE:CD1	1.93	0.99
1:G:295:LEU:HD22	1:G:342:ILE:CD1	1.93	0.99
1:E:295:LEU:HD22	1:E:342:ILE:CD1	1.93	0.99
1:E:513:LEU:O	1:F:49:ILE:HD11	1.60	0.99
1:F:295:LEU:HD22	1:F:342:ILE:CD1	1.93	0.99
1:G:200:LEU:HD11	1:G:254:VAL:CG2	1.91	0.99
1:G:200:LEU:CD1	1:G:254:VAL:HG21	1.93	0.98
1:K:301:ILE:HD12	1:K:309:LEU:HD23	1.41	0.98
1:J:301:ILE:HD11	1:J:312:ALA:HB2	1.46	0.98
1:L:301:ILE:HD12	1:L:309:LEU:HD23	1.44	0.97
1:N:301:ILE:HD11	1:N:312:ALA:HB2	1.47	0.96
1:M:301:ILE:HD11	1:M:312:ALA:HB2	1.48	0.95
1:M:301:ILE:HD12	1:M:309:LEU:HD23	1.48	0.95
1:I:301:ILE:HD11	1:I:312:ALA:HB2	1.47	0.95
1:J:136:VAL:HG21	1:J:489:ILE:HD13	1.49	0.94
1:N:220:ILE:HD12	1:N:296:THR:HG21	1.50	0.94
1:L:301:ILE:HD11	1:L:312:ALA:HB2	1.50	0.94
1:A:513:LEU:HB3	1:B:49:ILE:HD12	1.50	0.94
1:B:513:LEU:HB3	1:C:49:ILE:HD12	1.50	0.94
1:E:513:LEU:HB3	1:F:49:ILE:HD12	1.50	0.94
1:D:513:LEU:HB3	1:E:49:ILE:HD12	1.50	0.94
1:E:201:SER:HB3	1:E:204:PHE:CE1	2.04	0.93
1:K:227:ILE:CD1	1:K:233:MET:HE1	1.98	0.93
1:C:513:LEU:HB3	1:D:49:ILE:HD12	1.50	0.93
1:M:220:ILE:HD12	1:M:296:THR:HG21	1.48	0.93
1:G:200:LEU:N	1:G:200:LEU:HD12	1.83	0.93
1:K:301:ILE:CD1	1:K:309:LEU:HD23	1.97	0.93
1:I:220:ILE:HD12	1:I:296:THR:HG21	1.48	0.93
1:J:23:LEU:HA	1:J:60:ILE:HD13	1.51	0.93
1:H:220:ILE:HD12	1:H:296:THR:HG21	1.48	0.92
1:F:513:LEU:HB3	1:G:49:ILE:HD12	1.50	0.92
1:A:49:ILE:HD12	1:G:513:LEU:HB3	1.50	0.92
1:A:206:ASN:HB2	1:A:213:VAL:HG23	1.49	0.92
1:C:200:LEU:HD23	1:C:254:VAL:HG21	1.52	0.92
1:H:301:ILE:HD11	1:H:312:ALA:HB2	1.49	0.92
1:J:230:ILE:HD13	1:J:262:LEU:CG	2.00	0.92
1:D:213:VAL:CG1	1:D:325:ILE:HG12	2.00	0.92
1:F:213:VAL:CG1	1:F:325:ILE:HG12	2.00	0.92
1:C:213:VAL:CG1	1:C:325:ILE:HG12	2.00	0.91
1:D:200:LEU:HD23	1:D:254:VAL:HG21	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:301:ILE:HD11	1:K:312:ALA:HB2	1.51	0.91
1:B:200:LEU:HD23	1:B:254:VAL:HG21	1.52	0.91
1:K:220:ILE:HD12	1:K:296:THR:HG21	1.51	0.91
1:H:23:LEU:HA	1:H:60:ILE:HD13	1.51	0.91
1:H:230:ILE:HD12	1:H:262:LEU:HD12	1.51	0.91
1:M:220:ILE:HD12	1:M:296:THR:CG2	2.01	0.91
1:K:227:ILE:CD1	1:K:233:MET:CE	2.48	0.91
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.53	0.91
1:A:200:LEU:HD23	1:A:254:VAL:HG21	1.52	0.91
1:B:213:VAL:CG1	1:B:325:ILE:HG12	2.00	0.91
1:E:200:LEU:HD23	1:E:254:VAL:HG21	1.52	0.91
1:F:23:LEU:HA	1:F:60:ILE:HD13	1.53	0.91
1:G:213:VAL:CG1	1:G:325:ILE:HG12	2.00	0.91
1:J:220:ILE:HD12	1:J:296:THR:HG21	1.51	0.91
1:G:23:LEU:HA	1:G:60:ILE:HD13	1.53	0.90
1:B:220:ILE:HD13	1:B:332:ILE:HD13	1.54	0.90
1:E:213:VAL:CG1	1:E:325:ILE:HG12	2.00	0.90
1:F:295:LEU:HD22	1:F:342:ILE:HD11	1.54	0.90
1:L:301:ILE:CD1	1:L:309:LEU:HD23	2.00	0.90
1:B:295:LEU:HD22	1:B:342:ILE:HD11	1.53	0.90
1:F:220:ILE:HD13	1:F:332:ILE:HD13	1.53	0.90
1:G:220:ILE:HD13	1:G:332:ILE:HD13	1.54	0.90
1:L:220:ILE:HD12	1:L:296:THR:HG21	1.52	0.90
1:A:220:ILE:HD13	1:A:332:ILE:HD13	1.54	0.90
1:D:295:LEU:HD22	1:D:342:ILE:HD11	1.53	0.90
1:F:513:LEU:C	1:G:49:ILE:HD11	1.97	0.90
1:E:23:LEU:HA	1:E:60:ILE:HD13	1.53	0.90
1:A:23:LEU:HA	1:A:60:ILE:HD13	1.53	0.90
1:D:513:LEU:C	1:E:49:ILE:HD11	1.97	0.90
1:L:23:LEU:HA	1:L:60:ILE:HD13	1.53	0.90
1:M:230:ILE:HD13	1:M:262:LEU:CD1	1.96	0.90
1:N:136:VAL:HG21	1:N:489:ILE:HD13	1.53	0.90
1:I:220:ILE:HD12	1:I:296:THR:CG2	2.01	0.90
1:A:49:ILE:HD11	1:G:513:LEU:C	1.97	0.89
1:I:23:LEU:HA	1:I:60:ILE:HD13	1.54	0.89
1:M:136:VAL:HG21	1:M:489:ILE:HD13	1.54	0.89
1:C:220:ILE:HD13	1:C:332:ILE:HD13	1.53	0.89
1:K:230:ILE:HD12	1:K:262:LEU:HD12	1.55	0.89
1:D:23:LEU:HA	1:D:60:ILE:HD13	1.53	0.89
1:K:23:LEU:HA	1:K:60:ILE:HD13	1.54	0.89
1:E:513:LEU:C	1:F:49:ILE:HD11	1.97	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:295:LEU:HD22	1:G:342:ILE:HD11	1.54	0.89
1:A:295:LEU:HD22	1:A:342:ILE:HD11	1.54	0.89
1:C:23:LEU:HA	1:C:60:ILE:HD13	1.53	0.89
1:H:220:ILE:HD12	1:H:296:THR:CG2	2.01	0.89
1:C:513:LEU:C	1:D:49:ILE:HD11	1.97	0.89
1:E:220:ILE:HD13	1:E:332:ILE:HD13	1.54	0.89
1:D:220:ILE:HD13	1:D:332:ILE:HD13	1.53	0.88
1:J:220:ILE:HD12	1:J:296:THR:CG2	2.03	0.88
1:N:230:ILE:HD13	1:N:262:LEU:CG	2.01	0.88
1:B:23:LEU:HA	1:B:60:ILE:HD13	1.53	0.88
1:N:220:ILE:HD12	1:N:296:THR:CG2	2.03	0.88
1:L:220:ILE:HD12	1:L:296:THR:CG2	2.04	0.88
1:A:513:LEU:C	1:B:49:ILE:HD11	1.97	0.88
1:B:513:LEU:C	1:C:49:ILE:HD11	1.97	0.88
1:H:220:ILE:CD1	1:H:296:THR:CG2	2.51	0.88
1:I:230:ILE:HD13	1:I:262:LEU:CG	2.04	0.88
1:E:295:LEU:HD22	1:E:342:ILE:HD11	1.54	0.88
1:N:23:LEU:HA	1:N:60:ILE:HD13	1.55	0.88
1:C:200:LEU:HD12	1:C:275:ALA:HB3	1.55	0.88
1:I:220:ILE:CD1	1:I:296:THR:CG2	2.52	0.88
1:C:295:LEU:HD22	1:C:342:ILE:HD11	1.53	0.87
1:F:200:LEU:HD23	1:F:254:VAL:HG21	1.52	0.87
1:K:220:ILE:HD12	1:K:296:THR:CG2	2.04	0.87
1:F:200:LEU:HD12	1:F:275:ALA:HB3	1.55	0.87
1:D:200:LEU:HD12	1:D:275:ALA:HB3	1.54	0.87
1:M:220:ILE:CD1	1:M:296:THR:CG2	2.52	0.87
1:E:200:LEU:HD12	1:E:275:ALA:HB3	1.54	0.87
1:A:200:LEU:HD12	1:A:275:ALA:HB3	1.55	0.86
1:L:230:ILE:HD13	1:L:262:LEU:CG	2.04	0.86
1:B:200:LEU:HD12	1:B:275:ALA:HB3	1.55	0.86
1:L:227:ILE:HD13	1:L:233:MET:HE3	1.56	0.86
1:M:23:LEU:HA	1:M:60:ILE:HD13	1.55	0.86
1:H:230:ILE:HD11	1:H:262:LEU:CD1	2.05	0.86
1:D:190:VAL:CG1	1:D:334:ASP:HB2	2.05	0.86
1:G:23:LEU:HG	1:G:60:ILE:CD1	2.06	0.85
1:N:301:ILE:CD1	1:N:312:ALA:HB2	2.06	0.85
1:C:192:GLY:HA2	1:C:332:ILE:O	1.77	0.85
1:A:23:LEU:HG	1:A:60:ILE:CD1	2.06	0.85
1:H:230:ILE:HD13	1:H:262:LEU:CD1	2.02	0.85
1:M:230:ILE:HD13	1:M:262:LEU:CG	2.07	0.85
1:D:23:LEU:HG	1:D:60:ILE:CD1	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:301:ILE:HD12	1:H:309:LEU:HD23	1.56	0.85
1:J:220:ILE:HD13	1:J:296:THR:HG21	1.59	0.84
1:J:301:ILE:CD1	1:J:312:ALA:HB2	2.06	0.84
1:N:220:ILE:CD1	1:N:296:THR:CG2	2.55	0.84
1:L:220:ILE:HD13	1:L:296:THR:HG21	1.59	0.84
1:L:301:ILE:CD1	1:L:312:ALA:HB2	2.05	0.84
1:M:301:ILE:CD1	1:M:309:LEU:HD23	2.06	0.84
1:M:301:ILE:CD1	1:M:312:ALA:HB2	2.06	0.84
1:K:301:ILE:CD1	1:K:312:ALA:HB2	2.06	0.84
1:E:23:LEU:HG	1:E:60:ILE:CD1	2.06	0.84
1:I:301:ILE:CD1	1:I:312:ALA:HB2	2.06	0.84
1:L:220:ILE:CD1	1:L:296:THR:CG2	2.55	0.84
1:H:301:ILE:CD1	1:H:312:ALA:HB2	2.06	0.84
1:B:23:LEU:HG	1:B:60:ILE:CD1	2.06	0.84
1:F:23:LEU:HG	1:F:60:ILE:CD1	2.06	0.83
1:A:49:ILE:CD1	1:G:513:LEU:O	2.27	0.83
1:C:23:LEU:HG	1:C:60:ILE:CD1	2.08	0.83
1:F:150:ILE:HD11	1:F:493:ILE:HA	1.60	0.83
1:E:513:LEU:O	1:F:49:ILE:CD1	2.27	0.83
1:F:221:LEU:HD11	1:F:309:LEU:HD21	1.60	0.83
1:G:150:ILE:HD11	1:G:493:ILE:HA	1.60	0.83
1:K:230:ILE:HD11	1:K:262:LEU:CD1	2.09	0.83
1:E:221:LEU:HD11	1:E:309:LEU:HD21	1.60	0.83
1:K:230:ILE:HD13	1:K:262:LEU:CD1	1.99	0.83
1:N:220:ILE:HD13	1:N:296:THR:HG21	1.61	0.83
1:A:513:LEU:O	1:B:49:ILE:CD1	2.27	0.83
1:J:220:ILE:CD1	1:J:296:THR:CG2	2.54	0.83
1:D:513:LEU:HB3	1:E:49:ILE:CD1	2.09	0.82
1:M:230:ILE:HD12	1:M:262:LEU:HD12	1.59	0.82
1:G:221:LEU:HD11	1:G:309:LEU:HD21	1.60	0.82
1:H:230:ILE:CD1	1:H:262:LEU:CG	2.57	0.82
1:J:220:ILE:HD12	1:J:296:THR:CB	2.09	0.82
1:B:221:LEU:HD11	1:B:309:LEU:HD21	1.60	0.82
1:C:221:LEU:HD11	1:C:309:LEU:HD21	1.60	0.82
1:D:221:LEU:HD11	1:D:309:LEU:HD21	1.60	0.82
1:B:513:LEU:O	1:C:49:ILE:CD1	2.26	0.82
1:D:223:ALA:O	1:D:251:ALA:HA	1.80	0.82
1:M:220:ILE:HD13	1:M:296:THR:HG21	1.61	0.82
1:A:150:ILE:HD11	1:A:493:ILE:HA	1.61	0.82
1:A:221:LEU:HD11	1:A:309:LEU:HD21	1.60	0.82
1:K:230:ILE:HD13	1:K:262:LEU:CG	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ALA:O	1:C:251:ALA:HA	1.80	0.82
1:C:513:LEU:HB3	1:D:49:ILE:CD1	2.10	0.82
1:E:150:ILE:HD11	1:E:493:ILE:HA	1.61	0.82
1:B:223:ALA:O	1:B:251:ALA:HA	1.80	0.82
1:F:513:LEU:O	1:G:49:ILE:CD1	2.27	0.82
1:G:223:ALA:O	1:G:251:ALA:HA	1.80	0.82
1:A:513:LEU:HB3	1:B:49:ILE:CD1	2.10	0.82
1:D:513:LEU:O	1:E:49:ILE:CD1	2.28	0.82
1:C:513:LEU:O	1:D:49:ILE:CD1	2.27	0.81
1:B:513:LEU:HB3	1:C:49:ILE:CD1	2.11	0.81
1:E:513:LEU:HB3	1:F:49:ILE:CD1	2.10	0.81
1:B:150:ILE:HD11	1:B:493:ILE:HA	1.61	0.81
1:F:223:ALA:O	1:F:251:ALA:HA	1.80	0.81
1:H:230:ILE:HD13	1:H:262:LEU:CG	2.10	0.81
1:A:49:ILE:CD1	1:G:513:LEU:HB3	2.11	0.81
1:F:513:LEU:HB3	1:G:49:ILE:CD1	2.11	0.81
1:H:220:ILE:HD13	1:H:296:THR:HG21	1.60	0.81
1:D:150:ILE:HD11	1:D:493:ILE:HA	1.61	0.81
1:K:220:ILE:HD13	1:K:296:THR:HG21	1.61	0.81
1:A:223:ALA:O	1:A:251:ALA:HA	1.80	0.81
1:B:137:PRO:HA	1:B:410:GLY:HA2	1.63	0.80
1:C:150:ILE:HD11	1:C:493:ILE:HA	1.60	0.80
1:K:230:ILE:CD1	1:K:262:LEU:CG	2.59	0.80
1:K:220:ILE:HD12	1:K:296:THR:CB	2.12	0.80
1:L:220:ILE:HD12	1:L:296:THR:CB	2.11	0.80
1:N:220:ILE:HD12	1:N:296:THR:CB	2.11	0.80
1:A:137:PRO:HA	1:A:410:GLY:HA2	1.63	0.80
1:E:223:ALA:O	1:E:251:ALA:HA	1.80	0.80
1:G:200:LEU:CD1	1:G:254:VAL:HG11	2.11	0.80
1:K:220:ILE:CD1	1:K:296:THR:CG2	2.56	0.80
1:A:137:PRO:HA	1:A:410:GLY:CA	2.12	0.79
1:B:137:PRO:HA	1:B:410:GLY:CA	2.12	0.79
1:G:137:PRO:HA	1:G:410:GLY:HA2	1.63	0.79
1:C:193:MET:CE	1:C:296:THR:HG23	2.12	0.79
1:G:137:PRO:HA	1:G:410:GLY:CA	2.12	0.79
1:C:137:PRO:HA	1:C:410:GLY:HA2	1.63	0.79
1:G:199:TYR:C	1:G:200:LEU:HD12	2.07	0.79
1:F:137:PRO:HA	1:F:410:GLY:CA	2.12	0.79
1:A:513:LEU:CB	1:B:49:ILE:HD12	2.13	0.79
1:B:513:LEU:CB	1:C:49:ILE:HD12	2.13	0.79
1:D:137:PRO:HA	1:D:410:GLY:CA	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:LEU:HB2	1:D:259:LEU:HD13	1.65	0.79
1:C:513:LEU:CB	1:D:49:ILE:HD12	2.13	0.79
1:E:137:PRO:HA	1:E:410:GLY:HA2	1.63	0.79
1:E:137:PRO:HA	1:E:410:GLY:CA	2.12	0.79
1:F:295:LEU:HD22	1:F:342:ILE:HD13	1.64	0.78
1:E:295:LEU:HD22	1:E:342:ILE:HD13	1.64	0.78
1:C:137:PRO:HA	1:C:410:GLY:CA	2.12	0.78
1:C:295:LEU:HD22	1:C:342:ILE:HD13	1.64	0.78
1:D:513:LEU:CB	1:E:49:ILE:HD12	2.13	0.78
1:A:49:ILE:HD12	1:G:513:LEU:CB	2.13	0.78
1:B:194:GLN:CD	1:B:329:THR:HG21	2.09	0.78
1:D:137:PRO:HA	1:D:410:GLY:HA2	1.63	0.78
1:A:300:VAL:HG23	1:A:312:ALA:HB2	1.66	0.78
1:F:137:PRO:HA	1:F:410:GLY:HA2	1.63	0.78
1:G:200:LEU:HD22	1:G:254:VAL:HG11	1.66	0.78
1:B:295:LEU:HD22	1:B:342:ILE:HD13	1.64	0.78
1:C:300:VAL:HG23	1:C:312:ALA:HB2	1.66	0.78
1:G:300:VAL:HG23	1:G:312:ALA:HB2	1.66	0.78
1:I:220:ILE:HD13	1:I:296:THR:HG21	1.61	0.78
1:F:200:LEU:HB2	1:F:259:LEU:HD13	1.65	0.78
1:G:200:LEU:CD2	1:G:254:VAL:HG11	2.14	0.78
1:A:150:ILE:HD12	1:A:493:ILE:HA	1.65	0.78
1:I:301:ILE:HD12	1:I:309:LEU:HD23	1.64	0.78
1:D:295:LEU:HD22	1:D:342:ILE:HD13	1.64	0.77
1:D:300:VAL:HG23	1:D:312:ALA:HB2	1.66	0.77
1:B:300:VAL:HG23	1:B:312:ALA:HB2	1.66	0.77
1:E:150:ILE:HD12	1:E:493:ILE:HA	1.65	0.77
1:E:200:LEU:HB2	1:E:259:LEU:HD13	1.65	0.77
1:M:230:ILE:HD11	1:M:262:LEU:CD1	2.14	0.77
1:M:227:ILE:HD13	1:M:233:MET:HE3	1.66	0.77
1:D:150:ILE:HD12	1:D:493:ILE:HA	1.65	0.77
1:E:513:LEU:CB	1:F:49:ILE:HD12	2.13	0.77
1:F:300:VAL:HG23	1:F:312:ALA:HB2	1.66	0.77
1:F:513:LEU:CB	1:G:49:ILE:HD12	2.14	0.77
1:H:220:ILE:HD12	1:H:296:THR:CB	2.14	0.77
1:F:150:ILE:HD12	1:F:493:ILE:HA	1.65	0.77
1:G:192:GLY:HA2	1:G:332:ILE:O	1.85	0.77
1:F:199:TYR:HB3	1:F:325:ILE:CD1	2.14	0.77
1:G:295:LEU:HD22	1:G:342:ILE:HD13	1.64	0.77
1:I:220:ILE:HD12	1:I:296:THR:CB	2.15	0.77
1:M:230:ILE:CD1	1:M:262:LEU:CG	2.61	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLY:HA2	1:A:332:ILE:O	1.85	0.77
1:A:295:LEU:HD22	1:A:342:ILE:HD13	1.64	0.77
1:E:300:VAL:HG23	1:E:312:ALA:HB2	1.66	0.77
1:M:220:ILE:HD12	1:M:296:THR:CB	2.14	0.77
1:E:192:GLY:HA2	1:E:332:ILE:O	1.85	0.77
1:C:199:TYR:HB3	1:C:325:ILE:CD1	2.14	0.76
1:E:199:TYR:HB3	1:E:325:ILE:CD1	2.14	0.76
1:H:301:ILE:CD1	1:H:309:LEU:HD23	2.15	0.76
1:D:192:GLY:HA2	1:D:332:ILE:O	1.85	0.76
1:E:309:LEU:HD22	1:E:312:ALA:HB3	1.67	0.76
1:F:309:LEU:HD22	1:F:312:ALA:HB3	1.67	0.76
1:G:309:LEU:HD22	1:G:312:ALA:HB3	1.67	0.76
1:F:192:GLY:HA2	1:F:332:ILE:O	1.85	0.76
1:A:297:GLY:HA2	1:A:337:GLY:HA2	1.68	0.76
1:C:150:ILE:HD12	1:C:493:ILE:HA	1.64	0.76
1:D:297:GLY:HA2	1:D:337:GLY:HA2	1.68	0.76
1:E:297:GLY:HA2	1:E:337:GLY:HA2	1.68	0.76
1:B:192:GLY:HA2	1:B:332:ILE:O	1.85	0.76
1:B:200:LEU:HB2	1:B:259:LEU:HD13	1.65	0.76
1:J:136:VAL:HG21	1:J:489:ILE:CD1	2.15	0.76
1:C:200:LEU:HB2	1:C:259:LEU:HD13	1.65	0.76
1:D:309:LEU:HD22	1:D:312:ALA:HB3	1.67	0.76
1:B:297:GLY:HA2	1:B:337:GLY:HA2	1.68	0.76
1:G:297:GLY:HA2	1:G:337:GLY:HA2	1.68	0.76
1:K:227:ILE:HD12	1:K:233:MET:HE1	1.66	0.76
1:A:199:TYR:HB3	1:A:325:ILE:CD1	2.15	0.75
1:A:213:VAL:CG1	1:A:325:ILE:HG12	2.16	0.75
1:B:199:TYR:HB3	1:B:325:ILE:CD1	2.15	0.75
1:C:297:GLY:HA2	1:C:337:GLY:HA2	1.68	0.75
1:G:150:ILE:HD12	1:G:493:ILE:HA	1.65	0.75
1:A:200:LEU:HB2	1:A:259:LEU:HD13	1.65	0.75
1:B:150:ILE:HD12	1:B:493:ILE:HA	1.65	0.75
1:F:297:GLY:HA2	1:F:337:GLY:HA2	1.68	0.75
1:G:199:TYR:HB3	1:G:325:ILE:CD1	2.14	0.75
1:C:193:MET:CE	1:C:295:LEU:HD12	2.12	0.75
1:F:313:THR:H	1:F:316:ASP:HB3	1.52	0.75
1:B:313:THR:H	1:B:316:ASP:HB3	1.52	0.75
1:E:313:THR:H	1:E:316:ASP:HB3	1.52	0.75
1:D:313:THR:H	1:D:316:ASP:HB3	1.52	0.75
1:A:309:LEU:HD22	1:A:312:ALA:HB3	1.67	0.75
1:B:309:LEU:HD22	1:B:312:ALA:HB3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:LEU:HD22	1:C:312:ALA:HB3	1.67	0.74
1:E:200:LEU:HD12	1:E:275:ALA:CB	2.18	0.74
1:G:313:THR:H	1:G:316:ASP:HB3	1.52	0.74
1:N:100:ILE:HD13	1:N:514:MET:SD	2.27	0.74
1:K:100:ILE:HD13	1:K:514:MET:SD	2.28	0.74
1:A:240:VAL:HG11	1:A:247:LEU:HB2	1.69	0.74
1:A:313:THR:H	1:A:316:ASP:HB3	1.52	0.74
1:C:381:VAL:HG21	1:C:393:LYS:N	2.03	0.74
1:C:313:THR:H	1:C:316:ASP:HB3	1.52	0.74
1:F:200:LEU:HD12	1:F:275:ALA:CB	2.18	0.74
1:B:381:VAL:HG21	1:B:393:LYS:N	2.03	0.74
1:D:200:LEU:HD12	1:D:275:ALA:CB	2.18	0.74
1:G:240:VAL:HG11	1:G:247:LEU:HB2	1.69	0.74
1:B:240:VAL:HG11	1:B:247:LEU:HB2	1.69	0.73
1:J:100:ILE:HD13	1:J:514:MET:SD	2.28	0.73
1:D:381:VAL:HG21	1:D:393:LYS:N	2.03	0.73
1:G:381:VAL:HG21	1:G:393:LYS:N	2.03	0.73
1:L:100:ILE:HD13	1:L:514:MET:SD	2.28	0.73
1:E:381:VAL:HG21	1:E:393:LYS:N	2.03	0.73
1:A:381:VAL:HG21	1:A:393:LYS:N	2.03	0.73
1:C:200:LEU:HD12	1:C:275:ALA:CB	2.18	0.73
1:H:100:ILE:HD13	1:H:514:MET:SD	2.28	0.73
1:B:200:LEU:HD12	1:B:275:ALA:CB	2.18	0.73
1:A:200:LEU:HD12	1:A:275:ALA:CB	2.18	0.73
1:C:240:VAL:HG11	1:C:247:LEU:HB2	1.69	0.73
1:G:200:LEU:HD13	1:G:254:VAL:HG11	1.71	0.73
1:I:100:ILE:HD13	1:I:514:MET:SD	2.29	0.73
1:E:200:LEU:CB	1:E:259:LEU:HD13	2.19	0.72
1:D:200:LEU:CB	1:D:259:LEU:HD13	2.19	0.72
1:F:220:ILE:HD12	1:F:296:THR:HG21	1.71	0.72
1:D:240:VAL:HG11	1:D:247:LEU:HB2	1.69	0.72
1:F:381:VAL:HG21	1:F:393:LYS:N	2.03	0.72
1:E:220:ILE:HD12	1:E:296:THR:HG21	1.71	0.72
1:E:240:VAL:HG11	1:E:247:LEU:HB2	1.69	0.72
1:I:230:ILE:HD12	1:I:262:LEU:HD12	1.71	0.72
1:F:240:VAL:HG11	1:F:247:LEU:HB2	1.69	0.72
1:C:207:LYS:HB2	1:C:208:PRO:HD3	1.72	0.72
1:D:220:ILE:HD12	1:D:296:THR:HG21	1.71	0.72
1:B:200:LEU:CB	1:B:259:LEU:HD13	2.19	0.72
1:B:222:LEU:HD21	1:B:292:ILE:HG22	1.71	0.72
1:C:200:LEU:CB	1:C:259:LEU:HD13	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:301:ILE:HD11	1:N:312:ALA:CB	2.18	0.72
1:C:513:LEU:CA	1:D:49:ILE:CD1	2.68	0.72
1:G:220:ILE:HD12	1:G:296:THR:HG21	1.71	0.72
1:H:230:ILE:CD1	1:H:262:LEU:HG	2.20	0.72
1:I:301:ILE:HD11	1:I:312:ALA:CB	2.18	0.72
1:A:513:LEU:CA	1:B:49:ILE:CD1	2.68	0.71
1:C:312:ALA:HB1	1:C:316:ASP:CG	2.15	0.71
1:F:513:LEU:CA	1:G:49:ILE:CD1	2.68	0.71
1:M:301:ILE:HD11	1:M:312:ALA:CB	2.20	0.71
1:B:513:LEU:CA	1:C:49:ILE:CD1	2.68	0.71
1:E:513:LEU:CA	1:F:49:ILE:CD1	2.68	0.71
1:F:222:LEU:HD21	1:F:292:ILE:HG22	1.71	0.71
1:L:301:ILE:HD11	1:L:312:ALA:CB	2.21	0.71
1:B:312:ALA:HB1	1:B:316:ASP:CG	2.15	0.71
1:N:136:VAL:HG21	1:N:489:ILE:CD1	2.18	0.71
1:C:162:ILE:HD13	1:C:400:LEU:CA	2.20	0.71
1:C:220:ILE:HD12	1:C:296:THR:HG21	1.71	0.71
1:E:201:SER:HB3	1:E:204:PHE:CZ	2.25	0.71
1:A:162:ILE:HD13	1:A:400:LEU:CA	2.20	0.71
1:C:222:LEU:HD21	1:C:292:ILE:HG22	1.71	0.71
1:F:200:LEU:CB	1:F:259:LEU:HD13	2.19	0.71
1:A:222:LEU:HD21	1:A:292:ILE:HG22	1.71	0.71
1:D:513:LEU:CA	1:E:49:ILE:CD1	2.68	0.71
1:J:301:ILE:HD11	1:J:312:ALA:CB	2.18	0.71
1:B:213:VAL:HG13	1:B:325:ILE:HG12	1.73	0.71
1:D:312:ALA:HB1	1:D:316:ASP:CG	2.16	0.71
1:G:312:ALA:HB1	1:G:316:ASP:CG	2.15	0.71
1:E:162:ILE:HD13	1:E:400:LEU:CA	2.20	0.71
1:L:230:ILE:HD12	1:L:262:LEU:HD12	1.71	0.71
1:A:49:ILE:CD1	1:G:513:LEU:CA	2.68	0.71
1:G:222:LEU:HD21	1:G:292:ILE:HG22	1.71	0.71
1:A:312:ALA:HB1	1:A:316:ASP:CG	2.16	0.71
1:B:220:ILE:HD12	1:B:296:THR:HG21	1.71	0.71
1:D:162:ILE:HD13	1:D:400:LEU:CA	2.20	0.71
1:D:222:LEU:HD21	1:D:292:ILE:HG22	1.71	0.71
1:A:200:LEU:CB	1:A:259:LEU:HD13	2.19	0.70
1:E:222:LEU:HD21	1:E:292:ILE:HG22	1.71	0.70
1:G:213:VAL:HG13	1:G:325:ILE:HG12	1.73	0.70
1:F:162:ILE:HD13	1:F:400:LEU:CA	2.21	0.70
1:B:223:ALA:HA	1:B:309:LEU:HD23	1.72	0.70
2:C:1525:PO4:P	4:C:1527:ATP:O1G	2.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:VAL:HG13	1:E:325:ILE:HG12	1.73	0.70
1:G:162:ILE:HD13	1:G:400:LEU:CA	2.20	0.70
1:F:197:ARG:HG3	1:F:198:GLY:O	1.91	0.70
1:F:312:ALA:HB1	1:F:316:ASP:CG	2.15	0.70
2:G:1525:PO4:P	4:G:1527:ATP:O1G	2.50	0.70
1:K:301:ILE:HD11	1:K:312:ALA:CB	2.22	0.70
1:M:100:ILE:HD13	1:M:514:MET:SD	2.31	0.70
1:A:223:ALA:HA	1:A:309:LEU:HD23	1.72	0.70
1:E:312:ALA:HB1	1:E:316:ASP:CG	2.15	0.70
1:G:223:ALA:HA	1:G:309:LEU:HD23	1.72	0.70
1:G:270:ILE:HG22	1:G:271:VAL:HG23	1.74	0.70
1:H:301:ILE:HD11	1:H:312:ALA:CB	2.21	0.70
1:M:230:ILE:CD1	1:M:262:LEU:HG	2.22	0.70
1:B:162:ILE:HD13	1:B:400:LEU:CA	2.21	0.70
1:A:220:ILE:HD12	1:A:296:THR:HG21	1.71	0.70
1:F:270:ILE:HG22	1:F:271:VAL:HG23	1.74	0.70
1:K:301:ILE:HD12	1:K:309:LEU:CD2	2.18	0.70
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.74	0.70
1:B:113:PRO:HB2	1:B:516:THR:HG22	1.74	0.70
1:D:213:VAL:HG13	1:D:325:ILE:HG12	1.73	0.70
1:F:223:ALA:HA	1:F:309:LEU:HD23	1.72	0.70
1:E:270:ILE:HG22	1:E:271:VAL:HG23	1.74	0.70
1:D:270:ILE:HG22	1:D:271:VAL:HG23	1.74	0.69
2:F:1525:PO4:P	4:F:1527:ATP:O1G	2.50	0.69
1:F:207:LYS:HB2	1:F:208:PRO:HD3	1.74	0.69
1:G:200:LEU:HD22	1:G:259:LEU:HD22	1.74	0.69
1:A:38:VAL:HG11	1:A:56:VAL:HG22	1.74	0.69
2:B:1525:PO4:P	4:B:1527:ATP:O1G	2.50	0.69
1:C:223:ALA:HA	1:C:309:LEU:HD23	1.72	0.69
1:C:270:ILE:HG22	1:C:271:VAL:HG23	1.74	0.69
2:D:1525:PO4:P	4:D:1527:ATP:O1G	2.50	0.69
1:B:270:ILE:HG22	1:B:271:VAL:HG23	1.74	0.69
1:C:113:PRO:HB2	1:C:516:THR:HG22	1.75	0.69
1:E:202:PRO:O	1:E:205:ILE:HG13	1.92	0.69
1:G:271:VAL:HG12	1:G:273:VAL:CG2	2.23	0.69
1:A:271:VAL:HG12	1:A:273:VAL:CG2	2.23	0.69
1:I:301:ILE:CD1	1:I:309:LEU:HD23	2.21	0.69
1:K:230:ILE:CD1	1:K:262:LEU:HG	2.21	0.69
1:G:38:VAL:HG11	1:G:56:VAL:HG22	1.74	0.69
1:G:193:MET:CE	1:G:332:ILE:HD12	2.23	0.69
1:C:213:VAL:HG13	1:C:325:ILE:HG12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ALA:HA	1:D:309:LEU:HD23	1.72	0.69
1:E:38:VAL:HG11	1:E:56:VAL:HG22	1.73	0.69
1:D:199:TYR:HB3	1:D:325:ILE:CD1	2.19	0.69
1:E:223:ALA:HA	1:E:309:LEU:HD23	1.72	0.69
1:F:271:VAL:HG12	1:F:273:VAL:CG2	2.23	0.69
1:J:23:LEU:HA	1:J:60:ILE:CD1	2.21	0.69
1:C:38:VAL:HG11	1:C:56:VAL:HG22	1.73	0.69
2:E:1525:PO4:P	4:E:1527:ATP:O1G	2.50	0.69
1:B:271:VAL:HG12	1:B:273:VAL:CG2	2.23	0.68
1:D:271:VAL:HG12	1:D:273:VAL:CG2	2.23	0.68
1:F:38:VAL:HG11	1:F:56:VAL:HG22	1.74	0.68
1:D:38:VAL:HG11	1:D:56:VAL:HG22	1.74	0.68
1:B:38:VAL:HG11	1:B:56:VAL:HG22	1.74	0.68
1:F:213:VAL:HG13	1:F:325:ILE:HG12	1.73	0.68
2:A:1525:PO4:P	4:A:1527:ATP:O1G	2.50	0.68
1:G:197:ARG:HG3	1:G:198:GLY:O	1.92	0.68
1:I:23:LEU:HA	1:I:60:ILE:CD1	2.22	0.68
1:L:227:ILE:CD1	1:L:233:MET:CE	2.53	0.68
1:A:200:LEU:HB2	1:A:259:LEU:CD1	2.24	0.68
1:C:513:LEU:C	1:D:49:ILE:CD1	2.67	0.68
1:E:271:VAL:HG12	1:E:273:VAL:CG2	2.23	0.68
1:C:271:VAL:HG12	1:C:273:VAL:CG2	2.23	0.68
1:H:23:LEU:HA	1:H:60:ILE:CD1	2.22	0.68
1:M:136:VAL:HG21	1:M:489:ILE:CD1	2.21	0.68
1:D:183:LEU:HA	1:D:383:ALA:H	1.59	0.68
1:F:113:PRO:HB2	1:F:516:THR:HG22	1.75	0.68
1:J:301:ILE:HD12	1:J:309:LEU:HD23	1.74	0.68
1:G:113:PRO:HB2	1:G:516:THR:HG22	1.75	0.68
1:K:223:ALA:O	1:K:251:ALA:HA	1.94	0.68
1:D:513:LEU:C	1:E:49:ILE:CD1	2.67	0.67
1:E:183:LEU:HA	1:E:383:ALA:H	1.59	0.67
1:C:193:MET:SD	1:C:295:LEU:HB3	2.34	0.67
1:C:200:LEU:HB2	1:C:259:LEU:CD1	2.24	0.67
1:E:113:PRO:HB2	1:E:516:THR:HG22	1.75	0.67
1:L:23:LEU:HA	1:L:60:ILE:CD1	2.23	0.67
1:A:197:ARG:HG3	1:A:198:GLY:O	1.95	0.67
1:C:183:LEU:HA	1:C:383:ALA:H	1.59	0.67
1:A:513:LEU:C	1:B:49:ILE:CD1	2.67	0.67
1:B:200:LEU:HB2	1:B:259:LEU:CD1	2.24	0.67
1:B:183:LEU:HA	1:B:383:ALA:H	1.59	0.67
1:C:162:ILE:HD13	1:C:400:LEU:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:301:ILE:HD12	1:N:309:LEU:HD23	1.75	0.67
1:D:162:ILE:HD13	1:D:400:LEU:HA	1.77	0.67
1:E:513:LEU:C	1:F:49:ILE:CD1	2.67	0.67
1:F:183:LEU:HA	1:F:383:ALA:H	1.59	0.67
1:A:249:ILE:HD12	1:A:262:LEU:HD12	1.77	0.67
1:C:249:ILE:HD12	1:C:262:LEU:HD12	1.77	0.67
1:D:249:ILE:HD12	1:D:262:LEU:HD12	1.77	0.67
1:E:227:ILE:HB	1:E:258:ALA:HB2	1.77	0.67
1:G:279:PRO:O	1:G:285:ARG:HA	1.95	0.67
1:A:49:ILE:CD1	1:G:513:LEU:CB	2.73	0.67
1:B:249:ILE:HD12	1:B:262:LEU:HD12	1.77	0.67
1:B:513:LEU:C	1:C:49:ILE:CD1	2.67	0.67
1:E:513:LEU:CB	1:F:49:ILE:CD1	2.73	0.67
1:F:200:LEU:HB2	1:F:259:LEU:CD1	2.24	0.67
1:G:249:ILE:HD12	1:G:262:LEU:HD12	1.77	0.67
1:F:227:ILE:HB	1:F:258:ALA:HB2	1.77	0.66
1:M:223:ALA:O	1:M:251:ALA:HA	1.95	0.66
1:A:183:LEU:HA	1:A:383:ALA:H	1.59	0.66
1:C:279:PRO:O	1:C:285:ARG:HA	1.95	0.66
1:E:162:ILE:HD13	1:E:400:LEU:HA	1.77	0.66
1:E:200:LEU:HB2	1:E:259:LEU:CD1	2.24	0.66
1:F:249:ILE:HD12	1:F:262:LEU:HD12	1.77	0.66
1:L:230:ILE:HD13	1:L:262:LEU:HG	1.77	0.66
1:C:513:LEU:CB	1:D:49:ILE:CD1	2.73	0.66
1:D:227:ILE:HB	1:D:258:ALA:HB2	1.77	0.66
1:F:279:PRO:O	1:F:285:ARG:HA	1.95	0.66
1:I:223:ALA:O	1:I:251:ALA:HA	1.96	0.66
1:A:213:VAL:HG12	1:A:325:ILE:HG12	1.76	0.66
1:B:162:ILE:HD13	1:B:400:LEU:HA	1.77	0.66
1:N:23:LEU:HA	1:N:60:ILE:CD1	2.25	0.66
1:A:49:ILE:CD1	1:G:513:LEU:C	2.67	0.66
1:D:200:LEU:HB2	1:D:259:LEU:CD1	2.24	0.66
1:G:183:LEU:HA	1:G:383:ALA:H	1.59	0.66
1:F:513:LEU:C	1:G:49:ILE:CD1	2.67	0.66
1:H:230:ILE:HD11	1:H:262:LEU:CG	2.24	0.66
1:B:279:PRO:O	1:B:285:ARG:HA	1.95	0.66
1:B:194:GLN:OE1	1:B:329:THR:HG21	1.96	0.66
1:A:113:PRO:HB2	1:A:516:THR:HG22	1.75	0.66
1:A:279:PRO:O	1:A:285:ARG:HA	1.95	0.66
1:E:249:ILE:HD12	1:E:262:LEU:HD12	1.77	0.66
1:E:279:PRO:O	1:E:285:ARG:HA	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:513:LEU:CB	1:G:49:ILE:CD1	2.73	0.65
1:K:23:LEU:HA	1:K:60:ILE:CD1	2.24	0.65
1:C:227:ILE:HB	1:C:258:ALA:HB2	1.78	0.65
1:D:197:ARG:HG3	1:D:198:GLY:O	1.96	0.65
1:L:223:ALA:O	1:L:251:ALA:HA	1.95	0.65
1:G:227:ILE:HB	1:G:258:ALA:HB2	1.78	0.65
1:J:223:ALA:O	1:J:251:ALA:HA	1.96	0.65
1:E:162:ILE:HD13	1:E:400:LEU:N	2.12	0.65
1:A:162:ILE:HD13	1:A:400:LEU:HA	1.77	0.65
1:D:279:PRO:O	1:D:285:ARG:HA	1.95	0.65
1:G:162:ILE:HD13	1:G:400:LEU:HA	1.77	0.65
1:H:223:ALA:O	1:H:251:ALA:HA	1.95	0.65
1:N:223:ALA:O	1:N:251:ALA:HA	1.95	0.65
1:I:230:ILE:HD13	1:I:262:LEU:HG	1.77	0.65
1:I:230:ILE:CD1	1:I:262:LEU:CG	2.69	0.65
1:L:301:ILE:HD12	1:L:309:LEU:CD2	2.22	0.65
1:D:162:ILE:HD13	1:D:400:LEU:N	2.12	0.65
1:H:230:ILE:HD11	1:H:262:LEU:HG	1.77	0.64
1:A:227:ILE:HB	1:A:258:ALA:HB2	1.77	0.64
1:C:193:MET:HE1	1:C:296:THR:CG2	2.24	0.64
1:J:230:ILE:CD1	1:J:262:LEU:CG	2.69	0.64
1:L:230:ILE:CD1	1:L:262:LEU:CG	2.69	0.64
1:B:227:ILE:HB	1:B:258:ALA:HB2	1.78	0.64
1:F:162:ILE:HD13	1:F:400:LEU:HA	1.77	0.64
1:B:513:LEU:CB	1:C:49:ILE:CD1	2.73	0.64
1:D:513:LEU:CB	1:E:49:ILE:CD1	2.72	0.64
1:F:162:ILE:HD13	1:F:400:LEU:N	2.12	0.64
1:G:193:MET:HE1	1:G:332:ILE:HD12	1.79	0.64
1:G:200:LEU:CG	1:G:254:VAL:HG11	2.28	0.64
1:G:162:ILE:HD13	1:G:400:LEU:N	2.12	0.64
1:C:202:PRO:O	1:C:205:ILE:HG13	1.98	0.64
1:M:23:LEU:HA	1:M:60:ILE:CD1	2.26	0.64
1:C:196:ASP:HA	1:C:329:THR:HG22	1.80	0.64
1:G:202:PRO:O	1:G:205:ILE:HG13	1.98	0.63
1:A:162:ILE:HD13	1:A:400:LEU:N	2.12	0.63
1:C:162:ILE:HD13	1:C:400:LEU:N	2.12	0.63
1:C:297:GLY:CA	1:C:337:GLY:HA2	2.29	0.63
1:B:162:ILE:HD13	1:B:400:LEU:N	2.12	0.63
1:B:202:PRO:O	1:B:205:ILE:HG13	1.98	0.63
1:D:150:ILE:CD1	1:D:493:ILE:HG23	2.29	0.63
1:D:224:ASP:O	1:D:303:GLU:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:LEU:CD1	1:F:259:LEU:HD13	2.29	0.63
1:B:150:ILE:CD1	1:B:493:ILE:HG23	2.29	0.63
1:B:224:ASP:O	1:B:303:GLU:HB2	1.99	0.63
1:D:297:GLY:CA	1:D:337:GLY:HA2	2.29	0.63
1:B:297:GLY:CA	1:B:337:GLY:HA2	2.29	0.63
1:G:145:ALA:HA	1:G:159:GLY:O	1.99	0.63
1:A:200:LEU:CD1	1:A:259:LEU:HD13	2.29	0.62
1:B:145:ALA:HA	1:B:159:GLY:O	1.99	0.62
1:B:200:LEU:CD1	1:B:259:LEU:HD13	2.29	0.62
1:G:150:ILE:CD1	1:G:493:ILE:HG23	2.29	0.62
1:A:145:ALA:HA	1:A:159:GLY:O	1.99	0.62
1:A:513:LEU:CB	1:B:49:ILE:CD1	2.73	0.62
1:E:224:ASP:O	1:E:303:GLU:HB2	1.99	0.62
1:I:230:ILE:CD1	1:I:262:LEU:HG	2.29	0.62
1:C:145:ALA:HA	1:C:159:GLY:O	1.99	0.62
1:C:224:ASP:O	1:C:303:GLU:HB2	1.99	0.62
1:E:200:LEU:CD1	1:E:259:LEU:HD13	2.29	0.62
1:L:230:ILE:CD1	1:L:262:LEU:HG	2.29	0.62
1:A:150:ILE:CD1	1:A:493:ILE:HG23	2.29	0.62
1:C:150:ILE:CD1	1:C:493:ILE:HG23	2.29	0.62
1:C:200:LEU:CD1	1:C:259:LEU:HD13	2.29	0.62
1:D:202:PRO:O	1:D:205:ILE:HG13	1.98	0.62
1:E:150:ILE:HD13	1:E:493:ILE:HG23	1.81	0.62
1:E:297:GLY:CA	1:E:337:GLY:HA2	2.28	0.62
1:F:150:ILE:CD1	1:F:493:ILE:HG23	2.29	0.62
1:F:224:ASP:O	1:F:303:GLU:HB2	1.99	0.62
1:A:297:GLY:CA	1:A:337:GLY:HA2	2.29	0.62
1:C:193:MET:HE3	1:C:332:ILE:HG21	1.80	0.62
1:C:204:PHE:CE1	1:C:273:VAL:O	2.53	0.62
1:E:150:ILE:CD1	1:E:493:ILE:HG23	2.29	0.62
1:F:145:ALA:HA	1:F:159:GLY:O	2.00	0.62
1:A:224:ASP:O	1:A:303:GLU:HB2	1.99	0.62
1:B:204:PHE:CE1	1:B:273:VAL:O	2.53	0.62
1:D:145:ALA:HA	1:D:159:GLY:O	1.99	0.62
1:D:204:PHE:CE1	1:D:273:VAL:O	2.53	0.62
1:G:200:LEU:HD22	1:G:254:VAL:CG1	2.29	0.62
1:G:224:ASP:O	1:G:303:GLU:HB2	1.99	0.62
1:F:150:ILE:HD13	1:F:493:ILE:HG23	1.82	0.62
1:G:297:GLY:CA	1:G:337:GLY:HA2	2.29	0.62
1:I:230:ILE:HD11	1:I:262:LEU:CD1	2.27	0.62
1:G:150:ILE:HD13	1:G:493:ILE:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:MET:HE3	1:C:332:ILE:CG2	2.30	0.61
1:D:200:LEU:CD1	1:D:259:LEU:HD13	2.29	0.61
1:D:295:LEU:CD2	1:D:342:ILE:HD13	2.30	0.61
1:J:301:ILE:CD1	1:J:309:LEU:HD23	2.31	0.61
1:A:204:PHE:CE1	1:A:273:VAL:O	2.53	0.61
1:C:150:ILE:HD13	1:C:493:ILE:HG23	1.82	0.61
1:D:169:VAL:HB	1:D:173:GLY:HA3	1.81	0.61
1:E:145:ALA:HA	1:E:159:GLY:O	2.00	0.61
1:I:230:ILE:CD1	1:I:262:LEU:HD11	2.29	0.61
1:K:230:ILE:HD11	1:K:262:LEU:CG	2.30	0.61
1:F:297:GLY:CA	1:F:337:GLY:HA2	2.29	0.61
1:N:230:ILE:CD1	1:N:262:LEU:CG	2.70	0.61
1:A:169:VAL:HB	1:A:173:GLY:HA3	1.82	0.61
1:A:150:ILE:HD13	1:A:493:ILE:HG23	1.81	0.61
1:B:169:VAL:HB	1:B:173:GLY:HA3	1.82	0.61
1:C:169:VAL:HB	1:C:173:GLY:HA3	1.81	0.61
1:L:230:ILE:CD1	1:L:262:LEU:HD11	2.30	0.61
1:E:169:VAL:HB	1:E:173:GLY:HA3	1.82	0.61
1:F:295:LEU:CD2	1:F:342:ILE:HD13	2.30	0.61
1:D:150:ILE:HD13	1:D:493:ILE:HG23	1.82	0.60
1:F:204:PHE:CE1	1:F:273:VAL:O	2.53	0.60
1:G:169:VAL:HB	1:G:173:GLY:HA3	1.81	0.60
1:J:220:ILE:HD12	1:J:296:THR:HB	1.83	0.60
1:B:150:ILE:HD13	1:B:493:ILE:HG23	1.82	0.60
1:E:295:LEU:CD2	1:E:342:ILE:HD13	2.30	0.60
1:G:204:PHE:CE1	1:G:273:VAL:O	2.53	0.60
1:L:220:ILE:HD12	1:L:296:THR:HB	1.83	0.60
1:G:295:LEU:CD2	1:G:342:ILE:HD13	2.30	0.60
1:L:248:LEU:HD13	1:L:325:ILE:HD11	1.84	0.60
1:A:217:SER:HA	1:A:320:ALA:O	2.02	0.60
1:I:248:LEU:HD13	1:I:325:ILE:HD11	1.83	0.60
1:B:217:SER:HA	1:B:320:ALA:O	2.02	0.60
1:C:221:LEU:CD1	1:C:309:LEU:HD21	2.32	0.60
1:F:169:VAL:HB	1:F:173:GLY:HA3	1.82	0.60
1:L:230:ILE:HD11	1:L:262:LEU:CD1	2.27	0.60
1:N:301:ILE:CD1	1:N:309:LEU:HD23	2.31	0.60
1:G:240:VAL:CG1	1:G:271:VAL:HG13	2.32	0.59
1:H:103:GLY:HA3	1:H:515:ILE:HD11	1.84	0.59
1:A:295:LEU:CD2	1:A:342:ILE:HD13	2.30	0.59
1:E:240:VAL:CG1	1:E:271:VAL:HG13	2.32	0.59
1:G:217:SER:HA	1:G:320:ALA:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:CD1	1:B:309:LEU:HD21	2.32	0.59
1:B:295:LEU:CD2	1:B:342:ILE:HD13	2.30	0.59
1:D:221:LEU:CD1	1:D:309:LEU:HD21	2.32	0.59
1:E:189:VAL:HG13	1:E:376:VAL:O	2.02	0.59
1:F:240:VAL:CG1	1:F:271:VAL:HG13	2.32	0.59
1:F:240:VAL:HG21	1:F:247:LEU:HB2	1.85	0.59
1:F:217:SER:HA	1:F:320:ALA:O	2.02	0.59
1:C:240:VAL:CG1	1:C:271:VAL:HG13	2.32	0.59
1:E:217:SER:HA	1:E:320:ALA:O	2.02	0.59
1:E:240:VAL:HG21	1:E:247:LEU:HB2	1.85	0.59
1:F:227:ILE:HD12	1:F:258:ALA:CB	2.33	0.59
1:A:23:LEU:CG	1:A:60:ILE:HD12	2.20	0.59
1:A:511:ALA:O	1:A:515:ILE:HG13	2.03	0.59
1:B:240:VAL:CG1	1:B:271:VAL:HG13	2.32	0.59
1:C:207:LYS:CB	1:C:208:PRO:HD3	2.31	0.59
1:M:301:ILE:HD12	1:M:309:LEU:CD2	2.29	0.59
1:A:240:VAL:CG1	1:A:271:VAL:HG13	2.32	0.58
1:D:207:LYS:CB	1:D:208:PRO:HD3	2.33	0.58
1:D:300:VAL:CG2	1:D:312:ALA:HB2	2.33	0.58
1:E:300:VAL:CG2	1:E:312:ALA:HB2	2.33	0.58
1:G:227:ILE:HD12	1:G:258:ALA:CB	2.33	0.58
1:A:52:ASP:OD1	2:A:1525:PO4:P	2.61	0.58
1:D:217:SER:HA	1:D:320:ALA:O	2.02	0.58
1:E:227:ILE:HD12	1:E:258:ALA:CB	2.33	0.58
1:F:511:ALA:O	1:F:515:ILE:HG13	2.03	0.58
1:G:52:ASP:OD1	2:G:1525:PO4:P	2.61	0.58
1:G:193:MET:HE1	1:G:292:ILE:HG23	1.84	0.58
1:M:248:LEU:HD13	1:M:325:ILE:HD11	1.84	0.58
1:C:217:SER:HA	1:C:320:ALA:O	2.02	0.58
1:C:295:LEU:CD2	1:C:342:ILE:HD13	2.30	0.58
1:D:240:VAL:CG1	1:D:271:VAL:HG13	2.32	0.58
1:K:248:LEU:HD13	1:K:325:ILE:HD11	1.85	0.58
1:E:221:LEU:CD1	1:E:309:LEU:HD21	2.32	0.58
1:G:193:MET:SD	1:G:332:ILE:HB	2.43	0.58
1:J:248:LEU:HD13	1:J:325:ILE:HD11	1.85	0.58
1:A:227:ILE:HD12	1:A:258:ALA:CB	2.33	0.58
1:B:293:ALA:HB1	1:B:299:THR:HA	1.86	0.58
1:C:293:ALA:HB1	1:C:299:THR:HA	1.86	0.58
1:D:52:ASP:OD1	2:D:1525:PO4:P	2.61	0.58
1:D:293:ALA:HB1	1:D:299:THR:HA	1.86	0.58
1:H:248:LEU:HD13	1:H:325:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ASP:OD1	2:C:1525:PO4:P	2.61	0.58
1:C:224:ASP:HA	1:C:289:LEU:HD13	1.86	0.58
1:D:227:ILE:HD12	1:D:258:ALA:CB	2.33	0.58
1:E:224:ASP:HA	1:E:289:LEU:HD13	1.86	0.58
