



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:14 PM UTC

PDB ID : 4AB2 / pdb_00004ab2
EMDB ID : EMD-2002
Title : ATP-triggered molecular mechanics of the chaperonin GroEL
Authors : Clare, D.K.; Vasishtan, D.; Stagg, S.; Quispe, J.; Farr, G.W.; Topf, M.; Horwich, A.L.; Saibil, H.R.
Deposited on : 2011-12-06
Resolution : 8.50 Å(reported)
Based on initial model : 1OEL

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

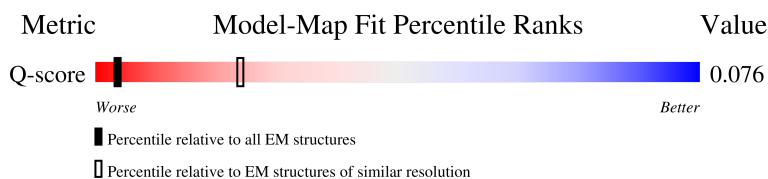
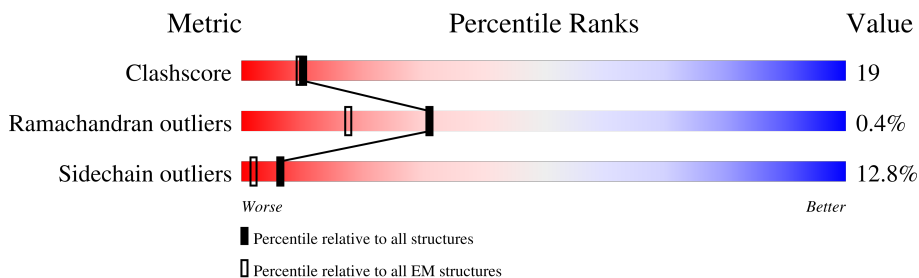
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	548	15% 49% 31% 14% • •
1	B	548	16% 49% 30% 15% • •
1	C	548	15% 49% 31% 15% • •
1	D	548	15% 50% 30% 15% • •

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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
4	PO4	A	1528	-	-	X	-
4	PO4	B	1528	-	-	X	-
4	PO4	C	1528	-	-	X	-
4	PO4	D	1528	-	-	X	-
4	PO4	E	1528	-	-	X	-
4	PO4	F	1528	-	-	X	-
4	PO4	G	1528	-	-	X	-
4	PO4	H	1528	-	-	X	-
4	PO4	I	1528	-	-	X	-
4	PO4	J	1528	-	-	X	-
4	PO4	K	1528	-	-	X	-
4	PO4	L	1528	-	-	X	-
4	PO4	M	1528	-	-	X	-
4	PO4	N	1528	-	-	X	-

2 Entry composition [i](#)

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

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 60 KDA CHAPERONIN.

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

There are 14 discrepancies between the modelled and reference sequences:

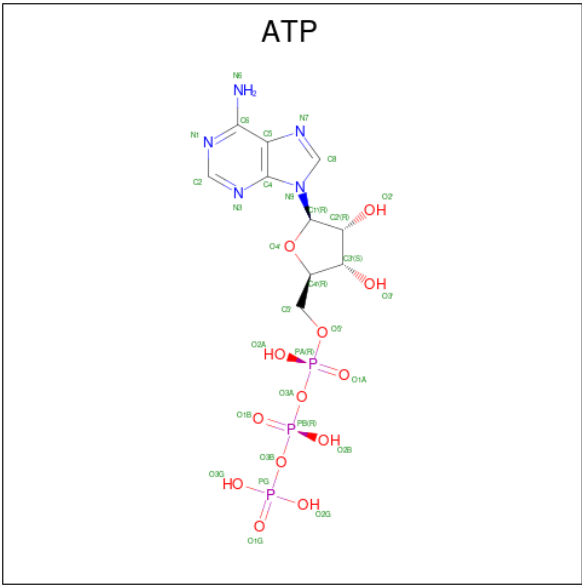
Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	engineered mutation	UNP P0A6F5
B	398	ALA	ASP	engineered mutation	UNP P0A6F5

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

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	E	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

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

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

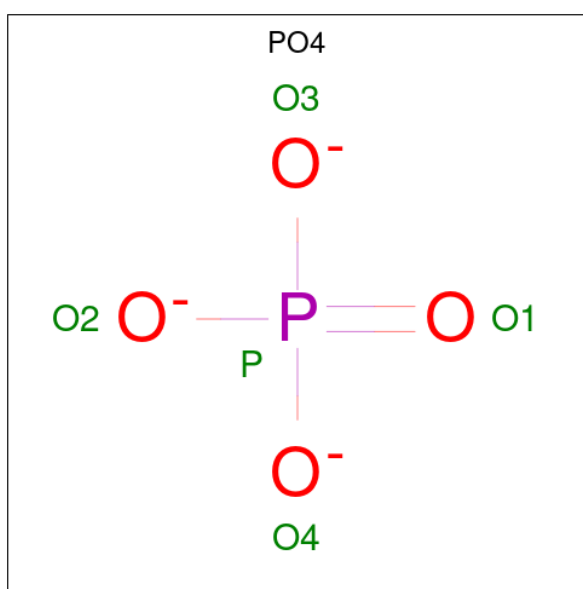
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Mg 1	0
3	B	1	Total 1	Mg 1	0
3	C	1	Total 1	Mg 1	0
3	D	1	Total 1	Mg 1	0
3	E	1	Total 1	Mg 1	0
3	F	1	Total 1	Mg 1	0
3	G	1	Total 1	Mg 1	0
3	H	1	Total 1	Mg 1	0
3	I	1	Total 1	Mg 1	0
3	J	1	Total 1	Mg 1	0

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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

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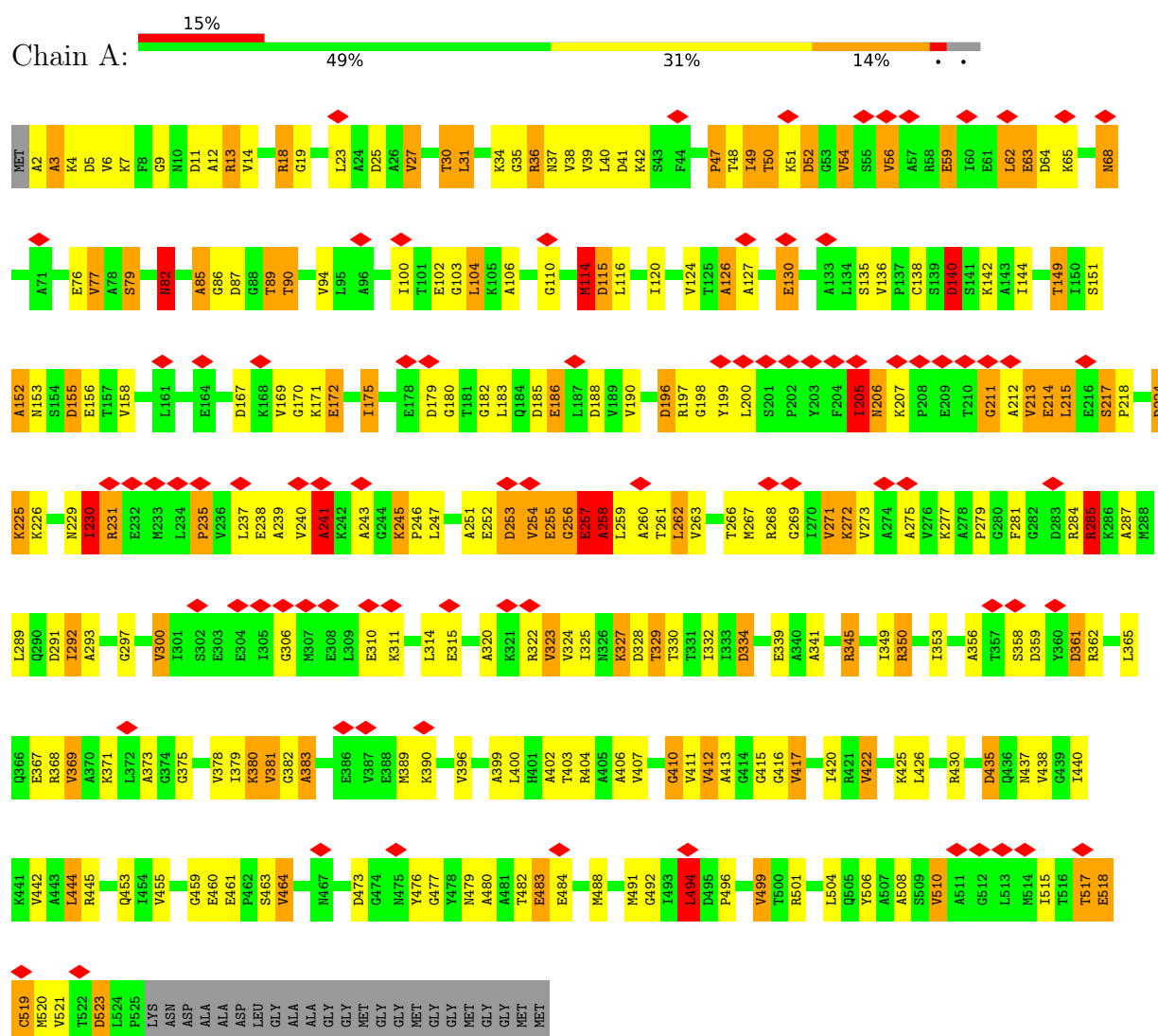
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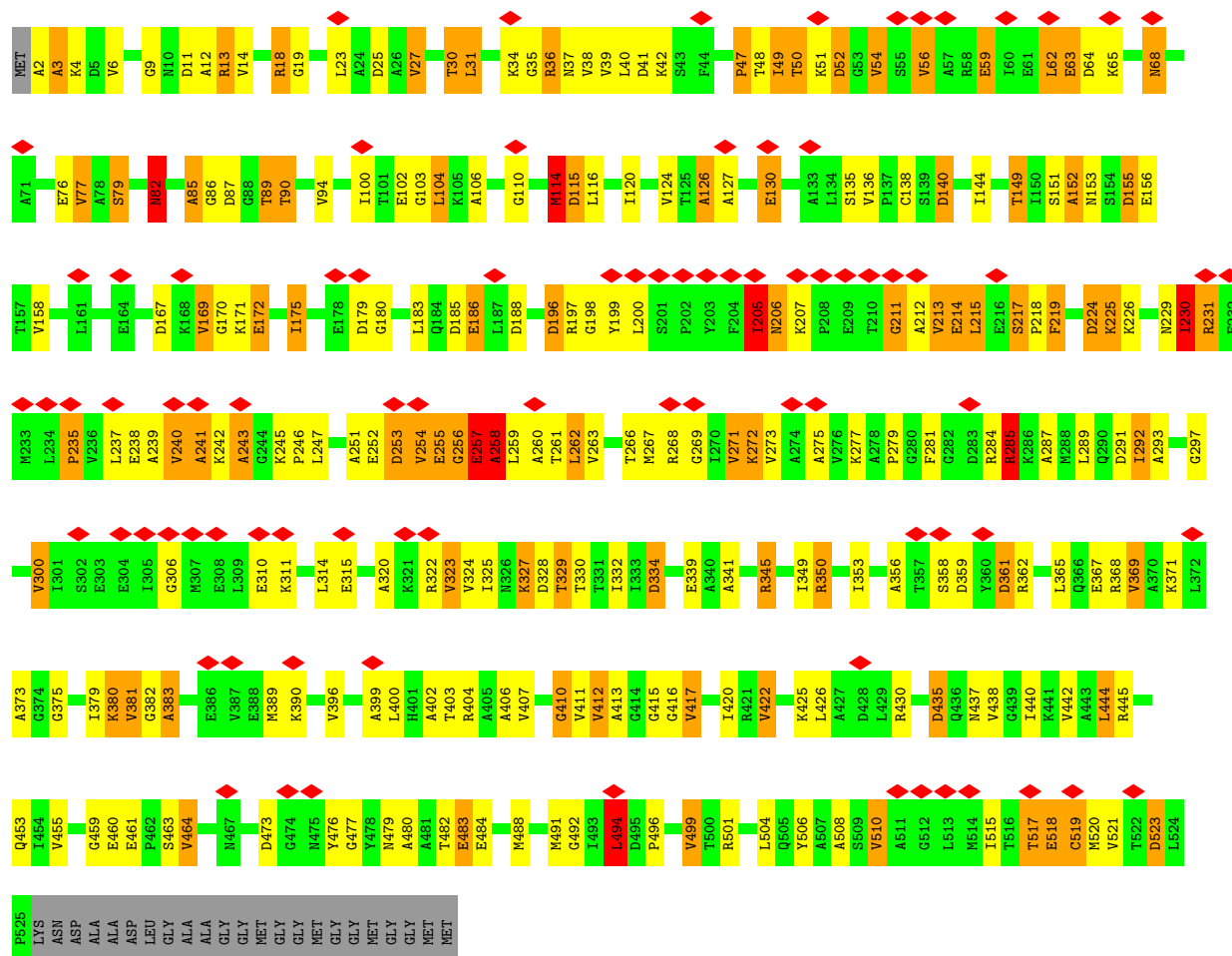
Mol	Chain	Residues	Atoms		AltConf
4	H	1	Total 1	P 1	0
4	I	1	Total 1	P 1	0
4	J	1	Total 1	P 1	0
4	K	1	Total 1	P 1	0
4	L	1	Total 1	P 1	0
4	M	1	Total 1	P 1	0
4	N	1	Total 1	P 1	0

3 Residue-property plots

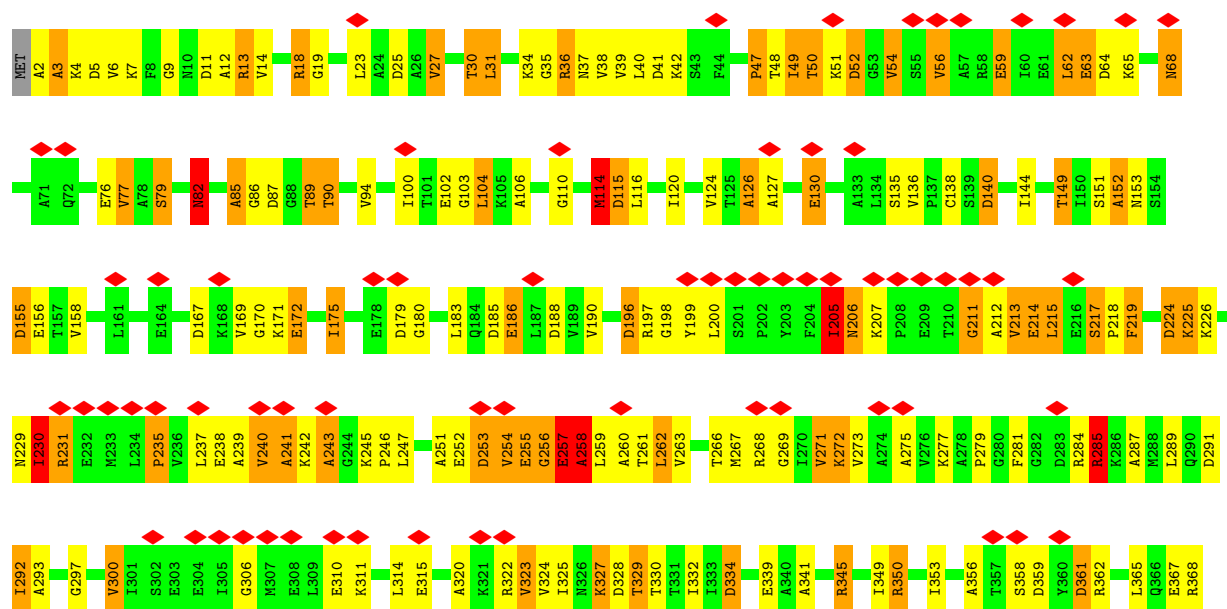
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

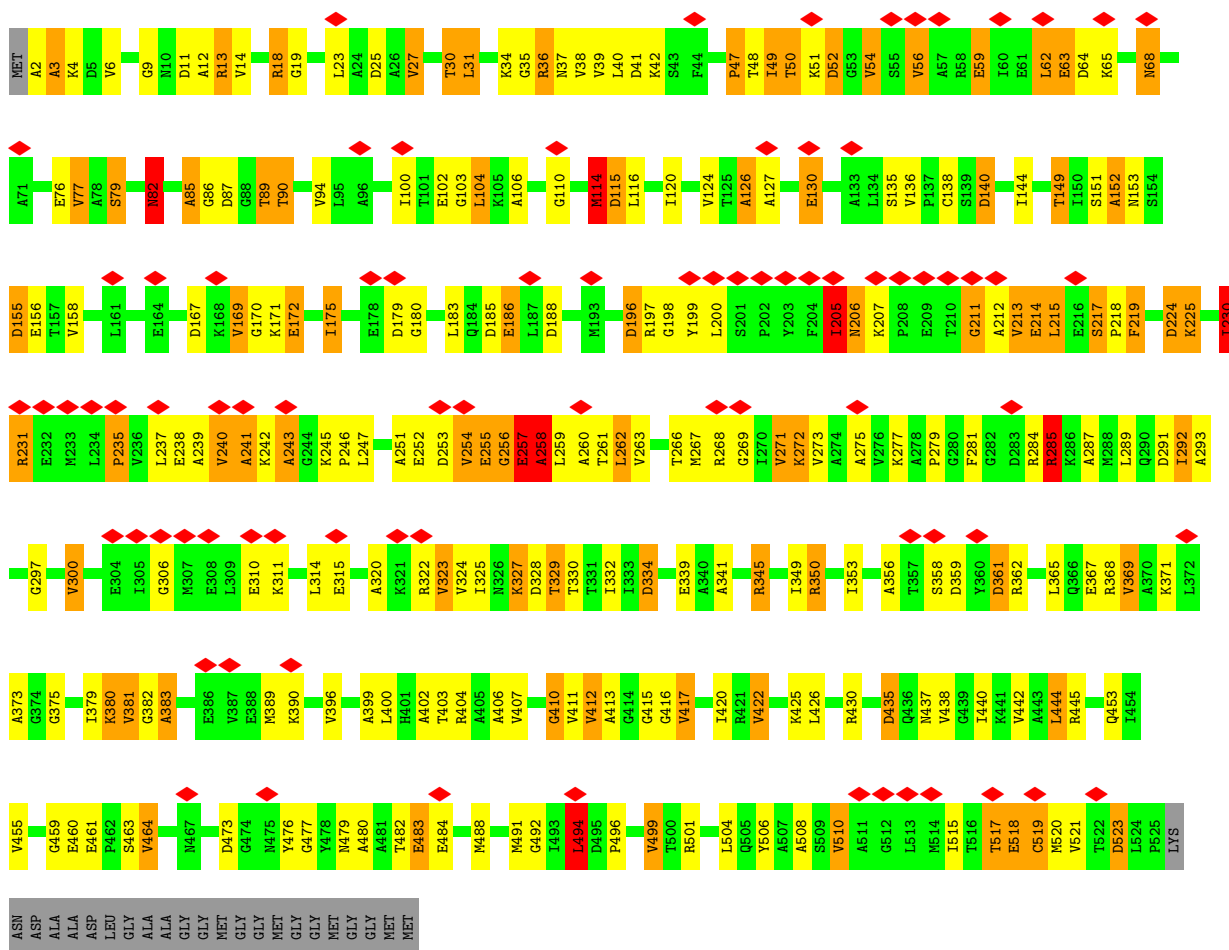




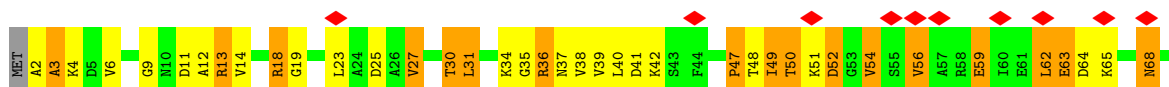
• Molecule 1: 60 KDA CHAPERONIN

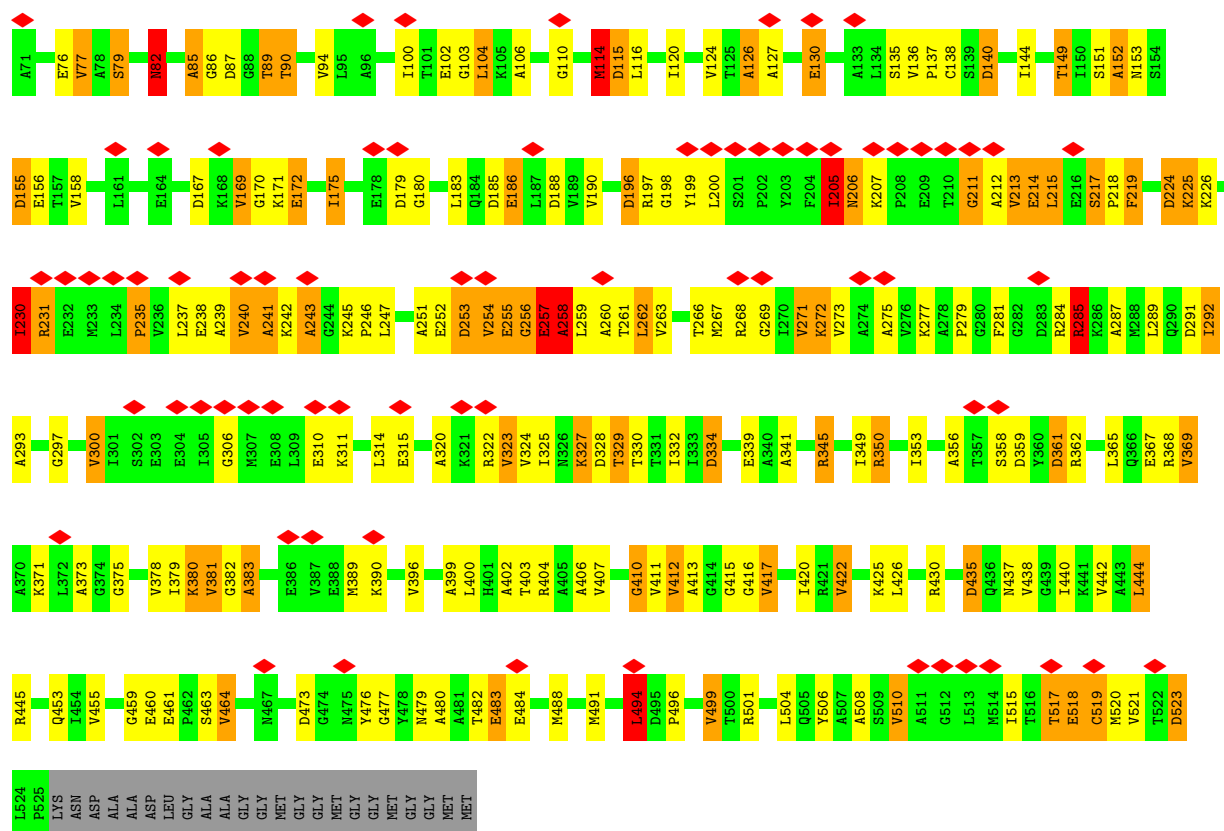


● Molecule 1: 60 KDA CHAPERONIN

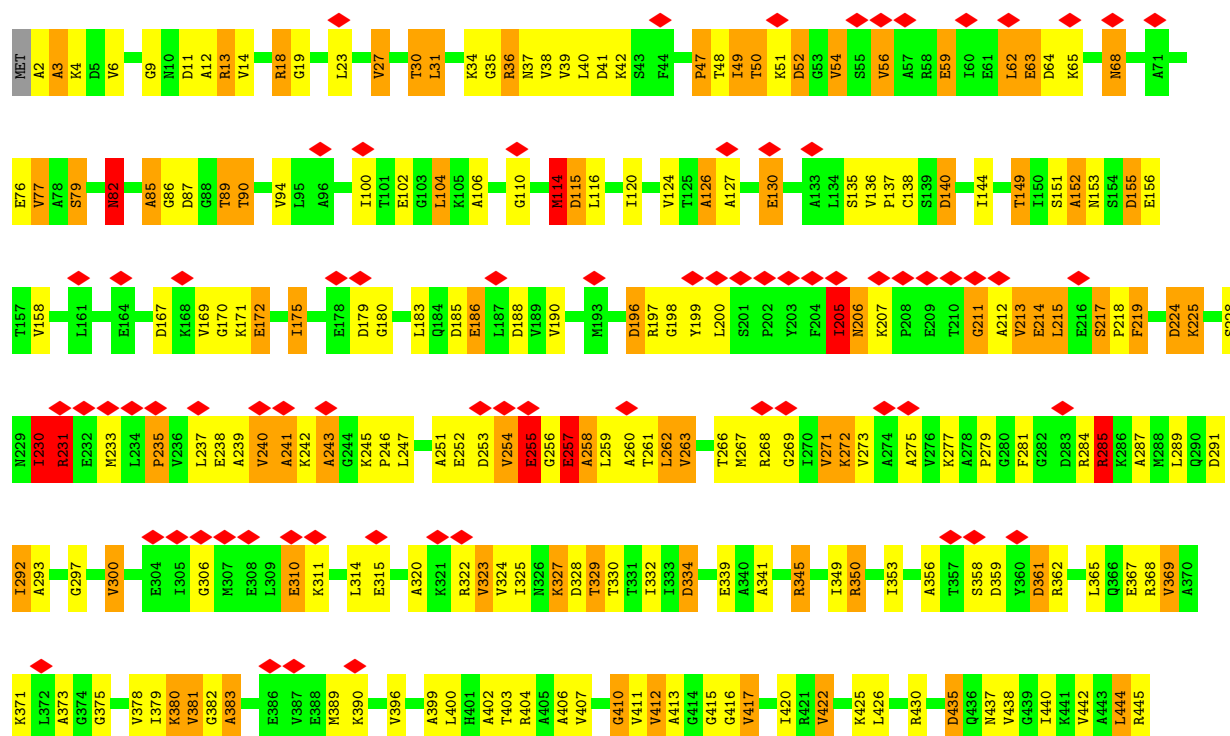


● Molecule 1: 60 KDA CHAPERONIN

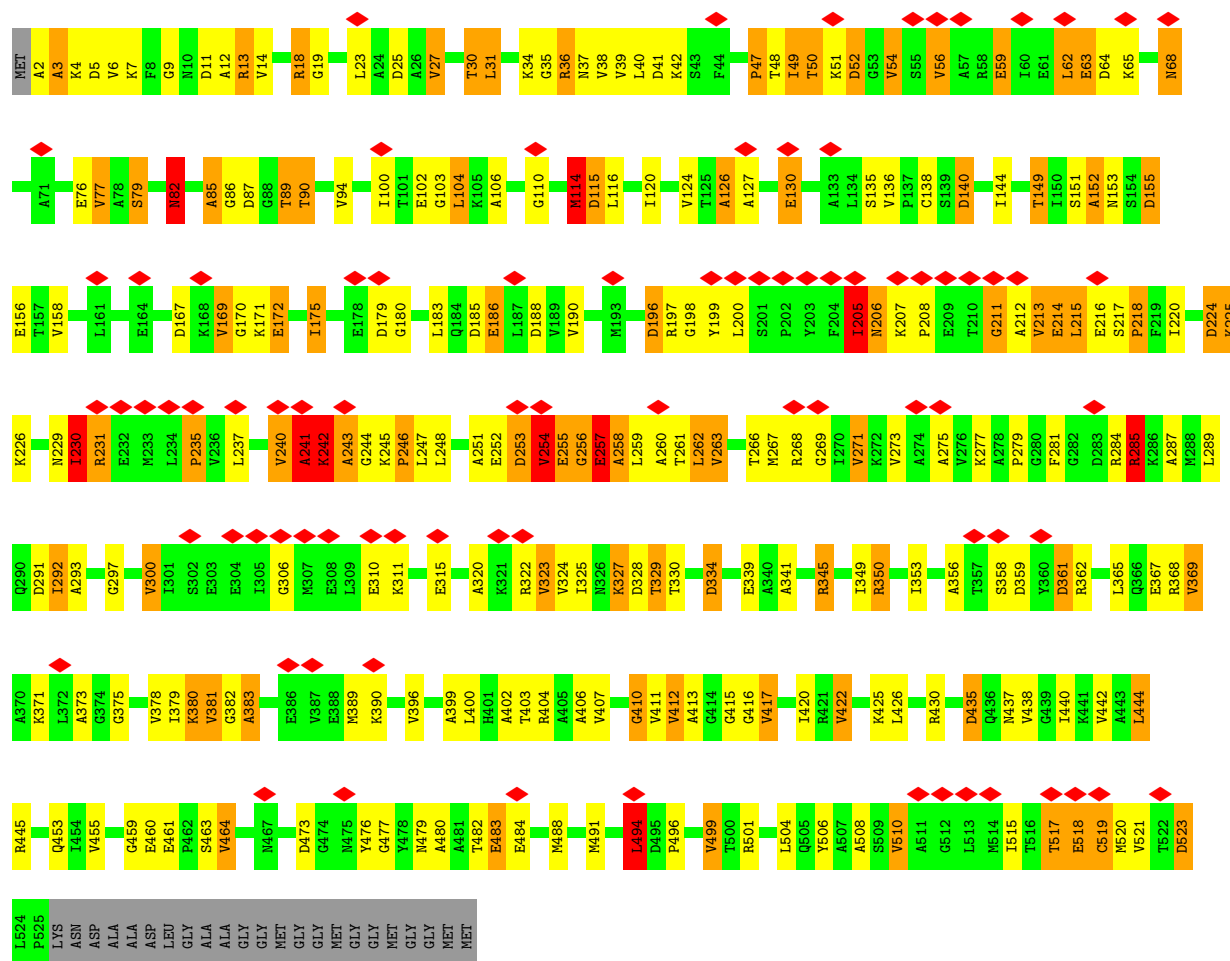




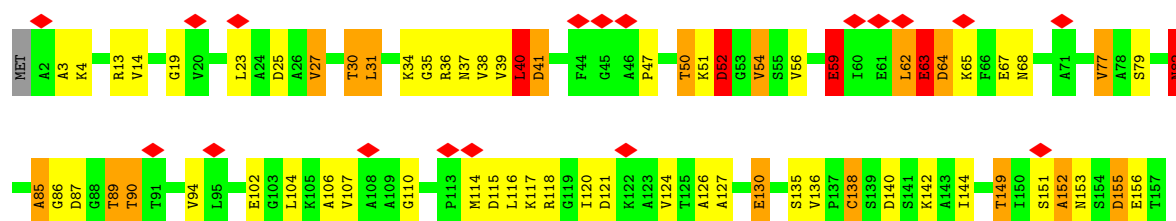
• Molecule 1: 60 KDA CHAPERONIN

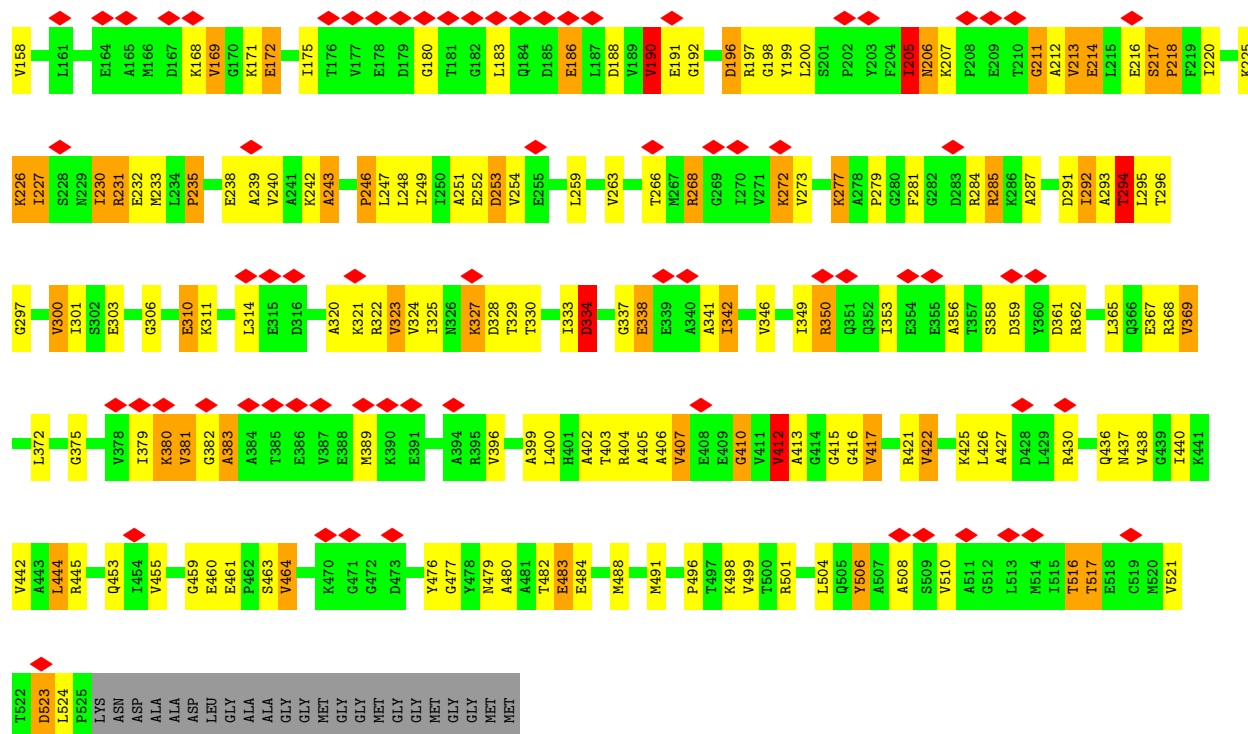


● Molecule 1: 60 KDA CHAPERONIN

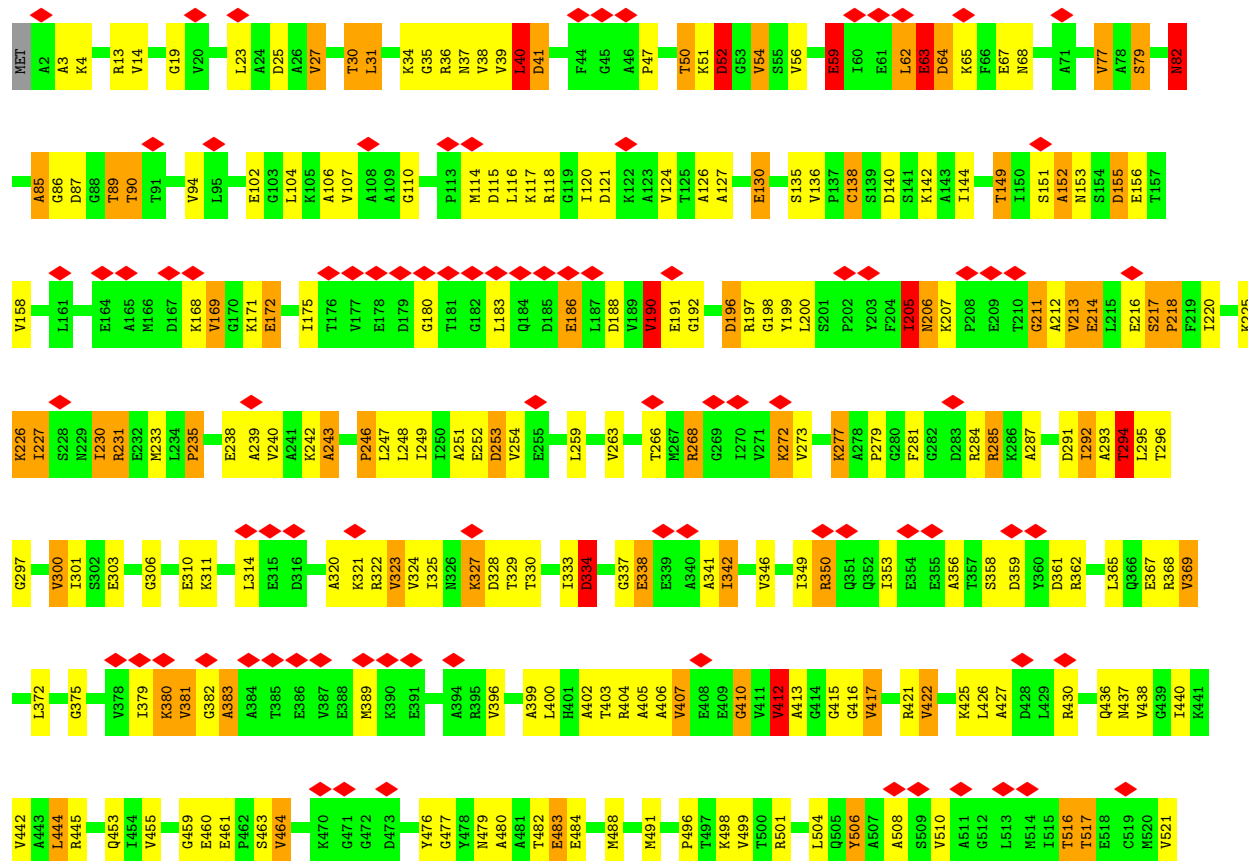


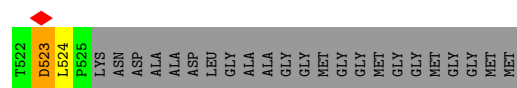
● Molecule 1: 60 KDA CHAPERONIN



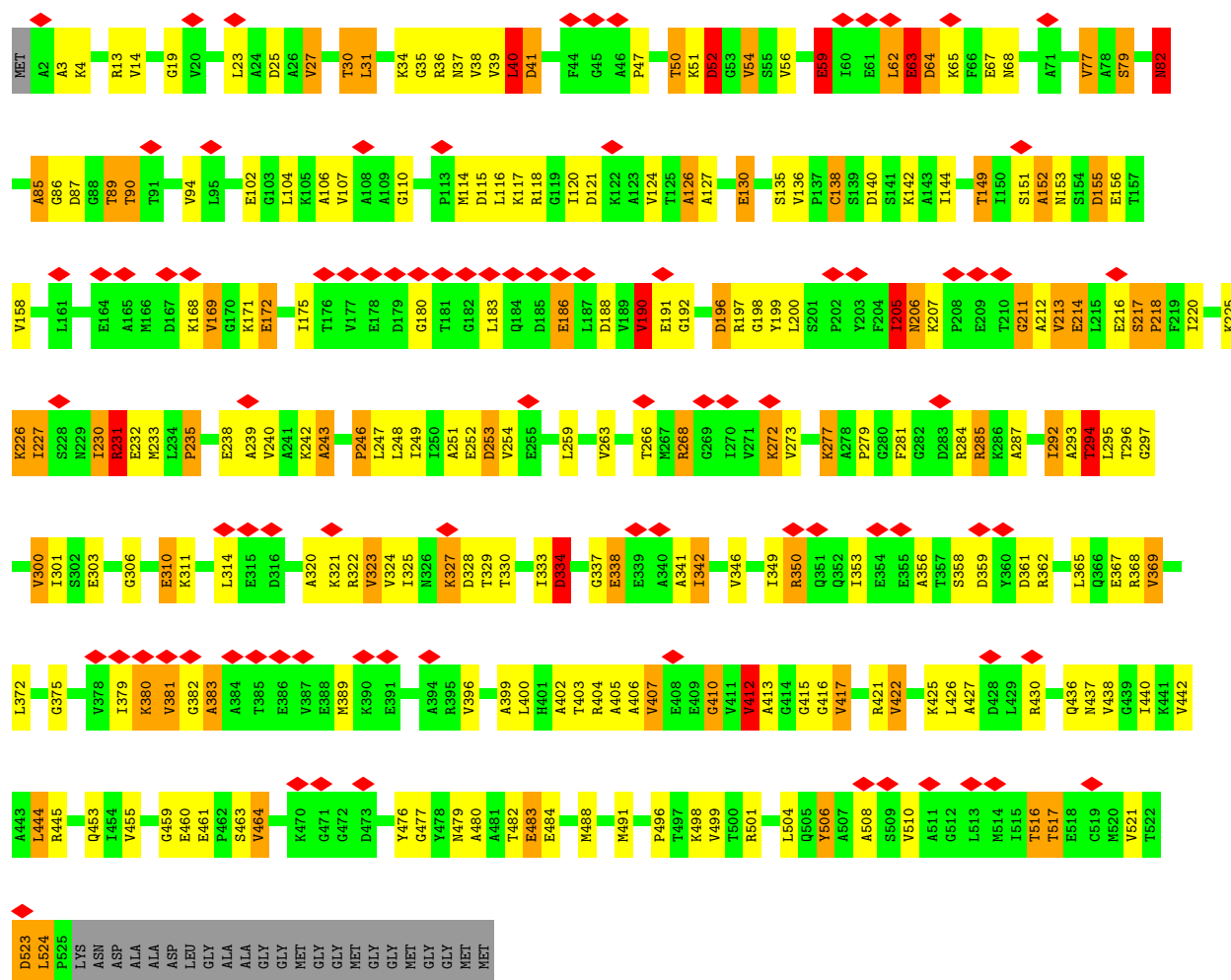


• Molecule 1: 60 KDA CHAPERONIN

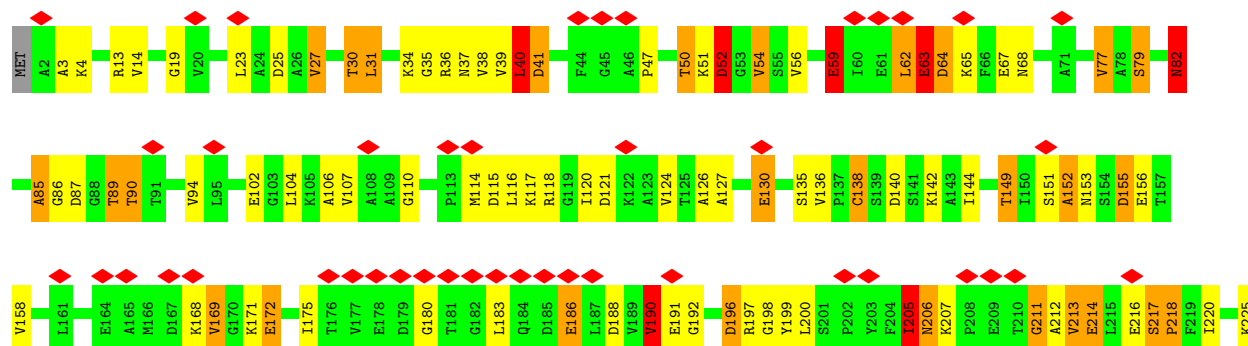




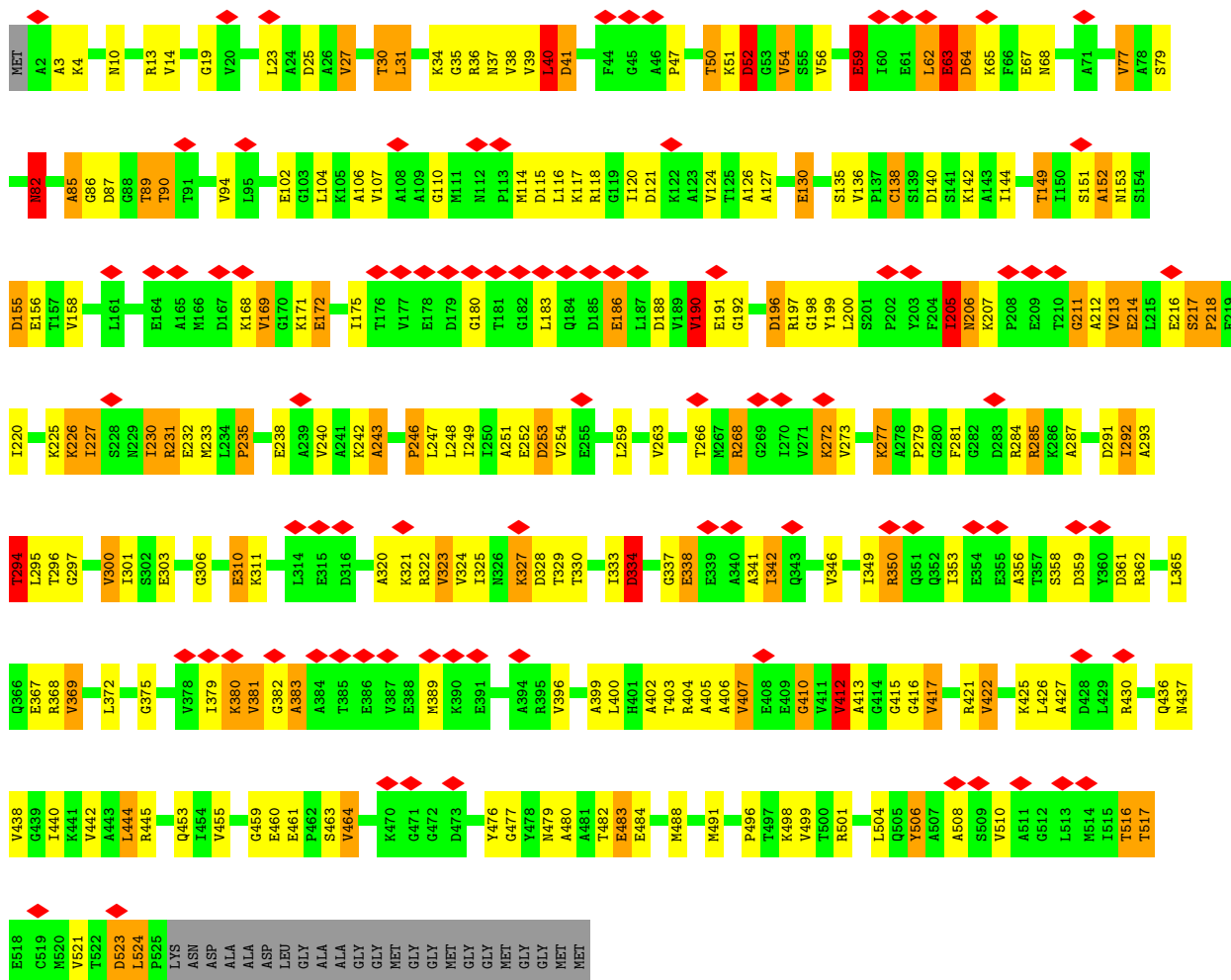
• Molecule 1: 60 KDA CHAPERONIN



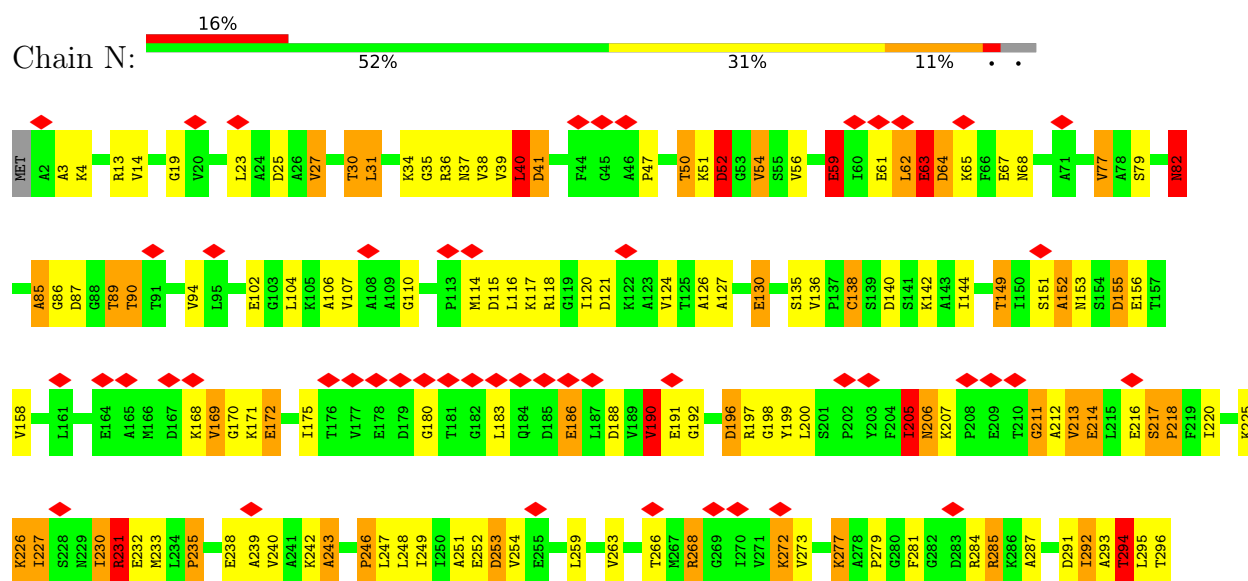
• Molecule 1: 60 KDA CHAPERONIN



- Molecule 1: 60 KDA CHAPERONIN



Chain M: 16% 52% 30% 11% . .





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D7	Depositor
Number of particles used	6500	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	3.092	Depositor
Minimum map value	-1.817	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.109	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: MG, ATP, PO4

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	1.49	2/3873 (0.1%)	1.95	142/5229 (2.7%)
1	B	1.49	2/3873 (0.1%)	1.95	143/5229 (2.7%)
1	C	1.49	2/3873 (0.1%)	1.95	143/5229 (2.7%)
1	D	1.49	2/3873 (0.1%)	1.95	143/5229 (2.7%)
1	E	1.49	2/3873 (0.1%)	1.95	142/5229 (2.7%)
1	F	1.49	1/3873 (0.0%)	1.94	138/5229 (2.6%)
1	G	1.49	3/3873 (0.1%)	1.94	141/5229 (2.7%)
1	H	1.48	1/3873 (0.0%)	1.86	116/5229 (2.2%)
1	I	1.48	1/3873 (0.0%)	1.86	118/5229 (2.3%)
1	J	1.48	2/3873 (0.1%)	1.86	119/5229 (2.3%)
1	K	1.48	1/3873 (0.0%)	1.86	117/5229 (2.2%)
1	L	1.48	2/3873 (0.1%)	1.86	118/5229 (2.3%)
1	M	1.48	1/3873 (0.0%)	1.86	118/5229 (2.3%)
1	N	1.48	1/3873 (0.0%)	1.86	118/5229 (2.3%)
All	All	1.48	23/54222 (0.0%)	1.91	1816/73206 (2.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	11
1	C	0	11
1	D	0	11
1	E	0	11
1	F	1	12
1	G	0	12
1	H	0	8
1	I	0	8

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

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	GLU	CA-CB	9.56	1.68	1.53
1	F	63	GLU	CA-CB	9.51	1.68	1.53
1	G	63	GLU	CA-CB	9.51	1.68	1.53
1	B	63	GLU	CA-CB	9.50	1.68	1.53
1	A	63	GLU	CA-CB	9.50	1.68	1.53
1	E	63	GLU	CA-CB	9.49	1.68	1.53
1	D	63	GLU	CA-CB	9.48	1.68	1.53
1	G	242	LYS	CA-CB	5.67	1.59	1.52
1	J	217	SER	CA-CB	5.53	1.56	1.52
1	L	217	SER	CA-CB	5.50	1.56	1.52
1	I	217	SER	CA-CB	5.46	1.56	1.52
1	N	217	SER	CA-CB	5.46	1.56	1.52
1	G	242	LYS	CA-C	5.43	1.59	1.53
1	H	217	SER	CA-CB	5.38	1.56	1.52
1	K	217	SER	CA-CB	5.38	1.56	1.52
1	M	217	SER	CA-CB	5.38	1.56	1.52
1	D	231	ARG	CD-NE	5.34	1.53	1.46
1	E	231	ARG	CD-NE	5.33	1.53	1.46
1	C	231	ARG	CD-NE	5.31	1.53	1.46
1	A	231	ARG	CD-NE	5.30	1.53	1.46
1	B	231	ARG	CD-NE	5.29	1.53	1.46
1	L	524	LEU	C-N	-5.05	1.26	1.34
1	J	524	LEU	C-N	-5.03	1.26	1.34

