



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:33 PM UTC

PDB ID : 4UUK / pdb_00004uuk
EMDB ID : EMD-2701
Title : Human dynamin 1 K44A superconstricted polymer stabilized with GTP strand 2
Authors : Sundborger, A.C.; Fang, S.; Heymann, J.A.; Ray, P.; Chappie, J.S.; Hinshaw, J.E.
Deposited on : 2014-07-29
Resolution : 12.50 Å(reported)
Based on initial models : 3SNH, 1DYN, 3ZYC

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
MolProbity : 4-5-2 with Phenix2.0
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

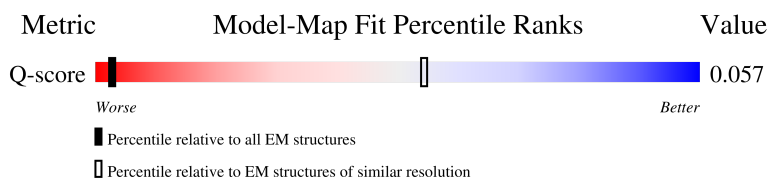
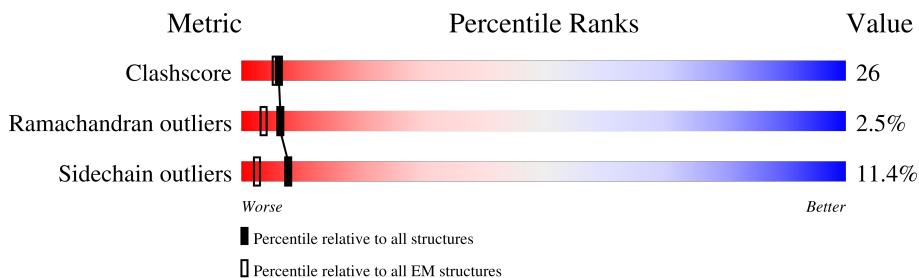
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.50 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	96 (12.00 - 13.00)

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	864	
1	D	864	
1	G	864	
1	K	864	

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Mol	Chain	Length	Quality of chain
2	B	864	8%7%6%.76%
2	C	864	6%5%..87%
2	E	864	7%9%5%.76%
2	F	864	6%5%..87%
2	H	864	6%5%..87%
2	I	864	8%8%5%.76%
2	J	864	7%9%5%.76%
2	L	864	6%5%..87%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 21116 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DYNAMIN-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	329	Total	C	N	O	S	0	0
			2567	1615	453	489	10		
1	D	337	Total	C	N	O	S	0	0
			2643	1664	466	503	10		
1	G	329	Total	C	N	O	S	0	0
			2567	1615	453	489	10		
1	K	337	Total	C	N	O	S	0	0
			2643	1664	466	503	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	744	ASN	ASP	variant	UNP Q05193
D	744	ASN	ASP	variant	UNP Q05193
G	744	ASN	ASP	variant	UNP Q05193
K	744	ASN	ASP	variant	UNP Q05193

- Molecule 2 is a protein called DYNAMIN-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	208	Total	C	N	O	S	0	0
			1728	1097	304	313	14		
2	C	113	Total	C	N	O	S	0	0
			946	609	158	175	4		
2	E	208	Total	C	N	O	S	0	0
			1728	1097	304	313	14		
2	F	113	Total	C	N	O	S	0	0
			946	609	158	175	4		
2	H	113	Total	C	N	O	S	0	0
			946	609	158	175	4		
2	I	208	Total	C	N	O	S	0	0
			1728	1097	304	313	14		
2	J	208	Total	C	N	O	S	0	0
			1728	1097	304	313	14		

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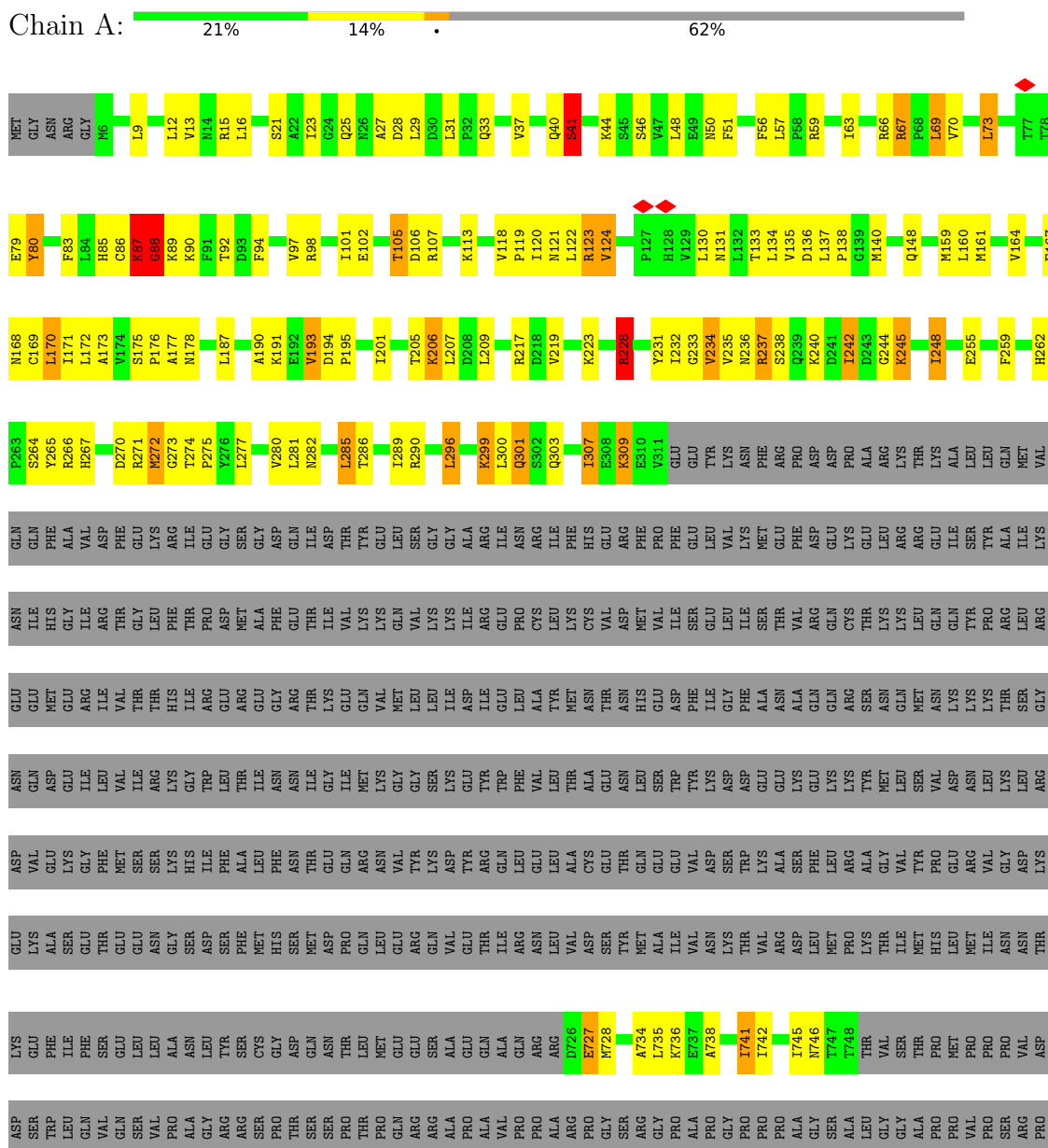
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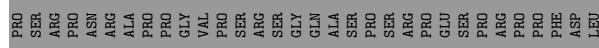
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	113	946	609	158	175	4	0	0

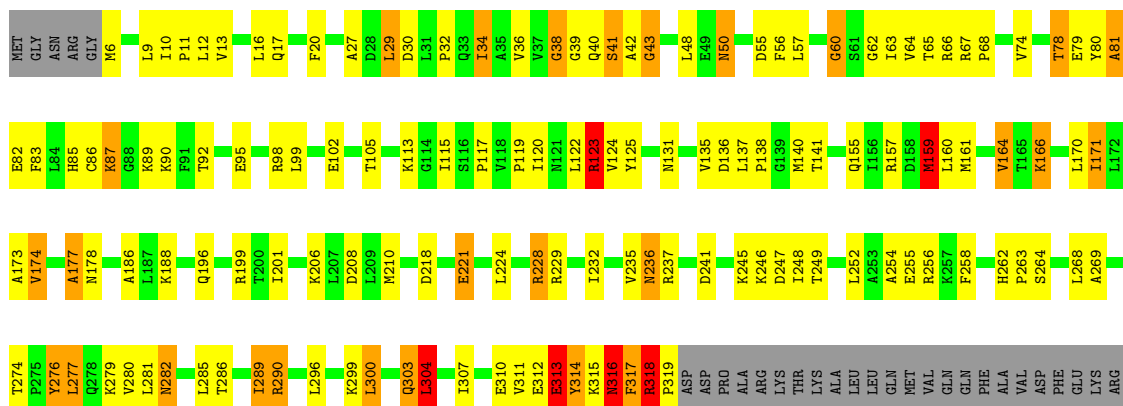
3 Residue-property plots

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: DYNAMIN-1









ASN	ASN	GLY	ASN	GLY	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN</
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GLY	ALA	PRO	PRO	PRO	VAL	PRO	SER	SER	ARG	GLY	ALA	SER	PRO	PRO	ASP	PHE	GLY	VAL	PRO	PRO	SER	SER	ARG	ARG	ARG	PRO	GLU	SER	GLY	GLN	ALA	SER	PRO	PRO	ARG	ARG	PRO	PRO	PHE	ASP	LEU
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Chain E: 76%

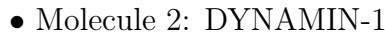
ASP
LEU

87%

- Molecule 2: DYNAMIN-1

87%

[illegible]