1:F:221:LEU:CD1	1:F:309:LEU:HD21	2.32	0.58
1:F:300:VAL:CG2	1:F:312:ALA:HB2	2.33	0.58
1:A:221:LEU:CD1	1:A:309:LEU:HD21	2.32	0.58
1:C:511:ALA:O	1:C:515:ILE:HG13	2.03	0.58
1:E:293:ALA:HB1	1:E:299:THR:HA	1.86	0.58
1:B:52:ASP:OD1	2:B:1525:PO4:P	2.61	0.58
1:B:224:ASP:HA	1:B:289:LEU:HD13	1.86	0.58
1:D:224:ASP:HA	1:D:289:LEU:HD13	1.86	0.58
1:F:52:ASP:OD1	2:F:1525:PO4:P	2.61	0.58
1:G:240:VAL:HG21	1:G:247:LEU:HB2	1.85	0.58
1:D:199:TYR:CB	1:D:325:ILE:HD11	2.22	0.58
1:D:240:VAL:HG21	1:D:247:LEU:HB2	1.85	0.58
1:F:224:ASP:HA	1:F:289:LEU:HD13	1.86	0.58
1:G:511:ALA:O	1:G:515:ILE:HG13	2.04	0.58
1:J:103:GLY:HA3	1:J:515:ILE:HD11	1.85	0.58
1:A:293:ALA:HB1	1:A:299:THR:HA	1.86	0.58
1:E:52:ASP:OD1	2:E:1525:PO4:P	2.62	0.58
1:E:189:VAL:HG22	1:E:376:VAL:O	2.03	0.58
1:G:221:LEU:CD1	1:G:309:LEU:HD21	2.32	0.58
1:M:229:ASN:HA	1:M:258:ALA:HB3	1.86	0.58
1:K:230:ILE:HD11	1:K:262:LEU:HG	1.84	0.57
1:N:248:LEU:HD13	1:N:325:ILE:HD11	1.84	0.57
1:B:300:VAL:CG2	1:B:312:ALA:HB2	2.33	0.57
1:C:227:ILE:HD12	1:C:258:ALA:CB	2.33	0.57
1:E:511:ALA:O	1:E:515:ILE:HG13	2.04	0.57
1:K:220:ILE:HD12	1:K:296:THR:HB	1.86	0.57
1:A:240:VAL:HG21	1:A:247:LEU:HB2	1.85	0.57
1:B:194:GLN:HG2	1:B:195:PHE:N	2.18	0.57
1:B:511:ALA:O	1:B:515:ILE:HG13	2.04	0.57
1:C:195:PHE:CE1	1:C:292:ILE:HD13	2.40	0.57
1:G:195:PHE:CE1	1:G:292:ILE:HD13	2.40	0.57
1:L:227:ILE:HD12	1:L:233:MET:HE1	1.77	0.57
1:A:224:ASP:HA	1:A:289:LEU:HD13	1.86	0.57
1:A:300:VAL:CG2	1:A:312:ALA:HB2	2.33	0.57
1:G:300:VAL:CG2	1:G:312:ALA:HB2	2.33	0.57
1:B:227:ILE:HD12	1:B:258:ALA:CB	2.33	0.57
1:B:240:VAL:HG21	1:B:247:LEU:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:PHE:CZ	1:E:262:LEU:HD21	2.40	0.57
1:J:85:ALA:HB1	1:J:499:VAL:HG12	1.86	0.57
1:A:195:PHE:CE1	1:A:292:ILE:HD13	2.40	0.57
1:C:240:VAL:HG21	1:C:247:LEU:HB2	1.85	0.57
1:C:381:VAL:HG22	1:C:382:GLY:N	2.20	0.57
1:B:381:VAL:HG22	1:B:382:GLY:N	2.20	0.57
1:C:300:VAL:CG2	1:C:312:ALA:HB2	2.33	0.57
1:D:195:PHE:CE1	1:D:292:ILE:HD13	2.39	0.57
1:E:517:THR:HG23	1:F:39:VAL:HG22	1.87	0.57
1:F:293:ALA:HB1	1:F:299:THR:HA	1.86	0.57
1:G:224:ASP:HA	1:G:289:LEU:HD13	1.86	0.57
1:L:248:LEU:CD1	1:L:325:ILE:HD11	2.35	0.57
1:G:293:ALA:HB1	1:G:299:THR:HA	1.86	0.57
1:A:193:MET:HE2	1:A:295:LEU:HD12	1.87	0.57
1:A:381:VAL:HG22	1:A:382:GLY:N	2.20	0.57
1:B:23:LEU:CG	1:B:60:ILE:HD12	2.20	0.57
1:K:229:ASN:HA	1:K:258:ALA:HB3	1.85	0.57
1:B:241:ALA:HA	1:B:271:VAL:HG22	1.87	0.56
1:D:517:THR:HG23	1:E:39:VAL:HG22	1.87	0.56
1:E:193:MET:HE2	1:E:295:LEU:HD12	1.88	0.56
1:A:199:TYR:CB	1:A:325:ILE:HD11	2.26	0.56
1:A:241:ALA:HA	1:A:271:VAL:HG22	1.88	0.56
1:C:517:THR:HG23	1:D:39:VAL:HG22	1.87	0.56
1:D:193:MET:HE2	1:D:295:LEU:HD12	1.87	0.56
1:E:241:ALA:HA	1:E:271:VAL:HG22	1.87	0.56
1:F:193:MET:HE2	1:F:295:LEU:HD12	1.87	0.56
1:F:241:ALA:HA	1:F:271:VAL:HG22	1.88	0.56
1:G:193:MET:CE	1:G:292:ILE:HG23	2.35	0.56
1:G:241:ALA:HA	1:G:271:VAL:HG22	1.87	0.56
1:A:39:VAL:HG22	1:G:517:THR:HG23	1.87	0.56
1:C:23:LEU:HA	1:C:60:ILE:CD1	2.33	0.56
1:C:193:MET:HE3	1:C:332:ILE:HB	1.86	0.56
1:C:241:ALA:HA	1:C:271:VAL:HG22	1.87	0.56
1:D:381:VAL:HG22	1:D:382:GLY:N	2.20	0.56
1:F:517:THR:HG23	1:G:39:VAL:HG22	1.87	0.56
1:G:192:GLY:HA3	1:G:376:VAL:HG23	1.87	0.56
1:H:229:ASN:HA	1:H:258:ALA:HB3	1.86	0.56
1:L:301:ILE:HD13	1:L:309:LEU:HD23	1.85	0.56
1:D:241:ALA:HA	1:D:271:VAL:HG22	1.87	0.56
1:E:195:PHE:CE1	1:E:292:ILE:HD13	2.40	0.56
1:G:200:LEU:CD1	1:G:200:LEU:N	2.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:103:GLY:HA3	1:I:515:ILE:HD11	1.88	0.56
1:I:248:LEU:CD1	1:I:325:ILE:HD11	2.35	0.56
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.86	0.56
1:M:230:ILE:HD11	1:M:262:LEU:CG	2.34	0.56
1:B:517:THR:HG23	1:C:39:VAL:HG22	1.87	0.56
1:E:223:ALA:CA	1:E:309:LEU:HD23	2.36	0.56
1:F:192:GLY:HA3	1:F:376:VAL:HG23	1.87	0.56
1:F:200:LEU:HB3	1:F:259:LEU:HD22	1.88	0.56
1:G:23:LEU:CG	1:G:60:ILE:HD12	2.20	0.56
1:L:103:GLY:HA3	1:L:515:ILE:HD11	1.87	0.56
1:A:192:GLY:HA3	1:A:376:VAL:HG23	1.87	0.56
1:B:193:MET:HE2	1:B:295:LEU:HD12	1.88	0.56
1:C:223:ALA:CA	1:C:309:LEU:HD23	2.36	0.56
1:D:100:ILE:HD13	1:D:514:MET:SD	2.46	0.56
1:F:100:ILE:HD13	1:F:514:MET:SD	2.46	0.56
1:B:200:LEU:HD12	1:B:259:LEU:HD13	1.87	0.56
1:F:200:LEU:CB	1:F:259:LEU:CD1	2.84	0.56
1:I:220:ILE:HD12	1:I:296:THR:HB	1.88	0.56
1:D:223:ALA:CA	1:D:309:LEU:HD23	2.36	0.56
1:E:192:GLY:HA3	1:E:376:VAL:HG23	1.87	0.56
1:E:200:LEU:HD12	1:E:259:LEU:HD13	1.87	0.56
1:F:200:LEU:HD12	1:F:259:LEU:HD13	1.87	0.56
1:H:220:ILE:HD12	1:H:296:THR:HB	1.87	0.56
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.87	0.56
1:N:248:LEU:CD1	1:N:325:ILE:HD11	2.36	0.56
1:B:195:PHE:CE1	1:B:292:ILE:HD13	2.41	0.56
1:E:199:TYR:CB	1:E:325:ILE:HD11	2.25	0.56
1:G:100:ILE:HD13	1:G:514:MET:SD	2.46	0.56
1:G:381:VAL:HG22	1:G:382:GLY:N	2.20	0.56
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.86	0.56
1:M:230:ILE:HD13	1:M:262:LEU:HG	1.83	0.56
1:A:200:LEU:HD12	1:A:259:LEU:HD13	1.87	0.56
1:A:517:THR:HG23	1:B:39:VAL:HG22	1.87	0.56
1:C:100:ILE:HD13	1:C:514:MET:SD	2.46	0.56
1:G:200:LEU:HD13	1:G:254:VAL:CG1	2.36	0.56
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.87	0.56
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.87	0.56
1:C:193:MET:O	1:C:193:MET:HG3	2.06	0.55
1:C:200:LEU:HD12	1:C:259:LEU:HD13	1.87	0.55
1:H:248:LEU:CD1	1:H:325:ILE:HD11	2.36	0.55
1:K:103:GLY:HA3	1:K:515:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:ILE:HD13	1:E:514:MET:SD	2.47	0.55
1:I:229:ASN:HA	1:I:258:ALA:HB3	1.87	0.55
1:D:200:LEU:CB	1:D:259:LEU:CD1	2.84	0.55
1:E:200:LEU:HB3	1:E:259:LEU:HD22	1.88	0.55
1:M:230:ILE:HD11	1:M:262:LEU:HG	1.88	0.55
1:N:229:ASN:HA	1:N:258:ALA:HB3	1.89	0.55
1:B:213:VAL:HG11	1:B:325:ILE:HG12	1.86	0.55
1:F:196:ASP:HA	1:F:329:THR:HG22	1.87	0.55
1:F:223:ALA:CA	1:F:309:LEU:HD23	2.36	0.55
1:J:248:LEU:CD1	1:J:325:ILE:HD11	2.36	0.55
1:K:301:ILE:HD13	1:K:309:LEU:HD23	1.84	0.55
1:A:406:ALA:HB1	1:A:411:VAL:HG13	1.89	0.55
1:B:406:ALA:HB1	1:B:411:VAL:HG13	1.89	0.55
1:C:193:MET:HE3	1:C:332:ILE:CB	2.37	0.55
1:A:200:LEU:HB3	1:A:259:LEU:HD22	1.88	0.55
1:B:192:GLY:HA3	1:B:376:VAL:HG23	1.87	0.55
1:D:192:GLY:HA3	1:D:376:VAL:HG23	1.88	0.55
1:D:200:LEU:HD12	1:D:259:LEU:HD13	1.87	0.55
1:G:213:VAL:HG11	1:G:325:ILE:HG12	1.86	0.55
1:M:248:LEU:CD1	1:M:325:ILE:HD11	2.35	0.55
1:N:103:GLY:HA3	1:N:515:ILE:HD11	1.89	0.55
1:A:100:ILE:HD13	1:A:514:MET:SD	2.46	0.55
1:F:381:VAL:HG22	1:F:382:GLY:N	2.20	0.55
1:M:227:ILE:HD12	1:M:233:MET:HE1	1.81	0.55
1:B:223:ALA:CA	1:B:309:LEU:HD23	2.35	0.55
1:D:200:LEU:HB3	1:D:259:LEU:HD22	1.88	0.55
1:E:381:VAL:HG22	1:E:382:GLY:N	2.20	0.55
1:G:199:TYR:CB	1:G:325:ILE:HD11	2.26	0.55
1:G:406:ALA:HB1	1:G:411:VAL:HG13	1.89	0.55
1:F:195:PHE:CZ	1:F:330:THR:HB	2.42	0.55
1:K:248:LEU:CD1	1:K:325:ILE:HD11	2.37	0.55
1:L:229:ASN:HA	1:L:258:ALA:HB3	1.89	0.55
1:G:223:ALA:CA	1:G:309:LEU:HD23	2.36	0.55
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.87	0.55
1:M:475:ASN:ND2	1:M:489:ILE:HD11	2.22	0.55
1:N:220:ILE:HD12	1:N:296:THR:HB	1.86	0.55
1:B:100:ILE:HD13	1:B:514:MET:SD	2.46	0.54
1:F:199:TYR:CB	1:F:325:ILE:HD11	2.25	0.54
1:M:220:ILE:HD12	1:M:296:THR:HB	1.87	0.54
1:N:475:ASN:ND2	1:N:489:ILE:HD11	2.22	0.54
1:A:150:ILE:CD1	1:A:493:ILE:CA	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ILE:CD1	1:C:262:LEU:HD12	2.37	0.54
1:E:249:ILE:CD1	1:E:262:LEU:HD12	2.37	0.54
1:C:34:LYS:HB3	1:C:457:ASN:O	2.08	0.54
1:D:137:PRO:HA	1:D:410:GLY:HA3	1.90	0.54
1:E:193:MET:SD	1:E:292:ILE:HG23	2.47	0.54
1:F:38:VAL:HG21	1:F:56:VAL:CG2	2.37	0.54
1:F:193:MET:SD	1:F:292:ILE:HG23	2.48	0.54
1:F:249:ILE:CD1	1:F:262:LEU:HD12	2.37	0.54
1:A:200:LEU:CB	1:A:259:LEU:CD1	2.84	0.54
1:A:200:LEU:HB3	1:A:259:LEU:CD2	2.38	0.54
1:D:31:LEU:HB2	1:D:90:THR:HG21	1.90	0.54
1:D:114:MET:HB2	1:E:36:ARG:HD2	1.88	0.54
1:A:223:ALA:CA	1:A:309:LEU:HD23	2.36	0.54
1:A:249:ILE:CD1	1:A:262:LEU:HD12	2.37	0.54
1:B:200:LEU:HB3	1:B:259:LEU:HD22	1.88	0.54
1:C:38:VAL:CG1	1:C:56:VAL:HG22	2.38	0.54
1:C:406:ALA:HB1	1:C:411:VAL:HG13	1.89	0.54
1:E:38:VAL:CG1	1:E:56:VAL:HG22	2.38	0.54
1:E:312:ALA:HB1	1:E:316:ASP:OD2	2.07	0.54
1:F:200:LEU:HD11	1:F:254:VAL:CA	2.12	0.54
1:D:38:VAL:CG1	1:D:56:VAL:HG22	2.38	0.54
1:D:193:MET:SD	1:D:292:ILE:HG23	2.48	0.54
1:G:150:ILE:CD1	1:G:493:ILE:CA	2.71	0.54
1:H:475:ASN:ND2	1:H:489:ILE:HD11	2.22	0.54
1:B:31:LEU:HB2	1:B:90:THR:HG21	1.90	0.54
1:C:200:LEU:HB3	1:C:259:LEU:HD22	1.88	0.54
1:C:312:ALA:HB1	1:C:316:ASP:OD2	2.07	0.54
1:D:38:VAL:HG21	1:D:56:VAL:CG2	2.38	0.54
1:D:249:ILE:CD1	1:D:262:LEU:HD12	2.37	0.54
1:F:406:ALA:HB1	1:F:411:VAL:HG13	1.88	0.54
1:G:31:LEU:HB2	1:G:90:THR:HG21	1.90	0.54
1:B:38:VAL:CG1	1:B:56:VAL:HG22	2.38	0.54
1:B:137:PRO:HA	1:B:410:GLY:HA3	1.90	0.54
1:F:31:LEU:HB2	1:F:90:THR:HG21	1.90	0.54
1:G:23:LEU:HA	1:G:60:ILE:CD1	2.33	0.54
1:A:38:VAL:HG21	1:A:56:VAL:CG2	2.38	0.54
1:B:23:LEU:HA	1:B:60:ILE:CD1	2.33	0.54
1:B:200:LEU:HB3	1:B:259:LEU:CD2	2.38	0.54
1:C:192:GLY:HA3	1:C:376:VAL:CG2	2.38	0.54
1:B:38:VAL:HG21	1:B:56:VAL:CG2	2.38	0.54
1:B:193:MET:SD	1:B:292:ILE:HG23	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LEU:HB2	1:C:90:THR:HG21	1.90	0.54
1:E:213:VAL:HG11	1:E:325:ILE:HG12	1.86	0.54
1:E:240:VAL:HG12	1:E:271:VAL:HG13	1.90	0.54
1:F:240:VAL:HG12	1:F:271:VAL:HG13	1.90	0.54
1:G:240:VAL:HG12	1:G:271:VAL:HG13	1.90	0.54
1:G:328:ASP:O	1:G:329:THR:HG23	2.08	0.54
1:B:249:ILE:CD1	1:B:262:LEU:HD12	2.37	0.53
1:E:31:LEU:HB2	1:E:90:THR:HG21	1.90	0.53
1:E:406:ALA:HB1	1:E:411:VAL:HG13	1.88	0.53
1:F:137:PRO:HA	1:F:410:GLY:HA3	1.90	0.53
1:F:144:ILE:HG23	1:F:403:THR:CG2	2.38	0.53
1:F:328:ASP:O	1:F:329:THR:HG23	2.08	0.53
1:G:249:ILE:CD1	1:G:262:LEU:HD12	2.37	0.53
1:G:312:ALA:HB1	1:G:316:ASP:OD2	2.07	0.53
1:H:23:LEU:CD1	1:H:60:ILE:HD12	2.24	0.53
1:A:31:LEU:HB2	1:A:90:THR:HG21	1.91	0.53
1:C:144:ILE:HG23	1:C:403:THR:CG2	2.39	0.53
1:C:224:ASP:CG	1:C:302:SER:HA	2.33	0.53
1:D:406:ALA:HB1	1:D:411:VAL:HG13	1.88	0.53
1:E:23:LEU:HA	1:E:60:ILE:CD1	2.33	0.53
1:E:144:ILE:HG23	1:E:403:THR:CG2	2.39	0.53
1:G:201:SER:OG	1:G:203:TYR:HB2	2.08	0.53
1:B:200:LEU:CB	1:B:259:LEU:CD1	2.84	0.53
1:D:144:ILE:HG23	1:D:403:THR:CG2	2.38	0.53
1:G:144:ILE:HG23	1:G:403:THR:CG2	2.39	0.53
1:A:23:LEU:HA	1:A:60:ILE:CD1	2.33	0.53
1:A:144:ILE:HG23	1:A:403:THR:CG2	2.38	0.53
1:A:240:VAL:HG12	1:A:271:VAL:HG13	1.90	0.53
1:B:144:ILE:HG23	1:B:403:THR:CG2	2.38	0.53
1:D:34:LYS:HB3	1:D:457:ASN:O	2.08	0.53
1:D:240:VAL:HG12	1:D:271:VAL:HG13	1.90	0.53
1:E:328:ASP:O	1:E:329:THR:HG23	2.08	0.53
1:A:38:VAL:CG1	1:A:56:VAL:HG22	2.38	0.53
1:A:193:MET:SD	1:A:292:ILE:HG23	2.48	0.53
1:B:224:ASP:CG	1:B:302:SER:HA	2.33	0.53
1:D:513:LEU:HD22	1:E:49:ILE:HD12	1.91	0.53
1:E:38:VAL:HG21	1:E:56:VAL:CG2	2.39	0.53
1:F:23:LEU:CG	1:F:60:ILE:HD12	2.20	0.53
1:F:213:VAL:HG11	1:F:325:ILE:HG12	1.86	0.53
1:F:224:ASP:CG	1:F:302:SER:HA	2.33	0.53
1:A:312:ALA:HB1	1:A:316:ASP:OD2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:LEU:HB3	1:C:259:LEU:CD2	2.38	0.53
1:C:213:VAL:HG11	1:C:325:ILE:HG12	1.86	0.53
1:D:328:ASP:O	1:D:329:THR:HG23	2.08	0.53
1:F:200:LEU:HB3	1:F:259:LEU:CD2	2.38	0.53
1:F:312:ALA:HB1	1:F:316:ASP:OD2	2.07	0.53
1:C:38:VAL:HG21	1:C:56:VAL:CG2	2.39	0.53
1:D:200:LEU:HB3	1:D:259:LEU:CD2	2.38	0.53
1:E:200:LEU:HB3	1:E:259:LEU:CD2	2.38	0.53
1:I:475:ASN:ND2	1:I:489:ILE:HD11	2.23	0.53
1:K:475:ASN:ND2	1:K:489:ILE:HD11	2.23	0.53
1:A:328:ASP:O	1:A:329:THR:HG23	2.08	0.53
1:G:224:ASP:CG	1:G:302:SER:HA	2.33	0.53
1:B:312:ALA:HB1	1:B:316:ASP:OD2	2.07	0.53
1:D:513:LEU:CD2	1:E:49:ILE:HD12	2.39	0.53
1:F:38:VAL:CG1	1:F:56:VAL:HG22	2.38	0.53
1:G:38:VAL:HG21	1:G:56:VAL:CG2	2.39	0.53
1:M:227:ILE:CD1	1:M:233:MET:CE	2.56	0.53
1:D:312:ALA:HB1	1:D:316:ASP:OD2	2.07	0.52
1:E:200:LEU:CB	1:E:259:LEU:CD1	2.84	0.52
1:A:224:ASP:CG	1:A:302:SER:HA	2.33	0.52
1:C:240:VAL:HG12	1:C:271:VAL:HG13	1.90	0.52
1:A:137:PRO:HA	1:A:410:GLY:HA3	1.90	0.52
1:G:38:VAL:CG1	1:G:56:VAL:HG22	2.38	0.52
1:A:193:MET:SD	1:A:292:ILE:HA	2.50	0.52
1:A:521:VAL:HG21	1:B:59:GLU:HB2	1.92	0.52
1:B:247:LEU:HB3	1:B:273:VAL:HG22	1.91	0.52
1:B:328:ASP:O	1:B:329:THR:HG23	2.08	0.52
1:C:137:PRO:HA	1:C:410:GLY:HA3	1.90	0.52
1:C:150:ILE:CD1	1:C:493:ILE:CA	2.71	0.52
1:C:513:LEU:HA	1:D:49:ILE:CD1	2.39	0.52
1:D:224:ASP:CG	1:D:302:SER:HA	2.33	0.52
1:J:229:ASN:HA	1:J:258:ALA:HB3	1.91	0.52
1:L:475:ASN:ND2	1:L:489:ILE:HD11	2.24	0.52
1:C:200:LEU:CB	1:C:259:LEU:CD1	2.84	0.52
1:C:328:ASP:O	1:C:329:THR:HG23	2.08	0.52
1:M:103:GLY:HA3	1:M:515:ILE:HD11	1.90	0.52
1:B:193:MET:SD	1:B:292:ILE:HA	2.50	0.52
1:C:207:LYS:HD3	1:C:207:LYS:N	2.25	0.52
1:D:250:ILE:HD11	1:D:332:ILE:HD11	1.92	0.52
1:E:521:VAL:HG21	1:F:59:GLU:HB2	1.92	0.52
1:F:513:LEU:CD2	1:G:49:ILE:HD12	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:475:ASN:ND2	1:J:489:ILE:HD11	2.23	0.52
1:A:247:LEU:HB3	1:A:273:VAL:HG22	1.91	0.52
1:A:513:LEU:HA	1:B:49:ILE:CD1	2.39	0.52
1:C:250:ILE:HD11	1:C:332:ILE:HD11	1.92	0.52
1:E:247:LEU:HB3	1:E:273:VAL:HG22	1.91	0.52
1:K:136:VAL:HG21	1:K:489:ILE:HD13	1.92	0.52
1:A:49:ILE:CD1	1:G:513:LEU:HA	2.39	0.52
1:A:250:ILE:HD11	1:A:332:ILE:HD11	1.92	0.52
1:C:247:LEU:HB3	1:C:273:VAL:HG22	1.91	0.52
1:D:191:GLU:OE1	1:D:191:GLU:HA	2.10	0.52
1:E:250:ILE:HD11	1:E:332:ILE:HD11	1.92	0.52
1:A:49:ILE:HD12	1:G:513:LEU:CD2	2.40	0.52
1:B:250:ILE:HD11	1:B:332:ILE:HD11	1.92	0.52
1:C:513:LEU:HD22	1:D:49:ILE:HD12	1.92	0.52
1:E:224:ASP:CG	1:E:302:SER:HA	2.34	0.52
1:G:193:MET:SD	1:G:332:ILE:HD12	2.50	0.52
1:I:475:ASN:ND2	1:I:489:ILE:CD1	2.73	0.52
1:A:59:GLU:HB2	1:G:521:VAL:HG21	1.92	0.52
1:B:240:VAL:HG12	1:B:271:VAL:HG13	1.90	0.52
1:C:183:LEU:HA	1:C:383:ALA:N	2.25	0.52
1:D:183:LEU:HA	1:D:383:ALA:N	2.25	0.52
1:E:513:LEU:CD2	1:F:49:ILE:HD12	2.40	0.52
1:F:247:LEU:HB3	1:F:273:VAL:HG22	1.91	0.52
1:F:521:VAL:HG21	1:G:59:GLU:HB2	1.92	0.52
1:G:250:ILE:HD11	1:G:332:ILE:HD11	1.92	0.52
1:A:254:VAL:H	1:A:277:LYS:HG2	1.76	0.51
1:B:199:TYR:CB	1:B:325:ILE:HD11	2.26	0.51
1:C:521:VAL:HG21	1:D:59:GLU:HB2	1.92	0.51
1:F:250:ILE:HD11	1:F:332:ILE:HD11	1.92	0.51
1:A:513:LEU:CD2	1:B:49:ILE:HD12	2.40	0.51
1:E:137:PRO:HA	1:E:410:GLY:HA3	1.90	0.51
1:E:338:GLU:HG2	1:E:340:ALA:HB3	1.93	0.51
1:E:513:LEU:HA	1:F:49:ILE:CD1	2.40	0.51
1:B:183:LEU:HA	1:B:383:ALA:N	2.25	0.51
1:B:200:LEU:HD11	1:B:254:VAL:CA	2.12	0.51
1:B:475:ASN:ND2	1:B:489:ILE:HD11	2.26	0.51
1:D:338:GLU:HG2	1:D:340:ALA:HB3	1.92	0.51
1:D:513:LEU:HA	1:E:49:ILE:CD1	2.39	0.51
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.93	0.51
1:G:34:LYS:HB2	1:G:458:CYS:HA	1.92	0.51
1:A:475:ASN:ND2	1:A:489:ILE:HD11	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ALA:HB1	1:B:361:ASP:HB2	1.93	0.51
1:C:199:TYR:CB	1:C:325:ILE:HD11	2.26	0.51
1:C:475:ASN:ND2	1:C:489:ILE:HD11	2.26	0.51
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.93	0.51
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.93	0.51
1:F:513:LEU:HA	1:G:49:ILE:CD1	2.39	0.51
1:A:34:LYS:HB2	1:A:458:CYS:HA	1.92	0.51
1:A:225:LYS:CB	1:A:308:GLU:HA	2.41	0.51
1:B:513:LEU:CD2	1:C:49:ILE:HD12	2.40	0.51
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.93	0.51
1:C:161:LEU:HD11	1:C:185:ASP:HB3	1.93	0.51
1:C:356:ALA:HB1	1:C:361:ASP:HB2	1.93	0.51
1:C:513:LEU:CD2	1:D:49:ILE:HD12	2.40	0.51
1:D:193:MET:SD	1:D:292:ILE:HA	2.50	0.51
1:D:475:ASN:ND2	1:D:489:ILE:HD11	2.26	0.51
1:E:193:MET:SD	1:E:292:ILE:HA	2.50	0.51
1:F:338:GLU:HG2	1:F:340:ALA:HB3	1.92	0.51
1:A:356:ALA:HB1	1:A:361:ASP:HB2	1.93	0.51
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.93	0.51
1:B:141:SER:O	1:B:163:ALA:HB1	2.11	0.51
1:C:206:ASN:CG	1:C:207:LYS:H	2.19	0.51
1:C:254:VAL:H	1:C:277:LYS:HG2	1.76	0.51
1:D:247:LEU:HB3	1:D:273:VAL:HG22	1.91	0.51
1:E:513:LEU:HD22	1:F:49:ILE:HD12	1.93	0.51
1:F:193:MET:SD	1:F:292:ILE:HA	2.50	0.51
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.93	0.51
1:G:247:LEU:HB3	1:G:273:VAL:HG22	1.91	0.51
1:A:49:ILE:HD12	1:G:513:LEU:HD22	1.92	0.51
1:B:161:LEU:HD11	1:B:185:ASP:HB3	1.93	0.51
1:B:224:ASP:HA	1:B:289:LEU:CD1	2.41	0.51
1:C:192:GLY:HA3	1:C:376:VAL:HG23	1.93	0.51
1:D:161:LEU:HD11	1:D:185:ASP:HB3	1.93	0.51
1:D:213:VAL:HG11	1:D:325:ILE:HG12	1.86	0.51
1:E:141:SER:O	1:E:163:ALA:HB1	2.11	0.51
1:E:150:ILE:CD1	1:E:493:ILE:CA	2.71	0.51
1:F:141:SER:O	1:F:163:ALA:HB1	2.11	0.51
1:F:475:ASN:ND2	1:F:489:ILE:HD11	2.26	0.51
1:G:141:SER:O	1:G:163:ALA:HB1	2.11	0.51
1:G:254:VAL:H	1:G:277:LYS:HG2	1.75	0.51
1:G:338:GLU:HG2	1:G:340:ALA:HB3	1.93	0.51
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:OD1	1:A:207:LYS:HD3	2.11	0.51
1:C:225:LYS:CB	1:C:308:GLU:HA	2.41	0.51
1:D:254:VAL:H	1:D:277:LYS:HG2	1.75	0.51
1:D:356:ALA:HB1	1:D:361:ASP:HB2	1.93	0.51
1:E:475:ASN:ND2	1:E:489:ILE:HD11	2.26	0.51
1:E:183:LEU:HA	1:E:383:ALA:N	2.25	0.51
1:G:158:VAL:HG22	1:G:396:VAL:HG22	1.93	0.51
1:G:225:LYS:CB	1:G:308:GLU:HA	2.41	0.51
1:J:103:GLY:HA3	1:J:515:ILE:CD1	2.41	0.51
1:B:52:ASP:CB	1:B:55:SER:H	2.24	0.50
1:C:141:SER:O	1:C:163:ALA:HB1	2.11	0.50
1:E:207:LYS:HB2	1:E:208:PRO:HD3	1.93	0.50
1:E:254:VAL:H	1:E:277:LYS:HG2	1.76	0.50
1:A:513:LEU:HD22	1:B:49:ILE:HD12	1.92	0.50
1:D:52:ASP:CB	1:D:55:SER:H	2.25	0.50
1:D:141:SER:O	1:D:163:ALA:HB1	2.11	0.50
1:E:158:VAL:HG22	1:E:396:VAL:HG22	1.94	0.50
1:E:225:LYS:CB	1:E:308:GLU:HA	2.41	0.50
1:F:164:GLU:HB3	1:F:187:LEU:HD21	1.93	0.50
1:G:199:TYR:HD1	1:G:200:LEU:O	1.94	0.50
1:J:475:ASN:ND2	1:J:489:ILE:CD1	2.75	0.50
1:A:52:ASP:CB	1:A:55:SER:H	2.25	0.50
1:A:158:VAL:HG22	1:A:396:VAL:HG22	1.94	0.50
1:A:183:LEU:HA	1:A:383:ALA:N	2.25	0.50
1:B:194:GLN:HE21	1:B:194:GLN:C	2.19	0.50
1:B:513:LEU:HA	1:C:49:ILE:CD1	2.39	0.50
1:C:200:LEU:HD11	1:C:254:VAL:HG22	1.92	0.50
1:C:338:GLU:HG2	1:C:340:ALA:HB3	1.93	0.50
1:D:521:VAL:HG21	1:E:59:GLU:HB2	1.92	0.50
1:F:158:VAL:HG22	1:F:396:VAL:HG22	1.93	0.50
1:F:224:ASP:HA	1:F:289:LEU:CD1	2.41	0.50
1:G:52:ASP:CB	1:G:55:SER:H	2.25	0.50
1:G:475:ASN:ND2	1:G:489:ILE:HD11	2.26	0.50
1:B:206:ASN:HB3	1:B:208:PRO:HD2	1.94	0.50
1:D:166:MET:O	1:D:170:GLY:HA2	2.12	0.50
1:E:161:LEU:HD11	1:E:185:ASP:HB3	1.93	0.50
1:E:200:LEU:HD11	1:E:254:VAL:CA	2.12	0.50
1:F:254:VAL:H	1:F:277:LYS:HG2	1.76	0.50
1:G:166:MET:O	1:G:170:GLY:HA2	2.12	0.50
1:K:475:ASN:ND2	1:K:489:ILE:CD1	2.75	0.50
1:A:161:LEU:HD11	1:A:185:ASP:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASP:HA	1:A:289:LEU:CD1	2.41	0.50
1:C:158:VAL:HG22	1:C:396:VAL:HG22	1.93	0.50
1:C:224:ASP:HA	1:C:289:LEU:CD1	2.41	0.50
1:D:224:ASP:HA	1:D:289:LEU:CD1	2.41	0.50
1:E:34:LYS:HB2	1:E:458:CYS:HA	1.92	0.50
1:F:34:LYS:HB2	1:F:458:CYS:HA	1.92	0.50
1:F:513:LEU:HD22	1:G:49:ILE:HD12	1.92	0.50
1:I:23:LEU:CD1	1:I:60:ILE:HD12	2.28	0.50
1:A:255:GLU:HB2	1:A:259:LEU:H	1.77	0.50
1:E:166:MET:O	1:E:170:GLY:HA2	2.12	0.50
1:G:356:ALA:HB1	1:G:361:ASP:HB2	1.93	0.50
1:H:99:ILE:CG2	1:H:120:ILE:HD13	2.42	0.50
1:J:23:LEU:CD1	1:J:60:ILE:HD12	2.27	0.50
1:L:475:ASN:ND2	1:L:489:ILE:CD1	2.74	0.50
1:A:338:GLU:HG2	1:A:340:ALA:HB3	1.93	0.50
1:A:382:GLY:O	1:A:389:MET:HA	2.12	0.50
1:B:166:MET:O	1:B:170:GLY:HA2	2.12	0.50
1:B:254:VAL:H	1:B:277:LYS:HG2	1.76	0.50
1:D:158:VAL:HG22	1:D:396:VAL:HG22	1.94	0.50
1:D:225:LYS:CB	1:D:308:GLU:HA	2.41	0.50
1:E:23:LEU:CG	1:E:60:ILE:HD12	2.20	0.50
1:F:52:ASP:CB	1:F:55:SER:H	2.25	0.50
1:F:225:LYS:CB	1:F:308:GLU:HA	2.41	0.50
1:A:141:SER:O	1:A:163:ALA:HB1	2.11	0.50
1:B:255:GLU:HB2	1:B:259:LEU:H	1.77	0.50
1:C:52:ASP:CB	1:C:55:SER:H	2.25	0.50
1:C:193:MET:CE	1:C:332:ILE:HG21	2.42	0.50
1:D:200:LEU:HD11	1:D:254:VAL:HG22	1.92	0.50
1:E:382:GLY:O	1:E:389:MET:HA	2.12	0.50
1:G:382:GLY:O	1:G:389:MET:HA	2.12	0.50
1:N:475:ASN:ND2	1:N:489:ILE:CD1	2.75	0.50
1:B:158:VAL:HG22	1:B:396:VAL:HG22	1.94	0.50
1:B:194:GLN:HG3	1:B:329:THR:OG1	2.11	0.50
1:C:147:VAL:HG22	1:C:494:LEU:HB2	1.94	0.50
1:D:23:LEU:HA	1:D:60:ILE:CD1	2.33	0.50
1:D:406:ALA:HB1	1:D:411:VAL:CG1	2.42	0.50
1:E:356:ALA:HB1	1:E:361:ASP:HB2	1.93	0.50
1:F:255:GLU:HB2	1:F:259:LEU:H	1.77	0.50
1:G:224:ASP:HA	1:G:289:LEU:CD1	2.41	0.50
1:G:225:LYS:HB2	1:G:308:GLU:HA	1.94	0.50
1:H:230:ILE:HD13	1:H:262:LEU:HG	1.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:103:GLY:HA3	1:L:515:ILE:CD1	2.41	0.50
1:A:166:MET:O	1:A:170:GLY:HA2	2.12	0.49
1:B:338:GLU:HG2	1:B:340:ALA:HB3	1.93	0.49
1:D:382:GLY:O	1:D:389:MET:HA	2.12	0.49
1:E:52:ASP:CB	1:E:55:SER:H	2.25	0.49
1:E:224:ASP:HA	1:E:289:LEU:CD1	2.41	0.49
1:F:147:VAL:HG22	1:F:494:LEU:HB2	1.94	0.49
1:F:183:LEU:HA	1:F:383:ALA:N	2.25	0.49
1:F:406:ALA:HB1	1:F:411:VAL:CG1	2.42	0.49
1:A:225:LYS:HB2	1:A:308:GLU:HA	1.94	0.49
1:B:147:VAL:HG22	1:B:494:LEU:HB2	1.94	0.49
1:B:192:GLY:HA3	1:B:376:VAL:CG2	2.42	0.49
1:C:166:MET:O	1:C:170:GLY:HA2	2.12	0.49
1:E:147:VAL:HG22	1:E:494:LEU:HB2	1.94	0.49
1:F:161:LEU:HD11	1:F:185:ASP:HB3	1.93	0.49
1:G:183:LEU:HA	1:G:383:ALA:N	2.25	0.49
1:H:320:ALA:HA	1:H:334:ASP:O	2.12	0.49
1:I:320:ALA:HA	1:I:334:ASP:O	2.12	0.49
1:B:34:LYS:HB2	1:B:458:CYS:HA	1.93	0.49
1:B:382:GLY:O	1:B:389:MET:HA	2.12	0.49
1:D:34:LYS:HB3	1:D:458:CYS:HA	1.94	0.49
1:F:240:VAL:HG11	1:F:247:LEU:CB	2.42	0.49
1:F:356:ALA:HB1	1:F:361:ASP:HB2	1.93	0.49
1:B:513:LEU:HD22	1:C:49:ILE:HD12	1.93	0.49
1:F:166:MET:O	1:F:170:GLY:HA2	2.12	0.49
1:H:475:ASN:ND2	1:H:489:ILE:CD1	2.75	0.49
1:M:103:GLY:HA3	1:M:515:ILE:CD1	2.43	0.49
1:M:320:ALA:HA	1:M:334:ASP:O	2.11	0.49
1:B:225:LYS:CB	1:B:308:GLU:HA	2.41	0.49
1:E:204:PHE:CZ	1:E:262:LEU:CD2	2.96	0.49
1:G:406:ALA:HB1	1:G:411:VAL:CG1	2.42	0.49
1:I:103:GLY:HA3	1:I:515:ILE:CD1	2.43	0.49
1:A:192:GLY:HA3	1:A:376:VAL:CG2	2.43	0.49
1:A:383:ALA:HA	1:A:389:MET:HB2	1.95	0.49
1:B:521:VAL:HG21	1:C:59:GLU:HB2	1.93	0.49
1:C:382:GLY:O	1:C:389:MET:HA	2.12	0.49
1:E:197:ARG:HG3	1:E:198:GLY:O	2.13	0.49
1:E:200:LEU:HD11	1:E:254:VAL:HG22	1.92	0.49
1:E:406:ALA:HB1	1:E:411:VAL:CG1	2.42	0.49
1:F:200:LEU:HD11	1:F:254:VAL:HA	1.94	0.49
1:F:381:VAL:HB	1:F:393:LYS:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:ALA:HB1	1:C:411:VAL:CG1	2.42	0.49
1:D:255:GLU:HB2	1:D:259:LEU:H	1.77	0.49
1:D:383:ALA:HA	1:D:389:MET:HB2	1.95	0.49
1:F:225:LYS:HB2	1:F:308:GLU:HA	1.94	0.49
1:F:382:GLY:O	1:F:389:MET:HA	2.12	0.49
1:G:196:ASP:HA	1:G:329:THR:HG22	1.95	0.49
1:B:225:LYS:HB2	1:B:308:GLU:HA	1.94	0.49
1:B:383:ALA:HA	1:B:389:MET:HB2	1.95	0.49
1:C:34:LYS:HB3	1:C:458:CYS:HA	1.95	0.49
1:C:241:ALA:CA	1:C:271:VAL:HG22	2.43	0.49
1:C:255:GLU:HB2	1:C:259:LEU:H	1.77	0.49
1:D:241:ALA:CA	1:D:271:VAL:HG22	2.43	0.49
1:E:255:GLU:HB2	1:E:259:LEU:H	1.77	0.49
1:G:383:ALA:HA	1:G:389:MET:HB2	1.95	0.49
1:N:320:ALA:HA	1:N:334:ASP:O	2.13	0.49
1:A:147:VAL:HG22	1:A:494:LEU:HB2	1.94	0.49
1:D:192:GLY:HA3	1:D:376:VAL:CG2	2.43	0.49
1:D:200:LEU:HD11	1:D:254:VAL:CG2	2.13	0.49
1:A:406:ALA:HB1	1:A:411:VAL:CG1	2.42	0.49
1:C:383:ALA:HA	1:C:389:MET:HB2	1.95	0.49
1:G:147:VAL:HG22	1:G:494:LEU:HB2	1.94	0.49
1:G:381:VAL:HB	1:G:393:LYS:HA	1.95	0.49
1:L:99:ILE:CG2	1:L:120:ILE:HD13	2.43	0.49
1:E:241:ALA:CA	1:E:271:VAL:HG22	2.43	0.48
1:E:383:ALA:HA	1:E:389:MET:HB2	1.95	0.48
1:F:200:LEU:HD11	1:F:254:VAL:HG22	1.92	0.48
1:M:475:ASN:ND2	1:M:489:ILE:CD1	2.76	0.48
1:B:406:ALA:HB1	1:B:411:VAL:CG1	2.42	0.48
1:D:147:VAL:HG22	1:D:494:LEU:HB2	1.94	0.48
1:F:192:GLY:HA3	1:F:376:VAL:CG2	2.43	0.48
1:F:195:PHE:O	1:F:329:THR:HB	2.13	0.48
1:G:221:LEU:HD13	1:G:236:VAL:HG21	1.96	0.48
1:H:103:GLY:HA3	1:H:515:ILE:CD1	2.43	0.48
1:L:320:ALA:HA	1:L:334:ASP:O	2.13	0.48
1:E:192:GLY:HA3	1:E:376:VAL:CG2	2.43	0.48
1:E:200:LEU:HD11	1:E:254:VAL:CG2	2.13	0.48
1:E:240:VAL:HG11	1:E:247:LEU:CB	2.42	0.48
1:F:207:LYS:HD3	1:F:207:LYS:H	1.78	0.48
1:F:383:ALA:HA	1:F:389:MET:HB2	1.95	0.48
1:G:137:PRO:HA	1:G:410:GLY:HA3	1.90	0.48
1:G:192:GLY:HA3	1:G:376:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:117:LYS:HZ2	1:H:121:ASP:CG	2.21	0.48
1:B:195:PHE:CE1	1:B:292:ILE:CD1	2.97	0.48
1:D:37:ASN:HD22	1:D:49:ILE:HG23	1.78	0.48
1:D:177:VAL:HG21	1:D:397:GLU:HG2	1.96	0.48
1:G:193:MET:HG2	1:G:295:LEU:HG	1.96	0.48
1:G:255:GLU:HB2	1:G:259:LEU:H	1.77	0.48
1:K:103:GLY:HA3	1:K:515:ILE:CD1	2.44	0.48
1:K:140:ASP:CG	1:K:142:LYS:HZ3	2.22	0.48
1:M:99:ILE:CG2	1:M:120:ILE:HD13	2.44	0.48
1:M:230:ILE:CD1	1:M:262:LEU:HD11	2.37	0.48
1:A:221:LEU:HD13	1:A:236:VAL:HG21	1.96	0.48
1:B:241:ALA:CA	1:B:271:VAL:HG22	2.43	0.48
1:C:162:ILE:CD1	1:C:400:LEU:N	2.77	0.48
1:C:225:LYS:HB2	1:C:308:GLU:HA	1.94	0.48
1:E:225:LYS:HB2	1:E:308:GLU:HA	1.94	0.48
1:E:381:VAL:HB	1:E:393:LYS:HA	1.95	0.48
1:F:221:LEU:HD13	1:F:236:VAL:HG21	1.96	0.48
1:H:230:ILE:HD13	1:H:262:LEU:CB	2.43	0.48
1:I:117:LYS:HZ2	1:I:121:ASP:CG	2.22	0.48
1:B:158:VAL:HG13	1:B:396:VAL:HA	1.96	0.48
1:B:177:VAL:HG21	1:B:397:GLU:HG2	1.96	0.48
1:K:23:LEU:CD1	1:K:60:ILE:HD12	2.29	0.48
1:A:158:VAL:HG13	1:A:396:VAL:HA	1.96	0.48
1:A:177:VAL:HG21	1:A:397:GLU:HG2	1.96	0.48
1:A:381:VAL:HB	1:A:393:LYS:HA	1.95	0.48
1:C:381:VAL:HB	1:C:393:LYS:HA	1.95	0.48
1:E:209:GLU:CD	1:E:209:GLU:H	2.22	0.48
1:F:241:ALA:CA	1:F:271:VAL:HG22	2.43	0.48
1:I:217:SER:HA	1:I:320:ALA:O	2.14	0.48
1:K:99:ILE:CG2	1:K:120:ILE:HD13	2.44	0.48
1:L:23:LEU:CD1	1:L:60:ILE:HD12	2.28	0.48
1:B:200:LEU:HD11	1:B:254:VAL:HG22	1.92	0.48
1:B:221:LEU:HD13	1:B:236:VAL:HG21	1.95	0.48
1:C:240:VAL:HG11	1:C:247:LEU:CB	2.42	0.48
1:D:225:LYS:HB2	1:D:308:GLU:HA	1.94	0.48
1:D:240:VAL:HG11	1:D:247:LEU:CB	2.42	0.48
1:F:162:ILE:CD1	1:F:400:LEU:N	2.77	0.48
1:G:162:ILE:CD1	1:G:400:LEU:N	2.77	0.48
1:C:158:VAL:HG13	1:C:396:VAL:HA	1.96	0.47
1:D:162:ILE:CD1	1:D:400:LEU:N	2.77	0.47
1:D:180:GLY:HA2	1:D:380:LYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:ILE:CG2	1:E:120:ILE:HD13	2.44	0.47
1:E:180:GLY:HA2	1:E:380:LYS:HB3	1.96	0.47
1:E:213:VAL:CG2	1:E:214:GLU:N	2.77	0.47
1:F:213:VAL:CG2	1:F:214:GLU:N	2.77	0.47
1:J:117:LYS:HZ2	1:J:121:ASP:CG	2.21	0.47
1:A:241:ALA:CA	1:A:271:VAL:HG22	2.43	0.47
1:D:99:ILE:CG2	1:D:120:ILE:HD13	2.45	0.47
1:I:246:PRO:HB3	1:I:272:LYS:HB2	1.97	0.47
1:C:37:ASN:HD22	1:C:49:ILE:HG23	1.79	0.47
1:F:23:LEU:HA	1:F:60:ILE:CD1	2.33	0.47
1:G:200:LEU:CD1	1:G:254:VAL:CG1	2.87	0.47
1:G:213:VAL:CG2	1:G:214:GLU:N	2.77	0.47
1:J:99:ILE:CG2	1:J:120:ILE:HD13	2.44	0.47
1:N:99:ILE:CG2	1:N:120:ILE:HD13	2.44	0.47
1:A:200:LEU:HD11	1:A:254:VAL:HA	1.94	0.47
1:B:195:PHE:O	1:B:329:THR:HB	2.15	0.47
1:B:381:VAL:HB	1:B:393:LYS:HA	1.95	0.47
1:D:158:VAL:HG13	1:D:396:VAL:HA	1.96	0.47
1:D:240:VAL:CG1	1:D:247:LEU:HB2	2.43	0.47
1:F:99:ILE:CG2	1:F:120:ILE:HD13	2.45	0.47
1:G:158:VAL:HG13	1:G:396:VAL:HA	1.96	0.47
1:G:241:ALA:CA	1:G:271:VAL:HG22	2.43	0.47
1:K:246:PRO:HB3	1:K:272:LYS:HB2	1.96	0.47
1:M:23:LEU:CD1	1:M:60:ILE:HD12	2.27	0.47
1:M:117:LYS:HZ2	1:M:121:ASP:CG	2.22	0.47
1:N:23:LEU:CD1	1:N:60:ILE:HD12	2.28	0.47
1:C:381:VAL:CG2	1:C:393:LYS:N	2.77	0.47
1:E:177:VAL:HG21	1:E:397:GLU:HG2	1.96	0.47
1:H:140:ASP:CG	1:H:142:LYS:HZ3	2.22	0.47
1:B:200:LEU:HD11	1:B:254:VAL:HA	1.94	0.47
1:B:213:VAL:O	1:B:324:VAL:HA	2.15	0.47
1:B:240:VAL:HG11	1:B:247:LEU:CB	2.42	0.47
1:C:99:ILE:CG2	1:C:120:ILE:HD13	2.45	0.47
1:C:193:MET:SD	1:C:295:LEU:HG	2.55	0.47
1:C:200:LEU:HD11	1:C:254:VAL:CA	2.12	0.47
1:E:221:LEU:HD13	1:E:236:VAL:HG21	1.95	0.47
1:F:180:GLY:HA2	1:F:380:LYS:HB3	1.96	0.47
1:F:200:LEU:HD11	1:F:254:VAL:CG2	2.14	0.47
1:M:217:SER:HA	1:M:320:ALA:O	2.14	0.47
1:N:103:GLY:HA3	1:N:515:ILE:CD1	2.44	0.47
1:A:37:ASN:HD22	1:A:49:ILE:HG23	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LEU:O	1:B:266:THR:HG23	2.15	0.47
1:C:177:VAL:HG21	1:C:397:GLU:HG2	1.96	0.47
1:C:200:LEU:HD11	1:C:254:VAL:HA	1.94	0.47
1:C:309:LEU:O	1:C:312:ALA:HB3	2.15	0.47
1:D:23:LEU:CG	1:D:60:ILE:HD12	2.20	0.47
1:D:262:LEU:O	1:D:266:THR:HG23	2.15	0.47
1:D:381:VAL:HB	1:D:393:LYS:HA	1.95	0.47
1:E:150:ILE:HG23	4:E:1527:ATP:H2'	1.97	0.47
1:E:240:VAL:HG21	1:E:247:LEU:HD13	1.97	0.47
1:G:209:GLU:H	1:G:209:GLU:CD	2.23	0.47
1:H:217:SER:HA	1:H:320:ALA:O	2.15	0.47
1:I:99:ILE:CG2	1:I:120:ILE:HD13	2.45	0.47
1:K:414:GLY:N	1:K:494:LEU:HA	2.30	0.47
1:L:217:SER:HA	1:L:320:ALA:O	2.14	0.47
1:M:246:PRO:HB3	1:M:272:LYS:HB2	1.97	0.47
1:M:479:ASN:O	1:M:483:GLU:N	2.47	0.47
1:N:117:LYS:HZ2	1:N:121:ASP:CG	2.23	0.47
1:C:213:VAL:O	1:C:324:VAL:HA	2.15	0.47
1:D:150:ILE:CD1	1:D:493:ILE:CA	2.71	0.47
1:D:240:VAL:HG21	1:D:247:LEU:HD13	1.97	0.47
1:E:200:LEU:CD1	1:E:254:VAL:CG2	2.60	0.47
1:F:272:LYS:CD	1:F:272:LYS:H	2.28	0.47
1:G:99:ILE:CG2	1:G:120:ILE:HD13	2.45	0.47
1:G:177:VAL:HG21	1:G:397:GLU:HG2	1.96	0.47
1:K:327:LYS:HZ2	1:K:328:ASP:CG	2.23	0.47
1:A:162:ILE:CD1	1:A:400:LEU:N	2.77	0.47
1:A:309:LEU:O	1:A:312:ALA:HB3	2.15	0.47
1:C:221:LEU:HD13	1:C:236:VAL:HG21	1.95	0.47
1:C:272:LYS:CD	1:C:272:LYS:H	2.28	0.47
1:E:37:ASN:HD22	1:E:49:ILE:HG23	1.79	0.47
1:E:158:VAL:HG13	1:E:396:VAL:HA	1.96	0.47
1:J:320:ALA:HA	1:J:334:ASP:O	2.15	0.47
1:K:181:THR:O	1:L:282:GLY:HA3	2.15	0.47
1:L:479:ASN:O	1:L:483:GLU:N	2.46	0.47
1:A:150:ILE:HD13	1:A:493:ILE:CG2	2.45	0.47
1:B:99:ILE:CG2	1:B:120:ILE:HD13	2.44	0.47
1:B:150:ILE:HD13	1:B:493:ILE:CG2	2.45	0.47
1:C:204:PHE:CD1	1:C:273:VAL:O	2.68	0.47
1:C:213:VAL:CG2	1:C:214:GLU:N	2.77	0.47
1:D:150:ILE:HG23	4:D:1527:ATP:H2'	1.97	0.47
1:E:272:LYS:H	1:E:272:LYS:CD	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:ASN:HD22	1:F:49:ILE:HG23	1.80	0.47
1:G:150:ILE:HG23	4:G:1527:ATP:H2'	1.97	0.47
1:G:180:GLY:HA2	1:G:380:LYS:HB3	1.96	0.47
1:G:201:SER:C	1:G:203:TYR:N	2.71	0.47
1:G:272:LYS:H	1:G:272:LYS:CD	2.28	0.47
1:A:150:ILE:HG23	4:A:1527:ATP:H2'	1.97	0.46
1:A:272:LYS:CD	1:A:272:LYS:H	2.28	0.46
1:B:37:ASN:HD22	1:B:49:ILE:HG23	1.79	0.46