All (1816) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	63	GLU	N-CA-CB	-22.43	77.15	110.12
1	F	63	GLU	N-CA-CB	-22.42	77.16	110.12
1	A	63	GLU	N-CA-CB	-22.42	77.16	110.12
1	C	63	GLU	N-CA-CB	-22.42	77.17	110.12
1	E	63	GLU	N-CA-CB	-22.41	77.17	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	GLU	N-CA-CB	-22.40	77.19	110.12
1	D	63	GLU	N-CA-CB	-22.39	77.21	110.12
1	A	206	ASN	CA-CB-CG	13.99	126.59	112.60
1	B	114	MET	N-CA-CB	13.99	130.68	110.12
1	C	114	MET	N-CA-CB	13.98	130.67	110.12
1	A	114	MET	N-CA-CB	13.97	130.66	110.12
1	D	114	MET	N-CA-CB	13.97	130.66	110.12
1	E	114	MET	N-CA-CB	13.97	130.65	110.12
1	G	114	MET	N-CA-CB	13.96	130.65	110.12
1	E	206	ASN	CA-CB-CG	13.96	126.56	112.60
1	F	114	MET	N-CA-CB	13.96	130.64	110.12
1	F	206	ASN	CA-CB-CG	13.92	126.52	112.60
1	D	206	ASN	CA-CB-CG	13.91	126.51	112.60
1	C	206	ASN	CA-CB-CG	13.90	126.50	112.60
1	B	206	ASN	CA-CB-CG	13.88	126.47	112.60
1	G	255	GLU	CB-CA-C	13.40	130.35	110.26
1	C	461	GLU	CB-CA-C	12.32	129.23	109.51
1	B	461	GLU	CB-CA-C	12.30	129.19	109.51
1	G	206	ASN	CA-CB-CG	12.28	124.88	112.60
1	A	461	GLU	CB-CA-C	12.22	129.06	109.51
1	G	461	GLU	CB-CA-C	12.15	128.96	109.51
1	D	461	GLU	CB-CA-C	12.15	128.95	109.51
1	D	230	ILE	CB-CA-C	-12.10	95.81	112.14
1	F	461	GLU	CB-CA-C	12.09	128.85	109.51
1	E	461	GLU	CB-CA-C	12.08	128.84	109.51
1	E	230	ILE	CB-CA-C	-12.08	95.84	112.14
1	C	230	ILE	CB-CA-C	-12.07	95.84	112.14
1	B	230	ILE	CB-CA-C	-12.07	95.84	112.14
1	A	230	ILE	CB-CA-C	-12.05	95.88	112.14
1	L	140	ASP	CA-CB-CG	11.75	124.35	112.60
1	H	140	ASP	CA-CB-CG	11.74	124.34	112.60
1	K	140	ASP	CA-CB-CG	11.74	124.34	112.60
1	J	140	ASP	CA-CB-CG	11.72	124.32	112.60
1	M	140	ASP	CA-CB-CG	11.72	124.32	112.60
1	I	140	ASP	CA-CB-CG	11.70	124.30	112.60
1	N	140	ASP	CA-CB-CG	11.68	124.28	112.60
1	C	231	ARG	CB-CA-C	-11.33	91.99	110.79
1	E	231	ARG	CB-CA-C	-11.32	91.99	110.79
1	A	231	ARG	CB-CA-C	-11.30	92.02	110.79
1	B	231	ARG	CB-CA-C	-11.30	92.03	110.79
1	D	231	ARG	CB-CA-C	-11.29	92.06	110.79
1	I	353	ILE	CB-CA-C	-10.96	97.94	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	353	ILE	CB-CA-C	-10.96	97.94	111.97
1	M	353	ILE	CB-CA-C	-10.95	97.96	111.97
1	J	353	ILE	CB-CA-C	-10.95	97.96	111.97
1	N	353	ILE	CB-CA-C	-10.94	97.97	111.97
1	G	230	ILE	CB-CA-C	-10.94	97.38	112.14
1	H	353	ILE	CB-CA-C	-10.93	97.98	111.97
1	K	353	ILE	CB-CA-C	-10.93	97.98	111.97
1	M	334	ASP	CA-CB-CG	10.56	123.16	112.60
1	N	334	ASP	CA-CB-CG	10.53	123.12	112.60
1	H	334	ASP	CA-CB-CG	10.52	123.12	112.60
1	K	334	ASP	CA-CB-CG	10.49	123.09	112.60
1	D	353	ILE	CB-CA-C	-10.49	98.54	111.97
1	J	334	ASP	CA-CB-CG	10.49	123.09	112.60
1	I	334	ASP	CA-CB-CG	10.49	123.09	112.60
1	L	334	ASP	CA-CB-CG	10.47	123.07	112.60
1	B	353	ILE	CB-CA-C	-10.45	98.59	111.97
1	E	353	ILE	CB-CA-C	-10.45	98.60	111.97
1	G	353	ILE	CB-CA-C	-10.43	98.62	111.97
1	C	353	ILE	CB-CA-C	-10.41	98.64	111.97
1	A	353	ILE	CB-CA-C	-10.40	98.65	111.97
1	F	353	ILE	CB-CA-C	-10.39	98.67	111.97
1	G	261	THR	N-CA-CB	10.18	124.84	110.07
1	M	115	ASP	CB-CA-C	9.89	127.21	110.79
1	H	115	ASP	CB-CA-C	9.89	127.20	110.79
1	I	115	ASP	CB-CA-C	9.89	127.20	110.79
1	L	115	ASP	CB-CA-C	9.88	127.19	110.79
1	J	115	ASP	CB-CA-C	9.87	127.18	110.79
1	N	115	ASP	CB-CA-C	9.86	127.16	110.79
1	K	115	ASP	CB-CA-C	9.86	127.15	110.79
1	B	261	THR	N-CA-CB	9.83	124.27	110.01
1	A	261	THR	N-CA-CB	9.82	124.25	110.01
1	E	261	THR	N-CA-CB	9.82	124.25	110.01
1	C	261	THR	N-CA-CB	9.80	124.22	110.01
1	A	285	ARG	CB-CA-C	-9.80	94.53	110.79
1	D	261	THR	N-CA-CB	9.79	124.21	110.01
1	D	285	ARG	CB-CA-C	-9.79	94.53	110.79
1	B	285	ARG	CB-CA-C	-9.79	94.54	110.79
1	E	285	ARG	CB-CA-C	-9.78	94.55	110.79
1	F	285	ARG	CB-CA-C	-9.77	94.57	110.79
1	J	369	VAL	N-CA-CB	9.77	123.83	110.54
1	G	285	ARG	CB-CA-C	-9.76	94.59	110.79
1	N	369	VAL	N-CA-CB	9.74	123.79	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	ARG	CB-CA-C	-9.74	94.62	110.79
1	H	369	VAL	N-CA-CB	9.73	123.77	110.54
1	L	369	VAL	N-CA-CB	9.73	123.77	110.54
1	H	285	ARG	CB-CA-C	-9.71	94.67	110.79
1	K	369	VAL	N-CA-CB	9.71	123.75	110.54
1	L	483	GLU	CB-CG-CD	9.71	129.11	112.60
1	K	285	ARG	CB-CA-C	-9.71	94.67	110.79
1	M	369	VAL	N-CA-CB	9.71	123.75	110.54
1	J	483	GLU	CB-CG-CD	9.70	129.09	112.60
1	I	369	VAL	N-CA-CB	9.70	123.73	110.54
1	M	285	ARG	CB-CA-C	-9.69	94.71	110.79
1	K	483	GLU	CB-CG-CD	9.69	129.07	112.60
1	H	483	GLU	CB-CG-CD	9.68	129.06	112.60
1	N	285	ARG	CB-CA-C	-9.68	94.73	110.79
1	I	285	ARG	CB-CA-C	-9.67	94.73	110.79
1	J	285	ARG	CB-CA-C	-9.67	94.74	110.79
1	N	483	GLU	CB-CG-CD	9.67	129.03	112.60
1	I	51	LYS	N-CA-CB	9.66	126.82	110.49
1	I	483	GLU	CB-CG-CD	9.66	129.03	112.60
1	L	285	ARG	CB-CA-C	-9.66	94.75	110.79
1	M	483	GLU	CB-CG-CD	9.66	129.03	112.60
1	H	51	LYS	N-CA-CB	9.66	126.81	110.49
1	J	51	LYS	N-CA-CB	9.66	126.81	110.49
1	M	51	LYS	N-CA-CB	9.66	126.81	110.49
1	K	51	LYS	N-CA-CB	9.66	126.81	110.49
1	L	51	LYS	N-CA-CB	9.64	126.78	110.49
1	N	51	LYS	N-CA-CB	9.63	126.76	110.49
1	F	261	THR	N-CA-CB	9.52	123.87	110.07
1	M	383	ALA	N-CA-CB	9.52	126.31	111.56
1	N	383	ALA	N-CA-CB	9.51	126.31	111.56
1	K	383	ALA	N-CA-CB	9.51	126.30	111.56
1	H	383	ALA	N-CA-CB	9.50	126.28	111.56
1	I	383	ALA	N-CA-CB	9.49	126.27	111.56
1	J	383	ALA	N-CA-CB	9.48	126.25	111.56
1	L	383	ALA	N-CA-CB	9.47	126.24	111.56
1	F	255	GLU	CB-CA-C	9.46	125.81	110.29
1	K	510	VAL	CB-CA-C	-9.46	99.86	111.97
1	M	510	VAL	CB-CA-C	-9.46	99.86	111.97
1	N	510	VAL	CB-CA-C	-9.45	99.87	111.97
1	L	510	VAL	CB-CA-C	-9.44	99.89	111.97
1	I	510	VAL	CB-CA-C	-9.43	99.90	111.97
1	H	510	VAL	CB-CA-C	-9.43	99.90	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	510	VAL	CB-CA-C	-9.43	99.91	111.97
1	C	383	ALA	N-CA-CB	9.16	125.75	111.56
1	D	383	ALA	N-CA-CB	9.15	125.74	111.56
1	E	383	ALA	N-CA-CB	9.15	125.74	111.56
1	G	383	ALA	N-CA-CB	9.15	125.74	111.56
1	F	383	ALA	N-CA-CB	9.14	125.73	111.56
1	B	383	ALA	N-CA-CB	9.13	125.72	111.56
1	F	115	ASP	CB-CA-C	9.12	125.93	110.79
1	C	115	ASP	CB-CA-C	9.11	125.91	110.79
1	B	115	ASP	CB-CA-C	9.10	125.90	110.79
1	A	383	ALA	N-CA-CB	9.10	125.67	111.56
1	B	510	VAL	CB-CA-C	-9.10	100.33	111.97
1	G	115	ASP	CB-CA-C	9.10	125.89	110.79
1	E	115	ASP	CB-CA-C	9.10	125.89	110.79
1	A	510	VAL	CB-CA-C	-9.09	100.33	111.97
1	G	510	VAL	CB-CA-C	-9.09	100.34	111.97
1	F	510	VAL	CB-CA-C	-9.08	100.34	111.97
1	J	82	ASN	CA-CB-CG	9.08	121.68	112.60
1	C	510	VAL	CB-CA-C	-9.08	100.34	111.97
1	D	510	VAL	CB-CA-C	-9.08	100.35	111.97
1	D	115	ASP	CB-CA-C	9.08	125.86	110.79
1	A	115	ASP	CB-CA-C	9.07	125.86	110.79
1	E	510	VAL	CB-CA-C	-9.06	100.37	111.97
1	N	82	ASN	CA-CB-CG	9.04	121.64	112.60
1	G	369	VAL	N-CA-CB	9.03	122.82	110.54
1	E	369	VAL	N-CA-CB	9.03	122.81	110.54
1	M	82	ASN	CA-CB-CG	9.03	121.63	112.60
1	K	82	ASN	CA-CB-CG	9.02	121.62	112.60
1	H	82	ASN	CA-CB-CG	9.02	121.61	112.60
1	I	82	ASN	CA-CB-CG	9.01	121.61	112.60
1	B	369	VAL	N-CA-CB	9.00	122.78	110.54
1	F	369	VAL	N-CA-CB	9.00	122.78	110.54
1	C	369	VAL	N-CA-CB	8.99	122.77	110.54
1	D	369	VAL	N-CA-CB	8.99	122.77	110.54
1	A	369	VAL	N-CA-CB	8.99	122.77	110.54
1	L	82	ASN	CA-CB-CG	8.96	121.56	112.60
1	H	41	ASP	CA-CB-CG	8.96	121.56	112.60
1	J	41	ASP	CA-CB-CG	8.92	121.52	112.60
1	C	230	ILE	N-CA-CB	8.91	122.65	110.54
1	M	41	ASP	CA-CB-CG	8.90	121.50	112.60
1	I	41	ASP	CA-CB-CG	8.90	121.50	112.60
1	K	41	ASP	CA-CB-CG	8.89	121.49	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ILE	N-CA-CB	8.88	122.61	110.54
1	L	41	ASP	CA-CB-CG	8.87	121.47	112.60
1	E	230	ILE	N-CA-CB	8.86	122.59	110.54
1	N	41	ASP	CA-CB-CG	8.86	121.46	112.60
1	B	230	ILE	N-CA-CB	8.85	122.58	110.54
1	E	482	THR	N-CA-CB	8.85	123.25	110.16
1	A	482	THR	N-CA-CB	8.84	123.24	110.16
1	C	482	THR	N-CA-CB	8.84	123.24	110.16
1	D	230	ILE	N-CA-CB	8.83	122.55	110.54
1	B	482	THR	N-CA-CB	8.83	123.23	110.16
1	G	482	THR	N-CA-CB	8.82	123.22	110.16
1	D	482	THR	N-CA-CB	8.81	123.20	110.16
1	F	482	THR	N-CA-CB	8.80	123.18	110.16
1	C	266	THR	N-CA-CB	8.76	122.78	110.07
1	E	266	THR	N-CA-CB	8.76	122.77	110.07
1	B	266	THR	N-CA-CB	8.74	122.75	110.07
1	D	266	THR	N-CA-CB	8.74	122.75	110.07
1	A	266	THR	N-CA-CB	8.74	122.74	110.07
1	H	482	THR	N-CA-CB	8.71	123.05	110.16
1	L	482	THR	N-CA-CB	8.69	123.02	110.16
1	N	482	THR	N-CA-CB	8.68	123.01	110.16
1	M	482	THR	N-CA-CB	8.68	123.00	110.16
1	J	482	THR	N-CA-CB	8.67	122.99	110.16
1	K	482	THR	N-CA-CB	8.67	122.99	110.16
1	I	482	THR	N-CA-CB	8.64	122.95	110.16
1	J	34	LYS	CB-CA-C	8.62	125.50	110.85
1	I	34	LYS	CB-CA-C	8.60	125.47	110.85
1	L	34	LYS	CB-CA-C	8.60	125.47	110.85
1	M	34	LYS	CB-CA-C	8.60	125.47	110.85
1	K	34	LYS	CB-CA-C	8.59	125.45	110.85
1	H	34	LYS	CB-CA-C	8.59	125.45	110.85
1	C	510	VAL	N-CA-CB	8.57	120.58	110.55
1	B	510	VAL	N-CA-CB	8.57	120.57	110.55
1	N	34	LYS	CB-CA-C	8.57	125.42	110.85
1	G	510	VAL	N-CA-CB	8.56	120.56	110.55
1	A	510	VAL	N-CA-CB	8.56	120.56	110.55
1	E	510	VAL	N-CA-CB	8.53	120.53	110.55
1	F	510	VAL	N-CA-CB	8.51	120.51	110.55
1	D	510	VAL	N-CA-CB	8.50	120.50	110.55
1	D	231	ARG	CA-CB-CG	8.48	131.06	114.10
1	B	231	ARG	CA-CB-CG	8.46	131.02	114.10
1	C	231	ARG	CA-CB-CG	8.43	130.96	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	257	GLU	CB-CA-C	8.43	126.12	110.10
1	A	231	ARG	CA-CB-CG	8.43	130.96	114.10
1	K	367	GLU	CB-CA-C	-8.43	96.80	110.79
1	E	231	ARG	CA-CB-CG	8.43	130.95	114.10
1	J	367	GLU	CB-CA-C	-8.41	96.83	110.79
1	N	367	GLU	CB-CA-C	-8.40	96.84	110.79
1	F	82	ASN	CA-CB-CG	8.40	121.00	112.60
1	L	367	GLU	CB-CA-C	-8.40	96.85	110.79
1	M	367	GLU	CB-CA-C	-8.39	96.86	110.79
1	I	367	GLU	CB-CA-C	-8.39	96.86	110.79
1	H	367	GLU	CB-CA-C	-8.39	96.87	110.79
1	G	82	ASN	CA-CB-CG	8.39	120.99	112.60
1	J	235	PRO	CB-CA-C	8.38	125.29	112.21
1	K	235	PRO	CB-CA-C	8.38	125.29	112.21
1	N	235	PRO	CB-CA-C	8.38	125.28	112.21
1	M	235	PRO	CB-CA-C	8.37	125.26	112.21
1	A	82	ASN	CA-CB-CG	8.35	120.95	112.60
1	D	82	ASN	CA-CB-CG	8.34	120.94	112.60
1	H	235	PRO	CB-CA-C	8.34	125.22	112.21
1	L	235	PRO	CB-CA-C	8.34	125.22	112.21
1	N	342	ILE	CB-CA-C	-8.34	101.30	111.97
1	B	82	ASN	CA-CB-CG	8.33	120.93	112.60
1	K	342	ILE	CB-CA-C	-8.33	101.31	111.97
1	C	104	LEU	CB-CA-C	8.33	124.61	110.79
1	L	342	ILE	CB-CA-C	-8.32	101.31	111.97
1	E	104	LEU	CB-CA-C	8.32	124.61	110.79
1	M	342	ILE	CB-CA-C	-8.32	101.32	111.97
1	C	82	ASN	CA-CB-CG	8.32	120.92	112.60
1	E	82	ASN	CA-CB-CG	8.32	120.92	112.60
1	G	104	LEU	CB-CA-C	8.32	124.59	110.79
1	M	190	VAL	CB-CA-C	8.31	123.00	110.62
1	D	104	LEU	CB-CA-C	8.31	124.58	110.79
1	H	342	ILE	CB-CA-C	-8.31	101.33	111.97
1	F	104	LEU	CB-CA-C	8.30	124.57	110.79
1	I	190	VAL	CB-CA-C	8.30	122.99	110.62
1	J	342	ILE	CB-CA-C	-8.30	101.34	111.97
1	A	104	LEU	CB-CA-C	8.30	124.57	110.79
1	J	190	VAL	CB-CA-C	8.29	122.98	110.62
1	I	342	ILE	CB-CA-C	-8.29	101.36	111.97
1	B	104	LEU	CB-CA-C	8.29	124.55	110.79
1	H	190	VAL	CB-CA-C	8.29	122.97	110.62
1	L	190	VAL	CB-CA-C	8.29	122.97	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	190	VAL	CB-CA-C	8.28	122.95	110.62
1	K	190	VAL	CB-CA-C	8.27	122.94	110.62
1	J	52	ASP	CA-CB-CG	-8.22	104.38	112.60
1	H	52	ASP	CA-CB-CG	-8.20	104.40	112.60
1	I	52	ASP	CA-CB-CG	-8.20	104.40	112.60
1	I	235	PRO	CB-CA-C	8.17	124.96	112.21
1	E	3	ALA	N-CA-CB	-8.17	98.41	110.17
1	K	52	ASP	CA-CB-CG	-8.17	104.43	112.60
1	B	3	ALA	N-CA-CB	-8.16	98.43	110.17
1	N	52	ASP	CA-CB-CG	-8.15	104.45	112.60
1	F	3	ALA	N-CA-CB	-8.15	98.43	110.17
1	A	14	VAL	N-CA-CB	8.15	121.62	110.54
1	A	255	GLU	CB-CA-C	8.14	123.65	110.29
1	C	14	VAL	N-CA-CB	8.14	121.62	110.54
1	D	3	ALA	N-CA-CB	-8.14	98.45	110.17
1	D	255	GLU	CB-CA-C	8.13	123.63	110.29
1	A	3	ALA	N-CA-CB	-8.13	98.46	110.17
1	C	3	ALA	N-CA-CB	-8.13	98.46	110.17
1	M	52	ASP	CA-CB-CG	-8.13	104.47	112.60
1	B	255	GLU	CB-CA-C	8.13	123.62	110.29
1	G	3	ALA	N-CA-CB	-8.13	98.47	110.17
1	C	255	GLU	CB-CA-C	8.12	123.61	110.29
1	D	14	VAL	N-CA-CB	8.12	121.59	110.54
1	L	52	ASP	CA-CB-CG	-8.12	104.48	112.60
1	E	255	GLU	CB-CA-C	8.11	123.60	110.29
1	F	14	VAL	N-CA-CB	8.11	121.57	110.54
1	G	14	VAL	N-CA-CB	8.10	121.55	110.54
1	E	14	VAL	N-CA-CB	8.09	121.54	110.54
1	B	14	VAL	N-CA-CB	8.08	121.53	110.54
1	F	260	ALA	N-CA-C	8.08	120.09	111.28
1	G	230	ILE	N-CA-CB	8.00	121.42	110.54
1	C	444	LEU	CB-CA-C	-7.91	97.66	110.79
1	A	444	LEU	CB-CA-C	-7.90	97.68	110.79
1	B	444	LEU	CB-CA-C	-7.89	97.69	110.79
1	G	444	LEU	CB-CA-C	-7.89	97.68	110.79
1	E	444	LEU	CB-CA-C	-7.89	97.69	110.79
1	F	444	LEU	CB-CA-C	-7.88	97.70	110.79
1	D	444	LEU	CB-CA-C	-7.88	97.71	110.79
1	L	140	ASP	N-CA-CB	-7.85	99.14	110.45
1	J	140	ASP	N-CA-CB	-7.84	99.16	110.45
1	N	140	ASP	N-CA-CB	-7.84	99.17	110.45
1	K	140	ASP	N-CA-CB	-7.83	99.17	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	140	ASP	N-CA-CB	-7.81	99.20	110.45
1	I	140	ASP	N-CA-CB	-7.81	99.21	110.45
1	M	140	ASP	N-CA-CB	-7.79	99.22	110.45
1	K	115	ASP	CA-CB-CG	-7.76	104.84	112.60
1	I	115	ASP	CA-CB-CG	-7.74	104.86	112.60
1	J	115	ASP	CA-CB-CG	-7.72	104.88	112.60
1	N	115	ASP	CA-CB-CG	-7.70	104.90	112.60
1	N	149	THR	N-CA-CB	7.69	121.43	110.12
1	I	149	THR	N-CA-CB	7.69	121.42	110.12
1	M	115	ASP	CA-CB-CG	-7.68	104.92	112.60
1	L	115	ASP	CA-CB-CG	-7.68	104.92	112.60
1	H	115	ASP	CA-CB-CG	-7.68	104.92	112.60
1	L	149	THR	N-CA-CB	7.68	121.41	110.12
1	K	149	THR	N-CA-CB	7.68	121.40	110.12
1	J	149	THR	N-CA-CB	7.67	121.40	110.12
1	H	149	THR	N-CA-CB	7.65	121.36	110.12
1	M	149	THR	N-CA-CB	7.64	121.36	110.12
1	N	153	ASN	CA-CB-CG	-7.61	104.99	112.60
1	C	412	VAL	CB-CA-C	-7.60	101.00	111.49
1	B	412	VAL	CB-CA-C	-7.59	101.02	111.49
1	E	412	VAL	CB-CA-C	-7.59	101.02	111.49
1	G	412	VAL	CB-CA-C	-7.57	101.05	111.49
1	A	412	VAL	CB-CA-C	-7.56	101.05	111.49
1	F	412	VAL	CB-CA-C	-7.55	101.07	111.49
1	D	412	VAL	CB-CA-C	-7.54	101.08	111.49
1	I	153	ASN	CA-CB-CG	-7.54	105.06	112.60
1	D	268	ARG	CB-CA-C	7.54	123.30	110.79
1	J	153	ASN	CA-CB-CG	-7.54	105.06	112.60
1	C	268	ARG	CB-CA-C	7.53	123.30	110.79
1	H	153	ASN	CA-CB-CG	-7.53	105.07	112.60
1	F	86	GLY	N-CA-C	-7.53	106.13	115.08
1	K	153	ASN	CA-CB-CG	-7.53	105.07	112.60
1	M	86	GLY	N-CA-C	-7.53	106.12	115.08
1	E	268	ARG	CB-CA-C	7.52	123.27	110.79
1	G	86	GLY	N-CA-C	-7.52	106.13	115.08
1	A	268	ARG	CB-CA-C	7.52	123.27	110.79
1	F	268	ARG	CB-CA-C	7.51	123.27	110.79
1	C	86	GLY	N-CA-C	-7.51	106.14	115.08
1	D	86	GLY	N-CA-C	-7.51	106.14	115.08
1	E	86	GLY	N-CA-C	-7.51	106.14	115.08
1	A	367	GLU	CB-CA-C	-7.51	98.33	110.79
1	B	268	ARG	CB-CA-C	7.51	123.26	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	86	GLY	N-CA-C	-7.51	106.15	115.08
1	M	153	ASN	CA-CB-CG	-7.51	105.09	112.60
1	A	86	GLY	N-CA-C	-7.50	106.15	115.08
1	D	367	GLU	CB-CA-C	-7.50	98.33	110.79
1	H	206	ASN	N-CA-CB	7.50	120.73	110.38
1	L	153	ASN	CA-CB-CG	-7.50	105.10	112.60
1	C	367	GLU	CB-CA-C	-7.50	98.34	110.79
1	H	86	GLY	N-CA-C	-7.50	106.16	115.08
1	J	86	GLY	N-CA-C	-7.50	106.16	115.08
1	K	206	ASN	N-CA-CB	7.50	120.73	110.38
1	F	367	GLU	CB-CA-C	-7.50	98.34	110.79
1	N	86	GLY	N-CA-C	-7.50	106.16	115.08
1	B	86	GLY	N-CA-C	-7.49	106.16	115.08
1	B	367	GLU	CB-CA-C	-7.49	98.36	110.79
1	M	206	ASN	N-CA-CB	7.49	120.71	110.38
1	G	268	ARG	CB-CA-C	7.48	123.21	110.79
1	E	367	GLU	CB-CA-C	-7.48	98.37	110.79
1	G	367	GLU	CB-CA-C	-7.48	98.37	110.79
1	L	86	GLY	N-CA-C	-7.48	106.18	115.08
1	I	86	GLY	N-CA-C	-7.48	106.18	115.08
1	K	138	CYS	N-CA-CB	7.47	120.93	110.17
1	N	206	ASN	N-CA-CB	7.47	120.69	110.38
1	L	206	ASN	N-CA-CB	7.46	120.67	110.38
1	I	206	ASN	N-CA-CB	7.45	120.66	110.38
1	J	206	ASN	N-CA-CB	7.45	120.66	110.38
1	J	138	CYS	N-CA-CB	7.44	120.88	110.17
1	M	138	CYS	N-CA-CB	7.43	120.86	110.17
1	L	138	CYS	N-CA-CB	7.42	120.86	110.17
1	I	138	CYS	N-CA-CB	7.42	120.85	110.17
1	H	138	CYS	N-CA-CB	7.41	120.84	110.17
1	N	138	CYS	N-CA-CB	7.41	120.84	110.17
1	C	499	VAL	N-CA-CB	7.38	119.19	110.55
1	D	410	GLY	N-CA-C	-7.36	104.04	112.29
1	C	381	VAL	N-CA-CB	-7.32	101.29	111.25
1	G	410	GLY	N-CA-C	-7.31	104.10	112.29
1	F	381	VAL	N-CA-CB	-7.29	101.33	111.25
1	C	410	GLY	N-CA-C	-7.29	104.12	112.29
1	A	256	GLY	N-CA-C	-7.28	105.79	115.32
1	A	381	VAL	N-CA-CB	-7.28	101.35	111.25
1	B	381	VAL	N-CA-CB	-7.28	101.35	111.25
1	G	381	VAL	N-CA-CB	-7.28	101.35	111.25
1	F	410	GLY	N-CA-C	-7.27	104.14	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	GLY	N-CA-C	-7.27	104.14	112.29
1	E	410	GLY	N-CA-C	-7.27	104.14	112.29
1	B	256	GLY	N-CA-C	-7.27	105.80	115.32
1	D	381	VAL	N-CA-CB	-7.27	101.36	111.25
1	B	410	GLY	N-CA-C	-7.25	104.17	112.29
1	E	381	VAL	N-CA-CB	-7.24	101.40	111.25
1	D	256	GLY	N-CA-C	-7.24	105.84	115.32
1	E	256	GLY	N-CA-C	-7.21	105.87	115.32
1	N	410	GLY	N-CA-C	-7.21	104.21	112.29
1	I	410	GLY	N-CA-C	-7.21	104.22	112.29
1	J	410	GLY	N-CA-C	-7.21	104.22	112.29
1	C	256	GLY	N-CA-C	-7.20	105.89	115.32
1	H	410	GLY	N-CA-C	-7.19	104.23	112.29
1	K	410	GLY	N-CA-C	-7.19	104.24	112.29
1	M	410	GLY	N-CA-C	-7.18	104.25	112.29
1	B	27	VAL	CB-CA-C	7.16	121.80	112.14
1	G	27	VAL	CB-CA-C	7.15	121.79	112.14
1	D	27	VAL	CB-CA-C	7.13	121.77	112.14
1	N	196	ASP	N-CA-CB	-7.13	99.90	110.24
1	J	196	ASP	N-CA-CB	-7.13	99.90	110.24
1	F	27	VAL	CB-CA-C	7.13	121.76	112.14
1	L	410	GLY	N-CA-C	-7.13	104.31	112.29
1	E	27	VAL	CB-CA-C	7.13	121.76	112.14
1	F	256	GLY	CA-C-N	7.13	134.53	121.70
1	F	256	GLY	C-N-CA	7.13	134.53	121.70
1	A	27	VAL	CB-CA-C	7.11	121.74	112.14
1	C	27	VAL	CB-CA-C	7.11	121.74	112.14
1	H	196	ASP	N-CA-CB	-7.10	99.95	110.24
1	K	523	ASP	CA-CB-CG	7.08	119.69	112.60
1	K	196	ASP	N-CA-CB	-7.08	99.97	110.24
1	M	196	ASP	N-CA-CB	-7.08	99.97	110.24
1	N	523	ASP	CA-CB-CG	7.07	119.67	112.60
1	L	196	ASP	N-CA-CB	-7.06	100.00	110.24
1	H	523	ASP	CA-CB-CG	7.06	119.66	112.60
1	I	196	ASP	N-CA-CB	-7.06	100.01	110.24
1	L	461	GLU	CB-CA-C	7.06	120.80	109.51
1	N	461	GLU	CB-CA-C	7.05	120.80	109.51
1	A	334	ASP	CA-CB-CG	7.05	119.65	112.60
1	I	523	ASP	CA-CB-CG	7.05	119.65	112.60
1	D	334	ASP	CA-CB-CG	7.05	119.65	112.60
1	J	523	ASP	CA-CB-CG	7.05	119.65	112.60
1	L	523	ASP	CA-CB-CG	7.05	119.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	334	ASP	CA-CB-CG	7.04	119.64	112.60
1	K	461	GLU	CB-CA-C	7.04	120.78	109.51
1	K	52	ASP	N-CA-CB	7.04	119.86	110.29
1	E	334	ASP	CA-CB-CG	7.04	119.64	112.60
1	I	52	ASP	N-CA-CB	7.04	119.86	110.29
1	M	461	GLU	CB-CA-C	7.03	120.76	109.51
1	M	523	ASP	CA-CB-CG	7.03	119.63	112.60
1	H	52	ASP	N-CA-CB	7.03	119.84	110.29
1	N	52	ASP	N-CA-CB	7.02	119.83	110.29
1	J	461	GLU	CB-CA-C	7.01	120.72	109.51
1	M	52	ASP	N-CA-CB	7.01	119.82	110.29
1	G	334	ASP	CA-CB-CG	7.00	119.60	112.60
1	B	334	ASP	CA-CB-CG	7.00	119.60	112.60
1	C	54	VAL	CB-CA-C	-6.99	103.03	111.97
1	G	54	VAL	CB-CA-C	-6.98	103.03	111.97
1	L	52	ASP	N-CA-CB	6.98	119.79	110.29
1	F	36	ARG	CB-CA-C	6.98	121.93	110.90
1	J	52	ASP	N-CA-CB	6.98	119.78	110.29
1	D	54	VAL	CB-CA-C	-6.97	103.04	111.97
1	A	54	VAL	CB-CA-C	-6.97	103.05	111.97
1	C	334	ASP	CA-CB-CG	6.97	119.57	112.60
1	F	54	VAL	CB-CA-C	-6.97	103.05	111.97
1	J	412	VAL	CB-CA-C	-6.97	101.88	111.49
1	D	36	ARG	CB-CA-C	6.96	121.90	110.90
1	G	36	ARG	CB-CA-C	6.96	121.90	110.90
1	J	54	VAL	CB-CA-C	-6.96	103.06	111.97
1	A	36	ARG	CB-CA-C	6.96	121.90	110.90
1	B	36	ARG	CB-CA-C	6.96	121.90	110.90
1	E	54	VAL	CB-CA-C	-6.96	103.06	111.97
1	I	54	VAL	CB-CA-C	-6.96	103.06	111.97
1	I	461	GLU	CB-CA-C	6.96	120.64	109.51
1	E	36	ARG	CB-CA-C	6.96	121.89	110.90
1	K	54	VAL	CB-CA-C	-6.96	103.07	111.97
1	L	412	VAL	CB-CA-C	-6.96	101.89	111.49
1	E	271	VAL	CB-CA-C	-6.95	100.69	111.26
1	H	461	GLU	CB-CA-C	6.95	120.63	109.51
1	L	54	VAL	CB-CA-C	-6.95	103.07	111.97
1	H	412	VAL	CB-CA-C	-6.95	101.90	111.49
1	A	369	VAL	CB-CA-C	-6.95	102.76	112.14
1	B	54	VAL	CB-CA-C	-6.95	103.08	111.97
1	B	271	VAL	CB-CA-C	-6.95	100.70	111.26
1	C	36	ARG	CB-CA-C	6.95	121.87	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	271	VAL	CB-CA-C	-6.94	100.71	111.26
1	G	369	VAL	CB-CA-C	-6.94	102.77	112.14
1	I	412	VAL	CB-CA-C	-6.94	101.91	111.49
1	N	85	ALA	N-CA-CB	-6.94	99.89	110.16
1	B	369	VAL	CB-CA-C	-6.94	102.77	112.14
1	H	54	VAL	CB-CA-C	-6.94	103.09	111.97
1	K	85	ALA	N-CA-CB	-6.93	99.90	110.16
1	I	85	ALA	N-CA-CB	-6.93	99.90	110.16
1	N	412	VAL	CB-CA-C	-6.93	101.92	111.49
1	F	369	VAL	CB-CA-C	-6.93	102.78	112.14
1	L	85	ALA	N-CA-CB	-6.93	99.90	110.16
1	M	54	VAL	CB-CA-C	-6.93	103.10	111.97
1	A	217	SER	CB-CA-C	-6.92	104.98	111.00
1	E	369	VAL	CB-CA-C	-6.92	102.80	112.14
1	J	85	ALA	N-CA-CB	-6.92	99.92	110.16
1	H	85	ALA	N-CA-CB	-6.92	99.92	110.16
1	C	271	VAL	CB-CA-C	-6.92	100.74	111.26
1	K	412	VAL	CB-CA-C	-6.92	101.94	111.49
1	N	27	VAL	CB-CA-C	6.92	121.47	112.14
1	D	271	VAL	CB-CA-C	-6.91	100.75	111.26
1	M	85	ALA	N-CA-CB	-6.91	99.93	110.16
1	D	369	VAL	CB-CA-C	-6.91	102.81	112.14
1	M	412	VAL	CB-CA-C	-6.91	101.96	111.49
1	N	54	VAL	CB-CA-C	-6.90	103.14	111.97
1	C	369	VAL	CB-CA-C	-6.89	102.83	112.14
1	F	230	ILE	CA-CB-CG1	6.88	122.09	110.40
1	H	27	VAL	CB-CA-C	6.86	121.41	112.14
1	K	27	VAL	CB-CA-C	6.86	121.41	112.14
1	I	226	LYS	N-CA-CB	-6.86	100.29	110.17
1	I	27	VAL	CB-CA-C	6.86	121.40	112.14
1	J	27	VAL	CB-CA-C	6.86	121.40	112.14
1	L	27	VAL	CB-CA-C	6.86	121.40	112.14
1	M	27	VAL	CB-CA-C	6.85	121.39	112.14
1	F	11	ASP	CB-CA-C	6.85	121.64	110.88
1	C	11	ASP	CB-CA-C	6.83	121.61	110.88
1	D	11	ASP	CB-CA-C	6.83	121.61	110.88
1	E	11	ASP	CB-CA-C	6.83	121.60	110.88
1	I	14	VAL	N-CA-CB	6.83	119.83	110.54
1	A	11	ASP	CB-CA-C	6.83	121.60	110.88
1	G	11	ASP	CB-CA-C	6.82	121.59	110.88
1	H	14	VAL	N-CA-CB	6.81	119.80	110.54
1	B	11	ASP	CB-CA-C	6.81	121.57	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	226	LYS	N-CA-CB	-6.81	100.36	110.17
1	M	226	LYS	N-CA-CB	-6.81	100.36	110.17
1	H	226	LYS	N-CA-CB	-6.81	100.37	110.17
1	L	226	LYS	N-CA-CB	-6.81	100.37	110.17
1	B	315	GLU	CB-CA-C	6.81	122.09	110.79
1	D	315	GLU	CB-CA-C	6.80	122.08	110.79
1	E	315	GLU	CB-CA-C	6.80	122.09	110.79
1	F	315	GLU	CB-CA-C	6.80	122.08	110.79
1	J	168	LYS	N-CA-CB	-6.80	100.14	110.01
1	C	315	GLU	CB-CA-C	6.80	122.08	110.79
1	H	168	LYS	N-CA-CB	-6.80	100.15	110.01
1	L	14	VAL	N-CA-CB	6.80	119.78	110.54
1	J	218	PRO	N-CA-CB	6.79	109.65	103.33
1	M	14	VAL	N-CA-CB	6.79	119.78	110.54
1	L	510	VAL	N-CA-CB	6.79	118.50	110.55
1	N	226	LYS	N-CA-CB	-6.79	100.39	110.17
1	I	168	LYS	N-CA-CB	-6.79	100.16	110.01
1	N	510	VAL	N-CA-CB	6.79	118.49	110.55
1	K	14	VAL	N-CA-CB	6.79	119.77	110.54
1	L	218	PRO	N-CA-CB	6.79	109.64	103.33
1	K	218	PRO	N-CA-CB	6.79	109.64	103.33
1	N	14	VAL	N-CA-CB	6.79	119.77	110.54
1	K	510	VAL	N-CA-CB	6.78	118.48	110.55
1	K	226	LYS	N-CA-CB	-6.78	100.41	110.17
1	N	218	PRO	N-CA-CB	6.78	109.63	103.33
1	N	168	LYS	N-CA-CB	-6.77	100.19	110.01
1	J	14	VAL	N-CA-CB	6.77	119.75	110.54
1	M	218	PRO	N-CA-CB	6.77	109.63	103.33
1	H	218	PRO	N-CA-CB	6.76	109.62	103.33
1	K	168	LYS	N-CA-CB	-6.76	100.20	110.01
1	M	168	LYS	N-CA-CB	-6.76	100.20	110.01
1	J	510	VAL	N-CA-CB	6.76	118.46	110.55
1	L	168	LYS	N-CA-CB	-6.75	100.22	110.01
1	F	262	LEU	CB-CA-C	6.75	121.47	110.88
1	G	245	LYS	CG-CD-CE	6.74	126.81	111.30
1	G	241	ALA	N-CA-C	-6.74	104.53	112.89
1	I	218	PRO	N-CA-CB	6.74	109.59	103.33
1	M	510	VAL	N-CA-CB	6.73	118.42	110.55
1	D	63	GLU	CA-CB-CG	6.72	127.54	114.10
1	H	510	VAL	N-CA-CB	6.72	118.41	110.55
1	A	63	GLU	CA-CB-CG	6.71	127.52	114.10
1	B	63	GLU	CA-CB-CG	6.71	127.52	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	284	ARG	CB-CA-C	-6.71	99.65	110.79
1	E	63	GLU	CA-CB-CG	6.71	127.51	114.10
1	I	510	VAL	N-CA-CB	6.71	118.39	110.55
1	I	284	ARG	CB-CA-C	-6.71	99.66	110.79
1	H	284	ARG	CB-CA-C	-6.70	99.67	110.79
1	G	63	GLU	CA-CB-CG	6.70	127.49	114.10
1	L	284	ARG	CB-CA-C	-6.70	99.67	110.79
1	F	63	GLU	CA-CB-CG	6.70	127.49	114.10
1	C	63	GLU	CA-CB-CG	6.69	127.49	114.10
1	N	284	ARG	CB-CA-C	-6.69	99.68	110.79
1	J	284	ARG	CB-CA-C	-6.68	99.70	110.79
1	M	284	ARG	CB-CA-C	-6.68	99.70	110.79
1	D	85	ALA	N-CA-CB	-6.67	100.28	110.16
1	F	85	ALA	N-CA-CB	-6.66	100.30	110.16
1	N	455	VAL	CB-CA-C	6.66	121.13	112.14
1	E	380	LYS	N-CA-CB	-6.66	99.97	110.69
1	A	85	ALA	N-CA-CB	-6.66	100.31	110.16
1	E	85	ALA	N-CA-CB	-6.65	100.31	110.16
1	B	85	ALA	N-CA-CB	-6.65	100.31	110.16
1	H	455	VAL	CB-CA-C	6.65	121.12	112.14
1	C	85	ALA	N-CA-CB	-6.64	100.33	110.16
1	G	85	ALA	N-CA-CB	-6.64	100.33	110.16
1	L	455	VAL	CB-CA-C	6.64	121.10	112.14
1	D	380	LYS	N-CA-CB	-6.63	100.02	110.69
1	M	455	VAL	CB-CA-C	6.62	121.08	112.14
1	G	380	LYS	N-CA-CB	-6.62	100.04	110.69
1	A	231	ARG	N-CA-CB	6.61	119.83	110.12
1	J	455	VAL	CB-CA-C	6.61	121.06	112.14
1	K	455	VAL	CB-CA-C	6.61	121.06	112.14
1	F	380	LYS	N-CA-CB	-6.61	100.06	110.69
1	B	380	LYS	N-CA-CB	-6.60	100.06	110.69
1	L	338	GLU	CB-CA-C	6.60	121.14	109.72
1	A	380	LYS	N-CA-CB	-6.59	100.08	110.69
1	A	315	GLU	CB-CA-C	6.59	121.73	110.79
1	C	380	LYS	N-CA-CB	-6.59	100.08	110.69
1	M	338	GLU	CB-CA-C	6.59	121.12	109.72
1	I	455	VAL	CB-CA-C	6.58	121.03	112.14
1	N	338	GLU	CB-CA-C	6.58	121.11	109.72
1	K	338	GLU	CB-CA-C	6.58	121.10	109.72
1	I	338	GLU	CB-CA-C	6.58	121.10	109.72
1	E	231	ARG	N-CA-CB	6.58	119.78	110.12
1	J	338	GLU	CB-CA-C	6.57	121.09	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	410	GLY	CA-C-N	-6.56	114.64	123.10
1	C	410	GLY	C-N-CA	-6.56	114.64	123.10
1	C	231	ARG	N-CA-CB	6.56	119.76	110.12
1	H	338	GLU	CB-CA-C	6.55	121.06	109.72
1	D	231	ARG	N-CA-CB	6.54	119.74	110.12
1	G	410	GLY	CA-C-N	-6.54	114.66	123.10
1	G	410	GLY	C-N-CA	-6.54	114.66	123.10
1	E	410	GLY	CA-C-N	-6.53	114.67	123.10
1	E	410	GLY	C-N-CA	-6.53	114.67	123.10
1	B	231	ARG	N-CA-CB	6.53	119.72	110.12
1	H	37	ASN	CA-CB-CG	6.53	119.13	112.60
1	J	37	ASN	CA-CB-CG	6.53	119.13	112.60
1	B	494	LEU	CB-CA-C	6.52	122.27	109.35
1	D	494	LEU	CB-CA-C	6.52	122.26	109.35
1	A	410	GLY	CA-C-N	-6.52	114.69	123.10
1	A	410	GLY	C-N-CA	-6.52	114.69	123.10
1	M	37	ASN	CA-CB-CG	6.51	119.11	112.60
1	D	300	VAL	CB-CA-C	-6.51	100.47	110.95
1	E	494	LEU	CB-CA-C	6.51	122.23	109.35
1	L	37	ASN	CA-CB-CG	6.51	119.11	112.60
1	D	257	GLU	CB-CA-C	6.50	123.36	110.42
1	G	494	LEU	CB-CA-C	6.50	122.23	109.35
1	A	257	GLU	CB-CA-C	6.50	123.36	110.42
1	F	494	LEU	CB-CA-C	6.50	122.22	109.35
1	B	300	VAL	CB-CA-C	-6.50	100.48	110.95
1	A	494	LEU	CB-CA-C	6.50	122.22	109.35
1	C	494	LEU	CB-CA-C	6.49	122.21	109.35
1	G	315	GLU	CB-CA-C	6.49	121.57	110.79
1	E	300	VAL	CB-CA-C	-6.49	100.50	110.95
1	D	410	GLY	CA-C-N	-6.49	114.73	123.10
1	D	410	GLY	C-N-CA	-6.49	114.73	123.10
1	E	257	GLU	CB-CA-C	6.49	123.33	110.42
1	B	257	GLU	CB-CA-C	6.49	123.33	110.42
1	C	257	GLU	CB-CA-C	6.49	123.33	110.42
1	N	37	ASN	CA-CB-CG	6.48	119.08	112.60
1	A	300	VAL	CB-CA-C	-6.48	100.52	110.95
1	F	300	VAL	CB-CA-C	-6.48	100.52	110.95
1	K	37	ASN	CA-CB-CG	6.47	119.07	112.60
1	G	300	VAL	CB-CA-C	-6.47	100.54	110.95
1	I	37	ASN	CA-CB-CG	6.47	119.07	112.60
1	F	410	GLY	CA-C-N	-6.46	114.77	123.10
1	F	410	GLY	C-N-CA	-6.46	114.77	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	300	VAL	CB-CA-C	-6.45	100.56	110.95
1	J	444	LEU	CB-CA-C	-6.45	100.09	110.79
1	I	444	LEU	CB-CA-C	-6.44	100.09	110.79
1	L	205	ILE	CB-CA-C	6.44	121.85	111.29
1	B	501	ARG	N-CA-CB	-6.43	100.68	110.01
1	D	501	ARG	N-CA-CB	-6.43	100.69	110.01
1	F	268	ARG	N-CA-CB	6.43	119.57	110.12
1	I	205	ILE	CB-CA-C	6.43	121.83	111.29
1	N	444	LEU	CB-CA-C	-6.43	100.12	110.79
1	F	501	ARG	N-CA-CB	-6.42	100.69	110.01
1	H	205	ILE	CB-CA-C	6.42	121.82	111.29
1	N	205	ILE	CB-CA-C	6.41	121.81	111.29
1	F	196	ASP	N-CA-CB	-6.41	99.69	109.94
1	G	501	ARG	N-CA-CB	-6.41	100.71	110.01
1	B	410	GLY	CA-C-N	-6.41	114.83	123.10
1	B	410	GLY	C-N-CA	-6.41	114.83	123.10
1	M	205	ILE	CB-CA-C	6.41	121.80	111.29
1	A	196	ASP	N-CA-CB	-6.40	99.70	109.94
1	H	444	LEU	CB-CA-C	-6.40	100.16	110.79
1	J	205	ILE	CB-CA-C	6.40	121.78	111.29
1	K	444	LEU	CB-CA-C	-6.40	100.17	110.79
1	A	501	ARG	N-CA-CB	-6.39	100.74	110.01
1	D	196	ASP	N-CA-CB	-6.39	99.71	109.94
1	E	196	ASP	N-CA-CB	-6.39	99.71	109.94
1	K	205	ILE	CB-CA-C	6.39	121.77	111.29
1	M	444	LEU	CB-CA-C	-6.39	100.18	110.79
1	A	499	VAL	N-CA-CB	6.38	119.22	110.54
1	C	501	ARG	N-CA-CB	-6.38	100.75	110.01
1	E	501	ARG	N-CA-CB	-6.38	100.75	110.01
1	G	196	ASP	N-CA-CB	-6.38	99.73	109.94
1	I	381	VAL	N-CA-CB	-6.38	102.57	111.25
1	C	196	ASP	N-CA-CB	-6.38	99.74	109.94
1	D	297	GLY	N-CA-C	-6.38	106.52	115.32
1	H	381	VAL	N-CA-CB	-6.37	102.58	111.25
1	L	444	LEU	CB-CA-C	-6.37	100.21	110.79
1	L	381	VAL	N-CA-CB	-6.37	102.59	111.25
1	E	297	GLY	N-CA-C	-6.36	106.54	115.32
1	J	381	VAL	N-CA-CB	-6.36	102.59	111.25
1	B	196	ASP	N-CA-CB	-6.36	99.76	109.94
1	M	381	VAL	N-CA-CB	-6.36	102.60	111.25
1	K	381	VAL	N-CA-CB	-6.36	102.60	111.25
1	A	271	VAL	CB-CA-C	-6.36	101.60	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	499	VAL	N-CA-CB	6.36	119.18	110.54
1	N	381	VAL	N-CA-CB	-6.35	102.61	111.25
1	L	369	VAL	CB-CA-C	-6.35	103.57	112.14
1	B	499	VAL	N-CA-CB	6.35	119.17	110.54
1	B	297	GLY	N-CA-C	-6.34	106.57	115.32
1	F	297	GLY	N-CA-C	-6.34	106.57	115.32
1	C	235	PRO	CB-CA-C	6.34	122.09	112.21
1	C	297	GLY	N-CA-C	-6.33	106.59	115.32
1	B	235	PRO	CB-CA-C	6.33	122.08	112.21
1	E	235	PRO	CB-CA-C	6.32	122.07	112.21
1	G	297	GLY	N-CA-C	-6.32	106.59	115.32
1	G	271	VAL	CB-CA-C	-6.32	101.65	111.26
1	B	149	THR	N-CA-CB	6.32	119.41	110.12
1	D	149	THR	N-CA-CB	6.32	119.41	110.12
1	G	256	GLY	N-CA-C	-6.32	107.04	115.32
1	A	235	PRO	CB-CA-C	6.32	122.06	112.21
1	D	499	VAL	N-CA-CB	6.32	119.13	110.54
1	D	235	PRO	CB-CA-C	6.31	122.06	112.21
1	A	297	GLY	N-CA-C	-6.31	106.61	115.32
1	E	499	VAL	N-CA-CB	6.31	119.12	110.54
1	J	369	VAL	CB-CA-C	-6.31	103.62	112.14
1	G	149	THR	N-CA-CB	6.31	119.40	110.12
1	G	268	ARG	N-CA-CB	6.31	119.40	110.12
1	C	149	THR	N-CA-CB	6.30	119.38	110.12
1	I	369	VAL	CB-CA-C	-6.30	103.63	112.14
1	K	369	VAL	CB-CA-C	-6.30	103.64	112.14
1	G	499	VAL	N-CA-CB	6.29	119.10	110.54
1	F	149	THR	N-CA-CB	6.29	119.36	110.12
1	A	149	THR	N-CA-CB	6.29	119.36	110.12
1	N	499	VAL	N-CA-CB	6.29	119.09	110.54
1	J	499	VAL	N-CA-CB	6.29	119.09	110.54
1	K	499	VAL	N-CA-CB	6.28	119.08	110.54
1	M	369	VAL	CB-CA-C	-6.28	103.66	112.14
1	G	235	PRO	CB-CA-C	6.28	122.00	112.21
1	N	369	VAL	CB-CA-C	-6.27	103.67	112.14
1	B	258	ALA	N-CA-C	6.27	124.16	110.80
1	E	149	THR	N-CA-CB	6.27	119.34	110.12
1	H	369	VAL	CB-CA-C	-6.27	103.68	112.14
1	H	268	ARG	N-CA-CB	6.26	119.32	110.12
1	I	499	VAL	N-CA-CB	6.25	119.05	110.54
1	E	258	ALA	N-CA-C	6.25	124.12	110.80
1	L	499	VAL	N-CA-CB	6.25	119.04	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	258	ALA	N-CA-C	6.25	124.11	110.80
1	I	334	ASP	CB-CA-C	6.25	119.47	110.79
1	A	59	GLU	CB-CA-C	6.24	121.15	110.79
1	L	297	GLY	N-CA-C	-6.24	106.71	115.32
1	M	499	VAL	N-CA-CB	6.24	119.03	110.54
1	N	268	ARG	N-CA-CB	6.24	119.29	110.12
1	C	59	GLU	CB-CA-C	6.24	121.14	110.79
1	F	59	GLU	CB-CA-C	6.24	121.14	110.79
1	G	253	ASP	CA-CB-CG	-6.23	106.37	112.60
1	I	268	ARG	N-CA-CB	6.23	119.28	110.12
1	A	284	ARG	CB-CA-C	-6.23	100.45	110.79
1	G	59	GLU	CB-CA-C	6.23	121.13	110.79
1	L	334	ASP	CB-CA-C	6.23	119.45	110.79
1	N	89	THR	CB-CA-C	-6.23	101.10	110.88
1	N	188	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	59	GLU	CB-CA-C	6.22	121.12	110.79
1	I	188	ASP	CA-CB-CG	6.22	118.83	112.60
1	D	258	ALA	N-CA-C	6.22	124.05	110.80
1	D	284	ARG	CB-CA-C	-6.22	100.46	110.79
1	J	268	ARG	N-CA-CB	6.22	119.26	110.12
1	A	258	ALA	N-CA-C	6.22	124.04	110.80
1	G	230	ILE	CA-CB-CG1	6.22	120.97	110.40
1	G	258	ALA	N-CA-C	6.22	124.04	110.80
1	H	334	ASP	CB-CA-C	6.22	119.43	110.79
1	H	499	VAL	N-CA-CB	6.22	118.99	110.54
1	L	188	ASP	CA-CB-CG	6.22	118.82	112.60
1	J	89	THR	CB-CA-C	-6.21	101.12	110.88
1	K	188	ASP	CA-CB-CG	6.21	118.81	112.60
1	N	334	ASP	CB-CA-C	6.21	119.42	110.79
1	K	268	ARG	N-CA-CB	6.21	119.24	110.12
1	M	334	ASP	CB-CA-C	6.21	119.42	110.79
1	D	59	GLU	CB-CA-C	6.21	121.09	110.79
1	M	188	ASP	CA-CB-CG	6.20	118.80	112.60
1	M	300	VAL	CB-CA-C	-6.20	100.96	110.95
1	G	491	MET	CB-CA-C	6.20	121.08	110.79
1	M	297	GLY	N-CA-C	-6.20	106.76	115.32
1	N	297	GLY	N-CA-C	-6.20	106.76	115.32
1	B	491	MET	CB-CA-C	6.20	121.08	110.79
1	D	491	MET	CB-CA-C	6.20	121.08	110.79
1	C	284	ARG	CB-CA-C	-6.20	100.50	110.79
1	H	188	ASP	CA-CB-CG	6.20	118.80	112.60
1	M	89	THR	CB-CA-C	-6.20	101.15	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	59	GLU	CB-CA-C	6.20	121.08	110.79
1	J	334	ASP	CB-CA-C	6.20	119.40	110.79
1	M	268	ARG	N-CA-CB	6.20	119.23	110.12
1	K	334	ASP	CB-CA-C	6.19	119.40	110.79
1	C	491	MET	CB-CA-C	6.19	121.07	110.79
1	L	268	ARG	N-CA-CB	6.19	119.22	110.12
1	F	284	ARG	CB-CA-C	-6.19	100.51	110.79
1	K	59	GLU	CB-CG-CD	6.19	123.12	112.60
1	F	235	PRO	CB-CA-C	6.19	121.86	112.21
1	I	297	GLY	N-CA-C	-6.19	106.78	115.32
1	I	300	VAL	CB-CA-C	-6.19	100.99	110.95
1	K	297	GLY	N-CA-C	-6.19	106.78	115.32
1	K	459	GLY	N-CA-C	-6.19	106.88	114.92
1	L	89	THR	CB-CA-C	-6.19	101.17	110.88
1	B	284	ARG	CB-CA-C	-6.18	100.52	110.79
1	E	284	ARG	CB-CA-C	-6.18	100.52	110.79
1	J	297	GLY	N-CA-C	-6.18	106.78	115.32
1	G	284	ARG	CB-CA-C	-6.18	100.53	110.79
1	H	297	GLY	N-CA-C	-6.18	106.79	115.32
1	H	300	VAL	CB-CA-C	-6.18	101.00	110.95
1	I	459	GLY	N-CA-C	-6.18	106.89	114.92
1	F	491	MET	CB-CA-C	6.18	121.04	110.79
1	H	89	THR	CB-CA-C	-6.18	101.18	110.88
1	K	89	THR	CB-CA-C	-6.18	101.18	110.88
1	B	345	ARG	CB-CA-C	6.17	121.04	110.79
1	G	345	ARG	CB-CA-C	6.17	121.04	110.79
1	N	300	VAL	CB-CA-C	-6.17	101.01	110.95
1	J	459	GLY	N-CA-C	-6.17	106.90	114.92
1	E	491	MET	CB-CA-C	6.17	121.03	110.79
1	I	89	THR	CB-CA-C	-6.17	101.20	110.88
1	C	345	ARG	CB-CA-C	6.16	121.02	110.79
1	J	59	GLU	CB-CG-CD	6.16	123.08	112.60
1	M	459	GLY	N-CA-C	-6.16	106.91	114.92
1	A	268	ARG	N-CA-CB	6.16	119.18	110.12
1	A	491	MET	CB-CA-C	6.16	121.02	110.79
1	E	345	ARG	CB-CA-C	6.16	121.02	110.79
1	L	300	VAL	CB-CA-C	-6.16	101.03	110.95
1	N	59	GLU	CB-CG-CD	6.16	123.07	112.60
1	M	59	GLU	CB-CG-CD	6.16	123.07	112.60
1	A	345	ARG	CB-CA-C	6.16	121.01	110.79
1	F	345	ARG	CB-CA-C	6.16	121.01	110.79
1	J	300	VAL	CB-CA-C	-6.16	101.04	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	59	GLU	CB-CG-CD	6.16	123.06	112.60
1	N	67	GLU	CB-CA-C	6.16	121.01	110.79
1	K	300	VAL	CB-CA-C	-6.15	101.04	110.95
1	B	268	ARG	N-CA-CB	6.15	119.16	110.12
1	D	345	ARG	CB-CA-C	6.15	121.00	110.79
1	I	59	GLU	CB-CG-CD	6.15	123.05	112.60
1	G	179	ASP	N-CA-CB	-6.15	101.32	110.17
1	H	59	GLU	CB-CG-CD	6.14	123.04	112.60
1	B	140	ASP	CA-CB-CG	6.14	118.74	112.60
1	F	420	ILE	CB-CA-C	6.14	120.43	112.14
1	J	188	ASP	CA-CB-CG	6.14	118.74	112.60
1	D	268	ARG	N-CA-CB	6.13	119.14	110.12
1	E	268	ARG	N-CA-CB	6.13	119.14	110.12
1	F	459	GLY	N-CA-C	-6.13	106.94	114.92
1	A	260	ALA	N-CA-C	6.13	117.63	111.07
1	E	140	ASP	CA-CB-CG	6.13	118.73	112.60
1	B	459	GLY	N-CA-C	-6.12	106.96	114.92
1	C	253	ASP	CA-CB-CG	-6.12	106.48	112.60
1	C	268	ARG	N-CA-CB	6.12	119.12	110.12
1	E	260	ALA	N-CA-C	6.12	117.62	111.07
1	G	37	ASN	CA-CB-CG	6.12	118.72	112.60
1	M	67	GLU	CB-CA-C	6.12	120.95	110.79
1	L	67	GLU	CB-CA-C	6.12	120.95	110.79
1	D	253	ASP	CA-CB-CG	-6.12	106.48	112.60
1	K	67	GLU	CB-CA-C	6.12	120.95	110.79
1	C	260	ALA	N-CA-C	6.12	117.61	111.07
1	H	459	GLY	N-CA-C	-6.12	106.97	114.92
1	E	253	ASP	CA-CB-CG	-6.11	106.49	112.60
1	G	140	ASP	CA-CB-CG	6.11	118.71	112.60
1	J	67	GLU	CB-CA-C	6.11	120.93	110.79
1	I	268	ARG	CB-CA-C	6.11	120.93	110.79
1	L	459	GLY	N-CA-C	-6.11	106.98	114.92
1	G	459	GLY	N-CA-C	-6.11	106.98	114.92
1	I	501	ARG	N-CA-CB	-6.11	101.14	110.12
1	D	235	PRO	N-CA-CB	6.10	109.98	103.39
1	L	501	ARG	N-CA-CB	-6.10	101.15	110.12
1	A	253	ASP	CA-CB-CG	-6.10	106.50	112.60
1	I	67	GLU	CB-CA-C	6.10	120.92	110.79
1	J	501	ARG	N-CA-CB	-6.10	101.16	110.12
1	N	459	GLY	N-CA-C	-6.10	106.99	114.92
1	N	501	ARG	N-CA-CB	-6.10	101.15	110.12
1	C	140	ASP	CA-CB-CG	6.10	118.70	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ASP	CA-CB-CG	6.09	118.69	112.60
1	E	420	ILE	CB-CA-C	6.09	120.37	112.14
1	B	260	ALA	N-CA-C	6.09	117.59	111.07
1	G	205	ILE	CB-CA-C	6.09	121.56	111.51
1	C	235	PRO	N-CA-CB	6.09	109.97	103.39
1	E	459	GLY	N-CA-C	-6.09	107.00	114.92
1	G	260	ALA	N-CA-C	6.09	117.58	111.07
1	A	179	ASP	N-CA-CB	-6.09	101.40	110.17
1	M	501	ARG	N-CA-CB	-6.09	101.17	110.12
1	B	235	PRO	N-CA-CB	6.08	109.96	103.39
1	C	37	ASN	CA-CB-CG	6.08	118.68	112.60
1	H	501	ARG	N-CA-CB	-6.08	101.18	110.12
1	A	235	PRO	N-CA-CB	6.08	109.96	103.39
1	E	235	PRO	N-CA-CB	6.08	109.96	103.39
1	F	205	ILE	CB-CA-C	6.08	121.55	111.51
1	A	459	GLY	N-CA-C	-6.08	107.02	114.92
1	B	205	ILE	CB-CA-C	6.08	121.54	111.51
1	C	459	GLY	N-CA-C	-6.08	107.02	114.92
1	A	205	ILE	CB-CA-C	6.08	121.54	111.51
1	F	140	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	89	THR	CB-CA-C	-6.08	101.34	110.88
1	B	179	ASP	N-CA-CB	-6.08	101.42	110.17
1	E	179	ASP	N-CA-CB	-6.08	101.42	110.17
1	G	89	THR	CB-CA-C	-6.08	101.34	110.88
1	N	268	ARG	CB-CA-C	6.08	120.88	110.79
1	D	205	ILE	CB-CA-C	6.07	121.53	111.51
1	K	268	ARG	CB-CA-C	6.07	120.87	110.79
1	L	268	ARG	CB-CA-C	6.07	120.87	110.79
1	C	205	ILE	CB-CA-C	6.07	121.53	111.51
1	F	37	ASN	CA-CB-CG	6.07	118.67	112.60
1	C	89	THR	CB-CA-C	-6.07	101.35	110.88
1	D	140	ASP	CA-CB-CG	6.07	118.67	112.60
1	E	89	THR	CB-CA-C	-6.07	101.35	110.88
1	C	179	ASP	N-CA-CB	-6.06	101.44	110.17
1	A	37	ASN	CA-CB-CG	6.06	118.66	112.60
1	B	253	ASP	CA-CB-CG	-6.06	106.54	112.60
1	D	179	ASP	N-CA-CB	-6.06	101.44	110.17
1	H	67	GLU	CB-CA-C	6.06	120.85	110.79
1	K	501	ARG	N-CA-CB	-6.06	101.21	110.12
1	M	268	ARG	CB-CA-C	6.06	120.85	110.79
1	B	89	THR	CB-CA-C	-6.06	101.37	110.88
1	D	37	ASN	CA-CB-CG	6.06	118.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	235	PRO	N-CA-CB	6.06	109.93	103.39
1	E	205	ILE	CB-CA-C	6.05	121.50	111.51
1	H	155	ASP	CB-CA-C	6.05	121.59	111.30
1	D	260	ALA	N-CA-C	6.05	117.55	111.07
1	B	37	ASN	CA-CB-CG	6.05	118.65	112.60
1	E	37	ASN	CA-CB-CG	6.04	118.64	112.60
1	F	179	ASP	N-CA-CB	-6.04	101.47	110.17
1	H	268	ARG	CB-CA-C	6.04	120.82	110.79
1	J	268	ARG	CB-CA-C	6.04	120.82	110.79
1	D	89	THR	CB-CA-C	-6.04	101.40	110.88
1	K	30	THR	N-CA-CB	6.04	118.99	110.12
1	F	89	THR	CB-CA-C	-6.03	101.41	110.88
1	D	459	GLY	N-CA-C	-6.03	107.08	114.92
1	K	155	ASP	CB-CA-C	6.03	121.54	111.30
1	N	155	ASP	CB-CA-C	6.02	121.53	111.30
1	F	266	THR	N-CA-CB	6.02	118.79	110.07
1	I	155	ASP	CB-CA-C	6.01	121.52	111.30
1	L	155	ASP	CB-CA-C	6.01	121.53	111.30
1	M	155	ASP	CB-CA-C	6.01	121.53	111.30
1	E	34	LYS	CB-CA-C	6.01	120.32	110.88