Chain J: 76%



ALA	GLY	SER	ALA	LEU	GLY	GLY	ALA	PRO	PRO	VAL	PRO	SER	ARG	PRO	GLY	ALA	SER	PRO	ASP	PRO	PHE	GLY	PRO	PRO	PRO	GLN	VAL	PRO	SER	ARG	PRO	ASN	ARG	ALA	PRO	PRO	GLY	VAL	PRO	SER	SER	GLY	GLN	ALA	SER	PRO	SER	ARG	PRO	GLU	SER	PRO	ARG	PRO	PHE	ASP	LEU
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4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	7525	Depositor
Resolution determination method	Not provided	
CTF correction method	INDIVIDUAL IMAGES	Depositor
Microscope	FEI/PHILIPS CM300FEG/HE	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	49000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	18.352	Depositor
Minimum map value	-18.065	Depositor
Average map value	0.361	Depositor
Map value standard deviation	3.624	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	510.0, 510.0, 510.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.55, 2.55, 2.55	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.06	6/2604 (0.2%)	1.76	88/3524 (2.5%)
1	D	1.26	14/2683 (0.5%)	2.06	112/3630 (3.1%)
1	G	1.06	7/2604 (0.3%)	1.76	88/3524 (2.5%)
1	K	1.26	14/2683 (0.5%)	2.06	112/3630 (3.1%)
2	B	1.86	31/1748 (1.8%)	3.16	156/2331 (6.7%)
2	C	1.20	11/966 (1.1%)	2.15	54/1298 (4.2%)
2	E	2.01	50/1748 (2.9%)	3.30	186/2331 (8.0%)
2	F	1.74	21/966 (2.2%)	2.60	80/1298 (6.2%)
2	H	1.20	11/966 (1.1%)	2.15	53/1298 (4.1%)
2	I	1.86	31/1748 (1.8%)	3.16	156/2331 (6.7%)
2	J	2.01	50/1748 (2.9%)	3.29	184/2331 (7.9%)
2	L	1.74	21/966 (2.2%)	2.60	80/1298 (6.2%)
All	All	1.51	267/21430 (1.2%)	2.50	1349/28824 (4.7%)

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	1	11
1	D	0	14
1	G	1	12
1	K	0	14
2	B	5	40
2	C	4	9
2	E	10	36
2	F	7	10
2	H	4	9
2	I	5	39
2	J	10	36
2	L	7	10
All	All	54	240