1:C:150:ILE:HD13	1:C:493:ILE:CG2	2.45	0.46
1:C:180:GLY:HA2	1:C:380:LYS:HB3	1.96	0.46
1:C:240:VAL:CG1	1:C:247:LEU:HB2	2.43	0.46
1:C:240:VAL:HG21	1:C:247:LEU:HD13	1.97	0.46
1:D:213:VAL:CG2	1:D:214:GLU:N	2.77	0.46
1:F:158:VAL:HG13	1:F:396:VAL:HA	1.96	0.46
1:F:204:PHE:CD1	1:F:273:VAL:O	2.69	0.46
1:G:278:ALA:HB2	1:G:289:LEU:CD1	2.46	0.46
1:L:117:LYS:HZ2	1:L:121:ASP:CG	2.22	0.46
1:L:414:GLY:N	1:L:494:LEU:HA	2.29	0.46
1:A:99:ILE:CG2	1:A:120:ILE:HD13	2.45	0.46
1:A:278:ALA:HB2	1:A:289:LEU:CD1	2.46	0.46
1:B:150:ILE:HG23	4:B:1527:ATP:H2'	1.97	0.46
1:D:221:LEU:HD13	1:D:236:VAL:HG21	1.95	0.46
1:D:309:LEU:O	1:D:312:ALA:HB3	2.15	0.46
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.96	0.46
1:A:204:PHE:CD1	1:A:273:VAL:O	2.68	0.46
1:B:203:TYR:N	1:B:203:TYR:CD1	2.84	0.46
1:B:204:PHE:CD1	1:B:273:VAL:O	2.69	0.46
1:B:213:VAL:CG2	1:B:214:GLU:N	2.77	0.46
1:C:150:ILE:HG23	4:C:1527:ATP:H2'	1.97	0.46
1:C:308:GLU:CD	1:C:311:LYS:HZ3	2.24	0.46
1:D:272:LYS:CD	1:D:272:LYS:H	2.28	0.46
1:D:278:ALA:HB2	1:D:289:LEU:CD1	2.46	0.46
1:E:162:ILE:CD1	1:E:400:LEU:N	2.77	0.46
1:F:150:ILE:HG23	4:F:1527:ATP:H2'	1.96	0.46
1:F:240:VAL:HG21	1:F:247:LEU:HD13	1.97	0.46
1:G:201:SER:C	1:G:203:TYR:H	2.22	0.46
1:G:309:LEU:O	1:G:312:ALA:HB3	2.15	0.46
1:A:402:ALA:HB1	1:A:496:PRO:HG2	1.98	0.46
1:C:197:ARG:HG3	1:C:198:GLY:O	2.15	0.46
1:C:200:LEU:HD11	1:C:254:VAL:CG2	2.13	0.46
1:C:262:LEU:O	1:C:266:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:THR:HG21	1:D:322:ARG:HH12	1.81	0.46
1:D:206:ASN:HB2	1:D:213:VAL:HG23	1.98	0.46
1:F:195:PHE:CD1	1:F:195:PHE:C	2.93	0.46
1:G:37:ASN:HD22	1:G:49:ILE:HG23	1.79	0.46
1:G:150:ILE:HD13	1:G:493:ILE:CG2	2.45	0.46
1:A:240:VAL:HG11	1:A:247:LEU:CB	2.42	0.46
1:A:311:LYS:HD3	1:A:311:LYS:HA	1.93	0.46
1:B:180:GLY:HA2	1:B:380:LYS:HB3	1.96	0.46
1:B:194:GLN:CG	1:B:329:THR:HG21	2.44	0.46
1:B:196:ASP:HA	1:B:329:THR:HG22	1.97	0.46
1:B:272:LYS:H	1:B:272:LYS:CD	2.28	0.46
1:C:271:VAL:O	1:C:273:VAL:HG23	2.16	0.46
1:D:381:VAL:CG2	1:D:393:LYS:N	2.77	0.46
1:E:65:LYS:NZ	1:E:524:LEU:O	2.49	0.46
1:E:213:VAL:O	1:E:324:VAL:HA	2.15	0.46
1:F:177:VAL:HG21	1:F:397:GLU:HG2	1.96	0.46
1:F:271:VAL:O	1:F:273:VAL:HG23	2.16	0.46
1:F:278:ALA:HB2	1:F:289:LEU:CD1	2.46	0.46
1:G:262:LEU:O	1:G:266:THR:HG23	2.15	0.46
1:N:414:GLY:N	1:N:494:LEU:HA	2.30	0.46
1:D:200:LEU:HD11	1:D:254:VAL:CA	2.12	0.46
1:D:271:VAL:O	1:D:273:VAL:HG23	2.16	0.46
1:G:240:VAL:HG21	1:G:247:LEU:HD13	1.97	0.46
1:G:402:ALA:HB1	1:G:496:PRO:HG2	1.98	0.46
1:A:65:LYS:NZ	1:A:524:LEU:O	2.49	0.46
1:B:402:ALA:HB1	1:B:496:PRO:HG2	1.98	0.46
1:D:213:VAL:O	1:D:324:VAL:HA	2.15	0.46
1:D:311:LYS:HD3	1:D:311:LYS:HA	1.93	0.46
1:E:262:LEU:O	1:E:266:THR:HG23	2.15	0.46
1:E:271:VAL:O	1:E:273:VAL:HG23	2.16	0.46
1:G:271:VAL:O	1:G:273:VAL:HG23	2.16	0.46
1:A:200:LEU:HD11	1:A:254:VAL:HG22	1.92	0.46
1:A:209:GLU:H	1:A:209:GLU:CD	2.23	0.46
1:B:240:VAL:HG21	1:B:247:LEU:HD13	1.97	0.46
1:C:278:ALA:HB2	1:C:289:LEU:CD1	2.45	0.46
1:E:309:LEU:O	1:E:312:ALA:HB3	2.15	0.46
1:F:65:LYS:NZ	1:F:524:LEU:O	2.49	0.46
1:H:414:GLY:N	1:H:494:LEU:HA	2.31	0.46
1:B:65:LYS:NZ	1:B:524:LEU:O	2.49	0.46
1:B:271:VAL:O	1:B:273:VAL:HG23	2.16	0.46
1:E:278:ALA:HB2	1:E:289:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:309:LEU:O	1:F:312:ALA:HB3	2.15	0.46
1:F:402:ALA:HB1	1:F:496:PRO:HG2	1.98	0.46
1:G:200:LEU:CD2	1:G:254:VAL:CG1	2.89	0.46
1:G:240:VAL:CG1	1:G:247:LEU:HB2	2.43	0.46
1:K:217:SER:HA	1:K:320:ALA:O	2.15	0.46
1:K:271:VAL:HG12	1:K:272:LYS:H	1.81	0.46
1:A:240:VAL:HG21	1:A:247:LEU:HD13	1.97	0.46
1:A:262:LEU:O	1:A:266:THR:HG23	2.15	0.46
1:B:309:LEU:O	1:B:312:ALA:HB3	2.15	0.46
1:C:65:LYS:NZ	1:C:524:LEU:O	2.49	0.46
1:D:65:LYS:NZ	1:D:524:LEU:O	2.49	0.46
1:F:176:THR:HG21	1:F:322:ARG:HH12	1.81	0.46
1:F:262:LEU:O	1:F:266:THR:HG23	2.15	0.46
1:F:381:VAL:CG2	1:F:393:LYS:N	2.77	0.46
1:G:65:LYS:NZ	1:G:524:LEU:O	2.49	0.46
1:G:204:PHE:CD1	1:G:273:VAL:O	2.69	0.46
1:K:149:THR:CG2	1:K:156:GLU:HA	2.46	0.46
1:B:278:ALA:HB2	1:B:289:LEU:CD1	2.46	0.45
1:D:204:PHE:CD1	1:D:273:VAL:O	2.69	0.45
1:K:117:LYS:HZ2	1:K:121:ASP:CG	2.23	0.45
1:B:227:ILE:HG12	1:B:309:LEU:HG	1.99	0.45
1:C:23:LEU:CG	1:C:60:ILE:HD12	2.21	0.45
1:H:479:ASN:O	1:H:483:GLU:N	2.47	0.45
1:I:230:ILE:HD11	1:I:262:LEU:HD11	1.96	0.45
1:J:149:THR:CG2	1:J:156:GLU:HA	2.46	0.45
1:K:320:ALA:HA	1:K:334:ASP:O	2.17	0.45
1:B:176:THR:HG21	1:B:322:ARG:HH12	1.81	0.45
1:C:176:THR:HG21	1:C:322:ARG:HH12	1.81	0.45
1:C:349:ILE:HG23	1:C:365:LEU:HD22	1.99	0.45
1:C:402:ALA:HB1	1:C:496:PRO:HG2	1.98	0.45
1:D:200:LEU:HD11	1:D:254:VAL:HA	1.94	0.45
1:F:150:ILE:HD13	1:F:493:ILE:CG2	2.46	0.45
1:F:384:ALA:HA	1:F:385:THR:HA	1.67	0.45
1:G:201:SER:HA	1:G:202:PRO:HD3	1.52	0.45
1:J:2:ALA:O	1:J:3:ALA:C	2.59	0.45
1:K:230:ILE:HD13	1:K:262:LEU:CB	2.47	0.45
1:M:301:ILE:HD13	1:M:309:LEU:HA	1.98	0.45
1:N:479:ASN:O	1:N:483:GLU:N	2.50	0.45
1:B:349:ILE:HG23	1:B:365:LEU:HD22	1.99	0.45
1:E:227:ILE:HG12	1:E:309:LEU:HG	1.98	0.45
1:F:213:VAL:O	1:F:324:VAL:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:479:ASN:O	1:J:483:GLU:N	2.49	0.45
1:A:176:THR:HG21	1:A:322:ARG:HH12	1.81	0.45
1:A:227:ILE:HG12	1:A:309:LEU:HG	1.99	0.45
1:A:271:VAL:O	1:A:273:VAL:HG23	2.16	0.45
1:B:240:VAL:CG1	1:B:247:LEU:HB2	2.43	0.45
1:B:289:LEU:O	1:B:289:LEU:HD23	2.17	0.45
1:B:297:GLY:CA	1:B:337:GLY:CA	2.95	0.45
1:C:227:ILE:HG12	1:C:309:LEU:HG	1.99	0.45
1:C:297:GLY:CA	1:C:337:GLY:CA	2.95	0.45
1:J:301:ILE:HD13	1:J:309:LEU:HA	1.99	0.45
1:M:65:LYS:H	1:M:65:LYS:HD2	1.82	0.45
1:A:297:GLY:CA	1:A:337:GLY:CA	2.95	0.45
1:D:226:LYS:HB2	1:D:252:GLU:HG3	1.99	0.45
1:D:227:ILE:HG12	1:D:309:LEU:HG	1.99	0.45
1:E:402:ALA:HB1	1:E:496:PRO:HG2	1.98	0.45
1:G:227:ILE:HG12	1:G:309:LEU:HG	1.99	0.45
1:H:65:LYS:HD2	1:H:65:LYS:H	1.82	0.45
1:I:271:VAL:HG12	1:I:272:LYS:H	1.82	0.45
1:B:278:ALA:HA	1:B:279:PRO:HD3	1.72	0.45
1:C:226:LYS:HB2	1:C:252:GLU:HG3	1.99	0.45
1:C:289:LEU:HD23	1:C:289:LEU:O	2.17	0.45
1:F:226:LYS:HB2	1:F:252:GLU:HG3	1.99	0.45
1:F:227:ILE:HG12	1:F:309:LEU:HG	1.99	0.45
1:G:213:VAL:O	1:G:324:VAL:HA	2.15	0.45
1:I:7:LYS:O	1:I:519:CYS:HA	2.15	0.45
1:I:479:ASN:O	1:I:483:GLU:N	2.48	0.45
1:A:205:ILE:HG23	1:A:212:ALA:O	2.16	0.45
1:B:162:ILE:CD1	1:B:400:LEU:N	2.77	0.45
1:F:186:GLU:HB2	1:F:380:LYS:CB	2.37	0.45
1:G:52:ASP:HB3	1:G:55:SER:H	1.82	0.45
1:G:297:GLY:CA	1:G:337:GLY:CA	2.95	0.45
1:H:7:LYS:O	1:H:519:CYS:HA	2.16	0.45
1:L:230:ILE:HD11	1:L:262:LEU:HD11	1.96	0.45
1:A:349:ILE:HG23	1:A:365:LEU:HD22	1.99	0.45
1:D:402:ALA:HB1	1:D:496:PRO:HG2	1.98	0.45
1:E:381:VAL:CG2	1:E:393:LYS:N	2.77	0.45
1:F:150:ILE:CD1	1:F:493:ILE:CA	2.71	0.45
1:F:248:LEU:HD23	1:F:332:ILE:HD11	1.98	0.45
1:G:200:LEU:CD1	1:G:254:VAL:CG2	2.74	0.45
1:G:226:LYS:HB2	1:G:252:GLU:HG3	1.99	0.45
1:H:149:THR:CG2	1:H:156:GLU:HA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:246:PRO:HB3	1:H:272:LYS:HB2	1.99	0.45
1:J:217:SER:HA	1:J:320:ALA:O	2.17	0.45
1:K:183:LEU:HA	1:K:383:ALA:O	2.17	0.45
1:K:191:GLU:O	1:K:334:ASP:HA	2.17	0.45
1:L:271:VAL:HG12	1:L:272:LYS:H	1.82	0.45
1:L:301:ILE:HD13	1:L:309:LEU:HA	1.99	0.45
1:N:65:LYS:H	1:N:65:LYS:HD2	1.82	0.45
1:A:196:ASP:HA	1:A:329:THR:HG22	1.98	0.45
1:A:200:LEU:HD11	1:A:254:VAL:CA	2.12	0.45
1:D:349:ILE:HG23	1:D:365:LEU:HD22	1.99	0.45
1:E:226:LYS:HB2	1:E:252:GLU:HG3	1.99	0.45
1:E:248:LEU:HD23	1:E:332:ILE:HD11	1.98	0.45
1:F:52:ASP:HB3	1:F:55:SER:H	1.82	0.45
1:F:207:LYS:HB2	1:F:208:PRO:CD	2.46	0.45
1:H:271:VAL:HG12	1:H:272:LYS:H	1.82	0.45
1:L:149:THR:CG2	1:L:156:GLU:HA	2.47	0.45
1:M:271:VAL:HG12	1:M:272:LYS:H	1.82	0.45
1:N:301:ILE:HD13	1:N:309:LEU:HA	1.99	0.45
1:A:278:ALA:HA	1:A:279:PRO:HD3	1.72	0.44
1:D:248:LEU:HD23	1:D:332:ILE:HD11	1.98	0.44
1:D:308:GLU:CD	1:D:311:LYS:HZ3	2.25	0.44
1:G:176:THR:HG21	1:G:322:ARG:HH12	1.81	0.44
1:J:191:GLU:O	1:J:334:ASP:HA	2.17	0.44
1:M:149:THR:CG2	1:M:156:GLU:HA	2.46	0.44
1:N:217:SER:HA	1:N:320:ALA:O	2.17	0.44
1:A:289:LEU:HD23	1:A:289:LEU:O	2.17	0.44
1:C:278:ALA:HB2	1:C:289:LEU:HD12	1.99	0.44
1:E:176:THR:HG21	1:E:322:ARG:HH12	1.81	0.44
1:E:308:GLU:CD	1:E:311:LYS:HZ3	2.25	0.44
1:G:240:VAL:HG11	1:G:247:LEU:CB	2.42	0.44
1:I:301:ILE:HD13	1:I:309:LEU:HA	2.00	0.44
1:J:230:ILE:HD11	1:J:262:LEU:CD2	2.46	0.44
1:J:414:GLY:N	1:J:494:LEU:HA	2.31	0.44
1:K:230:ILE:HD11	1:K:262:LEU:HD11	1.94	0.44
1:M:414:GLY:N	1:M:494:LEU:HA	2.32	0.44
1:N:230:ILE:HD11	1:N:262:LEU:CD2	2.47	0.44
1:B:226:LYS:HB2	1:B:252:GLU:HG3	1.99	0.44
1:C:278:ALA:CB	1:C:289:LEU:HD12	2.47	0.44
1:D:240:VAL:HG13	1:D:245:LYS:O	2.18	0.44
1:F:278:ALA:CB	1:F:289:LEU:HD12	2.48	0.44
1:G:240:VAL:HG13	1:G:245:LYS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:65:LYS:H	1:I:65:LYS:HD2	1.82	0.44
1:I:414:GLY:N	1:I:494:LEU:HA	2.32	0.44
1:K:165:ALA:HA	1:K:187:LEU:HD21	1.99	0.44
1:L:215:LEU:O	1:L:218:PRO:HD3	2.18	0.44
1:A:240:VAL:HG13	1:A:245:LYS:O	2.18	0.44
1:B:177:VAL:HA	1:B:379:ILE:O	2.18	0.44
1:C:384:ALA:HA	1:C:385:THR:HA	1.67	0.44
1:D:297:GLY:CA	1:D:337:GLY:CA	2.95	0.44
1:E:205:ILE:O	1:E:205:ILE:HG22	2.17	0.44
1:E:278:ALA:CB	1:E:289:LEU:HD12	2.48	0.44
1:E:297:GLY:CA	1:E:337:GLY:CA	2.95	0.44
1:E:349:ILE:HG23	1:E:365:LEU:HD22	1.99	0.44
1:F:240:VAL:HG13	1:F:245:LYS:O	2.18	0.44
1:F:297:GLY:CA	1:F:337:GLY:CA	2.95	0.44
1:G:152:ALA:HB2	1:G:399:ALA:HB2	2.00	0.44
1:G:381:VAL:HG11	1:G:393:LYS:HB2	2.00	0.44
1:J:8:PHE:HA	1:J:518:GLU:O	2.18	0.44
1:M:215:LEU:O	1:M:218:PRO:HD3	2.18	0.44
1:N:271:VAL:HG12	1:N:272:LYS:H	1.82	0.44
1:A:381:VAL:HG11	1:A:393:LYS:HB2	2.00	0.44
1:B:117:LYS:HZ2	1:B:121:ASP:CG	2.26	0.44
1:B:308:GLU:CD	1:B:311:LYS:HZ3	2.25	0.44
1:B:384:ALA:HA	1:B:385:THR:HA	1.68	0.44
1:E:289:LEU:O	1:E:289:LEU:HD23	2.17	0.44
1:E:524:LEU:HG	1:E:525:PRO:N	2.33	0.44
1:F:152:ALA:HB2	1:F:399:ALA:HB2	2.00	0.44
1:F:289:LEU:HD23	1:F:289:LEU:O	2.17	0.44
1:F:349:ILE:HG23	1:F:365:LEU:HD22	1.99	0.44
1:G:227:ILE:HD12	1:G:258:ALA:HB1	2.00	0.44
1:G:278:ALA:CB	1:G:289:LEU:HD12	2.48	0.44
1:G:311:LYS:HD3	1:G:311:LYS:HA	1.93	0.44
1:G:349:ILE:HG23	1:G:365:LEU:HD22	1.99	0.44
1:I:149:THR:CG2	1:I:156:GLU:HA	2.47	0.44
1:J:183:LEU:HA	1:J:383:ALA:O	2.18	0.44
1:A:226:LYS:HB2	1:A:252:GLU:HG3	1.99	0.44
1:A:227:ILE:HD12	1:A:258:ALA:HB1	2.00	0.44
1:A:278:ALA:HB2	1:A:289:LEU:HD12	2.00	0.44
1:A:524:LEU:HG	1:A:525:PRO:N	2.33	0.44
1:B:248:LEU:HD23	1:B:332:ILE:HD11	1.98	0.44
1:D:100:ILE:CD1	1:D:514:MET:SD	3.06	0.44
1:D:150:ILE:HD13	1:D:493:ILE:CG2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:MET:CB	1:F:36:ARG:HD2	2.48	0.44
1:E:222:LEU:CD2	1:E:292:ILE:HG22	2.45	0.44
1:E:240:VAL:HG13	1:E:245:LYS:O	2.18	0.44
1:F:117:LYS:HZ2	1:F:121:ASP:CG	2.26	0.44
1:F:381:VAL:HG11	1:F:393:LYS:HB2	2.00	0.44
1:I:216:GLU:H	1:I:216:GLU:CD	2.24	0.44
1:K:216:GLU:H	1:K:216:GLU:CD	2.25	0.44
1:K:301:ILE:HD13	1:K:309:LEU:HA	2.00	0.44
1:K:479:ASN:O	1:K:483:GLU:N	2.50	0.44
1:N:2:ALA:O	1:N:3:ALA:C	2.61	0.44
1:N:149:THR:CG2	1:N:156:GLU:HA	2.46	0.44
1:A:381:VAL:CG2	1:A:393:LYS:N	2.77	0.44
1:B:278:ALA:HB2	1:B:289:LEU:HD12	2.00	0.44
1:B:278:ALA:CB	1:B:289:LEU:HD12	2.47	0.44
1:C:150:ILE:HD11	1:C:493:ILE:HG23	1.99	0.44
1:D:289:LEU:HD23	1:D:289:LEU:O	2.17	0.44
1:E:152:ALA:HB2	1:E:399:ALA:HB2	2.00	0.44
1:E:381:VAL:HG11	1:E:393:LYS:HB2	2.00	0.44
1:F:100:ILE:CD1	1:F:514:MET:SD	3.06	0.44
1:F:207:LYS:CB	1:F:208:PRO:HD3	2.47	0.44
1:F:240:VAL:CG1	1:F:247:LEU:HB2	2.43	0.44
1:F:524:LEU:HG	1:F:525:PRO:N	2.33	0.44
1:G:524:LEU:HG	1:G:525:PRO:N	2.33	0.44
1:A:152:ALA:HB2	1:A:399:ALA:HB2	2.00	0.44
1:A:248:LEU:HD23	1:A:332:ILE:HD11	1.98	0.44
1:B:150:ILE:CD1	1:B:493:ILE:CA	2.71	0.44
1:C:248:LEU:HD23	1:C:332:ILE:HD11	1.98	0.44
1:D:381:VAL:HG11	1:D:393:LYS:HB2	2.00	0.44
1:D:524:LEU:HG	1:D:525:PRO:N	2.33	0.44
1:F:195:PHE:C	1:F:329:THR:HG22	2.43	0.44
1:F:227:ILE:HD12	1:F:258:ALA:HB1	2.00	0.44
1:G:100:ILE:CD1	1:G:514:MET:SD	3.06	0.44
1:A:36:ARG:HD2	1:G:114:MET:CB	2.48	0.44
1:A:100:ILE:CD1	1:A:514:MET:SD	3.06	0.44
1:B:227:ILE:HD12	1:B:258:ALA:HB1	2.00	0.44
1:B:240:VAL:HG13	1:B:245:LYS:O	2.18	0.44
1:B:524:LEU:HG	1:B:525:PRO:N	2.33	0.44
1:D:209:GLU:H	1:D:209:GLU:CD	2.26	0.44
1:D:278:ALA:CB	1:D:289:LEU:HD12	2.48	0.44
1:E:177:VAL:HA	1:E:379:ILE:O	2.18	0.44
1:G:117:LYS:HZ2	1:G:121:ASP:CG	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:MET:H	1:G:193:MET:HG3	1.58	0.44
1:G:278:ALA:HB2	1:G:289:LEU:HD12	2.00	0.44
1:K:230:ILE:HG23	1:K:259:LEU:HD12	2.00	0.44
1:L:2:ALA:O	1:L:3:ALA:C	2.61	0.44
1:N:7:LYS:O	1:N:519:CYS:HA	2.17	0.44
1:A:240:VAL:CG1	1:A:247:LEU:HB2	2.43	0.43
1:B:381:VAL:HG11	1:B:393:LYS:HB2	2.00	0.43
1:C:227:ILE:HD12	1:C:258:ALA:HB1	2.00	0.43
1:C:524:LEU:HG	1:C:525:PRO:N	2.33	0.43
1:D:152:ALA:HB2	1:D:399:ALA:HB2	2.00	0.43
1:D:227:ILE:HD12	1:D:258:ALA:HB1	2.00	0.43
1:E:52:ASP:HB3	1:E:55:SER:H	1.83	0.43
1:H:215:LEU:O	1:H:218:PRO:HD3	2.18	0.43
1:A:177:VAL:HA	1:A:379:ILE:O	2.18	0.43
1:C:52:ASP:HB3	1:C:55:SER:H	1.82	0.43
1:C:177:VAL:HA	1:C:379:ILE:O	2.18	0.43
1:C:240:VAL:HG13	1:C:245:LYS:O	2.18	0.43
1:D:117:LYS:HZ2	1:D:121:ASP:CG	2.26	0.43
1:G:289:LEU:O	1:G:289:LEU:HD23	2.17	0.43
1:J:271:VAL:HG12	1:J:272:LYS:H	1.83	0.43
1:A:213:VAL:HG22	1:A:214:GLU:N	2.32	0.43
1:A:278:ALA:CB	1:A:289:LEU:HD12	2.48	0.43
1:B:100:ILE:CD1	1:B:514:MET:SD	3.06	0.43
1:B:150:ILE:HD11	1:B:493:ILE:HG23	1.99	0.43
1:B:152:ALA:HB2	1:B:399:ALA:HB2	2.00	0.43
1:E:150:ILE:HD13	1:E:493:ILE:CG2	2.45	0.43
1:G:248:LEU:HD23	1:G:332:ILE:HD11	1.98	0.43
1:G:381:VAL:CG2	1:G:393:LYS:N	2.77	0.43
1:G:460:GLU:CD	1:G:461:GLU:H	2.26	0.43
1:K:62:LEU:H	1:K:68:ASN:HD22	1.65	0.43
1:M:7:LYS:O	1:M:519:CYS:HA	2.18	0.43
1:A:117:LYS:HZ2	1:A:121:ASP:CG	2.26	0.43
1:A:278:ALA:HB2	1:A:289:LEU:CG	2.49	0.43
1:B:114:MET:CB	1:C:36:ARG:HD2	2.49	0.43
1:C:262:LEU:CD1	1:C:275:ALA:HB2	2.48	0.43
1:C:381:VAL:HG11	1:C:393:LYS:HB2	2.00	0.43
1:D:150:ILE:HD11	1:D:493:ILE:HG23	2.00	0.43
1:E:278:ALA:HB2	1:E:289:LEU:CG	2.49	0.43
1:I:2:ALA:O	1:I:3:ALA:C	2.60	0.43
1:I:8:PHE:HA	1:I:518:GLU:O	2.19	0.43
1:J:7:LYS:O	1:J:519:CYS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:65:LYS:H	1:J:65:LYS:HD2	1.82	0.43
1:A:114:MET:CB	1:B:36:ARG:HD2	2.49	0.43
1:C:100:ILE:CD1	1:C:514:MET:SD	3.06	0.43
1:D:262:LEU:CD1	1:D:275:ALA:HB2	2.48	0.43
1:E:200:LEU:HD13	1:E:259:LEU:HB2	2.00	0.43
1:F:262:LEU:CD1	1:F:275:ALA:HB2	2.48	0.43
1:G:177:VAL:HA	1:G:379:ILE:O	2.18	0.43
1:G:262:LEU:CD1	1:G:275:ALA:HB2	2.48	0.43
1:G:278:ALA:HB2	1:G:289:LEU:CG	2.49	0.43
1:H:301:ILE:HD13	1:H:309:LEU:HA	2.00	0.43
1:L:183:LEU:HA	1:L:383:ALA:O	2.18	0.43
1:A:460:GLU:CD	1:A:461:GLU:H	2.26	0.43
1:E:100:ILE:CD1	1:E:514:MET:SD	3.06	0.43
1:E:262:LEU:CD1	1:E:275:ALA:HB2	2.48	0.43
1:E:278:ALA:HA	1:E:279:PRO:HD3	1.72	0.43
1:F:195:PHE:CE2	1:F:292:ILE:HD13	2.54	0.43
1:I:49:ILE:HD11	1:J:73:MET:HE3	2.00	0.43
1:C:152:ALA:HB2	1:C:399:ALA:HB2	2.00	0.43
1:D:73:MET:CG	1:E:47:PRO:HD2	2.49	0.43
1:D:177:VAL:HA	1:D:379:ILE:O	2.18	0.43
1:D:200:LEU:HD13	1:D:259:LEU:HB2	2.00	0.43
1:F:460:GLU:CD	1:F:461:GLU:H	2.27	0.43
1:H:183:LEU:HA	1:H:383:ALA:O	2.19	0.43
1:K:254:VAL:CG1	1:K:259:LEU:HD23	2.49	0.43
1:M:49:ILE:HD11	1:N:73:MET:HE3	1.99	0.43
1:M:183:LEU:HA	1:M:383:ALA:O	2.19	0.43
1:A:73:MET:CG	1:B:47:PRO:HD2	2.49	0.43
1:B:52:ASP:HB3	1:B:55:SER:H	1.82	0.43
1:B:311:LYS:HD3	1:B:311:LYS:HA	1.93	0.43
1:F:177:VAL:HA	1:F:379:ILE:O	2.18	0.43
1:H:8:PHE:HA	1:H:518:GLU:O	2.19	0.43
1:I:191:GLU:O	1:I:334:ASP:HA	2.19	0.43
1:K:230:ILE:HD13	1:K:262:LEU:HG	1.86	0.43
1:A:262:LEU:CD1	1:A:275:ALA:HB2	2.48	0.43
1:B:262:LEU:CD1	1:B:275:ALA:HB2	2.48	0.43
1:D:200:LEU:CD1	1:D:254:VAL:HG22	2.47	0.43
1:D:278:ALA:HB2	1:D:289:LEU:HG	2.01	0.43
1:E:144:ILE:CG2	1:E:163:ALA:HA	2.49	0.43
1:F:144:ILE:CG2	1:F:163:ALA:HA	2.49	0.43
1:F:193:MET:HE3	1:F:332:ILE:HD12	2.01	0.43
1:F:200:LEU:HD13	1:F:259:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:GLU:CD	1:F:311:LYS:HZ3	2.26	0.43
1:G:144:ILE:CG2	1:G:163:ALA:HA	2.49	0.43
1:K:34:LYS:HZ3	1:K:483:GLU:CD	2.26	0.43
1:A:34:LYS:NZ	1:A:483:GLU:OE2	2.52	0.43
1:A:384:ALA:HA	1:A:385:THR:HA	1.67	0.43
1:D:52:ASP:HB3	1:D:55:SER:H	1.83	0.43
1:D:223:ALA:HB3	1:D:251:ALA:HA	2.01	0.43
1:E:460:GLU:CD	1:E:461:GLU:H	2.26	0.43
1:F:114:MET:CB	1:G:36:ARG:HD2	2.49	0.43
1:L:353:ILE:HG12	1:L:365:LEU:HB3	2.00	0.43
1:N:162:ILE:HD11	1:N:399:ALA:CB	2.49	0.43
1:A:308:GLU:CD	1:A:311:LYS:HZ3	2.27	0.42
1:B:278:ALA:HB2	1:B:289:LEU:CG	2.49	0.42
1:C:166:MET:HE3	1:C:175:ILE:HD12	2.02	0.42
1:C:278:ALA:HB2	1:C:289:LEU:CG	2.49	0.42
1:C:278:ALA:HB2	1:C:289:LEU:HG	2.01	0.42
1:D:196:ASP:HA	1:D:329:THR:HG22	2.00	0.42
1:D:278:ALA:HB2	1:D:289:LEU:HD12	2.00	0.42
1:E:200:LEU:HD11	1:E:254:VAL:HA	1.94	0.42
1:E:223:ALA:HB3	1:E:251:ALA:HA	2.01	0.42
1:E:227:ILE:HD12	1:E:258:ALA:HB1	2.00	0.42
1:F:513:LEU:HB3	1:G:49:ILE:HD11	1.98	0.42
1:I:183:LEU:HA	1:I:383:ALA:O	2.18	0.42
1:M:353:ILE:HG12	1:M:365:LEU:HB3	2.00	0.42
1:A:207:LYS:N	1:A:208:PRO:HD2	2.34	0.42
1:B:193:MET:HE3	1:B:332:ILE:HD12	2.01	0.42
1:C:114:MET:CB	1:D:36:ARG:HD2	2.49	0.42
1:C:117:LYS:HZ2	1:C:121:ASP:CG	2.27	0.42
1:C:200:LEU:HD13	1:C:259:LEU:HB2	2.00	0.42
1:C:311:LYS:HD3	1:C:311:LYS:HA	1.93	0.42
1:D:278:ALA:HB2	1:D:289:LEU:CG	2.49	0.42
1:E:193:MET:HE3	1:E:332:ILE:HD12	2.01	0.42
1:F:200:LEU:CD1	1:F:254:VAL:HG22	2.47	0.42
1:K:215:LEU:O	1:K:218:PRO:HD3	2.19	0.42
1:K:219:PHE:O	1:K:247:LEU:HD12	2.19	0.42
1:L:8:PHE:HA	1:L:518:GLU:O	2.20	0.42
1:A:47:PRO:HD2	1:G:73:MET:CG	2.49	0.42
1:B:144:ILE:CG2	1:B:163:ALA:HA	2.49	0.42
1:C:220:ILE:CD1	1:C:296:THR:HG21	2.47	0.42
1:D:166:MET:HE3	1:D:175:ILE:HD12	2.02	0.42
1:E:278:ALA:HB2	1:E:289:LEU:HD12	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:ALA:HB2	1:F:289:LEU:HD12	2.00	0.42
1:H:301:ILE:HD13	1:H:309:LEU:HD23	2.00	0.42
1:A:144:ILE:CG2	1:A:163:ALA:HA	2.49	0.42
1:A:223:ALA:HB3	1:A:251:ALA:HA	2.01	0.42
1:B:209:GLU:H	1:B:209:GLU:CD	2.26	0.42
1:D:384:ALA:HA	1:D:385:THR:HA	1.68	0.42
1:E:117:LYS:HZ2	1:E:121:ASP:CG	2.26	0.42
1:F:73:MET:CG	1:G:47:PRO:HD2	2.49	0.42
1:I:219:PHE:O	1:I:247:LEU:HD12	2.19	0.42
1:I:353:ILE:HG12	1:I:365:LEU:HB3	2.01	0.42
1:J:215:LEU:O	1:J:218:PRO:HD3	2.18	0.42
1:L:13:ARG:HH21	1:L:518:GLU:CD	2.26	0.42
1:M:230:ILE:HD11	1:M:262:LEU:HD11	1.95	0.42
1:B:73:MET:CG	1:C:47:PRO:HD2	2.49	0.42
1:B:200:LEU:HD13	1:B:259:LEU:HB2	2.00	0.42
1:C:144:ILE:CG2	1:C:163:ALA:HA	2.49	0.42
1:D:144:ILE:CG2	1:D:163:ALA:HA	2.49	0.42
1:E:166:MET:HE3	1:E:175:ILE:HD12	2.02	0.42
1:F:150:ILE:HD11	1:F:493:ILE:HG23	1.99	0.42
1:G:461:GLU:HA	1:G:462:PRO:HD3	1.93	0.42
1:K:62:LEU:H	1:K:68:ASN:ND2	2.17	0.42
1:K:166:MET:O	1:K:170:GLY:N	2.51	0.42
1:M:301:ILE:HD13	1:M:309:LEU:HD23	1.93	0.42
1:N:215:LEU:O	1:N:218:PRO:HD3	2.19	0.42
1:N:353:ILE:HG12	1:N:365:LEU:HB3	2.01	0.42
1:B:166:MET:HE3	1:B:175:ILE:HD12	2.02	0.42
1:B:278:ALA:HB2	1:B:289:LEU:HG	2.01	0.42
1:C:223:ALA:HB3	1:C:251:ALA:HA	2.01	0.42
1:E:278:ALA:HB2	1:E:289:LEU:HG	2.01	0.42
1:F:209:GLU:H	1:F:209:GLU:CD	2.27	0.42
1:F:311:LYS:HD3	1:F:311:LYS:HA	1.93	0.42
1:G:193:MET:HE3	1:G:332:ILE:HG21	2.01	0.42
1:K:488:MET:HE2	1:K:488:MET:HA	2.02	0.42
1:A:222:LEU:CD2	1:A:292:ILE:HG22	2.45	0.42
1:C:165:ALA:HB2	1:C:187:LEU:HD13	2.02	0.42
1:D:222:LEU:CD2	1:D:292:ILE:HG22	2.45	0.42
1:E:73:MET:CG	1:F:47:PRO:HD2	2.49	0.42
1:G:223:ALA:HB3	1:G:251:ALA:HA	2.01	0.42
1:I:166:MET:O	1:I:170:GLY:N	2.53	0.42
1:L:219:PHE:O	1:L:247:LEU:HD12	2.20	0.42
1:A:200:LEU:HD13	1:A:259:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:CD2	1:B:292:ILE:HG22	2.45	0.42
1:C:73:MET:CG	1:D:47:PRO:HD2	2.49	0.42
1:D:165:ALA:HB2	1:D:187:LEU:HD13	2.02	0.42
1:E:204:PHE:CD1	1:E:204:PHE:N	2.85	0.42
1:F:164:GLU:CB	1:F:187:LEU:HD21	2.50	0.42
1:F:278:ALA:HB2	1:F:289:LEU:CG	2.49	0.42
1:F:409:GLU:CD	1:F:501:ARG:HH22	2.28	0.42
1:G:34:LYS:NZ	1:G:483:GLU:OE2	2.52	0.42
1:G:384:ALA:HA	1:G:385:THR:HA	1.67	0.42
1:L:136:VAL:HG21	1:L:489:ILE:HD13	2.02	0.42
1:L:162:ILE:HD11	1:L:399:ALA:CB	2.50	0.42
1:L:209:GLU:CD	1:L:209:GLU:H	2.28	0.42
1:C:52:ASP:HB2	1:C:55:SER:HB2	2.02	0.42
1:D:52:ASP:HB2	1:D:55:SER:HB2	2.01	0.42
1:D:223:ALA:HB3	1:D:251:ALA:CA	2.50	0.42
1:D:513:LEU:HA	1:E:49:ILE:HD13	2.02	0.42
1:F:223:ALA:HB3	1:F:251:ALA:HA	2.01	0.42
1:H:253:ASP:CG	1:H:277:LYS:HZ3	2.27	0.42
1:I:335:GLY:C	1:I:337:GLY:H	2.28	0.42
1:J:219:PHE:O	1:J:247:LEU:HD12	2.20	0.42
1:J:488:MET:HE2	1:J:488:MET:HA	2.02	0.42
1:K:162:ILE:HD11	1:K:399:ALA:CB	2.50	0.42
1:L:166:MET:O	1:L:170:GLY:N	2.51	0.42
1:A:513:LEU:HA	1:B:49:ILE:HD13	2.02	0.42
1:B:409:GLU:CD	1:B:501:ARG:HH22	2.28	0.42
1:C:223:ALA:HB3	1:C:251:ALA:CA	2.50	0.42
1:D:409:GLU:CD	1:D:501:ARG:HH22	2.28	0.42
1:E:165:ALA:HB2	1:E:187:LEU:HD13	2.02	0.42
1:E:223:ALA:HB3	1:E:251:ALA:CA	2.50	0.42
1:E:240:VAL:CG1	1:E:247:LEU:HB2	2.43	0.42
1:E:262:LEU:HD13	1:E:275:ALA:HB2	2.02	0.42
1:F:215:LEU:HB3	1:F:246:PRO:HG2	2.02	0.42
1:G:215:LEU:HB3	1:G:246:PRO:HG2	2.02	0.42
1:J:353:ILE:HG12	1:J:365:LEU:HB3	2.01	0.42
1:A:52:ASP:HB3	1:A:55:SER:H	1.83	0.41
1:A:193:MET:HE3	1:A:332:ILE:HD12	2.01	0.41
1:A:215:LEU:HB3	1:A:246:PRO:HG2	2.02	0.41
1:A:278:ALA:HB2	1:A:289:LEU:HG	2.01	0.41
1:A:409:GLU:CD	1:A:501:ARG:HH22	2.28	0.41
1:B:513:LEU:HA	1:C:49:ILE:HD13	2.02	0.41
1:C:513:LEU:HA	1:D:49:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:MET:HE3	1:F:175:ILE:HD12	2.02	0.41
1:F:201:SER:C	1:F:203:TYR:H	2.26	0.41
1:F:262:LEU:HD13	1:F:275:ALA:HB2	2.02	0.41
1:G:278:ALA:HB2	1:G:289:LEU:HG	2.01	0.41
1:G:409:GLU:CD	1:G:501:ARG:HH22	2.28	0.41
1:H:2:ALA:O	1:H:3:ALA:C	2.61	0.41
1:H:219:PHE:O	1:H:247:LEU:HD12	2.19	0.41
1:N:183:LEU:HA	1:N:383:ALA:O	2.20	0.41
1:A:326:ASN:HB2	1:A:327:LYS:H	1.78	0.41
1:D:513:LEU:HB3	1:E:49:ILE:HD11	1.96	0.41
2:D:1525:PO4:P	4:D:1527:ATP:PG	3.19	0.41
1:E:150:ILE:HD11	1:E:493:ILE:HG23	2.01	0.41
1:F:278:ALA:HB2	1:F:289:LEU:HG	2.01	0.41
1:K:8:PHE:HA	1:K:518:GLU:O	2.21	0.41
1:K:65:LYS:NZ	1:K:524:LEU:O	2.49	0.41
1:L:65:LYS:NZ	1:L:524:LEU:O	2.49	0.41
1:M:219:PHE:O	1:M:247:LEU:HD12	2.21	0.41
1:M:230:ILE:HG23	1:M:259:LEU:HD12	2.02	0.41
1:A:223:ALA:HB3	1:A:251:ALA:CA	2.50	0.41
1:B:52:ASP:HB2	1:B:55:SER:HB2	2.01	0.41
1:B:215:LEU:HB3	1:B:246:PRO:HG2	2.02	0.41
1:B:223:ALA:HB3	1:B:251:ALA:CA	2.50	0.41
1:C:248:LEU:HD22	1:C:323:VAL:HG21	2.03	0.41
1:D:193:MET:HE3	1:D:332:ILE:HD12	2.01	0.41
1:E:311:LYS:HD3	1:E:311:LYS:HA	1.93	0.41
1:E:513:LEU:HB3	1:F:49:ILE:HD11	1.98	0.41
1:G:161:LEU:CD1	1:G:185:ASP:HB3	2.30	0.41
1:G:166:MET:HE3	1:G:175:ILE:HD12	2.02	0.41
1:G:308:GLU:CD	1:G:311:LYS:HZ3	2.28	0.41
2:G:1525:PO4:P	4:G:1527:ATP:PG	3.18	0.41
1:H:488:MET:HE2	1:H:488:MET:HA	2.01	0.41
1:L:206:ASN:HB2	1:L:213:VAL:HG23	2.02	0.41
1:L:488:MET:HA	1:L:488:MET:HE2	2.03	0.41
1:N:219:PHE:O	1:N:247:LEU:HD12	2.20	0.41
1:D:248:LEU:HD22	1:D:323:VAL:HG21	2.03	0.41
1:D:262:LEU:HD13	1:D:275:ALA:HB2	2.02	0.41
1:F:52:ASP:HB2	1:F:55:SER:HB2	2.01	0.41
1:G:165:ALA:HB2	1:G:187:LEU:HD13	2.02	0.41
1:H:19:GLY:HA3	1:H:67:GLU:O	2.21	0.41
1:H:162:ILE:HD11	1:H:399:ALA:CB	2.51	0.41
1:H:191:GLU:O	1:H:334:ASP:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:417:VAL:HA	1:H:420:ILE:HG22	2.01	0.41
1:M:335:GLY:C	1:M:337:GLY:H	2.28	0.41
1:A:49:ILE:HD13	1:G:513:LEU:O	2.18	0.41
1:A:166:MET:HE3	1:A:175:ILE:HD12	2.02	0.41
1:B:223:ALA:HB3	1:B:251:ALA:HA	2.01	0.41
2:C:1525:PO4:P	4:C:1527:ATP:PG	3.18	0.41
1:E:52:ASP:HB2	1:E:55:SER:HB2	2.02	0.41
1:F:223:ALA:HB3	1:F:251:ALA:CA	2.50	0.41
1:G:250:ILE:HD13	1:G:292:ILE:HG21	2.02	0.41
1:I:19:GLY:HA3	1:I:67:GLU:O	2.21	0.41
1:J:13:ARG:HH21	1:J:518:GLU:CD	2.28	0.41
1:K:182:GLY:HA2	1:L:284:ARG:NH2	2.35	0.41
1:M:254:VAL:CG1	1:M:259:LEU:HD23	2.50	0.41
1:A:219:PHE:HB3	1:A:317:LEU:HD11	2.03	0.41
1:A:521:VAL:O	1:B:41:ASP:HB3	2.21	0.41
1:B:195:PHE:N	1:B:195:PHE:CD1	2.88	0.41
1:C:409:GLU:CD	1:C:501:ARG:HH22	2.28	0.41
1:F:195:PHE:O	1:F:329:THR:HG22	2.19	0.41
1:F:271:VAL:HG12	1:F:273:VAL:HG23	2.03	0.41
1:G:150:ILE:HD11	1:G:493:ILE:HG23	2.00	0.41
1:H:230:ILE:HG23	1:H:259:LEU:HD12	2.01	0.41
1:K:301:ILE:CD1	1:K:312:ALA:CB	2.89	0.41
1:N:191:GLU:O	1:N:334:ASP:HA	2.19	0.41
1:A:150:ILE:HD11	1:A:493:ILE:HG23	2.01	0.41
1:A:250:ILE:HD13	1:A:292:ILE:HG21	2.02	0.41
1:B:381:VAL:CG2	1:B:393:LYS:N	2.77	0.41
1:D:220:ILE:CD1	1:D:296:THR:HG21	2.47	0.41
1:E:52:ASP:O	1:E:53:GLY:C	2.59	0.41
1:E:196:ASP:HA	1:E:329:THR:HG22	2.02	0.41
1:E:219:PHE:HB3	1:E:317:LEU:HD11	2.03	0.41
1:E:409:GLU:CD	1:E:501:ARG:HH22	2.28	0.41
1:E:521:VAL:O	1:F:41:ASP:HB3	2.21	0.41
1:H:353:ILE:HG12	1:H:365:LEU:HB3	2.03	0.41
1:J:49:ILE:HD11	1:K:73:MET:HE3	2.02	0.41
1:N:19:GLY:HA3	1:N:67:GLU:O	2.21	0.41
1:N:488:MET:HE2	1:N:488:MET:HA	2.03	0.41
1:A:52:ASP:O	1:A:53:GLY:C	2.59	0.41
1:B:262:LEU:HD13	1:B:275:ALA:HB2	2.02	0.41
1:C:222:LEU:CD2	1:C:292:ILE:HG22	2.45	0.41
1:E:215:LEU:HB3	1:E:246:PRO:HG2	2.02	0.41
1:F:513:LEU:O	1:G:49:ILE:HD13	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:ASP:HB2	1:G:55:SER:HB2	2.02	0.41
1:G:219:PHE:HB3	1:G:317:LEU:HD11	2.03	0.41
1:G:278:ALA:HA	1:G:279:PRO:HD3	1.72	0.41
1:H:206:ASN:HB2	1:H:213:VAL:HG23	2.03	0.41
1:I:263:VAL:O	1:I:267:MET:HB3	2.21	0.41
1:K:2:ALA:O	1:K:3:ALA:C	2.63	0.41
1:M:488:MET:HE2	1:M:488:MET:HA	2.02	0.41
1:A:52:ASP:HB2	1:A:55:SER:HB2	2.02	0.41
1:A:165:ALA:HB2	1:A:187:LEU:HD13	2.02	0.41
1:A:311:LYS:O	1:A:313:THR:HG23	2.21	0.41
1:B:248:LEU:HD22	1:B:323:VAL:HG21	2.03	0.41
1:B:250:ILE:HD13	1:B:292:ILE:HG21	2.02	0.41
1:C:215:LEU:HB3	1:C:246:PRO:HG2	2.02	0.41
1:C:219:PHE:HB3	1:C:317:LEU:HD11	2.03	0.41
1:C:250:ILE:HD13	1:C:292:ILE:HG21	2.02	0.41
1:C:262:LEU:HD13	1:C:275:ALA:HB2	2.02	0.41
1:D:219:PHE:HB3	1:D:317:LEU:HD11	2.03	0.41
1:D:250:ILE:HD13	1:D:292:ILE:HG21	2.02	0.41
1:E:262:LEU:HD23	1:E:262:LEU:C	2.46	0.41
1:F:219:PHE:HB3	1:F:317:LEU:HD11	2.03	0.41
1:F:250:ILE:HD13	1:F:292:ILE:HG21	2.02	0.41
1:F:262:LEU:HD23	1:F:262:LEU:C	2.46	0.41
1:F:521:VAL:O	1:G:41:ASP:HB3	2.21	0.41
2:F:1525:PO4:P	4:F:1527:ATP:PG	3.19	0.41
1:G:207:LYS:N	1:G:208:PRO:HD2	2.36	0.41
1:G:223:ALA:HB3	1:G:251:ALA:CA	2.50	0.41
1:G:262:LEU:HD13	1:G:275:ALA:HB2	2.02	0.41
1:J:162:ILE:HD11	1:J:399:ALA:CB	2.51	0.41
1:J:246:PRO:HB3	1:J:272:LYS:HB2	2.03	0.41
1:K:321:LYS:HB3	1:K:334:ASP:CG	2.46	0.41
1:K:417:VAL:HA	1:K:420:ILE:HG22	2.02	0.41
1:L:417:VAL:HA	1:L:420:ILE:HG22	2.03	0.41
2:A:1525:PO4:P	4:A:1527:ATP:PG	3.19	0.41
1:B:165:ALA:HB2	1:B:187:LEU:HD13	2.02	0.41
1:B:219:PHE:HB3	1:B:317:LEU:HD11	2.03	0.41
1:C:209:GLU:H	1:C:209:GLU:CD	2.29	0.41
1:D:207:LYS:HB3	1:D:208:PRO:HD3	2.02	0.41
1:D:262:LEU:C	1:D:262:LEU:HD23	2.46	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:PG	3.18	0.41
1:L:7:LYS:O	1:L:519:CYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:8:PHE:HA	1:N:518:GLU:O	2.21	0.41
1:N:206:ASN:HB2	1:N:213:VAL:HG23	2.03	0.41
1:A:41:ASP:HB3	1:G:521:VAL:O	2.21	0.40
1:A:49:ILE:HD13	1:G:513:LEU:HA	2.03	0.40
2:B:1525:PO4:P	4:B:1527:ATP:PG	3.18	0.40
1:C:262:LEU:HD23	1:C:262:LEU:C	2.46	0.40
1:D:215:LEU:HB3	1:D:246:PRO:HG2	2.02	0.40
1:D:326:ASN:HB2	1:D:327:LYS:H	1.78	0.40
1:E:248:LEU:HD22	1:E:323:VAL:HG21	2.03	0.40
1:F:270:ILE:O	1:F:271:VAL:HB	2.21	0.40
1:G:311:LYS:O	1:G:313:THR:HG23	2.21	0.40
1:J:263:VAL:O	1:J:267:MET:HB3	2.21	0.40
1:K:326:ASN:HD22	1:K:327:LYS:HD3	1.86	0.40
1:K:353:ILE:HG12	1:K:365:LEU:HB3	2.02	0.40
1:N:166:MET:O	1:N:170:GLY:N	2.54	0.40
1:A:262:LEU:HD13	1:A:275:ALA:HB2	2.02	0.40
1:B:311:LYS:O	1:B:313:THR:HG23	2.21	0.40
1:B:460:GLU:CD	1:B:461:GLU:H	2.29	0.40
1:E:49:ILE:HD13	1:E:49:ILE:HG21	1.93	0.40
1:F:144:ILE:HG23	1:F:403:THR:HG23	2.04	0.40
1:F:248:LEU:HD22	1:F:323:VAL:HG21	2.03	0.40
1:I:162:ILE:HD11	1:I:399:ALA:CB	2.51	0.40
1:L:19:GLY:HA3	1:L:67:GLU:O	2.22	0.40
1:N:263:VAL:O	1:N:267:MET:HB3	2.21	0.40
1:B:194:GLN:CG	1:B:329:THR:CB	3.00	0.40
1:E:295:LEU:O	1:E:337:GLY:HA3	2.22	0.40
1:G:248:LEU:HD22	1:G:323:VAL:HG21	2.03	0.40
1:H:263:VAL:O	1:H:267:MET:HB3	2.21	0.40
1:A:248:LEU:HD22	1:A:323:VAL:HG21	2.03	0.40
1:C:193:MET:CE	1:C:332:ILE:CG2	2.97	0.40
1:C:513:LEU:HB3	1:D:49:ILE:HD11	1.98	0.40
1:D:270:ILE:O	1:D:271:VAL:HB	2.21	0.40
1:E:203:TYR:N	1:E:203:TYR:CD1	2.90	0.40
1:G:203:TYR:N	1:G:203:TYR:CD1	2.90	0.40
1:G:222:LEU:CD2	1:G:292:ILE:HG22	2.45	0.40
1:G:295:LEU:O	1:G:337:GLY:HA3	2.22	0.40
1:I:215:LEU:O	1:I:218:PRO:HD3	2.21	0.40
1:L:191:GLU:O	1:L:334:ASP:HA	2.22	0.40
1:B:262:LEU:C	1:B:262:LEU:HD23	2.46	0.40
1:B:338:GLU:O	1:B:342:ILE:HG13	2.21	0.40
1:D:521:VAL:O	1:E:41:ASP:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:VAL:HG12	1:E:273:VAL:HG23	2.02	0.40
1:E:383:ALA:HA	1:E:389:MET:CB	2.52	0.40
1:G:338:GLU:O	1:G:342:ILE:HG13	2.21	0.40
1:J:335:GLY:C	1:J:337:GLY:H	2.29	0.40
1:M:191:GLU:O	1:M:334:ASP:HA	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	496 (95%)	23 (4%)	3 (1%)	21	59
1	B	522/548 (95%)	495 (95%)	23 (4%)	4 (1%)	16	54
1	C	522/548 (95%)	497 (95%)	22 (4%)	3 (1%)	21	59
1	D	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	30	67
1	E	522/548 (95%)	494 (95%)	23 (4%)	5 (1%)	12	49
1	F	522/548 (95%)	495 (95%)	24 (5%)	3 (1%)	21	59
1	G	522/548 (95%)	494 (95%)	23 (4%)	5 (1%)	12	49
1	H	522/548 (95%)	496 (95%)	24 (5%)	2 (0%)	30	67
1	I	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	30	67
1	J	522/548 (95%)	497 (95%)	23 (4%)	2 (0%)	30	67
1	K	522/548 (95%)	497 (95%)	24 (5%)	1 (0%)	43	78
1	L	522/548 (95%)	497 (95%)	22 (4%)	3 (1%)	21	59
1	M	522/548 (95%)	497 (95%)	24 (5%)	1 (0%)	43	78
1	N	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	30	67
All	All	7308/7672 (95%)	6949 (95%)	321 (4%)	38 (0%)	26	63