1	C	34	LYS	CB-CA-C	6.01	120.31	110.88
1	J	30	THR	N-CA-CB	6.01	118.95	110.12
1	L	30	THR	N-CA-CB	6.01	118.95	110.12
1	A	34	LYS	CB-CA-C	6.00	120.30	110.88
1	G	34	LYS	CB-CA-C	6.00	120.29	110.88
1	J	155	ASP	CB-CA-C	5.99	121.49	111.30
1	L	63	GLU	N-CA-CB	-5.99	101.31	110.12
1	F	310	GLU	N-CA-CB	-5.99	101.32	110.12
1	M	30	THR	N-CA-CB	5.98	118.92	110.12
1	H	30	THR	N-CA-CB	5.98	118.91	110.12
1	N	30	THR	N-CA-CB	5.98	118.91	110.12
1	F	34	LYS	CB-CA-C	5.98	120.27	110.88
1	D	34	LYS	CB-CA-C	5.97	120.26	110.88
1	C	30	THR	N-CA-CB	5.97	118.89	110.12
1	I	30	THR	N-CA-CB	5.97	118.89	110.12
1	H	63	GLU	N-CA-CB	-5.96	101.35	110.12
1	K	63	GLU	N-CA-CB	-5.96	101.35	110.12
1	D	420	ILE	CB-CA-C	5.96	120.45	112.22
1	J	63	GLU	N-CA-CB	-5.96	101.36	110.12
1	B	34	LYS	CB-CA-C	5.96	120.24	110.88
1	M	63	GLU	N-CA-CB	-5.96	101.36	110.12
1	N	63	GLU	N-CA-CB	-5.96	101.36	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	63	GLU	N-CA-CB	-5.96	101.37	110.12
1	A	30	THR	N-CA-CB	5.95	118.86	110.12
1	B	30	THR	N-CA-CB	5.95	118.86	110.12
1	E	30	THR	N-CA-CB	5.95	118.86	110.12
1	G	30	THR	N-CA-CB	5.95	118.86	110.12
1	D	30	THR	N-CA-CB	5.94	118.85	110.12
1	G	218	PRO	N-CA-CB	5.94	109.62	103.38
1	M	152	ALA	CB-CA-C	5.94	121.62	110.63
1	A	420	ILE	CB-CA-C	5.94	120.41	112.22
1	D	59	GLU	N-CA-CB	5.94	118.84	110.12
1	B	420	ILE	CB-CA-C	5.93	120.41	112.22
1	G	341	ALA	N-CA-CB	5.93	118.84	110.12
1	H	104	LEU	CB-CA-C	5.93	120.64	110.79
1	C	420	ILE	CB-CA-C	5.93	120.40	112.22
1	B	341	ALA	N-CA-CB	5.93	118.83	110.12
1	G	215	LEU	N-CA-CB	-5.93	101.14	110.69
1	F	59	GLU	N-CA-CB	5.93	118.83	110.12
1	L	104	LEU	CB-CA-C	5.92	120.62	110.79
1	C	59	GLU	N-CA-CB	5.92	118.82	110.12
1	D	341	ALA	N-CA-CB	5.92	118.82	110.12
1	B	59	GLU	N-CA-CB	5.92	118.82	110.12
1	F	30	THR	N-CA-CB	5.92	118.82	110.12
1	I	104	LEU	CB-CA-C	5.92	120.61	110.79
1	N	104	LEU	CB-CA-C	5.92	120.62	110.79
1	K	152	ALA	CB-CA-C	5.92	121.58	110.63
1	G	420	ILE	CB-CA-C	5.91	120.38	112.22
1	G	254	VAL	N-CA-CB	-5.91	103.25	111.41
1	I	152	ALA	CB-CA-C	5.91	121.57	110.63
1	N	152	ALA	CB-CA-C	5.91	121.57	110.63
1	K	104	LEU	CB-CA-C	5.91	120.60	110.79
1	M	104	LEU	CB-CA-C	5.91	120.60	110.79
1	J	104	LEU	CB-CA-C	5.91	120.59	110.79
1	L	152	ALA	CB-CA-C	5.91	121.55	110.63
1	B	517	THR	CB-CA-C	-5.90	101.44	110.88
1	F	341	ALA	N-CA-CB	5.90	118.80	110.12
1	A	341	ALA	N-CA-CB	5.90	118.80	110.12
1	E	59	GLU	N-CA-CB	5.90	118.79	110.12
1	E	62	LEU	CB-CA-C	5.90	120.00	109.38
1	H	152	ALA	CB-CA-C	5.90	121.54	110.63
1	N	67	GLU	CB-CG-CD	5.90	122.63	112.60
1	A	62	LEU	CB-CA-C	5.89	119.99	109.38
1	D	517	THR	CB-CA-C	-5.89	101.45	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	62	LEU	CB-CA-C	5.89	119.99	109.38
1	E	341	ALA	N-CA-CB	5.89	118.78	110.12
1	J	152	ALA	CB-CA-C	5.89	121.53	110.63
1	G	59	GLU	N-CA-CB	5.89	118.78	110.12
1	M	67	GLU	CB-CG-CD	5.89	122.61	112.60
1	C	517	THR	CB-CA-C	-5.89	101.46	110.88
1	G	243	ALA	O-C-N	-5.89	117.08	123.26
1	D	62	LEU	CB-CA-C	5.88	119.97	109.38
1	I	380	LYS	N-CA-CB	-5.88	101.22	110.69
1	C	341	ALA	N-CA-CB	5.88	118.76	110.12
1	H	67	GLU	CB-CG-CD	5.88	122.59	112.60
1	F	517	THR	CB-CA-C	-5.88	101.48	110.88
1	L	235	PRO	N-CA-CB	5.88	109.73	103.39
1	G	62	LEU	CB-CA-C	5.87	119.95	109.38
1	L	67	GLU	CB-CG-CD	5.87	122.58	112.60
1	A	455	VAL	CB-CA-C	5.87	120.06	112.14
1	A	517	THR	CB-CA-C	-5.87	101.49	110.88
1	J	294	THR	N-CA-CB	5.87	118.75	110.12
1	M	235	PRO	N-CA-CB	5.87	109.73	103.39
1	H	235	PRO	N-CA-CB	5.87	109.72	103.39
1	F	455	VAL	CB-CA-C	5.86	120.06	112.14
1	H	294	THR	N-CA-CB	5.86	118.74	110.12
1	E	517	THR	CB-CA-C	-5.86	101.50	110.88
1	L	294	THR	N-CA-CB	5.86	118.74	110.12
1	B	62	LEU	CB-CA-C	5.86	119.92	109.38
1	B	455	VAL	CB-CA-C	5.86	120.05	112.14
1	C	62	LEU	CB-CA-C	5.86	119.93	109.38
1	L	380	LYS	N-CA-CB	-5.86	101.26	110.69
1	A	59	GLU	N-CA-CB	5.86	118.73	110.12
1	G	455	VAL	CB-CA-C	5.86	120.05	112.14
1	G	517	THR	CB-CA-C	-5.86	101.51	110.88
1	M	294	THR	N-CA-CB	5.86	118.73	110.12
1	I	294	THR	N-CA-CB	5.85	118.73	110.12
1	K	380	LYS	N-CA-CB	-5.85	101.27	110.69
1	H	380	LYS	N-CA-CB	-5.85	101.27	110.69
1	K	67	GLU	CB-CG-CD	5.85	122.55	112.60
1	J	67	GLU	CB-CG-CD	5.85	122.54	112.60
1	K	294	THR	N-CA-CB	5.85	118.72	110.12
1	I	67	GLU	CB-CG-CD	5.85	122.54	112.60
1	C	455	VAL	CB-CA-C	5.84	120.03	112.14
1	M	380	LYS	N-CA-CB	-5.84	101.28	110.69
1	N	294	THR	N-CA-CB	5.84	118.71	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	455	VAL	CB-CA-C	5.84	120.03	112.14
1	N	380	LYS	N-CA-CB	-5.83	101.30	110.69
1	J	380	LYS	N-CA-CB	-5.83	101.31	110.69
1	E	455	VAL	CB-CA-C	5.82	120.00	112.14
1	N	169	VAL	N-CA-CB	5.82	119.31	110.58
1	J	235	PRO	N-CA-CB	5.82	109.68	103.39
1	M	407	VAL	N-CA-CB	5.82	117.36	110.55
1	K	407	VAL	N-CA-CB	5.82	117.36	110.55
1	K	235	PRO	N-CA-CB	5.81	109.67	103.39
1	B	464	VAL	CB-CA-C	-5.81	104.53	111.97
1	N	407	VAL	N-CA-CB	5.81	117.35	110.55
1	N	235	PRO	N-CA-CB	5.81	109.67	103.39
1	C	464	VAL	CB-CA-C	-5.80	104.54	111.97
1	G	266	THR	N-CA-CB	5.80	118.48	110.07
1	H	407	VAL	N-CA-CB	5.80	117.34	110.55
1	L	407	VAL	N-CA-CB	5.80	117.34	110.55
1	A	211	GLY	N-CA-C	-5.80	107.38	114.92
1	J	407	VAL	N-CA-CB	5.80	117.34	110.55
1	L	169	VAL	N-CA-CB	5.79	119.27	110.58
1	H	169	VAL	N-CA-CB	5.79	119.27	110.58
1	G	235	PRO	N-CA-CB	5.79	109.64	103.39
1	E	260	ALA	CA-C-N	5.79	127.96	120.44
1	E	260	ALA	C-N-CA	5.79	127.96	120.44
1	K	169	VAL	N-CA-CB	5.79	119.26	110.58
1	I	407	VAL	N-CA-CB	5.78	117.32	110.55
1	I	169	VAL	N-CA-CB	5.78	119.25	110.58
1	J	517	THR	CA-CB-CG2	5.78	120.33	110.50
1	M	169	VAL	N-CA-CB	5.78	119.25	110.58
1	M	296	THR	N-CA-CB	5.78	118.72	110.16
1	A	464	VAL	CB-CA-C	-5.78	104.57	111.97
1	G	464	VAL	CB-CA-C	-5.78	104.58	111.97
1	K	296	THR	N-CA-CB	5.78	118.71	110.16
1	A	260	ALA	CA-C-N	5.77	127.95	120.44
1	A	260	ALA	C-N-CA	5.77	127.95	120.44
1	H	517	THR	CA-CB-CG2	5.77	120.32	110.50
1	L	296	THR	N-CA-CB	5.77	118.70	110.16
1	F	3	ALA	CB-CA-C	-5.77	98.92	109.54
1	E	175	ILE	CB-CA-C	-5.77	102.02	110.62
1	J	169	VAL	N-CA-CB	5.77	119.23	110.58
1	D	3	ALA	CB-CA-C	-5.77	98.93	109.54
1	C	175	ILE	CB-CA-C	-5.77	102.03	110.62
1	C	211	GLY	N-CA-C	-5.77	107.42	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	517	THR	CA-CB-CG2	5.77	120.30	110.50
1	J	25	ASP	CA-CB-CG	-5.76	106.84	112.60
1	G	175	ILE	CB-CA-C	-5.76	102.04	110.62
1	L	216	GLU	N-CA-CB	-5.76	101.04	110.43
1	K	517	THR	CA-CB-CG2	5.76	120.28	110.50
1	M	216	GLU	N-CA-CB	-5.76	101.05	110.43
1	B	3	ALA	CB-CA-C	-5.75	98.95	109.54
1	G	211	GLY	N-CA-C	-5.75	107.44	114.92
1	H	211	GLY	N-CA-C	-5.75	107.44	114.92
1	E	3	ALA	CB-CA-C	-5.75	98.95	109.54
1	L	517	THR	CA-CB-CG2	5.75	120.28	110.50
1	N	517	THR	CA-CB-CG2	5.75	120.28	110.50
1	H	216	GLU	N-CA-CB	-5.75	101.05	110.43
1	B	211	GLY	N-CA-C	-5.75	107.44	114.92
1	A	285	ARG	N-CA-CB	5.75	118.57	110.12
1	B	260	ALA	CA-C-N	5.75	127.91	120.44
1	B	260	ALA	C-N-CA	5.75	127.91	120.44
1	F	175	ILE	CB-CA-C	-5.75	102.05	110.62
1	N	216	GLU	N-CA-CB	-5.75	101.06	110.43
1	D	175	ILE	CB-CA-C	-5.75	102.06	110.62
1	E	211	GLY	N-CA-C	-5.75	107.45	114.92
1	J	296	THR	N-CA-CB	5.75	118.67	110.16
1	I	296	THR	N-CA-CB	5.74	118.66	110.16
1	G	3	ALA	CB-CA-C	-5.74	98.98	109.54
1	J	216	GLU	N-CA-CB	-5.74	101.07	110.43
1	K	211	GLY	N-CA-C	-5.74	107.46	114.92
1	K	491	MET	CB-CA-C	5.74	120.32	110.79
1	C	260	ALA	CA-C-N	5.74	127.90	120.44
1	C	260	ALA	C-N-CA	5.74	127.90	120.44
1	M	517	THR	CA-CB-CG2	5.74	120.25	110.50
1	C	3	ALA	CB-CA-C	-5.74	98.98	109.54
1	B	175	ILE	CB-CA-C	-5.74	102.08	110.62
1	G	255	GLU	N-CA-C	-5.73	101.16	109.59
1	A	3	ALA	CB-CA-C	-5.73	98.99	109.54
1	A	175	ILE	CB-CA-C	-5.73	102.08	110.62
1	I	216	GLU	N-CA-CB	-5.73	101.09	110.43
1	A	56	VAL	CB-CA-C	-5.73	104.64	111.97
1	F	285	ARG	N-CA-CB	5.73	118.54	110.12
1	D	56	VAL	CB-CA-C	-5.73	104.64	111.97
1	K	216	GLU	N-CA-CB	-5.73	101.10	110.43
1	D	330	THR	CB-CA-C	-5.72	99.24	109.71
1	H	491	MET	CB-CA-C	5.72	120.29	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	330	THR	CB-CA-C	-5.72	99.24	109.71
1	J	211	GLY	N-CA-C	-5.72	107.48	114.92
1	A	215	LEU	N-CA-CB	-5.72	101.48	110.69
1	F	211	GLY	N-CA-C	-5.72	107.49	114.92
1	L	491	MET	CB-CA-C	5.72	120.28	110.79
1	N	296	THR	N-CA-CB	5.72	118.62	110.16
1	C	285	ARG	N-CA-CB	5.71	118.52	110.12
1	D	464	VAL	CB-CA-C	-5.71	104.66	111.97
1	F	56	VAL	CB-CA-C	-5.71	104.66	111.97
1	C	56	VAL	CB-CA-C	-5.71	104.66	111.97
1	D	211	GLY	N-CA-C	-5.71	107.49	114.92
1	I	491	MET	CB-CA-C	5.71	120.27	110.79
1	N	491	MET	CB-CA-C	5.71	120.27	110.79
1	I	211	GLY	N-CA-C	-5.71	107.49	114.92
1	D	260	ALA	CA-C-N	5.71	127.86	120.44
1	D	260	ALA	C-N-CA	5.71	127.86	120.44
1	B	330	THR	CB-CA-C	-5.71	99.27	109.71
1	C	330	THR	CB-CA-C	-5.71	99.27	109.71
1	D	285	ARG	N-CA-CB	5.71	118.51	110.12
1	I	285	ARG	N-CA-CB	5.71	118.51	110.12
1	M	25	ASP	CA-CB-CG	-5.71	106.89	112.60
1	A	330	THR	CB-CA-C	-5.70	99.27	109.71
1	H	296	THR	N-CA-CB	5.70	118.60	110.16
1	K	25	ASP	CA-CB-CG	-5.70	106.90	112.60
1	L	211	GLY	N-CA-C	-5.70	107.51	114.92
1	G	285	ARG	N-CA-CB	5.70	118.50	110.12
1	B	56	VAL	CB-CA-C	-5.70	104.67	111.97
1	B	285	ARG	N-CA-CB	5.70	118.50	110.12
1	N	211	GLY	N-CA-C	-5.70	107.51	114.92
1	B	523	ASP	N-CA-CB	5.70	118.38	110.17
1	C	523	ASP	N-CA-CB	5.70	118.38	110.17
1	G	523	ASP	N-CA-CB	5.70	118.38	110.17
1	F	464	VAL	CB-CA-C	-5.70	104.68	111.97
1	G	56	VAL	CB-CA-C	-5.70	104.68	111.97
1	I	416	GLY	N-CA-C	-5.70	106.31	115.08
1	J	416	GLY	N-CA-C	-5.69	106.31	115.08
1	E	285	ARG	N-CA-CB	5.69	118.49	110.12
1	G	330	THR	CB-CA-C	-5.69	99.29	109.71
1	H	25	ASP	CA-CB-CG	-5.69	106.91	112.60
1	M	211	GLY	N-CA-C	-5.69	107.52	114.92
1	M	285	ARG	N-CA-CB	5.69	118.49	110.12
1	B	153	ASN	CA-CB-CG	-5.69	106.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	523	ASP	N-CA-CB	5.69	118.36	110.17
1	H	285	ARG	N-CA-CB	5.69	118.48	110.12
1	E	523	ASP	N-CA-CB	5.69	118.36	110.17
1	E	330	THR	CB-CA-C	-5.68	99.31	109.71
1	J	285	ARG	N-CA-CB	5.68	118.48	110.12
1	M	416	GLY	N-CA-C	-5.68	106.33	115.08
1	E	56	VAL	CB-CA-C	-5.68	104.70	111.97
1	F	263	VAL	N-CA-CB	5.68	117.20	110.55
1	A	422	VAL	N-CA-CB	5.68	118.27	110.54
1	J	491	MET	CB-CA-C	5.68	120.22	110.79
1	M	491	MET	CB-CA-C	5.68	120.22	110.79
1	B	272	LYS	CB-CA-C	5.68	119.36	109.65
1	D	523	ASP	N-CA-CB	5.67	118.34	110.17
1	F	306	GLY	N-CA-C	-5.67	107.49	115.32
1	K	416	GLY	N-CA-C	-5.67	106.34	115.08
1	L	285	ARG	N-CA-CB	5.67	118.46	110.12
1	C	272	LYS	CB-CA-C	5.67	119.35	109.65
1	E	422	VAL	N-CA-CB	5.67	118.25	110.54
1	C	153	ASN	CA-CB-CG	-5.67	106.93	112.60
1	D	306	GLY	N-CA-C	-5.67	107.50	115.32
1	N	285	ARG	N-CA-CB	5.67	118.45	110.12
1	B	422	VAL	N-CA-CB	5.67	118.25	110.54
1	F	153	ASN	CA-CB-CG	-5.67	106.93	112.60
1	N	25	ASP	CA-CB-CG	-5.67	106.93	112.60
1	D	153	ASN	CA-CB-CG	-5.67	106.94	112.60
1	F	422	VAL	N-CA-CB	5.66	118.24	110.54
1	C	422	VAL	N-CA-CB	5.66	118.24	110.54
1	E	306	GLY	N-CA-C	-5.66	107.51	115.32
1	H	416	GLY	N-CA-C	-5.66	106.36	115.08
1	N	416	GLY	N-CA-C	-5.66	106.36	115.08
1	G	153	ASN	CA-CB-CG	-5.66	106.94	112.60
1	D	422	VAL	N-CA-CB	5.66	118.24	110.54
1	B	306	GLY	N-CA-C	-5.66	107.51	115.32
1	K	285	ARG	N-CA-CB	5.66	118.43	110.12
1	E	272	LYS	CB-CA-C	5.65	119.32	109.65
1	G	306	GLY	N-CA-C	-5.65	107.52	115.32
1	L	25	ASP	CA-CB-CG	-5.65	106.95	112.60
1	L	306	GLY	N-CA-C	-5.65	107.46	115.43
1	A	523	ASP	N-CA-CB	5.65	118.31	110.17
1	E	464	VAL	CB-CA-C	-5.65	104.74	111.97
1	I	25	ASP	CA-CB-CG	-5.65	106.95	112.60
1	F	272	LYS	CB-CA-C	5.65	119.31	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	416	GLY	N-CA-C	-5.65	106.38	115.08
1	A	306	GLY	N-CA-C	-5.64	107.53	115.32
1	D	272	LYS	CB-CA-C	5.64	119.30	109.65
1	E	153	ASN	CA-CB-CG	-5.64	106.96	112.60
1	C	306	GLY	N-CA-C	-5.64	107.54	115.32
1	J	306	GLY	N-CA-C	-5.63	107.48	115.43
1	A	361	ASP	CB-CA-C	5.63	120.13	110.79
1	F	361	ASP	CB-CA-C	5.62	120.13	110.79
1	E	258	ALA	O-C-N	-5.62	115.11	122.59
1	M	306	GLY	N-CA-C	-5.62	107.50	115.43
1	D	479	ASN	CB-CA-C	5.62	119.29	110.19
1	F	230	ILE	CA-CB-CG2	-5.62	100.95	110.50
1	F	253	ASP	CA-CB-CG	-5.62	106.98	112.60
1	G	361	ASP	CB-CA-C	5.62	120.11	110.79
1	G	422	VAL	N-CA-CB	5.62	118.18	110.54
1	A	479	ASN	CB-CA-C	5.61	119.28	110.19
1	K	306	GLY	N-CA-C	-5.61	107.52	115.43
1	N	272	LYS	N-CA-CB	5.61	118.22	109.97
1	A	241	ALA	N-CA-C	-5.61	106.79	113.97
1	H	272	LYS	N-CA-CB	5.61	118.22	109.97
1	I	272	LYS	N-CA-CB	5.61	118.22	109.97
1	L	272	LYS	N-CA-CB	5.61	118.21	109.97
1	L	310	GLU	N-CA-CB	-5.61	101.88	110.12
1	L	107	VAL	N-CA-CB	5.60	118.16	110.54
1	N	306	GLY	N-CA-C	-5.60	107.53	115.43
1	C	361	ASP	CB-CA-C	5.60	120.09	110.79
1	D	361	ASP	CB-CA-C	5.60	120.09	110.79
1	H	306	GLY	N-CA-C	-5.60	107.53	115.43
1	J	107	VAL	N-CA-CB	5.60	118.16	110.54
1	M	107	VAL	N-CA-CB	5.60	118.15	110.54
1	A	153	ASN	CA-CB-CG	-5.60	107.00	112.60
1	A	272	LYS	CB-CA-C	5.60	119.22	109.65
1	C	479	ASN	CB-CA-C	5.60	119.26	110.19
1	K	62	LEU	CB-CA-C	5.60	119.45	109.38
1	K	107	VAL	N-CA-CB	5.60	118.15	110.54
1	B	479	ASN	CB-CA-C	5.60	119.25	110.19
1	B	215	LEU	N-CA-CB	-5.59	101.68	110.69
1	B	361	ASP	CB-CA-C	5.59	120.08	110.79
1	F	215	LEU	N-CA-CB	-5.59	101.68	110.69
1	I	306	GLY	N-CA-C	-5.59	107.54	115.43
1	D	215	LEU	N-CA-CB	-5.59	101.69	110.69
1	E	479	ASN	CB-CA-C	5.59	119.25	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	107	VAL	N-CA-CB	5.59	118.15	110.54
1	M	272	LYS	N-CA-CB	5.59	118.19	109.97
1	E	215	LEU	N-CA-CB	-5.59	101.69	110.69
1	E	361	ASP	CB-CA-C	5.59	120.07	110.79
1	F	479	ASN	CB-CA-C	5.59	119.24	110.19
1	N	107	VAL	N-CA-CB	5.59	118.14	110.54
1	I	62	LEU	CB-CA-C	5.58	119.43	109.38
1	J	272	LYS	N-CA-CB	5.58	118.17	109.97
1	G	479	ASN	CB-CA-C	5.58	119.22	110.19
1	I	107	VAL	N-CA-CB	5.58	118.12	110.54
1	C	215	LEU	N-CA-CB	-5.57	101.72	110.69
1	H	310	GLU	N-CA-CB	-5.57	101.93	110.12
1	J	62	LEU	CB-CA-C	5.57	119.41	109.38
1	K	272	LYS	N-CA-CB	5.57	118.15	109.97
1	M	310	GLU	N-CA-CB	-5.57	101.94	110.12
1	D	47	PRO	N-CA-CB	-5.56	98.51	103.35
1	F	311	LYS	N-CA-CB	5.56	118.29	110.12
1	H	62	LEU	CB-CA-C	5.56	119.39	109.38
1	J	310	GLU	N-CA-CB	-5.56	101.95	110.12
1	K	310	GLU	N-CA-CB	-5.56	101.95	110.12
1	M	62	LEU	CB-CA-C	5.55	119.38	109.38
1	L	200	LEU	CB-CA-C	-5.55	102.17	110.88
1	H	200	LEU	CB-CA-C	-5.55	102.17	110.88
1	N	62	LEU	CB-CA-C	5.55	119.37	109.38
1	C	258	ALA	O-C-N	-5.54	115.22	122.59
1	N	310	GLU	N-CA-CB	-5.54	101.97	110.12
1	A	258	ALA	O-C-N	-5.54	115.22	122.59
1	G	311	LYS	N-CA-CB	5.54	118.26	110.12
1	I	227	ILE	N-CA-CB	5.54	117.97	111.66
1	K	200	LEU	CB-CA-C	-5.54	102.19	110.88
1	B	258	ALA	O-C-N	-5.54	115.23	122.59
1	N	200	LEU	CB-CA-C	-5.54	102.19	110.88
1	J	200	LEU	CB-CA-C	-5.53	102.19	110.88
1	L	77	VAL	CB-CA-C	5.53	119.61	112.14
1	A	63	GLU	CB-CA-C	-5.53	101.61	110.79
1	G	47	PRO	N-CA-CB	-5.53	98.54	103.35
1	L	359	ASP	CA-CB-CG	-5.53	107.07	112.60
1	I	200	LEU	CB-CA-C	-5.53	102.20	110.88
1	L	62	LEU	CB-CA-C	5.53	119.33	109.38
1	B	47	PRO	N-CA-CB	-5.53	98.54	103.35
1	K	77	VAL	CB-CA-C	5.53	119.60	112.14
1	M	359	ASP	CA-CB-CG	-5.52	107.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	479	ASN	CB-CA-C	5.52	119.14	110.19
1	C	185	ASP	N-CA-CB	-5.52	102.22	110.17
1	D	311	LYS	N-CA-CB	5.52	118.23	110.12
1	E	63	GLU	CB-CA-C	-5.52	101.63	110.79
1	M	77	VAL	CB-CA-C	5.52	119.59	112.14
1	K	479	ASN	CB-CA-C	5.52	119.13	110.19
1	M	200	LEU	CB-CA-C	-5.52	102.22	110.88
1	B	63	GLU	CB-CA-C	-5.51	101.64	110.79
1	C	63	GLU	CB-CA-C	-5.51	101.63	110.79
1	L	479	ASN	CB-CA-C	5.51	119.12	110.19
1	D	416	GLY	N-CA-C	-5.51	106.59	115.08
1	N	77	VAL	CB-CA-C	5.51	119.58	112.14
1	D	63	GLU	CB-CA-C	-5.51	101.64	110.79
1	D	258	ALA	O-C-N	-5.51	115.26	122.59
1	F	185	ASP	N-CA-CB	-5.51	102.24	110.17
1	H	479	ASN	CB-CA-C	5.51	119.12	110.19
1	I	479	ASN	CB-CA-C	5.51	119.12	110.19
1	G	416	GLY	N-CA-C	-5.51	106.60	115.08
1	I	77	VAL	CB-CA-C	5.50	119.57	112.14
1	G	63	GLU	CB-CA-C	-5.50	101.66	110.79
1	H	77	VAL	CB-CA-C	5.50	119.57	112.14
1	M	479	ASN	CB-CA-C	5.50	119.10	110.19
1	B	185	ASP	N-CA-CB	-5.50	102.25	110.17
1	J	479	ASN	CB-CA-C	5.50	119.10	110.19
1	E	185	ASP	N-CA-CB	-5.50	102.26	110.17
1	G	185	ASP	N-CA-CB	-5.50	102.26	110.17
1	I	359	ASP	CA-CB-CG	-5.50	107.11	112.60
1	B	311	LYS	N-CA-CB	5.49	118.20	110.12
1	C	311	LYS	N-CA-CB	5.49	118.19	110.12
1	G	262	LEU	CB-CA-C	5.49	119.50	110.88
1	A	185	ASP	N-CA-CB	-5.49	102.26	110.17
1	D	185	ASP	N-CA-CB	-5.49	102.26	110.17
1	D	90	THR	N-CA-CB	5.49	118.19	110.12
1	F	416	GLY	N-CA-C	-5.49	106.62	115.08
1	B	416	GLY	N-CA-C	-5.49	106.63	115.08
1	E	417	VAL	CA-CB-CG2	-5.49	101.07	110.40
1	F	63	GLU	CB-CA-C	-5.49	101.68	110.79
1	F	417	VAL	CA-CB-CG2	-5.49	101.07	110.40
1	E	416	GLY	N-CA-C	-5.49	106.63	115.08
1	L	227	ILE	N-CA-CB	5.49	117.91	111.66
1	A	311	LYS	N-CA-CB	5.48	118.18	110.12
1	A	416	GLY	N-CA-C	-5.48	106.64	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	PRO	N-CA-CB	-5.48	98.58	103.35
1	H	417	VAL	CA-CB-CG2	-5.48	101.08	110.40
1	J	77	VAL	CB-CA-C	5.48	119.54	112.14
1	N	359	ASP	CA-CB-CG	-5.48	107.12	112.60
1	K	417	VAL	CA-CB-CG2	-5.48	101.08	110.40
1	F	47	PRO	N-CA-CB	-5.48	98.58	103.35
1	L	277	LYS	CB-CA-C	5.48	119.54	109.46
1	C	47	PRO	N-CA-CB	-5.48	98.58	103.35
1	E	47	PRO	N-CA-CB	-5.48	98.58	103.35
1	H	359	ASP	CA-CB-CG	-5.47	107.13	112.60
1	J	277	LYS	CB-CA-C	5.47	119.53	109.46
1	K	277	LYS	CB-CA-C	5.47	119.53	109.46
1	D	417	VAL	CA-CB-CG2	-5.47	101.09	110.40
1	H	227	ILE	N-CA-CB	5.47	117.90	111.66
1	I	417	VAL	CA-CB-CG2	-5.47	101.10	110.40
1	J	359	ASP	CA-CB-CG	-5.47	107.13	112.60
1	J	417	VAL	CA-CB-CG2	-5.47	101.10	110.40
1	K	359	ASP	CA-CB-CG	-5.47	107.13	112.60
1	C	152	ALA	CB-CA-C	5.47	120.75	110.63
1	C	90	THR	N-CA-CB	5.47	118.16	110.12
1	E	311	LYS	N-CA-CB	5.46	118.15	110.12
1	M	277	LYS	CB-CA-C	5.46	119.52	109.46
1	N	277	LYS	CB-CA-C	5.46	119.51	109.46
1	M	417	VAL	CA-CB-CG2	-5.46	101.12	110.40
1	B	90	THR	N-CA-CB	5.46	118.14	110.12
1	B	417	VAL	CA-CB-CG2	-5.46	101.12	110.40
1	N	422	VAL	N-CA-CB	5.46	117.96	110.54
1	H	277	LYS	CB-CA-C	5.46	119.50	109.46
1	G	152	ALA	CB-CA-C	5.46	120.72	110.63
1	J	422	VAL	N-CA-CB	5.46	117.96	110.54
1	L	417	VAL	CA-CB-CG2	-5.45	101.13	110.40
1	E	152	ALA	CB-CA-C	5.45	120.71	110.63
1	F	152	ALA	CB-CA-C	5.45	120.71	110.63
1	H	422	VAL	N-CA-CB	5.45	117.95	110.54
1	J	227	ILE	N-CA-CB	5.45	117.87	111.66
1	K	227	ILE	N-CA-CB	5.45	117.87	111.66
1	K	422	VAL	N-CA-CB	5.45	117.95	110.54
1	F	90	THR	N-CA-CB	5.45	118.13	110.12
1	E	68	ASN	CA-CB-CG	5.45	118.05	112.60
1	N	227	ILE	N-CA-CB	5.44	117.86	111.66
1	A	417	VAL	CA-CB-CG2	-5.44	101.15	110.40
1	B	152	ALA	CB-CA-C	5.44	120.69	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	416	GLY	N-CA-C	-5.44	106.70	115.08
1	G	417	VAL	CA-CB-CG2	-5.44	101.15	110.40
1	I	277	LYS	CB-CA-C	5.44	119.47	109.46
1	A	152	ALA	CB-CA-C	5.44	120.69	110.63
1	M	227	ILE	N-CA-CB	5.44	117.86	111.66
1	A	90	THR	N-CA-CB	5.44	118.11	110.12
1	C	417	VAL	CA-CB-CG2	-5.44	101.16	110.40
1	M	422	VAL	N-CA-CB	5.44	117.93	110.54
1	N	417	VAL	CA-CB-CG2	-5.44	101.16	110.40
1	I	422	VAL	N-CA-CB	5.43	117.93	110.54
1	M	330	THR	CB-CA-C	-5.43	99.76	109.71
1	D	152	ALA	CB-CA-C	5.43	120.68	110.63
1	G	90	THR	N-CA-CB	5.43	118.11	110.12
1	C	461	GLU	CB-CG-CD	5.43	121.83	112.60
1	L	330	THR	CB-CA-C	-5.43	99.78	109.71
1	J	330	THR	CB-CA-C	-5.43	99.78	109.71
1	E	90	THR	N-CA-CB	5.43	118.10	110.12
1	E	225	LYS	CB-CA-C	5.43	119.44	109.46
1	H	330	THR	CB-CA-C	-5.43	99.78	109.71
1	I	311	LYS	N-CA-CB	5.43	118.10	110.12
1	B	461	GLU	CB-CG-CD	5.42	121.82	112.60
1	K	330	THR	CB-CA-C	-5.42	99.78	109.71
1	A	225	LYS	CB-CA-C	5.42	119.43	109.46
1	A	68	ASN	CA-CB-CG	5.42	118.02	112.60
1	G	68	ASN	CA-CB-CG	5.42	118.02	112.60
1	I	330	THR	CB-CA-C	-5.42	99.79	109.71
1	L	422	VAL	N-CA-CB	5.42	117.91	110.54
1	F	68	ASN	CA-CB-CG	5.42	118.02	112.60
1	C	68	ASN	CA-CB-CG	5.42	118.02	112.60
1	F	225	LYS	CB-CA-C	5.42	119.42	109.46
1	N	266	THR	N-CA-CB	5.41	117.91	110.07
1	H	266	THR	N-CA-CB	5.41	117.91	110.07
1	G	263	VAL	CB-CA-C	-5.41	105.05	111.97
1	D	225	LYS	CB-CA-C	5.40	119.40	109.46
1	G	225	LYS	CB-CA-C	5.40	119.40	109.46
1	B	68	ASN	CA-CB-CG	5.40	118.00	112.60
1	J	266	THR	N-CA-CB	5.40	117.90	110.07
1	L	266	THR	N-CA-CB	5.40	117.89	110.07
1	N	330	THR	CB-CA-C	-5.40	99.84	109.71
1	K	266	THR	N-CA-CB	5.39	117.89	110.07
1	G	461	GLU	CB-CG-CD	5.39	121.77	112.60
1	M	266	THR	N-CA-CB	5.39	117.88	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	440	ILE	CB-CA-C	-5.39	104.87	112.14
1	F	461	GLU	CB-CG-CD	5.38	121.75	112.60
1	D	68	ASN	CA-CB-CG	5.38	117.98	112.60
1	A	461	GLU	CB-CG-CD	5.38	121.75	112.60
1	I	266	THR	N-CA-CB	5.38	117.87	110.07
1	L	253	ASP	CA-C-N	-5.38	116.12	123.12
1	L	253	ASP	C-N-CA	-5.38	116.12	123.12
1	D	461	GLU	CB-CG-CD	5.38	121.75	112.60
1	B	225	LYS	CB-CA-C	5.37	119.34	109.46
1	C	292	ILE	N-CA-CB	5.37	117.85	110.54
1	C	225	LYS	CB-CA-C	5.37	119.34	109.46
1	A	440	ILE	CB-CA-C	-5.37	104.89	112.14
1	F	292	ILE	N-CA-CB	5.37	117.84	110.54
1	I	292	ILE	N-CA-CB	5.37	117.84	110.54
1	E	292	ILE	N-CA-CB	5.36	117.83	110.54
1	E	461	GLU	CB-CG-CD	5.36	121.71	112.60
1	N	253	ASP	CA-C-N	-5.36	116.15	123.12
1	N	253	ASP	C-N-CA	-5.36	116.15	123.12
1	C	155	ASP	CB-CA-C	5.36	120.41	111.30
1	I	253	ASP	CA-C-N	-5.36	116.16	123.12
1	I	253	ASP	C-N-CA	-5.36	116.16	123.12
1	D	240	VAL	CA-C-N	5.35	130.77	122.26
1	D	240	VAL	C-N-CA	5.35	130.77	122.26
1	M	253	ASP	CA-C-N	-5.35	116.16	123.12
1	M	253	ASP	C-N-CA	-5.35	116.16	123.12
1	A	483	GLU	N-CA-CB	5.35	120.43	112.30
1	D	56	VAL	N-CA-CB	5.35	116.81	110.55
1	G	246	PRO	N-CA-C	5.35	119.43	111.41
1	G	292	ILE	N-CA-CB	5.35	117.81	110.54
1	B	483	GLU	N-CA-CB	5.34	120.42	112.30
1	C	188	ASP	CA-CB-CG	5.34	117.94	112.60
1	D	292	ILE	N-CA-CB	5.34	117.81	110.54
1	G	483	GLU	N-CA-CB	5.34	120.42	112.30
1	C	483	GLU	N-CA-CB	5.34	120.42	112.30
1	F	483	GLU	N-CA-CB	5.34	120.42	112.30
1	K	253	ASP	CA-C-N	-5.34	116.17	123.12
1	K	253	ASP	C-N-CA	-5.34	116.17	123.12
1	D	155	ASP	CB-CA-C	5.34	120.38	111.30
1	D	483	GLU	N-CA-CB	5.34	120.42	112.30
1	A	155	ASP	CB-CA-C	5.34	120.38	111.30
1	G	155	ASP	CB-CA-C	5.34	120.37	111.30
1	K	292	ILE	N-CA-CB	5.34	117.80	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	77	VAL	CB-CA-C	5.33	119.34	112.14
1	E	77	VAL	CB-CA-C	5.33	119.34	112.14
1	E	440	ILE	CB-CA-C	-5.33	104.94	112.14
1	L	292	ILE	N-CA-CB	5.33	117.79	110.54
1	A	56	VAL	N-CA-CB	5.33	116.79	110.55
1	E	483	GLU	N-CA-CB	5.33	120.41	112.30
1	F	77	VAL	CB-CA-C	5.33	119.34	112.14
1	F	440	ILE	CB-CA-C	-5.33	104.94	112.14
1	J	253	ASP	CA-C-N	-5.33	116.19	123.12
1	J	253	ASP	C-N-CA	-5.33	116.19	123.12
1	M	110	GLY	N-CA-C	-5.33	107.92	115.43
1	F	155	ASP	CB-CA-C	5.33	120.36	111.30
1	C	240	VAL	CA-C-N	5.33	130.73	122.26
1	C	240	VAL	C-N-CA	5.33	130.73	122.26
1	L	440	ILE	CB-CA-C	-5.33	104.95	112.14
1	B	77	VAL	CB-CA-C	5.32	119.33	112.14
1	E	155	ASP	CB-CA-C	5.32	120.35	111.30
1	H	110	GLY	N-CA-C	-5.32	107.92	115.43
1	B	240	VAL	CA-C-N	5.32	130.72	122.26
1	B	240	VAL	C-N-CA	5.32	130.72	122.26
1	I	110	GLY	N-CA-C	-5.32	107.93	115.43
1	G	440	ILE	CB-CA-C	-5.32	104.96	112.14
1	E	240	VAL	CA-C-N	5.32	130.71	122.26
1	E	240	VAL	C-N-CA	5.32	130.71	122.26
1	G	77	VAL	CB-CA-C	5.32	119.32	112.14
1	B	292	ILE	N-CA-CB	5.32	117.77	110.54
1	C	440	ILE	CB-CA-C	-5.32	104.96	112.14
1	I	440	ILE	CB-CA-C	-5.32	104.96	112.14
1	M	292	ILE	N-CA-CB	5.32	117.77	110.54
1	N	292	ILE	N-CA-CB	5.32	117.77	110.54
1	C	77	VAL	CB-CA-C	5.31	119.31	112.14
1	C	435	ASP	CA-CB-CG	5.31	117.91	112.60
1	H	253	ASP	CA-C-N	-5.31	116.21	123.12
1	H	253	ASP	C-N-CA	-5.31	116.21	123.12
1	A	292	ILE	N-CA-CB	5.31	117.77	110.54
1	E	188	ASP	CA-CB-CG	5.31	117.91	112.60
1	G	435	ASP	CA-CB-CG	5.31	117.91	112.60
1	F	435	ASP	CA-CB-CG	5.31	117.91	112.60
1	G	56	VAL	N-CA-CB	5.31	116.76	110.55
1	H	292	ILE	N-CA-CB	5.31	117.76	110.54
1	N	110	GLY	N-CA-C	-5.31	107.95	115.43
1	A	77	VAL	CB-CA-C	5.30	119.30	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	ILE	CB-CA-C	-5.30	104.98	112.14
1	J	292	ILE	N-CA-CB	5.30	117.75	110.54
1	B	435	ASP	CA-CB-CG	5.30	117.90	112.60
1	J	110	GLY	N-CA-C	-5.30	107.95	115.43
1	K	110	GLY	N-CA-C	-5.30	107.95	115.43
1	B	56	VAL	N-CA-CB	5.30	116.75	110.55
1	B	155	ASP	CB-CA-C	5.30	120.31	111.30
1	D	126	ALA	CB-CA-C	5.30	119.58	110.79
1	E	126	ALA	CB-CA-C	5.30	119.58	110.79
1	F	240	VAL	CA-C-N	5.30	130.68	122.26
1	F	240	VAL	C-N-CA	5.30	130.68	122.26
1	K	440	ILE	CB-CA-C	-5.30	104.99	112.14
1	L	110	GLY	N-CA-C	-5.30	107.96	115.43
1	N	440	ILE	CB-CA-C	-5.30	104.99	112.14
1	F	126	ALA	CB-CA-C	5.29	119.58	110.79
1	C	126	ALA	CB-CA-C	5.29	119.57	110.79
1	H	311	LYS	N-CA-CB	5.29	117.90	110.12
1	J	440	ILE	CB-CA-C	-5.29	105.00	112.14
1	A	126	ALA	CB-CA-C	5.29	119.56	110.79
1	B	126	ALA	CB-CA-C	5.29	119.56	110.79
1	D	188	ASP	CA-CB-CG	5.28	117.88	112.60
1	G	126	ALA	CB-CA-C	5.28	119.56	110.79
1	A	188	ASP	CA-CB-CG	5.28	117.88	112.60
1	K	230	ILE	CB-CA-C	-5.28	105.01	112.14
1	F	359	ASP	CA-CB-CG	-5.28	107.32	112.60
1	E	56	VAL	N-CA-CB	5.27	116.72	110.55
1	I	235	PRO	N-CA-CB	5.27	109.08	103.39
1	H	440	ILE	CB-CA-C	-5.27	105.03	112.14
1	D	435	ASP	CA-CB-CG	5.27	117.87	112.60
1	M	440	ILE	CB-CA-C	-5.27	105.03	112.14
1	N	311	LYS	N-CA-CB	5.27	117.86	110.12
1	J	230	ILE	CB-CA-C	-5.26	105.03	112.14
1	C	56	VAL	N-CA-CB	5.26	116.71	110.55
1	F	188	ASP	CA-CB-CG	5.26	117.86	112.60
1	M	311	LYS	N-CA-CB	5.26	117.85	110.12
1	E	435	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	435	ASP	CA-CB-CG	5.25	117.86	112.60
1	F	56	VAL	N-CA-CB	5.25	116.70	110.55
1	J	311	LYS	N-CA-CB	5.25	117.84	110.12
1	L	311	LYS	N-CA-CB	5.25	117.84	110.12
1	N	230	ILE	CB-CA-C	-5.25	105.05	112.14
1	E	359	ASP	CA-CB-CG	-5.25	107.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	230	ILE	CB-CA-C	-5.25	105.05	112.14
1	C	359	ASP	CA-CB-CG	-5.25	107.35	112.60
1	B	188	ASP	CA-CB-CG	5.25	117.85	112.60
1	G	359	ASP	CA-CB-CG	-5.25	107.35	112.60
1	H	230	ILE	CB-CA-C	-5.25	105.06	112.14
1	K	311	LYS	N-CA-CB	5.24	117.83	110.12
1	B	359	ASP	CA-CB-CG	-5.24	107.36	112.60
1	L	230	ILE	CB-CA-C	-5.24	105.07	112.14
1	G	188	ASP	CA-CB-CG	5.22	117.83	112.60
1	F	291	ASP	CA-CB-CG	-5.22	107.38	112.60
1	L	40	LEU	N-CA-CB	-5.22	102.47	111.55
1	M	40	LEU	N-CA-CB	-5.22	102.47	111.55
1	A	359	ASP	CA-CB-CG	-5.22	107.38	112.60
1	K	483	GLU	N-CA-CB	5.22	120.23	112.30
1	N	40	LEU	N-CA-CB	-5.22	102.47	111.55
1	A	291	ASP	CA-CB-CG	-5.22	107.38	112.60
1	H	40	LEU	N-CA-CB	-5.21	102.48	111.55
1	J	40	LEU	N-CA-CB	-5.21	102.48	111.55
1	B	375	GLY	N-CA-C	-5.21	106.88	114.90
1	D	359	ASP	CA-CB-CG	-5.21	107.39	112.60
1	E	438	VAL	N-CA-CB	5.21	117.63	110.54
1	G	291	ASP	CA-CB-CG	-5.21	107.39	112.60
1	G	375	GLY	N-CA-C	-5.21	106.87	114.90
1	B	291	ASP	CA-CB-CG	-5.21	107.39	112.60
1	E	49	ILE	N-CA-CB	-5.21	102.33	111.39
1	I	483	GLU	N-CA-CB	5.21	120.21	112.30
1	M	90	THR	N-CA-CB	5.21	117.77	110.12
1	J	415	GLY	N-CA-C	-5.21	108.14	115.32
1	D	438	VAL	N-CA-CB	5.20	117.62	110.54
1	F	196	ASP	CB-CA-C	5.20	119.46	110.77
1	F	375	GLY	N-CA-C	-5.20	106.89	114.90
1	F	438	VAL	N-CA-CB	5.20	117.62	110.54
1	M	64	ASP	CB-CA-C	5.20	118.55	109.65
1	M	483	GLU	N-CA-CB	5.20	120.21	112.30
1	N	483	GLU	N-CA-CB	5.20	120.21	112.30
1	D	291	ASP	CA-CB-CG	-5.20	107.40	112.60
1	B	196	ASP	CB-CA-C	5.20	119.45	110.77
1	I	40	LEU	N-CA-CB	-5.20	102.50	111.55
1	C	49	ILE	N-CA-CB	-5.20	102.35	111.39
1	K	40	LEU	N-CA-CB	-5.20	102.50	111.55
1	N	64	ASP	CB-CA-C	5.20	118.54	109.65
1	C	291	ASP	CA-CB-CG	-5.20	107.41	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	49	ILE	N-CA-CB	-5.20	102.35	111.39
1	H	436	GLN	N-CA-CB	5.20	117.76	110.12
1	A	49	ILE	N-CA-CB	-5.19	102.35	111.39
1	F	49	ILE	N-CA-CB	-5.19	102.36	111.39
1	C	438	VAL	N-CA-CB	5.19	117.60	110.54
1	G	49	ILE	N-CA-CB	-5.19	102.36	111.39
1	K	64	ASP	CB-CA-C	5.19	118.53	109.65
1	L	438	VAL	N-CA-CB	5.19	117.60	110.54
1	L	483	GLU	N-CA-CB	5.19	120.19	112.30
1	E	196	ASP	CB-CA-C	5.19	119.43	110.77
1	H	64	ASP	CB-CA-C	5.19	118.52	109.65
1	G	196	ASP	CB-CA-C	5.19	119.43	110.77
1	E	291	ASP	CA-CB-CG	-5.18	107.42	112.60
1	I	438	VAL	N-CA-CB	5.18	117.59	110.54
1	H	438	VAL	N-CA-CB	5.18	117.58	110.54
1	L	64	ASP	CB-CA-C	5.18	118.51	109.65
1	B	49	ILE	N-CA-CB	-5.18	102.38	111.39
1	C	519	CYS	N-CA-CB	-5.18	102.23	111.08
1	F	110	GLY	N-CA-C	-5.18	108.08	115.64
1	J	64	ASP	CB-CA-C	5.18	118.50	109.65
1	C	375	GLY	N-CA-C	-5.17	106.93	114.90
1	H	483	GLU	N-CA-CB	5.17	120.16	112.30
1	J	483	GLU	N-CA-CB	5.17	120.17	112.30
1	G	519	CYS	N-CA-CB	-5.17	102.23	111.08
1	D	375	GLY	N-CA-C	-5.17	106.94	114.90
1	I	415	GLY	N-CA-C	-5.17	108.19	115.32
1	B	438	VAL	N-CA-CB	5.17	117.57	110.54
1	D	110	GLY	N-CA-C	-5.17	108.10	115.64
1	A	196	ASP	CB-CA-C	5.16	119.39	110.77
1	D	519	CYS	N-CA-CB	-5.16	102.25	111.08
1	I	230	ILE	CB-CA-C	-5.16	105.17	112.14
1	K	415	GLY	N-CA-C	-5.16	108.19	115.32
1	K	436	GLN	N-CA-CB	5.16	117.71	110.12
1	E	437	ASN	N-CA-CB	5.16	117.49	110.01
1	K	90	THR	N-CA-CB	5.16	117.71	110.12
1	A	519	CYS	N-CA-CB	-5.16	102.26	111.08
1	C	196	ASP	CB-CA-C	5.16	119.38	110.77
1	I	64	ASP	CB-CA-C	5.16	118.47	109.65
1	J	436	GLN	N-CA-CB	5.16	117.70	110.12
1	J	438	VAL	N-CA-CB	5.16	117.56	110.54
1	N	438	VAL	N-CA-CB	5.16	117.56	110.54
1	E	110	GLY	N-CA-C	-5.16	108.11	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	519	CYS	N-CA-CB	-5.16	102.26	111.08
1	I	90	THR	N-CA-CB	5.16	117.70	110.12
1	F	437	ASN	N-CA-CB	5.15	117.48	110.01
1	G	169	VAL	CB-CA-C	5.15	119.09	112.14
1	H	415	GLY	N-CA-C	-5.15	108.21	115.32
1	L	415	GLY	N-CA-C	-5.15	108.21	115.32
1	M	436	GLN	N-CA-CB	5.15	117.69	110.12
1	D	437	ASN	N-CA-CB	5.15	117.48	110.01
1	I	436	GLN	N-CA-CB	5.15	117.69	110.12
1	J	90	THR	N-CA-CB	5.15	117.69	110.12
1	L	90	THR	N-CA-CB	5.15	117.69	110.12
1	E	519	CYS	N-CA-CB	-5.15	102.28	111.08
1	I	263	VAL	N-CA-CB	5.15	116.58	110.55
1	B	373	ALA	N-CA-C	-5.15	105.56	111.07
1	D	196	ASP	CB-CA-C	5.15	119.37	110.77
1	G	373	ALA	N-CA-C	-5.15	105.56	111.07
1	G	438	VAL	N-CA-CB	5.15	117.54	110.54
1	A	375	GLY	N-CA-C	-5.15	106.97	114.90
1	N	436	GLN	N-CA-CB	5.15	117.69	110.12
1	A	437	ASN	N-CA-CB	5.14	117.47	110.01
1	D	169	VAL	CB-CA-C	5.14	119.08	112.14
1	G	437	ASN	N-CA-CB	5.14	117.47	110.01
1	M	415	GLY	N-CA-C	-5.14	108.22	115.32
1	K	438	VAL	N-CA-CB	5.14	117.53	110.54
1	M	438	VAL	N-CA-CB	5.14	117.53	110.54
1	A	438	VAL	N-CA-CB	5.14	117.53	110.54
1	B	437	ASN	N-CA-CB	5.14	117.46	110.01
1	C	437	ASN	N-CA-CB	5.14	117.47	110.01
1	A	371	LYS	CB-CA-C	5.14	119.32	110.79
1	H	63	GLU	CA-CB-CG	5.14	124.38	114.10
1	K	63	GLU	CA-CB-CG	5.14	124.38	114.10
1	B	230	ILE	CA-CB-CG1	5.14	119.13	110.40
1	E	375	GLY	N-CA-C	-5.14	106.99	114.90
1	N	506	TYR	CB-CA-C	5.14	119.31	110.79
1	B	519	CYS	N-CA-CB	-5.13	102.30	111.08
1	C	353	ILE	N-CA-CB	5.13	116.56	110.55
1	E	169	VAL	CB-CA-C	5.13	119.07	112.14
1	L	436	GLN	N-CA-CB	5.13	117.67	110.12
1	C	110	GLY	N-CA-C	-5.13	108.14	115.64
1	G	371	LYS	CB-CA-C	5.13	119.31	110.79
1	A	230	ILE	CA-CB-CG1	5.13	119.12	110.40
1	B	110	GLY	N-CA-C	-5.13	108.15	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	63	GLU	CA-CB-CG	5.13	124.36	114.10
1	N	90	THR	N-CA-CB	5.13	117.67	110.12
1	G	110	GLY	N-CA-C	-5.13	108.15	115.64
1	M	63	GLU	CA-CB-CG	5.13	124.36	114.10
1	D	230	ILE	CA-CB-CG1	5.13	119.11	110.40
1	K	506	TYR	CB-CA-C	5.13	119.30	110.79
1	E	371	LYS	CB-CA-C	5.12	119.30	110.79
1	E	373	ALA	N-CA-C	-5.12	105.59	111.07
1	G	208	PRO	CA-N-CD	-5.12	104.83	112.00
1	J	63	GLU	CA-CB-CG	5.12	124.35	114.10
1	A	373	ALA	N-CA-C	-5.12	105.59	111.07
1	B	169	VAL	CB-CA-C	5.12	119.05	112.14
1	B	379	ILE	N-CA-CB	5.12	118.48	111.41
1	C	371	LYS	CB-CA-C	5.12	119.29	110.79
1	E	332	ILE	N-CA-CB	-5.12	105.01	111.46
1	C	415	GLY	N-CA-C	-5.12	108.25	115.32
1	D	373	ALA	N-CA-C	-5.12	105.59	111.07
1	H	90	THR	N-CA-CB	5.12	117.65	110.12
1	F	373	ALA	N-CA-C	-5.12	105.59	111.07
1	M	263	VAL	N-CA-CB	5.12	116.54	110.55
1	A	110	GLY	N-CA-C	-5.12	108.17	115.64
1	C	230	ILE	CA-CB-CG1	5.11	119.09	110.40
1	E	379	ILE	N-CA-CB	5.11	118.47	111.41
1	F	371	LYS	CB-CA-C	5.11	119.28	110.79
1	H	506	TYR	CB-CA-C	5.11	119.28	110.79
1	I	506	TYR	CB-CA-C	5.11	119.28	110.79
1	D	371	LYS	CB-CA-C	5.11	119.28	110.79
1	N	63	GLU	CA-CB-CG	5.11	124.33	114.10
1	E	167	ASP	CB-CA-C	5.11	118.90	110.88
1	E	230	ILE	CA-CB-CG1	5.11	119.08	110.40
1	I	63	GLU	CA-CB-CG	5.11	124.32	114.10
1	N	415	GLY	N-CA-C	-5.11	108.27	115.32
1	D	379	ILE	N-CA-CB	5.11	118.46	111.41
1	M	379	ILE	CB-CA-C	-5.11	103.01	110.62
1	B	332	ILE	N-CA-CB	-5.11	105.03	111.46
1	D	167	ASP	CB-CA-C	5.11	118.90	110.88
1	I	379	ILE	CB-CA-C	-5.11	103.01	110.62
1	A	379	ILE	N-CA-CB	5.10	118.45	111.41
1	B	371	LYS	CB-CA-C	5.10	119.26	110.79
1	E	415	GLY	N-CA-C	-5.10	108.28	115.32
1	K	263	VAL	N-CA-CB	5.10	116.52	110.55
1	B	415	GLY	N-CA-C	-5.10	108.29	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	506	TYR	CB-CA-C	5.10	119.25	110.79
1	L	506	TYR	CB-CA-C	5.10	119.25	110.79
1	M	63	GLU	CB-CG-CD	5.10	121.27	112.60
1	A	353	ILE	N-CA-CB	5.09	116.51	110.55
1	C	25	ASP	CA-CB-CG	-5.09	107.51	112.60
1	D	415	GLY	N-CA-C	-5.09	108.29	115.32
1	E	353	ILE	N-CA-CB	5.09	116.51	110.55
1	F	332	ILE	N-CA-CB	-5.09	105.04	111.46
1	C	167	ASP	CB-CA-C	5.09	118.87	110.88
1	G	353	ILE	N-CA-CB	5.09	116.51	110.55
1	J	379	ILE	CB-CA-C	-5.09	103.03	110.62
1	D	353	ILE	N-CA-CB	5.09	116.50	110.55
1	K	379	ILE	CB-CA-C	-5.09	103.04	110.62
1	N	63	GLU	CB-CG-CD	5.09	121.25	112.60
1	E	473	ASP	N-CA-CB	5.09	118.15	110.42
1	L	379	ILE	CB-CA-C	-5.09	103.04	110.62
1	L	63	GLU	CB-CG-CD	5.09	121.25	112.60
1	C	379	ILE	N-CA-CB	5.08	118.43	111.41
1	C	373	ALA	N-CA-C	-5.08	105.63	111.07
1	F	353	ILE	N-CA-CB	5.08	116.50	110.55
1	G	473	ASP	N-CA-CB	5.08	118.15	110.42
1	J	263	VAL	N-CA-CB	5.08	116.50	110.55
1	A	473	ASP	N-CA-CB	5.08	118.14	110.42
1	F	167	ASP	CB-CA-C	5.08	118.85	110.88
1	J	63	GLU	CB-CG-CD	5.08	121.23	112.60
1	L	263	VAL	N-CA-CB	5.08	116.49	110.55
1	N	263	VAL	N-CA-CB	5.08	116.49	110.55
1	A	167	ASP	CB-CA-C	5.08	118.85	110.88
1	B	167	ASP	CB-CA-C	5.08	118.85	110.88
1	C	473	ASP	N-CA-CB	5.08	118.13	110.42
1	G	167	ASP	CB-CA-C	5.07	118.84	110.88
1	G	25	ASP	CA-CB-CG	-5.07	107.53	112.60
1	H	379	ILE	CB-CA-C	-5.07	103.06	110.62
1	I	263	VAL	CB-CA-C	-5.07	105.48	111.97
1	M	506	TYR	CB-CA-C	5.07	119.21	110.79
1	A	379	ILE	CB-CA-C	-5.07	103.13	110.63
1	D	332	ILE	N-CA-CB	-5.07	105.07	111.46
1	G	379	ILE	N-CA-CB	5.07	118.41	111.41
1	B	353	ILE	N-CA-CB	5.07	116.48	110.55
1	D	473	ASP	N-CA-CB	5.07	118.12	110.42
1	A	332	ILE	N-CA-CB	-5.07	105.08	111.46
1	A	415	GLY	N-CA-C	-5.07	108.33	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	415	GLY	N-CA-C	-5.07	108.33	115.32
1	G	329	THR	CA-CB-CG2	5.07	119.12	110.50
1	I	63	GLU	CB-CG-CD	5.07	121.21	112.60
1	J	367	GLU	CA-CB-CG	5.07	124.23	114.10
1	G	379	ILE	CB-CA-C	-5.07	103.13	110.63
1	E	25	ASP	CA-CB-CG	-5.06	107.54	112.60
1	H	196	ASP	CB-CA-C	5.06	119.61	111.05
1	B	329	THR	CA-CB-CG2	5.06	119.11	110.50
1	C	332	ILE	N-CA-CB	-5.06	105.08	111.46
1	D	492	GLY	N-CA-C	-5.06	108.33	115.32
1	E	379	ILE	CB-CA-C	-5.06	103.14	110.63
1	F	379	ILE	N-CA-CB	5.06	118.40	111.41
1	I	437	ASN	N-CA-CB	5.06	117.35	110.01
1	A	492	GLY	N-CA-C	-5.06	108.33	115.32
1	K	196	ASP	CB-CA-C	5.06	119.60	111.05
1	D	329	THR	CA-CB-CG2	5.06	119.10	110.50
1	H	437	ASN	N-CA-CB	5.06	117.34	110.01
1	C	329	THR	CA-CB-CG2	5.06	119.10	110.50
1	F	79	SER	N-CA-CB	5.06	117.56	110.12
1	B	473	ASP	N-CA-CB	5.06	118.11	110.42
1	H	63	GLU	CB-CG-CD	5.06	121.20	112.60
1	L	196	ASP	CB-CA-C	5.06	119.59	111.05
1	L	367	GLU	CA-CB-CG	5.06	124.21	114.10
1	N	379	ILE	CB-CA-C	-5.06	103.09	110.62
1	N	196	ASP	CB-CA-C	5.05	119.59	111.05
1	B	79	SER	N-CA-CB	5.05	117.55	110.12
1	C	379	ILE	CB-CA-C	-5.05	103.16	110.63
1	G	415	GLY	N-CA-C	-5.05	108.35	115.32
1	A	329	THR	CA-CB-CG2	5.05	119.08	110.50
1	D	379	ILE	CB-CA-C	-5.05	103.16	110.63
1	G	79	SER	N-CA-CB	5.05	117.54	110.12
1	J	196	ASP	CB-CA-C	5.05	119.58	111.05
1	D	34	LYS	N-CA-CB	5.05	117.33	110.01
1	F	379	ILE	CB-CA-C	-5.05	103.16	110.63
1	A	79	SER	N-CA-CB	5.05	117.54	110.12
1	H	263	VAL	N-CA-CB	5.05	116.45	110.55
1	F	473	ASP	N-CA-CB	5.04	118.09	110.42
1	I	196	ASP	CB-CA-C	5.04	119.58	111.05
1	A	25	ASP	CA-CB-CG	-5.04	107.56	112.60
1	B	25	ASP	CA-CB-CG	-5.04	107.56	112.60
1	B	492	GLY	N-CA-C	-5.04	108.36	115.32
1	D	79	SER	N-CA-CB	5.04	117.53	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	492	GLY	N-CA-C	-5.04	108.36	115.32
1	I	367	GLU	CA-CB-CG	5.04	124.18	114.10
1	M	196	ASP	CB-CA-C	5.04	119.57	111.05
1	M	367	GLU	CA-CB-CG	5.04	124.18	114.10
1	K	63	GLU	CB-CG-CD	5.04	121.17	112.60
1	E	79	SER	N-CA-CB	5.04	117.53	110.12
1	H	367	GLU	CA-CB-CG	5.04	124.17	114.10
1	C	79	SER	N-CA-CB	5.04	117.52	110.12
1	B	34	LYS	N-CA-CB	5.04	117.31	110.01
1	E	329	THR	CA-CB-CG2	5.04	119.06	110.50
1	B	379	ILE	CB-CA-C	-5.03	103.18	110.63
1	I	169	VAL	CB-CA-C	5.03	119.17	112.22
1	L	169	VAL	CB-CA-C	5.03	119.17	112.22
1	F	315	GLU	CB-CG-CD	5.03	121.16	112.60
1	L	437	ASN	N-CA-CB	5.03	117.31	110.01
1	M	437	ASN	N-CA-CB	5.03	117.30	110.01
1	M	79	SER	N-CA-CB	5.03	117.51	110.12
1	D	315	GLU	CB-CG-CD	5.03	121.14	112.60
1	F	483	GLU	CB-CG-CD	5.03	121.14	112.60
1	C	315	GLU	CB-CG-CD	5.02	121.14	112.60
1	N	437	ASN	N-CA-CB	5.02	117.29	110.01
1	J	437	ASN	N-CA-CB	5.02	117.29	110.01
1	G	483	GLU	CB-CG-CD	5.02	121.13	112.60
1	N	367	GLU	CA-CB-CG	5.02	124.14	114.10
1	C	492	GLY	N-CA-C	-5.02	108.39	115.32
1	A	483	GLU	CB-CG-CD	5.01	121.12	112.60
1	K	367	GLU	CA-CB-CG	5.01	124.13	114.10
1	L	10	ASN	CA-CB-CG	-5.01	107.59	112.60
1	C	34	LYS	N-CA-CB	5.01	117.28	110.01
1	C	483	GLU	CB-CG-CD	5.01	121.12	112.60
1	E	315	GLU	CB-CG-CD	5.01	121.12	112.60
1	E	483	GLU	CB-CG-CD	5.01	121.12	112.60
1	F	329	THR	CA-CB-CG2	5.01	119.02	110.50
1	G	34	LYS	N-CA-CB	5.01	117.27	110.01
1	I	79	SER	N-CA-CB	5.01	117.48	110.12
1	J	126	ALA	CB-CA-C	5.01	119.11	110.79
1	J	79	SER	N-CA-CB	5.01	117.48	110.12
1	K	437	ASN	N-CA-CB	5.01	117.27	110.01
1	K	79	SER	N-CA-CB	5.01	117.48	110.12
1	B	483	GLU	CB-CG-CD	5.00	121.11	112.60
1	M	10	ASN	CA-CB-CG	-5.00	107.59	112.60
1	A	34	LYS	N-CA-CB	5.00	117.26	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	34	LYS	N-CA-CB	5.00	117.26	110.01
1	N	170	GLY	N-CA-C	-5.00	105.47	112.18
1	N	263	VAL	CB-CA-C	-5.00	105.56	111.97
1	D	25	ASP	CA-CB-CG	-5.00	107.60	112.60
1	J	263	VAL	CB-CA-C	-5.00	105.57	111.97