All (267) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	492	ASP	C-O	-22.46	0.95	1.24
2	B	492	ASP	C-O	-22.46	0.95	1.24
2	E	492	ASP	C-O	-22.01	0.96	1.24
2	J	492	ASP	C-O	-22.00	0.96	1.24
2	E	490	HIS	CG-CD2	-19.26	1.14	1.35
2	J	490	HIS	CG-CD2	-19.24	1.14	1.35
1	K	317	PHE	C-O	-17.77	1.03	1.23
1	D	317	PHE	C-O	-17.76	1.03	1.23
2	E	490	HIS	C-O	-17.61	1.01	1.24
2	J	490	HIS	C-O	-17.59	1.01	1.24
2	B	489	ASN	CA-C	-16.74	1.30	1.52
2	I	489	ASN	CA-C	-16.68	1.30	1.52
2	B	488	THR	C-O	-16.44	0.99	1.23
2	I	488	THR	C-O	-16.43	0.99	1.23
2	B	490	HIS	C-O	-16.24	0.91	1.23
2	I	490	HIS	C-O	-16.24	0.91	1.23
2	E	449	TYR	CA-CB	-15.72	1.28	1.53
2	J	449	TYR	CA-CB	-15.71	1.28	1.53
2	E	490	HIS	CA-C	-14.72	1.33	1.52
2	J	490	HIS	CA-C	-14.71	1.33	1.52
1	G	245	LYS	CA-CB	-14.08	1.32	1.53
1	A	245	LYS	CA-CB	-14.08	1.32	1.53
2	J	490	HIS	ND1-CE1	-13.93	1.18	1.32
2	E	490	HIS	ND1-CE1	-13.92	1.18	1.32
2	L	577	LYS	C-N	-13.78	1.23	1.33
2	F	577	LYS	C-N	-13.77	1.23	1.33
2	E	491	GLU	CA-CB	13.30	1.74	1.53
2	J	491	GLU	CA-CB	13.30	1.74	1.53
2	L	569	ASN	CA-CB	-12.91	1.35	1.53
2	F	569	ASN	CA-CB	-12.89	1.35	1.53
2	F	628	GLU	CA-C	-12.77	1.46	1.53
2	L	628	GLU	CA-C	-12.73	1.46	1.53
1	D	318	ARG	CB-CG	-12.38	1.15	1.52
1	K	318	ARG	CB-CG	-12.38	1.15	1.52
2	L	628	GLU	CA-CB	-12.25	1.34	1.53
2	F	628	GLU	CA-CB	-12.24	1.34	1.53
2	I	487	ASN	C-N	11.94	1.52	1.33
2	B	487	ASN	C-N	11.92	1.52	1.33
1	D	313	GLU	C-O	-11.52	1.09	1.24
1	K	313	GLU	C-O	-11.49	1.09	1.24
2	I	489	ASN	C-N	-11.38	1.17	1.33
2	E	491	GLU	CA-C	-11.37	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	491	GLU	CA-C	-11.37	1.39	1.52
2	B	489	ASN	C-N	-11.35	1.17	1.33
2	I	489	ASN	N-CA	-11.13	1.31	1.46
2	B	489	ASN	N-CA	-11.11	1.31	1.46
2	I	491	GLU	CA-C	-10.88	1.38	1.52
2	B	491	GLU	CA-C	-10.85	1.38	1.52
2	L	627	PRO	C-N	-10.48	1.24	1.33
1	D	318	ARG	N-CA	-10.48	1.31	1.46
1	K	318	ARG	N-CA	-10.46	1.31	1.46
2	B	699	SER	CB-OG	-10.44	1.21	1.42
2	J	442	CYS	N-CA	-10.40	1.33	1.46
2	I	699	SER	CB-OG	-10.39	1.21	1.42
2	E	442	CYS	N-CA	-10.39	1.33	1.46
2	F	627	PRO	C-N	-10.36	1.24	1.33
2	I	490	HIS	CA-C	-10.06	1.31	1.52
2	B	490	HIS	CA-C	-10.04	1.31	1.52
2	E	451	ARG	CA-C	-9.97	1.43	1.53
2	J	451	ARG	CA-C	-9.95	1.44	1.53
2	F	560	GLU	CA-C	-9.95	1.44	1.53
2	L	560	GLU	CA-C	-9.90	1.44	1.53
2	I	442	CYS	N-CA	-9.45	1.33	1.46
2	B	442	CYS	N-CA	-9.42	1.34	1.46
2	J	490	HIS	CG-ND1	-9.37	1.27	1.38
2	E	490	HIS	CG-ND1	-9.35	1.27	1.38
1	D	316	ASN	C-O	9.19	1.35	1.24
1	K	316	ASN	C-O	9.17	1.35	1.24
2	B	487	ASN	C-O	-9.01	1.12	1.24
2	I	487	ASN	C-O	-8.97	1.12	1.24
2	L	529	ASN	CA-CB	-8.80	1.39	1.53
2	F	529	ASN	CA-CB	-8.78	1.39	1.53
1	D	316	ASN	C-N	-8.60	1.18	1.33
1	K	316	ASN	C-N	-8.59	1.18	1.33
2	E	452	LEU	N-CA	-8.50	1.35	1.46
2	J	452	LEU	N-CA	-8.49	1.35	1.46
1	K	317	PHE	CA-C	-8.49	1.42	1.53
1	D	317	PHE	CA-C	-8.48	1.42	1.53
2	E	490	HIS	CE1-NE2	8.47	1.41	1.32
2	J	490	HIS	CE1-NE2	8.43	1.41	1.32
1	A	88	GLY	N-CA	-8.42	1.33	1.45
1	G	88	GLY	N-CA	-8.41	1.33	1.45
2	F	561	LYS	N-CA	-8.32	1.35	1.46
2	F	581	SER	N-CA	-8.27	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	581	SER	N-CA	-8.25	1.34	1.46
2	L	561	LYS	N-CA	-8.23	1.35	1.46
2	H	561	LYS	N-CA	-8.19	1.35	1.46
2	C	561	LYS	N-CA	-8.16	1.35	1.46
2	E	491	GLU	C-O	-7.96	1.13	1.23
2	J	491	GLU	C-O	-7.95	1.13	1.23
2	L	534	MET	N-CA	-7.93	1.35	1.46
2	F	534	MET	N-CA	-7.90	1.35	1.46
2	J	699	SER	CB-OG	-7.89	1.26	1.42
2	E	699	SER	CB-OG	-7.87	1.26	1.42
2	E	453	ARG	C-O	-7.86	1.14	1.24
2	J	453	ARG	C-O	-7.83	1.14	1.24
1	K	90	LYS	N-CA	-7.68	1.37	1.46
1	D	90	LYS	N-CA	-7.67	1.37	1.46
2	E	490	HIS	CD2-NE2	-7.65	1.29	1.37
2	J	490	HIS	CD2-NE2	-7.64	1.29	1.37
2	E	672	ILE	CB-CG1	-7.61	1.38	1.53
2	J	672	ILE	CB-CG1	-7.61	1.38	1.53
2	J	454	GLU	N-CA	-7.50	1.36	1.46
2	E	454	GLU	N-CA	-7.49	1.36	1.46
2	B	413	VAL	C-O	-7.46	1.15	1.24
2	I	413	VAL	C-O	-7.43	1.15	1.24
2	E	491	GLU	N-CA	-7.34	1.36	1.46
2	J	491	GLU	N-CA	-7.32	1.36	1.46
2	H	577	LYS	C-N	-7.32	1.24	1.32
2	C	577	LYS	C-N	-7.26	1.24	1.32
2	I	491	GLU	N-CA	-7.20	1.37	1.46
2	I	488	THR	CA-CB	7.18	1.63	1.53
2	B	491	GLU	N-CA	-7.17	1.37	1.46
2	B	488	THR	CA-CB	7.16	1.63	1.53
2	B	490	HIS	CG-ND1	-7.13	1.30	1.38
2	H	534	MET	N-CA	-7.01	1.37	1.46
2	C	534	MET	N-CA	-7.01	1.37	1.46
2	I	490	HIS	CG-ND1	-7.01	1.30	1.38
2	J	453	ARG	CA-C	-6.78	1.43	1.52
2	B	339	ASP	CA-CB	-6.78	1.42	1.53
2	I	339	ASP	CA-CB	-6.77	1.42	1.53
2	E	453	ARG	CA-C	-6.76	1.43	1.52
2	H	560	GLU	N-CA	-6.74	1.39	1.46
2	C	560	GLU	N-CA	-6.74	1.39	1.46
2	L	602	GLN	N-CA	-6.73	1.37	1.45
2	E	339	ASP	N-CA	-6.72	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	451	ARG	N-CA	-6.72	1.39	1.47
2	J	491	GLU	CB-CG	-6.71	1.32	1.52
2	F	602	GLN	N-CA	-6.71	1.37	1.45
2	E	451	ARG	N-CA	-6.70	1.39	1.47
2	E	491	GLU	CB-CG	-6.69	1.32	1.52
2	C	560	GLU	CA-C	-6.67	1.46	1.53
2	J	339	ASP	N-CA	-6.67	1.38	1.46
1	K	316	ASN	N-CA	-6.66	1.37	1.46
2	H	560	GLU	CA-C	-6.66	1.46	1.53
1	D	316	ASN	N-CA	-6.66	1.37	1.46
2	C	578	GLY	N-CA	-6.59	1.39	1.45
2	H	578	GLY	N-CA	-6.58	1.39	1.45
2	L	560	GLU	N-CA	-6.53	1.39	1.47
2	F	560	GLU	N-CA	-6.52	1.39	1.47
2	J	456	MET	CG-SD	-6.42	1.64	1.80
2	E	456	MET	CG-SD	-6.41	1.64	1.80
2	J	452	LEU	CA-CB	-6.37	1.42	1.53
2	E	452	LEU	CA-CB	-6.36	1.42	1.53
2	F	574	ASP	CA-C	-6.36	1.44	1.52
2	J	492	ASP	N-CA	-6.35	1.38	1.46
2	E	492	ASP	N-CA	-6.35	1.38	1.46
2	L	574	ASP	CA-C	-6.33	1.44	1.52
2	I	491	GLU	CA-CB	6.31	1.63	1.53
2	F	558	GLU	CA-CB	-6.29	1.44	1.53
2	F	574	ASP	N-CA	-6.28	1.38	1.46
2	L	558	GLU	CA-CB	-6.27	1.44	1.53
2	J	449	TYR	C-O	-6.26	1.16	1.24
2	L	574	ASP	N-CA	-6.26	1.38	1.46
2	B	491	GLU	CA-CB	6.25	1.63	1.53
2	E	449	TYR	C-O	-6.24	1.16	1.24
2	I	490	HIS	N-CA	-6.20	1.34	1.46
2	B	490	HIS	N-CA	-6.16	1.34	1.46
2	E	453	ARG	N-CA	-6.05	1.38	1.46
2	F	601	ARG	C-N	-6.05	1.26	1.33
2	B	342	LYS	N-CA	-6.04	1.38	1.46
2	I	342	LYS	N-CA	-6.03	1.38	1.46
2	F	575	VAL	N-CA	-6.02	1.38	1.46
2	L	575	VAL	N-CA	-6.01	1.38	1.46
2	J	453	ARG	N-CA	-6.01	1.38	1.46
2	H	564	MET	C-O	-6.00	1.16	1.24
2	L	601	ARG	C-N	-5.98	1.26	1.33
2	C	602	GLN	N-CA	-5.97	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	564	MET	C-O	-5.97	1.16	1.24
2	E	489	ASN	C-N	-5.97	1.25	1.33
2	J	449	TYR	C-N	5.96	1.47	1.33
2	E	449	TYR	C-N	5.96	1.47	1.33
2	E	492	ASP	CA-C	-5.95	1.44	1.52
2	J	492	ASP	CA-C	-5.94	1.44	1.52
2	I	488	THR	CB-OG1	-5.94	1.34	1.43
2	J	489	ASN	C-N	-5.93	1.25	1.33
2	H	602	GLN	N-CA	-5.92	1.38	1.45
2	B	679	ASP	C-N	-5.92	1.25	1.33
2	E	494	ILE	CA-CB	-5.91	1.48	1.54
2	B	488	THR	CB-OG1	-5.91	1.34	1.43
2	J	339	ASP	CA-CB	-5.90	1.44	1.53
2	J	705	LEU	N-CA	-5.90	1.39	1.46
2	I	679	ASP	C-N	-5.90	1.25	1.33
2	B	339	ASP	N-CA	-5.90	1.39	1.46
2	E	705	LEU	N-CA	-5.89	1.39	1.46
2	E	339	ASP	CA-CB	-5.89	1.44	1.53
2	I	339	ASP	N-CA	-5.89	1.39	1.46
2	J	494	ILE	CA-CB	-5.88	1.48	1.54
1	G	234	VAL	N-CA	-5.83	1.39	1.46
1	G	73	LEU	CA-CB	-5.83	1.45	1.53
2	J	450	PRO	CA-C	-5.83	1.44	1.52
2	E	450	PRO	CA-C	-5.82	1.44	1.52
1	A	234	VAL	N-CA	-5.78	1.39	1.46
2	J	699	SER	CA-C	-5.77	1.45	1.52
1	D	303	GLN	CA-CB	-5.76	1.44	1.53
2	E	699	SER	CA-C	-5.76	1.45	1.52
2	J	492	ASP	CG-OD1	-5.75	1.14	1.25
1	A	73	LEU	CA-CB	-5.75	1.45	1.53
1	K	303	GLN	CA-CB	-5.75	1.44	1.53
2	E	492	ASP	CG-OD1	-5.74	1.14	1.25
2	E	699	SER	N-CA	-5.73	1.40	1.46
2	J	699	SER	N-CA	-5.72	1.40	1.46
2	F	529	ASN	N-CA	-5.66	1.39	1.46
1	D	316	ASN	CG-ND2	-5.64	1.21	1.33
1	K	316	ASN	CG-ND2	-5.63	1.21	1.33
2	E	442	CYS	CA-CB	-5.63	1.44	1.53
2	J	451	ARG	C-O	-5.63	1.19	1.23
2	L	529	ASN	N-CA	-5.63	1.39	1.46
2	J	442	CYS	CA-CB	-5.62	1.44	1.53
1	D	317	PHE	N-CA	-5.62	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	317	PHE	N-CA	-5.62	1.38	1.46
2	L	580	MET	C-N	-5.62	1.26	1.33
2	E	451	ARG	C-O	-5.62	1.19	1.23
2	C	630	VAL	N-CA	-5.61	1.35	1.46
2	H	630	VAL	N-CA	-5.60	1.35	1.46
2	F	580	MET	C-N	-5.59	1.26	1.33
2	F	574	ASP	CA-CB	-5.56	1.44	1.53
2	L	574	ASP	CA-CB	-5.55	1.44	1.53
2	I	490	HIS	C-N	5.52	1.41	1.33
2	B	490	HIS	C-N	5.51	1.41	1.33
2	E	451	ARG	C-N	-5.47	1.26	1.33
2	I	469	GLY	N-CA	-5.45	1.38	1.45
2	C	584	HIS	CA-CB	-5.45	1.46	1.53
2	J	451	ARG	C-N	-5.45	1.26	1.33
2	C	601	ARG	C-N	-5.43	1.26	1.33
2	J	489	ASN	N-CA	5.43	1.53	1.46
2	H	584	HIS	CA-CB	-5.42	1.46	1.53
2	E	489	ASN	N-CA	5.42	1.53	1.46
2	B	469	GLY	N-CA	-5.42	1.38	1.45
2	H	601	ARG	C-N	-5.41	1.26	1.33
2	B	492	ASP	CA-C	-5.36	1.45	1.52
2	J	700	GLU	CB-CG	-5.35	1.36	1.52
2	E	700	GLU	CB-CG	-5.34	1.36	1.52
2	B	490	HIS	ND1-CE1	5.33	1.37	1.32
1	A	89	LYS	N-CA	-5.32	1.39	1.46
2	E	488	THR	N-CA	-5.31	1.39	1.46
2	I	492	ASP	CA-C	-5.30	1.45	1.52
1	G	87	LYS	CG-CD	-5.30	1.36	1.52
1	G	89	LYS	N-CA	-5.29	1.39	1.46
2	E	456	MET	CA-CB	-5.29	1.44	1.53
1	A	87	LYS	CG-CD	-5.28	1.36	1.52
2	J	456	MET	CA-CB	-5.26	1.44	1.53
2	J	488	THR	N-CA	-5.26	1.39	1.46
1	D	315	LYS	C-N	-5.24	1.26	1.33
1	K	315	LYS	C-N	-5.23	1.26	1.33
2	B	485	TYR	N-CA	5.21	1.52	1.46
2	F	564	MET	C-O	-5.21	1.18	1.23
2	I	490	HIS	ND1-CE1	5.21	1.37	1.32
2	I	485	TYR	N-CA	5.20	1.52	1.46
2	E	669	TYR	C-O	-5.17	1.18	1.24
2	J	669	TYR	C-O	-5.13	1.18	1.24
1	K	89	LYS	CA-C	-5.12	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	693	THR	C-O	-5.12	1.18	1.24
2	E	453	ARG	C-N	-5.11	1.26	1.33
2	L	564	MET	C-O	-5.11	1.18	1.23
1	D	89	LYS	CA-C	-5.10	1.46	1.52
2	J	452	LEU	CA-C	-5.09	1.46	1.52
2	I	344	ILE	CA-CB	-5.09	1.48	1.54
2	B	693	THR	C-O	-5.09	1.18	1.24
2	J	453	ARG	C-N	-5.09	1.26	1.33
2	E	452	LEU	CA-C	-5.08	1.46	1.52
2	I	693	THR	C-N	-5.06	1.27	1.33
2	J	449	TYR	CA-C	-5.05	1.46	1.52
2	B	693	THR	C-N	-5.03	1.27	1.33
2	E	449	TYR	CA-C	-5.03	1.46	1.52
2	B	344	ILE	CA-CB	-5.01	1.48	1.54
1	G	293	LEU	C-O	-5.01	1.20	1.24