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	199	TYR
1	E	205	ILE
1	G	199	TYR
1	A	384	ALA
1	B	384	ALA
1	C	199	TYR
1	C	384	ALA
1	D	384	ALA
1	E	199	TYR
1	E	384	ALA
1	F	384	ALA
1	G	384	ALA
1	A	271	VAL
1	B	271	VAL
1	C	271	VAL
1	D	271	VAL
1	E	271	VAL
1	F	271	VAL
1	G	271	VAL
1	A	208	PRO
1	E	208	PRO
1	G	202	PRO
1	G	208	PRO
1	L	426	LEU
1	H	426	LEU
1	H	269	GLY
1	K	269	GLY
1	L	269	GLY
1	M	269	GLY
1	B	208	PRO
1	F	208	PRO
1	I	269	GLY
1	J	269	GLY
1	N	269	GLY
1	I	336	VAL
1	J	336	VAL
1	N	336	VAL
1	L	336	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	360 (90%)	42 (10%)	7	22
1	C	402/414 (97%)	360 (90%)	42 (10%)	7	22
1	D	402/414 (97%)	359 (89%)	43 (11%)	6	21
1	E	402/414 (97%)	360 (90%)	42 (10%)	7	22
1	F	402/414 (97%)	360 (90%)	42 (10%)	7	22
1	G	402/414 (97%)	358 (89%)	44 (11%)	6	21
1	H	402/414 (97%)	369 (92%)	33 (8%)	10	31
1	I	402/414 (97%)	363 (90%)	39 (10%)	8	24
1	J	402/414 (97%)	365 (91%)	37 (9%)	8	27
1	K	402/414 (97%)	370 (92%)	32 (8%)	11	31
1	L	402/414 (97%)	363 (90%)	39 (10%)	8	24
1	M	402/414 (97%)	363 (90%)	39 (10%)	8	24
1	N	402/414 (97%)	367 (91%)	35 (9%)	9	29
All	All	5628/5796 (97%)	5078 (90%)	550 (10%)	10	24