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	257	GLU	CA

All (135) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
1	C	345	ARG	Sidechain
1	C	350	ARG	Sidechain
1	C	362	ARG	Sidechain
1	C	404	ARG	Sidechain
1	C	445	ARG	Sidechain
1	D	18	ARG	Sidechain
1	D	197	ARG	Sidechain
1	D	241	ALA	Peptide
1	D	245	LYS	Peptide
1	D	256	GLY	Peptide
1	D	285	ARG	Sidechain
1	D	345	ARG	Sidechain
1	D	350	ARG	Sidechain
1	D	362	ARG	Sidechain
1	D	404	ARG	Sidechain
1	D	445	ARG	Sidechain
1	E	18	ARG	Sidechain
1	E	197	ARG	Sidechain
1	E	241	ALA	Peptide
1	E	245	LYS	Peptide
1	E	256	GLY	Peptide
1	E	285	ARG	Sidechain
1	E	345	ARG	Sidechain
1	E	350	ARG	Sidechain
1	E	362	ARG	Sidechain
1	E	404	ARG	Sidechain
1	E	445	ARG	Sidechain
1	F	18	ARG	Sidechain
1	F	197	ARG	Sidechain
1	F	231	ARG	Sidechain
1	F	241	ALA	Peptide
1	F	245	LYS	Peptide
1	F	255	GLU	Peptide
1	F	285	ARG	Sidechain
1	F	345	ARG	Sidechain
1	F	350	ARG	Sidechain
1	F	362	ARG	Sidechain
1	F	404	ARG	Sidechain
1	F	445	ARG	Sidechain
1	G	18	ARG	Sidechain
1	G	197	ARG	Sidechain
1	G	231	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	G	241	ALA	Peptide
1	G	244	GLY	Peptide
1	G	256	GLY	Peptide
1	G	285	ARG	Sidechain
1	G	345	ARG	Sidechain
1	G	350	ARG	Sidechain
1	G	362	ARG	Sidechain
1	G	404	ARG	Sidechain
1	G	445	ARG	Sidechain
1	H	118	ARG	Sidechain
1	H	13	ARG	Sidechain
1	H	197	ARG	Sidechain
1	H	231	ARG	Sidechain
1	H	350	ARG	Sidechain
1	H	362	ARG	Sidechain
1	H	404	ARG	Sidechain
1	H	445	ARG	Sidechain
1	I	118	ARG	Sidechain
1	I	13	ARG	Sidechain
1	I	197	ARG	Sidechain
1	I	231	ARG	Sidechain
1	I	350	ARG	Sidechain
1	I	362	ARG	Sidechain
1	I	404	ARG	Sidechain
1	I	445	ARG	Sidechain
1	J	118	ARG	Sidechain
1	J	13	ARG	Sidechain
1	J	197	ARG	Sidechain
1	J	231	ARG	Sidechain
1	J	350	ARG	Sidechain
1	J	362	ARG	Sidechain
1	J	404	ARG	Sidechain
1	J	445	ARG	Sidechain
1	K	118	ARG	Sidechain
1	K	13	ARG	Sidechain
1	K	197	ARG	Sidechain
1	K	231	ARG	Sidechain
1	K	350	ARG	Sidechain
1	K	362	ARG	Sidechain
1	K	404	ARG	Sidechain
1	K	445	ARG	Sidechain
1	L	118	ARG	Sidechain

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3846	0	3970	188	0
1	B	3846	0	3970	186	0
1	C	3846	0	3970	186	0
1	D	3846	0	3970	186	0
1	E	3846	0	3970	187	0
1	F	3846	0	3970	189	0
1	G	3846	0	3970	187	0
1	H	3846	0	3970	134	0
1	I	3846	0	3970	135	0
1	J	3846	0	3970	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	3846	0	3970	133	0
1	L	3846	0	3970	132	0
1	M	3846	0	3970	135	0
1	N	3846	0	3970	137	0
2	A	31	12	12	3	0
2	B	31	12	12	3	0
2	C	31	12	12	3	0
2	D	31	12	12	3	0
2	E	31	12	12	3	0
2	F	31	12	12	3	0
2	G	31	12	12	3	0
2	H	31	12	12	3	0
2	I	31	12	12	3	0
2	J	31	12	12	3	0
2	K	31	12	12	3	0
2	L	31	12	12	3	0
2	M	31	12	12	3	0
2	N	31	12	12	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	1	0	0	4	0
4	B	1	0	0	4	0
4	C	1	0	0	4	0
4	D	1	0	0	4	0
4	E	1	0	0	4	0
4	F	1	0	0	4	0
4	G	1	0	0	4	0
4	H	1	0	0	4	0
4	I	1	0	0	4	0
4	J	1	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	1	0	0	4	0
4	L	1	0	0	4	0
4	M	1	0	0	4	0
4	N	1	0	0	4	0
All	All	54306	168	55748	2107	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 (2107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:ALA:HA	1:F:63:GLU:CA	1.69	1.23
1:D:3:ALA:HA	1:E:63:GLU:CA	1.69	1.22
1:F:3:ALA:HA	1:G:63:GLU:CA	1.69	1.22
1:C:3:ALA:HA	1:D:63:GLU:CA	1.69	1.22
1:N:30:THR:HA	1:N:35:GLY:HA3	1.22	1.21
1:A:63:GLU:CA	1:G:3:ALA:HA	1.69	1.20
1:B:3:ALA:HA	1:C:63:GLU:CA	1.69	1.20
1:A:3:ALA:HA	1:B:63:GLU:CA	1.69	1.20
1:H:30:THR:HA	1:H:35:GLY:HA3	1.23	1.17
1:M:30:THR:HA	1:M:35:GLY:HA3	1.22	1.16
1:I:30:THR:HA	1:I:35:GLY:HA3	1.22	1.14
1:J:30:THR:HA	1:J:35:GLY:HA3	1.22	1.12
1:L:30:THR:HA	1:L:35:GLY:HA3	1.23	1.11
1:K:30:THR:HA	1:K:35:GLY:HA3	1.23	1.10
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.44	1.00
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.44	1.00
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.43	1.00
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.44	1.00
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.44	1.00
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.44	1.00
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.44	0.99
1:A:3:ALA:CA	1:B:63:GLU:HA	1.93	0.99
1:F:3:ALA:CA	1:G:63:GLU:HA	1.93	0.99
1:E:3:ALA:CA	1:F:63:GLU:HA	1.93	0.99
1:A:63:GLU:HA	1:G:3:ALA:CA	1.93	0.98
1:D:3:ALA:CA	1:E:63:GLU:HA	1.93	0.98
1:B:3:ALA:CA	1:C:63:GLU:HA	1.93	0.98
1:C:3:ALA:CA	1:D:63:GLU:HA	1.93	0.98
1:B:3:ALA:HA	1:C:63:GLU:HA	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ALA:HA	1:B:63:GLU:HA	1.46	0.97
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.47	0.95
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.47	0.95
1:E:3:ALA:HA	1:F:63:GLU:HA	1.45	0.95
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.47	0.95
1:A:63:GLU:HA	1:G:3:ALA:HA	1.46	0.94
1:D:3:ALA:HA	1:E:63:GLU:HA	1.46	0.94
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.47	0.94
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.47	0.94
1:C:3:ALA:HA	1:D:63:GLU:HA	1.46	0.93
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.47	0.93
1:F:3:ALA:HA	1:G:63:GLU:HA	1.46	0.92
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.47	0.92
1:F:30:THR:HA	1:F:35:GLY:HA3	1.52	0.92
1:G:30:THR:HA	1:G:35:GLY:HA3	1.52	0.91
1:C:30:THR:HA	1:C:35:GLY:HA3	1.52	0.91
1:B:30:THR:HA	1:B:35:GLY:HA3	1.51	0.90
1:A:3:ALA:CA	1:B:63:GLU:CA	2.49	0.90
1:E:30:THR:HA	1:E:35:GLY:HA3	1.52	0.90
1:A:63:GLU:CA	1:G:3:ALA:CA	2.49	0.90
1:B:3:ALA:CA	1:C:63:GLU:CA	2.49	0.89
1:D:30:THR:HA	1:D:35:GLY:HA3	1.52	0.89
1:A:30:THR:HA	1:A:35:GLY:HA3	1.52	0.89
1:F:3:ALA:CA	1:G:63:GLU:CA	2.49	0.89
1:E:3:ALA:CA	1:F:63:GLU:CA	2.49	0.88
1:C:3:ALA:CA	1:D:63:GLU:CA	2.49	0.87
1:D:3:ALA:CA	1:E:63:GLU:CA	2.49	0.87
1:E:3:ALA:HA	1:F:63:GLU:C	2.00	0.86
1:A:3:ALA:HA	1:B:63:GLU:C	2.00	0.86
1:A:63:GLU:C	1:G:3:ALA:HA	2.00	0.86
1:F:3:ALA:HA	1:G:63:GLU:C	2.00	0.86
1:B:3:ALA:HA	1:C:63:GLU:C	2.00	0.86
1:D:3:ALA:HA	1:E:63:GLU:C	2.00	0.86
1:C:3:ALA:HA	1:D:63:GLU:C	2.00	0.85
1:K:30:THR:CA	1:K:35:GLY:HA3	2.07	0.85
1:J:30:THR:CA	1:J:35:GLY:HA3	2.07	0.84
1:I:30:THR:CA	1:I:35:GLY:HA3	2.07	0.84
1:H:30:THR:CA	1:H:35:GLY:HA3	2.07	0.82
1:N:30:THR:CA	1:N:35:GLY:HA3	2.07	0.81
1:J:39:VAL:HB	1:K:517:THR:HG23	1.62	0.81
1:M:30:THR:CA	1:M:35:GLY:HA3	2.07	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:VAL:HB	1:J:517:THR:HG23	1.62	0.80
1:K:39:VAL:HB	1:L:517:THR:HG23	1.62	0.80
1:D:183:LEU:O	1:D:382:GLY:HA3	1.82	0.80
1:H:517:THR:HG23	1:N:39:VAL:HB	1.62	0.80
1:B:183:LEU:O	1:B:382:GLY:HA3	1.82	0.80
1:C:183:LEU:O	1:C:382:GLY:HA3	1.82	0.80
1:A:183:LEU:O	1:A:382:GLY:HA3	1.82	0.80
1:H:39:VAL:HB	1:I:517:THR:HG23	1.62	0.80
1:D:138:CYS:N	1:D:410:GLY:HA2	1.97	0.79
1:E:183:LEU:O	1:E:382:GLY:HA3	1.82	0.79
1:G:183:LEU:O	1:G:382:GLY:HA3	1.82	0.79
1:L:39:VAL:HB	1:M:517:THR:HG23	1.62	0.79
1:E:138:CYS:N	1:E:410:GLY:HA2	1.97	0.79
1:L:30:THR:CA	1:L:35:GLY:HA3	2.07	0.79
1:C:138:CYS:N	1:C:410:GLY:HA2	1.97	0.79
1:C:240:VAL:HA	1:C:243:ALA:HB3	1.65	0.79
1:D:240:VAL:HA	1:D:243:ALA:HB3	1.65	0.79
1:F:183:LEU:O	1:F:382:GLY:HA3	1.82	0.79
1:J:183:LEU:O	1:J:382:GLY:HA3	1.83	0.79
1:K:183:LEU:O	1:K:382:GLY:HA3	1.83	0.79
1:B:240:VAL:HA	1:B:243:ALA:HB3	1.65	0.79
1:A:138:CYS:N	1:A:410:GLY:HA2	1.97	0.78
1:D:127:ALA:HB2	1:D:426:LEU:HD11	1.65	0.78
1:G:138:CYS:N	1:G:410:GLY:HA2	1.97	0.78
1:B:138:CYS:N	1:B:410:GLY:HA2	1.97	0.78
1:C:127:ALA:HB2	1:C:426:LEU:HD11	1.65	0.78
1:F:138:CYS:N	1:F:410:GLY:HA2	1.97	0.78
1:M:39:VAL:HB	1:N:517:THR:HG23	1.62	0.78
1:A:127:ALA:HB2	1:A:426:LEU:HD11	1.65	0.78
1:E:127:ALA:HB2	1:E:426:LEU:HD11	1.66	0.78
1:M:183:LEU:O	1:M:382:GLY:HA3	1.83	0.78
1:E:240:VAL:HA	1:E:243:ALA:HB3	1.65	0.78
1:I:183:LEU:O	1:I:382:GLY:HA3	1.83	0.78
1:N:183:LEU:O	1:N:382:GLY:HA3	1.83	0.78
1:F:127:ALA:HB2	1:F:426:LEU:HD11	1.65	0.78
1:F:240:VAL:HA	1:F:243:ALA:HB3	1.65	0.77
1:G:127:ALA:HB2	1:G:426:LEU:HD11	1.65	0.77
1:H:183:LEU:O	1:H:382:GLY:HA3	1.83	0.77
1:J:85:ALA:O	1:J:402:ALA:HA	1.85	0.77
1:K:85:ALA:O	1:K:402:ALA:HA	1.84	0.77
1:L:183:LEU:O	1:L:382:GLY:HA3	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:85:ALA:O	1:L:402:ALA:HA	1.85	0.77
1:I:85:ALA:O	1:I:402:ALA:HA	1.85	0.77
1:N:85:ALA:O	1:N:402:ALA:HA	1.85	0.77
1:B:214:GLU:HA	1:B:323:VAL:O	1.85	0.77
1:E:214:GLU:HA	1:E:323:VAL:O	1.85	0.77
1:M:85:ALA:O	1:M:402:ALA:HA	1.84	0.77
1:F:214:GLU:HA	1:F:323:VAL:O	1.85	0.77
1:H:85:ALA:O	1:H:402:ALA:HA	1.85	0.77
1:A:214:GLU:HA	1:A:323:VAL:O	1.85	0.77
2:A:1525:ATP:O1A	4:A:1528:PO4:P	2.44	0.77
2:B:1525:ATP:O1G	4:B:1528:PO4:P	2.43	0.76
2:C:1526:ATP:O1G	4:C:1528:PO4:P	2.44	0.76
2:E:1525:ATP:O1A	4:E:1528:PO4:P	2.43	0.76
1:D:214:GLU:HA	1:D:323:VAL:O	1.85	0.76
1:G:214:GLU:HA	1:G:323:VAL:O	1.85	0.76
2:B:1525:ATP:O1A	4:B:1528:PO4:P	2.43	0.76
1:C:214:GLU:HA	1:C:323:VAL:O	1.85	0.76
1:B:127:ALA:HB2	1:B:426:LEU:HD11	1.65	0.76
2:F:1525:ATP:O1A	4:F:1528:PO4:P	2.43	0.76
2:G:1525:ATP:O1A	4:G:1528:PO4:P	2.43	0.76
1:D:4:LYS:H	1:E:63:GLU:HB2	1.51	0.76
2:D:1525:ATP:O1G	4:D:1528:PO4:P	2.44	0.76
1:C:4:LYS:H	1:D:63:GLU:HB2	1.51	0.76
1:E:4:LYS:H	1:F:63:GLU:HB2	1.51	0.76
1:F:4:LYS:H	1:G:63:GLU:HB2	1.51	0.76
2:A:1525:ATP:O1G	4:A:1528:PO4:P	2.44	0.75
2:D:1525:ATP:O1A	4:D:1528:PO4:P	2.43	0.75
1:H:480:ALA:O	1:H:483:GLU:HG2	1.86	0.75
1:A:4:LYS:H	1:B:63:GLU:HB2	1.51	0.75
1:B:4:LYS:H	1:C:63:GLU:HB2	1.51	0.75
2:G:1525:ATP:O1G	4:G:1528:PO4:P	2.44	0.75
1:I:480:ALA:O	1:I:483:GLU:HG2	1.86	0.75
2:F:1525:ATP:O1G	4:F:1528:PO4:P	2.44	0.75
1:L:480:ALA:O	1:L:483:GLU:HG2	1.86	0.75
1:A:63:GLU:HB2	1:G:4:LYS:H	1.51	0.75
1:H:138:CYS:N	1:H:410:GLY:HA2	2.02	0.75
1:I:138:CYS:N	1:I:410:GLY:HA2	2.02	0.75
2:E:1525:ATP:O1G	4:E:1528:PO4:P	2.44	0.75
1:K:138:CYS:N	1:K:410:GLY:HA2	2.02	0.75
1:J:480:ALA:O	1:J:483:GLU:HG2	1.86	0.75
1:N:480:ALA:O	1:N:483:GLU:HG2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:HB2	1:A:213:VAL:HA	1.69	0.74
2:C:1526:ATP:O1A	4:C:1528:PO4:P	2.43	0.74
1:B:206:ASN:HB2	1:B:213:VAL:HA	1.70	0.74
1:C:206:ASN:HB2	1:C:213:VAL:HA	1.69	0.74
1:J:138:CYS:N	1:J:410:GLY:HA2	2.02	0.74
1:N:127:ALA:HB2	1:N:426:LEU:HD11	1.70	0.74
1:N:138:CYS:N	1:N:410:GLY:HA2	2.02	0.74
1:M:480:ALA:O	1:M:483:GLU:HG2	1.86	0.74
1:I:198:GLY:HA2	1:I:327:LYS:O	1.88	0.74
1:J:198:GLY:HA2	1:J:327:LYS:O	1.88	0.74
1:K:480:ALA:O	1:K:483:GLU:HG2	1.86	0.74
1:M:198:GLY:HA2	1:M:327:LYS:O	1.88	0.74
1:H:127:ALA:HB2	1:H:426:LEU:HD11	1.70	0.74
1:K:198:GLY:HA2	1:K:327:LYS:O	1.88	0.74
1:L:127:ALA:HB2	1:L:426:LEU:HD11	1.70	0.74
1:L:138:CYS:N	1:L:410:GLY:HA2	2.02	0.74
1:D:206:ASN:HB2	1:D:213:VAL:HA	1.69	0.73
1:I:127:ALA:HB2	1:I:426:LEU:HD11	1.70	0.73
1:K:127:ALA:HB2	1:K:426:LEU:HD11	1.70	0.73
1:G:206:ASN:HB2	1:G:213:VAL:HA	1.70	0.73
1:G:255:GLU:HB2	1:G:258:ALA:HB3	1.70	0.73
1:I:191:GLU:O	1:I:334:ASP:HA	1.89	0.73
1:H:198:GLY:HA2	1:H:327:LYS:O	1.88	0.73
1:F:206:ASN:HB2	1:F:213:VAL:HA	1.69	0.73
1:H:191:GLU:O	1:H:334:ASP:HA	1.89	0.73
1:M:138:CYS:N	1:M:410:GLY:HA2	2.02	0.73
1:J:191:GLU:O	1:J:334:ASP:HA	1.89	0.73
1:J:127:ALA:HB2	1:J:426:LEU:HD11	1.70	0.73
2:K:1527:ATP:O1G	4:K:1528:PO4:P	2.47	0.73
1:L:198:GLY:HA2	1:L:327:LYS:O	1.88	0.72
2:M:1527:ATP:O1G	4:M:1528:PO4:P	2.47	0.72
1:N:191:GLU:O	1:N:334:ASP:HA	1.89	0.72
1:N:198:GLY:HA2	1:N:327:LYS:O	1.88	0.72
1:E:4:LYS:H	1:F:63:GLU:CB	2.03	0.72
1:A:4:LYS:H	1:B:63:GLU:CB	2.03	0.72
2:H:1527:ATP:O1G	4:H:1528:PO4:P	2.47	0.72
1:M:127:ALA:HB2	1:M:426:LEU:HD11	1.70	0.72
1:D:198:GLY:HA2	1:D:327:LYS:O	1.90	0.72
1:E:206:ASN:HB2	1:E:213:VAL:HA	1.69	0.72
2:J:1526:ATP:O1G	4:J:1528:PO4:P	2.47	0.72
1:F:4:LYS:H	1:G:63:GLU:CB	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:198:GLY:HA2	1:G:327:LYS:O	1.90	0.72
2:I:1525:ATP:O1G	4:I:1528:PO4:P	2.47	0.72
1:L:191:GLU:O	1:L:334:ASP:HA	1.88	0.72
1:A:198:GLY:HA2	1:A:327:LYS:O	1.90	0.72
2:L:1527:ATP:O1G	4:L:1528:PO4:P	2.47	0.72
1:C:4:LYS:H	1:D:63:GLU:CB	2.03	0.72
1:C:198:GLY:HA2	1:C:327:LYS:O	1.90	0.72
1:K:191:GLU:O	1:K:334:ASP:HA	1.89	0.72
1:M:191:GLU:O	1:M:334:ASP:HA	1.89	0.72
1:A:63:GLU:CB	1:G:4:LYS:H	2.03	0.72
1:B:2:ALA:O	1:C:63:GLU:HA	1.90	0.72
1:E:198:GLY:HA2	1:E:327:LYS:O	1.90	0.72
2:H:1527:ATP:O1A	4:H:1528:PO4:P	2.48	0.72
2:N:1527:ATP:O1G	4:N:1528:PO4:P	2.47	0.72
1:D:4:LYS:H	1:E:63:GLU:CB	2.03	0.72
1:F:2:ALA:O	1:G:63:GLU:HA	1.90	0.71
1:A:2:ALA:O	1:B:63:GLU:HA	1.90	0.71
1:A:63:GLU:HA	1:G:2:ALA:O	1.90	0.71
2:M:1527:ATP:O1A	4:M:1528:PO4:P	2.48	0.71
2:J:1526:ATP:O1A	4:J:1528:PO4:P	2.48	0.71
2:K:1527:ATP:O1A	4:K:1528:PO4:P	2.48	0.71
1:L:214:GLU:HA	1:L:323:VAL:O	1.91	0.71
1:M:199:TYR:CD2	1:M:205:ILE:HD11	2.25	0.71
1:I:199:TYR:CD2	1:I:205:ILE:HD11	2.25	0.71
1:J:38:VAL:HB	1:J:56:VAL:HG22	1.71	0.71
1:J:199:TYR:CD2	1:J:205:ILE:HD11	2.25	0.71
1:K:38:VAL:HB	1:K:56:VAL:HG22	1.71	0.71
1:H:214:GLU:HA	1:H:323:VAL:O	1.90	0.71
1:N:199:TYR:CD2	1:N:205:ILE:HD11	2.25	0.71
1:N:214:GLU:HA	1:N:323:VAL:O	1.91	0.71
2:N:1527:ATP:O1A	4:N:1528:PO4:P	2.48	0.71
1:D:2:ALA:O	1:E:63:GLU:HA	1.90	0.71
1:H:38:VAL:HB	1:H:56:VAL:HG22	1.71	0.71
1:I:214:GLU:HA	1:I:323:VAL:O	1.91	0.71
2:I:1525:ATP:O1A	4:I:1528:PO4:P	2.48	0.71
1:K:214:GLU:HA	1:K:323:VAL:O	1.91	0.71
1:A:243:ALA:HA	1:G:258:ALA:HA	1.72	0.70
1:B:4:LYS:H	1:C:63:GLU:CB	2.03	0.70
1:B:198:GLY:HA2	1:B:327:LYS:O	1.90	0.70
1:E:2:ALA:O	1:F:63:GLU:HA	1.90	0.70
2:L:1527:ATP:O1A	4:L:1528:PO4:P	2.48	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:199:TYR:CD2	1:H:205:ILE:HD11	2.25	0.70
1:A:39:VAL:HB	1:G:517:THR:HG23	1.73	0.70
1:L:199:TYR:CD2	1:L:205:ILE:HD11	2.26	0.70
1:F:517:THR:HG23	1:G:39:VAL:HB	1.73	0.70
1:I:38:VAL:HB	1:I:56:VAL:HG22	1.72	0.70
1:K:199:TYR:CD2	1:K:205:ILE:HD11	2.25	0.70
1:L:38:VAL:HB	1:L:56:VAL:HG22	1.71	0.70
1:N:38:VAL:HB	1:N:56:VAL:HG22	1.71	0.70
1:F:198:GLY:HA2	1:F:327:LYS:O	1.90	0.70
1:J:214:GLU:HA	1:J:323:VAL:O	1.91	0.70
1:M:214:GLU:HA	1:M:323:VAL:O	1.91	0.70
1:E:517:THR:HG23	1:F:39:VAL:HB	1.73	0.70
1:A:517:THR:HG23	1:B:39:VAL:HB	1.73	0.69
1:C:2:ALA:O	1:D:63:GLU:HA	1.90	0.69
1:M:38:VAL:HB	1:M:56:VAL:HG22	1.71	0.69
1:C:517:THR:HG23	1:D:39:VAL:HB	1.73	0.69
1:I:30:THR:HA	1:I:35:GLY:CA	2.14	0.69
1:D:517:THR:HG23	1:E:39:VAL:HB	1.73	0.69
1:B:517:THR:HG23	1:C:39:VAL:HB	1.73	0.68
1:A:240:VAL:HA	1:A:243:ALA:HB3	1.75	0.68
1:F:180:GLY:HA2	1:F:380:LYS:HB3	1.76	0.68
1:H:30:THR:HA	1:H:35:GLY:CA	2.14	0.68
1:J:30:THR:HA	1:J:35:GLY:CA	2.14	0.68
1:E:180:GLY:HA2	1:E:380:LYS:HB3	1.76	0.68
1:D:180:GLY:HA2	1:D:380:LYS:HB3	1.76	0.67
1:C:3:ALA:C	1:D:63:GLU:HA	2.19	0.67
1:D:3:ALA:C	1:E:63:GLU:HA	2.19	0.67
1:D:199:TYR:CD2	1:D:205:ILE:HD11	2.30	0.67
1:C:199:TYR:CD2	1:C:205:ILE:HD11	2.30	0.67
1:E:199:TYR:CD2	1:E:205:ILE:HD11	2.30	0.67
1:L:30:THR:HA	1:L:35:GLY:CA	2.14	0.67
1:C:180:GLY:HA2	1:C:380:LYS:HB3	1.76	0.67
1:C:41:ASP:HA	1:C:47:PRO:HB3	1.77	0.67
1:B:3:ALA:C	1:C:63:GLU:HA	2.19	0.67
1:B:41:ASP:HA	1:B:47:PRO:HB3	1.77	0.67
1:D:41:ASP:HA	1:D:47:PRO:HB3	1.77	0.67
1:G:180:GLY:HA2	1:G:380:LYS:HB3	1.76	0.67
1:H:287:ALA:HB1	1:H:368:ARG:CZ	2.25	0.67
1:K:30:THR:HA	1:K:35:GLY:CA	2.14	0.67
1:N:287:ALA:HB1	1:N:368:ARG:CZ	2.25	0.67
1:B:199:TYR:CD2	1:B:205:ILE:HD11	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:287:ALA:HB1	1:I:368:ARG:CZ	2.25	0.67
1:K:287:ALA:HB1	1:K:368:ARG:CZ	2.25	0.67
1:M:287:ALA:HB1	1:M:368:ARG:CZ	2.25	0.67
1:E:3:ALA:C	1:F:63:GLU:HA	2.19	0.67
1:B:180:GLY:HA2	1:B:380:LYS:HB3	1.76	0.67
1:F:199:TYR:CD2	1:F:205:ILE:HD11	2.30	0.67
1:J:287:ALA:HB1	1:J:368:ARG:CZ	2.25	0.67
1:L:287:ALA:HB1	1:L:368:ARG:CZ	2.25	0.67
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.76	0.66
1:A:41:ASP:HA	1:A:47:PRO:HB3	1.77	0.66
1:E:41:ASP:HA	1:E:47:PRO:HB3	1.77	0.66
1:I:39:VAL:CB	1:J:517:THR:HG23	2.26	0.66
1:L:27:VAL:HG12	1:L:90:THR:CG2	2.25	0.66
1:M:27:VAL:HG12	1:M:90:THR:CG2	2.25	0.66
1:H:3:ALA:HB3	1:H:524:LEU:HB3	1.78	0.66
1:I:3:ALA:HB3	1:I:524:LEU:HB3	1.78	0.66
1:J:39:VAL:CB	1:K:517:THR:HG23	2.26	0.66
1:L:39:VAL:CB	1:M:517:THR:HG23	2.26	0.66
1:F:41:ASP:HA	1:F:47:PRO:HB3	1.77	0.66
1:A:3:ALA:C	1:B:63:GLU:HA	2.19	0.66
1:A:199:TYR:CD2	1:A:205:ILE:HD11	2.30	0.66
1:F:3:ALA:C	1:G:63:GLU:HA	2.19	0.66
1:G:41:ASP:HA	1:G:47:PRO:HB3	1.77	0.66
1:M:30:THR:HA	1:M:35:GLY:CA	2.14	0.66
1:N:27:VAL:HG12	1:N:90:THR:CG2	2.25	0.66
1:A:63:GLU:HA	1:G:3:ALA:C	2.19	0.65
1:D:251:ALA:O	1:D:277:LYS:HA	1.96	0.65
1:G:199:TYR:CD2	1:G:205:ILE:HD11	2.30	0.65
1:G:257:GLU:H	1:G:257:GLU:CD	2.03	0.65
1:E:251:ALA:O	1:E:277:LYS:HA	1.96	0.65
1:G:251:ALA:O	1:G:277:LYS:HA	1.96	0.65
1:H:517:THR:HG23	1:N:39:VAL:CB	2.26	0.65
1:J:3:ALA:HB3	1:J:524:LEU:HB3	1.77	0.65
1:C:251:ALA:O	1:C:277:LYS:HA	1.96	0.65
1:F:251:ALA:O	1:F:277:LYS:HA	1.96	0.65
1:H:39:VAL:CB	1:I:517:THR:HG23	2.26	0.65
1:K:27:VAL:HG12	1:K:90:THR:CG2	2.25	0.65
1:K:39:VAL:CB	1:L:517:THR:HG23	2.26	0.65
1:B:251:ALA:O	1:B:277:LYS:HA	1.96	0.65
1:A:251:ALA:O	1:A:277:LYS:HA	1.96	0.65
1:G:135:SER:HA	1:G:412:VAL:HG12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:39:VAL:CB	1:N:517:THR:HG23	2.26	0.65
1:A:200:LEU:HD13	1:A:254:VAL:HG11	1.80	0.64
1:B:200:LEU:HD13	1:B:254:VAL:HG11	1.79	0.64
1:G:218:PRO:HG2	1:G:320:ALA:HB3	1.78	0.64
1:H:27:VAL:HG12	1:H:90:THR:CG2	2.25	0.64
1:A:135:SER:HA	1:A:412:VAL:HG12	1.79	0.64
1:F:135:SER:HA	1:F:412:VAL:HG12	1.80	0.64
1:M:3:ALA:HB3	1:M:524:LEU:HB3	1.78	0.64
1:N:3:ALA:HB3	1:N:524:LEU:HB3	1.78	0.64
1:K:3:ALA:HB3	1:K:524:LEU:HB3	1.78	0.64
1:N:30:THR:HA	1:N:35:GLY:CA	2.14	0.64
1:A:130:GLU:HB3	1:A:422:VAL:HG12	1.80	0.64
1:D:135:SER:HA	1:D:412:VAL:HG12	1.79	0.64
1:E:135:SER:HA	1:E:412:VAL:HG12	1.80	0.64
1:F:130:GLU:HB3	1:F:422:VAL:HG12	1.80	0.64
1:G:130:GLU:HB3	1:G:422:VAL:HG12	1.80	0.64
1:L:3:ALA:HB3	1:L:524:LEU:HB3	1.78	0.64
1:C:200:LEU:HD13	1:C:254:VAL:HG11	1.80	0.64
1:F:200:LEU:HD13	1:F:254:VAL:HG11	1.80	0.64
1:B:130:GLU:HB3	1:B:422:VAL:HG12	1.80	0.63
1:C:135:SER:HA	1:C:412:VAL:HG12	1.79	0.63
1:D:50:THR:HG21	1:D:56:VAL:HA	1.80	0.63
1:D:138:CYS:HB3	1:D:407:VAL:HA	1.81	0.63
1:C:50:THR:HG21	1:C:56:VAL:HA	1.80	0.63
1:E:52:ASP:O	1:E:56:VAL:HG23	1.98	0.63
1:E:200:LEU:HD13	1:E:254:VAL:HG11	1.80	0.63
1:D:27:VAL:HG12	1:D:90:THR:CG2	2.26	0.63
1:E:130:GLU:HB3	1:E:422:VAL:HG12	1.80	0.63
1:A:52:ASP:O	1:A:56:VAL:HG23	1.98	0.63
1:D:200:LEU:HD13	1:D:254:VAL:HG11	1.80	0.63
1:E:138:CYS:HB3	1:E:407:VAL:HA	1.81	0.63
1:B:135:SER:HA	1:B:412:VAL:HG12	1.80	0.63
1:E:50:THR:HG21	1:E:56:VAL:HA	1.80	0.63
1:G:52:ASP:O	1:G:56:VAL:HG23	1.98	0.63
1:J:27:VAL:HG12	1:J:90:THR:CG2	2.25	0.63
1:C:138:CYS:HB3	1:C:407:VAL:HA	1.81	0.63
1:D:52:ASP:O	1:D:56:VAL:HG23	1.98	0.63
1:F:138:CYS:HB3	1:F:407:VAL:HA	1.81	0.63
1:B:52:ASP:O	1:B:56:VAL:HG23	1.98	0.62
1:C:130:GLU:HB3	1:C:422:VAL:HG12	1.80	0.62
1:A:50:THR:HG21	1:A:56:VAL:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:THR:HG21	1:B:56:VAL:HA	1.80	0.62
1:D:130:GLU:HB3	1:D:422:VAL:HG12	1.80	0.62
1:G:200:LEU:HD13	1:G:254:VAL:HG11	1.81	0.62
1:I:180:GLY:HA2	1:I:380:LYS:HB3	1.82	0.62
1:F:50:THR:HG21	1:F:56:VAL:HA	1.80	0.62
1:G:50:THR:HG21	1:G:56:VAL:HA	1.80	0.62
1:H:180:GLY:HA2	1:H:380:LYS:HB3	1.82	0.62
1:J:180:GLY:HA2	1:J:380:LYS:HB3	1.82	0.62
1:C:52:ASP:O	1:C:56:VAL:HG23	1.98	0.62
1:G:138:CYS:HB3	1:G:407:VAL:HA	1.81	0.62
1:F:52:ASP:O	1:F:56:VAL:HG23	1.98	0.62
1:N:180:GLY:HA2	1:N:380:LYS:HB3	1.82	0.62
1:B:138:CYS:HB3	1:B:407:VAL:HA	1.81	0.62
1:E:27:VAL:HG12	1:E:90:THR:CG2	2.26	0.62
1:M:227:ILE:HG21	1:M:233:MET:HE3	1.82	0.62
1:N:227:ILE:HG21	1:N:233:MET:HE3	1.82	0.62
1:A:138:CYS:HB3	1:A:407:VAL:HA	1.81	0.61
1:D:54:VAL:HG13	1:D:89:THR:HG21	1.83	0.61
1:E:54:VAL:HG13	1:E:89:THR:HG21	1.83	0.61
1:I:27:VAL:HG12	1:I:90:THR:CG2	2.25	0.61
1:K:180:GLY:HA2	1:K:380:LYS:HB3	1.82	0.61
1:L:227:ILE:HG21	1:L:233:MET:HE3	1.82	0.61
1:C:54:VAL:HG13	1:C:89:THR:HG21	1.83	0.61
1:G:240:VAL:HG11	1:G:247:LEU:HD22	1.83	0.61
1:M:149:THR:HA	1:M:152:ALA:HB3	1.83	0.61
1:F:54:VAL:HG13	1:F:89:THR:HG21	1.83	0.61
1:H:227:ILE:HG21	1:H:233:MET:HE3	1.82	0.61
1:J:149:THR:HA	1:J:152:ALA:HB3	1.83	0.61
1:F:149:THR:HA	1:F:152:ALA:HB3	1.83	0.61
1:M:180:GLY:HA2	1:M:380:LYS:HB3	1.82	0.61
1:E:149:THR:HA	1:E:152:ALA:HB3	1.83	0.61
1:F:27:VAL:HG12	1:F:90:THR:CG2	2.26	0.61
1:H:149:THR:HA	1:H:152:ALA:HB3	1.83	0.61
1:I:149:THR:HA	1:I:152:ALA:HB3	1.83	0.61
1:D:149:THR:HA	1:D:152:ALA:HB3	1.83	0.61
1:F:267:MET:HE3	1:F:269:GLY:HA2	1.83	0.61
1:L:149:THR:HA	1:L:152:ALA:HB3	1.83	0.61
1:M:52:ASP:OD1	4:M:1528:PO4:P	2.59	0.61
1:N:149:THR:HA	1:N:152:ALA:HB3	1.83	0.61
1:C:149:THR:HA	1:C:152:ALA:HB3	1.83	0.60
1:H:426:LEU:HB2	1:H:444:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:PRO:HG2	1:B:320:ALA:HB3	1.84	0.60
1:C:218:PRO:HG2	1:C:320:ALA:HB3	1.84	0.60
1:I:426:LEU:HB2	1:I:444:LEU:HD22	1.83	0.60
1:K:40:LEU:HD13	1:K:41:ASP:O	2.01	0.60
1:J:426:LEU:HB2	1:J:444:LEU:HD22	1.83	0.60
1:K:149:THR:HA	1:K:152:ALA:HB3	1.83	0.60
1:K:227:ILE:HG21	1:K:233:MET:HE3	1.82	0.60
1:L:52:ASP:OD1	4:L:1528:PO4:P	2.59	0.60
1:A:218:PRO:HG2	1:A:320:ALA:HB3	1.84	0.60
1:B:54:VAL:HG13	1:B:89:THR:HG21	1.83	0.60
1:H:52:ASP:OD1	4:H:1528:PO4:P	2.59	0.60
1:E:464:VAL:HG22	1:L:464:VAL:HG22	1.83	0.60
1:G:54:VAL:HG13	1:G:89:THR:HG21	1.83	0.60
1:I:227:ILE:HG21	1:I:233:MET:HE3	1.82	0.60
1:L:40:LEU:HD13	1:L:41:ASP:O	2.02	0.60
1:L:180:GLY:HA2	1:L:380:LYS:HB3	1.82	0.60
1:N:52:ASP:OD1	4:N:1528:PO4:P	2.59	0.60
1:B:217:SER:HA	1:B:320:ALA:O	2.02	0.60
1:G:149:THR:HA	1:G:152:ALA:HB3	1.83	0.60
1:H:3:ALA:O	1:H:523:ASP:HA	2.02	0.60
1:J:40:LEU:HD13	1:J:41:ASP:O	2.02	0.60
1:K:426:LEU:HB2	1:K:444:LEU:HD22	1.83	0.60
1:N:426:LEU:HB2	1:N:444:LEU:HD22	1.83	0.60
1:F:218:PRO:HG2	1:F:320:ALA:HB3	1.84	0.60
1:J:227:ILE:HG21	1:J:233:MET:HE3	1.82	0.60
1:A:54:VAL:HG13	1:A:89:THR:HG21	1.83	0.60
1:D:218:PRO:HG2	1:D:320:ALA:HB3	1.84	0.60
1:I:3:ALA:O	1:I:523:ASP:HA	2.02	0.60
1:I:52:ASP:OD1	4:I:1528:PO4:P	2.59	0.60
1:G:27:VAL:HG12	1:G:90:THR:CG2	2.26	0.60
1:B:31:LEU:HA	4:B:1528:PO4:P	2.42	0.60
1:H:40:LEU:HD13	1:H:41:ASP:O	2.02	0.60
1:I:40:LEU:HD13	1:I:41:ASP:O	2.02	0.60
1:D:31:LEU:HA	4:D:1528:PO4:P	2.42	0.59
1:E:218:PRO:HG2	1:E:320:ALA:HB3	1.84	0.59
1:F:464:VAL:HG22	1:M:464:VAL:HG22	1.83	0.59
1:L:426:LEU:HB2	1:L:444:LEU:HD22	1.83	0.59
1:A:149:THR:HA	1:A:152:ALA:HB3	1.83	0.59
1:B:40:LEU:HD11	1:B:59:GLU:O	2.03	0.59
1:B:149:THR:HA	1:B:152:ALA:HB3	1.83	0.59
1:D:31:LEU:CB	1:D:90:THR:HG21	2.32	0.59