All (1349) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	489	ASN	O-C-N	-36.81	73.63	122.59
2	I	489	ASN	O-C-N	-36.79	73.66	122.59
2	J	490	HIS	ND1-CG-CD2	-31.84	74.26	106.10
2	E	490	HIS	ND1-CG-CD2	-31.83	74.27	106.10
2	E	491	GLU	O-C-N	-29.54	83.49	122.19
2	J	491	GLU	O-C-N	-29.53	83.50	122.19
2	I	489	ASN	CA-C-N	28.41	172.83	121.70
2	I	489	ASN	C-N-CA	28.41	172.83	121.70
2	B	489	ASN	CA-C-N	28.40	172.83	121.70
2	B	489	ASN	C-N-CA	28.40	172.83	121.70
2	B	488	THR	CA-C-N	27.93	174.88	121.54
2	B	488	THR	C-N-CA	27.93	174.88	121.54
2	I	488	THR	CA-C-N	27.90	174.83	121.54
2	I	488	THR	C-N-CA	27.90	174.83	121.54
2	E	491	GLU	N-CA-C	27.42	149.15	112.68
2	J	491	GLU	N-CA-C	27.40	149.13	112.68
2	B	490	HIS	ND1-CE1-NE2	-27.36	81.04	108.40
2	I	490	HIS	ND1-CE1-NE2	-27.34	81.06	108.40
2	L	569	ASN	CA-CB-CG	26.04	138.64	112.60
2	F	569	ASN	CA-CB-CG	26.03	138.63	112.60
2	J	449	TYR	CA-CB-CG	25.87	160.47	113.90
2	E	449	TYR	CA-CB-CG	25.85	160.43	113.90
2	E	490	HIS	ND1-CE1-NE2	-25.08	83.32	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	490	HIS	ND1-CE1-NE2	-25.08	83.32	108.40
1	K	317	PHE	O-C-N	-22.98	93.14	123.01
1	D	317	PHE	O-C-N	-22.97	93.15	123.01
2	E	490	HIS	CG-CD2-NE2	22.79	129.99	107.20
2	J	490	HIS	CG-CD2-NE2	22.76	129.96	107.20
2	I	491	GLU	N-CA-C	22.06	138.31	111.40
2	B	491	GLU	N-CA-C	22.05	138.30	111.40
2	H	577	LYS	CA-C-N	21.20	139.88	121.86
2	H	577	LYS	C-N-CA	21.20	139.88	121.86
2	C	577	LYS	CA-C-N	21.16	139.85	121.86
2	C	577	LYS	C-N-CA	21.16	139.85	121.86
2	I	491	GLU	O-C-N	-21.01	96.75	122.17
2	B	491	GLU	O-C-N	-20.95	96.82	122.17
2	J	492	ASP	O-C-N	-20.81	94.91	122.59
2	E	492	ASP	O-C-N	-20.80	94.93	122.59
2	J	490	HIS	CG-ND1-CE1	20.45	144.07	109.30
2	E	490	HIS	CG-ND1-CE1	20.44	144.04	109.30
2	B	492	ASP	O-C-N	-20.29	95.60	122.59
2	I	492	ASP	O-C-N	-20.21	95.71	122.59
2	B	488	THR	CA-C-O	-19.58	97.42	120.53
2	I	488	THR	CA-C-O	-19.58	97.43	120.53
2	J	362	ILE	N-CA-C	-18.98	93.47	110.74
2	E	362	ILE	N-CA-C	-18.96	93.48	110.74
2	E	338	VAL	CA-C-N	18.83	144.93	120.44
2	E	338	VAL	C-N-CA	18.83	144.93	120.44
2	B	362	ILE	N-CA-C	-18.60	93.81	110.74
2	I	362	ILE	N-CA-C	-18.56	93.85	110.74
1	K	316	ASN	CB-CG-ND2	-18.32	88.91	116.40
1	D	316	ASN	CB-CG-ND2	-18.30	88.95	116.40
2	J	699	SER	N-CA-C	18.24	135.41	114.62
2	E	699	SER	N-CA-C	18.23	135.41	114.62
2	J	338	VAL	CA-C-N	18.09	144.96	120.54
2	J	338	VAL	C-N-CA	18.09	144.96	120.54
2	B	338	VAL	CA-C-N	17.44	144.09	120.54
2	B	338	VAL	C-N-CA	17.44	144.09	120.54
2	I	338	VAL	CA-C-N	17.41	144.04	120.54
2	I	338	VAL	C-N-CA	17.41	144.04	120.54
2	E	441	GLN	CA-C-N	17.36	149.68	122.60
2	E	441	GLN	C-N-CA	17.36	149.68	122.60
2	J	441	GLN	CA-C-N	17.34	149.66	122.60
2	J	441	GLN	C-N-CA	17.34	149.66	122.60
2	E	672	ILE	CB-CG1-CD1	16.95	149.40	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	672	ILE	CB-CG1-CD1	16.95	149.39	113.80
2	B	699	SER	N-CA-C	16.79	134.59	113.43
2	I	699	SER	N-CA-C	16.77	134.56	113.43
2	E	451	ARG	O-C-N	-16.76	104.28	122.38
2	J	451	ARG	O-C-N	-16.74	104.30	122.38
2	E	490	HIS	CB-CG-ND1	16.68	147.72	122.70
2	J	490	HIS	CB-CG-ND1	16.68	147.72	122.70
2	J	449	TYR	CB-CA-C	16.25	142.19	110.17
2	E	449	TYR	CB-CA-C	16.24	142.17	110.17
2	J	491	GLU	CA-C-N	15.80	151.72	121.54
2	J	491	GLU	C-N-CA	15.80	151.72	121.54
2	E	491	GLU	CA-C-N	15.80	151.71	121.54
2	E	491	GLU	C-N-CA	15.80	151.71	121.54
1	D	313	GLU	O-C-N	-15.61	100.91	122.46
1	K	313	GLU	O-C-N	-15.60	100.93	122.46
2	F	529	ASN	CA-CB-CG	15.55	128.15	112.60
2	L	529	ASN	CA-CB-CG	15.54	128.14	112.60
1	K	316	ASN	CB-CG-OD1	15.42	151.65	120.80
1	D	316	ASN	CB-CG-OD1	15.41	151.62	120.80
2	I	491	GLU	CA-C-N	15.36	150.87	121.54
2	I	491	GLU	C-N-CA	15.36	150.87	121.54
2	B	491	GLU	CA-C-N	15.32	150.81	121.54
2	B	491	GLU	C-N-CA	15.32	150.81	121.54
2	F	580	MET	CA-C-N	15.13	148.95	122.32
2	F	580	MET	C-N-CA	15.13	148.95	122.32
2	L	580	MET	CA-C-N	15.12	148.93	122.32
2	L	580	MET	C-N-CA	15.12	148.93	122.32
1	K	316	ASN	CA-C-N	14.85	145.11	123.14
1	K	316	ASN	C-N-CA	14.85	145.11	123.14
1	D	316	ASN	CA-C-N	14.83	145.09	123.14
1	D	316	ASN	C-N-CA	14.83	145.09	123.14
2	J	449	TYR	O-C-N	-14.59	104.54	121.32
2	E	449	TYR	O-C-N	-14.56	104.58	121.32
1	D	317	PHE	CA-C-N	14.47	157.12	121.80
1	D	317	PHE	C-N-CA	14.47	157.12	121.80
1	K	317	PHE	CA-C-N	14.46	157.08	121.80
1	K	317	PHE	C-N-CA	14.46	157.08	121.80
2	I	441	GLN	CA-C-N	14.38	149.01	121.54
2	I	441	GLN	C-N-CA	14.38	149.01	121.54
2	B	441	GLN	CA-C-N	14.36	148.97	121.54
2	B	441	GLN	C-N-CA	14.36	148.97	121.54
2	E	339	ASP	N-CA-CB	14.34	130.81	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	451	ARG	CA-C-N	14.24	148.73	121.54
2	E	451	ARG	C-N-CA	14.24	148.73	121.54
2	J	451	ARG	CA-C-N	14.22	148.70	121.54
2	J	451	ARG	C-N-CA	14.22	148.70	121.54
2	J	339	ASP	N-CA-CB	14.00	130.80	109.94
1	K	314	TYR	O-C-N	-13.86	107.43	122.12
2	I	339	ASP	N-CA-CB	13.84	130.56	109.94
1	D	314	TYR	O-C-N	-13.84	107.45	122.12
2	B	339	ASP	N-CA-CB	13.84	130.55	109.94
2	E	492	ASP	CA-C-N	13.81	146.11	120.97
2	E	492	ASP	C-N-CA	13.81	146.11	120.97
2	J	492	ASP	CA-C-N	13.80	146.09	120.97
2	J	492	ASP	C-N-CA	13.80	146.09	120.97
2	I	492	ASP	CB-CG-OD2	13.34	149.09	118.40
2	B	492	ASP	CB-CG-OD2	13.34	149.07	118.40
2	C	629	ARG	CA-C-N	13.27	145.58	121.70
2	C	629	ARG	C-N-CA	13.27	145.58	121.70
2	H	629	ARG	CA-C-N	13.25	145.55	121.70
2	H	629	ARG	C-N-CA	13.25	145.55	121.70
1	D	317	PHE	N-CA-C	13.13	133.49	107.62
1	K	317	PHE	N-CA-C	13.12	133.47	107.62
2	B	490	HIS	N-CA-CB	12.97	132.55	110.50
2	I	490	HIS	N-CA-CB	12.97	132.55	110.50
2	J	453	ARG	O-C-N	-12.96	105.35	122.59
2	E	453	ARG	O-C-N	-12.95	105.37	122.59
2	E	494	ILE	CA-C-O	-12.90	109.33	121.97
2	J	494	ILE	CA-C-O	-12.88	109.35	121.97
2	I	490	HIS	ND1-CG-CD2	-12.87	93.23	106.10
2	B	490	HIS	ND1-CG-CD2	-12.81	93.29	106.10