All (550) 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	47	PRO
1	A	169	VAL
1	A	171	LYS
1	A	176	THR
1	A	177	VAL
1	A	181	THR
1	A	183	LEU

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Mol	Chain	Res	Type
1	A	188	ASP
1	A	190	VAL
1	A	194	GLN
1	A	207	LYS
1	A	225	LYS
1	A	226	LYS
1	A	242	LYS
1	A	252	GLU
1	A	262	LEU
1	A	272	LYS
1	A	296	THR
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	364	LYS
1	A	376	VAL
1	A	404	ARG
1	A	428	ASP
1	A	453	GLN
1	A	460	GLU
1	A	499	VAL
1	A	518	GLU
1	A	521	VAL
1	B	8	PHE
1	B	18	ARG
1	B	34	LYS
1	B	36	ARG
1	B	37	ASN
1	B	47	PRO
1	B	169	VAL
1	B	171	LYS
1	B	176	THR
1	B	177	VAL
1	B	181	THR
1	B	183	LEU

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Mol	Chain	Res	Type
1	B	188	ASP
1	B	190	VAL
1	B	194	GLN
1	B	213	VAL
1	B	225	LYS
1	B	226	LYS
1	B	242	LYS
1	B	252	GLU
1	B	262	LEU
1	B	272	LYS
1	B	296	THR
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
1	B	364	LYS
1	B	376	VAL
1	B	404	ARG
1	B	428	ASP
1	B	453	GLN
1	B	460	GLU
1	B	499	VAL
1	B	518	GLU
1	B	521	VAL
1	C	18	ARG
1	C	34	LYS
1	C	36	ARG
1	C	37	ASN
1	C	47	PRO
1	C	169	VAL
1	C	171	LYS
1	C	176	THR
1	C	177	VAL
1	C	181	THR
1	C	183	LEU
1	C	188	ASP