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:130:GLU:HB3	1:I:422:VAL:HG12	1.84	0.59
2:J:1526:ATP:PG	4:J:1528:PO4:P	3.01	0.59
1:D:38:VAL:HB	1:D:56:VAL:HG22	1.85	0.59
1:E:217:SER:HA	1:E:320:ALA:O	2.02	0.59
1:F:230:ILE:HG22	1:F:263:VAL:HG23	1.84	0.59
1:G:464:VAL:HG22	1:N:464:VAL:HG22	1.84	0.59
1:D:217:SER:HA	1:D:320:ALA:O	2.02	0.59
1:G:31:LEU:CB	1:G:90:THR:HG21	2.33	0.59
1:G:40:LEU:HD11	1:G:59:GLU:O	2.03	0.59
2:M:1527:ATP:PG	4:M:1528:PO4:P	3.01	0.59
1:N:130:GLU:HB3	1:N:422:VAL:HG12	1.83	0.59
1:D:212:ALA:HA	1:D:325:ILE:O	2.03	0.58
2:H:1527:ATP:PG	4:H:1528:PO4:P	3.01	0.58
1:I:30:THR:HG21	1:I:56:VAL:HG21	1.85	0.58
1:J:3:ALA:O	1:J:523:ASP:HA	2.02	0.58
2:K:1527:ATP:PG	4:K:1528:PO4:P	3.01	0.58
1:M:3:ALA:O	1:M:523:ASP:HA	2.02	0.58
1:A:212:ALA:HA	1:A:325:ILE:O	2.03	0.58
1:B:31:LEU:CB	1:B:90:THR:HG21	2.33	0.58
1:K:235:PRO:HB2	1:K:310:GLU:HA	1.85	0.58
1:A:31:LEU:HA	4:A:1528:PO4:P	2.42	0.58
1:A:230:ILE:CG2	1:A:263:VAL:HA	2.34	0.58
1:B:519:CYS:O	1:C:39:VAL:O	2.21	0.58
1:M:235:PRO:HB2	1:M:310:GLU:HA	1.85	0.58
1:N:30:THR:HG21	1:N:56:VAL:HG21	1.85	0.58
1:A:186:GLU:H	1:A:380:LYS:HB2	1.67	0.58
1:B:464:VAL:HG22	1:I:464:VAL:HG22	1.84	0.58
1:C:85:ALA:O	1:C:402:ALA:HA	2.03	0.58
1:D:85:ALA:O	1:D:402:ALA:HA	2.04	0.58
1:D:186:GLU:H	1:D:380:LYS:HB2	1.67	0.58
1:F:186:GLU:H	1:F:380:LYS:HB2	1.67	0.58
2:L:1527:ATP:PG	4:L:1528:PO4:P	3.01	0.58
1:M:130:GLU:HB3	1:M:422:VAL:HG12	1.83	0.58
1:B:230:ILE:CG2	1:B:263:VAL:HA	2.34	0.58
1:C:186:GLU:H	1:C:380:LYS:HB2	1.67	0.58
1:C:217:SER:HA	1:C:320:ALA:O	2.02	0.58
1:E:230:ILE:CG2	1:E:263:VAL:HA	2.34	0.58
1:F:217:SER:HA	1:F:320:ALA:O	2.02	0.58
1:G:5:ASP:CG	1:G:7:LYS:HZ3	2.12	0.58
1:H:130:GLU:HB3	1:H:422:VAL:HG12	1.83	0.58
1:H:30:THR:HG21	1:H:56:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ALA:HA	1:B:325:ILE:O	2.03	0.58
1:C:31:LEU:CB	1:C:90:THR:HG21	2.32	0.58
1:D:169:VAL:HG11	1:D:175:ILE:HG12	1.85	0.58
1:E:169:VAL:HG11	1:E:175:ILE:HG12	1.86	0.58
1:C:230:ILE:CG2	1:C:263:VAL:HA	2.34	0.58
1:E:212:ALA:HA	1:E:325:ILE:O	2.03	0.58
1:F:212:ALA:HA	1:F:325:ILE:O	2.03	0.58
1:G:169:VAL:HG11	1:G:175:ILE:CG1	2.34	0.58
2:I:1525:ATP:PG	4:I:1528:PO4:P	3.01	0.58
1:J:30:THR:HG21	1:J:56:VAL:HG21	1.85	0.58
1:M:279:PRO:HG3	1:M:292:ILE:HD11	1.85	0.58
1:A:267:MET:HE3	1:A:269:GLY:HA2	1.86	0.58
1:D:169:VAL:HG11	1:D:175:ILE:CG1	2.34	0.58
1:J:279:PRO:HG3	1:J:292:ILE:HD11	1.85	0.58
1:L:235:PRO:HB2	1:L:310:GLU:HA	1.85	0.58
1:N:251:ALA:O	1:N:277:LYS:HA	2.04	0.58
1:E:519:CYS:O	1:F:39:VAL:O	2.21	0.58
1:F:169:VAL:HG11	1:F:175:ILE:CG1	2.34	0.58
1:N:279:PRO:HG3	1:N:292:ILE:HD11	1.86	0.58
1:A:4:LYS:N	1:B:63:GLU:CA	2.67	0.57
1:A:464:VAL:HG22	1:H:464:VAL:HG22	1.84	0.57
1:B:4:LYS:N	1:C:63:GLU:CA	2.67	0.57
1:C:4:LYS:N	1:D:63:GLU:CA	2.67	0.57
1:C:169:VAL:HG11	1:C:175:ILE:CG1	2.34	0.57
1:C:212:ALA:HA	1:C:325:ILE:O	2.03	0.57
1:D:4:LYS:N	1:E:63:GLU:CA	2.67	0.57
1:E:169:VAL:HG11	1:E:175:ILE:CG1	2.34	0.57
1:E:172:GLU:CD	1:E:172:GLU:H	2.12	0.57
1:G:85:ALA:O	1:G:402:ALA:HA	2.04	0.57
1:G:217:SER:HA	1:G:320:ALA:O	2.04	0.57
1:I:279:PRO:HG3	1:I:292:ILE:HD11	1.85	0.57
1:K:251:ALA:O	1:K:277:LYS:HA	2.04	0.57
1:M:30:THR:HG21	1:M:56:VAL:HG21	1.85	0.57
1:A:85:ALA:O	1:A:402:ALA:HA	2.04	0.57
1:A:519:CYS:O	1:B:39:VAL:O	2.21	0.57
1:B:267:MET:HE3	1:B:269:GLY:HA2	1.86	0.57
1:D:172:GLU:H	1:D:172:GLU:CD	2.12	0.57
1:G:267:MET:HE3	1:G:269:GLY:HA2	1.87	0.57
1:H:251:ALA:O	1:H:277:LYS:HA	2.04	0.57
1:A:169:VAL:HG11	1:A:175:ILE:HG12	1.86	0.57
1:F:4:LYS:N	1:G:63:GLU:CA	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ALA:O	1:B:402:ALA:HA	2.04	0.57
1:D:519:CYS:O	1:E:39:VAL:O	2.21	0.57
1:F:85:ALA:O	1:F:402:ALA:HA	2.03	0.57
1:F:169:VAL:HG11	1:F:175:ILE:HG12	1.86	0.57
1:F:172:GLU:H	1:F:172:GLU:CD	2.12	0.57
1:A:5:ASP:CG	1:A:7:LYS:HZ3	2.13	0.57
1:A:169:VAL:HG11	1:A:175:ILE:CG1	2.34	0.57
1:C:5:ASP:CG	1:C:7:LYS:HZ3	2.12	0.57
1:C:169:VAL:HG11	1:C:175:ILE:HG12	1.85	0.57
1:D:230:ILE:CG2	1:D:263:VAL:HA	2.34	0.57
1:F:519:CYS:O	1:G:39:VAL:O	2.21	0.57
1:K:279:PRO:HG3	1:K:292:ILE:HD11	1.85	0.57
1:L:279:PRO:HG3	1:L:292:ILE:HD11	1.85	0.57
1:A:63:GLU:CA	1:G:4:LYS:N	2.67	0.57
1:C:519:CYS:O	1:D:39:VAL:O	2.21	0.57
1:E:4:LYS:N	1:F:63:GLU:CA	2.67	0.57
1:E:267:MET:HE3	1:E:269:GLY:HA2	1.86	0.57
1:G:169:VAL:HG11	1:G:175:ILE:HG12	1.85	0.57
1:G:230:ILE:CG2	1:G:263:VAL:HA	2.35	0.57
1:J:251:ALA:O	1:J:277:LYS:HA	2.04	0.57
1:K:30:THR:HG21	1:K:56:VAL:HG21	1.85	0.57
1:L:251:ALA:O	1:L:277:LYS:HA	2.04	0.57
1:M:251:ALA:O	1:M:277:LYS:HA	2.04	0.57
1:A:39:VAL:O	1:G:519:CYS:O	2.21	0.57
1:C:267:MET:HE3	1:C:269:GLY:HA2	1.86	0.57
1:E:85:ALA:O	1:E:402:ALA:HA	2.04	0.57
1:I:251:ALA:O	1:I:277:LYS:HA	2.04	0.57
1:L:30:THR:HG21	1:L:56:VAL:HG21	1.85	0.57
1:H:212:ALA:HA	1:H:325:ILE:O	2.05	0.57
1:H:279:PRO:HG3	1:H:292:ILE:HD11	1.85	0.57
1:I:235:PRO:HB2	1:I:310:GLU:HA	1.87	0.57
1:B:169:VAL:HG11	1:B:175:ILE:CG1	2.34	0.56
1:M:212:ALA:HA	1:M:325:ILE:O	2.05	0.56
1:A:127:ALA:N	1:A:426:LEU:HD21	2.21	0.56
1:A:172:GLU:H	1:A:172:GLU:CD	2.12	0.56
1:C:27:VAL:HG12	1:C:90:THR:CG2	2.26	0.56
1:G:12:ALA:HB2	1:G:520:MET:H	1.71	0.56
1:B:172:GLU:CD	1:B:172:GLU:H	2.12	0.56
1:C:127:ALA:N	1:C:426:LEU:HD21	2.20	0.56
1:D:267:MET:HE3	1:D:269:GLY:HA2	1.86	0.56
1:B:169:VAL:HG11	1:B:175:ILE:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:ALA:HB2	1:F:520:MET:H	1.71	0.56
1:N:212:ALA:HA	1:N:325:ILE:O	2.05	0.56
1:A:12:ALA:HB2	1:A:520:MET:H	1.71	0.56
1:C:151:SER:CB	1:C:399:ALA:HA	2.36	0.56
1:F:127:ALA:N	1:F:426:LEU:HD21	2.20	0.56
1:G:127:ALA:N	1:G:426:LEU:HD21	2.20	0.56
1:A:151:SER:CB	1:A:399:ALA:HA	2.36	0.56
1:C:172:GLU:H	1:C:172:GLU:CD	2.12	0.56
1:E:12:ALA:HB2	1:E:520:MET:H	1.70	0.56
1:J:212:ALA:HA	1:J:325:ILE:O	2.06	0.56
1:K:212:ALA:HA	1:K:325:ILE:O	2.05	0.56
1:C:240:VAL:HG11	1:C:247:LEU:HD22	1.88	0.56
1:D:127:ALA:N	1:D:426:LEU:HD21	2.20	0.56
1:F:240:VAL:HG11	1:F:247:LEU:HD22	1.88	0.56
1:G:172:GLU:CD	1:G:172:GLU:H	2.12	0.56
1:H:227:ILE:H	1:H:251:ALA:HB1	1.71	0.56
1:B:12:ALA:HB2	1:B:520:MET:H	1.71	0.56
1:B:127:ALA:N	1:B:426:LEU:HD21	2.20	0.56
1:D:12:ALA:HB2	1:D:520:MET:H	1.70	0.56
1:D:240:VAL:HG11	1:D:247:LEU:HD22	1.88	0.56
1:I:212:ALA:HA	1:I:325:ILE:O	2.05	0.56
1:C:12:ALA:HB2	1:C:520:MET:H	1.70	0.56
1:E:151:SER:CB	1:E:399:ALA:HA	2.36	0.56
1:E:240:VAL:HG11	1:E:247:LEU:HD22	1.88	0.56
1:F:151:SER:CB	1:F:399:ALA:HA	2.36	0.56
1:B:240:VAL:HG11	1:B:247:LEU:HD22	1.88	0.56
1:G:151:SER:CB	1:G:399:ALA:HA	2.36	0.56
1:G:240:VAL:O	1:G:271:VAL:HG21	2.06	0.56
1:J:138:CYS:CB	1:J:407:VAL:HA	2.36	0.55
1:J:151:SER:CB	1:J:399:ALA:HA	2.36	0.55
1:H:31:LEU:CB	1:H:90:THR:HG21	2.37	0.55
1:L:138:CYS:CB	1:L:407:VAL:HA	2.37	0.55
1:M:516:THR:O	1:M:517:THR:HB	2.06	0.55
1:D:151:SER:CB	1:D:399:ALA:HA	2.36	0.55
1:L:212:ALA:HA	1:L:325:ILE:O	2.05	0.55
1:M:227:ILE:H	1:M:251:ALA:HB1	1.71	0.55
1:N:138:CYS:CB	1:N:407:VAL:HA	2.36	0.55
1:N:227:ILE:H	1:N:251:ALA:HB1	1.71	0.55
1:B:151:SER:CB	1:B:399:ALA:HA	2.36	0.55
1:I:31:LEU:CB	1:I:90:THR:HG21	2.37	0.55
1:E:127:ALA:N	1:E:426:LEU:HD21	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:138:CYS:CB	1:K:407:VAL:HA	2.36	0.55
1:L:151:SER:CB	1:L:399:ALA:HA	2.36	0.55
1:H:138:CYS:CB	1:H:407:VAL:HA	2.36	0.55
1:I:151:SER:CB	1:I:399:ALA:HA	2.36	0.55
1:L:227:ILE:H	1:L:251:ALA:HB1	1.71	0.55
1:M:138:CYS:CB	1:M:407:VAL:HA	2.36	0.55
1:M:151:SER:CB	1:M:399:ALA:HA	2.36	0.55
1:N:31:LEU:CB	1:N:90:THR:HG21	2.37	0.55
1:N:516:THR:O	1:N:517:THR:HB	2.06	0.55
1:J:227:ILE:H	1:J:251:ALA:HB1	1.71	0.55
1:N:172:GLU:H	1:N:172:GLU:CD	2.15	0.55
1:M:196:ASP:HA	1:M:329:THR:HA	1.89	0.55
1:H:151:SER:CB	1:H:399:ALA:HA	2.36	0.55
1:B:144:ILE:HG23	1:B:403:THR:CG2	2.37	0.54
1:I:227:ILE:H	1:I:251:ALA:HB1	1.71	0.54
1:J:196:ASP:HA	1:J:329:THR:HA	1.89	0.54
1:K:151:SER:CB	1:K:399:ALA:HA	2.36	0.54
1:K:196:ASP:HA	1:K:329:THR:HA	1.90	0.54
1:L:516:THR:O	1:L:517:THR:HB	2.06	0.54
1:M:233:MET:HE1	1:M:259:LEU:HD21	1.90	0.54
1:N:151:SER:CB	1:N:399:ALA:HA	2.36	0.54
1:N:196:ASP:HA	1:N:329:THR:HA	1.89	0.54
1:A:4:LYS:H	1:B:63:GLU:CA	2.21	0.54
1:C:144:ILE:HG23	1:C:403:THR:CG2	2.37	0.54
1:D:4:LYS:H	1:E:63:GLU:CA	2.21	0.54
1:L:144:ILE:HG23	1:L:403:THR:CG2	2.38	0.54
1:I:144:ILE:HG23	1:I:403:THR:CG2	2.38	0.54
1:I:516:THR:O	1:I:517:THR:HB	2.06	0.54
1:J:31:LEU:CB	1:J:90:THR:HG21	2.37	0.54
1:M:144:ILE:HG23	1:M:403:THR:CG2	2.38	0.54
1:H:172:GLU:H	1:H:172:GLU:CD	2.15	0.54
1:J:233:MET:HE1	1:J:259:LEU:HD21	1.90	0.54
1:K:31:LEU:CB	1:K:90:THR:HG21	2.37	0.54
1:L:196:ASP:HA	1:L:329:THR:HA	1.89	0.54
1:M:172:GLU:CD	1:M:172:GLU:H	2.15	0.54
1:A:206:ASN:CB	1:A:213:VAL:HA	2.37	0.54
1:H:196:ASP:HA	1:H:329:THR:HA	1.89	0.54
1:H:233:MET:HE1	1:H:259:LEU:HD21	1.89	0.54
1:I:172:GLU:H	1:I:172:GLU:CD	2.15	0.54
1:J:172:GLU:CD	1:J:172:GLU:H	2.15	0.54
1:J:516:THR:O	1:J:517:THR:HB	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:144:ILE:HG23	1:K:403:THR:CG2	2.38	0.54
1:L:31:LEU:CB	1:L:90:THR:HG21	2.37	0.54
1:N:233:MET:HE1	1:N:259:LEU:HD21	1.90	0.54
1:E:144:ILE:HG23	1:E:403:THR:CG2	2.37	0.54
1:F:4:LYS:H	1:G:63:GLU:CA	2.21	0.54
1:H:144:ILE:HG23	1:H:403:THR:CG2	2.38	0.54
1:I:233:MET:HE1	1:I:259:LEU:HD21	1.90	0.54
1:K:227:ILE:H	1:K:251:ALA:HB1	1.71	0.54
1:C:4:LYS:H	1:D:63:GLU:CA	2.21	0.54
1:F:31:LEU:HB2	1:F:90:THR:HG21	1.89	0.54
1:F:144:ILE:HG23	1:F:403:THR:CG2	2.37	0.54
1:J:144:ILE:HG23	1:J:403:THR:CG2	2.38	0.54
1:L:233:MET:HE1	1:L:259:LEU:HD21	1.90	0.54
1:A:63:GLU:CA	1:G:4:LYS:H	2.21	0.54
1:A:255:GLU:HB2	1:A:258:ALA:HB3	1.90	0.54
1:E:12:ALA:HB2	1:E:520:MET:N	2.23	0.54
1:I:138:CYS:CB	1:I:407:VAL:HA	2.37	0.54
1:I:196:ASP:HA	1:I:329:THR:HA	1.89	0.54
1:B:4:LYS:H	1:C:63:GLU:CA	2.21	0.54
1:E:31:LEU:HB2	1:E:90:THR:HG21	1.89	0.54
1:H:349:ILE:HG22	1:H:369:VAL:HG13	1.90	0.54
1:M:31:LEU:CB	1:M:90:THR:HG21	2.37	0.54
1:D:144:ILE:HG23	1:D:403:THR:CG2	2.37	0.54
1:G:12:ALA:HB2	1:G:520:MET:N	2.23	0.54
1:K:516:THR:O	1:K:517:THR:HB	2.06	0.54
1:A:144:ILE:HG23	1:A:403:THR:CG2	2.37	0.53
1:H:218:PRO:HG2	1:H:320:ALA:HB3	1.90	0.53
1:I:218:PRO:HG2	1:I:320:ALA:HB3	1.90	0.53
1:N:144:ILE:HG23	1:N:403:THR:CG2	2.38	0.53
1:B:255:GLU:HB2	1:B:258:ALA:HB3	1.90	0.53
1:M:349:ILE:HG22	1:M:369:VAL:HG13	1.90	0.53
1:N:218:PRO:HG2	1:N:320:ALA:HB3	1.90	0.53
1:G:31:LEU:HB2	1:G:90:THR:HG21	1.89	0.53
1:I:349:ILE:HG22	1:I:369:VAL:HG13	1.91	0.53
1:K:172:GLU:H	1:K:172:GLU:CD	2.15	0.53
1:N:349:ILE:HG22	1:N:369:VAL:HG13	1.91	0.53
1:B:206:ASN:CB	1:B:213:VAL:HA	2.37	0.53
1:H:516:THR:O	1:H:517:THR:HB	2.06	0.53
1:L:349:ILE:HG22	1:L:369:VAL:HG13	1.90	0.53
1:N:217:SER:HA	1:N:320:ALA:O	2.09	0.53
1:D:31:LEU:HB2	1:D:90:THR:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:258:ALA:HA	1:G:242:LYS:C	2.34	0.53
1:I:206:ASN:HB2	1:I:213:VAL:HA	1.90	0.53
1:J:217:SER:HA	1:J:320:ALA:O	2.09	0.53
1:E:4:LYS:H	1:F:63:GLU:CA	2.21	0.53
1:F:258:ALA:HA	1:G:242:LYS:CA	2.39	0.53
1:K:349:ILE:HG22	1:K:369:VAL:HG13	1.90	0.53
1:A:217:SER:HA	1:A:320:ALA:O	2.08	0.53
1:A:257:GLU:CD	1:A:257:GLU:H	2.17	0.53
1:F:12:ALA:HB2	1:F:520:MET:N	2.23	0.53
1:G:183:LEU:C	1:G:382:GLY:HA3	2.34	0.53
1:K:233:MET:HE1	1:K:259:LEU:HD21	1.90	0.53
1:L:172:GLU:H	1:L:172:GLU:CD	2.15	0.53
1:C:257:GLU:CD	1:C:257:GLU:H	2.17	0.53
1:J:218:PRO:HG2	1:J:320:ALA:HB3	1.90	0.53
1:L:206:ASN:HB2	1:L:213:VAL:HA	1.90	0.53
1:B:31:LEU:HB2	1:B:90:THR:HG21	1.89	0.53
1:C:31:LEU:HB2	1:C:90:THR:HG21	1.89	0.53
1:D:257:GLU:CD	1:D:257:GLU:H	2.17	0.53
1:J:206:ASN:HB2	1:J:213:VAL:HA	1.90	0.53
1:C:206:ASN:CB	1:C:213:VAL:HA	2.37	0.53
1:D:12:ALA:HB2	1:D:520:MET:N	2.23	0.53
1:F:41:ASP:HA	1:F:47:PRO:CB	2.39	0.53
1:F:183:LEU:C	1:F:382:GLY:HA3	2.34	0.53
1:G:144:ILE:HG23	1:G:403:THR:CG2	2.37	0.53
1:J:142:LYS:H	1:J:142:LYS:HD2	1.74	0.53
1:C:12:ALA:HB2	1:C:520:MET:N	2.23	0.52
1:C:255:GLU:HB2	1:C:258:ALA:HB3	1.90	0.52
1:D:255:GLU:HB2	1:D:258:ALA:HB3	1.90	0.52
1:H:106:ALA:CB	1:H:116:LEU:HD21	2.40	0.52
1:H:206:ASN:HB2	1:H:213:VAL:HA	1.90	0.52
1:J:349:ILE:HG22	1:J:369:VAL:HG13	1.91	0.52
1:M:106:ALA:CB	1:M:116:LEU:HD21	2.39	0.52
1:M:206:ASN:HB2	1:M:213:VAL:HA	1.90	0.52
1:N:106:ALA:CB	1:N:116:LEU:HD21	2.40	0.52
1:A:41:ASP:HA	1:A:47:PRO:CB	2.39	0.52
1:L:142:LYS:H	1:L:142:LYS:HD2	1.74	0.52
1:M:142:LYS:H	1:M:142:LYS:HD2	1.75	0.52
1:M:217:SER:HA	1:M:320:ALA:O	2.09	0.52
1:M:218:PRO:HG2	1:M:320:ALA:HB3	1.90	0.52
1:A:183:LEU:C	1:A:382:GLY:HA3	2.34	0.52
1:E:257:GLU:H	1:E:257:GLU:CD	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:106:ALA:CB	1:K:116:LEU:HD21	2.40	0.52
1:A:12:ALA:HB2	1:A:520:MET:N	2.23	0.52
1:A:31:LEU:HB2	1:A:90:THR:HG21	1.89	0.52
1:B:257:GLU:H	1:B:257:GLU:CD	2.17	0.52
1:F:255:GLU:HB2	1:F:258:ALA:HB3	1.91	0.52
1:H:142:LYS:H	1:H:142:LYS:HD2	1.74	0.52
1:K:206:ASN:HB2	1:K:213:VAL:HA	1.90	0.52
1:K:217:SER:HA	1:K:320:ALA:O	2.09	0.52
1:D:41:ASP:HA	1:D:47:PRO:CB	2.39	0.52
1:E:255:GLU:HB2	1:E:258:ALA:HB3	1.90	0.52
1:G:254:VAL:HG23	1:G:259:LEU:HB3	1.92	0.52
1:H:217:SER:HA	1:H:320:ALA:O	2.09	0.52
1:K:142:LYS:H	1:K:142:LYS:HD2	1.75	0.52
1:L:217:SER:HA	1:L:320:ALA:O	2.09	0.52
1:A:169:VAL:HG13	1:A:170:GLY:O	2.10	0.52
1:B:183:LEU:C	1:B:382:GLY:HA3	2.34	0.52
1:C:124:VAL:HG21	1:C:508:ALA:CB	2.40	0.52
1:I:217:SER:HA	1:I:320:ALA:O	2.09	0.52
1:J:106:ALA:CB	1:J:116:LEU:HD21	2.40	0.52
1:K:218:PRO:HG2	1:K:320:ALA:HB3	1.90	0.52
1:L:106:ALA:CB	1:L:116:LEU:HD21	2.40	0.52
1:A:254:VAL:HG23	1:A:259:LEU:HB3	1.91	0.52
1:F:206:ASN:HB2	1:F:213:VAL:CB	2.40	0.52
1:B:12:ALA:HB2	1:B:520:MET:N	2.23	0.52
1:B:254:VAL:HG23	1:B:259:LEU:HB3	1.91	0.52
1:C:183:LEU:C	1:C:382:GLY:HA3	2.34	0.52
1:D:124:VAL:HG21	1:D:508:ALA:CB	2.40	0.52
1:E:183:LEU:C	1:E:382:GLY:HA3	2.34	0.52
1:L:427:ALA:HA	1:L:444:LEU:HD11	1.92	0.52
1:N:206:ASN:HB2	1:N:213:VAL:HA	1.90	0.52
1:C:41:ASP:HA	1:C:47:PRO:CB	2.39	0.52
1:J:226:LYS:HA	1:J:253:ASP:H	1.75	0.52
1:M:427:ALA:HA	1:M:444:LEU:HD11	1.92	0.52
1:A:4:LYS:HZ2	1:A:523:ASP:CG	2.18	0.52
1:B:124:VAL:HG21	1:B:508:ALA:CB	2.40	0.52
1:B:206:ASN:HB2	1:B:213:VAL:CB	2.40	0.52
1:C:180:GLY:HA3	1:C:381:VAL:O	2.11	0.52
1:D:206:ASN:CB	1:D:213:VAL:HA	2.37	0.52
1:E:206:ASN:HB2	1:E:213:VAL:CB	2.40	0.52
1:F:206:ASN:CB	1:F:213:VAL:HA	2.37	0.52
1:G:169:VAL:HG13	1:G:170:GLY:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:226:LYS:HA	1:I:253:ASP:H	1.75	0.52
1:M:226:LYS:HA	1:M:253:ASP:H	1.75	0.52
1:N:142:LYS:H	1:N:142:LYS:HD2	1.75	0.52
1:B:169:VAL:HG13	1:B:170:GLY:O	2.10	0.51
1:I:190:VAL:HG13	1:I:333:ILE:O	2.10	0.51
1:K:427:ALA:HA	1:K:444:LEU:HD11	1.92	0.51
1:A:199:TYR:CE2	1:A:327:LYS:HB3	2.46	0.51
1:B:180:GLY:HA3	1:B:381:VAL:O	2.10	0.51
1:G:206:ASN:CB	1:G:213:VAL:HA	2.37	0.51
1:H:427:ALA:HA	1:H:444:LEU:HD11	1.92	0.51
1:L:190:VAL:HG13	1:L:333:ILE:O	2.10	0.51
1:N:190:VAL:HG13	1:N:333:ILE:O	2.10	0.51
1:N:427:ALA:HA	1:N:444:LEU:HD11	1.92	0.51
1:D:180:GLY:HA3	1:D:381:VAL:O	2.10	0.51
1:F:257:GLU:HG2	1:F:258:ALA:H	1.75	0.51
1:J:190:VAL:HG13	1:J:333:ILE:O	2.10	0.51
1:K:190:VAL:HG13	1:K:333:ILE:O	2.10	0.51
1:L:218:PRO:HG2	1:L:320:ALA:HB3	1.90	0.51
1:L:417:VAL:HG21	1:L:477:GLY:HA3	1.91	0.51
1:M:190:VAL:HG13	1:M:333:ILE:O	2.10	0.51
1:G:199:TYR:CE2	1:G:327:LYS:HB3	2.46	0.51
1:K:417:VAL:HG21	1:K:477:GLY:HA3	1.91	0.51
1:M:417:VAL:HG21	1:M:477:GLY:HA3	1.91	0.51
1:B:199:TYR:CE2	1:B:327:LYS:HB3	2.46	0.51
1:C:169:VAL:HG13	1:C:170:GLY:O	2.10	0.51
1:D:183:LEU:C	1:D:382:GLY:HA3	2.34	0.51
1:D:206:ASN:HB2	1:D:213:VAL:CB	2.40	0.51
1:E:124:VAL:HG21	1:E:508:ALA:CB	2.40	0.51
1:E:169:VAL:HG13	1:E:170:GLY:O	2.10	0.51
1:F:169:VAL:HG13	1:F:170:GLY:O	2.10	0.51
1:I:127:ALA:N	1:I:426:LEU:HD21	2.26	0.51
1:J:417:VAL:HG21	1:J:477:GLY:HA3	1.91	0.51
1:K:226:LYS:HA	1:K:253:ASP:H	1.75	0.51
1:L:247:LEU:O	1:L:273:VAL:HA	2.11	0.51
1:C:206:ASN:HB2	1:C:213:VAL:CB	2.40	0.51
1:H:190:VAL:HG13	1:H:333:ILE:O	2.10	0.51
1:H:226:LYS:HA	1:H:253:ASP:H	1.75	0.51
1:N:417:VAL:HG21	1:N:477:GLY:HA3	1.91	0.51
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.40	0.51
1:B:258:ALA:HA	1:C:243:ALA:HA	1.92	0.51
1:D:169:VAL:HG13	1:D:170:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:VAL:HG23	1:E:259:LEU:HB3	1.91	0.51
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.40	0.51
1:F:199:TYR:CE2	1:F:327:LYS:HB3	2.46	0.51
1:H:127:ALA:N	1:H:426:LEU:HD21	2.26	0.51
1:H:417:VAL:HG21	1:H:477:GLY:HA3	1.91	0.51
1:J:127:ALA:N	1:J:426:LEU:HD21	2.26	0.51
1:N:226:LYS:HA	1:N:253:ASP:H	1.75	0.51
1:A:218:PRO:HA	1:A:246:PRO:O	2.10	0.51
1:A:240:VAL:O	1:A:271:VAL:HG21	2.11	0.51
1:A:240:VAL:HG11	1:A:247:LEU:HD22	1.92	0.51
1:B:41:ASP:HA	1:B:47:PRO:CB	2.39	0.51
1:B:293:ALA:HB2	1:B:300:VAL:CG2	2.41	0.51
1:C:254:VAL:HG23	1:C:259:LEU:HB3	1.91	0.51
1:F:293:ALA:HB2	1:F:300:VAL:CG2	2.41	0.51
1:G:124:VAL:HG21	1:G:508:ALA:CB	2.40	0.51
1:G:206:ASN:HB2	1:G:213:VAL:CB	2.41	0.51
1:I:106:ALA:CB	1:I:116:LEU:HD21	2.40	0.51
1:I:417:VAL:HG21	1:I:477:GLY:HA3	1.91	0.51
1:M:127:ALA:N	1:M:426:LEU:HD21	2.26	0.51
1:N:127:ALA:N	1:N:426:LEU:HD21	2.26	0.51
1:I:124:VAL:HG21	1:I:508:ALA:CB	2.41	0.51
1:I:427:ALA:HA	1:I:444:LEU:HD11	1.93	0.51
1:L:127:ALA:N	1:L:426:LEU:HD21	2.26	0.51
1:A:206:ASN:HB2	1:A:213:VAL:CB	2.40	0.51
1:A:258:ALA:HA	1:B:243:ALA:HA	1.93	0.51
1:C:199:TYR:CE2	1:C:327:LYS:HB3	2.46	0.51
1:D:254:VAL:HG23	1:D:259:LEU:HB3	1.91	0.51
1:E:406:ALA:HB2	1:E:496:PRO:HG3	1.93	0.51
1:G:180:GLY:HA3	1:G:381:VAL:O	2.10	0.51
1:I:142:LYS:H	1:I:142:LYS:HD2	1.75	0.51
1:K:124:VAL:HG21	1:K:508:ALA:CB	2.41	0.51
1:K:127:ALA:N	1:K:426:LEU:HD21	2.26	0.51
1:A:180:GLY:HA3	1:A:381:VAL:O	2.10	0.50
1:C:4:LYS:N	1:D:63:GLU:HA	2.26	0.50
1:D:4:LYS:N	1:E:63:GLU:HA	2.26	0.50
1:E:41:ASP:HA	1:E:47:PRO:CB	2.39	0.50
1:F:4:LYS:N	1:G:63:GLU:HA	2.26	0.50
1:F:180:GLY:HA3	1:F:381:VAL:O	2.11	0.50
1:G:41:ASP:HA	1:G:47:PRO:CB	2.39	0.50
1:J:427:ALA:HA	1:J:444:LEU:HD11	1.93	0.50
1:K:247:LEU:O	1:K:273:VAL:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:VAL:HG21	1:L:508:ALA:CB	2.41	0.50
1:E:180:GLY:HA3	1:E:381:VAL:O	2.11	0.50
1:E:206:ASN:CB	1:E:213:VAL:HA	2.37	0.50
1:H:247:LEU:O	1:H:273:VAL:HA	2.11	0.50
1:J:124:VAL:HG21	1:J:508:ALA:CB	2.41	0.50
1:B:196:ASP:HA	1:B:329:THR:HA	1.94	0.50
1:D:106:ALA:CB	1:D:116:LEU:HD21	2.42	0.50
1:D:293:ALA:HB2	1:D:300:VAL:CG2	2.41	0.50
1:I:247:LEU:O	1:I:273:VAL:HA	2.11	0.50
1:M:124:VAL:HG21	1:M:508:ALA:CB	2.41	0.50
1:M:247:LEU:O	1:M:273:VAL:HA	2.11	0.50
1:C:106:ALA:CB	1:C:116:LEU:HD21	2.42	0.50
1:C:258:ALA:HA	1:D:243:ALA:HA	1.92	0.50
1:C:496:PRO:HB2	1:C:499:VAL:HG13	1.93	0.50
1:D:199:TYR:CE2	1:D:327:LYS:HB3	2.46	0.50
1:D:406:ALA:HB2	1:D:496:PRO:HG3	1.94	0.50
1:J:138:CYS:HB2	1:J:407:VAL:HA	1.94	0.50
1:H:293:ALA:HB2	1:H:300:VAL:CG2	2.42	0.50
1:I:138:CYS:HB2	1:I:407:VAL:HA	1.94	0.50
1:J:40:LEU:O	1:J:47:PRO:HB2	2.12	0.50
1:L:226:LYS:HA	1:L:253:ASP:H	1.75	0.50
1:N:349:ILE:HG23	1:N:365:LEU:HD13	1.93	0.50
2:B:1525:ATP:PG	4:B:1528:PO4:P	3.10	0.50
1:C:31:LEU:HB3	1:C:90:THR:HG21	1.94	0.50
1:G:106:ALA:CB	1:G:116:LEU:HD21	2.42	0.50
1:J:293:ALA:HB2	1:J:300:VAL:CG2	2.42	0.50
1:L:293:ALA:HB2	1:L:300:VAL:CG2	2.42	0.50
1:N:293:ALA:HB2	1:N:300:VAL:CG2	2.42	0.50
1:B:496:PRO:HB2	1:B:499:VAL:HG13	1.93	0.50
1:C:4:LYS:HZ2	1:C:523:ASP:CG	2.19	0.50
1:D:496:PRO:HB2	1:D:499:VAL:HG13	1.93	0.50
2:D:1525:ATP:PG	4:D:1528:PO4:P	3.10	0.50
1:E:199:TYR:CE2	1:E:327:LYS:HB3	2.46	0.50
1:E:262:LEU:HB2	1:F:242:LYS:HA	1.94	0.50
1:E:293:ALA:HB2	1:E:300:VAL:CG2	2.41	0.50
1:E:383:ALA:HB3	1:E:389:MET:HB2	1.94	0.50
1:F:406:ALA:HB2	1:F:496:PRO:HG3	1.93	0.50
1:G:4:LYS:HZ2	1:G:523:ASP:CG	2.20	0.50
1:H:349:ILE:HG23	1:H:365:LEU:HD13	1.93	0.50
1:I:40:LEU:O	1:I:47:PRO:HB2	2.12	0.50
1:A:196:ASP:HA	1:A:329:THR:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LYS:N	1:C:63:GLU:HA	2.26	0.50
1:C:196:ASP:HA	1:C:329:THR:HA	1.94	0.50
2:C:1526:ATP:PG	4:C:1528:PO4:P	3.10	0.50
1:E:4:LYS:N	1:F:63:GLU:HA	2.26	0.50
1:E:258:ALA:HA	1:F:243:ALA:HA	1.93	0.50
2:E:1525:ATP:PG	4:E:1528:PO4:P	3.10	0.50
1:H:124:VAL:HG21	1:H:508:ALA:CB	2.41	0.50
1:J:247:LEU:O	1:J:273:VAL:HA	2.11	0.50
1:K:293:ALA:HB2	1:K:300:VAL:CG2	2.42	0.50
1:N:124:VAL:HG21	1:N:508:ALA:CB	2.41	0.50
1:N:247:LEU:O	1:N:273:VAL:HA	2.11	0.50
1:B:31:LEU:HB3	1:B:90:THR:HG21	1.94	0.49
1:B:106:ALA:CB	1:B:116:LEU:HD21	2.42	0.49
1:B:262:LEU:HB2	1:C:242:LYS:HA	1.94	0.49
1:B:383:ALA:HB3	1:B:389:MET:HB2	1.94	0.49
1:B:406:ALA:HB2	1:B:496:PRO:HG3	1.94	0.49
1:C:126:ALA:HB3	1:C:426:LEU:HD22	1.94	0.49
1:D:258:ALA:HA	1:E:243:ALA:HA	1.93	0.49
1:D:262:LEU:HB2	1:E:242:LYS:HA	1.94	0.49
1:D:383:ALA:HB3	1:D:389:MET:HB2	1.94	0.49
1:G:293:ALA:HB2	1:G:300:VAL:CG2	2.41	0.49
1:A:106:ALA:CB	1:A:116:LEU:HD21	2.42	0.49
1:A:140:ASP:CG	1:A:142:LYS:HZ3	2.20	0.49
1:B:126:ALA:HB3	1:B:426:LEU:HD22	1.95	0.49
1:C:262:LEU:HB2	1:D:242:LYS:HA	1.94	0.49
1:C:293:ALA:HB2	1:C:300:VAL:CG2	2.41	0.49
1:D:126:ALA:HB3	1:D:426:LEU:HD22	1.94	0.49
1:E:349:ILE:HG22	1:E:369:VAL:HG13	1.95	0.49
1:F:31:LEU:HB3	1:F:90:THR:HG21	1.94	0.49
1:F:106:ALA:CB	1:F:116:LEU:HD21	2.42	0.49
1:G:496:PRO:HB2	1:G:499:VAL:HG13	1.93	0.49
1:K:40:LEU:O	1:K:47:PRO:HB2	2.12	0.49
1:M:349:ILE:HG23	1:M:365:LEU:HD13	1.93	0.49
1:A:126:ALA:HB3	1:A:426:LEU:HD22	1.94	0.49
1:A:262:LEU:HB2	1:B:242:LYS:HA	1.94	0.49
1:A:496:PRO:HB2	1:A:499:VAL:HG13	1.93	0.49
1:E:106:ALA:CB	1:E:116:LEU:HD21	2.42	0.49
1:E:496:PRO:HB2	1:E:499:VAL:HG13	1.93	0.49
1:F:383:ALA:HB3	1:F:389:MET:HB2	1.94	0.49
1:G:383:ALA:HB3	1:G:389:MET:HB2	1.94	0.49
1:J:356:ALA:HB1	1:J:361:ASP:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:186:GLU:H	1:N:380:LYS:HB2	1.77	0.49
1:A:31:LEU:HB3	1:A:90:THR:HG21	1.94	0.49
1:A:349:ILE:HG22	1:A:369:VAL:HG13	1.94	0.49
1:E:196:ASP:HA	1:E:329:THR:HA	1.93	0.49
1:F:496:PRO:HB2	1:F:499:VAL:HG13	1.93	0.49
2:F:1525:ATP:PG	4:F:1528:PO4:P	3.10	0.49
1:G:349:ILE:HG22	1:G:369:VAL:HG13	1.95	0.49
1:L:356:ALA:HB1	1:L:361:ASP:HB2	1.95	0.49
1:A:293:ALA:HB2	1:A:300:VAL:CG2	2.41	0.49
1:D:349:ILE:HG22	1:D:369:VAL:HG13	1.95	0.49
1:E:126:ALA:HB3	1:E:426:LEU:HD22	1.94	0.49
1:F:257:GLU:HA	1:G:243:ALA:C	2.38	0.49
1:F:349:ILE:HG22	1:F:369:VAL:HG13	1.95	0.49
1:H:186:GLU:H	1:H:380:LYS:HB2	1.77	0.49
1:K:356:ALA:HB1	1:K:361:ASP:HB2	1.95	0.49
1:M:293:ALA:HB2	1:M:300:VAL:CG2	2.42	0.49
1:A:406:ALA:HB2	1:A:496:PRO:HG3	1.93	0.49
1:D:31:LEU:HB3	1:D:90:THR:HG21	1.94	0.49
1:D:237:LEU:O	1:D:241:ALA:N	2.46	0.49
1:H:40:LEU:O	1:H:47:PRO:HB2	2.12	0.49
1:K:138:CYS:HB2	1:K:407:VAL:HA	1.94	0.49
1:L:349:ILE:HG23	1:L:365:LEU:HD13	1.93	0.49
2:A:1525:ATP:PG	4:A:1528:PO4:P	3.10	0.49
1:B:82:ASN:HB2	1:B:89:THR:HG23	1.95	0.49
1:C:406:ALA:HB2	1:C:496:PRO:HG3	1.93	0.49
1:E:31:LEU:HB3	1:E:90:THR:HG21	1.94	0.49
1:I:293:ALA:HB2	1:I:300:VAL:CG2	2.42	0.49
1:L:40:LEU:O	1:L:47:PRO:HB2	2.12	0.49
1:L:186:GLU:H	1:L:380:LYS:HB2	1.77	0.49
1:B:349:ILE:HG22	1:B:369:VAL:HG13	1.94	0.49
1:C:349:ILE:HG22	1:C:369:VAL:HG13	1.94	0.49
1:G:406:ALA:HB2	1:G:496:PRO:HG3	1.94	0.49
1:H:31:LEU:HB2	1:H:90:THR:HG21	1.95	0.49
1:H:190:VAL:HG11	1:H:333:ILE:HG23	1.95	0.49
1:H:337:GLY:HA3	1:H:342:ILE:HD11	1.94	0.49
1:I:31:LEU:HB2	1:I:90:THR:HG21	1.95	0.49
1:I:337:GLY:HA3	1:I:342:ILE:HD11	1.94	0.49
1:I:349:ILE:HG23	1:I:365:LEU:HD13	1.93	0.49
1:L:190:VAL:HG11	1:L:333:ILE:HG23	1.94	0.49
1:M:356:ALA:HB1	1:M:361:ASP:HB2	1.95	0.49
1:N:31:LEU:HB2	1:N:90:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASN:HB2	1:A:89:THR:HG23	1.95	0.49
1:C:237:LEU:O	1:C:241:ALA:N	2.46	0.49
2:G:1525:ATP:PG	4:G:1528:PO4:P	3.10	0.49
1:J:349:ILE:HG23	1:J:365:LEU:HD13	1.93	0.49
1:K:186:GLU:H	1:K:380:LYS:HB2	1.77	0.49
1:A:281:PHE:CA	1:A:285:ARG:HB2	2.43	0.49
1:C:82:ASN:HB2	1:C:89:THR:HG23	1.95	0.49
1:C:383:ALA:HB3	1:C:389:MET:HB2	1.94	0.49
1:E:114:MET:CB	1:F:36:ARG:HD2	2.43	0.49
1:F:196:ASP:HA	1:F:329:THR:HA	1.94	0.49
1:F:230:ILE:HG21	1:F:262:LEU:C	2.38	0.49
1:H:138:CYS:HB2	1:H:407:VAL:HA	1.94	0.49
1:H:199:TYR:CE2	1:H:327:LYS:HB3	2.48	0.49
1:I:190:VAL:HG11	1:I:333:ILE:HG23	1.95	0.49
1:I:199:TYR:CE2	1:I:327:LYS:HB3	2.48	0.49
1:A:36:ARG:HD2	1:G:114:MET:CB	2.43	0.48
1:A:138:CYS:CB	1:A:407:VAL:HA	2.43	0.48
1:D:196:ASP:HA	1:D:329:THR:HA	1.94	0.48
1:F:254:VAL:HG23	1:F:259:LEU:HB2	1.95	0.48
1:G:126:ALA:HB3	1:G:426:LEU:HD22	1.94	0.48
1:I:356:ALA:HB1	1:I:361:ASP:HB2	1.95	0.48
1:L:337:GLY:HA3	1:L:342:ILE:HD11	1.94	0.48
1:A:383:ALA:HB3	1:A:389:MET:HB2	1.94	0.48
1:A:411:VAL:HG12	1:A:494:LEU:HB2	1.95	0.48
1:D:3:ALA:HA	1:E:63:GLU:CB	2.42	0.48
1:E:230:ILE:HG12	1:E:262:LEU:HD12	1.95	0.48
1:E:237:LEU:O	1:E:241:ALA:N	2.46	0.48
1:F:114:MET:CB	1:G:36:ARG:HD2	2.43	0.48
1:G:138:CYS:CB	1:G:407:VAL:HA	2.43	0.48
1:G:229:ASN:ND2	1:G:230:ILE:H	2.10	0.48
1:J:180:GLY:HA3	1:J:381:VAL:O	2.14	0.48
1:K:349:ILE:HG23	1:K:365:LEU:HD13	1.93	0.48
1:N:40:LEU:O	1:N:47:PRO:HB2	2.12	0.48
1:N:180:GLY:HA3	1:N:381:VAL:O	2.14	0.48
1:N:199:TYR:CE2	1:N:327:LYS:HB3	2.48	0.48
1:A:4:LYS:N	1:B:63:GLU:HA	2.26	0.48
1:B:138:CYS:CB	1:B:407:VAL:HA	2.43	0.48
1:C:411:VAL:HG12	1:C:494:LEU:HB2	1.95	0.48
1:D:411:VAL:HG12	1:D:494:LEU:HB2	1.96	0.48
1:G:411:VAL:HG12	1:G:494:LEU:HB2	1.95	0.48
1:J:337:GLY:HA3	1:J:342:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:31:LEU:HB2	1:K:90:THR:HG21	1.94	0.48
1:K:180:GLY:HA3	1:K:381:VAL:O	2.14	0.48
1:M:40:LEU:O	1:M:47:PRO:HB2	2.12	0.48
1:N:138:CYS:HB2	1:N:407:VAL:HA	1.94	0.48
1:N:337:GLY:HA3	1:N:342:ILE:HD11	1.94	0.48
1:D:4:LYS:HZ2	1:D:523:ASP:CG	2.20	0.48
1:E:411:VAL:HG12	1:E:494:LEU:HB2	1.96	0.48
1:F:267:MET:HE3	1:F:269:GLY:CA	2.43	0.48
1:F:281:PHE:CA	1:F:285:ARG:HB2	2.43	0.48
1:G:31:LEU:HB3	1:G:90:THR:HG21	1.94	0.48
1:I:186:GLU:H	1:I:380:LYS:HB2	1.77	0.48
1:J:186:GLU:H	1:J:380:LYS:HB2	1.77	0.48
1:L:31:LEU:HB2	1:L:90:THR:HG21	1.95	0.48
1:L:138:CYS:HB2	1:L:407:VAL:HA	1.94	0.48
1:M:199:TYR:CE2	1:M:327:LYS:HB3	2.48	0.48
1:M:205:ILE:HD12	1:M:211:GLY:O	2.13	0.48
1:M:337:GLY:HA3	1:M:342:ILE:HD11	1.94	0.48
1:N:356:ALA:HB1	1:N:361:ASP:HB2	1.95	0.48
1:C:138:CYS:CB	1:C:407:VAL:HA	2.43	0.48
1:F:411:VAL:HG12	1:F:494:LEU:HB2	1.96	0.48
1:G:196:ASP:HA	1:G:329:THR:HA	1.93	0.48
1:G:218:PRO:HA	1:G:246:PRO:O	2.13	0.48
1:H:356:ALA:HB1	1:H:361:ASP:HB2	1.95	0.48
1:I:180:GLY:HA3	1:I:381:VAL:O	2.14	0.48
1:J:31:LEU:HB2	1:J:90:THR:HG21	1.94	0.48
1:K:190:VAL:HG11	1:K:333:ILE:HG23	1.95	0.48
1:K:383:ALA:HB3	1:K:389:MET:HB2	1.95	0.48
1:M:190:VAL:HG11	1:M:333:ILE:HG23	1.95	0.48
1:M:383:ALA:HB3	1:M:389:MET:HB2	1.95	0.48
1:N:205:ILE:HD12	1:N:211:GLY:O	2.13	0.48
1:A:114:MET:CB	1:B:36:ARG:HD2	2.43	0.48
1:B:114:MET:CB	1:C:36:ARG:HD2	2.43	0.48
1:D:230:ILE:HG12	1:D:262:LEU:HD12	1.95	0.48
1:D:240:VAL:O	1:D:271:VAL:HG21	2.14	0.48
1:D:281:PHE:CA	1:D:285:ARG:HB2	2.43	0.48
1:F:200:LEU:CD1	1:F:254:VAL:HG11	2.44	0.48
1:K:199:TYR:CE2	1:K:327:LYS:HB3	2.48	0.48
1:K:205:ILE:HD12	1:K:211:GLY:O	2.13	0.48
1:L:199:TYR:CE2	1:L:327:LYS:HB3	2.48	0.48
1:L:205:ILE:HD12	1:L:211:GLY:O	2.13	0.48
1:A:63:GLU:HA	1:G:4:LYS:N	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:CD1	1:A:254:VAL:HG11	2.44	0.48
1:B:281:PHE:CA	1:B:285:ARG:HB2	2.43	0.48
1:E:281:PHE:CA	1:E:285:ARG:HB2	2.43	0.48
1:H:205:ILE:HD12	1:H:211:GLY:O	2.13	0.48
1:L:180:GLY:HA3	1:L:381:VAL:O	2.14	0.48
1:M:31:LEU:HB2	1:M:90:THR:HG21	1.95	0.48
1:M:138:CYS:HB2	1:M:407:VAL:HA	1.94	0.48
1:A:23:LEU:O	1:A:27:VAL:HG23	2.14	0.48
1:A:115:ASP:HB2	1:A:435:ASP:HB2	1.96	0.48
1:B:219:PHE:CE2	1:B:314:LEU:HD22	2.49	0.48
1:B:230:ILE:HG12	1:B:262:LEU:HD12	1.95	0.48
1:B:411:VAL:HG12	1:B:494:LEU:HB2	1.96	0.48
1:E:82:ASN:HB2	1:E:89:THR:HG23	1.95	0.48
1:F:82:ASN:HB2	1:F:89:THR:HG23	1.95	0.48
1:F:138:CYS:CB	1:F:407:VAL:HA	2.43	0.48
1:F:219:PHE:CE2	1:F:314:LEU:HD22	2.49	0.48
1:J:383:ALA:HB3	1:J:389:MET:HB2	1.95	0.48
1:N:190:VAL:HG11	1:N:333:ILE:HG23	1.95	0.48
1:N:383:ALA:HB3	1:N:389:MET:HB2	1.95	0.48
1:A:237:LEU:O	1:A:241:ALA:N	2.46	0.48
1:C:281:PHE:CA	1:C:285:ARG:HB2	2.43	0.48
1:D:138:CYS:CB	1:D:407:VAL:HA	2.43	0.48
1:D:224:ASP:HA	1:D:289:LEU:CD1	2.44	0.48
1:D:426:LEU:HB2	1:D:444:LEU:HD22	1.96	0.48
1:E:3:ALA:HA	1:F:63:GLU:CB	2.42	0.48
1:E:219:PHE:CE2	1:E:314:LEU:HD22	2.49	0.48
1:F:426:LEU:HB2	1:F:444:LEU:HD22	1.96	0.48
1:I:54:VAL:HG13	1:I:89:THR:HG21	1.96	0.48
1:J:190:VAL:HG11	1:J:333:ILE:HG23	1.95	0.48
1:J:199:TYR:CE2	1:J:327:LYS:HB3	2.48	0.48
1:B:136:VAL:O	1:B:410:GLY:HA3	2.14	0.48
1:C:3:ALA:HA	1:D:63:GLU:CB	2.42	0.48
1:C:219:PHE:CE2	1:C:314:LEU:HD22	2.49	0.48
1:C:426:LEU:HB2	1:C:444:LEU:HD22	1.96	0.48
1:D:158:VAL:HG22	1:D:396:VAL:HG22	1.96	0.48
1:E:224:ASP:HA	1:E:289:LEU:CD1	2.44	0.48
1:E:240:VAL:O	1:E:271:VAL:HG21	2.14	0.48
1:F:4:LYS:HD3	1:F:523:ASP:HA	1.95	0.48
1:G:4:LYS:HD3	1:G:523:ASP:HA	1.95	0.48
1:G:19:GLY:HA2	1:G:62:LEU:HD13	1.96	0.48
1:K:337:GLY:HA3	1:K:342:ILE:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:61:GLU:CD	1:N:4:LYS:HZ3	2.22	0.48
1:A:19:GLY:HA2	1:A:62:LEU:HD13	1.96	0.47
1:B:224:ASP:HA	1:B:289:LEU:CD1	2.44	0.47
1:C:4:LYS:HD3	1:C:523:ASP:HA	1.95	0.47
1:C:23:LEU:O	1:C:27:VAL:HG23	2.14	0.47
1:C:114:MET:CB	1:D:36:ARG:HD2	2.43	0.47
1:C:115:ASP:HB2	1:C:435:ASP:HB2	1.96	0.47
1:C:224:ASP:HA	1:C:289:LEU:CD1	2.44	0.47
1:C:240:VAL:O	1:C:271:VAL:HG21	2.14	0.47
1:D:23:LEU:O	1:D:27:VAL:HG23	2.14	0.47
1:D:114:MET:CB	1:E:36:ARG:HD2	2.43	0.47
1:F:228:SER:O	1:F:258:ALA:HB1	2.14	0.47
1:J:54:VAL:HG13	1:J:89:THR:HG21	1.96	0.47
1:A:4:LYS:HD3	1:A:523:ASP:HA	1.95	0.47
1:A:158:VAL:HG22	1:A:396:VAL:HG22	1.96	0.47
1:A:224:ASP:HA	1:A:289:LEU:CD1	2.44	0.47
1:B:4:LYS:HZ2	1:B:523:ASP:CG	2.21	0.47
1:B:115:ASP:HB2	1:B:435:ASP:HB2	1.96	0.47
1:D:219:PHE:CE2	1:D:314:LEU:HD22	2.49	0.47
1:E:23:LEU:O	1:E:27:VAL:HG23	2.14	0.47
1:E:138:CYS:CB	1:E:407:VAL:HA	2.43	0.47
1:E:426:LEU:HB2	1:E:444:LEU:HD22	1.96	0.47
1:F:126:ALA:HB3	1:F:426:LEU:HD22	1.95	0.47
1:G:82:ASN:HB2	1:G:89:THR:HG23	1.95	0.47
1:G:115:ASP:HB2	1:G:435:ASP:HB2	1.96	0.47
1:A:136:VAL:O	1:A:410:GLY:HA3	2.14	0.47
1:B:152:ALA:HB1	1:B:155:ASP:O	2.15	0.47
1:B:200:LEU:CD1	1:B:254:VAL:HG11	2.44	0.47
1:B:237:LEU:O	1:B:241:ALA:N	2.46	0.47
1:E:4:LYS:HD3	1:E:523:ASP:HA	1.95	0.47
1:F:19:GLY:HA2	1:F:62:LEU:HD13	1.96	0.47
1:F:237:LEU:O	1:F:241:ALA:N	2.46	0.47
1:F:240:VAL:O	1:F:271:VAL:HG21	2.14	0.47
1:G:281:PHE:CA	1:G:285:ARG:HB2	2.43	0.47
1:G:426:LEU:HB2	1:G:444:LEU:HD22	1.96	0.47
1:I:383:ALA:HB3	1:I:389:MET:HB2	1.95	0.47
1:L:31:LEU:HB3	1:L:90:THR:HG21	1.96	0.47
1:M:180:GLY:HA3	1:M:381:VAL:O	2.14	0.47
1:N:126:ALA:HB3	1:N:426:LEU:HD22	1.97	0.47
1:A:287:ALA:HB1	1:A:368:ARG:CZ	2.44	0.47
1:B:23:LEU:O	1:B:27:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:HG22	1:B:396:VAL:HG22	1.96	0.47
1:B:281:PHE:HA	1:B:285:ARG:HB2	1.96	0.47
1:B:287:ALA:HB1	1:B:368:ARG:CZ	2.44	0.47
1:B:426:LEU:HB2	1:B:444:LEU:HD22	1.96	0.47
1:C:158:VAL:HG22	1:C:396:VAL:HG22	1.96	0.47
1:D:4:LYS:HD3	1:D:523:ASP:HA	1.95	0.47
1:E:151:SER:HB3	1:E:399:ALA:HA	1.97	0.47
1:G:23:LEU:O	1:G:27:VAL:HG23	2.14	0.47
1:K:31:LEU:HB3	1:K:90:THR:HG21	1.97	0.47
1:L:383:ALA:HB3	1:L:389:MET:HB2	1.95	0.47
1:B:19:GLY:HA2	1:B:62:LEU:HD13	1.96	0.47
1:C:230:ILE:HG12	1:C:262:LEU:HD12	1.95	0.47
1:C:287:ALA:HB1	1:C:368:ARG:CZ	2.44	0.47
1:D:82:ASN:HB2	1:D:89:THR:HG23	1.95	0.47
1:D:279:PRO:HG3	1:D:292:ILE:HD11	1.97	0.47
1:F:206:ASN:HB2	1:F:213:VAL:HB	1.96	0.47
1:F:287:ALA:HB1	1:F:368:ARG:CZ	2.44	0.47
1:G:287:ALA:HB1	1:G:368:ARG:CZ	2.44	0.47
1:H:180:GLY:HA3	1:H:381:VAL:O	2.14	0.47
1:K:213:VAL:HG13	1:K:325:ILE:HB	1.97	0.47
1:M:186:GLU:H	1:M:380:LYS:HB2	1.77	0.47
1:A:230:ILE:HG12	1:A:262:LEU:HD12	1.95	0.47
1:A:426:LEU:HB2	1:A:444:LEU:HD22	1.96	0.47
1:C:152:ALA:HB1	1:C:155:ASP:O	2.14	0.47
1:C:281:PHE:HA	1:C:285:ARG:HB2	1.96	0.47
1:F:224:ASP:HA	1:F:289:LEU:CD1	2.44	0.47
1:H:4:LYS:HZ3	1:N:61:GLU:CD	2.21	0.47
1:H:213:VAL:HG13	1:H:325:ILE:HB	1.97	0.47
1:B:4:LYS:HD3	1:B:523:ASP:HA	1.95	0.47
1:B:206:ASN:HB2	1:B:213:VAL:HB	1.96	0.47
1:C:279:PRO:HG3	1:C:292:ILE:HD11	1.97	0.47
1:D:115:ASP:HB2	1:D:435:ASP:HB2	1.96	0.47
1:F:4:LYS:HZ2	1:F:523:ASP:CG	2.23	0.47
1:F:115:ASP:HB2	1:F:435:ASP:HB2	1.96	0.47
1:F:136:VAL:O	1:F:410:GLY:HA3	2.14	0.47
1:G:136:VAL:O	1:G:410:GLY:HA3	2.14	0.47
1:H:54:VAL:HG13	1:H:89:THR:HG21	1.96	0.47
1:H:383:ALA:HB3	1:H:389:MET:HB2	1.95	0.47
1:I:205:ILE:HD12	1:I:211:GLY:O	2.13	0.47
1:I:213:VAL:HG13	1:I:325:ILE:HB	1.97	0.47
1:J:31:LEU:HB3	1:J:90:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:183:LEU:C	1:J:382:GLY:HA3	2.40	0.47
1:J:205:ILE:HD12	1:J:211:GLY:O	2.13	0.47
1:J:213:VAL:HG13	1:J:325:ILE:HB	1.97	0.47
1:K:87:ASP:CG	1:K:151:SER:HA	2.40	0.47
1:K:183:LEU:C	1:K:382:GLY:HA3	2.40	0.47
1:L:54:VAL:HG13	1:L:89:THR:HG21	1.96	0.47
1:L:213:VAL:HG13	1:L:325:ILE:HB	1.97	0.47
1:M:126:ALA:HB3	1:M:426:LEU:HD22	1.97	0.47
1:M:152:ALA:HB1	1:M:155:ASP:HB3	1.97	0.47
1:N:213:VAL:HG13	1:N:325:ILE:HB	1.97	0.47
1:A:281:PHE:HA	1:A:285:ARG:HB2	1.96	0.47
1:D:281:PHE:HA	1:D:285:ARG:HB2	1.96	0.47
1:E:279:PRO:HG3	1:E:292:ILE:HD11	1.97	0.47
1:F:151:SER:HB3	1:F:399:ALA:HA	1.97	0.47
1:H:126:ALA:HB3	1:H:426:LEU:HD22	1.97	0.47
1:L:183:LEU:C	1:L:382:GLY:HA3	2.40	0.47
1:N:87:ASP:CG	1:N:151:SER:HA	2.40	0.47
1:N:152:ALA:HB1	1:N:155:ASP:HB3	1.97	0.47
1:A:267:MET:HE3	1:A:269:GLY:CA	2.45	0.47
1:B:240:VAL:O	1:B:271:VAL:HG21	2.14	0.47
1:D:12:ALA:HB3	1:D:518:GLU:O	2.15	0.47
1:E:4:LYS:HZ2	1:E:523:ASP:CG	2.23	0.47
1:E:12:ALA:HB3	1:E:518:GLU:O	2.15	0.47
1:E:136:VAL:O	1:E:410:GLY:HA3	2.14	0.47
1:F:152:ALA:HB1	1:F:155:ASP:O	2.14	0.47
1:F:233:MET:HE3	1:F:259:LEU:HD11	1.97	0.47
1:G:158:VAL:HG22	1:G:396:VAL:HG22	1.96	0.47
1:G:224:ASP:HA	1:G:289:LEU:CD1	2.44	0.47
1:M:31:LEU:HB3	1:M:90:THR:HG21	1.97	0.47
1:A:206:ASN:HB2	1:A:213:VAL:HB	1.97	0.47
1:B:218:PRO:HA	1:B:246:PRO:O	2.15	0.47
1:C:136:VAL:O	1:C:410:GLY:HA3	2.14	0.47
1:D:287:ALA:HB1	1:D:368:ARG:CZ	2.44	0.47
1:E:19:GLY:HA2	1:E:62:LEU:HD13	1.96	0.47
1:E:287:ALA:HB1	1:E:368:ARG:CZ	2.44	0.47
1:G:206:ASN:HB2	1:G:213:VAL:HB	1.97	0.47
1:K:152:ALA:HB1	1:K:155:ASP:HB3	1.97	0.47
1:L:152:ALA:HB1	1:L:155:ASP:HB3	1.97	0.47
1:C:12:ALA:HB3	1:C:518:GLU:O	2.16	0.46
1:C:206:ASN:HB2	1:C:213:VAL:HB	1.96	0.46
1:D:200:LEU:CD1	1:D:254:VAL:HG11	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:233:MET:HE2	1:J:249:ILE:HD13	1.97	0.46
1:M:87:ASP:CG	1:M:151:SER:HA	2.40	0.46
1:A:152:ALA:HB1	1:A:155:ASP:O	2.14	0.46
1:B:12:ALA:HB3	1:B:518:GLU:O	2.15	0.46
1:C:19:GLY:HA2	1:C:62:LEU:HD13	1.96	0.46
1:C:218:PRO:HA	1:C:246:PRO:O	2.15	0.46
1:D:136:VAL:O	1:D:410:GLY:HA3	2.14	0.46
1:E:152:ALA:HB1	1:E:155:ASP:O	2.14	0.46
1:E:158:VAL:HG22	1:E:396:VAL:HG22	1.96	0.46
1:E:206:ASN:HB2	1:E:213:VAL:HB	1.97	0.46
1:F:417:VAL:HG21	1:F:477:GLY:HA3	1.97	0.46
1:G:255:GLU:HB3	1:G:257:GLU:HG2	1.96	0.46
1:I:183:LEU:C	1:I:382:GLY:HA3	2.40	0.46
1:J:87:ASP:CG	1:J:151:SER:HA	2.40	0.46
1:K:54:VAL:HG13	1:K:89:THR:HG21	1.96	0.46
1:K:233:MET:HE2	1:K:249:ILE:HD13	1.97	0.46
1:M:54:VAL:HG13	1:M:89:THR:HG21	1.96	0.46
1:A:102:GLU:HB2	1:A:442:VAL:HG13	1.97	0.46
1:B:267:MET:HE3	1:B:269:GLY:CA	2.45	0.46
1:E:115:ASP:HB2	1:E:435:ASP:HB2	1.96	0.46
1:E:281:PHE:HA	1:E:285:ARG:HB2	1.96	0.46
1:G:151:SER:HB3	1:G:399:ALA:HA	1.97	0.46
1:H:151:SER:HB3	1:H:399:ALA:HA	1.98	0.46
1:I:31:LEU:HB3	1:I:90:THR:HG21	1.97	0.46
1:I:87:ASP:CG	1:I:151:SER:HA	2.40	0.46
1:C:40:LEU:HD21	1:C:59:GLU:C	2.41	0.46
1:D:19:GLY:HA2	1:D:62:LEU:HD13	1.96	0.46
1:D:151:SER:HB3	1:D:399:ALA:HA	1.97	0.46
1:G:152:ALA:HB1	1:G:155:ASP:O	2.15	0.46
1:G:281:PHE:HA	1:G:285:ARG:HB2	1.96	0.46
1:A:120:ILE:O	1:A:124:VAL:HG23	2.16	0.46
1:B:3:ALA:HA	1:C:63:GLU:CB	2.42	0.46
1:D:40:LEU:HD21	1:D:59:GLU:C	2.41	0.46
1:D:206:ASN:HB2	1:D:213:VAL:HB	1.97	0.46
1:E:417:VAL:HG21	1:E:477:GLY:HA3	1.97	0.46
1:F:3:ALA:HA	1:G:63:GLU:CB	2.42	0.46
1:F:23:LEU:O	1:F:27:VAL:HG23	2.14	0.46
1:F:158:VAL:HG22	1:F:396:VAL:HG22	1.96	0.46
1:G:279:PRO:HG3	1:G:292:ILE:HD11	1.96	0.46
1:J:120:ILE:O	1:J:124:VAL:HG23	2.16	0.46
1:K:346:VAL:HG22	1:K:372:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:87:ASP:CG	1:L:151:SER:HA	2.40	0.46
1:M:213:VAL:HG13	1:M:325:ILE:HB	1.97	0.46
1:B:40:LEU:HD21	1:B:59:GLU:C	2.41	0.46
1:B:114:MET:H	1:C:36:ARG:HG3	1.80	0.46
1:B:120:ILE:O	1:B:124:VAL:HG23	2.16	0.46