2	J	492	ASP	CB-CG-OD2	12.77	147.76	118.40
2	E	492	ASP	CB-CG-OD2	12.76	147.75	118.40
2	I	488	THR	O-C-N	-12.73	105.13	122.19
2	B	488	THR	O-C-N	-12.70	105.17	122.19
1	K	318	ARG	CB-CG-CD	12.68	140.46	111.30
2	J	491	GLU	CB-CA-C	-12.66	89.09	110.24
2	E	491	GLU	CB-CA-C	-12.66	89.10	110.24
1	D	318	ARG	CB-CG-CD	12.66	140.41	111.30
2	E	339	ASP	O-C-N	-12.33	109.37	122.07
2	B	441	GLN	O-C-N	-12.27	108.16	122.15
2	I	441	GLN	O-C-N	-12.26	108.17	122.15
1	K	316	ASN	CA-C-O	-12.26	102.98	120.51
1	D	316	ASN	CA-C-O	-12.26	102.98	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	339	ASP	O-C-N	-12.21	109.39	122.09
1	D	318	ARG	CA-C-O	-12.11	103.56	120.16
1	K	318	ARG	CA-C-O	-12.09	103.60	120.16
2	B	489	ASN	N-CA-C	12.02	136.41	110.80
2	I	489	ASN	N-CA-C	11.99	136.34	110.80
2	L	569	ASN	OD1-CG-ND2	-11.63	110.97	122.60
2	F	569	ASN	OD1-CG-ND2	-11.62	110.98	122.60
2	J	454	GLU	N-CA-CB	11.60	130.09	110.49
2	E	454	GLU	N-CA-CB	11.59	130.08	110.49
2	I	488	THR	N-CA-C	11.58	127.54	111.56
2	B	488	THR	N-CA-C	11.57	127.52	111.56
2	H	559	LYS	CA-C-N	11.55	138.21	120.89
2	H	559	LYS	C-N-CA	11.55	138.21	120.89
2	C	559	LYS	CA-C-N	11.54	138.20	120.89
2	C	559	LYS	C-N-CA	11.54	138.20	120.89
2	B	492	ASP	OD1-CG-OD2	-11.36	95.63	122.90
2	I	492	ASP	OD1-CG-OD2	-11.36	95.63	122.90
1	A	228	ARG	CB-CG-CD	11.34	137.38	111.30
1	G	228	ARG	CB-CG-CD	11.32	137.34	111.30
2	L	628	GLU	CB-CA-C	11.29	133.33	117.07
2	F	628	GLU	CB-CA-C	11.26	133.28	117.07
2	J	340	PHE	N-CA-C	11.19	124.80	111.82
2	E	340	PHE	N-CA-C	11.17	124.78	111.82
2	B	467	ARG	NE-CZ-NH2	11.07	129.16	119.20
2	I	467	ARG	NE-CZ-NH2	11.05	129.15	119.20
2	L	628	GLU	N-CA-C	11.00	117.80	108.78
2	F	628	GLU	N-CA-C	10.99	117.79	108.78
2	F	581	SER	N-CA-CB	10.79	127.80	110.97
2	L	581	SER	N-CA-CB	10.79	127.80	110.97
1	D	314	TYR	CA-C-O	10.73	132.22	120.63
1	K	314	TYR	CA-C-O	10.73	132.22	120.63
2	F	601	ARG	CA-C-N	10.71	140.81	121.85
2	F	601	ARG	C-N-CA	10.71	140.81	121.85
2	L	601	ARG	CA-C-N	10.70	140.78	121.85
2	L	601	ARG	C-N-CA	10.70	140.78	121.85
2	F	569	ASN	CB-CG-ND2	-10.53	100.61	116.40
2	L	569	ASN	CB-CG-ND2	-10.52	100.62	116.40
1	A	245	LYS	CB-CA-C	10.49	126.63	111.73
1	G	245	LYS	CB-CA-C	10.48	126.61	111.73
2	E	490	HIS	CE1-NE2-CD2	-10.47	98.53	109.00
2	J	490	HIS	CE1-NE2-CD2	-10.46	98.54	109.00
2	B	339	ASP	CA-CB-CG	10.41	123.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	339	ASP	CA-CB-CG	10.37	122.97	112.60
2	L	559	LYS	CA-C-N	10.36	136.10	121.71
2	L	559	LYS	C-N-CA	10.36	136.10	121.71
2	I	490	HIS	O-C-N	-10.34	106.46	123.00
2	F	559	LYS	CA-C-N	10.33	136.07	121.71
2	F	559	LYS	C-N-CA	10.33	136.07	121.71
2	B	490	HIS	O-C-N	-10.31	106.51	123.00
2	F	528	ILE	CA-C-N	10.13	133.86	120.28
2	F	528	ILE	C-N-CA	10.13	133.86	120.28
2	L	528	ILE	CA-C-N	10.12	133.84	120.28
2	L	528	ILE	C-N-CA	10.12	133.84	120.28
2	F	573	ARG	CA-C-N	10.12	140.87	121.54
2	F	573	ARG	C-N-CA	10.12	140.87	121.54
2	F	560	GLU	CA-C-N	10.11	140.85	121.54
2	F	560	GLU	C-N-CA	10.11	140.85	121.54
2	J	491	GLU	CA-C-O	10.11	134.28	120.13
2	E	491	GLU	CA-C-O	10.10	134.28	120.13
2	L	573	ARG	CA-C-N	10.10	140.83	121.54
2	L	573	ARG	C-N-CA	10.10	140.83	121.54
2	L	560	GLU	CA-C-N	10.08	140.80	121.54
2	L	560	GLU	C-N-CA	10.08	140.80	121.54
2	E	448	GLN	O-C-N	-9.95	107.07	123.00
2	J	448	GLN	O-C-N	-9.94	107.09	123.00
2	H	560	GLU	CA-C-N	9.94	140.52	121.54
2	H	560	GLU	C-N-CA	9.94	140.52	121.54
2	C	560	GLU	CA-C-N	9.94	140.52	121.54
2	C	560	GLU	C-N-CA	9.94	140.52	121.54
2	L	577	LYS	CA-C-N	9.89	132.81	122.63
2	L	577	LYS	C-N-CA	9.89	132.81	122.63
2	F	577	LYS	CA-C-N	9.88	132.81	122.63
2	F	577	LYS	C-N-CA	9.88	132.81	122.63
2	E	452	LEU	N-CA-C	9.84	131.76	110.80
2	J	452	LEU	N-CA-C	9.84	131.77	110.80
2	I	340	PHE	N-CA-C	9.82	125.06	112.89
2	B	340	PHE	N-CA-C	9.80	125.04	112.89
2	E	492	ASP	OD1-CG-OD2	-9.74	99.52	122.90
2	J	492	ASP	OD1-CG-OD2	-9.74	99.53	122.90
2	J	492	ASP	N-CA-CB	9.71	126.90	110.49
2	E	492	ASP	N-CA-CB	9.70	126.89	110.49
1	G	87	LYS	CG-CD-CE	9.68	133.56	111.30
1	D	303	GLN	CA-CB-CG	9.67	133.45	114.10
1	K	303	GLN	CA-CB-CG	9.67	133.44	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	LYS	CG-CD-CE	9.66	133.53	111.30
2	L	533	ILE	CA-C-N	9.54	139.77	121.54
2	L	533	ILE	C-N-CA	9.54	139.77	121.54
1	A	87	LYS	CA-C-N	9.54	140.11	121.41
1	A	87	LYS	C-N-CA	9.54	140.11	121.41
2	F	533	ILE	CA-C-N	9.54	139.76	121.54
2	F	533	ILE	C-N-CA	9.54	139.76	121.54
1	G	87	LYS	CA-C-N	9.53	140.09	121.41
1	G	87	LYS	C-N-CA	9.53	140.09	121.41
2	E	457	GLU	CA-C-N	9.44	133.31	120.38
2	E	457	GLU	C-N-CA	9.44	133.31	120.38
2	J	457	GLU	CA-C-N	9.44	133.31	120.38
2	J	457	GLU	C-N-CA	9.44	133.31	120.38
2	B	346	GLY	CA-C-O	9.43	140.61	120.80
2	I	346	GLY	CA-C-O	9.43	140.61	120.80
1	G	73	LEU	N-CA-CB	9.41	125.21	109.87
1	A	73	LEU	N-CA-CB	9.39	125.18	109.87
2	E	456	MET	CA-CB-CG	9.38	132.85	114.10
2	J	456	MET	CA-CB-CG	9.37	132.83	114.10
1	G	245	LYS	CA-CB-CG	9.36	132.82	114.10
1	A	245	LYS	CA-CB-CG	9.36	132.81	114.10
2	I	679	ASP	CA-C-N	9.35	133.56	120.29
2	I	679	ASP	C-N-CA	9.35	133.56	120.29
2	J	491	GLU	CB-CG-CD	9.34	128.47	112.60
2	B	679	ASP	CA-C-N	9.34	133.55	120.29
2	B	679	ASP	C-N-CA	9.34	133.55	120.29
2	E	450	PRO	O-C-N	-9.33	110.05	122.64
2	E	491	GLU	CB-CG-CD	9.33	128.46	112.60
2	L	581	SER	CA-CB-OG	-9.33	92.44	111.10
2	F	581	SER	CA-CB-OG	-9.33	92.45	111.10
2	J	450	PRO	O-C-N	-9.31	110.07	122.64
2	C	600	TYR	N-CA-C	9.31	125.58	114.04
2	B	339	ASP	O-C-N	-9.31	112.41	122.09
2	I	339	ASP	O-C-N	-9.30	112.41	122.09
2	E	493	PHE	CA-C-N	9.30	134.82	120.13
2	E	493	PHE	C-N-CA	9.30	134.82	120.13
2	H	600	TYR	N-CA-C	9.30	125.57	114.04
2	J	493	PHE	CA-C-N	9.29	134.82	120.13
2	J	493	PHE	C-N-CA	9.29	134.82	120.13
2	E	341	GLU	N-CA-C	-9.27	100.74	111.03
2	J	341	GLU	N-CA-C	-9.27	100.74	111.03