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Mol	Chain	Res	Type
1	C	190	VAL
1	C	194	GLN
1	C	207	LYS
1	C	213	VAL
1	C	225	LYS
1	C	226	LYS
1	C	242	LYS
1	C	252	GLU
1	C	262	LEU
1	C	272	LYS
1	C	296	THR
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	364	LYS
1	C	376	VAL
1	C	404	ARG
1	C	428	ASP
1	C	453	GLN
1	C	460	GLU
1	C	499	VAL
1	C	518	GLU
1	C	521	VAL
1	D	18	ARG
1	D	34	LYS
1	D	36	ARG
1	D	37	ASN
1	D	47	PRO
1	D	169	VAL
1	D	171	LYS
1	D	176	THR
1	D	177	VAL
1	D	181	THR
1	D	183	LEU
1	D	188	ASP

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Mol	Chain	Res	Type
1	D	190	VAL
1	D	194	GLN
1	D	207	LYS
1	D	213	VAL
1	D	225	LYS
1	D	226	LYS
1	D	242	LYS
1	D	252	GLU
1	D	262	LEU
1	D	272	LYS
1	D	296	THR
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	364	LYS
1	D	376	VAL
1	D	404	ARG
1	D	428	ASP
1	D	453	GLN
1	D	460	GLU
1	D	499	VAL
1	D	516	THR
1	D	518	GLU
1	D	521	VAL
1	E	18	ARG
1	E	34	LYS
1	E	36	ARG
1	E	37	ASN
1	E	47	PRO
1	E	169	VAL
1	E	171	LYS
1	E	176	THR
1	E	177	VAL
1	E	181	THR
1	E	183	LEU

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Mol	Chain	Res	Type
1	E	189	VAL
1	E	190	VAL
1	E	194	GLN
1	E	204	PHE
1	E	213	VAL
1	E	225	LYS
1	E	226	LYS
1	E	242	LYS
1	E	252	GLU
1	E	262	LEU
1	E	272	LYS
1	E	296	THR
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	364	LYS
1	E	376	VAL
1	E	404	ARG
1	E	428	ASP
1	E	453	GLN
1	E	460	GLU
1	E	499	VAL
1	E	518	GLU
1	E	521	VAL
1	F	18	ARG
1	F	34	LYS
1	F	36	ARG
1	F	37	ASN
1	F	47	PRO
1	F	169	VAL
1	F	171	LYS
1	F	176	THR
1	F	177	VAL
1	F	181	THR
1	F	183	LEU

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Mol	Chain	Res	Type
1	F	188	ASP
1	F	190	VAL
1	F	194	GLN
1	F	207	LYS
1	F	213	VAL
1	F	225	LYS
1	F	226	LYS
1	F	242	LYS
1	F	252	GLU
1	F	262	LEU
1	F	272	LYS
1	F	296	THR
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	364	LYS
1	F	376	VAL
1	F	404	ARG
1	F	428	ASP
1	F	453	GLN
1	F	460	GLU
1	F	499	VAL
1	F	518	GLU
1	F	521	VAL
1	G	18	ARG
1	G	34	LYS
1	G	36	ARG
1	G	37	ASN
1	G	47	PRO
1	G	169	VAL
1	G	171	LYS
1	G	176	THR
1	G	177	VAL
1	G	181	THR
1	G	183	LEU

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Mol	Chain	Res	Type
1	G	188	ASP
1	G	190	VAL
1	G	193	MET
1	G	194	GLN
1	G	201	SER
1	G	207	LYS
1	G	213	VAL
1	G	225	LYS
1	G	226	LYS
1	G	242	LYS
1	G	252	GLU
1	G	262	LEU
1	G	272	LYS
1	G	296	THR
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	364	LYS
1	G	376	VAL
1	G	404	ARG
1	G	428	ASP
1	G	453	GLN
1	G	460	GLU
1	G	499	VAL
1	G	518	GLU
1	G	521	VAL
1	H	65	LYS
1	H	82	ASN
1	H	130	GLU
1	H	142	LYS
1	H	153	ASN
1	H	169	VAL
1	H	171	LYS
1	H	172	GLU
1	H	174	VAL

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Mol	Chain	Res	Type
1	H	184	GLN
1	H	187	LEU
1	H	196	ASP
1	H	213	VAL
1	H	214	GLU
1	H	230	ILE
1	H	231	ARG
1	H	271	VAL
1	H	290	GLN
1	H	313	THR
1	H	321	LYS
1	H	329	THR
1	H	334	ASP
1	H	338	GLU
1	H	350	ARG
1	H	390	LYS
1	H	404	ARG
1	H	460	GLU
1	H	483	GLU
1	H	484	GLU
1	H	494	LEU
1	H	500	THR
1	H	504	LEU
1	H	510	VAL
1	I	63	GLU
1	I	65	LYS
1	I	82	ASN
1	I	130	GLU
1	I	140	ASP
1	I	142	LYS
1	I	153	ASN
1	I	169	VAL
1	I	171	LYS
1	I	172	GLU
1	I	174	VAL
1	I	184	GLN
1	I	187	LEU
1	I	196	ASP
1	I	213	VAL
1	I	214	GLU
1	I	216	GLU
1	I	226	LYS

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Mol	Chain	Res	Type
1	I	229	ASN
1	I	230	ILE
1	I	232	GLU
1	I	271	VAL
1	I	290	GLN
1	I	313	THR
1	I	326	ASN
1	I	329	THR
1	I	334	ASP
1	I	338	GLU
1	I	350	ARG
1	I	390	LYS
1	I	404	ARG
1	I	460	GLU
1	I	461	GLU
1	I	483	GLU
1	I	484	GLU
1	I	494	LEU
1	I	500	THR
1	I	504	LEU
1	I	510	VAL
1	J	65	LYS
1	J	82	ASN
1	J	142	LYS
1	J	153	ASN
1	J	171	LYS
1	J	172	GLU
1	J	174	VAL
1	J	184	GLN
1	J	187	LEU
1	J	196	ASP
1	J	206	ASN
1	J	213	VAL
1	J	214	GLU
1	J	228	SER
1	J	229	ASN
1	J	230	ILE
1	J	271	VAL
1	J	290	GLN
1	J	313	THR
1	J	321	LYS
1	J	326	ASN

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Mol	Chain	Res	Type
1	J	329	THR
1	J	334	ASP
1	J	338	GLU
1	J	350	ARG
1	J	390	LYS
1	J	404	ARG
1	J	411	VAL
1	J	460	GLU
1	J	461	GLU
1	J	473	ASP
1	J	483	GLU
1	J	484	GLU
1	J	494	LEU
1	J	500	THR
1	J	504	LEU
1	J	510	VAL
1	K	82	ASN
1	K	130	GLU
1	K	142	LYS
1	K	153	ASN
1	K	164	GLU
1	K	169	VAL
1	K	171	LYS
1	K	172	GLU
1	K	174	VAL
1	K	184	GLN
1	K	196	ASP
1	K	213	VAL
1	K	214	GLU
1	K	216	GLU
1	K	230	ILE
1	K	271	VAL
1	K	290	GLN
1	K	313	THR
1	K	327	LYS
1	K	329	THR
1	K	334	ASP
1	K	338	GLU
1	K	350	ARG
1	K	390	LYS
1	K	404	ARG
1	K	460	GLU

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Mol	Chain	Res	Type
1	K	483	GLU
1	K	484	GLU
1	K	494	LEU
1	K	500	THR
1	K	504	LEU
1	K	510	VAL
1	L	63	GLU
1	L	82	ASN
1	L	130	GLU
1	L	142	LYS
1	L	153	ASN
1	L	169	VAL
1	L	171	LYS
1	L	172	GLU
1	L	174	VAL
1	L	184	GLN
1	L	186	GLU
1	L	187	LEU
1	L	196	ASP
1	L	213	VAL
1	L	228	SER
1	L	229	ASN
1	L	230	ILE
1	L	262	LEU
1	L	271	VAL
1	L	290	GLN
1	L	313	THR
1	L	322	ARG
1	L	326	ASN
1	L	329	THR
1	L	334	ASP
1	L	338	GLU
1	L	339	GLU
1	L	350	ARG
1	L	390	LYS
1	L	404	ARG
1	L	411	VAL
1	L	421	ARG
1	L	460	GLU
1	L	483	GLU
1	L	484	GLU
1	L	494	LEU