1:B:417:VAL:HG21	1:B:477:GLY:HA3	1.97	0.46
1:C:417:VAL:HG21	1:C:477:GLY:HA3	1.97	0.46
1:D:206:ASN:HB2	1:D:213:VAL:CA	2.43	0.46
1:E:120:ILE:O	1:E:124:VAL:HG23	2.16	0.46
1:F:235:PRO:HB2	1:F:310:GLU:HA	1.97	0.46
1:I:151:SER:HB3	1:I:399:ALA:HA	1.97	0.46
1:J:152:ALA:HB1	1:J:155:ASP:HB3	1.97	0.46
1:A:19:GLY:HA2	1:A:62:LEU:CD1	2.46	0.46
1:A:151:SER:HB3	1:A:399:ALA:HA	1.97	0.46
1:B:151:SER:HB3	1:B:399:ALA:HA	1.97	0.46
1:B:279:PRO:HG3	1:B:292:ILE:HD11	1.97	0.46
1:C:19:GLY:HA2	1:C:62:LEU:CD1	2.46	0.46
1:C:267:MET:HE3	1:C:269:GLY:CA	2.45	0.46
1:D:152:ALA:HB1	1:D:155:ASP:O	2.14	0.46
1:F:12:ALA:HB3	1:F:518:GLU:O	2.15	0.46
1:G:102:GLU:HB2	1:G:442:VAL:HG13	1.97	0.46
1:G:120:ILE:O	1:G:124:VAL:HG23	2.16	0.46
1:L:120:ILE:O	1:L:124:VAL:HG23	2.16	0.46
1:N:54:VAL:HG13	1:N:89:THR:HG21	1.96	0.46
1:D:19:GLY:HA2	1:D:62:LEU:CD1	2.46	0.46
1:E:267:MET:HE3	1:E:269:GLY:CA	2.45	0.46
1:F:218:PRO:HA	1:F:246:PRO:O	2.15	0.46
1:F:281:PHE:HA	1:F:285:ARG:HB2	1.96	0.46
1:H:38:VAL:HG21	1:H:56:VAL:HG13	1.98	0.46
1:H:152:ALA:HB1	1:H:155:ASP:HB3	1.97	0.46
1:I:406:ALA:HB2	1:I:496:PRO:HG3	1.97	0.46
1:J:126:ALA:HB3	1:J:426:LEU:HD22	1.97	0.46
1:J:406:ALA:HB2	1:J:496:PRO:HG3	1.97	0.46
1:L:151:SER:HB3	1:L:399:ALA:HA	1.97	0.46
1:L:346:VAL:HG22	1:L:372:LEU:HD13	1.98	0.46
1:M:183:LEU:C	1:M:382:GLY:HA3	2.40	0.46
1:A:12:ALA:HB3	1:A:518:GLU:O	2.15	0.46
1:B:205:ILE:HD12	1:B:211:GLY:O	2.16	0.46
1:C:200:LEU:CD1	1:C:254:VAL:HG11	2.44	0.46
1:C:240:VAL:HA	1:C:243:ALA:CB	2.43	0.46
1:D:90:THR:HG22	1:D:94:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ILE:O	1:D:124:VAL:HG23	2.16	0.46
1:D:267:MET:HE3	1:D:269:GLY:CA	2.45	0.46
1:E:90:THR:HG22	1:E:94:VAL:HG23	1.98	0.46
1:E:102:GLU:HB2	1:E:442:VAL:HG13	1.97	0.46
1:E:218:PRO:HA	1:E:246:PRO:O	2.15	0.46
1:F:19:GLY:HA2	1:F:62:LEU:CD1	2.46	0.46
1:G:267:MET:HE3	1:G:269:GLY:CA	2.45	0.46
1:G:417:VAL:HG21	1:G:477:GLY:HA3	1.97	0.46
1:J:152:ALA:HB1	1:J:155:ASP:CA	2.46	0.46
1:K:126:ALA:HB3	1:K:426:LEU:HD22	1.97	0.46
1:K:152:ALA:HB1	1:K:155:ASP:CA	2.46	0.46
1:N:38:VAL:HG21	1:N:56:VAL:HG13	1.98	0.46
1:N:158:VAL:HG22	1:N:396:VAL:HG22	1.98	0.46
1:B:19:GLY:HA2	1:B:62:LEU:CD1	2.46	0.46
1:B:235:PRO:HB2	1:B:310:GLU:HA	1.98	0.46
1:C:120:ILE:O	1:C:124:VAL:HG23	2.16	0.46
1:C:205:ILE:HD12	1:C:211:GLY:O	2.16	0.46
1:D:218:PRO:HA	1:D:246:PRO:O	2.15	0.46
1:G:230:ILE:HG21	1:G:263:VAL:HA	1.97	0.46
1:I:152:ALA:HB1	1:I:155:ASP:CA	2.46	0.46
1:A:235:PRO:HB2	1:A:310:GLU:HA	1.98	0.45
1:A:279:PRO:HG3	1:A:292:ILE:HD11	1.97	0.45
1:D:102:GLU:HB2	1:D:442:VAL:HG13	1.97	0.45
1:D:240:VAL:HA	1:D:243:ALA:CB	2.43	0.45
1:E:40:LEU:HD21	1:E:59:GLU:C	2.41	0.45
1:F:114:MET:H	1:G:36:ARG:HG3	1.80	0.45
1:F:120:ILE:O	1:F:124:VAL:HG23	2.16	0.45
1:G:40:LEU:HD21	1:G:59:GLU:C	2.41	0.45
1:J:151:SER:HB3	1:J:399:ALA:HA	1.97	0.45
1:L:126:ALA:HB3	1:L:426:LEU:HD22	1.97	0.45
1:L:152:ALA:HB1	1:L:155:ASP:CA	2.46	0.45
1:L:233:MET:HE2	1:L:249:ILE:HD13	1.97	0.45
1:N:31:LEU:HB3	1:N:90:THR:HG21	1.97	0.45
1:N:120:ILE:O	1:N:124:VAL:HG23	2.16	0.45
1:N:233:MET:HE2	1:N:249:ILE:HD13	1.97	0.45
1:H:31:LEU:HB3	1:H:90:THR:HG21	1.96	0.45
1:H:120:ILE:O	1:H:124:VAL:HG23	2.16	0.45
1:H:158:VAL:HG22	1:H:396:VAL:HG22	1.98	0.45
1:H:183:LEU:C	1:H:382:GLY:HA3	2.40	0.45
1:I:120:ILE:O	1:I:124:VAL:HG23	2.16	0.45
1:K:120:ILE:O	1:K:124:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:120:ILE:O	1:M:124:VAL:HG23	2.16	0.45
1:N:151:SER:HB3	1:N:399:ALA:HA	1.97	0.45
1:A:36:ARG:HG3	1:G:114:MET:H	1.80	0.45
1:A:205:ILE:HD12	1:A:211:GLY:O	2.16	0.45
1:C:151:SER:HB3	1:C:399:ALA:HA	1.97	0.45
1:G:19:GLY:HA2	1:G:62:LEU:CD1	2.46	0.45
1:H:87:ASP:CG	1:H:151:SER:HA	2.40	0.45
1:I:126:ALA:HB3	1:I:426:LEU:HD22	1.97	0.45
1:I:233:MET:HE2	1:I:249:ILE:HD13	1.98	0.45
1:K:151:SER:HB3	1:K:399:ALA:HA	1.97	0.45
1:M:158:VAL:HG22	1:M:396:VAL:HG22	1.98	0.45
1:M:346:VAL:HG22	1:M:372:LEU:HD13	1.98	0.45
1:N:240:VAL:HG21	1:N:247:LEU:HD22	1.98	0.45
1:A:114:MET:H	1:B:36:ARG:HG3	1.80	0.45
1:B:102:GLU:HB2	1:B:442:VAL:HG13	1.98	0.45
1:B:206:ASN:HB2	1:B:213:VAL:CA	2.43	0.45
1:D:213:VAL:O	1:D:324:VAL:HA	2.17	0.45
1:E:206:ASN:HB2	1:E:213:VAL:CA	2.43	0.45
1:G:237:LEU:O	1:G:241:ALA:N	2.50	0.45
1:H:152:ALA:HB1	1:H:155:ASP:CA	2.46	0.45
1:I:102:GLU:HB2	1:I:442:VAL:HG13	1.99	0.45
1:J:346:VAL:HG22	1:J:372:LEU:HD13	1.98	0.45
1:M:406:ALA:HB2	1:M:496:PRO:HG3	1.97	0.45
1:N:152:ALA:HB1	1:N:155:ASP:CA	2.46	0.45
1:A:40:LEU:HD21	1:A:59:GLU:C	2.41	0.45
1:A:90:THR:HG22	1:A:94:VAL:HG23	1.98	0.45
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.97	0.45
1:C:114:MET:H	1:D:36:ARG:HG3	1.81	0.45
1:C:213:VAL:O	1:C:324:VAL:HA	2.17	0.45
1:D:114:MET:H	1:E:36:ARG:HG3	1.81	0.45
1:D:417:VAL:HG21	1:D:477:GLY:HA3	1.97	0.45
1:E:19:GLY:HA2	1:E:62:LEU:CD1	2.46	0.45
1:E:205:ILE:HD12	1:E:211:GLY:O	2.16	0.45
1:F:90:THR:HG22	1:F:94:VAL:HG23	1.98	0.45
1:F:205:ILE:HD12	1:F:211:GLY:O	2.16	0.45
1:F:279:PRO:HG3	1:F:292:ILE:HD11	1.97	0.45
1:G:90:THR:HG22	1:G:94:VAL:HG23	1.98	0.45
1:H:102:GLU:HB2	1:H:442:VAL:HG13	1.99	0.45
1:I:152:ALA:HB1	1:I:155:ASP:HB3	1.97	0.45
1:J:102:GLU:HB2	1:J:442:VAL:HG13	1.99	0.45
1:J:240:VAL:HG21	1:J:247:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:151:SER:HB3	1:M:399:ALA:HA	1.97	0.45
1:M:233:MET:HE2	1:M:249:ILE:HD13	1.97	0.45
1:N:406:ALA:HB2	1:N:496:PRO:HG3	1.97	0.45
1:A:206:ASN:HB2	1:A:213:VAL:CA	2.43	0.45
1:C:90:THR:HG22	1:C:94:VAL:HG23	1.98	0.45
1:F:102:GLU:HB2	1:F:442:VAL:HG13	1.97	0.45
1:G:12:ALA:HB3	1:G:518:GLU:O	2.15	0.45
1:H:233:MET:HE2	1:H:249:ILE:HD13	1.97	0.45
1:H:240:VAL:HG21	1:H:247:LEU:HD22	1.98	0.45
1:K:240:VAL:HG21	1:K:247:LEU:HD22	1.98	0.45
1:K:406:ALA:HB2	1:K:496:PRO:HG3	1.97	0.45
1:N:102:GLU:HB2	1:N:442:VAL:HG13	1.99	0.45
1:N:183:LEU:C	1:N:382:GLY:HA3	2.40	0.45
1:E:200:LEU:CD1	1:E:254:VAL:HG11	2.44	0.45
1:E:235:PRO:HB2	1:E:310:GLU:HA	1.98	0.45
1:F:206:ASN:HB2	1:F:213:VAL:CA	2.43	0.45
1:G:213:VAL:O	1:G:324:VAL:HA	2.16	0.45
1:H:406:ALA:HB2	1:H:496:PRO:HG3	1.97	0.45
1:K:158:VAL:HG22	1:K:396:VAL:HG22	1.98	0.45
1:B:240:VAL:HA	1:B:243:ALA:CB	2.43	0.45
1:D:205:ILE:HD12	1:D:211:GLY:O	2.16	0.45
1:F:40:LEU:HD21	1:F:59:GLU:C	2.41	0.45
1:G:205:ILE:HD12	1:G:211:GLY:O	2.16	0.45
1:G:255:GLU:HB3	1:G:258:ALA:H	1.81	0.45
1:H:346:VAL:HG22	1:H:372:LEU:HD13	1.98	0.45
1:I:346:VAL:HG22	1:I:372:LEU:HD13	1.98	0.45
1:J:64:ASP:O	1:J:68:ASN:HB2	2.17	0.45
1:J:158:VAL:HG22	1:J:396:VAL:HG22	1.98	0.45
1:K:102:GLU:HB2	1:K:442:VAL:HG13	1.99	0.45
1:B:39:VAL:HG22	1:B:49:ILE:HG23	1.99	0.45
1:F:213:VAL:O	1:F:324:VAL:HA	2.17	0.45
1:G:200:LEU:CD1	1:G:254:VAL:HG11	2.45	0.45
1:I:281:PHE:HA	1:I:285:ARG:HB2	1.99	0.45
1:K:199:TYR:CD2	1:K:327:LYS:HA	2.52	0.45
1:L:406:ALA:HB2	1:L:496:PRO:HG3	1.97	0.45
1:M:192:GLY:O	1:M:375:GLY:HA2	2.17	0.45
1:A:3:ALA:HA	1:B:63:GLU:CB	2.42	0.45
1:A:63:GLU:CB	1:G:3:ALA:HA	2.42	0.45
1:C:102:GLU:HB2	1:C:442:VAL:HG13	1.97	0.45
1:E:213:VAL:O	1:E:324:VAL:HA	2.17	0.45
1:G:9:GLY:HA2	1:G:518:GLU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:23:LEU:O	1:I:27:VAL:HG23	2.17	0.45
1:I:38:VAL:HG21	1:I:56:VAL:HG13	1.98	0.45
1:K:23:LEU:O	1:K:27:VAL:HG23	2.17	0.45
1:M:23:LEU:O	1:M:27:VAL:HG23	2.17	0.45
1:M:38:VAL:HG21	1:M:56:VAL:HG13	1.98	0.45
1:M:64:ASP:O	1:M:68:ASN:HB2	2.17	0.45
1:M:175:ILE:HD12	1:M:400:LEU:CD1	2.47	0.45
1:M:240:VAL:HG21	1:M:247:LEU:HD22	1.98	0.45
1:N:64:ASP:O	1:N:68:ASN:HB2	2.17	0.45
1:N:192:GLY:O	1:N:375:GLY:HA2	2.17	0.45
1:B:90:THR:HG22	1:B:94:VAL:HG23	1.98	0.44
1:B:213:VAL:O	1:B:324:VAL:HA	2.17	0.44
1:C:235:PRO:HB2	1:C:310:GLU:HA	1.98	0.44
1:D:235:PRO:HB2	1:D:310:GLU:HA	1.98	0.44
1:E:114:MET:H	1:F:36:ARG:HG3	1.81	0.44
1:H:281:PHE:HA	1:H:285:ARG:HB2	1.99	0.44
1:J:175:ILE:HD12	1:J:400:LEU:CD1	2.47	0.44
1:L:175:ILE:HD12	1:L:400:LEU:CD1	2.47	0.44
1:M:152:ALA:HB1	1:M:155:ASP:CA	2.46	0.44
1:C:231:ARG:O	1:C:235:PRO:HD2	2.18	0.44
1:E:9:GLY:HA2	1:E:518:GLU:C	2.42	0.44
1:F:215:LEU:HD22	1:F:246:PRO:HB2	1.99	0.44
1:H:64:ASP:O	1:H:68:ASN:HB2	2.17	0.44
1:J:199:TYR:CD2	1:J:327:LYS:HA	2.53	0.44
1:K:220:ILE:HD12	1:K:248:LEU:HD23	2.00	0.44
1:L:192:GLY:O	1:L:375:GLY:HA2	2.17	0.44
1:M:102:GLU:HB2	1:M:442:VAL:HG13	1.99	0.44
1:C:39:VAL:HG22	1:C:49:ILE:HG23	1.99	0.44
1:D:9:GLY:HA2	1:D:518:GLU:C	2.42	0.44
1:G:235:PRO:HB2	1:G:310:GLU:HA	1.99	0.44
1:J:192:GLY:O	1:J:375:GLY:HA2	2.17	0.44
1:J:220:ILE:HD12	1:J:248:LEU:HD23	2.00	0.44
1:J:349:ILE:HG23	1:J:365:LEU:CD1	2.48	0.44
1:K:64:ASP:O	1:K:68:ASN:HB2	2.17	0.44
1:K:90:THR:HG22	1:K:94:VAL:HG23	1.99	0.44
1:L:240:VAL:HG21	1:L:247:LEU:HD22	1.98	0.44
1:M:117:LYS:HZ2	1:M:121:ASP:CG	2.26	0.44
1:N:281:PHE:HA	1:N:285:ARG:HB2	1.99	0.44
1:N:346:VAL:HG22	1:N:372:LEU:HD13	1.98	0.44
1:A:9:GLY:HA2	1:A:518:GLU:C	2.42	0.44
1:A:230:ILE:HG22	1:A:263:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:O	1:A:235:PRO:HD2	2.18	0.44
1:B:231:ARG:O	1:B:235:PRO:HD2	2.18	0.44
1:C:206:ASN:HB2	1:C:213:VAL:CA	2.43	0.44
1:D:215:LEU:HD22	1:D:246:PRO:HB2	1.99	0.44
1:D:231:ARG:O	1:D:235:PRO:HD2	2.18	0.44
1:E:230:ILE:HG22	1:E:263:VAL:HG22	1.99	0.44
1:H:82:ASN:HB2	1:H:89:THR:HG23	1.99	0.44
1:H:117:LYS:HZ2	1:H:121:ASP:CG	2.26	0.44
1:H:521:VAL:O	1:N:41:ASP:HB2	2.18	0.44
1:J:38:VAL:HG21	1:J:56:VAL:HG13	1.98	0.44
1:J:90:THR:HG22	1:J:94:VAL:HG23	1.99	0.44
1:L:23:LEU:O	1:L:27:VAL:HG23	2.17	0.44
1:L:41:ASP:HB2	1:M:521:VAL:O	2.17	0.44
1:A:213:VAL:O	1:A:324:VAL:HA	2.17	0.44
1:A:349:ILE:HG23	1:A:365:LEU:CD1	2.48	0.44
1:C:215:LEU:HD22	1:C:246:PRO:HB2	1.99	0.44
1:D:230:ILE:HG22	1:D:263:VAL:HG22	1.99	0.44
1:I:192:GLY:O	1:I:375:GLY:HA2	2.17	0.44
1:J:281:PHE:HA	1:J:285:ARG:HB2	1.99	0.44
1:L:102:GLU:HB2	1:L:442:VAL:HG13	1.99	0.44
1:L:106:ALA:HB1	1:L:116:LEU:HD21	2.00	0.44
1:L:413:ALA:HB1	1:L:488:MET:HB2	2.00	0.44
1:M:106:ALA:HB1	1:M:116:LEU:HD21	2.00	0.44
1:M:413:ALA:HB1	1:M:488:MET:HB2	2.00	0.44
1:N:106:ALA:HB1	1:N:116:LEU:HD21	2.00	0.44
1:E:240:VAL:HA	1:E:243:ALA:CB	2.43	0.44
1:E:255:GLU:HB3	1:E:257:GLU:HG2	2.00	0.44
1:H:106:ALA:HB1	1:H:116:LEU:HD21	2.00	0.44
1:I:158:VAL:HG22	1:I:396:VAL:HG22	1.98	0.44
1:I:240:VAL:HG21	1:I:247:LEU:HD22	1.98	0.44
1:K:38:VAL:HG21	1:K:56:VAL:HG13	1.98	0.44
1:K:175:ILE:HD12	1:K:400:LEU:CD1	2.48	0.44
1:L:38:VAL:HG21	1:L:56:VAL:HG13	1.98	0.44
1:L:199:TYR:CD2	1:L:327:LYS:HA	2.53	0.44
1:M:199:TYR:CD2	1:M:327:LYS:HA	2.52	0.44
1:M:349:ILE:HG23	1:M:365:LEU:CD1	2.48	0.44
1:A:255:GLU:HB3	1:A:257:GLU:HG2	2.00	0.44
1:B:6:VAL:HG22	1:B:521:VAL:HG13	2.00	0.44
1:B:230:ILE:HG22	1:B:263:VAL:HG22	1.99	0.44
1:E:9:GLY:HA2	1:E:518:GLU:O	2.18	0.44
1:E:349:ILE:HG23	1:E:365:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:LEU:O	1:H:27:VAL:HG23	2.17	0.44
1:H:41:ASP:HB2	1:I:521:VAL:O	2.18	0.44
1:H:349:ILE:HG23	1:H:365:LEU:CD1	2.48	0.44
1:I:82:ASN:HB2	1:I:89:THR:HG23	1.99	0.44
1:I:199:TYR:CD2	1:I:327:LYS:HA	2.52	0.44
1:I:413:ALA:HB1	1:I:488:MET:HB2	2.00	0.44
1:J:413:ALA:HB1	1:J:488:MET:HB2	2.00	0.44
1:L:281:PHE:HA	1:L:285:ARG:HB2	1.99	0.44
1:M:152:ALA:HB1	1:M:155:ASP:O	2.18	0.44
1:N:199:TYR:CD2	1:N:327:LYS:HA	2.53	0.44
1:A:9:GLY:HA2	1:A:518:GLU:O	2.18	0.44
1:A:39:VAL:HG22	1:A:49:ILE:HG23	1.99	0.44
1:C:9:GLY:HA2	1:C:518:GLU:C	2.42	0.44
1:E:246:PRO:HB3	1:E:272:LYS:HB2	2.00	0.44
1:G:206:ASN:HB2	1:G:213:VAL:CA	2.44	0.44
1:H:175:ILE:HD12	1:H:400:LEU:CD1	2.48	0.44
1:I:152:ALA:HB1	1:I:155:ASP:O	2.18	0.44
1:I:220:ILE:HD12	1:I:248:LEU:HD23	2.00	0.44
1:I:349:ILE:HG23	1:I:365:LEU:CD1	2.48	0.44
1:J:417:VAL:HG13	1:J:476:TYR:O	2.18	0.44
1:K:192:GLY:O	1:K:375:GLY:HA2	2.17	0.44
1:K:281:PHE:HA	1:K:285:ARG:HB2	1.99	0.44
1:L:158:VAL:HG22	1:L:396:VAL:HG22	1.98	0.44
1:L:220:ILE:HD12	1:L:248:LEU:HD23	2.00	0.44
1:M:41:ASP:HB2	1:N:521:VAL:O	2.17	0.44
1:M:281:PHE:HA	1:M:285:ARG:HB2	1.99	0.44
1:N:23:LEU:O	1:N:27:VAL:HG23	2.17	0.44
1:B:9:GLY:HA2	1:B:518:GLU:C	2.42	0.44
1:C:9:GLY:HA2	1:C:518:GLU:O	2.18	0.44
1:C:230:ILE:HG22	1:C:263:VAL:HG22	1.99	0.44
1:C:349:ILE:HG23	1:C:365:LEU:CD1	2.48	0.44
1:F:152:ALA:HB1	1:F:155:ASP:CA	2.48	0.44
1:F:246:PRO:HB3	1:F:272:LYS:HB2	2.00	0.44
1:F:349:ILE:HG23	1:F:365:LEU:CD1	2.48	0.44
1:J:117:LYS:HZ2	1:J:121:ASP:CG	2.25	0.44
1:K:413:ALA:HB1	1:K:488:MET:HB2	2.00	0.44
1:L:136:VAL:O	1:L:410:GLY:HA3	2.18	0.44
1:B:349:ILE:HG23	1:B:365:LEU:CD1	2.48	0.43
1:E:231:ARG:O	1:E:235:PRO:HD2	2.18	0.43
1:F:9:GLY:HA2	1:F:518:GLU:C	2.42	0.43
1:F:175:ILE:HD12	1:F:400:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:ALA:HB1	1:G:155:ASP:CA	2.48	0.43
1:H:192:GLY:O	1:H:375:GLY:HA2	2.17	0.43
1:H:199:TYR:CD2	1:H:327:LYS:HA	2.52	0.43
1:J:152:ALA:HB1	1:J:155:ASP:O	2.18	0.43
1:K:349:ILE:HG23	1:K:365:LEU:CD1	2.48	0.43
1:K:417:VAL:HG13	1:K:476:TYR:O	2.18	0.43
1:N:82:ASN:HB2	1:N:89:THR:HG23	1.99	0.43
1:A:152:ALA:HB1	1:A:155:ASP:CA	2.48	0.43
1:B:152:ALA:HB1	1:B:155:ASP:CA	2.48	0.43
1:C:6:VAL:HG22	1:C:521:VAL:HG13	2.00	0.43
1:C:13:ARG:HG3	1:C:13:ARG:HH11	1.84	0.43
1:E:215:LEU:HD22	1:E:246:PRO:HB2	1.99	0.43
1:F:39:VAL:HG22	1:F:49:ILE:HG23	1.99	0.43
1:G:349:ILE:HG23	1:G:365:LEU:CD1	2.48	0.43
1:L:338:GLU:HB3	1:L:341:ALA:HB3	2.00	0.43
1:N:90:THR:HG22	1:N:94:VAL:HG23	1.99	0.43
1:N:338:GLU:HB3	1:N:341:ALA:HB3	2.00	0.43
1:A:480:ALA:O	1:A:483:GLU:HG2	2.19	0.43
1:C:199:TYR:CD2	1:C:327:LYS:HA	2.54	0.43
1:D:9:GLY:HA2	1:D:518:GLU:O	2.18	0.43
1:D:199:TYR:CD2	1:D:327:LYS:HA	2.54	0.43
1:E:39:VAL:HG22	1:E:49:ILE:HG23	1.99	0.43
1:E:175:ILE:HD12	1:E:400:LEU:CD1	2.48	0.43
1:G:254:VAL:HG23	1:G:259:LEU:CB	2.49	0.43
1:I:41:ASP:HB2	1:J:521:VAL:O	2.18	0.43
1:J:136:VAL:O	1:J:410:GLY:HA3	2.18	0.43
1:K:41:ASP:HB2	1:L:521:VAL:O	2.17	0.43
1:K:152:ALA:HB1	1:K:155:ASP:O	2.18	0.43
1:L:152:ALA:HB1	1:L:155:ASP:O	2.18	0.43
1:L:295:LEU:HA	1:L:342:ILE:HG12	2.00	0.43
1:L:417:VAL:HG13	1:L:476:TYR:O	2.18	0.43
1:M:90:THR:HG22	1:M:94:VAL:HG23	1.99	0.43
1:N:136:VAL:O	1:N:410:GLY:HA3	2.18	0.43
1:N:175:ILE:HD12	1:N:400:LEU:CD1	2.47	0.43
1:B:9:GLY:HA2	1:B:518:GLU:O	2.18	0.43
1:B:199:TYR:CD2	1:B:327:LYS:HA	2.53	0.43
1:D:255:GLU:HB3	1:D:257:GLU:HG2	2.00	0.43
1:E:199:TYR:CD2	1:E:327:LYS:HA	2.53	0.43
1:E:480:ALA:O	1:E:483:GLU:HG2	2.19	0.43
1:F:9:GLY:HA2	1:F:518:GLU:O	2.18	0.43
1:F:77:VAL:HG12	1:F:506:TYR:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:TYR:CD2	1:F:327:LYS:HA	2.53	0.43
1:H:90:THR:HG22	1:H:94:VAL:HG23	1.99	0.43
1:H:413:ALA:HB1	1:H:488:MET:HB2	2.00	0.43
1:I:90:THR:HG22	1:I:94:VAL:HG23	1.99	0.43
1:J:23:LEU:O	1:J:27:VAL:HG23	2.17	0.43
1:L:64:ASP:O	1:L:68:ASN:HB2	2.17	0.43
1:L:82:ASN:HB2	1:L:89:THR:HG23	1.99	0.43
1:L:349:ILE:HG23	1:L:365:LEU:CD1	2.48	0.43
1:M:82:ASN:HB2	1:M:89:THR:HG23	1.99	0.43
1:M:338:GLU:HB3	1:M:341:ALA:HB3	2.00	0.43
1:N:413:ALA:HB1	1:N:488:MET:HB2	2.00	0.43
1:B:215:LEU:HD22	1:B:246:PRO:HB2	1.99	0.43
1:B:255:GLU:HB3	1:B:257:GLU:HG2	2.00	0.43
1:C:77:VAL:HG12	1:C:506:TYR:HB3	2.01	0.43
1:C:240:VAL:CA	1:C:243:ALA:HB3	2.43	0.43
1:D:246:PRO:HB3	1:D:272:LYS:HB2	2.00	0.43
1:D:349:ILE:HG23	1:D:365:LEU:CD1	2.48	0.43
1:G:231:ARG:O	1:G:235:PRO:HD2	2.18	0.43
1:H:417:VAL:HG13	1:H:476:TYR:O	2.18	0.43
1:I:64:ASP:O	1:I:68:ASN:HB2	2.17	0.43
1:I:106:ALA:HB1	1:I:116:LEU:HD21	2.00	0.43
1:I:175:ILE:HD12	1:I:400:LEU:CD1	2.47	0.43
1:J:41:ASP:HB2	1:K:521:VAL:O	2.17	0.43
1:J:405:ALA:HB1	1:J:498:LYS:HD2	2.01	0.43
1:K:136:VAL:O	1:K:410:GLY:HA3	2.18	0.43
1:K:405:ALA:HB1	1:K:498:LYS:HD2	2.00	0.43
1:B:152:ALA:HB1	1:B:155:ASP:HB3	2.01	0.43
1:C:246:PRO:HB3	1:C:272:LYS:HB2	2.00	0.43
1:D:39:VAL:HG22	1:D:49:ILE:HG23	1.99	0.43
1:D:152:ALA:HB1	1:D:155:ASP:CA	2.48	0.43
1:D:175:ILE:HD12	1:D:400:LEU:CD1	2.48	0.43
1:F:480:ALA:O	1:F:483:GLU:HG2	2.19	0.43
1:G:9:GLY:HA2	1:G:518:GLU:O	2.18	0.43
1:G:77:VAL:HG12	1:G:506:TYR:HB3	2.01	0.43
1:I:417:VAL:HG13	1:I:476:TYR:O	2.18	0.43
1:K:106:ALA:HB1	1:K:116:LEU:HD21	2.00	0.43
1:K:117:LYS:HZ2	1:K:121:ASP:CG	2.26	0.43
1:K:295:LEU:HA	1:K:342:ILE:HG12	2.00	0.43
1:L:90:THR:HG22	1:L:94:VAL:HG23	1.99	0.43
1:N:349:ILE:HG23	1:N:365:LEU:CD1	2.48	0.43
1:A:6:VAL:HG22	1:A:521:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:ALA:HB1	1:F:155:ASP:HB3	2.01	0.43
1:G:175:ILE:HD12	1:G:400:LEU:CD1	2.48	0.43
1:H:152:ALA:HB1	1:H:155:ASP:O	2.18	0.43
1:I:488:MET:HA	1:I:488:MET:HE2	2.01	0.43
1:J:82:ASN:HB2	1:J:89:THR:HG23	1.99	0.43
1:J:240:VAL:HA	1:J:243:ALA:HB3	2.01	0.43
1:K:338:GLU:HB3	1:K:341:ALA:HB3	2.00	0.43
1:A:152:ALA:HB1	1:A:155:ASP:HB3	2.01	0.43
1:B:175:ILE:HD12	1:B:400:LEU:CD1	2.48	0.43
1:C:255:GLU:HB3	1:C:257:GLU:HG2	2.00	0.43
1:D:77:VAL:HG12	1:D:506:TYR:HB3	2.01	0.43
1:D:480:ALA:O	1:D:483:GLU:HG2	2.18	0.43
1:E:77:VAL:HG12	1:E:506:TYR:HB3	2.01	0.43
1:G:152:ALA:HB1	1:G:155:ASP:HB3	2.01	0.43
1:H:338:GLU:HB3	1:H:341:ALA:HB3	2.00	0.43
1:I:117:LYS:HZ2	1:I:121:ASP:CG	2.26	0.43
1:K:218:PRO:HG2	1:K:323:VAL:HG23	2.01	0.43
1:L:218:PRO:HG2	1:L:323:VAL:HG23	2.00	0.43
1:M:220:ILE:HD12	1:M:248:LEU:HD23	2.00	0.43
1:N:152:ALA:HB1	1:N:155:ASP:O	2.18	0.43
1:N:405:ALA:HB1	1:N:498:LYS:HD2	2.00	0.43
1:N:417:VAL:HG13	1:N:476:TYR:O	2.18	0.43
1:C:480:ALA:O	1:C:483:GLU:HG2	2.19	0.43
1:G:39:VAL:HG22	1:G:49:ILE:HG23	1.99	0.43
1:G:417:VAL:HG13	1:G:476:TYR:O	2.19	0.43
1:I:405:ALA:HB1	1:I:498:LYS:HD2	2.00	0.43
1:J:3:ALA:C	1:J:524:LEU:H	2.27	0.43
1:K:213:VAL:O	1:K:324:VAL:HA	2.19	0.43
1:K:240:VAL:HA	1:K:243:ALA:HB3	2.01	0.43
1:K:488:MET:HE2	1:K:488:MET:HA	2.01	0.43
1:N:281:PHE:CA	1:N:285:ARG:HB2	2.49	0.43
1:A:243:ALA:HA	1:G:258:ALA:CA	2.46	0.43
1:B:13:ARG:HH11	1:B:13:ARG:HG3	1.84	0.43
1:B:77:VAL:HG12	1:B:506:TYR:HB3	2.01	0.43
1:B:356:ALA:HB1	1:B:361:ASP:HB2	2.01	0.43
1:B:426:LEU:HB2	1:B:444:LEU:CD2	2.49	0.43
1:C:356:ALA:HB1	1:C:361:ASP:HB2	2.01	0.43
1:D:6:VAL:HG22	1:D:521:VAL:HG13	2.00	0.43
1:D:13:ARG:HH11	1:D:13:ARG:HG3	1.83	0.43
1:E:6:VAL:HG22	1:E:521:VAL:HG13	2.00	0.43
1:E:152:ALA:HB1	1:E:155:ASP:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:ILE:HG21	1:E:263:VAL:HA	2.00	0.43
1:E:417:VAL:HG13	1:E:476:TYR:O	2.19	0.43
1:G:199:TYR:CD2	1:G:327:LYS:HA	2.53	0.43
1:H:206:ASN:HB2	1:H:213:VAL:CB	2.49	0.43
1:H:220:ILE:HD12	1:H:248:LEU:HD23	2.00	0.43
1:K:206:ASN:HB2	1:K:213:VAL:CB	2.49	0.43
1:L:213:VAL:O	1:L:324:VAL:HA	2.19	0.43
1:M:417:VAL:HG13	1:M:476:TYR:O	2.18	0.43
1:A:175:ILE:HD12	1:A:400:LEU:CD1	2.48	0.42
1:B:413:ALA:HB1	1:B:488:MET:HB2	2.01	0.42
1:C:152:ALA:HB1	1:C:155:ASP:HB3	2.01	0.42
1:D:240:VAL:CA	1:D:243:ALA:HB3	2.43	0.42
1:E:426:LEU:HB2	1:E:444:LEU:CD2	2.49	0.42
1:F:231:ARG:O	1:F:235:PRO:HD2	2.18	0.42
1:F:417:VAL:HG13	1:F:476:TYR:O	2.19	0.42
1:G:13:ARG:HH11	1:G:13:ARG:HG3	1.83	0.42
1:G:480:ALA:O	1:G:483:GLU:HG2	2.19	0.42
1:H:281:PHE:CA	1:H:285:ARG:HB2	2.49	0.42
1:H:295:LEU:HA	1:H:342:ILE:HG12	2.00	0.42
1:I:405:ALA:HB1	1:I:498:LYS:CD	2.49	0.42
1:J:206:ASN:HB2	1:J:213:VAL:CB	2.49	0.42
1:J:218:PRO:HG2	1:J:323:VAL:HG23	2.00	0.42
1:K:3:ALA:C	1:K:524:LEU:H	2.27	0.42
1:K:82:ASN:HB2	1:K:89:THR:HG23	1.99	0.42
1:K:281:PHE:CA	1:K:285:ARG:HB2	2.49	0.42
1:L:405:ALA:HB1	1:L:498:LYS:HD2	2.00	0.42
1:M:218:PRO:HG2	1:M:323:VAL:HG23	2.00	0.42
1:N:251:ALA:HB3	1:N:254:VAL:HG23	2.02	0.42
1:A:199:TYR:CD2	1:A:327:LYS:HA	2.53	0.42
1:A:215:LEU:O	1:A:322:ARG:HA	2.19	0.42
1:A:230:ILE:HG21	1:A:263:VAL:HA	2.00	0.42
1:C:114:MET:HB3	1:D:36:ARG:HD2	2.01	0.42
1:C:215:LEU:O	1:C:322:ARG:HA	2.19	0.42
1:C:413:ALA:HB1	1:C:488:MET:HB2	2.01	0.42
1:C:417:VAL:HG13	1:C:476:TYR:O	2.19	0.42
1:C:426:LEU:HB2	1:C:444:LEU:CD2	2.49	0.42
1:E:13:ARG:HH11	1:E:13:ARG:HG3	1.83	0.42
1:F:6:VAL:HG22	1:F:521:VAL:HG13	2.00	0.42
1:G:215:LEU:O	1:G:322:ARG:HA	2.19	0.42
1:H:136:VAL:O	1:H:410:GLY:HA3	2.18	0.42
1:H:251:ALA:HB3	1:H:254:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:251:ALA:HB3	1:I:254:VAL:HG23	2.02	0.42
1:I:281:PHE:CA	1:I:285:ARG:HB2	2.49	0.42
1:L:117:LYS:HZ2	1:L:121:ASP:CG	2.27	0.42
1:M:281:PHE:CA	1:M:285:ARG:HB2	2.49	0.42
1:M:295:LEU:HA	1:M:342:ILE:HG12	2.00	0.42
1:M:405:ALA:HB1	1:M:498:LYS:CD	2.49	0.42
1:N:117:LYS:HZ2	1:N:121:ASP:CG	2.26	0.42
1:N:218:PRO:HG2	1:N:323:VAL:HG23	2.00	0.42
1:A:77:VAL:HG12	1:A:506:TYR:HB3	2.01	0.42
1:A:426:LEU:HB2	1:A:444:LEU:CD2	2.49	0.42
1:B:240:VAL:CA	1:B:243:ALA:HB3	2.43	0.42
1:D:64:ASP:O	1:D:68:ASN:HB2	2.20	0.42
1:D:356:ALA:HB1	1:D:361:ASP:HB2	2.01	0.42
1:H:294:THR:HB	1:H:342:ILE:HA	2.01	0.42
1:I:206:ASN:HB2	1:I:213:VAL:CB	2.49	0.42
1:I:295:LEU:HA	1:I:342:ILE:HG12	2.00	0.42
1:M:206:ASN:HB2	1:M:213:VAL:CB	2.49	0.42
1:M:405:ALA:HB1	1:M:498:LYS:HD2	2.00	0.42
1:N:220:ILE:HD12	1:N:248:LEU:HD23	2.00	0.42
1:N:294:THR:HB	1:N:342:ILE:HA	2.01	0.42
1:N:405:ALA:HB1	1:N:498:LYS:CD	2.49	0.42
1:A:13:ARG:HH11	1:A:13:ARG:HG3	1.83	0.42
1:B:64:ASP:O	1:B:68:ASN:HB2	2.20	0.42
1:B:114:MET:HB3	1:C:36:ARG:HD2	2.01	0.42
1:B:215:LEU:O	1:B:322:ARG:HA	2.19	0.42
1:B:230:ILE:HG21	1:B:263:VAL:HA	2.00	0.42
1:B:246:PRO:HB3	1:B:272:LYS:HB2	2.00	0.42
1:C:230:ILE:HG21	1:C:263:VAL:HA	2.00	0.42
1:D:152:ALA:HB1	1:D:155:ASP:HB3	2.01	0.42
1:D:215:LEU:O	1:D:322:ARG:HA	2.19	0.42
1:E:215:LEU:O	1:E:322:ARG:HA	2.19	0.42
1:G:6:VAL:HG22	1:G:521:VAL:HG13	2.00	0.42
1:G:230:ILE:HG22	1:G:263:VAL:HG22	2.01	0.42
1:H:218:PRO:HG2	1:H:323:VAL:HG23	2.00	0.42
1:L:206:ASN:HB2	1:L:213:VAL:CB	2.49	0.42
1:L:240:VAL:HA	1:L:243:ALA:HB3	2.01	0.42
1:M:136:VAL:O	1:M:410:GLY:HA3	2.18	0.42
1:M:251:ALA:HB3	1:M:254:VAL:HG23	2.01	0.42
1:N:206:ASN:HB2	1:N:213:VAL:CB	2.50	0.42
1:B:417:VAL:HG13	1:B:476:TYR:O	2.19	0.42
1:C:175:ILE:HD12	1:C:400:LEU:CD1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:ALA:HB1	1:D:116:LEU:HD21	2.02	0.42
1:E:152:ALA:HB1	1:E:155:ASP:CA	2.48	0.42
1:F:240:VAL:HA	1:F:243:ALA:CB	2.43	0.42
1:G:64:ASP:O	1:G:68:ASN:HB2	2.20	0.42
1:G:506:TYR:O	1:G:510:VAL:HG23	2.20	0.42
1:H:3:ALA:C	1:H:524:LEU:H	2.27	0.42
1:H:405:ALA:HB1	1:H:498:LYS:HD2	2.00	0.42
1:I:19:GLY:HA2	1:I:62:LEU:CD1	2.50	0.42
1:I:218:PRO:HG2	1:I:323:VAL:HG23	2.00	0.42
1:I:240:VAL:HA	1:I:243:ALA:HB3	2.01	0.42
1:I:338:GLU:HB3	1:I:341:ALA:HB3	2.00	0.42
1:J:77:VAL:HG12	1:J:506:TYR:HB3	2.02	0.42
1:J:251:ALA:HB3	1:J:254:VAL:HG23	2.02	0.42
1:L:281:PHE:CA	1:L:285:ARG:HB2	2.49	0.42
1:N:77:VAL:HG12	1:N:506:TYR:HB3	2.02	0.42
1:N:295:LEU:HA	1:N:342:ILE:HG12	2.00	0.42
1:A:40:LEU:HG	1:A:59:GLU:HB3	2.02	0.42
1:A:413:ALA:HB1	1:A:488:MET:HB2	2.01	0.42
1:D:230:ILE:HG21	1:D:263:VAL:HA	2.00	0.42
1:D:506:TYR:O	1:D:510:VAL:HG23	2.20	0.42
1:F:426:LEU:HB2	1:F:444:LEU:CD2	2.50	0.42
1:H:19:GLY:HA2	1:H:62:LEU:CD1	2.50	0.42
1:I:136:VAL:O	1:I:410:GLY:HA3	2.18	0.42
1:J:338:GLU:HB3	1:J:341:ALA:HB3	2.00	0.42
1:L:488:MET:HA	1:L:488:MET:HE2	2.01	0.42
1:M:19:GLY:HA2	1:M:62:LEU:CD1	2.50	0.42
1:N:3:ALA:C	1:N:524:LEU:H	2.27	0.42
1:B:480:ALA:O	1:B:483:GLU:HG2	2.19	0.42
1:C:200:LEU:HD22	1:C:254:VAL:HG11	2.01	0.42
1:F:506:TYR:O	1:F:510:VAL:HG23	2.20	0.42
1:I:294:THR:HB	1:I:342:ILE:HA	2.01	0.42
1:J:213:VAL:O	1:J:324:VAL:HA	2.19	0.42
1:J:405:ALA:HB1	1:J:498:LYS:CD	2.49	0.42
1:L:3:ALA:C	1:L:524:LEU:H	2.27	0.42
1:L:218:PRO:HA	1:L:246:PRO:O	2.20	0.42
1:M:240:VAL:HA	1:M:243:ALA:HB3	2.01	0.42
1:D:417:VAL:HG13	1:D:476:TYR:O	2.19	0.42
1:D:426:LEU:HB2	1:D:444:LEU:CD2	2.49	0.42
1:G:426:LEU:HB2	1:G:444:LEU:CD2	2.49	0.42
1:H:213:VAL:CG1	1:H:325:ILE:HB	2.50	0.42
1:H:488:MET:HE2	1:H:488:MET:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:19:GLY:HA2	1:I:62:LEU:HD13	2.02	0.42
1:I:50:THR:HG21	1:I:59:GLU:HG2	2.01	0.42
1:I:213:VAL:O	1:I:324:VAL:HA	2.19	0.42
1:J:19:GLY:HA2	1:J:62:LEU:CD1	2.50	0.42
1:J:218:PRO:HA	1:J:246:PRO:O	2.20	0.42
1:M:77:VAL:HG12	1:M:506:TYR:HB3	2.02	0.42
1:N:19:GLY:HA2	1:N:62:LEU:CD1	2.50	0.42
1:N:213:VAL:CG1	1:N:325:ILE:HB	2.50	0.42
1:N:218:PRO:HA	1:N:246:PRO:O	2.20	0.42
1:A:103:GLY:HA3	1:A:515:ILE:HG12	2.02	0.42
1:A:114:MET:HB3	1:B:36:ARG:HD2	2.01	0.42
1:A:417:VAL:HG13	1:A:476:TYR:O	2.19	0.42
1:B:103:GLY:HA3	1:B:515:ILE:HG12	2.02	0.42
1:B:200:LEU:HD22	1:B:254:VAL:HG11	2.01	0.42
1:C:152:ALA:HB1	1:C:155:ASP:CA	2.48	0.42
1:F:64:ASP:O	1:F:68:ASN:HB2	2.19	0.42
1:F:114:MET:HB3	1:G:36:ARG:HD2	2.01	0.42
1:G:40:LEU:HG	1:G:59:GLU:HB3	2.02	0.42
1:H:77:VAL:HG12	1:H:506:TYR:HB3	2.02	0.42
1:H:213:VAL:O	1:H:324:VAL:HA	2.19	0.42
1:K:19:GLY:HA2	1:K:62:LEU:CD1	2.50	0.42
1:L:19:GLY:HA2	1:L:62:LEU:CD1	2.50	0.42
1:M:213:VAL:O	1:M:324:VAL:HA	2.19	0.42
1:N:50:THR:HG21	1:N:59:GLU:HG2	2.02	0.42
1:A:64:ASP:O	1:A:68:ASN:HB2	2.20	0.42
1:A:200:LEU:HD22	1:A:254:VAL:HG11	2.01	0.42
1:A:239:ALA:HB1	1:A:314:LEU:HG	2.02	0.42
1:A:356:ALA:HB1	1:A:361:ASP:HB2	2.01	0.42
1:B:40:LEU:HG	1:B:59:GLU:HB3	2.02	0.42
1:B:106:ALA:HB1	1:B:116:LEU:HD21	2.02	0.42
1:C:506:TYR:O	1:C:510:VAL:HG23	2.20	0.42
1:D:200:LEU:HD22	1:D:254:VAL:HG11	2.01	0.42
1:E:114:MET:HB3	1:F:36:ARG:HD2	2.01	0.42
1:E:247:LEU:O	1:E:273:VAL:HA	2.20	0.42
1:F:13:ARG:HG3	1:F:13:ARG:HH11	1.83	0.42
1:F:215:LEU:O	1:F:322:ARG:HA	2.19	0.42
1:I:77:VAL:HG12	1:I:506:TYR:HB3	2.02	0.42
1:I:517:THR:HG22	1:I:517:THR:O	2.20	0.42
1:J:213:VAL:CG1	1:J:325:ILE:HB	2.50	0.42
1:J:488:MET:HE2	1:J:488:MET:HA	2.01	0.42
1:J:517:THR:O	1:J:517:THR:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:383:ALA:HB3	1:K:389:MET:N	2.35	0.42
1:L:383:ALA:HB3	1:L:389:MET:N	2.35	0.42
1:N:240:VAL:HA	1:N:243:ALA:HB3	2.01	0.42
1:A:488:MET:HA	1:A:488:MET:HE2	2.02	0.41
1:D:100:ILE:O	1:D:104:LEU:HG	2.20	0.41
1:D:114:MET:HB3	1:E:36:ARG:HD2	2.01	0.41
1:E:64:ASP:O	1:E:68:ASN:HB2	2.19	0.41
1:F:200:LEU:CD1	1:F:275:ALA:HB3	2.50	0.41
1:G:200:LEU:HD22	1:G:254:VAL:HG11	2.00	0.41
1:G:488:MET:HE2	1:G:488:MET:HA	2.02	0.41
1:I:3:ALA:C	1:I:524:LEU:H	2.27	0.41
1:I:213:VAL:CG1	1:I:325:ILE:HB	2.50	0.41
1:J:19:GLY:HA2	1:J:62:LEU:HD13	2.02	0.41
1:K:294:THR:HB	1:K:342:ILE:HA	2.01	0.41
1:L:251:ALA:HB3	1:L:254:VAL:HG23	2.02	0.41
1:A:349:ILE:HG23	1:A:365:LEU:HD13	2.02	0.41
1:A:506:TYR:O	1:A:510:VAL:HG23	2.20	0.41
1:B:87:ASP:CG	1:B:151:SER:HA	2.46	0.41
1:C:103:GLY:HA3	1:C:515:ILE:HG12	2.02	0.41
1:C:106:ALA:HB1	1:C:116:LEU:HD21	2.02	0.41
1:D:413:ALA:HB1	1:D:488:MET:HB2	2.01	0.41
1:F:213:VAL:CG1	1:F:325:ILE:HB	2.50	0.41
1:G:103:GLY:HA3	1:G:515:ILE:HG12	2.02	0.41
1:H:19:GLY:HA2	1:H:62:LEU:HD13	2.02	0.41
1:J:63:GLU:HB3	1:K:4:LYS:O	2.21	0.41
1:J:295:LEU:HA	1:J:342:ILE:HG12	2.00	0.41
1:K:77:VAL:HG12	1:K:506:TYR:HB3	2.02	0.41
1:K:218:PRO:HA	1:K:246:PRO:O	2.20	0.41
1:K:251:ALA:HB3	1:K:254:VAL:HG23	2.02	0.41
1:L:517:THR:O	1:L:517:THR:HG22	2.20	0.41
1:M:50:THR:HG21	1:M:59:GLU:HG2	2.02	0.41
1:M:294:THR:HB	1:M:342:ILE:HA	2.01	0.41
1:A:106:ALA:HB1	1:A:116:LEU:HD21	2.02	0.41
1:B:411:VAL:HG13	1:B:496:PRO:HA	2.02	0.41
1:C:64:ASP:O	1:C:68:ASN:HB2	2.20	0.41
1:C:213:VAL:CG1	1:C:325:ILE:HB	2.50	0.41
1:D:87:ASP:CG	1:D:151:SER:HA	2.46	0.41
1:E:100:ILE:O	1:E:104:LEU:HG	2.21	0.41
1:E:106:ALA:HB1	1:E:116:LEU:HD21	2.02	0.41
1:E:506:TYR:O	1:E:510:VAL:HG23	2.20	0.41
1:F:413:ALA:HB1	1:F:488:MET:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:488:MET:HE2	1:F:488:MET:HA	2.02	0.41
1:G:190:VAL:HB	1:G:378:VAL:HG23	2.02	0.41
1:G:220:ILE:HD12	1:G:248:LEU:HD23	2.02	0.41
1:I:63:GLU:HB3	1:J:4:LYS:O	2.21	0.41
1:J:50:THR:HG21	1:J:59:GLU:HG2	2.02	0.41
1:J:106:ALA:HB1	1:J:116:LEU:HD21	2.00	0.41
1:J:383:ALA:HB3	1:J:389:MET:N	2.35	0.41
1:K:63:GLU:HB3	1:L:4:LYS:O	2.21	0.41
1:K:383:ALA:HB3	1:K:389:MET:CA	2.51	0.41
1:L:294:THR:HB	1:L:342:ILE:HA	2.01	0.41
1:M:383:ALA:HB3	1:M:389:MET:N	2.35	0.41
1:A:87:ASP:CG	1:A:151:SER:HA	2.46	0.41
1:B:213:VAL:CG1	1:B:325:ILE:HB	2.50	0.41
1:B:506:TYR:O	1:B:510:VAL:HG23	2.20	0.41
1:C:411:VAL:HG13	1:C:496:PRO:HA	2.02	0.41
1:E:200:LEU:CD1	1:E:275:ALA:HB3	2.50	0.41
1:E:200:LEU:HD22	1:E:254:VAL:HG11	2.01	0.41
1:F:40:LEU:HG	1:F:59:GLU:HB3	2.02	0.41
1:F:247:LEU:O	1:F:273:VAL:HA	2.20	0.41
1:G:247:LEU:O	1:G:273:VAL:HA	2.20	0.41
1:I:383:ALA:HB3	1:I:389:MET:N	2.35	0.41
1:J:135:SER:HA	1:J:412:VAL:HG12	2.03	0.41
1:J:281:PHE:CA	1:J:285:ARG:HB2	2.49	0.41
1:K:19:GLY:HA2	1:K:62:LEU:HD13	2.02	0.41
1:K:213:VAL:CG1	1:K:325:ILE:HB	2.50	0.41
1:K:405:ALA:HB1	1:K:498:LYS:CD	2.49	0.41
1:L:405:ALA:HB1	1:L:498:LYS:CD	2.49	0.41
1:M:3:ALA:C	1:M:524:LEU:H	2.27	0.41
1:M:488:MET:HE2	1:M:488:MET:HA	2.01	0.41
1:N:383:ALA:HB3	1:N:389:MET:CA	2.51	0.41
1:N:417:VAL:CG2	1:N:477:GLY:HA3	2.50	0.41
1:N:488:MET:HE2	1:N:488:MET:HA	2.01	0.41
1:B:488:MET:HE2	1:B:488:MET:HA	2.02	0.41
1:C:87:ASP:CG	1:C:151:SER:HA	2.46	0.41
1:C:226:LYS:HB2	1:C:253:ASP:O	2.20	0.41
1:E:413:ALA:HB1	1:E:488:MET:HB2	2.01	0.41
1:H:240:VAL:HA	1:H:243:ALA:HB3	2.01	0.41
1:H:517:THR:O	1:H:517:THR:HG22	2.20	0.41
1:I:218:PRO:HA	1:I:246:PRO:O	2.20	0.41
1:I:417:VAL:CG2	1:I:477:GLY:HA3	2.50	0.41
1:J:383:ALA:HB3	1:J:389:MET:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:383:ALA:HB3	1:L:389:MET:CA	2.51	0.41
1:M:63:GLU:HB3	1:N:4:LYS:O	2.21	0.41
1:M:213:VAL:CG1	1:M:325:ILE:HB	2.50	0.41
1:M:383:ALA:HB3	1:M:389:MET:CA	2.50	0.41
1:N:135:SER:HA	1:N:412:VAL:HG12	2.03	0.41
1:B:349:ILE:HG23	1:B:365:LEU:HD13	2.02	0.41
1:E:213:VAL:CG1	1:E:325:ILE:HB	2.51	0.41
1:F:100:ILE:O	1:F:104:LEU:HG	2.21	0.41
1:F:190:VAL:HB	1:F:378:VAL:HG23	2.02	0.41
1:G:106:ALA:HB1	1:G:116:LEU:HD21	2.02	0.41
1:G:413:ALA:HB1	1:G:488:MET:HB2	2.01	0.41
1:H:135:SER:HA	1:H:412:VAL:HG12	2.03	0.41
1:H:405:ALA:HB1	1:H:498:LYS:CD	2.49	0.41
1:I:106:ALA:HB3	1:I:116:LEU:HD21	2.03	0.41
1:J:106:ALA:HB3	1:J:116:LEU:HD21	2.03	0.41
1:K:106:ALA:HB3	1:K:116:LEU:HD21	2.03	0.41
1:M:106:ALA:HB3	1:M:116:LEU:HD21	2.03	0.41
1:M:218:PRO:HA	1:M:246:PRO:O	2.20	0.41
1:N:517:THR:O	1:N:517:THR:HG22	2.20	0.41
1:A:36:ARG:HD2	1:G:114:MET:HB3	2.01	0.41
1:A:200:LEU:CD1	1:A:275:ALA:HB3	2.50	0.41
1:C:100:ILE:O	1:C:104:LEU:HG	2.21	0.41
1:D:239:ALA:HB1	1:D:314:LEU:HG	2.03	0.41
1:E:40:LEU:HG	1:E:59:GLU:HB3	2.02	0.41
1:E:239:ALA:HB1	1:E:314:LEU:HG	2.03	0.41
1:E:356:ALA:HB1	1:E:361:ASP:HB2	2.01	0.41
1:F:115:ASP:CB	1:F:435:ASP:HB2	2.51	0.41
1:G:200:LEU:CD1	1:G:275:ALA:HB3	2.50	0.41
1:G:349:ILE:HG23	1:G:365:LEU:HD13	2.02	0.41
1:H:239:ALA:HB1	1:H:314:LEU:HG	2.02	0.41
1:I:135:SER:HA	1:I:412:VAL:HG12	2.03	0.41
1:J:294:THR:HB	1:J:342:ILE:HA	2.01	0.41
1:K:50:THR:HG21	1:K:59:GLU:HG2	2.02	0.41
1:K:517:THR:O	1:K:517:THR:HG22	2.20	0.41
1:L:50:THR:HG21	1:L:59:GLU:HG2	2.02	0.41
1:L:77:VAL:HG12	1:L:506:TYR:HB3	2.02	0.41
1:M:417:VAL:CG2	1:M:477:GLY:HA3	2.51	0.41
1:N:383:ALA:HB3	1:N:389:MET:N	2.35	0.41
1:A:226:LYS:HB2	1:A:253:ASP:O	2.20	0.41
1:D:115:ASP:CB	1:D:435:ASP:HB2	2.51	0.41
1:E:190:VAL:HB	1:E:378:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:ALA:HB1	1:F:116:LEU:HD21	2.02	0.41
1:G:356:ALA:HB1	1:G:361:ASP:HB2	2.01	0.41
1:H:50:THR:HG21	1:H:59:GLU:HG2	2.01	0.41
1:K:135:SER:HA	1:K:412:VAL:HG12	2.03	0.41
1:L:63:GLU:HB3	1:M:4:LYS:O	2.20	0.41
1:N:239:ALA:HB1	1:N:314:LEU:HG	2.02	0.41
1:A:215:LEU:HD22	1:A:246:PRO:HB2	2.02	0.41
1:A:247:LEU:O	1:A:273:VAL:HA	2.20	0.41
1:A:411:VAL:HG13	1:A:496:PRO:HA	2.02	0.41
1:B:100:ILE:O	1:B:104:LEU:HG	2.20	0.41
1:B:115:ASP:CB	1:B:435:ASP:HB2	2.51	0.41
1:B:200:LEU:CD1	1:B:275:ALA:HB3	2.50	0.41
1:B:239:ALA:HB1	1:B:314:LEU:HG	2.03	0.41
1:D:13:ARG:HB2	1:D:104:LEU:HD22	2.03	0.41
1:D:103:GLY:HA3	1:D:515:ILE:HG12	2.02	0.41
1:D:200:LEU:CD1	1:D:275:ALA:HB3	2.50	0.41
1:D:247:LEU:O	1:D:273:VAL:HA	2.20	0.41
1:D:257:GLU:C	1:E:243:ALA:HA	2.46	0.41
1:E:115:ASP:CB	1:E:435:ASP:HB2	2.51	0.41
1:E:226:LYS:HB2	1:E:253:ASP:O	2.20	0.41
1:F:77:VAL:CB	1:F:510:VAL:HG22	2.51	0.41
1:F:239:ALA:HB1	1:F:314:LEU:HG	2.03	0.41
1:F:349:ILE:HG23	1:F:365:LEU:HD13	2.02	0.41
1:F:356:ALA:HB1	1:F:361:ASP:HB2	2.01	0.41
1:G:87:ASP:CG	1:G:151:SER:HA	2.46	0.41
1:G:100:ILE:O	1:G:104:LEU:HG	2.20	0.41
1:G:115:ASP:CB	1:G:435:ASP:HB2	2.51	0.41
1:H:4:LYS:O	1:N:63:GLU:HB3	2.20	0.41
1:H:63:GLU:HB3	1:I:4:LYS:O	2.21	0.41
1:H:106:ALA:HB3	1:H:116:LEU:HD21	2.03	0.41
1:H:218:PRO:HA	1:H:246:PRO:O	2.20	0.41
1:H:291:ASP:OD1	1:H:349:ILE:HD11	2.21	0.41
1:H:383:ALA:HB3	1:H:389:MET:N	2.35	0.41
1:H:417:VAL:CG2	1:H:477:GLY:HA3	2.50	0.41
1:I:291:ASP:OD1	1:I:349:ILE:HD11	2.21	0.41
1:I:383:ALA:HB3	1:I:389:MET:CA	2.51	0.41
1:K:239:ALA:HB1	1:K:314:LEU:HG	2.02	0.41
1:L:135:SER:HA	1:L:412:VAL:HG12	2.03	0.41
1:L:213:VAL:CG1	1:L:325:ILE:HB	2.50	0.41
1:M:135:SER:HA	1:M:412:VAL:HG12	2.03	0.41
1:M:239:ALA:HB1	1:M:314:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:291:ASP:OD1	1:M:349:ILE:HD11	2.21	0.41
1:M:517:THR:O	1:M:517:THR:HG22	2.20	0.41
1:N:213:VAL:O	1:N:324:VAL:HA	2.19	0.41
1:N:291:ASP:OD1	1:N:349:ILE:HD11	2.21	0.41
1:A:100:ILE:O	1:A:104:LEU:HG	2.21	0.41
1:B:226:LYS:HB2	1:B:253:ASP:O	2.20	0.41
1:B:247:LEU:O	1:B:273:VAL:HA	2.20	0.41
1:C:40:LEU:HG	1:C:59:GLU:HB3	2.02	0.41
1:C:190:VAL:HB	1:C:378:VAL:HG23	2.02	0.41
1:C:200:LEU:CD1	1:C:275:ALA:HB3	2.50	0.41
1:D:40:LEU:HG	1:D:59:GLU:HB3	2.02	0.41
1:E:13:ARG:HB2	1:E:104:LEU:HD22	2.03	0.41
1:E:349:ILE:HG23	1:E:365:LEU:HD13	2.02	0.41
1:E:411:VAL:HG13	1:E:496:PRO:HA	2.02	0.41
1:G:240:VAL:HG21	1:G:247:LEU:HD22	2.03	0.41
1:L:19:GLY:HA2	1:L:62:LEU:HD13	2.02	0.41
1:N:19:GLY:HA2	1:N:62:LEU:HD13	2.02	0.41
1:A:190:VAL:HB	1:A:378:VAL:HG23	2.03	0.40
1:A:229:ASN:CG	1:A:230:ILE:H	2.29	0.40
1:C:239:ALA:HB1	1:C:314:LEU:HG	2.03	0.40
1:E:240:VAL:CA	1:E:243:ALA:HB3	2.43	0.40
1:F:87:ASP:CG	1:F:151:SER:HA	2.46	0.40
1:J:239:ALA:HB1	1:J:314:LEU:HG	2.02	0.40
1:A:36:ARG:HD2	1:G:114:MET:HB2	2.04	0.40
1:A:213:VAL:CG1	1:A:325:ILE:HB	2.50	0.40
1:B:229:ASN:CG	1:B:230:ILE:H	2.29	0.40
1:C:349:ILE:HG23	1:C:365:LEU:HD13	2.02	0.40
1:E:257:GLU:C	1:F:243:ALA:HA	2.46	0.40
1:F:411:VAL:HG13	1:F:496:PRO:HA	2.02	0.40
1:G:226:LYS:HB2	1:G:253:ASP:O	2.21	0.40
1:I:239:ALA:HB1	1:I:314:LEU:HG	2.03	0.40
1:N:106:ALA:HB3	1:N:116:LEU:HD21	2.03	0.40
1:N:231:ARG:O	1:N:235:PRO:HD2	2.21	0.40
1:A:182:GLY:O	1:A:382:GLY:HA2	2.22	0.40
1:B:77:VAL:CB	1:B:510:VAL:HG22	2.51	0.40
1:C:247:LEU:O	1:C:273:VAL:HA	2.20	0.40
1:C:257:GLU:C	1:D:243:ALA:HA	2.46	0.40
1:D:383:ALA:HB3	1:D:389:MET:CA	2.52	0.40
1:D:383:ALA:HB3	1:D:389:MET:N	2.36	0.40
1:F:137:PRO:HA	1:F:410:GLY:HA3	2.04	0.40
1:F:254:VAL:HG23	1:F:259:LEU:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:77:VAL:CB	1:G:510:VAL:HG22	2.52	0.40
1:M:231:ARG:O	1:M:235:PRO:HD2	2.21	0.40
1:A:77:VAL:CB	1:A:510:VAL:HG22	2.52	0.40
1:C:229:ASN:CG	1:C:230:ILE:H	2.29	0.40
1:D:213:VAL:CG1	1:D:325:ILE:HB	2.51	0.40
1:D:411:VAL:HG13	1:D:496:PRO:HA	2.02	0.40
1:E:87:ASP:CG	1:E:151:SER:HA	2.46	0.40
1:E:103:GLY:HA3	1:E:515:ILE:HG12	2.02	0.40
1:F:169:VAL:HG11	1:F:175:ILE:HG13	2.04	0.40
1:F:200:LEU:HD22	1:F:254:VAL:HG11	2.02	0.40
1:G:262:LEU:HD12	1:G:262:LEU:HA	1.98	0.40
1:G:411:VAL:CG1	1:G:494:LEU:HB2	2.52	0.40
1:I:144:ILE:HG23	1:I:403:THR:HG21	2.04	0.40
1:K:417:VAL:CG2	1:K:477:GLY:HA3	2.51	0.40
1:L:106:ALA:HB3	1:L:116:LEU:HD21	2.03	0.40
1:A:114:MET:HB2	1:B:36:ARG:HD2	2.04	0.40
1:A:115:ASP:CB	1:A:435:ASP:HB2	2.51	0.40
1:A:246:PRO:HB3	1:A:272:LYS:HB2	2.03	0.40
1:C:488:MET:HA	1:C:488:MET:HE2	2.02	0.40
1:D:349:ILE:HG23	1:D:365:LEU:HD13	2.02	0.40
1:E:137:PRO:HA	1:E:410:GLY:HA3	2.04	0.40
1:F:13:ARG:HB2	1:F:104:LEU:HD22	2.03	0.40
1:F:114:MET:HB2	1:G:36:ARG:HD2	2.04	0.40
1:F:138:CYS:CA	1:F:410:GLY:HA2	2.52	0.40
1:G:138:CYS:CA	1:G:410:GLY:HA2	2.52	0.40
1:J:144:ILE:HG23	1:J:403:THR:HG21	2.04	0.40
1:J:231:ARG:O	1:J:235:PRO:HD2	2.21	0.40
1:L:291:ASP:OD1	1:L:349:ILE:HD11	2.21	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%)	516 (99%)	4 (1%)	2 (0%)	30	67
1	B	522/548 (95%)	516 (99%)	3 (1%)	3 (1%)	21	59
1	C	522/548 (95%)	516 (99%)	3 (1%)	3 (1%)	21	59
1	D	522/548 (95%)	516 (99%)	3 (1%)	3 (1%)	21	59
1	E	522/548 (95%)	515 (99%)	4 (1%)	3 (1%)	21	59
1	F	522/548 (95%)	516 (99%)	3 (1%)	3 (1%)	21	59
1	G	522/548 (95%)	518 (99%)	3 (1%)	1 (0%)	43	78
1	H	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	30	67
1	I	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	30	67
1	J	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	30	67
1	K	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	30	67
1	L	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	30	67
1	M	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	30	67
1	N	522/548 (95%)	518 (99%)	2 (0%)	2 (0%)	30	67
All	All	7308/7672 (95%)	7239 (99%)	37 (0%)	32 (0%)	31	67