2	J	705	LEU	N-CA-CB	9.27	123.44	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	581	SER	N-CA-C	9.26	120.47	108.24
2	E	705	LEU	N-CA-CB	9.26	123.43	109.91
2	F	581	SER	N-CA-C	9.26	120.46	108.24
2	H	601	ARG	CA-C-N	9.15	138.04	121.85
2	H	601	ARG	C-N-CA	9.15	138.04	121.85
2	B	464	ILE	CB-CG1-CD1	9.13	132.98	113.80
2	I	464	ILE	CB-CG1-CD1	9.13	132.97	113.80
2	C	601	ARG	CA-C-N	9.12	138.00	121.85
2	C	601	ARG	C-N-CA	9.12	138.00	121.85
2	J	452	LEU	CB-CG-CD2	-9.05	83.55	110.70
2	E	452	LEU	CB-CG-CD2	-9.05	83.56	110.70
1	K	228	ARG	CB-CG-CD	9.03	132.07	111.30
1	D	228	ARG	CB-CG-CD	9.02	132.04	111.30
2	J	490	HIS	CA-CB-CG	-9.02	104.78	113.80
2	E	490	HIS	CA-CB-CG	-9.01	104.79	113.80
2	C	560	GLU	N-CA-C	9.01	125.00	111.04
2	H	560	GLU	N-CA-C	9.00	125.00	111.04
2	J	416	GLN	CA-C-N	9.00	132.78	120.46
2	J	416	GLN	C-N-CA	9.00	132.78	120.46
2	E	416	GLN	CA-C-N	8.98	132.77	120.46
2	E	416	GLN	C-N-CA	8.98	132.77	120.46
1	K	310	GLU	O-C-N	-8.94	112.64	122.12
2	J	453	ARG	CA-C-N	8.93	138.59	121.54
2	J	453	ARG	C-N-CA	8.93	138.59	121.54
2	E	453	ARG	CA-C-N	8.92	138.57	121.54
2	E	453	ARG	C-N-CA	8.92	138.57	121.54
1	D	310	GLU	O-C-N	-8.89	112.70	122.12
2	B	494	ILE	CA-CB-CG1	8.83	125.40	110.40
2	I	494	ILE	CA-CB-CG1	8.80	125.35	110.40
2	B	341	GLU	N-CA-C	-8.79	101.27	111.03
2	I	490	HIS	CA-C-O	-8.77	105.90	120.80
2	E	442	CYS	N-CA-C	8.76	124.18	112.88
2	I	341	GLU	N-CA-C	-8.76	101.30	111.03
2	B	490	HIS	CA-C-O	-8.76	105.92	120.80
2	J	442	CYS	N-CA-C	8.76	124.18	112.88
2	I	700	GLU	CA-CB-CG	8.63	131.37	114.10
2	B	700	GLU	CA-CB-CG	8.62	131.35	114.10
2	L	600	TYR	N-CA-C	8.62	125.44	114.31
2	F	600	TYR	N-CA-C	8.62	125.42	114.31
2	L	574	ASP	N-CA-CB	8.60	125.03	110.49
2	F	574	ASP	N-CA-CB	8.59	125.01	110.49
2	J	700	GLU	CB-CG-CD	8.57	127.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	700	GLU	CB-CG-CD	8.55	127.14	112.60
2	E	490	HIS	CA-C-O	-8.54	108.30	120.51
2	J	490	HIS	CA-C-O	-8.54	108.30	120.51
1	K	316	ASN	O-C-N	-8.48	111.31	122.59
1	D	316	ASN	O-C-N	-8.47	111.32	122.59
1	K	316	ASN	N-CA-C	8.44	128.78	110.80
1	D	316	ASN	N-CA-C	8.44	128.77	110.80
2	E	448	GLN	CA-C-N	8.39	142.26	121.80
2	E	448	GLN	C-N-CA	8.39	142.26	121.80
2	J	448	GLN	CA-C-N	8.38	142.24	121.80
2	J	448	GLN	C-N-CA	8.38	142.24	121.80
2	H	533	ILE	CA-C-N	8.35	137.49	121.54
2	H	533	ILE	C-N-CA	8.35	137.49	121.54
2	C	533	ILE	CA-C-N	8.34	137.47	121.54
2	C	533	ILE	C-N-CA	8.34	137.47	121.54
2	B	488	THR	OG1-CB-CG2	8.30	125.90	109.30
2	I	488	THR	OG1-CB-CG2	8.29	125.89	109.30
1	D	726	ASP	CA-C-N	8.29	131.71	120.44
1	D	726	ASP	C-N-CA	8.29	131.71	120.44
1	K	726	ASP	CA-C-N	8.28	131.70	120.44
1	K	726	ASP	C-N-CA	8.28	131.70	120.44
2	I	414	LYS	N-CA-CB	8.24	124.41	110.49
2	B	414	LYS	N-CA-CB	8.24	124.41	110.49
2	F	574	ASP	CA-CB-CG	8.09	120.69	112.60
2	L	574	ASP	CA-CB-CG	8.08	120.68	112.60
2	B	488	THR	CB-CA-C	-8.08	98.58	111.18
1	A	270	ASP	CA-C-N	8.07	135.50	122.67
1	A	270	ASP	C-N-CA	8.07	135.50	122.67
1	G	88	GLY	N-CA-C	8.06	132.28	113.18
2	I	488	THR	CB-CA-C	-8.06	98.61	111.18
1	A	88	GLY	N-CA-C	8.05	132.26	113.18
2	J	669	TYR	O-C-N	-8.05	113.59	122.12
2	E	669	TYR	O-C-N	-8.04	113.59	122.12
1	G	270	ASP	CA-C-N	8.05	135.46	122.67
1	G	270	ASP	C-N-CA	8.05	135.46	122.67
2	B	489	ASN	OD1-CG-ND2	8.01	130.61	122.60
2	E	339	ASP	CA-CB-CG	8.00	120.60	112.60
2	B	487	ASN	CA-C-O	-7.99	109.08	120.51
2	I	489	ASN	OD1-CG-ND2	7.99	130.59	122.60
2	I	487	ASN	CA-C-O	-7.97	109.11	120.51
2	J	339	ASP	CA-CB-CG	7.97	120.57	112.60
2	I	449	TYR	CA-C-O	-7.97	111.70	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	449	TYR	CA-C-O	-7.96	111.71	119.51
2	J	488	THR	O-C-N	-7.92	112.61	122.19
2	E	488	THR	O-C-N	-7.91	112.62	122.19
2	F	601	ARG	O-C-N	-7.89	112.09	122.59
2	L	601	ARG	O-C-N	-7.89	112.10	122.59
2	I	677	VAL	N-CA-C	7.89	119.61	110.62
2	H	601	ARG	O-C-N	-7.88	112.11	122.59
2	B	677	VAL	N-CA-C	7.88	119.60	110.62
2	C	561	LYS	N-CA-CB	7.87	123.80	110.49
2	H	561	LYS	N-CA-CB	7.85	123.76	110.49
2	B	670	MET	O-C-N	-7.84	113.99	122.07
1	D	178	ASN	CA-C-N	7.81	135.18	122.29
1	D	178	ASN	C-N-CA	7.81	135.18	122.29
2	C	601	ARG	O-C-N	-7.80	112.22	122.59
2	I	675	LYS	N-CA-CB	7.80	122.98	109.72
2	B	675	LYS	N-CA-CB	7.79	122.97	109.72
1	K	178	ASN	CA-C-N	7.79	135.15	122.29
1	K	178	ASN	C-N-CA	7.79	135.15	122.29
2	I	670	MET	O-C-N	-7.78	114.05	122.07
2	J	450	PRO	CA-N-CD	-7.78	101.11	112.00
2	E	450	PRO	CA-N-CD	-7.78	101.11	112.00
1	D	90	LYS	CB-CG-CD	7.75	129.12	111.30
2	J	453	ARG	NH1-CZ-NH2	-7.73	109.25	119.30
2	B	486	MET	O-C-N	-7.73	112.31	122.59
2	E	453	ARG	NH1-CZ-NH2	-7.73	109.25	119.30
1	K	90	LYS	CB-CG-CD	7.73	129.08	111.30
2	E	489	ASN	N-CA-C	-7.73	103.65	113.23
2	J	489	ASN	N-CA-C	-7.72	103.66	113.23
2	L	575	VAL	CA-C-N	7.71	136.27	121.54
2	L	575	VAL	C-N-CA	7.71	136.27	121.54
2	I	486	MET	O-C-N	-7.71	112.34	122.59
2	F	575	VAL	CA-C-N	7.70	136.24	121.54
2	F	575	VAL	C-N-CA	7.70	136.24	121.54
2	J	454	GLU	CA-CB-CG	7.67	129.44	114.10
2	E	454	GLU	CA-CB-CG	7.66	129.43	114.10
2	I	490	HIS	CB-CG-ND1	7.66	134.19	122.70
2	H	534	MET	N-CA-CB	7.66	123.43	110.49
2	L	575	VAL	N-CA-CB	7.66	123.86	111.23
2	F	575	VAL	N-CA-CB	7.65	123.85	111.23
2	I	674	ASN	O-C-N	-7.65	114.14	122.09
2	C	534	MET	N-CA-CB	7.64	123.40	110.49
2	B	674	ASN	O-C-N	-7.64	114.15	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	490	HIS	CB-CG-ND1	7.64	134.16	122.70
2	L	628	GLU	CA-CB-CG	7.63	129.37	114.10
2	E	441	GLN	O-C-N	-7.63	112.89	122.27
2	B	489	ASN	CA-C-O	7.62	131.41	120.51
2	F	628	GLU	CA-CB-CG	7.62	129.34	114.10
2	J	441	GLN	O-C-N	-7.62	112.90	122.27
2	L	533	ILE	O-C-N	-7.62	114.44	121.91
2	F	533	ILE	O-C-N	-7.61	114.45	121.91
1	G	741	ILE	CB-CG1-CD1	-7.61	97.83	113.80
2	C	584	HIS	CB-CG-CD2	-7.60	121.31	131.20
1	A	741	ILE	CB-CG1-CD1	-7.60	97.85	113.80
2	I	489	ASN	CA-C-O	7.60	131.37	120.51
2	E	492	ASP	N-CA-C	7.59	126.98	110.80