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Mol	Chain	Res	Type
1	L	500	THR
1	L	504	LEU
1	L	510	VAL
1	M	65	LYS
1	M	82	ASN
1	M	130	GLU
1	M	142	LYS
1	M	153	ASN
1	M	169	VAL
1	M	171	LYS
1	M	172	GLU
1	M	174	VAL
1	M	184	GLN
1	M	187	LEU
1	M	196	ASP
1	M	206	ASN
1	M	213	VAL
1	M	214	GLU
1	M	216	GLU
1	M	230	ILE
1	M	232	GLU
1	M	262	LEU
1	M	271	VAL
1	M	290	GLN
1	M	313	THR
1	M	321	LYS
1	M	326	ASN
1	M	329	THR
1	M	334	ASP
1	M	338	GLU
1	M	350	ARG
1	M	390	LYS
1	M	404	ARG
1	M	411	VAL
1	M	460	GLU
1	M	461	GLU
1	M	483	GLU
1	M	484	GLU
1	M	494	LEU
1	M	500	THR
1	M	504	LEU
1	M	510	VAL

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Mol	Chain	Res	Type
1	N	65	LYS
1	N	82	ASN
1	N	130	GLU
1	N	142	LYS
1	N	153	ASN
1	N	171	LYS
1	N	172	GLU
1	N	174	VAL
1	N	186	GLU
1	N	187	LEU
1	N	196	ASP
1	N	213	VAL
1	N	229	ASN
1	N	230	ILE
1	N	271	VAL
1	N	290	GLN
1	N	313	THR
1	N	322	ARG
1	N	326	ASN
1	N	327	LYS
1	N	328	ASP
1	N	329	THR
1	N	334	ASP
1	N	338	GLU
1	N	339	GLU
1	N	350	ARG
1	N	390	LYS
1	N	404	ARG
1	N	460	GLU
1	N	483	GLU
1	N	484	GLU
1	N	494	LEU
1	N	500	THR
1	N	504	LEU
1	N	510	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	194	GLN
1	A	351	GLN

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Mol	Chain	Res	Type
1	B	37	ASN
1	B	351	GLN
1	C	37	ASN
1	C	194	GLN
1	C	351	GLN
1	C	401	HIS
1	D	37	ASN
1	D	194	GLN
1	D	351	GLN
1	D	401	HIS
1	E	194	GLN
1	E	351	GLN
1	F	194	GLN
1	F	351	GLN
1	F	401	HIS
1	G	37	ASN
1	G	194	GLN
1	G	351	GLN
1	H	68	ASN
1	H	352	GLN
1	H	475	ASN
1	I	68	ASN
1	I	229	ASN
1	I	352	GLN
1	I	475	ASN
1	J	68	ASN
1	J	229	ASN
1	J	352	GLN
1	J	475	ASN
1	K	68	ASN
1	K	326	ASN
1	K	352	GLN
1	K	475	ASN
1	L	68	ASN
1	L	352	GLN
1	L	475	ASN
1	M	68	ASN
1	M	352	GLN
1	M	475	ASN
1	N	68	ASN
1	N	352	GLN
1	N	475	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 7 are modelled with single atom and 7 are monoatomic - leaving 7 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	A	1527	3	32,33,33	1.83	3 (9%)	48,52,52	0.98	3 (6%)
4	ATP	F	1527	3	32,33,33	1.82	3 (9%)	48,52,52	0.99	3 (6%)
4	ATP	D	1527	3	32,33,33	1.84	3 (9%)	48,52,52	0.99	3 (6%)
4	ATP	G	1527	3	32,33,33	1.84	3 (9%)	48,52,52	0.99	3 (6%)
4	ATP	B	1527	3	32,33,33	1.83	3 (9%)	48,52,52	0.99	3 (6%)
4	ATP	C	1527	3	32,33,33	1.83	3 (9%)	48,52,52	0.99	3 (6%)
4	ATP	E	1527	3	32,33,33	1.82	3 (9%)	48,52,52	0.98	3 (6%)

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	A	1527	3	-	1/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	F	1527	3	-	1/22/38/38	0/3/3/3
4	ATP	D	1527	3	-	1/22/38/38	0/3/3/3
4	ATP	G	1527	3	-	1/22/38/38	0/3/3/3
4	ATP	B	1527	3	-	1/22/38/38	0/3/3/3
4	ATP	C	1527	3	-	1/22/38/38	0/3/3/3
4	ATP	E	1527	3	-	1/22/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1527	ATP	PA-O3A	-8.97	1.49	1.59
4	G	1527	ATP	PA-O3A	-8.94	1.49	1.59
4	C	1527	ATP	PA-O3A	-8.93	1.49	1.59
4	A	1527	ATP	PA-O3A	-8.92	1.49	1.59
4	B	1527	ATP	PA-O3A	-8.91	1.49	1.59
4	F	1527	ATP	PA-O3A	-8.90	1.49	1.59
4	E	1527	ATP	PA-O3A	-8.86	1.49	1.59
4	B	1527	ATP	PB-O3B	2.73	1.62	1.59
4	D	1527	ATP	PB-O3B	2.71	1.62	1.59
4	C	1527	ATP	PB-O3B	2.70	1.62	1.59
4	E	1527	ATP	PB-O3B	2.69	1.62	1.59
4	F	1527	ATP	PB-O3B	2.68	1.62	1.59
4	G	1527	ATP	PB-O3B	2.65	1.62	1.59
4	G	1527	ATP	PB-O3A	-2.64	1.56	1.59
4	A	1527	ATP	PB-O3B	2.61	1.62	1.59
4	D	1527	ATP	PB-O3A	-2.61	1.56	1.59
4	B	1527	ATP	PB-O3A	-2.56	1.56	1.59
4	E	1527	ATP	PB-O3A	-2.54	1.56	1.59
4	C	1527	ATP	PB-O3A	-2.53	1.56	1.59
4	F	1527	ATP	PB-O3A	-2.52	1.56	1.59
4	A	1527	ATP	PB-O3A	-2.49	1.56	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1527	ATP	O2A-PA-O3A	3.51	116.77	107.27
4	B	1527	ATP	O2A-PA-O3A	3.51	116.75	107.27
4	G	1527	ATP	O2A-PA-O3A	3.51	116.75	107.27
4	C	1527	ATP	O2A-PA-O3A	3.49	116.72	107.27
4	A	1527	ATP	O2A-PA-O3A	3.49	116.71	107.27
4	D	1527	ATP	O2A-PA-O3A	3.49	116.71	107.27
4	F	1527	ATP	O2A-PA-O3A	3.49	116.70	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1527	ATP	O4'-C1'-N9	2.50	112.89	108.09
4	B	1527	ATP	O4'-C1'-N9	2.49	112.87	108.09
4	D	1527	ATP	O4'-C1'-N9	2.49	112.87	108.09
4	C	1527	ATP	O4'-C1'-N9	2.48	112.86	108.09
4	F	1527	ATP	O4'-C1'-N9	2.48	112.85	108.09
4	E	1527	ATP	O4'-C1'-N9	2.46	112.82	108.09
4	A	1527	ATP	O4'-C1'-N9	2.45	112.80	108.09
4	D	1527	ATP	O3'-C3'-C4'	2.42	118.03	111.08
4	G	1527	ATP	O3'-C3'-C4'	2.42	118.02	111.08
4	B	1527	ATP	O3'-C3'-C4'	2.41	118.01	111.08
4	C	1527	ATP	O3'-C3'-C4'	2.41	117.99	111.08
4	F	1527	ATP	O3'-C3'-C4'	2.40	117.98	111.08
4	E	1527	ATP	O3'-C3'-C4'	2.38	117.91	111.08
4	A	1527	ATP	O3'-C3'-C4'	2.37	117.90	111.08

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1527	ATP	PG-O3B-PB-O2B
4	B	1527	ATP	PG-O3B-PB-O2B
4	C	1527	ATP	PG-O3B-PB-O2B
4	D	1527	ATP	PG-O3B-PB-O2B
4	E	1527	ATP	PG-O3B-PB-O2B
4	F	1527	ATP	PG-O3B-PB-O2B
4	G	1527	ATP	PG-O3B-PB-O2B

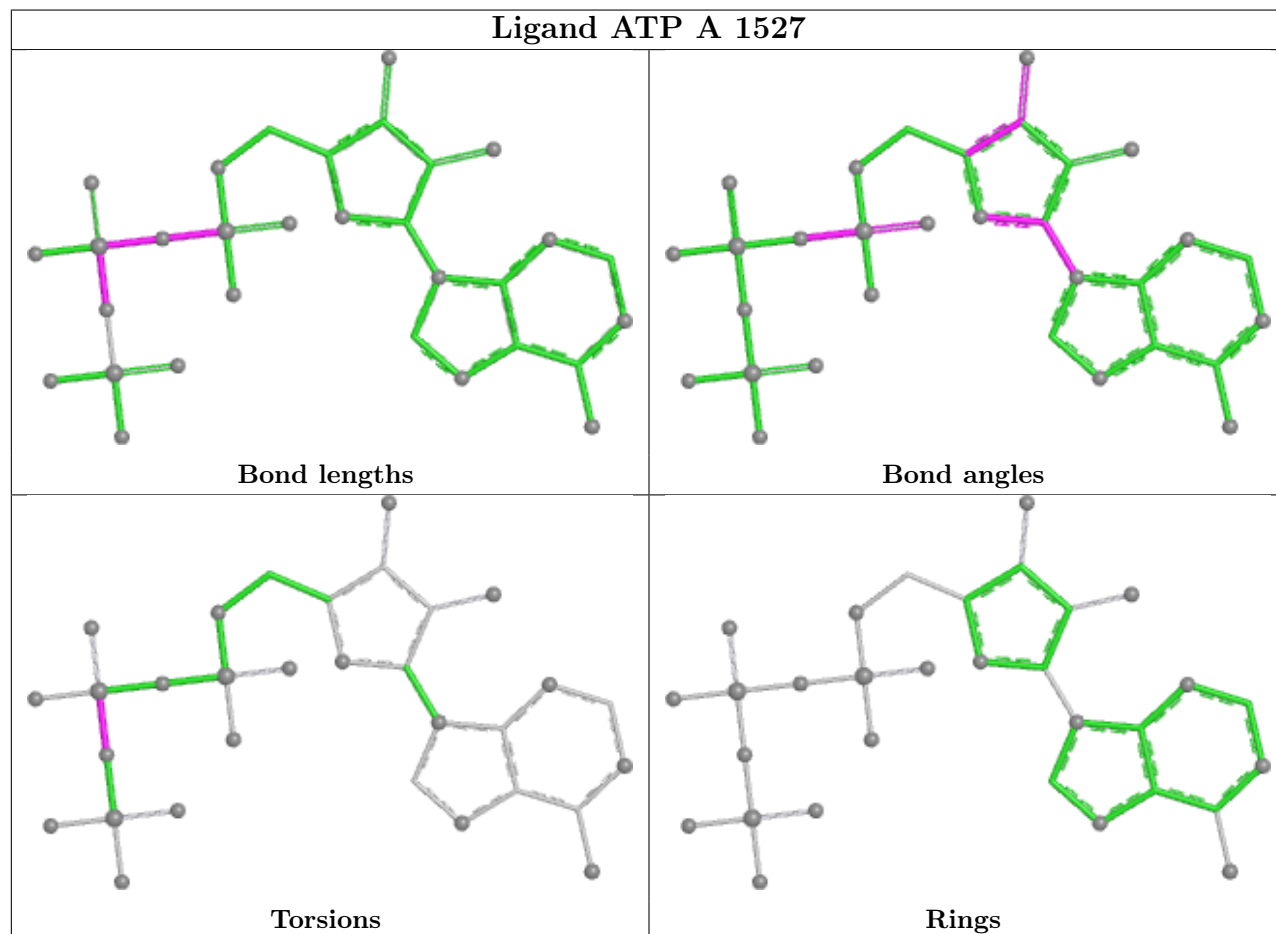
There are no ring outliers.

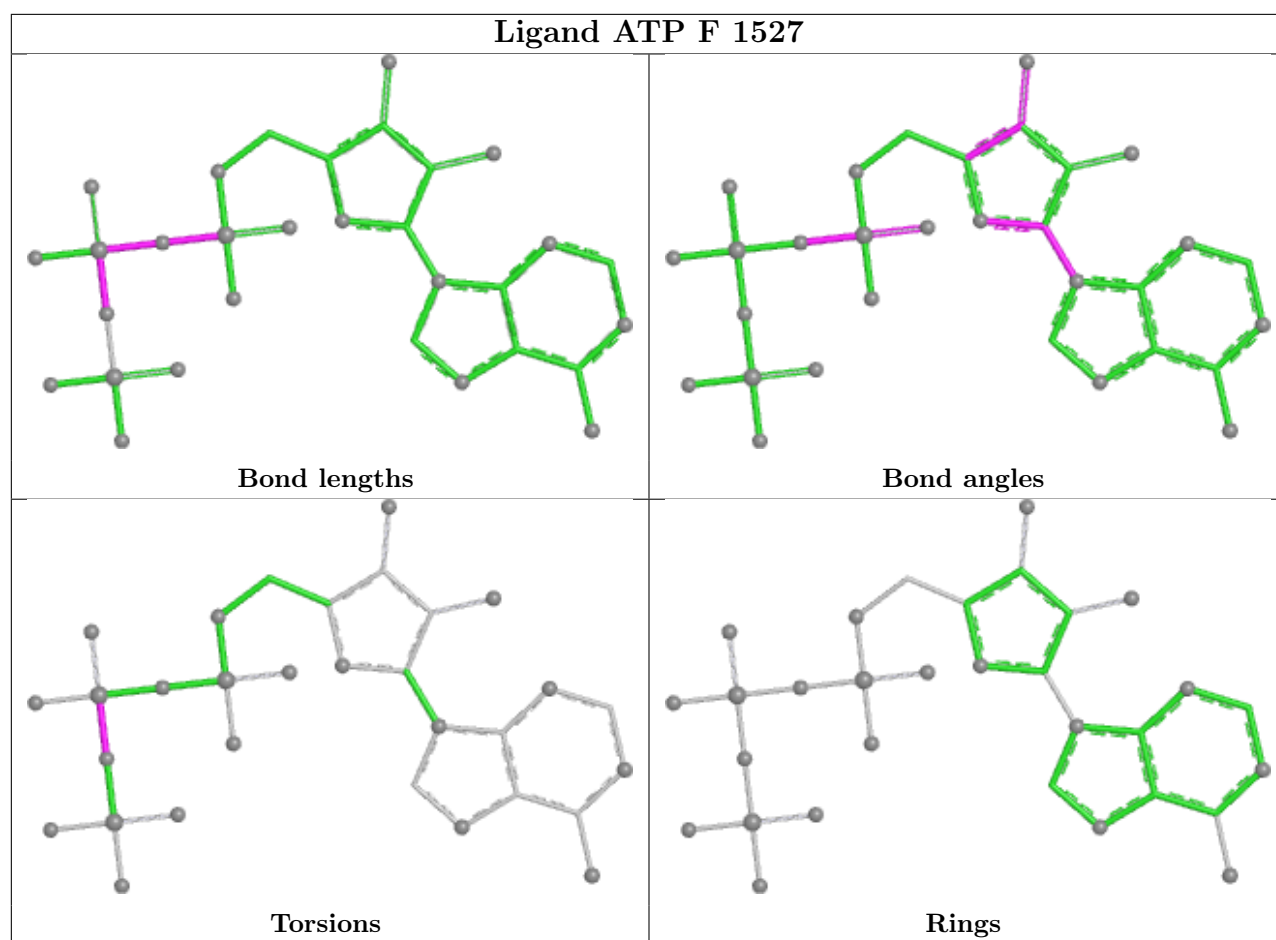
7 monomers are involved in 21 short contacts:

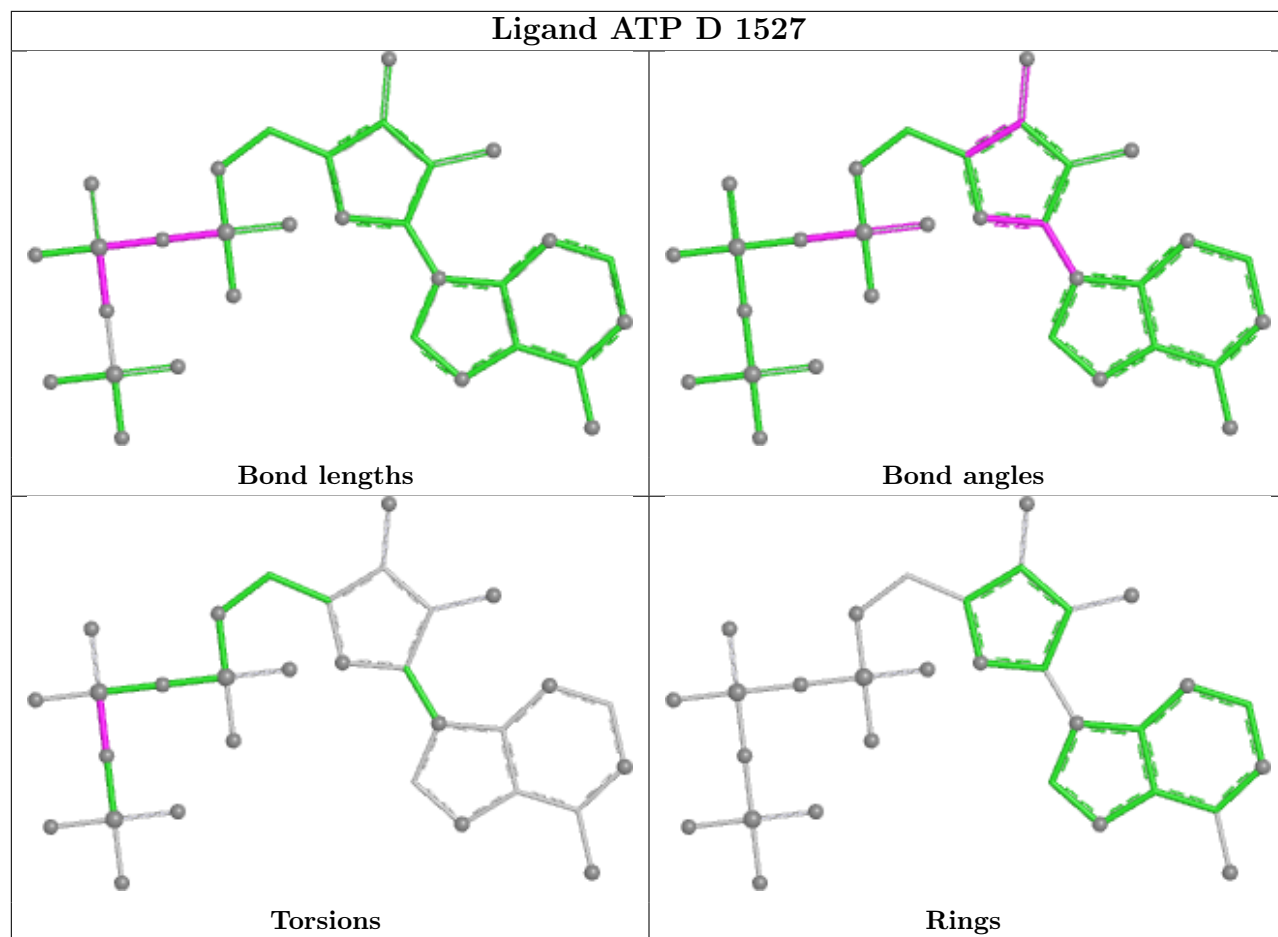
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1527	ATP	3	0
4	F	1527	ATP	3	0
4	D	1527	ATP	3	0
4	G	1527	ATP	3	0
4	B	1527	ATP	3	0
4	C	1527	ATP	3	0
4	E	1527	ATP	3	0

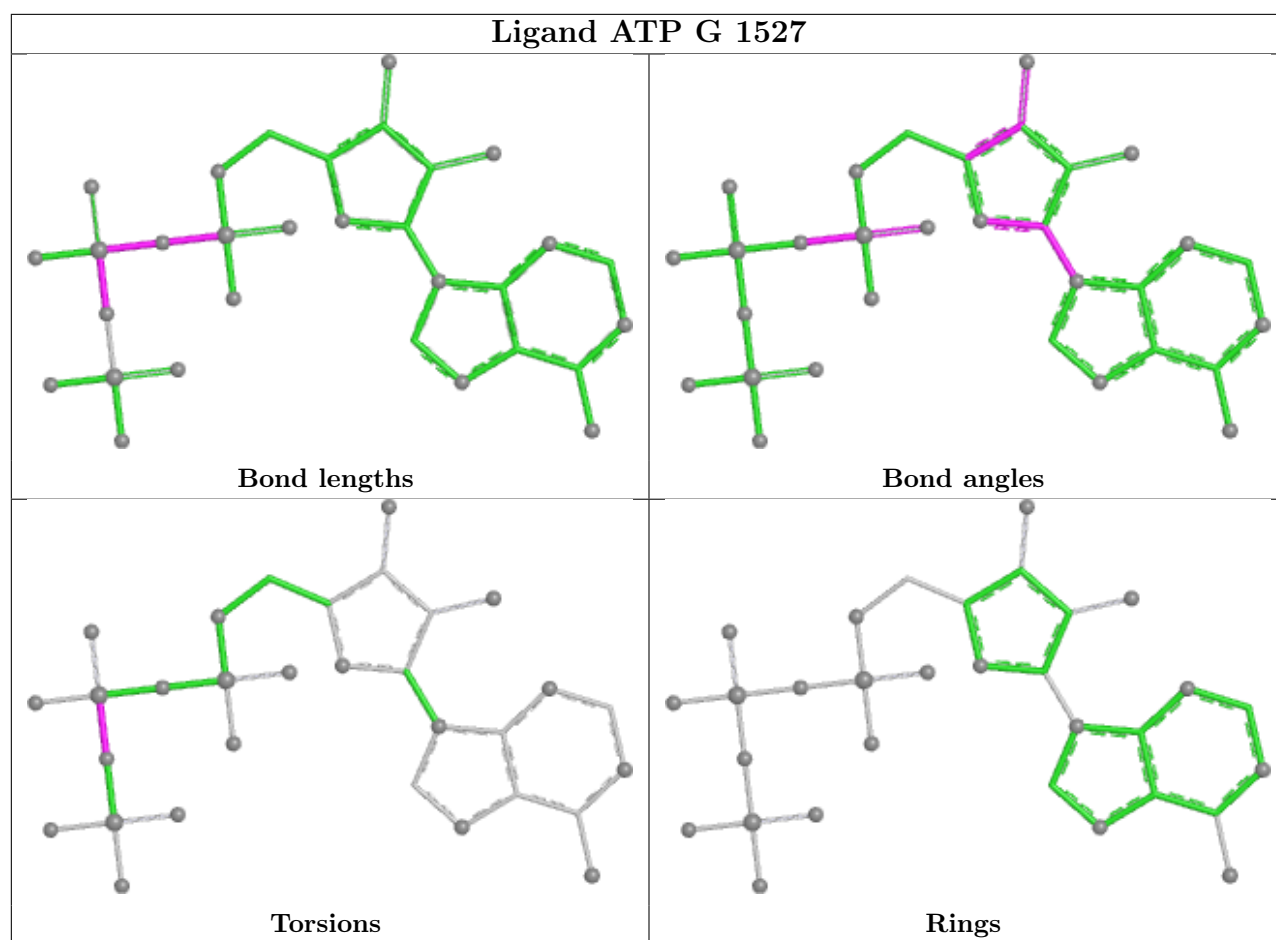
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

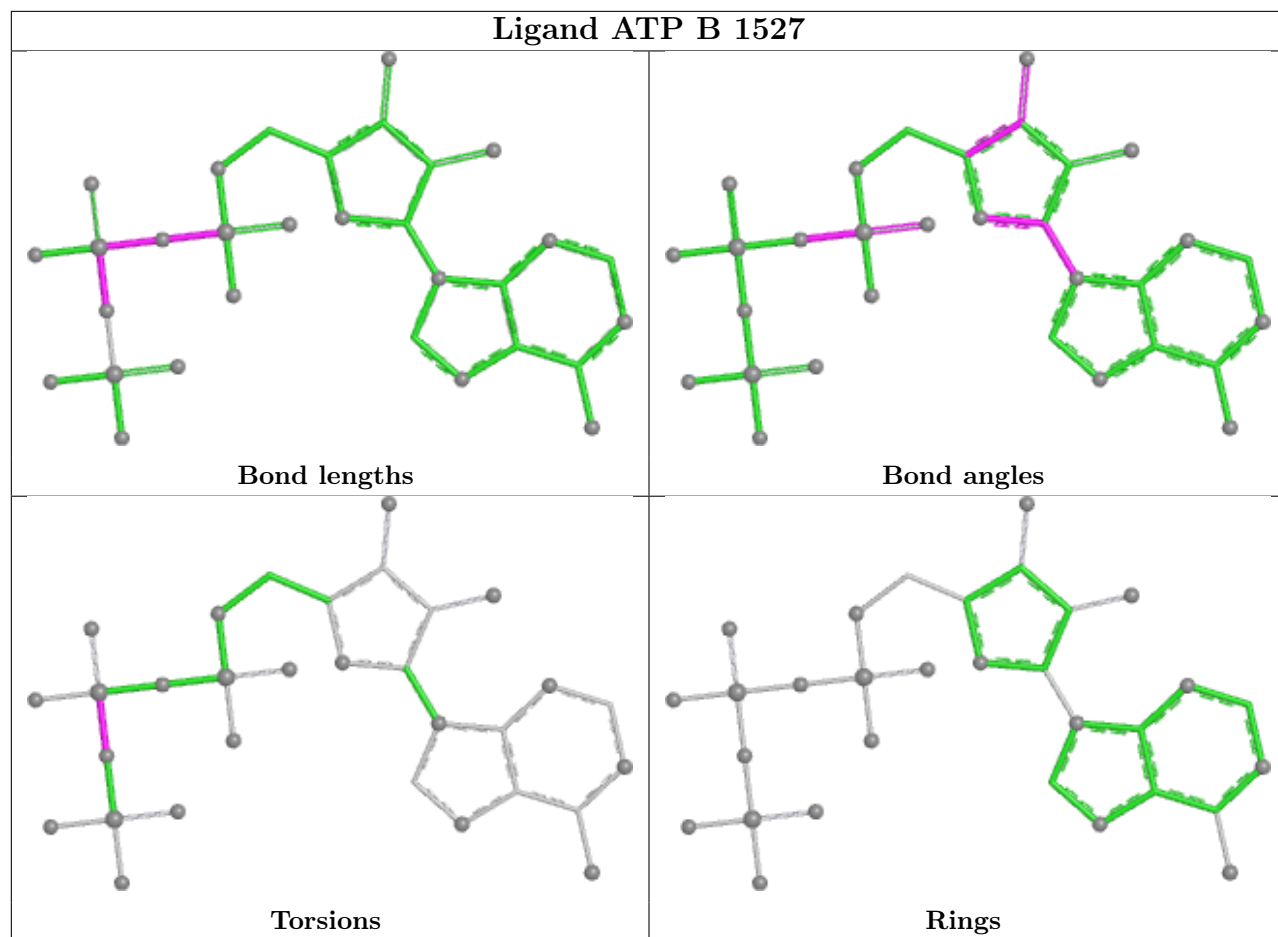
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