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	GLU
1	B	257	GLU
1	C	257	GLU
1	D	257	GLU
1	E	257	GLU
1	F	257	GLU
1	G	257	GLU
1	H	243	ALA
1	I	243	ALA
1	J	243	ALA
1	K	243	ALA
1	L	243	ALA
1	M	243	ALA
1	N	243	ALA
1	H	516	THR
1	I	516	THR
1	J	516	THR
1	K	516	THR
1	L	516	THR

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Mol	Chain	Res	Type
1	M	516	THR
1	N	516	THR
1	A	258	ALA
1	B	258	ALA
1	C	258	ALA
1	D	258	ALA
1	E	258	ALA
1	B	243	ALA
1	C	243	ALA
1	D	243	ALA
1	E	243	ALA
1	F	243	ALA
1	F	258	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	402/414 (97%)	353 (88%)	49 (12%)	5	17
1	B	402/414 (97%)	352 (88%)	50 (12%)	4	17
1	C	402/414 (97%)	352 (88%)	50 (12%)	4	17
1	D	402/414 (97%)	352 (88%)	50 (12%)	4	17
1	E	402/414 (97%)	352 (88%)	50 (12%)	4	17
1	F	402/414 (97%)	352 (88%)	50 (12%)	4	17
1	G	402/414 (97%)	353 (88%)	49 (12%)	5	17
1	H	402/414 (97%)	349 (87%)	53 (13%)	4	15
1	I	402/414 (97%)	350 (87%)	52 (13%)	4	15
1	J	402/414 (97%)	349 (87%)	53 (13%)	4	15
1	K	402/414 (97%)	349 (87%)	53 (13%)	4	15
1	L	402/414 (97%)	349 (87%)	53 (13%)	4	15
1	M	402/414 (97%)	349 (87%)	53 (13%)	4	15
1	N	402/414 (97%)	349 (87%)	53 (13%)	4	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5628/5796 (97%)	4910 (87%)	718 (13%)	6 15

All (718) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	18	ARG
1	A	31	LEU
1	A	42	LYS
1	A	48	THR
1	A	50	THR
1	A	51	LYS
1	A	52	ASP
1	A	65	LYS
1	A	76	GLU
1	A	79	SER
1	A	82	ASN
1	A	114	MET
1	A	130	GLU
1	A	140	ASP
1	A	156	GLU
1	A	171	LYS
1	A	172	GLU
1	A	186	GLU
1	A	205	ILE
1	A	207	LYS
1	A	213	VAL
1	A	214	GLU
1	A	224	ASP
1	A	225	LYS
1	A	230	ILE
1	A	238	GLU
1	A	245	LYS
1	A	252	GLU
1	A	254	VAL
1	A	257	GLU
1	A	262	LEU
1	A	323	VAL
1	A	327	LYS
1	A	328	ASP
1	A	334	ASP
1	A	339	GLU

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Mol	Chain	Res	Type
1	A	350	ARG
1	A	358	SER
1	A	390	LYS
1	A	425	LYS
1	A	430	ARG
1	A	453	GLN
1	A	460	GLU
1	A	463	SER
1	A	484	GLU
1	A	494	LEU
1	A	504	LEU
1	A	518	GLU
1	B	13	ARG
1	B	18	ARG
1	B	31	LEU
1	B	42	LYS
1	B	48	THR
1	B	50	THR
1	B	51	LYS
1	B	52	ASP
1	B	65	LYS
1	B	76	GLU
1	B	79	SER
1	B	82	ASN
1	B	114	MET
1	B	130	GLU
1	B	140	ASP
1	B	156	GLU
1	B	171	LYS
1	B	172	GLU
1	B	186	GLU
1	B	205	ILE
1	B	207	LYS
1	B	213	VAL
1	B	214	GLU
1	B	217	SER
1	B	219	PHE
1	B	224	ASP
1	B	225	LYS
1	B	230	ILE
1	B	238	GLU
1	B	252	GLU

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Mol	Chain	Res	Type
1	B	254	VAL
1	B	257	GLU
1	B	262	LEU
1	B	323	VAL
1	B	327	LYS
1	B	328	ASP
1	B	334	ASP
1	B	339	GLU
1	B	350	ARG
1	B	358	SER
1	B	390	LYS
1	B	425	LYS
1	B	430	ARG
1	B	453	GLN
1	B	460	GLU
1	B	463	SER
1	B	484	GLU
1	B	494	LEU
1	B	504	LEU
1	B	518	GLU
1	C	13	ARG
1	C	18	ARG
1	C	31	LEU
1	C	42	LYS
1	C	48	THR
1	C	50	THR
1	C	51	LYS
1	C	52	ASP
1	C	65	LYS
1	C	76	GLU
1	C	79	SER
1	C	82	ASN
1	C	114	MET
1	C	130	GLU
1	C	140	ASP
1	C	156	GLU
1	C	171	LYS
1	C	172	GLU
1	C	186	GLU
1	C	205	ILE
1	C	207	LYS
1	C	213	VAL

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Mol	Chain	Res	Type
1	C	214	GLU
1	C	217	SER
1	C	219	PHE
1	C	224	ASP
1	C	225	LYS
1	C	230	ILE
1	C	238	GLU
1	C	252	GLU
1	C	254	VAL
1	C	257	GLU
1	C	262	LEU
1	C	323	VAL
1	C	327	LYS
1	C	328	ASP
1	C	334	ASP
1	C	339	GLU
1	C	350	ARG
1	C	358	SER
1	C	390	LYS
1	C	425	LYS
1	C	430	ARG
1	C	453	GLN
1	C	460	GLU
1	C	463	SER
1	C	484	GLU
1	C	494	LEU
1	C	504	LEU
1	C	518	GLU
1	D	13	ARG
1	D	18	ARG
1	D	31	LEU
1	D	42	LYS
1	D	48	THR
1	D	50	THR
1	D	51	LYS
1	D	52	ASP
1	D	65	LYS
1	D	76	GLU
1	D	79	SER
1	D	82	ASN
1	D	114	MET
1	D	130	GLU

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Mol	Chain	Res	Type
1	D	140	ASP
1	D	156	GLU
1	D	171	LYS
1	D	172	GLU
1	D	186	GLU
1	D	205	ILE
1	D	207	LYS
1	D	213	VAL
1	D	214	GLU
1	D	217	SER
1	D	219	PHE
1	D	224	ASP
1	D	225	LYS
1	D	230	ILE
1	D	238	GLU
1	D	252	GLU
1	D	254	VAL
1	D	257	GLU
1	D	262	LEU
1	D	323	VAL
1	D	327	LYS
1	D	328	ASP
1	D	334	ASP
1	D	339	GLU
1	D	350	ARG
1	D	358	SER
1	D	390	LYS
1	D	425	LYS
1	D	430	ARG
1	D	453	GLN
1	D	460	GLU
1	D	463	SER
1	D	484	GLU
1	D	494	LEU
1	D	504	LEU
1	D	518	GLU
1	E	13	ARG
1	E	18	ARG
1	E	31	LEU
1	E	42	LYS
1	E	48	THR
1	E	50	THR

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Mol	Chain	Res	Type
1	E	51	LYS
1	E	52	ASP
1	E	65	LYS
1	E	76	GLU
1	E	79	SER
1	E	82	ASN
1	E	114	MET
1	E	130	GLU
1	E	140	ASP
1	E	156	GLU
1	E	171	LYS
1	E	172	GLU
1	E	186	GLU
1	E	205	ILE
1	E	207	LYS
1	E	213	VAL
1	E	214	GLU
1	E	217	SER
1	E	219	PHE
1	E	224	ASP
1	E	225	LYS
1	E	230	ILE
1	E	238	GLU
1	E	252	GLU
1	E	254	VAL
1	E	257	GLU
1	E	262	LEU
1	E	323	VAL
1	E	327	LYS
1	E	328	ASP
1	E	334	ASP
1	E	339	GLU
1	E	350	ARG
1	E	358	SER
1	E	390	LYS
1	E	425	LYS
1	E	430	ARG
1	E	453	GLN
1	E	460	GLU
1	E	463	SER
1	E	484	GLU
1	E	494	LEU

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Mol	Chain	Res	Type
1	E	504	LEU
1	E	518	GLU
1	F	13	ARG
1	F	18	ARG
1	F	31	LEU
1	F	42	LYS
1	F	48	THR
1	F	50	THR
1	F	51	LYS
1	F	52	ASP
1	F	65	LYS
1	F	76	GLU
1	F	79	SER
1	F	82	ASN
1	F	114	MET
1	F	130	GLU
1	F	140	ASP
1	F	156	GLU
1	F	171	LYS
1	F	172	GLU
1	F	186	GLU
1	F	205	ILE
1	F	207	LYS
1	F	213	VAL
1	F	214	GLU
1	F	217	SER
1	F	219	PHE
1	F	224	ASP
1	F	225	LYS
1	F	230	ILE
1	F	231	ARG
1	F	238	GLU
1	F	252	GLU
1	F	254	VAL
1	F	257	GLU
1	F	323	VAL
1	F	327	LYS
1	F	328	ASP
1	F	334	ASP
1	F	339	GLU
1	F	350	ARG
1	F	358	SER

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Mol	Chain	Res	Type
1	F	390	LYS
1	F	425	LYS
1	F	430	ARG
1	F	453	GLN
1	F	460	GLU
1	F	463	SER
1	F	484	GLU
1	F	494	LEU
1	F	504	LEU
1	F	518	GLU
1	G	13	ARG
1	G	18	ARG
1	G	31	LEU
1	G	42	LYS
1	G	48	THR
1	G	50	THR
1	G	51	LYS
1	G	52	ASP
1	G	65	LYS
1	G	76	GLU
1	G	79	SER
1	G	82	ASN
1	G	114	MET
1	G	130	GLU
1	G	140	ASP
1	G	156	GLU
1	G	171	LYS
1	G	172	GLU
1	G	186	GLU
1	G	205	ILE
1	G	207	LYS
1	G	213	VAL
1	G	214	GLU
1	G	216	GLU
1	G	224	ASP
1	G	225	LYS
1	G	230	ILE
1	G	240	VAL
1	G	242	LYS
1	G	252	GLU
1	G	254	VAL
1	G	257	GLU

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Mol	Chain	Res	Type
1	G	323	VAL
1	G	327	LYS
1	G	328	ASP
1	G	334	ASP
1	G	339	GLU
1	G	350	ARG
1	G	358	SER
1	G	390	LYS
1	G	425	LYS
1	G	430	ARG
1	G	453	GLN
1	G	460	GLU
1	G	463	SER
1	G	484	GLU
1	G	494	LEU
1	G	504	LEU
1	G	518	GLU
1	H	31	LEU
1	H	36	ARG
1	H	40	LEU
1	H	50	THR
1	H	52	ASP
1	H	59	GLU
1	H	63	GLU
1	H	65	LYS
1	H	79	SER
1	H	82	ASN
1	H	114	MET
1	H	130	GLU
1	H	156	GLU
1	H	169	VAL
1	H	171	LYS
1	H	172	GLU
1	H	186	GLU
1	H	190	VAL
1	H	205	ILE
1	H	207	LYS
1	H	213	VAL
1	H	214	GLU
1	H	225	LYS
1	H	230	ILE
1	H	231	ARG

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Mol	Chain	Res	Type
1	H	232	GLU
1	H	238	GLU
1	H	242	LYS
1	H	246	PRO
1	H	252	GLU
1	H	268	ARG
1	H	272	LYS
1	H	294	THR
1	H	301	ILE
1	H	303	GLU
1	H	321	LYS
1	H	322	ARG
1	H	323	VAL
1	H	327	LYS
1	H	328	ASP
1	H	334	ASP
1	H	350	ARG
1	H	358	SER
1	H	412	VAL
1	H	421	ARG
1	H	425	LYS
1	H	430	ARG
1	H	453	GLN
1	H	460	GLU
1	H	463	SER
1	H	464	VAL
1	H	484	GLU
1	H	504	LEU
1	I	31	LEU
1	I	36	ARG
1	I	40	LEU
1	I	50	THR
1	I	52	ASP
1	I	59	GLU
1	I	63	GLU
1	I	65	LYS
1	I	79	SER
1	I	82	ASN
1	I	114	MET
1	I	130	GLU
1	I	156	GLU
1	I	169	VAL

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Mol	Chain	Res	Type
1	I	171	LYS
1	I	172	GLU
1	I	186	GLU
1	I	190	VAL
1	I	205	ILE
1	I	207	LYS
1	I	213	VAL
1	I	214	GLU
1	I	225	LYS
1	I	230	ILE
1	I	231	ARG
1	I	238	GLU
1	I	242	LYS
1	I	246	PRO
1	I	252	GLU
1	I	268	ARG
1	I	272	LYS
1	I	294	THR
1	I	301	ILE
1	I	303	GLU
1	I	321	LYS
1	I	322	ARG
1	I	323	VAL
1	I	327	LYS
1	I	328	ASP
1	I	334	ASP
1	I	350	ARG
1	I	358	SER
1	I	412	VAL
1	I	421	ARG
1	I	425	LYS
1	I	430	ARG
1	I	453	GLN
1	I	460	GLU
1	I	463	SER
1	I	464	VAL
1	I	484	GLU
1	I	504	LEU
1	J	31	LEU
1	J	36	ARG
1	J	40	LEU
1	J	50	THR

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Mol	Chain	Res	Type
1	J	52	ASP
1	J	59	GLU
1	J	63	GLU
1	J	65	LYS
1	J	79	SER
1	J	82	ASN
1	J	114	MET
1	J	130	GLU
1	J	156	GLU
1	J	169	VAL
1	J	171	LYS
1	J	172	GLU
1	J	186	GLU
1	J	190	VAL
1	J	205	ILE
1	J	207	LYS
1	J	213	VAL
1	J	214	GLU
1	J	225	LYS
1	J	230	ILE
1	J	231	ARG
1	J	232	GLU
1	J	238	GLU
1	J	242	LYS
1	J	246	PRO
1	J	252	GLU
1	J	268	ARG
1	J	272	LYS
1	J	294	THR
1	J	301	ILE
1	J	303	GLU
1	J	321	LYS
1	J	322	ARG
1	J	323	VAL
1	J	327	LYS
1	J	328	ASP
1	J	334	ASP
1	J	350	ARG
1	J	358	SER
1	J	412	VAL
1	J	421	ARG
1	J	425	LYS

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Mol	Chain	Res	Type
1	J	430	ARG
1	J	453	GLN
1	J	460	GLU
1	J	463	SER
1	J	464	VAL
1	J	484	GLU
1	J	504	LEU
1	K	31	LEU
1	K	36	ARG
1	K	40	LEU
1	K	50	THR
1	K	52	ASP
1	K	59	GLU
1	K	63	GLU
1	K	65	LYS
1	K	79	SER
1	K	82	ASN
1	K	114	MET
1	K	130	GLU
1	K	156	GLU
1	K	169	VAL
1	K	171	LYS
1	K	172	GLU
1	K	186	GLU
1	K	190	VAL
1	K	205	ILE
1	K	207	LYS
1	K	213	VAL
1	K	214	GLU
1	K	225	LYS
1	K	230	ILE
1	K	231	ARG
1	K	232	GLU
1	K	238	GLU
1	K	242	LYS
1	K	246	PRO
1	K	252	GLU
1	K	268	ARG
1	K	272	LYS
1	K	294	THR
1	K	301	ILE
1	K	303	GLU

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Mol	Chain	Res	Type
1	K	321	LYS
1	K	322	ARG
1	K	323	VAL
1	K	327	LYS
1	K	328	ASP
1	K	334	ASP
1	K	350	ARG
1	K	358	SER
1	K	412	VAL
1	K	421	ARG
1	K	425	LYS
1	K	430	ARG
1	K	453	GLN
1	K	460	GLU
1	K	463	SER
1	K	464	VAL
1	K	484	GLU
1	K	504	LEU
1	L	31	LEU
1	L	36	ARG
1	L	40	LEU
1	L	50	THR
1	L	52	ASP
1	L	59	GLU
1	L	63	GLU
1	L	65	LYS
1	L	79	SER
1	L	82	ASN
1	L	114	MET
1	L	130	GLU
1	L	156	GLU
1	L	169	VAL
1	L	171	LYS
1	L	172	GLU
1	L	186	GLU
1	L	190	VAL
1	L	205	ILE
1	L	207	LYS
1	L	213	VAL
1	L	214	GLU
1	L	225	LYS
1	L	230	ILE

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Mol	Chain	Res	Type
1	L	231	ARG
1	L	232	GLU
1	L	238	GLU
1	L	242	LYS
1	L	246	PRO
1	L	252	GLU
1	L	268	ARG
1	L	272	LYS
1	L	294	THR
1	L	301	ILE
1	L	303	GLU
1	L	321	LYS
1	L	322	ARG
1	L	323	VAL
1	L	327	LYS
1	L	328	ASP
1	L	334	ASP
1	L	350	ARG
1	L	358	SER
1	L	412	VAL
1	L	421	ARG
1	L	425	LYS
1	L	430	ARG
1	L	453	GLN
1	L	460	GLU
1	L	463	SER
1	L	464	VAL
1	L	484	GLU
1	L	504	LEU
1	M	31	LEU
1	M	36	ARG
1	M	40	LEU
1	M	50	THR
1	M	52	ASP
1	M	59	GLU
1	M	63	GLU
1	M	65	LYS
1	M	79	SER
1	M	82	ASN
1	M	114	MET
1	M	130	GLU
1	M	156	GLU

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Mol	Chain	Res	Type
1	M	169	VAL
1	M	171	LYS
1	M	172	GLU
1	M	186	GLU
1	M	190	VAL
1	M	205	ILE
1	M	207	LYS
1	M	213	VAL
1	M	214	GLU
1	M	225	LYS
1	M	230	ILE
1	M	231	ARG
1	M	232	GLU
1	M	238	GLU
1	M	242	LYS
1	M	246	PRO
1	M	252	GLU
1	M	268	ARG
1	M	272	LYS
1	M	294	THR
1	M	301	ILE
1	M	303	GLU
1	M	321	LYS
1	M	322	ARG
1	M	323	VAL
1	M	327	LYS
1	M	328	ASP
1	M	334	ASP
1	M	350	ARG
1	M	358	SER
1	M	412	VAL
1	M	421	ARG
1	M	425	LYS
1	M	430	ARG
1	M	453	GLN
1	M	460	GLU
1	M	463	SER
1	M	464	VAL
1	M	484	GLU
1	M	504	LEU
1	N	31	LEU
1	N	36	ARG

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Mol	Chain	Res	Type
1	N	40	LEU
1	N	50	THR
1	N	52	ASP
1	N	59	GLU
1	N	63	GLU
1	N	65	LYS
1	N	79	SER
1	N	82	ASN
1	N	114	MET
1	N	130	GLU
1	N	156	GLU
1	N	169	VAL
1	N	171	LYS
1	N	172	GLU
1	N	186	GLU
1	N	190	VAL
1	N	205	ILE
1	N	207	LYS
1	N	213	VAL
1	N	214	GLU
1	N	225	LYS
1	N	230	ILE
1	N	231	ARG
1	N	232	GLU
1	N	238	GLU
1	N	242	LYS
1	N	246	PRO
1	N	252	GLU
1	N	268	ARG
1	N	272	LYS
1	N	294	THR
1	N	301	ILE
1	N	303	GLU
1	N	321	LYS
1	N	322	ARG
1	N	323	VAL
1	N	327	LYS
1	N	328	ASP
1	N	334	ASP
1	N	350	ARG
1	N	358	SER
1	N	412	VAL

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Mol	Chain	Res	Type
1	N	421	ARG
1	N	425	LYS
1	N	430	ARG
1	N	453	GLN
1	N	460	GLU
1	N	463	SER
1	N	464	VAL
1	N	484	GLU
1	N	504	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	229	ASN
1	A	265	ASN
1	A	453	GLN
1	A	475	ASN
1	B	97	GLN
1	B	229	ASN
1	B	265	ASN
1	B	453	GLN
1	B	475	ASN
1	C	97	GLN
1	C	229	ASN
1	C	265	ASN
1	C	453	GLN
1	C	475	ASN
1	D	97	GLN
1	D	229	ASN
1	D	265	ASN
1	D	453	GLN
1	D	475	ASN
1	E	97	GLN
1	E	229	ASN
1	E	265	ASN
1	E	453	GLN
1	E	475	ASN
1	F	97	GLN
1	F	265	ASN
1	F	453	GLN
1	F	475	ASN

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Mol	Chain	Res	Type
1	G	97	GLN
1	G	265	ASN
1	G	453	GLN
1	G	475	ASN
1	H	453	GLN
1	H	475	ASN
1	I	453	GLN
1	I	475	ASN
1	J	453	GLN
1	J	475	ASN
1	K	453	GLN
1	K	475	ASN
1	L	453	GLN
1	L	475	ASN
1	M	453	GLN
1	M	475	ASN
1	N	453	GLN
1	N	475	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ATP	C	1526	3	32,33,33	1.81	3 (9%)	48,52,52	0.99	4 (8%)
2	ATP	H	1527	3	32,33,33	1.74	1 (3%)	48,52,52	0.97	3 (6%)
2	ATP	N	1527	3	32,33,33	1.73	1 (3%)	48,52,52	0.97	4 (8%)
2	ATP	B	1525	3	32,33,33	1.81	3 (9%)	48,52,52	0.99	4 (8%)
2	ATP	D	1525	3	32,33,33	1.81	3 (9%)	48,52,52	0.99	4 (8%)
2	ATP	E	1525	3	32,33,33	1.82	3 (9%)	48,52,52	0.99	4 (8%)
2	ATP	F	1525	3	32,33,33	1.82	3 (9%)	48,52,52	0.99	4 (8%)
2	ATP	J	1526	3	32,33,33	1.72	1 (3%)	48,52,52	0.97	4 (8%)
2	ATP	A	1525	3	32,33,33	1.83	3 (9%)	48,52,52	0.99	4 (8%)
2	ATP	K	1527	3	32,33,33	1.75	1 (3%)	48,52,52	0.97	4 (8%)
2	ATP	G	1525	3	32,33,33	1.83	3 (9%)	48,52,52	0.99	4 (8%)
2	ATP	M	1527	3	32,33,33	1.73	1 (3%)	48,52,52	0.97	3 (6%)
2	ATP	I	1525	3	32,33,33	1.73	1 (3%)	48,52,52	0.96	3 (6%)
2	ATP	L	1527	3	32,33,33	1.74	1 (3%)	48,52,52	0.96	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	C	1526	3	-	1/22/38/38	0/3/3/3
2	ATP	H	1527	3	-	2/22/38/38	0/3/3/3
2	ATP	N	1527	3	-	2/22/38/38	0/3/3/3
2	ATP	B	1525	3	-	1/22/38/38	0/3/3/3
2	ATP	D	1525	3	-	1/22/38/38	0/3/3/3
2	ATP	E	1525	3	-	1/22/38/38	0/3/3/3
2	ATP	F	1525	3	-	1/22/38/38	0/3/3/3
2	ATP	J	1526	3	-	2/22/38/38	0/3/3/3
2	ATP	A	1525	3	-	1/22/38/38	0/3/3/3
2	ATP	K	1527	3	-	2/22/38/38	0/3/3/3
2	ATP	G	1525	3	-	1/22/38/38	0/3/3/3
2	ATP	M	1527	3	-	2/22/38/38	0/3/3/3
2	ATP	I	1525	3	-	2/22/38/38	0/3/3/3
2	ATP	L	1527	3	-	2/22/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1525	ATP	PA-O3A	-9.29	1.49	1.59
2	G	1525	ATP	PA-O3A	-9.27	1.49	1.59
2	F	1525	ATP	PA-O3A	-9.25	1.49	1.59
2	E	1525	ATP	PA-O3A	-9.22	1.49	1.59
2	C	1526	ATP	PA-O3A	-9.21	1.49	1.59
2	B	1525	ATP	PA-O3A	-9.17	1.49	1.59
2	D	1525	ATP	PA-O3A	-9.13	1.49	1.59
2	K	1527	ATP	PA-O3A	-9.02	1.49	1.59
2	L	1527	ATP	PA-O3A	-9.00	1.49	1.59
2	H	1527	ATP	PA-O3A	-8.93	1.49	1.59
2	M	1527	ATP	PA-O3A	-8.93	1.49	1.59
2	N	1527	ATP	PA-O3A	-8.90	1.49	1.59
2	J	1526	ATP	PA-O3A	-8.88	1.49	1.59
2	I	1525	ATP	PA-O3A	-8.87	1.49	1.59
2	B	1525	ATP	PB-O3B	2.48	1.62	1.59
2	E	1525	ATP	PB-O3B	2.48	1.62	1.59
2	D	1525	ATP	PB-O3B	2.47	1.62	1.59
2	G	1525	ATP	PB-O3B	2.46	1.62	1.59
2	F	1525	ATP	PB-O3B	2.44	1.62	1.59
2	C	1526	ATP	PB-O3B	2.42	1.62	1.59
2	A	1525	ATP	PB-O3B	2.39	1.62	1.59
2	B	1525	ATP	PB-O3A	-2.25	1.57	1.59
2	E	1525	ATP	PB-O3A	-2.24	1.57	1.59
2	D	1525	ATP	PB-O3A	-2.24	1.57	1.59
2	G	1525	ATP	PB-O3A	-2.21	1.57	1.59
2	A	1525	ATP	PB-O3A	-2.20	1.57	1.59
2	F	1525	ATP	PB-O3A	-2.18	1.57	1.59
2	C	1526	ATP	PB-O3A	-2.16	1.57	1.59

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1527	ATP	O2A-PA-O3A	2.87	115.03	107.27
2	H	1527	ATP	O2A-PA-O3A	2.86	115.01	107.27
2	M	1527	ATP	O2A-PA-O3A	2.86	115.00	107.27
2	J	1526	ATP	O2A-PA-O3A	2.84	114.95	107.27
2	I	1525	ATP	O2A-PA-O3A	2.83	114.92	107.27
2	K	1527	ATP	O2A-PA-O3A	2.83	114.92	107.27
2	L	1527	ATP	O2A-PA-O3A	2.83	114.92	107.27
2	B	1525	ATP	C5'-C4'-C3'	-2.73	105.40	115.21
2	F	1525	ATP	C5'-C4'-C3'	-2.72	105.43	115.21
2	D	1525	ATP	C5'-C4'-C3'	-2.71	105.45	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1525	ATP	C5'-C4'-C3'	-2.71	105.46	115.21
2	C	1526	ATP	C5'-C4'-C3'	-2.71	105.47	115.21
2	E	1525	ATP	C5'-C4'-C3'	-2.71	105.47	115.21
2	A	1525	ATP	C5'-C4'-C3'	-2.70	105.48	115.21
2	H	1527	ATP	C5'-C4'-C3'	-2.68	105.56	115.21
2	N	1527	ATP	C5'-C4'-C3'	-2.68	105.56	115.21
2	M	1527	ATP	C5'-C4'-C3'	-2.68	105.57	115.21
2	J	1526	ATP	C5'-C4'-C3'	-2.68	105.57	115.21
2	L	1527	ATP	C5'-C4'-C3'	-2.68	105.57	115.21
2	K	1527	ATP	C5'-C4'-C3'	-2.68	105.58	115.21
2	I	1525	ATP	C5'-C4'-C3'	-2.68	105.58	115.21
2	G	1525	ATP	O2A-PA-O3A	2.60	114.31	107.27
2	C	1526	ATP	O2A-PA-O3A	2.58	114.24	107.27
2	E	1525	ATP	O2A-PA-O3A	2.58	114.23	107.27
2	A	1525	ATP	O2A-PA-O3A	2.57	114.23	107.27
2	D	1525	ATP	O2A-PA-O3A	2.57	114.21	107.27
2	B	1525	ATP	O2A-PA-O3A	2.57	114.21	107.27
2	F	1525	ATP	O2A-PA-O3A	2.56	114.20	107.27
2	C	1526	ATP	O3B-PG-O1G	-2.43	98.27	111.04
2	B	1525	ATP	O3B-PG-O1G	-2.42	98.28	111.04
2	D	1525	ATP	O3B-PG-O1G	-2.42	98.29	111.04
2	G	1525	ATP	O3B-PG-O1G	-2.42	98.30	111.04
2	F	1525	ATP	O3B-PG-O1G	-2.42	98.30	111.04
2	E	1525	ATP	O3B-PG-O1G	-2.42	98.30	111.04
2	A	1525	ATP	O3B-PG-O1G	-2.42	98.31	111.04
2	L	1527	ATP	O3B-PG-O1G	-2.37	98.54	111.04
2	K	1527	ATP	O3B-PG-O1G	-2.37	98.54	111.04
2	I	1525	ATP	O3B-PG-O1G	-2.37	98.55	111.04
2	N	1527	ATP	O3B-PG-O1G	-2.37	98.55	111.04
2	J	1526	ATP	O3B-PG-O1G	-2.37	98.58	111.04
2	M	1527	ATP	O3B-PG-O1G	-2.37	98.58	111.04
2	H	1527	ATP	O3B-PG-O1G	-2.37	98.59	111.04
2	C	1526	ATP	O3G-PG-O2G	2.13	115.80	107.80
2	B	1525	ATP	O3G-PG-O2G	2.13	115.78	107.80
2	E	1525	ATP	O3G-PG-O2G	2.12	115.74	107.80
2	A	1525	ATP	O3G-PG-O2G	2.11	115.73	107.80
2	G	1525	ATP	O3G-PG-O2G	2.11	115.73	107.80
2	D	1525	ATP	O3G-PG-O2G	2.11	115.72	107.80
2	F	1525	ATP	O3G-PG-O2G	2.11	115.71	107.80
2	K	1527	ATP	O3G-PG-O2G	2.02	115.36	107.80
2	J	1526	ATP	O3G-PG-O2G	2.01	115.35	107.80
2	N	1527	ATP	O3G-PG-O2G	2.01	115.33	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1527	ATP	O3G-PG-O2G	2.00	115.30	107.80

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1525	ATP	PG-O3B-PB-O2B
2	B	1525	ATP	PG-O3B-PB-O2B
2	C	1526	ATP	PG-O3B-PB-O2B
2	D	1525	ATP	PG-O3B-PB-O2B
2	E	1525	ATP	PG-O3B-PB-O2B
2	F	1525	ATP	PG-O3B-PB-O2B
2	G	1525	ATP	PG-O3B-PB-O2B
2	H	1527	ATP	PG-O3B-PB-O1B
2	I	1525	ATP	PG-O3B-PB-O1B
2	J	1526	ATP	PG-O3B-PB-O1B
2	K	1527	ATP	PG-O3B-PB-O1B
2	L	1527	ATP	PG-O3B-PB-O1B
2	M	1527	ATP	PG-O3B-PB-O1B
2	N	1527	ATP	PG-O3B-PB-O1B
2	H	1527	ATP	PG-O3B-PB-O2B
2	I	1525	ATP	PG-O3B-PB-O2B
2	J	1526	ATP	PG-O3B-PB-O2B
2	K	1527	ATP	PG-O3B-PB-O2B
2	L	1527	ATP	PG-O3B-PB-O2B
2	M	1527	ATP	PG-O3B-PB-O2B
2	N	1527	ATP	PG-O3B-PB-O2B

There are no ring outliers.

14 monomers are involved in 42 short contacts:

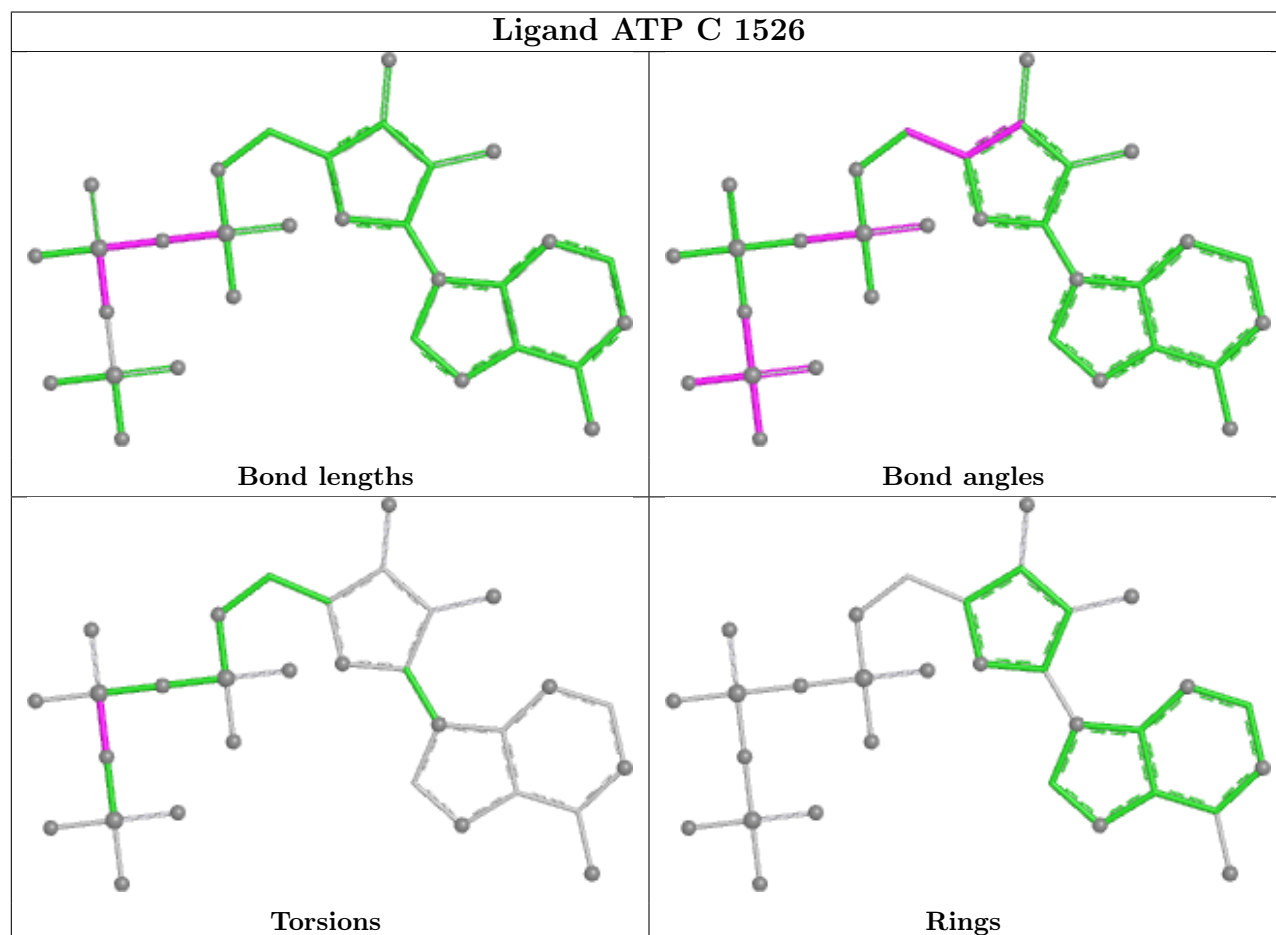
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1526	ATP	3	0
2	H	1527	ATP	3	0
2	N	1527	ATP	3	0
2	B	1525	ATP	3	0
2	D	1525	ATP	3	0
2	E	1525	ATP	3	0
2	F	1525	ATP	3	0
2	J	1526	ATP	3	0
2	A	1525	ATP	3	0

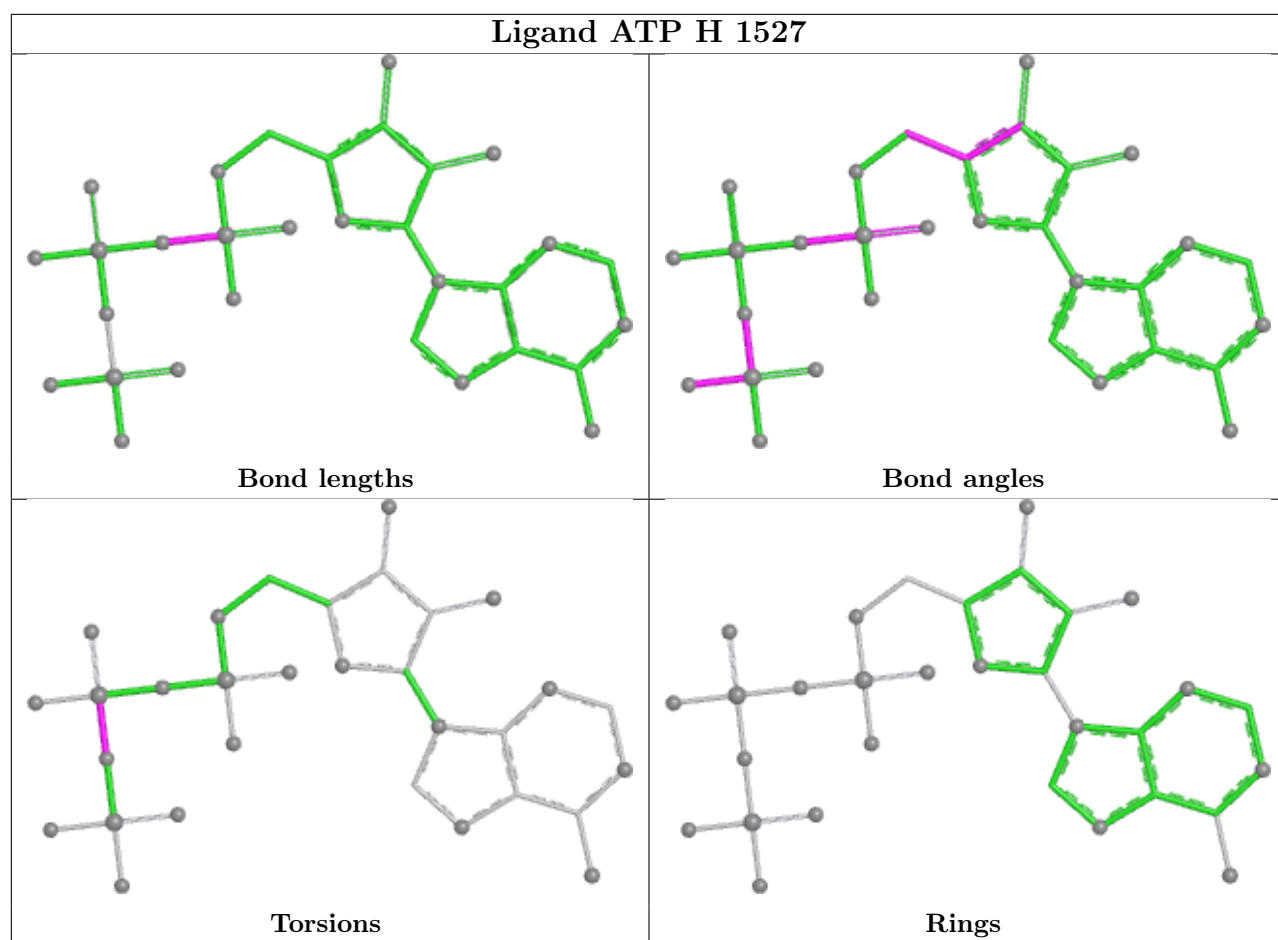
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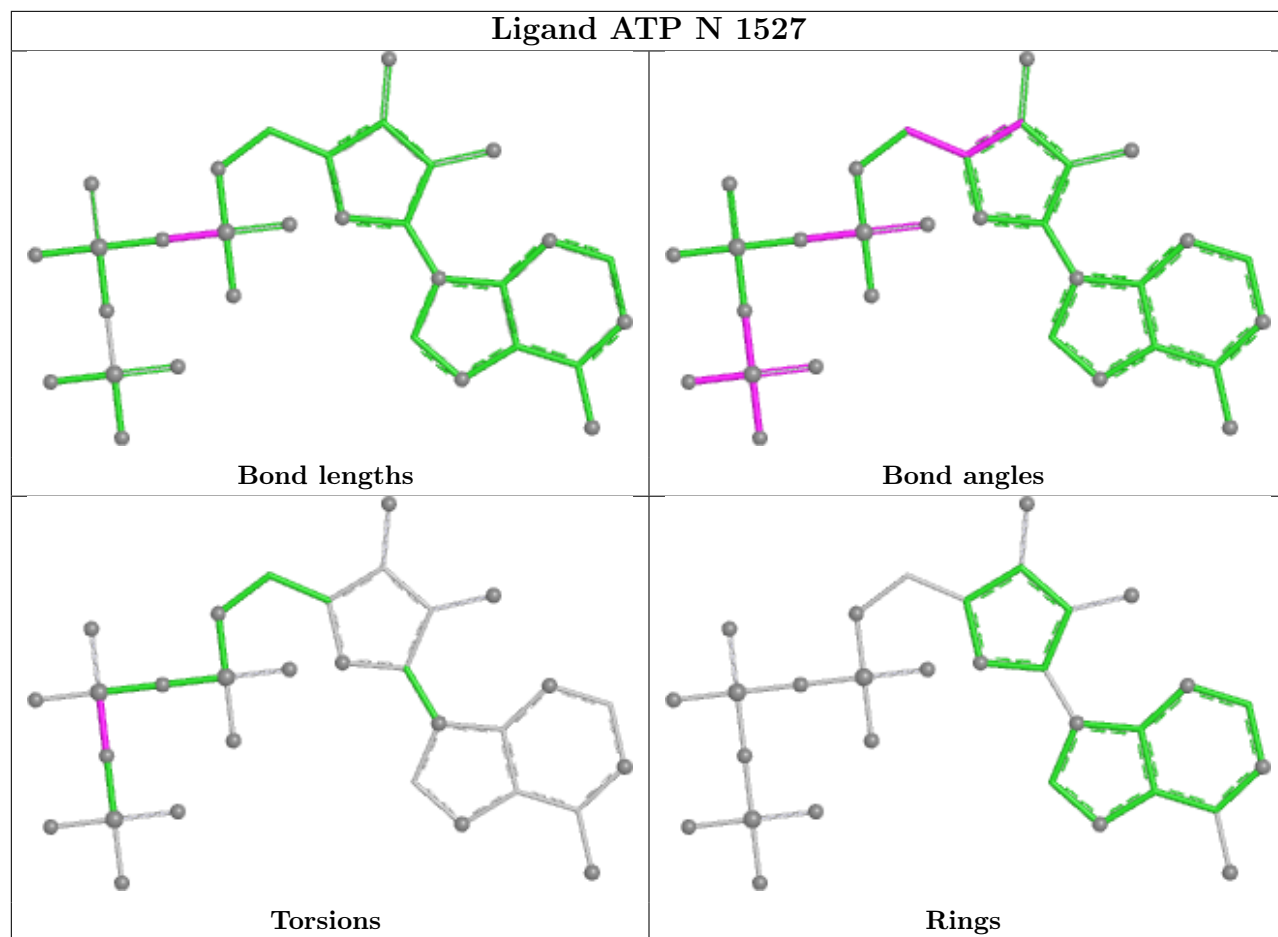
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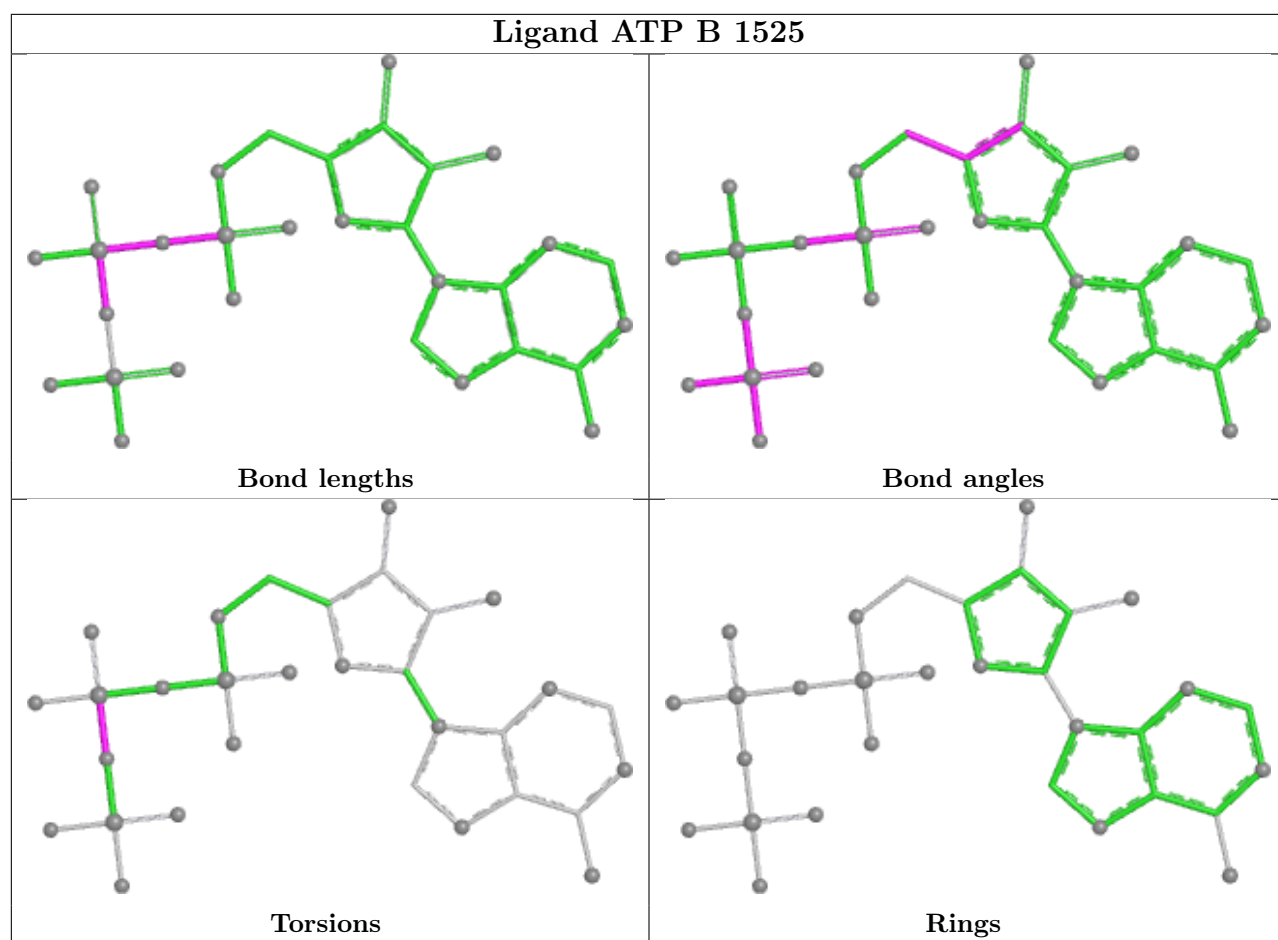
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1527	ATP	3	0
2	G	1525	ATP	3	0
2	M	1527	ATP	3	0
2	I	1525	ATP	3	0
2	L	1527	ATP	3	0

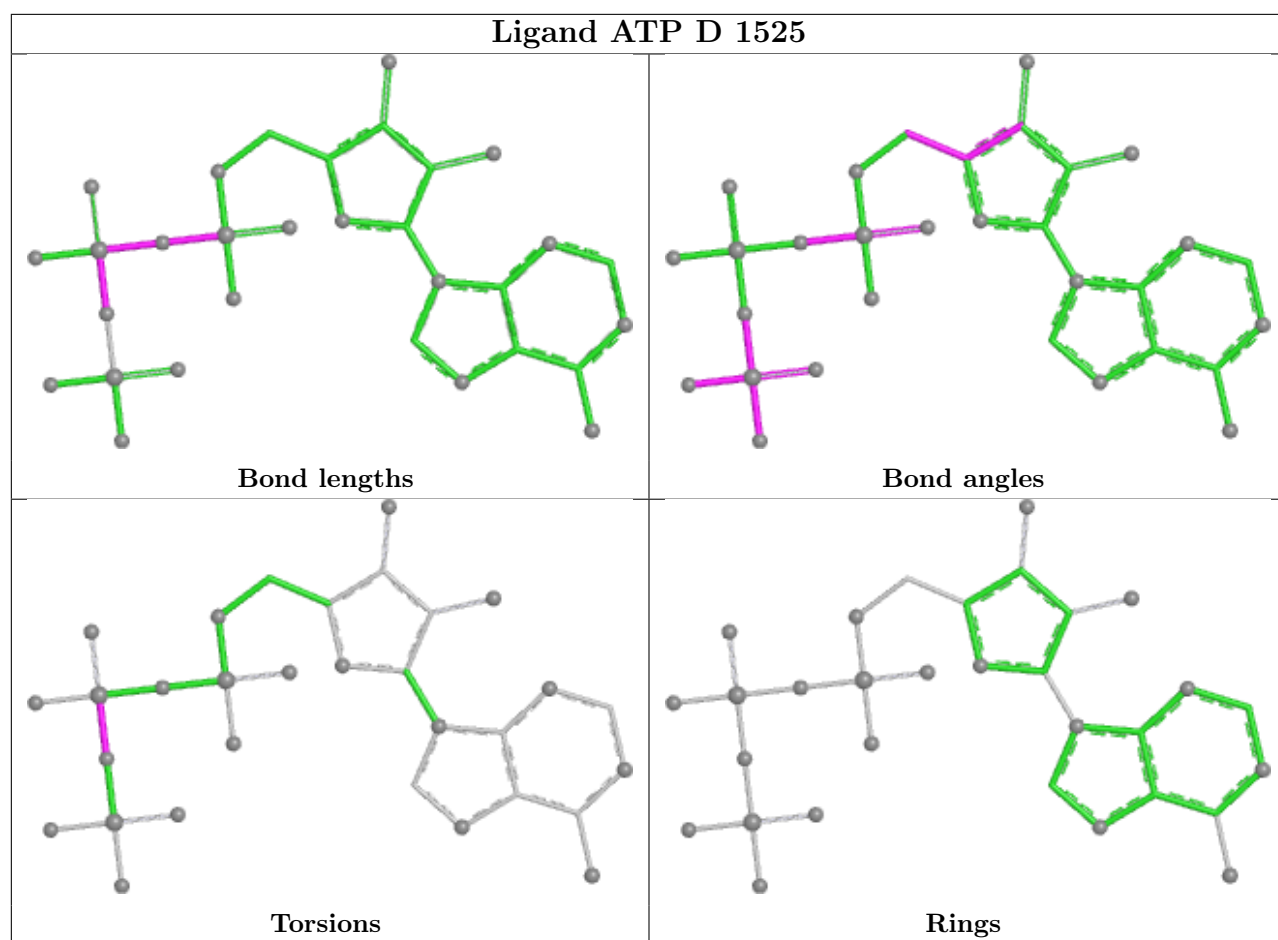
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