2	H	584	HIS	CB-CG-CD2	-7.59	121.33	131.20
2	J	492	ASP	N-CA-C	7.59	126.97	110.80
1	D	131	ASN	CA-C-N	7.58	134.50	122.59
1	D	131	ASN	C-N-CA	7.58	134.50	122.59
1	K	131	ASN	CA-C-N	7.58	134.50	122.59
1	K	131	ASN	C-N-CA	7.58	134.50	122.59
1	D	289	ILE	CA-C-N	7.58	130.76	120.38
1	D	289	ILE	C-N-CA	7.58	130.76	120.38
2	L	569	ASN	CB-CA-C	7.57	124.92	111.06
2	F	529	ASN	N-CA-CB	7.57	121.24	110.12
1	G	282	ASN	CA-C-N	7.56	130.41	120.28
1	G	282	ASN	C-N-CA	7.56	130.41	120.28
1	K	289	ILE	CA-C-N	7.56	130.73	120.38
1	K	289	ILE	C-N-CA	7.56	130.73	120.38
1	D	313	GLU	CA-C-O	7.55	128.87	119.05
2	F	569	ASN	CB-CA-C	7.55	124.88	111.06
2	L	529	ASN	N-CA-CB	7.54	121.21	110.12
2	B	336	PHE	CA-C-N	7.54	130.72	120.38
2	B	336	PHE	C-N-CA	7.54	130.72	120.38
1	A	282	ASN	CA-C-N	7.54	130.38	120.28
1	A	282	ASN	C-N-CA	7.54	130.38	120.28
1	K	313	GLU	CA-C-O	7.54	128.85	119.05
2	I	336	PHE	CA-C-N	7.53	130.70	120.38
2	I	336	PHE	C-N-CA	7.53	130.70	120.38
2	B	442	CYS	N-CA-C	7.51	126.80	110.80
2	F	558	GLU	CA-CB-CG	7.51	129.12	114.10
2	I	442	CYS	N-CA-C	7.50	126.77	110.80
2	I	702	LEU	CA-C-N	7.49	131.21	120.79
2	I	702	LEU	C-N-CA	7.49	131.21	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	456	MET	CG-SD-CE	7.49	117.39	100.90
2	E	494	ILE	CA-CB-CG1	7.49	123.14	110.40
2	F	560	GLU	N-CA-C	7.48	125.08	110.56
2	L	558	GLU	CA-CB-CG	7.48	129.06	114.10
2	B	702	LEU	CA-C-N	7.48	131.19	120.79
2	B	702	LEU	C-N-CA	7.48	131.19	120.79
2	J	494	ILE	CA-CB-CG1	7.48	123.11	110.40
2	E	456	MET	CG-SD-CE	7.47	117.34	100.90
2	L	560	GLU	N-CA-C	7.47	125.05	110.56
1	G	303	GLN	CA-C-N	7.47	132.02	120.82
1	G	303	GLN	C-N-CA	7.47	132.02	120.82
1	A	303	GLN	CA-C-N	7.46	132.02	120.82
1	A	303	GLN	C-N-CA	7.46	132.02	120.82
2	H	554	LYS	CB-CG-CD	7.46	128.45	111.30
2	C	554	LYS	CB-CG-CD	7.45	128.44	111.30
2	C	630	VAL	N-CA-CB	7.41	124.09	111.50
2	H	630	VAL	N-CA-CB	7.40	124.09	111.50
2	B	472	LYS	CA-C-N	7.40	130.52	120.38
2	B	472	LYS	C-N-CA	7.40	130.52	120.38
1	A	193	VAL	CA-C-N	7.39	129.24	122.37
1	A	193	VAL	C-N-CA	7.39	129.24	122.37
1	G	193	VAL	CA-C-N	7.39	129.24	122.37
1	G	193	VAL	C-N-CA	7.39	129.24	122.37
2	B	460	VAL	N-CA-C	7.39	117.46	110.74
2	E	671	ALA	CA-C-N	7.39	132.14	120.47
2	E	671	ALA	C-N-CA	7.39	132.14	120.47
2	J	671	ALA	CA-C-N	7.38	132.14	120.47
2	J	671	ALA	C-N-CA	7.38	132.14	120.47
2	E	448	GLN	N-CA-CB	-7.38	97.96	110.50
2	I	472	LYS	CA-C-N	7.37	130.48	120.38
2	I	472	LYS	C-N-CA	7.37	130.48	120.38
2	I	414	LYS	CA-CB-CG	7.37	128.84	114.10
2	I	460	VAL	N-CA-C	7.37	117.44	110.74
2	J	448	GLN	N-CA-CB	-7.37	97.97	110.50
1	D	316	ASN	OD1-CG-ND2	-7.37	115.23	122.60
2	J	455	GLU	CA-C-N	7.36	135.60	121.54
2	J	455	GLU	C-N-CA	7.36	135.60	121.54
2	L	569	ASN	CB-CG-OD1	7.35	135.51	120.80
2	F	569	ASN	CB-CG-OD1	7.35	135.50	120.80
2	B	414	LYS	CA-CB-CG	7.35	128.79	114.10
2	E	455	GLU	CA-C-N	7.35	135.57	121.54
2	E	455	GLU	C-N-CA	7.35	135.57	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	296	LEU	CA-C-N	7.34	130.45	120.54
1	D	296	LEU	C-N-CA	7.34	130.45	120.54
1	K	296	LEU	CA-C-N	7.34	130.45	120.54
1	K	296	LEU	C-N-CA	7.34	130.45	120.54
1	K	315	LYS	CA-C-N	7.33	135.54	121.54
1	K	315	LYS	C-N-CA	7.33	135.54	121.54
1	D	315	LYS	CA-C-N	7.33	135.53	121.54
1	D	315	LYS	C-N-CA	7.33	135.53	121.54
1	K	316	ASN	OD1-CG-ND2	-7.32	115.28	122.60
2	I	700	GLU	N-CA-CB	7.31	121.48	110.22
2	B	700	GLU	N-CA-CB	7.31	121.48	110.22
1	G	285	LEU	CA-C-N	7.30	129.93	120.44
1	G	285	LEU	C-N-CA	7.30	129.93	120.44
2	J	490	HIS	CB-CG-CD2	-7.29	121.72	131.20
1	A	307	ILE	CA-C-N	7.28	129.91	120.44
1	A	307	ILE	C-N-CA	7.28	129.91	120.44
2	F	558	GLU	CB-CG-CD	7.27	124.95	112.60
2	E	490	HIS	CB-CG-CD2	-7.26	121.76	131.20
1	A	285	LEU	CA-C-N	7.26	129.88	120.44
1	A	285	LEU	C-N-CA	7.26	129.88	120.44
2	L	558	GLU	CB-CG-CD	7.24	124.91	112.60
2	I	462	THR	N-CA-C	7.23	119.16	111.28
1	G	307	ILE	CA-C-N	7.22	129.83	120.44
1	G	307	ILE	C-N-CA	7.22	129.83	120.44
2	B	462	THR	N-CA-C	7.21	119.14	111.28
1	G	178	ASN	CA-C-N	7.19	134.16	122.29
1	G	178	ASN	C-N-CA	7.19	134.16	122.29
2	F	529	ASN	N-CA-C	7.19	119.12	111.28
1	A	178	ASN	CA-C-N	7.19	134.15	122.29
1	A	178	ASN	C-N-CA	7.19	134.15	122.29
2	B	372	PHE	CA-C-N	7.17	130.22	120.54
2	B	372	PHE	C-N-CA	7.17	130.22	120.54
2	L	529	ASN	N-CA-C	7.16	119.09	111.28
1	G	267	HIS	CA-C-N	7.14	134.07	122.65
1	G	267	HIS	C-N-CA	7.14	134.07	122.65
2	I	372	PHE	CA-C-N	7.13	130.17	120.54
2	I	372	PHE	C-N-CA	7.13	130.17	120.54
1	A	267	HIS	CA-C-N	7.13	134.06	122.65
1	A	267	HIS	C-N-CA	7.13	134.06	122.65
1	D	317	PHE	CA-CB-CG	7.13	120.93	113.80
1	K	315	LYS	N-CA-C	7.12	121.81	113.20
1	K	317	PHE	CA-CB-CG	7.12	120.92	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	315	LYS	N-CA-C	7.11	121.80	113.20
2	E	452	LEU	CA-C-N	7.10	135.11	121.54
2	E	452	LEU	C-N-CA	7.10	135.11	121.54
2	C	577	LYS	O-C-N	-7.10	113.15	122.59
2	H	577	LYS	O-C-N	-7.10	113.15	122.59
2	J	452	LEU	CA-C-N	7.09	135.09	121.54
2	J	452	LEU	C-N-CA	7.09	135.09	121.54
2	F	563	TYR	O-C-N	-7.08	116.45	123.46
2	E	487	ASN	CA-C-N	7.08	133.28	122.37
2	E	487	ASN	C-N-CA	7.08	133.28	122.37
2	J	487	ASN	CA-C-N	7.08	133.27	122.37
2	J	487	ASN	C-N-CA	7.08	133.27	122.37
2	L	563	TYR	O-C-N	-7.08	116.45	123.46
2	J	662	ILE	CA-C-N	7.07	131.43	120.82
2	J	662	ILE	C-N-CA	7.07	131.43	120.82
2	E	662	ILE	CA-C-N	7.07	131.43	120.82
2	E	662	ILE	C-N-CA	7.07	131.43	120.82
1	D	174	VAL	O-C-N	-7.07	114.89	122.95
1	K	174	VAL	O-C-N	-7.04	114.93	122.95
1	K	29	LEU	CA-C-N	7.00	133.96	122.07
1	K	29	LEU	C-N-CA	7.00	133.96	122.07
1	A	88	GLY	CA-C-N	6.99	134.06	121.97
1	A	88	GLY	C-N-CA	6.99	134.06	121.97
2	B	413	VAL	CA-C-N	6.99	134.89	121.54
2	B	413	VAL	C-N-CA	6.99	134.89	121.54
2	I	413	VAL	CA-C-N	6.99	134.88	121.54
2	I	413	VAL	C-N-CA	6.99	134.88	121.54
2	C	576	GLU	CA-C-N	6.99	134.88	121.54