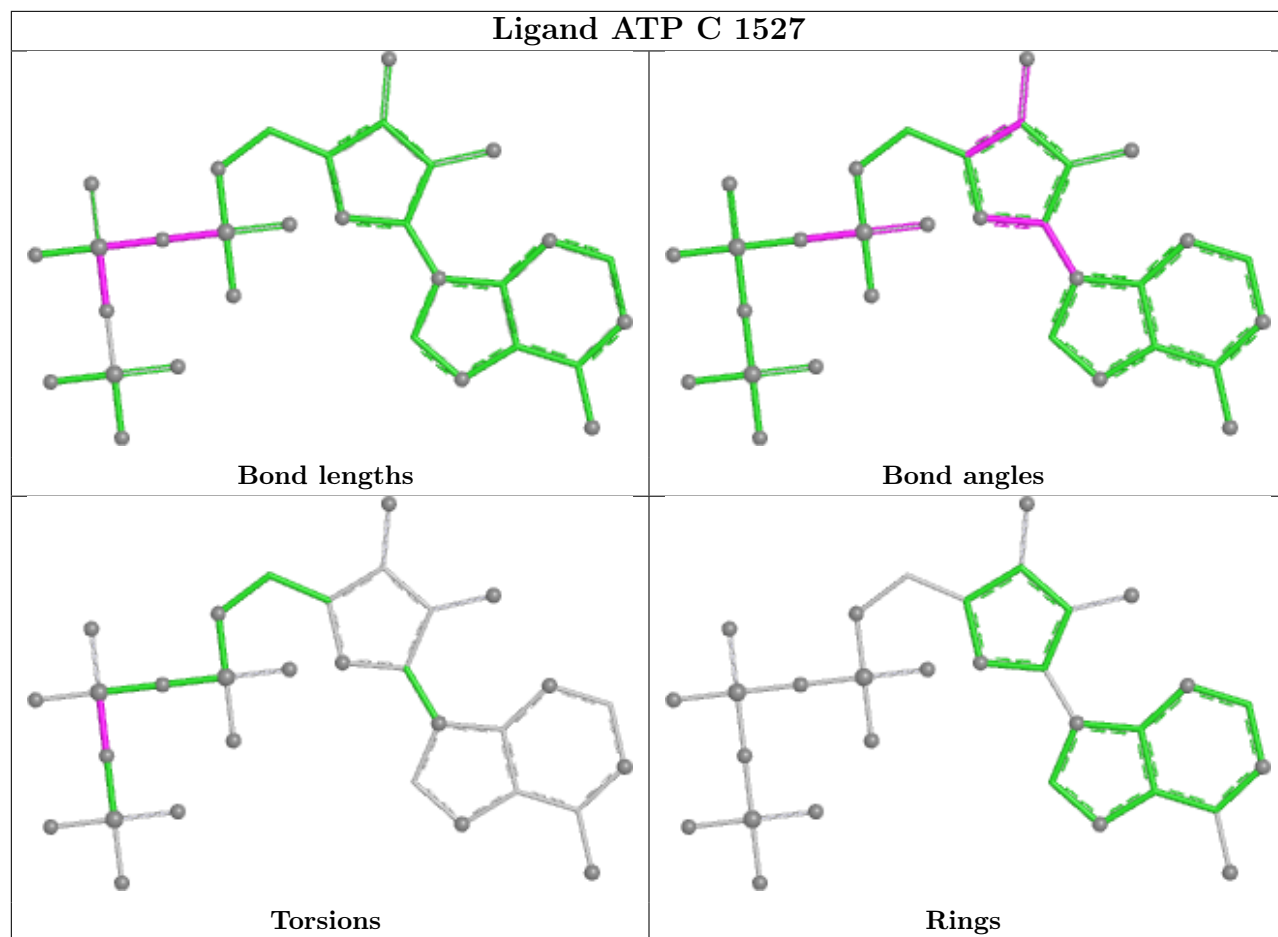


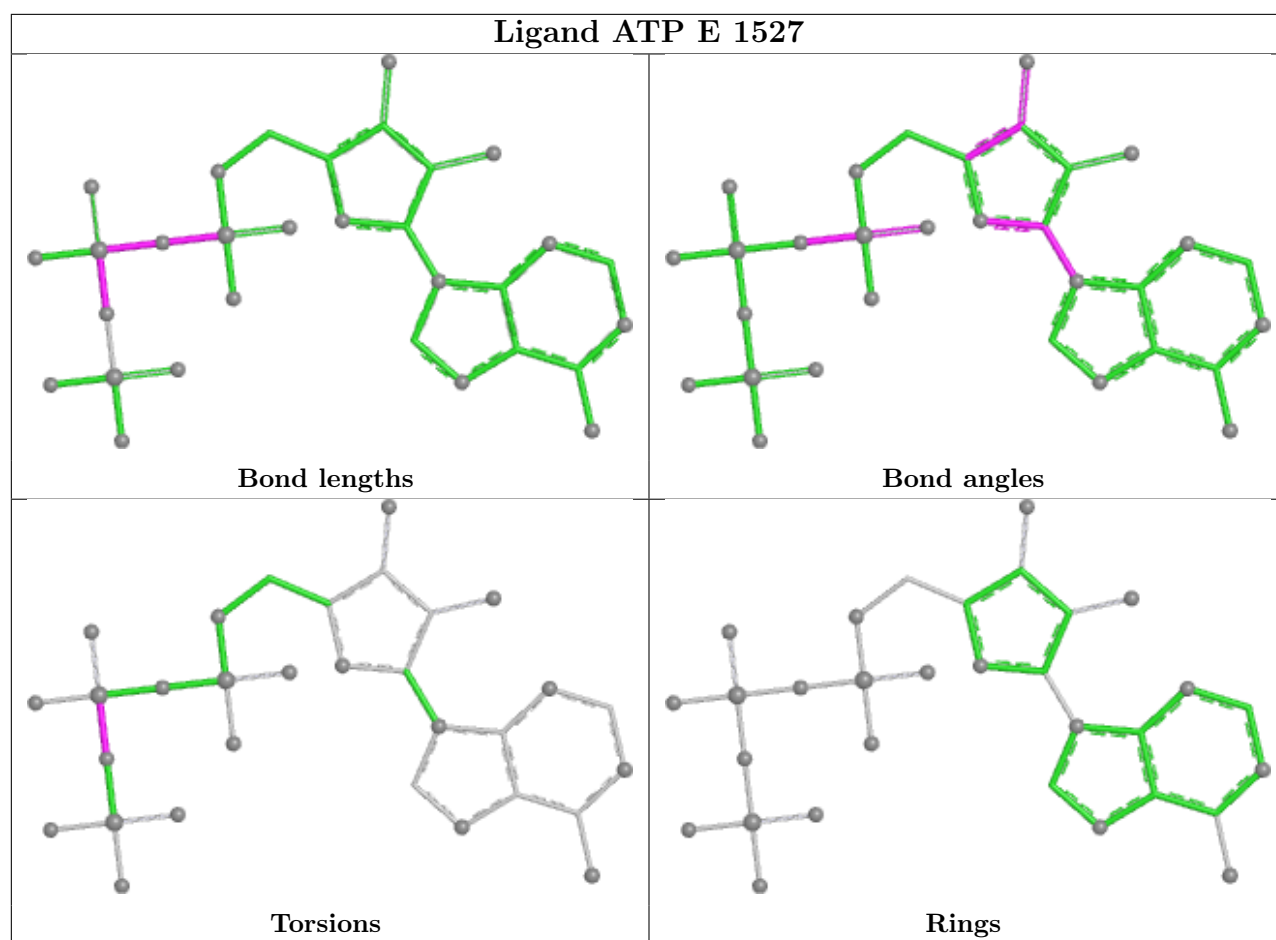












5.7 Other polymers [i](#)

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	513:LEU	C	514:MET	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	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	C	513:LEU	C	514:MET	N	1.18
1	D	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-2000. 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: 128

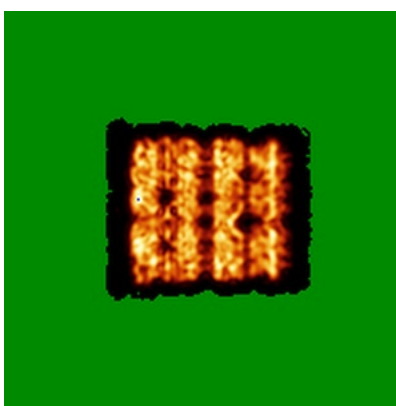
The images above show the largest variance slices of the map in three orthogonal directions.

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

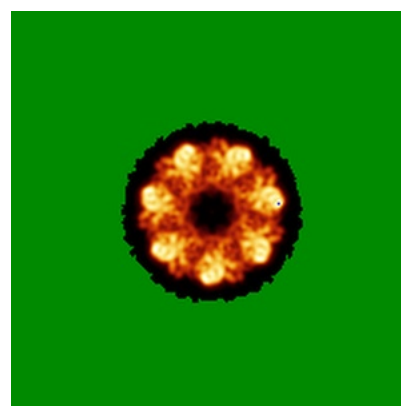
6.4.1 Primary map



X



Y

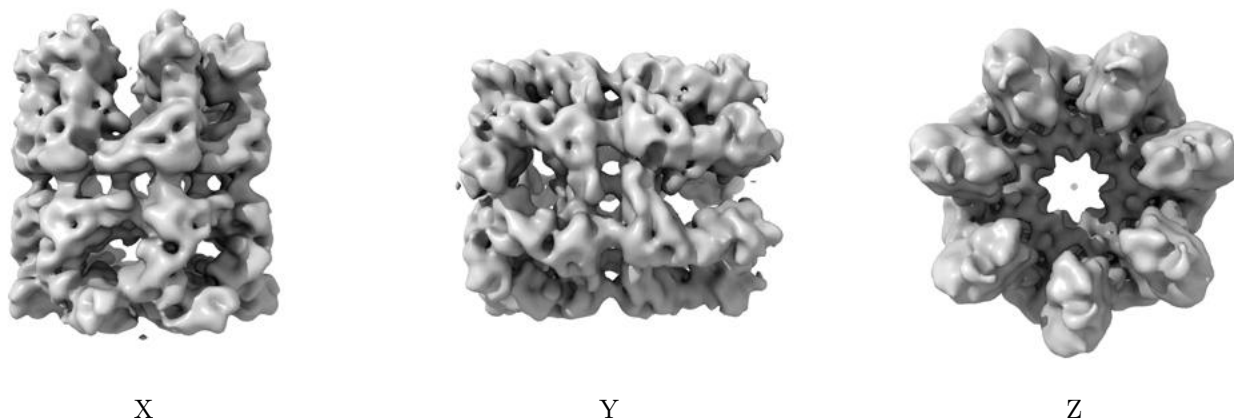


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

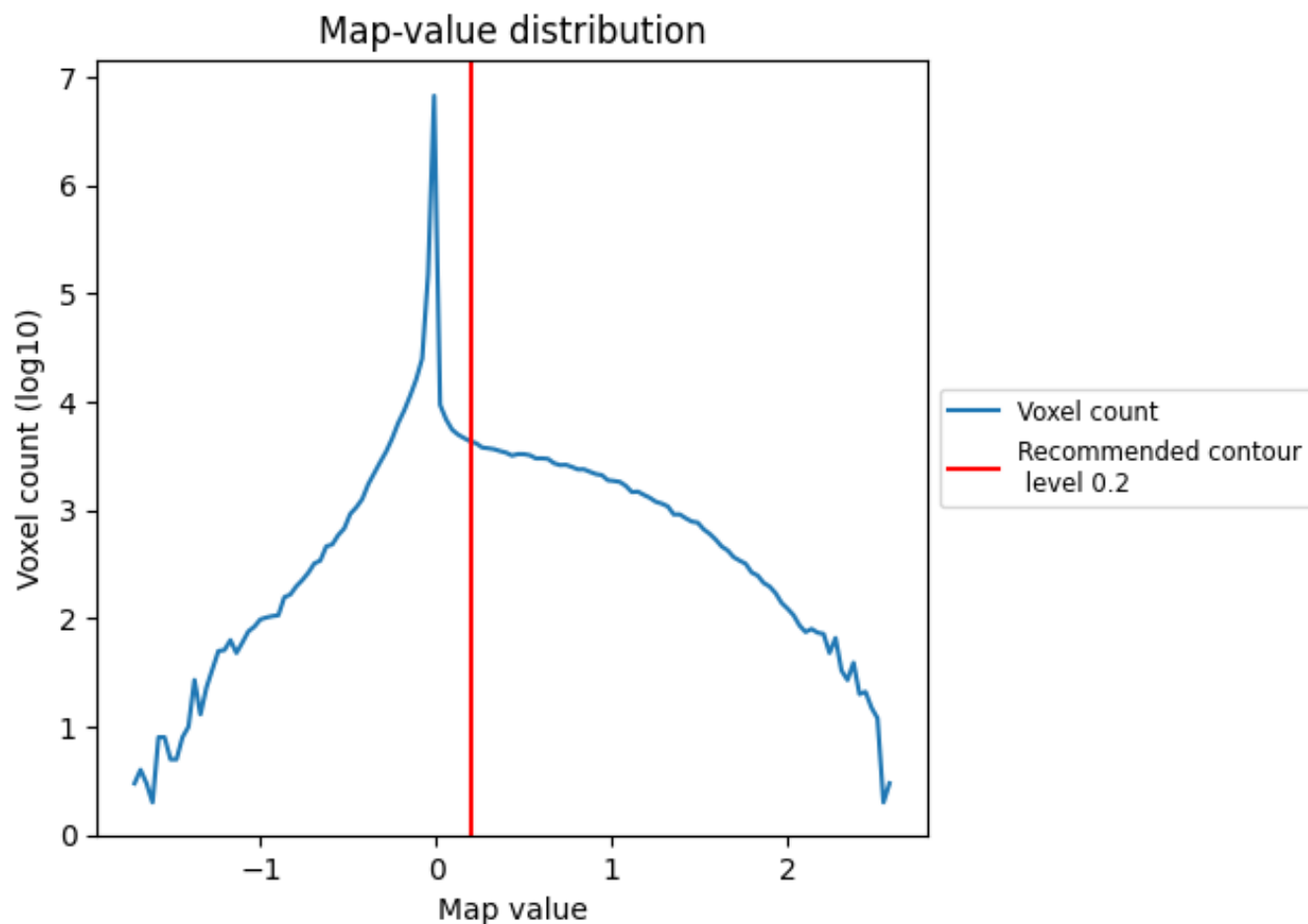
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

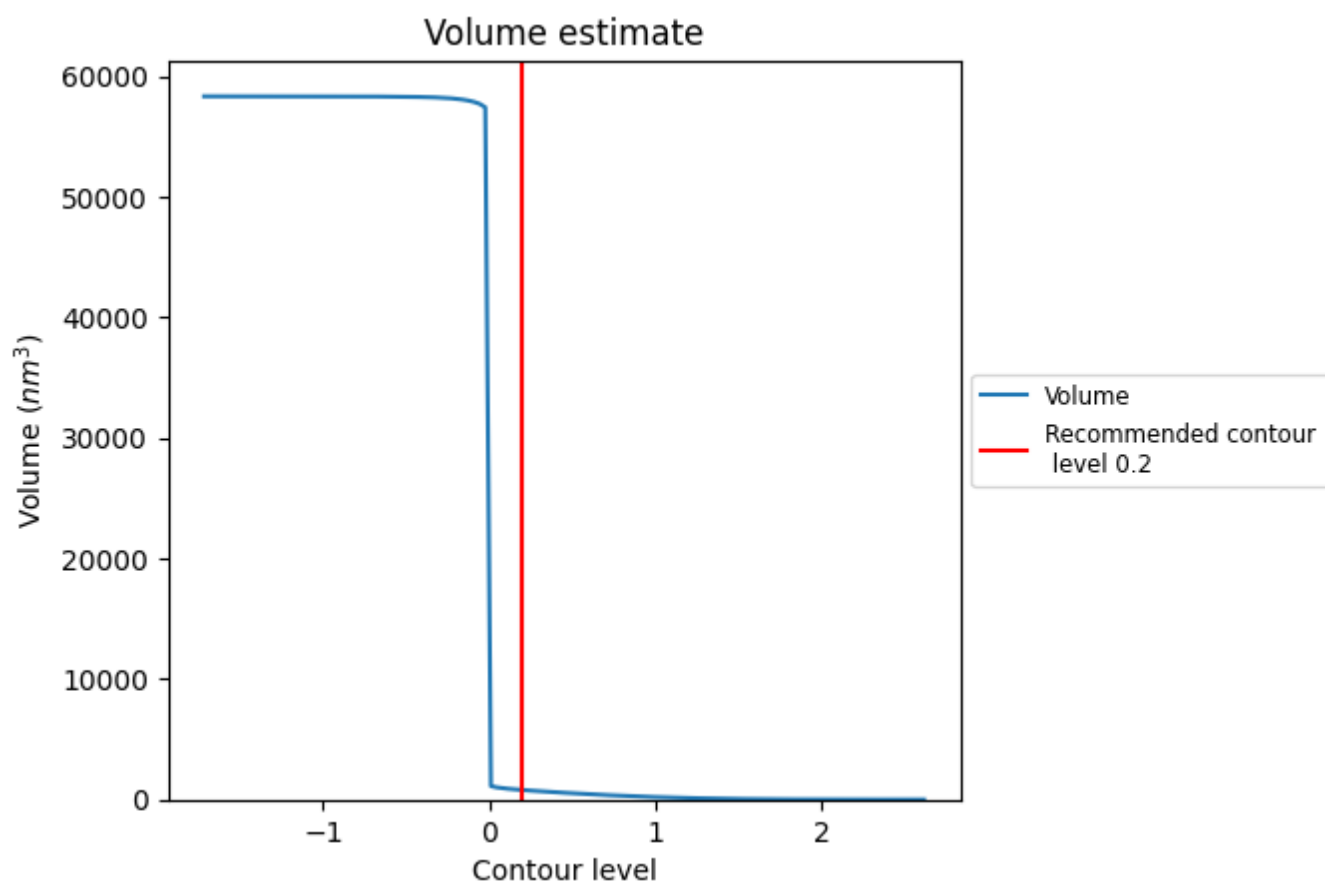
This section contains the results of statistical analysis of the map.

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.

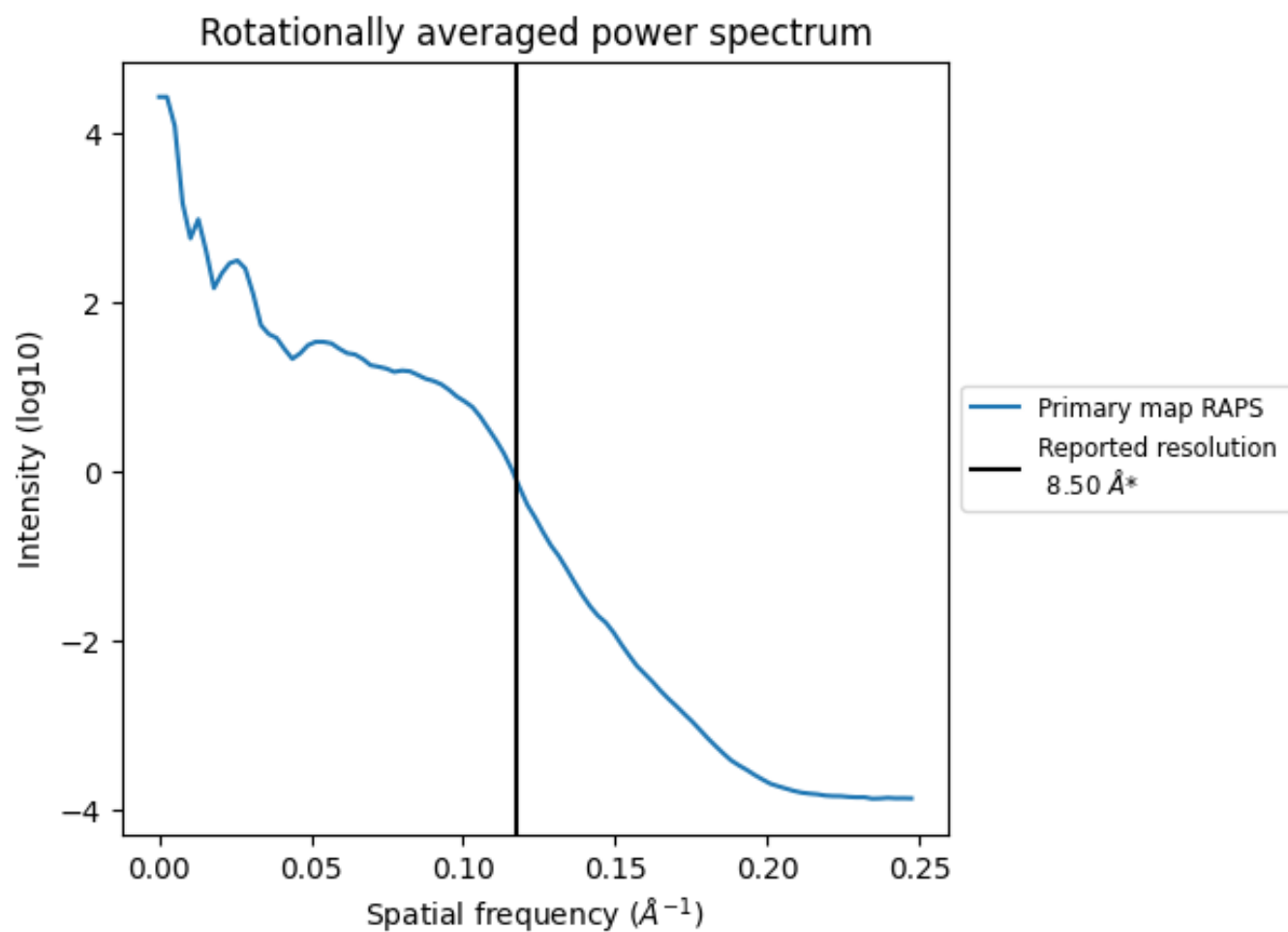
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 793 nm³; this corresponds to an approximate mass of 716 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

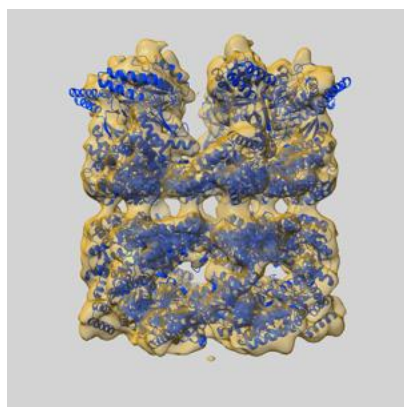
8 Fourier-Shell correlation

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

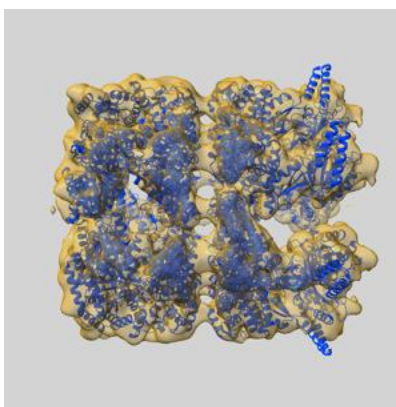
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2000 and PDB model 4AAS. Per-residue inclusion information can be found in section 3 on page 8.

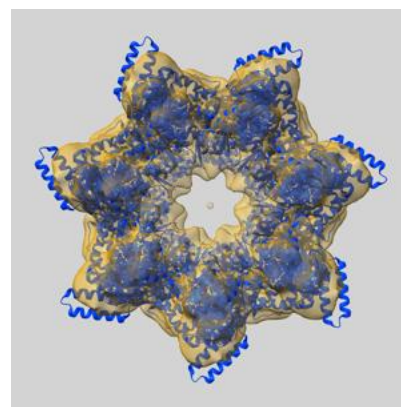
9.1 Map-model overlay [i](#)



X



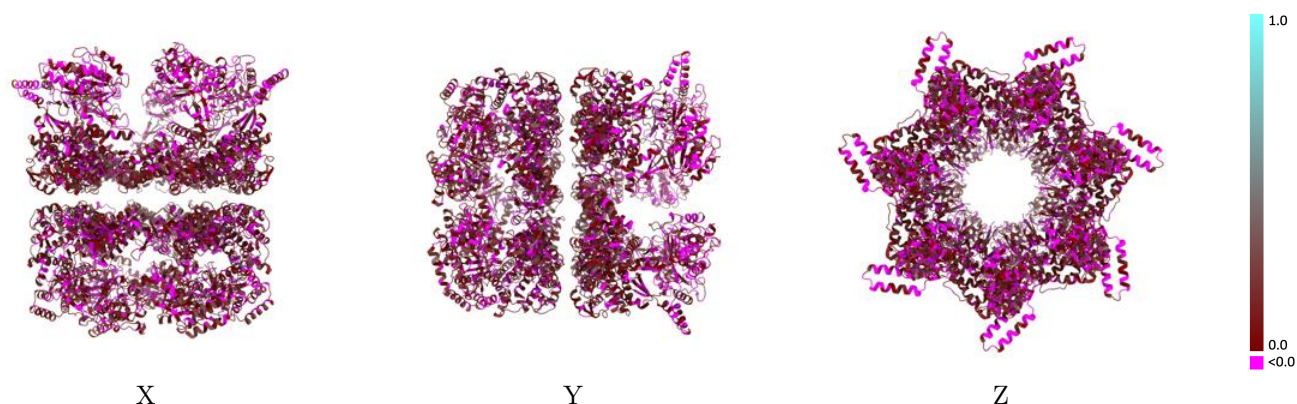
Y



Z

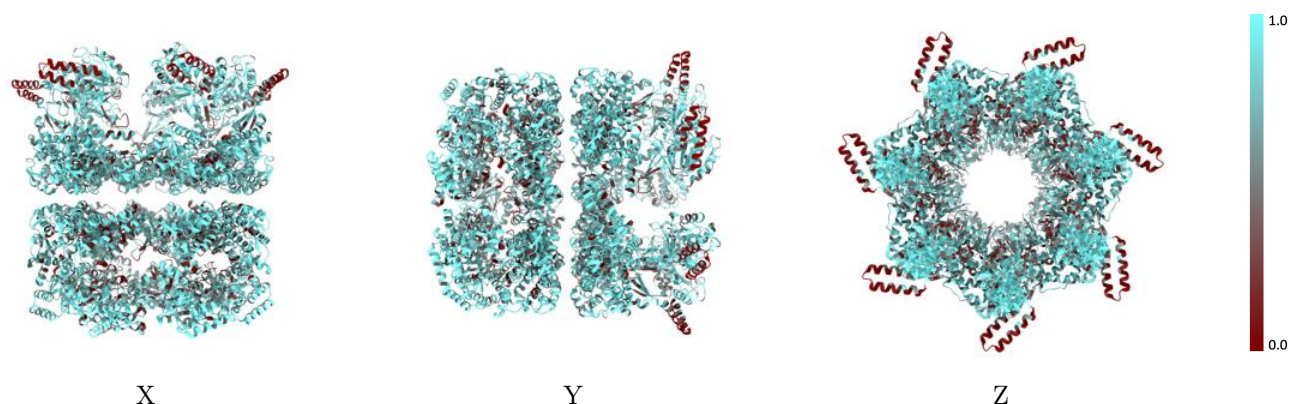
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



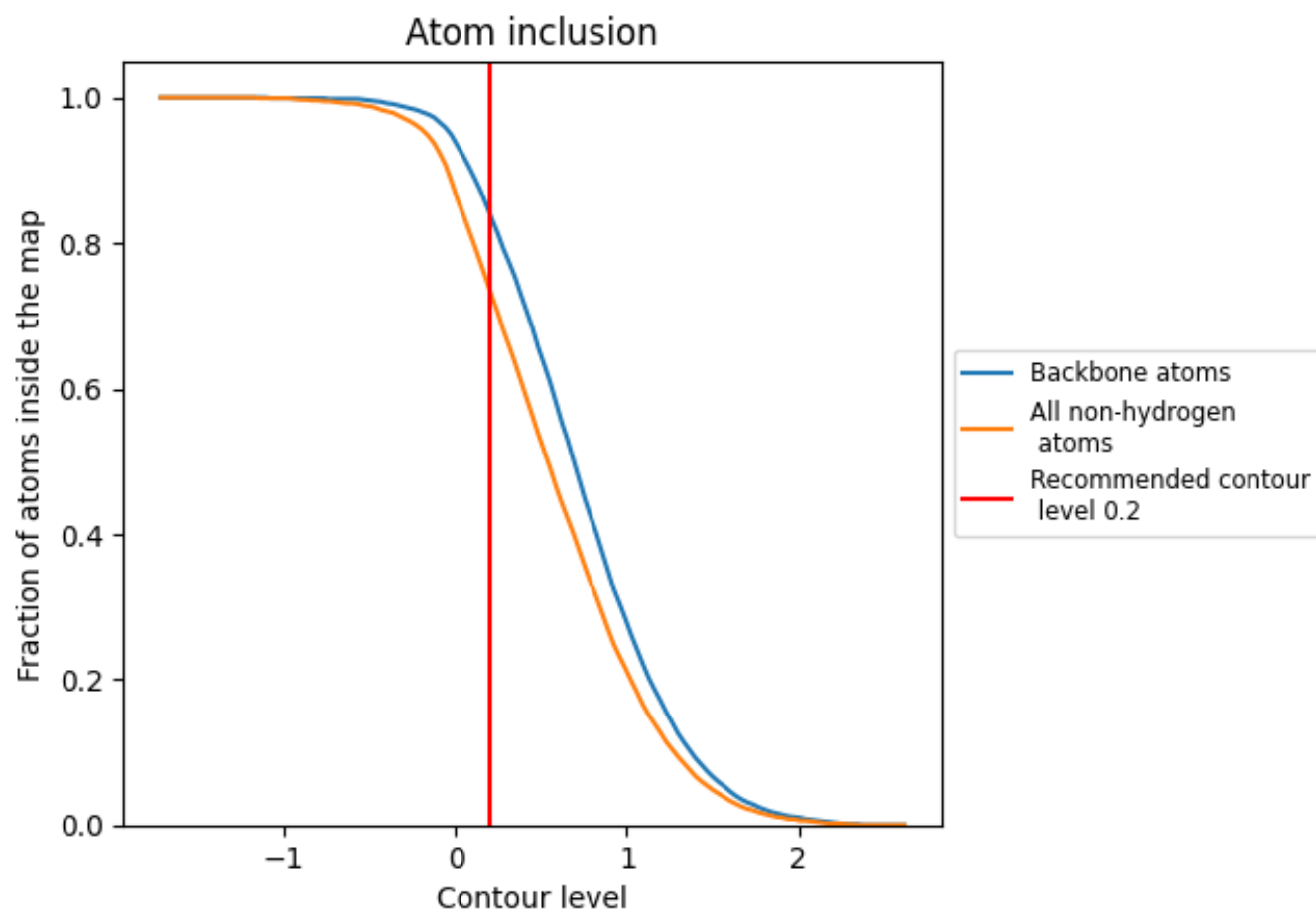
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 84% of all backbone atoms, 74% 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	0.7370	0.0790
A	0.7430	0.0740
B	0.7410	0.0760
C	0.7430	0.0750
D	0.7420	0.0750
E	0.7410	0.0730
F	0.7420	0.0730
G	0.7430	0.0740
H	0.7300	0.0860
I	0.7330	0.0860
J	0.7350	0.0860
K	0.7260	0.0800
L	0.7360	0.0850
M	0.7300	0.0820
N	0.7380	0.0860