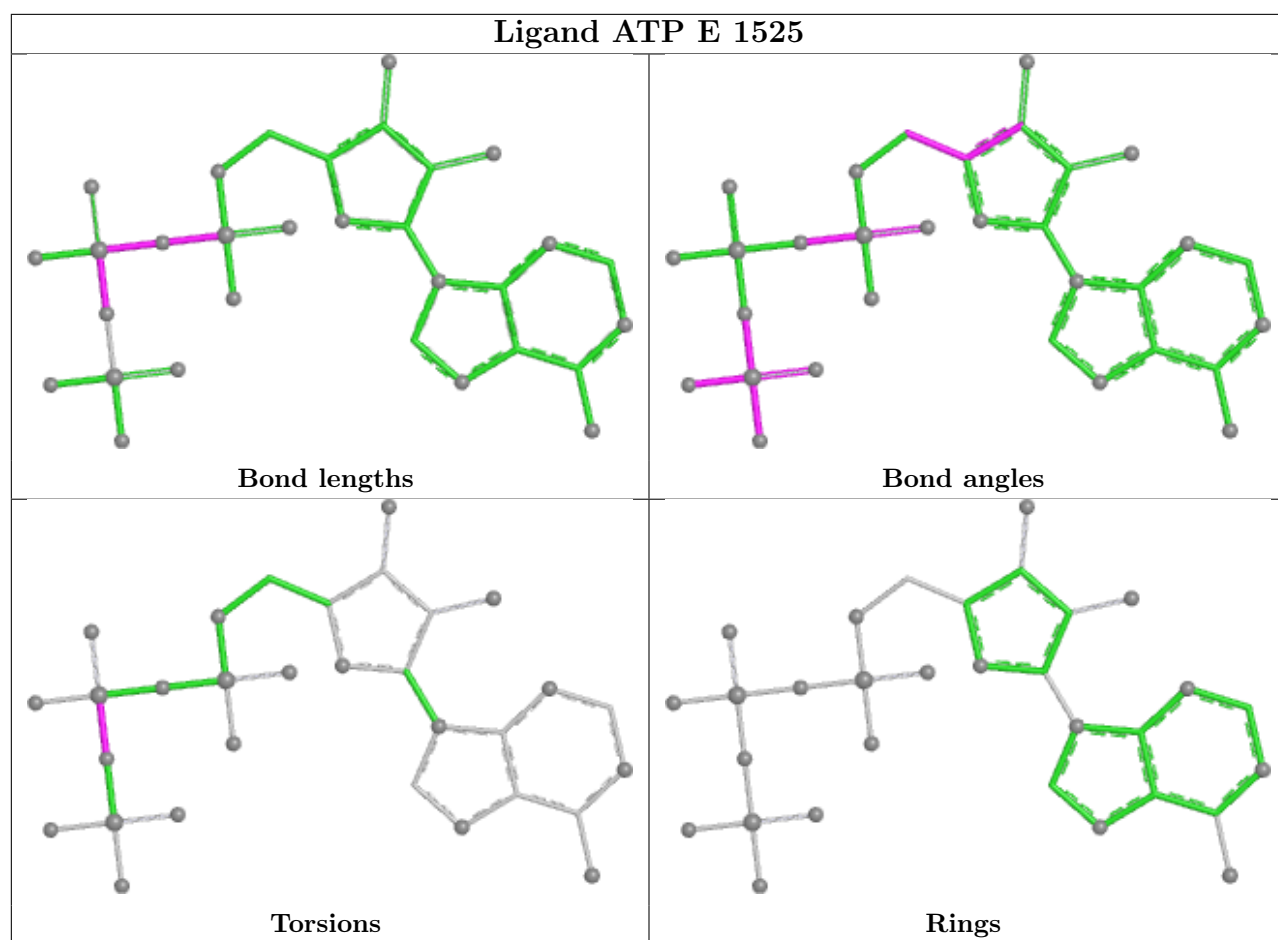


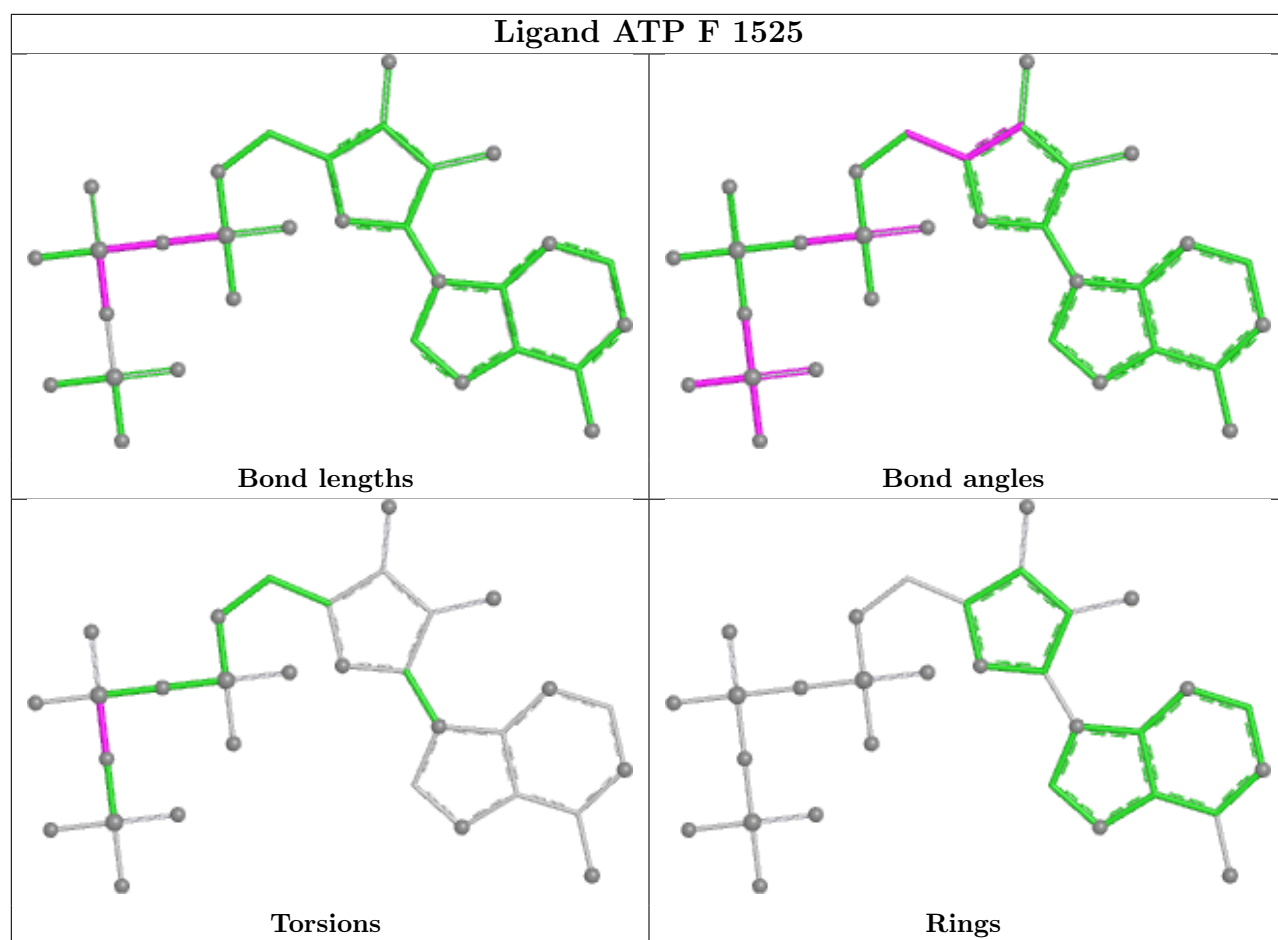


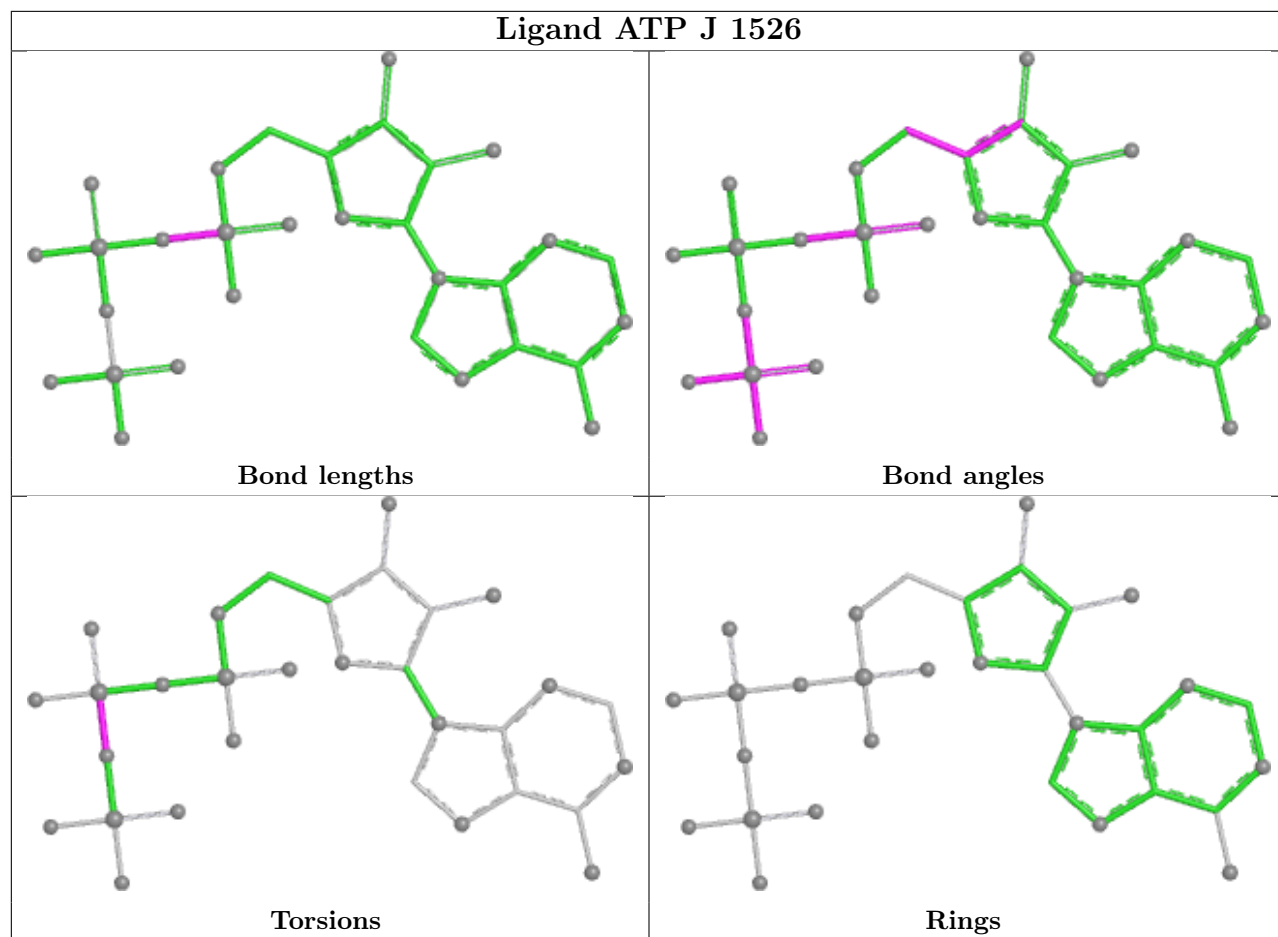


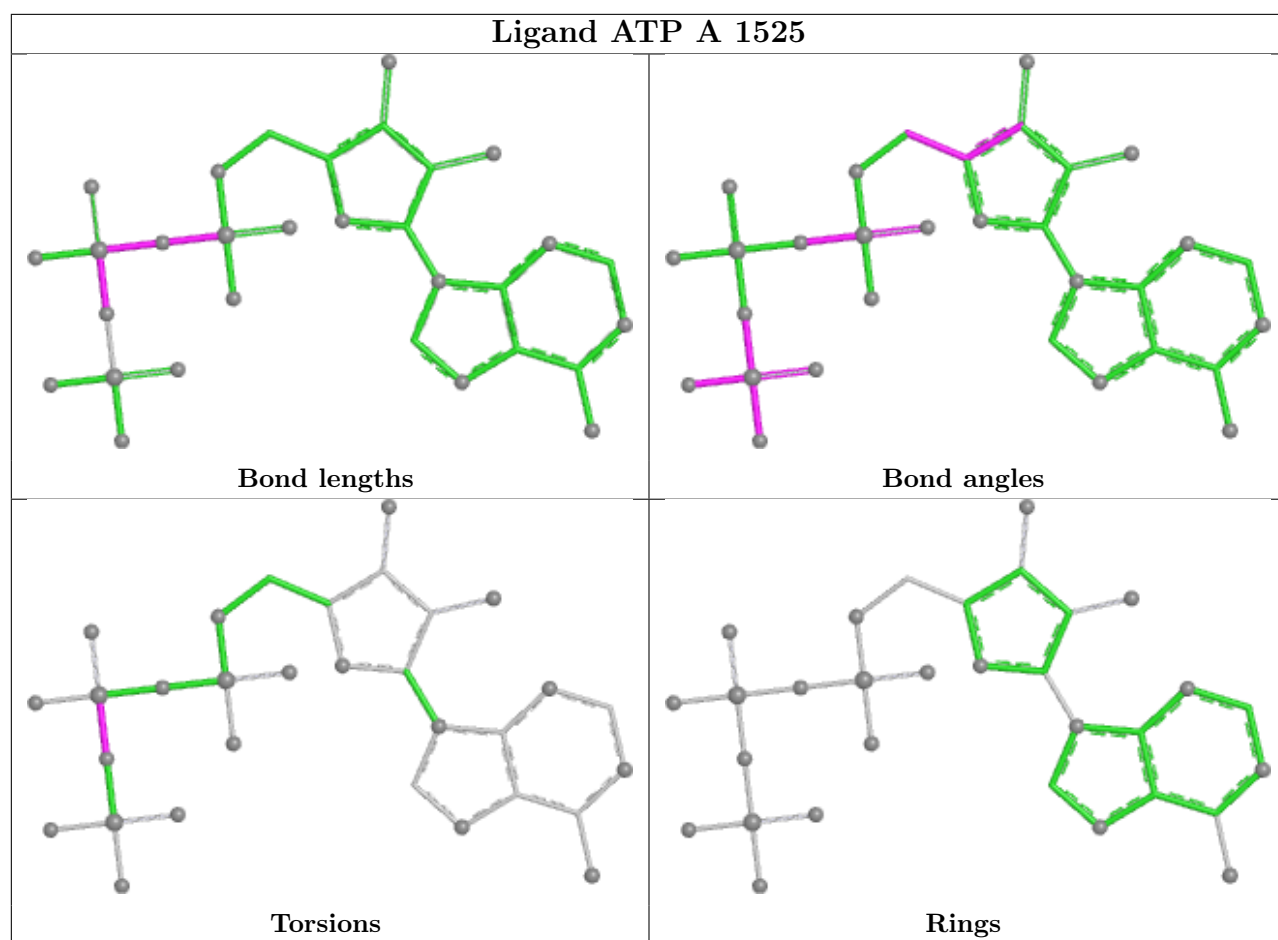


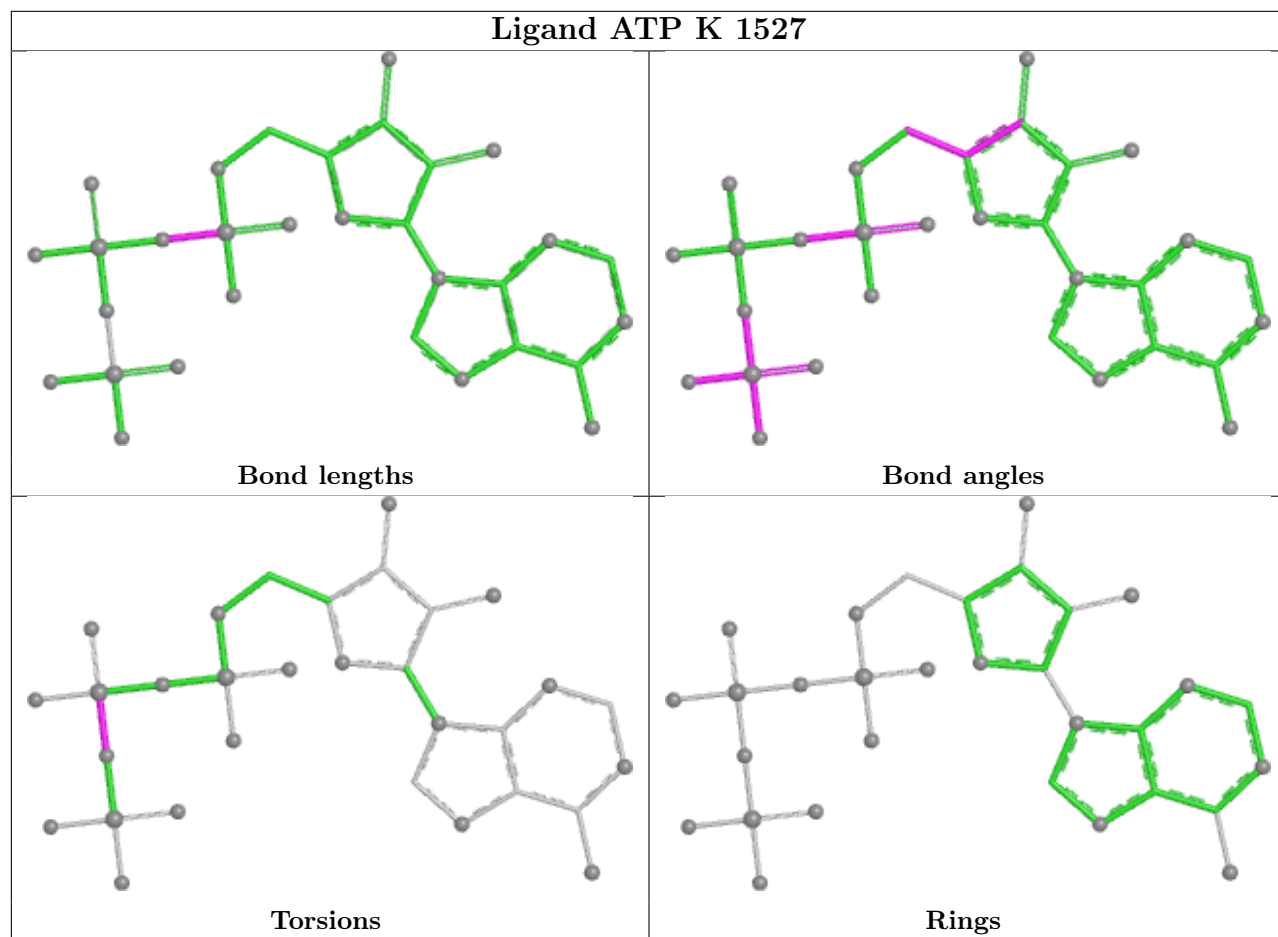


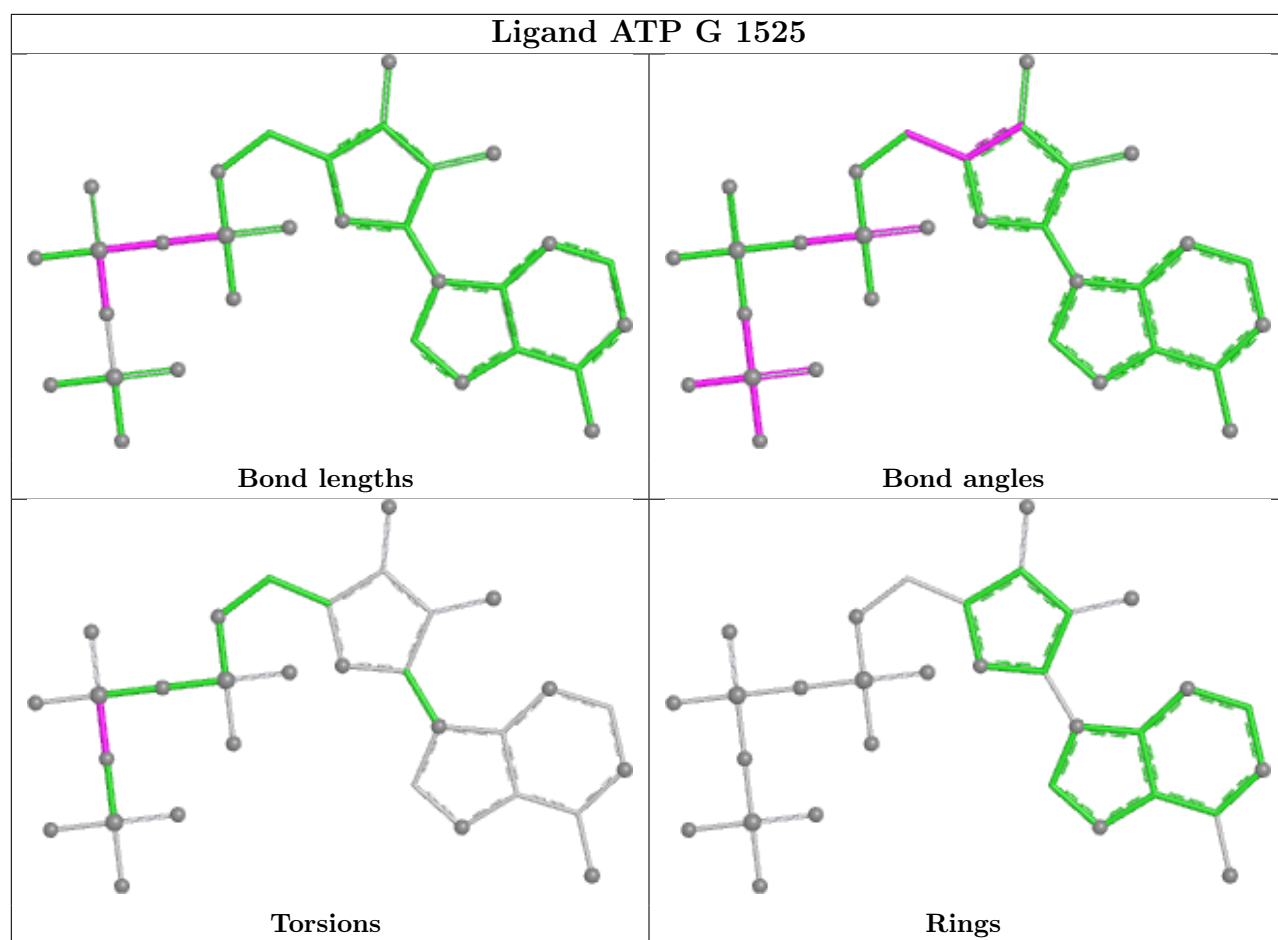


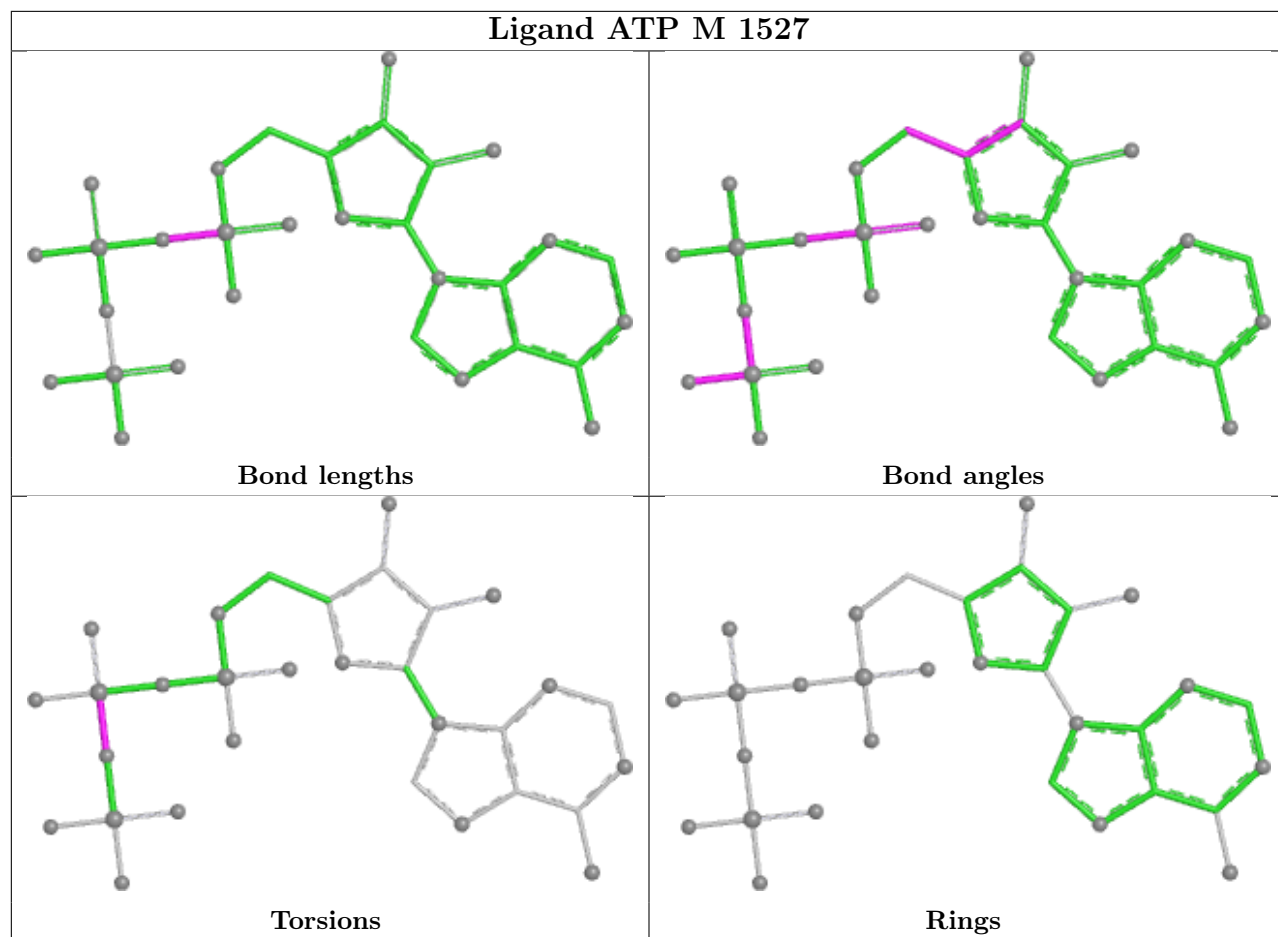


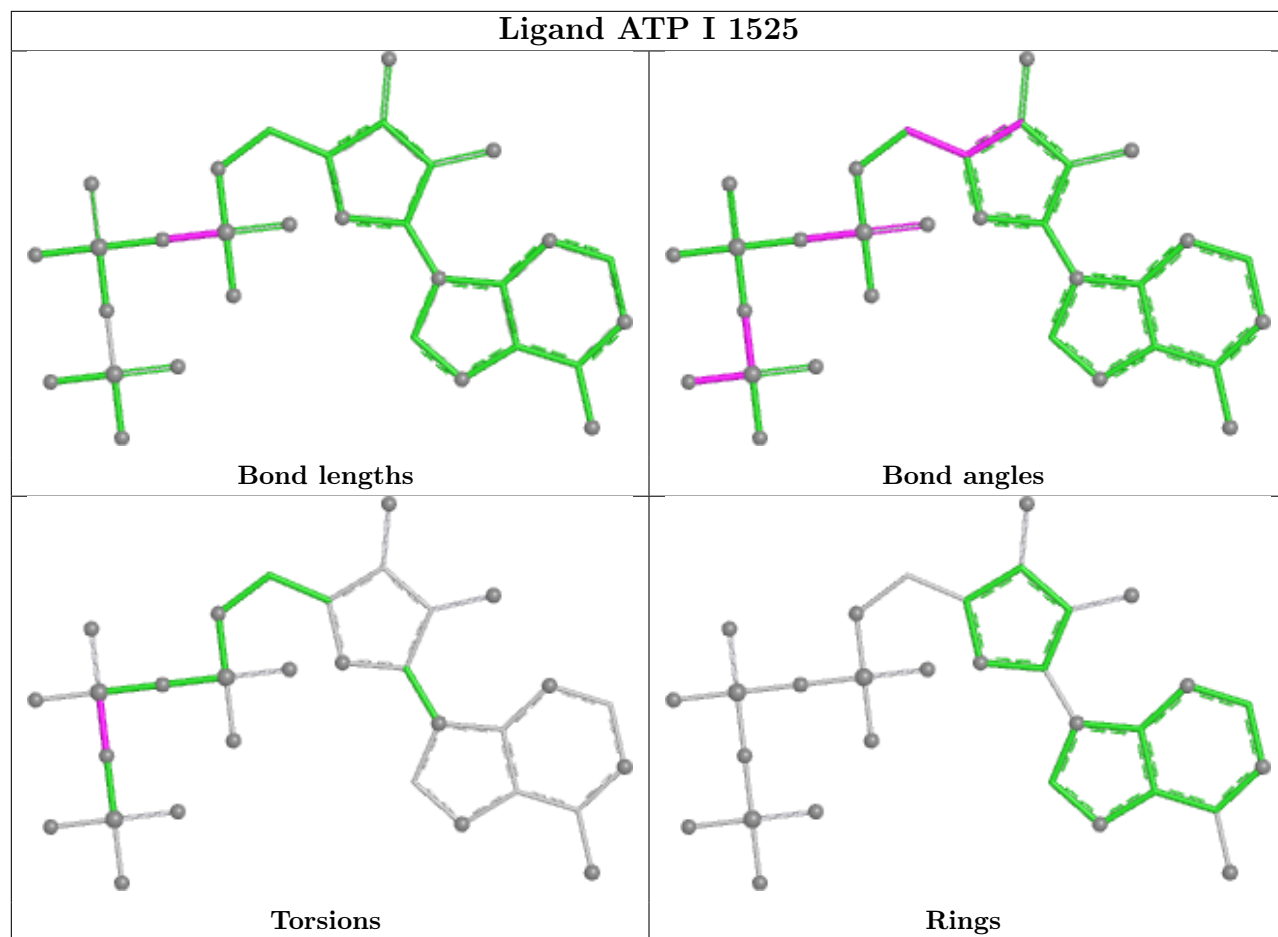


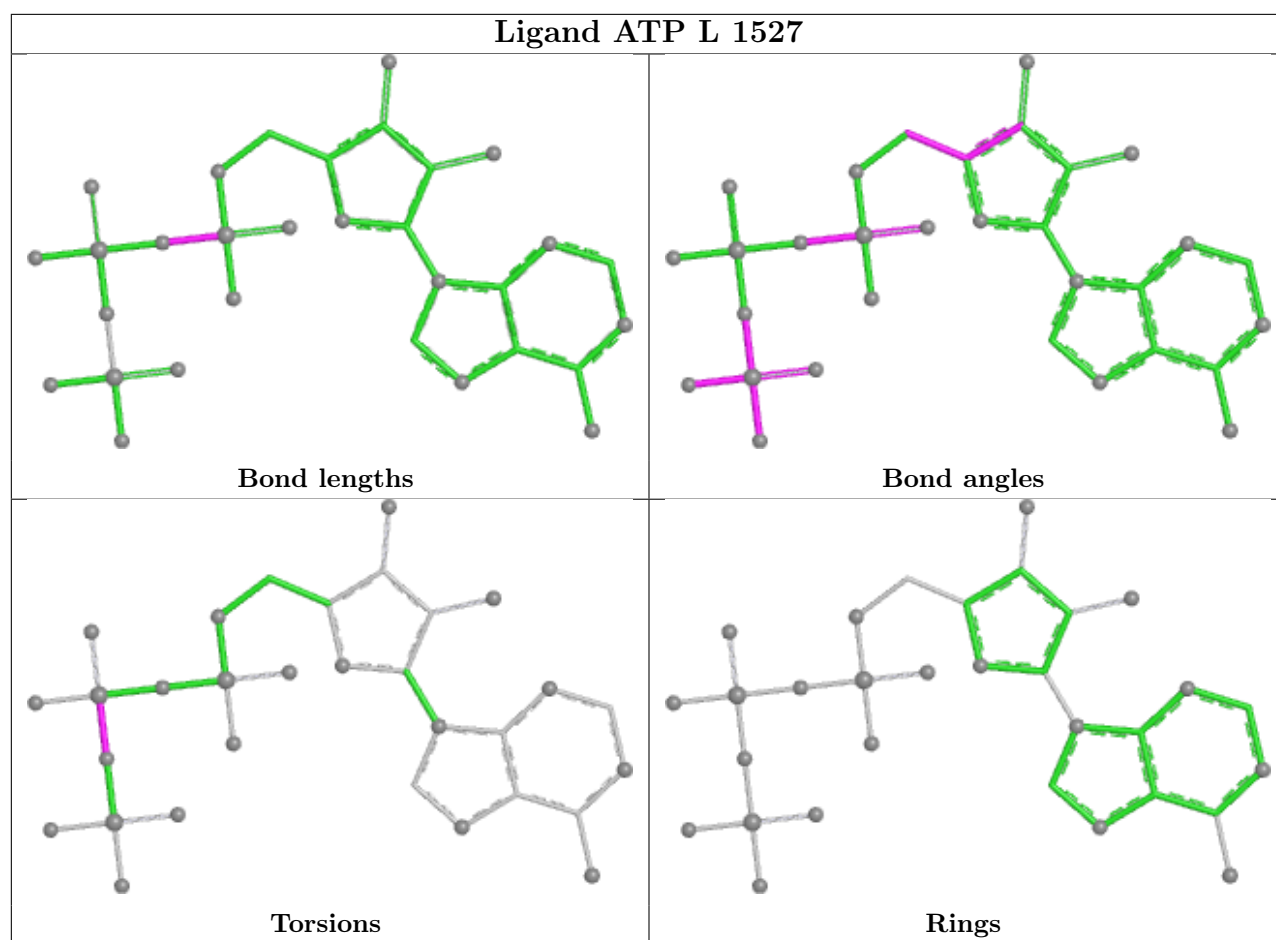












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2002. 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: 73



Y Index: 76

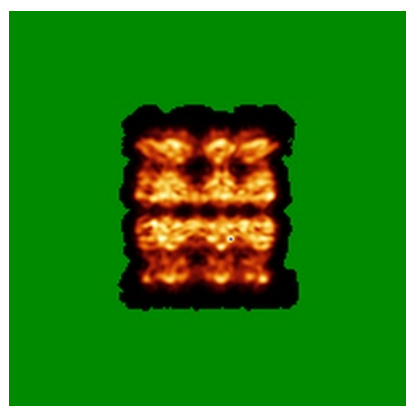


Z Index: 89

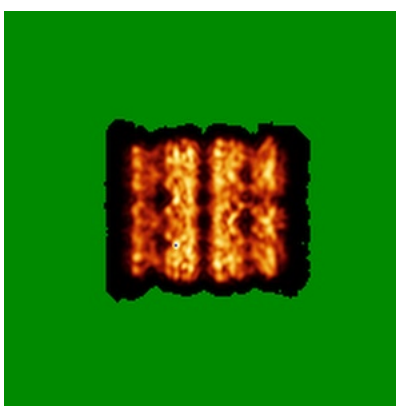
The images above show the largest variance slices of the map in three orthogonal directions.

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

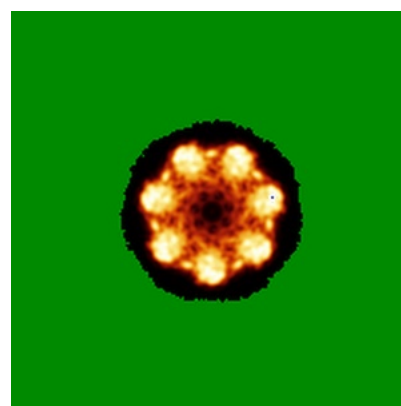
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

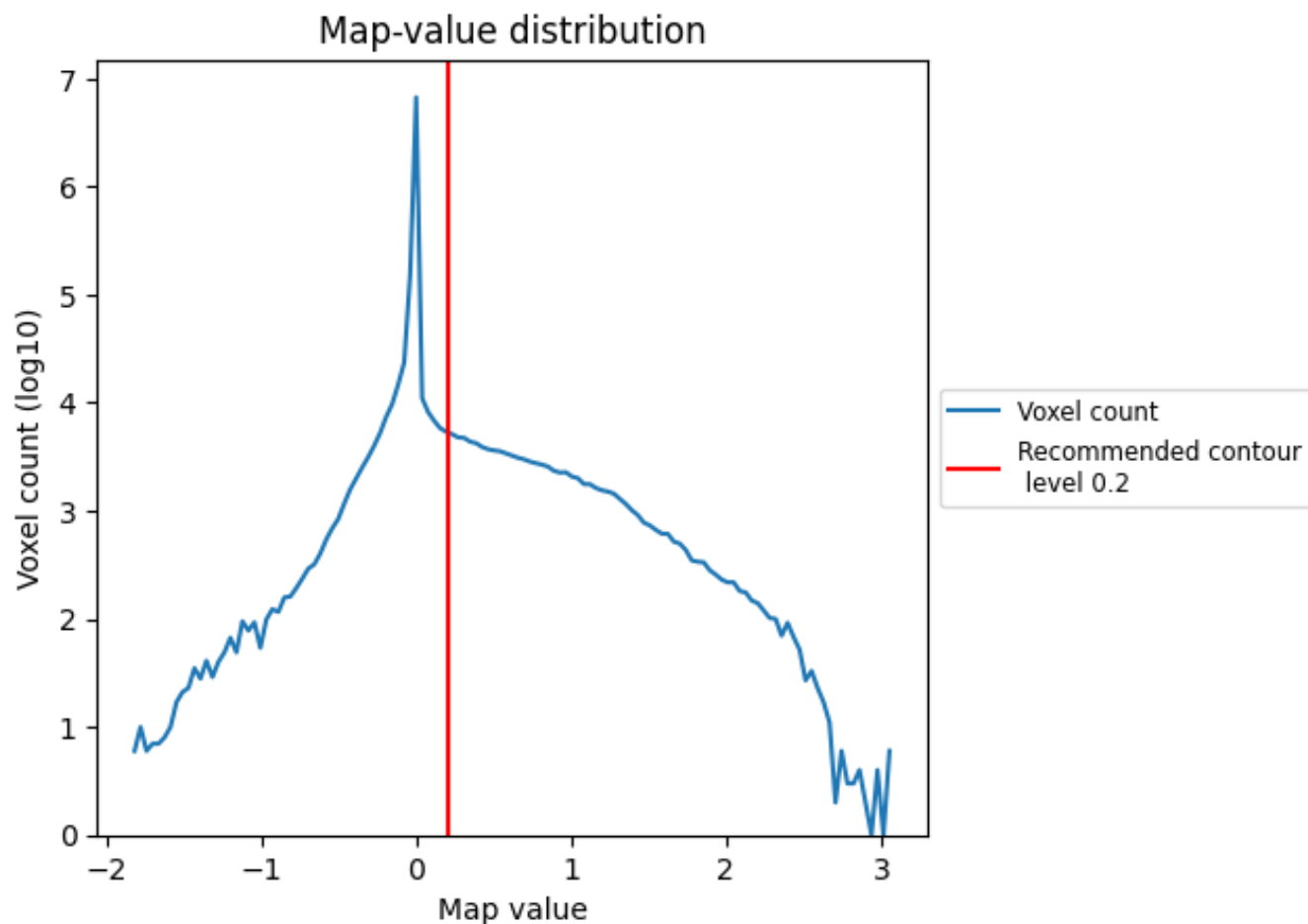
6.6 Mask visualisation

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

7 Map analysis [i](#)

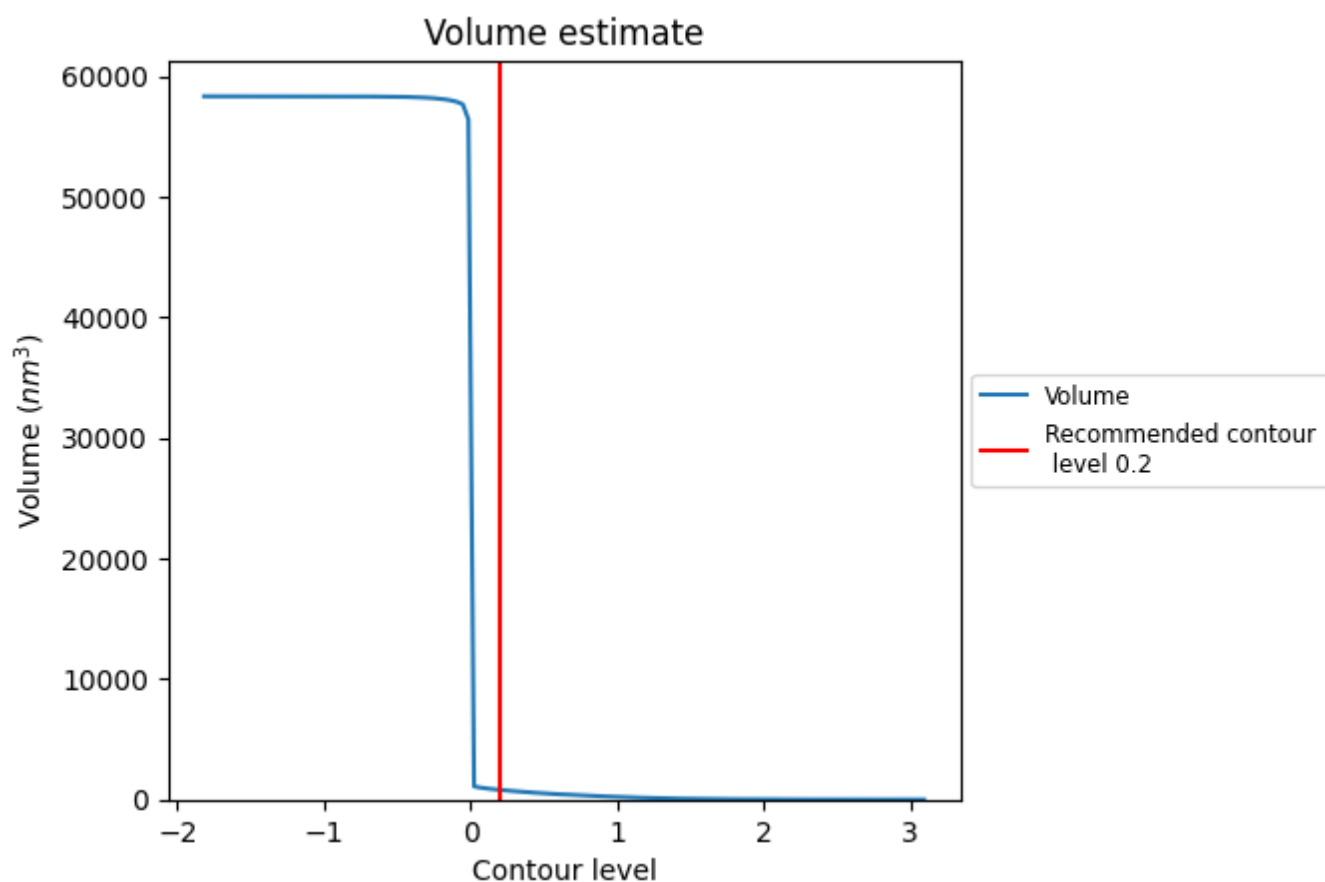
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

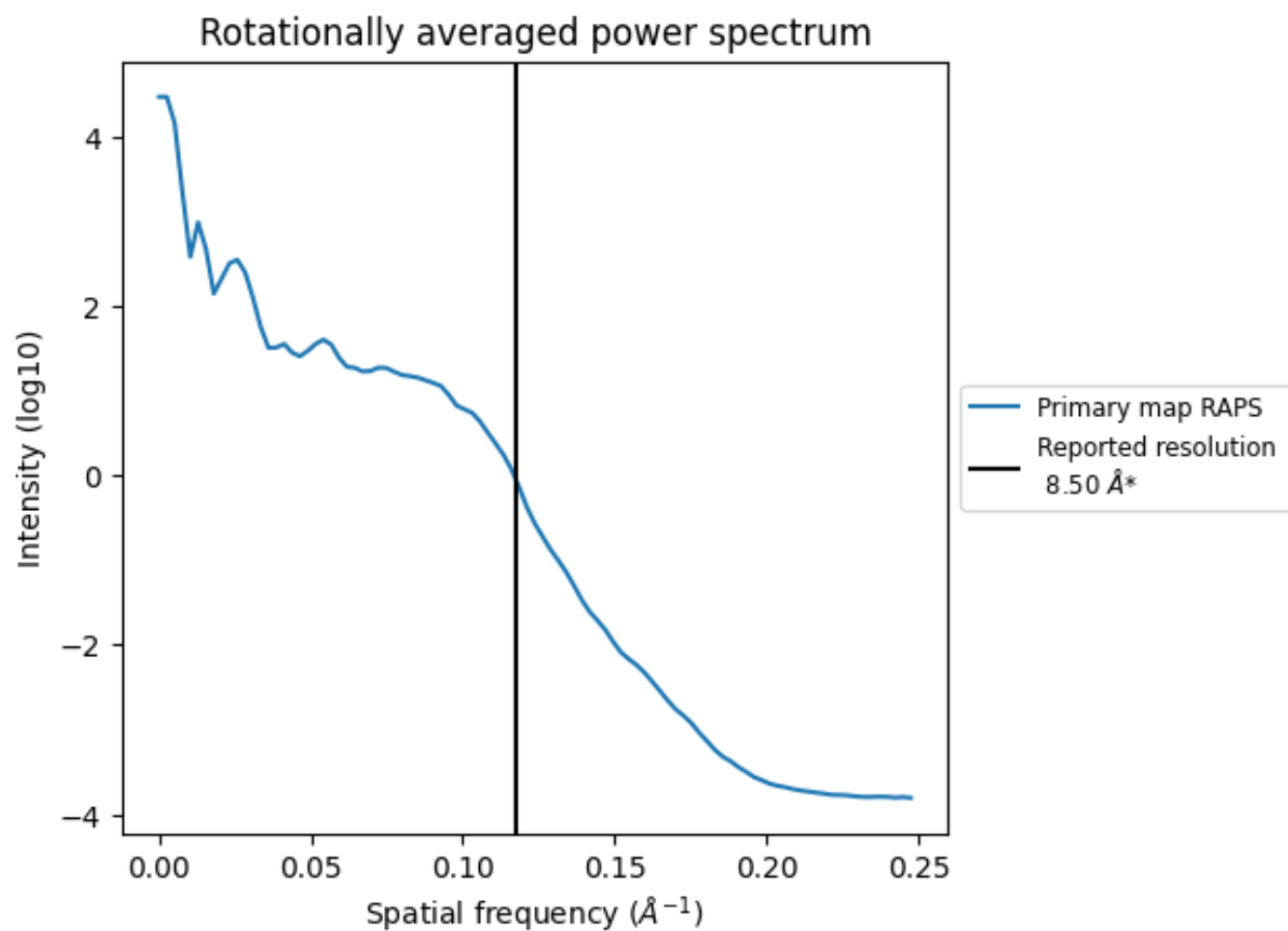
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 802 nm³; this corresponds to an approximate mass of 725 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

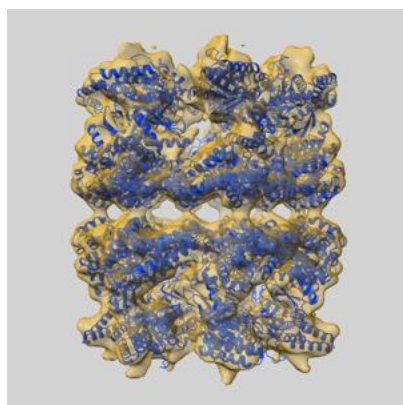
8 Fourier-Shell correlation

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

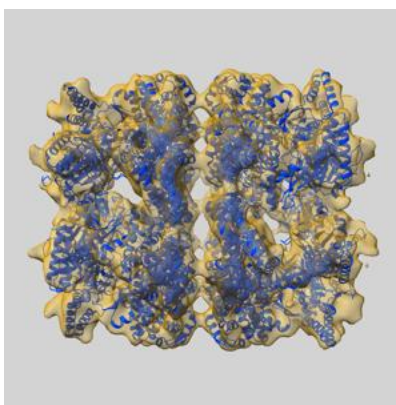
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2002 and PDB model 4AB2. Per-residue inclusion information can be found in section [3](#) on page [9](#).

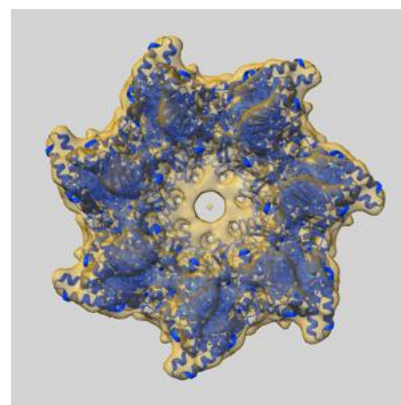
9.1 Map-model overlay [i](#)



X



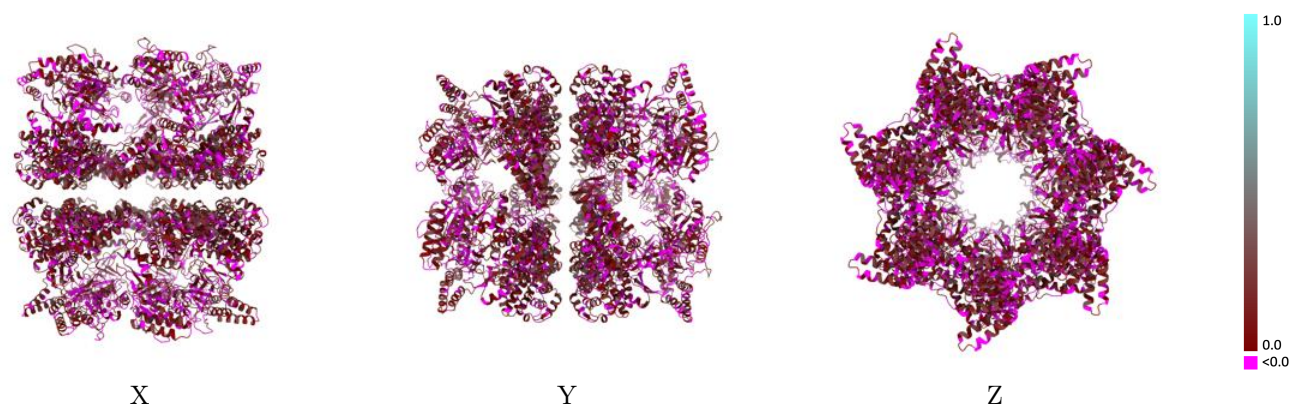
Y



Z

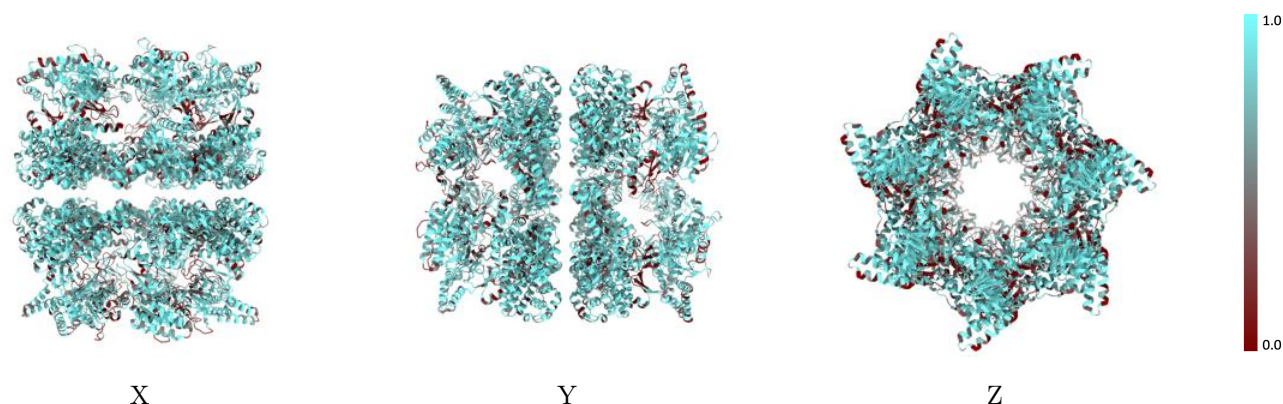
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



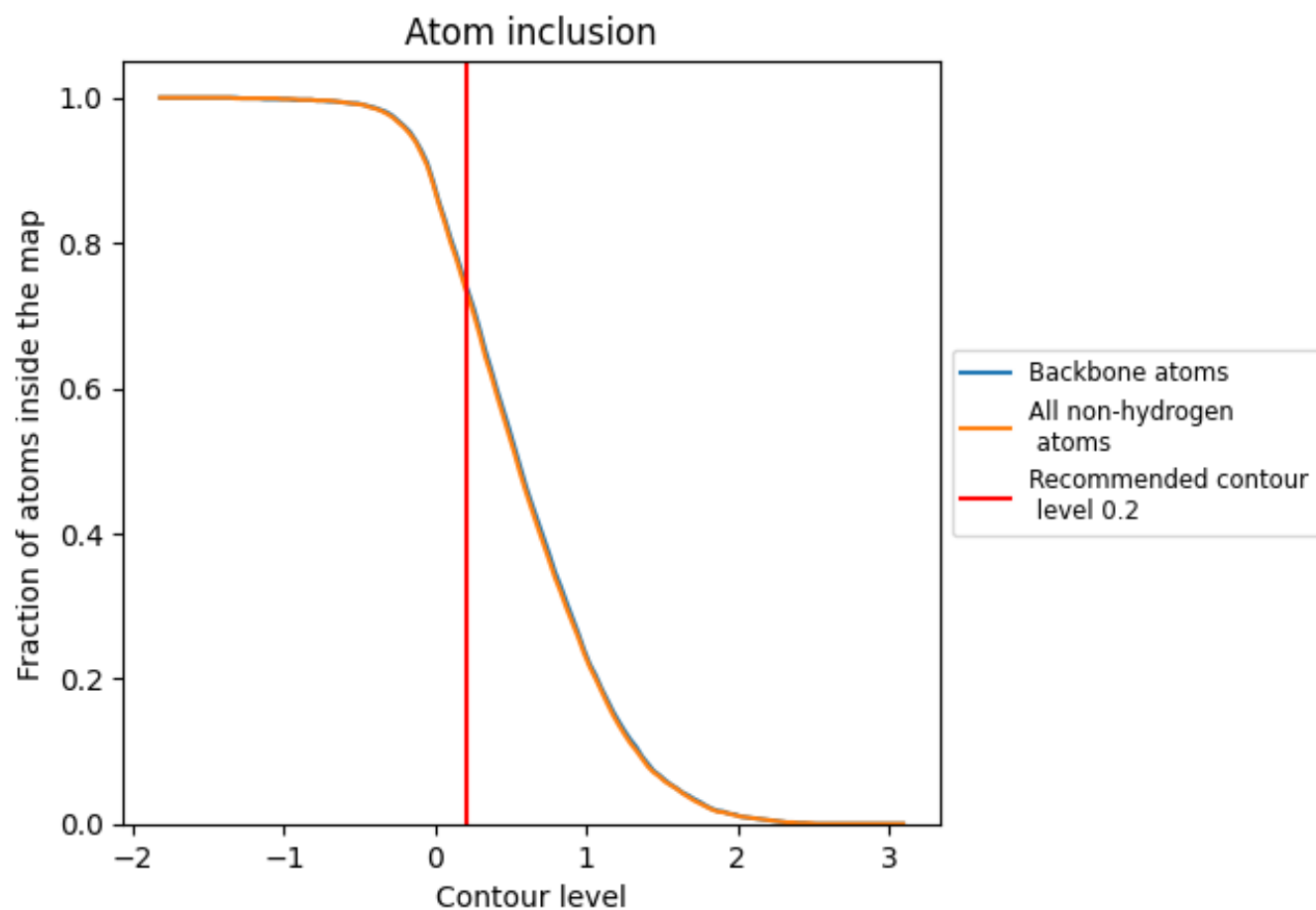
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 74% 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	0.7360	0.0760
A	0.7360	0.0790
B	0.7350	0.0780
C	0.7360	0.0780
D	0.7350	0.0780
E	0.7370	0.0780
F	0.7340	0.0770
G	0.7370	0.0780
H	0.7430	0.0760
I	0.7440	0.0750
J	0.7450	0.0760
K	0.7450	0.0750
L	0.7460	0.0730
M	0.7450	0.0730
N	0.7440	0.0750