2	C	576	GLU	C-N-CA	6.99	134.88	121.54
1	D	29	LEU	CA-C-N	6.99	133.95	122.07
1	D	29	LEU	C-N-CA	6.99	133.95	122.07
1	G	88	GLY	CA-C-N	6.98	134.05	121.97
1	G	88	GLY	C-N-CA	6.98	134.05	121.97
2	I	327	LYS	CB-CG-CD	6.98	127.34	111.30
2	B	327	LYS	CB-CG-CD	6.97	127.34	111.30
2	H	576	GLU	CA-C-N	6.97	134.86	121.54
2	H	576	GLU	C-N-CA	6.97	134.86	121.54
2	F	580	MET	O-C-N	-6.96	114.02	122.71
2	L	580	MET	O-C-N	-6.92	114.05	122.71
1	K	171	ILE	N-CA-C	6.92	118.53	107.73
1	D	171	ILE	N-CA-C	6.92	118.52	107.73
2	L	563	TYR	CA-C-O	-6.92	113.49	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	273	GLY	CA-C-N	6.92	132.48	121.62
1	G	273	GLY	C-N-CA	6.92	132.48	121.62
1	D	303	GLN	CA-C-N	6.91	129.77	120.65
1	D	303	GLN	C-N-CA	6.91	129.77	120.65
2	B	670	MET	CA-C-N	6.90	131.17	120.82
2	B	670	MET	C-N-CA	6.90	131.17	120.82
1	A	273	GLY	CA-C-N	6.90	132.45	121.62
1	A	273	GLY	C-N-CA	6.90	132.45	121.62
2	L	575	VAL	CA-C-O	-6.89	112.16	120.78
2	J	387	GLU	CA-C-N	6.88	130.24	120.53
2	J	387	GLU	C-N-CA	6.88	130.24	120.53
2	F	563	TYR	CA-C-O	-6.88	113.53	121.10
2	I	670	MET	CA-C-N	6.88	131.14	120.82
2	I	670	MET	C-N-CA	6.88	131.14	120.82
2	E	387	GLU	CA-C-N	6.88	130.22	120.53
2	E	387	GLU	C-N-CA	6.88	130.22	120.53
2	F	575	VAL	CA-C-O	-6.87	112.19	120.78
2	J	490	HIS	N-CA-C	6.86	125.42	110.80
1	A	219	VAL	CB-CA-C	-6.86	103.19	111.97
2	B	409	PHE	CA-C-N	6.86	129.77	120.38
2	B	409	PHE	C-N-CA	6.86	129.77	120.38
1	A	296	LEU	CA-C-N	6.86	130.32	120.79
1	A	296	LEU	C-N-CA	6.86	130.32	120.79
2	E	490	HIS	N-CA-C	6.85	125.39	110.80
1	G	219	VAL	CB-CA-C	-6.85	103.20	111.97
1	K	90	LYS	CA-C-N	6.83	132.73	121.39
1	K	90	LYS	C-N-CA	6.83	132.73	121.39
1	K	311	VAL	CA-C-N	6.82	129.75	120.54
1	K	311	VAL	C-N-CA	6.82	129.75	120.54
1	D	311	VAL	CA-C-N	6.81	129.73	120.54
1	D	311	VAL	C-N-CA	6.81	129.73	120.54
2	F	573	ARG	O-C-N	-6.81	114.86	123.24
2	I	409	PHE	CA-C-N	6.81	129.71	120.38
2	I	409	PHE	C-N-CA	6.81	129.71	120.38
1	D	90	LYS	CA-C-N	6.81	132.69	121.39
1	D	90	LYS	C-N-CA	6.81	132.69	121.39
1	G	296	LEU	CA-C-N	6.81	130.25	120.79
1	G	296	LEU	C-N-CA	6.81	130.25	120.79
2	F	573	ARG	CD-NE-CZ	6.80	133.92	124.40
2	E	487	ASN	O-C-N	-6.80	114.66	122.68
2	L	573	ARG	CD-NE-CZ	6.80	133.92	124.40
2	L	573	ARG	O-C-N	-6.80	114.88	123.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	487	ASN	O-C-N	-6.80	114.66	122.68
2	B	484	ALA	N-CA-C	6.77	121.86	112.45
2	L	581	SER	CA-C-O	-6.77	113.94	121.05
2	I	484	ALA	N-CA-C	6.76	121.85	112.45
2	J	468	GLU	N-CA-C	-6.76	103.37	111.69
2	F	581	SER	CA-C-O	-6.76	113.95	121.05
2	E	468	GLU	N-CA-C	-6.76	103.38	111.69
2	H	629	ARG	O-C-N	-6.74	113.57	122.47
1	D	50	ASN	OD1-CG-ND2	-6.74	115.86	122.60
2	J	453	ARG	N-CA-CB	6.73	121.87	110.49
2	J	672	ILE	CA-CB-CG1	6.73	121.85	110.40
2	C	629	ARG	O-C-N	-6.73	113.58	122.47
2	E	453	ARG	N-CA-CB	6.73	121.86	110.49
1	D	727	GLU	N-CA-C	-6.72	103.88	111.14
2	E	672	ILE	CA-CB-CG1	6.72	121.83	110.40
1	K	314	TYR	N-CA-C	6.72	119.46	111.33
1	K	50	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	D	314	TYR	N-CA-C	6.71	119.45	111.33
2	F	574	ASP	CA-C-O	-6.71	110.92	120.51
1	K	727	GLU	N-CA-C	-6.71	103.90	111.14
1	D	277	LEU	CA-C-N	6.70	129.15	120.44
1	D	277	LEU	C-N-CA	6.70	129.15	120.44
2	B	694	LYS	CA-C-N	6.70	130.87	120.82
2	B	694	LYS	C-N-CA	6.70	130.87	120.82
1	K	277	LEU	CA-C-N	6.70	129.15	120.44
1	K	277	LEU	C-N-CA	6.70	129.15	120.44
2	J	696	PHE	CA-C-N	6.70	129.97	120.53
2	J	696	PHE	C-N-CA	6.70	129.97	120.53
2	J	451	ARG	CA-CB-CG	6.70	127.49	114.10
2	E	696	PHE	CA-C-N	6.69	129.96	120.53
2	E	696	PHE	C-N-CA	6.69	129.96	120.53
2	E	451	ARG	CA-CB-CG	6.69	127.47	114.10
2	I	694	LYS	CA-C-N	6.69	130.85	120.82
2	I	694	LYS	C-N-CA	6.69	130.85	120.82
2	L	574	ASP	CA-C-O	-6.68	110.96	120.51
2	H	560	GLU	N-CA-CB	6.67	119.57	110.10
2	C	560	GLU	N-CA-CB	6.66	119.56	110.10
2	I	435	LEU	CA-C-N	6.65	129.57	120.46
2	I	435	LEU	C-N-CA	6.65	129.57	120.46
2	F	561	LYS	N-CA-CB	6.65	121.72	110.49
1	K	32	PRO	CA-C-N	6.64	131.35	121.72
1	K	32	PRO	C-N-CA	6.64	131.35	121.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	435	LEU	CA-C-N	6.64	129.56	120.46
2	B	435	LEU	C-N-CA	6.64	129.56	120.46
1	D	32	PRO	CA-C-N	6.64	131.35	121.72
1	D	32	PRO	C-N-CA	6.64	131.35	121.72
1	A	223	LYS	CB-CG-CD	6.63	126.56	111.30
2	E	677	VAL	N-CA-C	6.63	118.18	110.62
2	L	561	LYS	N-CA-CB	6.63	121.70	110.49
2	I	440	ARG	CA-C-N	6.63	129.70	120.29
2	I	440	ARG	C-N-CA	6.63	129.70	120.29
2	B	440	ARG	CA-C-N	6.61	129.68	120.29
2	B	440	ARG	C-N-CA	6.61	129.68	120.29
1	G	223	LYS	CB-CG-CD	6.61	126.50	111.30
2	B	707	SER	CB-CA-C	6.60	122.65	110.10
2	I	707	SER	CB-CA-C	6.60	122.64	110.10
2	E	443	THR	N-CA-CB	6.60	119.84	110.67
2	J	677	VAL	N-CA-C	6.60	118.14	110.62
1	A	738	ALA	CA-C-N	6.60	129.42	120.38
1	A	738	ALA	C-N-CA	6.60	129.42	120.38
2	J	443	THR	N-CA-CB	6.59	119.83	110.67
2	I	685	ILE	CA-C-N	6.57	129.41	120.54
2	I	685	ILE	C-N-CA	6.57	129.41	120.54
1	K	159	MET	CA-CB-CG	6.56	127.23	114.10
1	D	159	MET	CA-CB-CG	6.56	127.23	114.10
2	J	491	GLU	N-CA-CB	6.56	121.35	110.33
2	I	362	ILE	N-CA-CB	6.56	118.51	110.64
2	L	573	ARG	CG-CD-NE	-6.55	97.58	112.00
2	B	685	ILE	CA-C-N	6.55	129.38	120.54
2	B	685	ILE	C-N-CA	6.55	129.38	120.54
2	F	528	ILE	N-CA-CB	6.55	118.97	111.90
2	F	573	ARG	CG-CD-NE	-6.54	97.61	112.00
2	E	491	GLU	N-CA-CB	6.54	121.32	110.33
1	G	738	ALA	CA-C-N	6.53	129.33	120.38
1	G	738	ALA	C-N-CA	6.53	129.33	120.38
2	B	362	ILE	N-CA-CB	6.53	118.47	110.64
2	L	528	ILE	N-CA-CB	6.52	118.95	111.90
2	L	534	MET	N-CA-CB	6.52	121.52	110.49
2	E	450	PRO	CA-C-N	6.52	130.78	121.71
2	E	450	PRO	C-N-CA	6.52	130.78	121.71
2	J	450	PRO	CA-C-N	6.51	130.76	121.71
2	J	450	PRO	C-N-CA	6.51	130.76	121.71
2	B	455	GLU	CA-C-N	6.50	129.29	120.38
2	B	455	GLU	C-N-CA	6.50	129.29	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	455	GLU	CA-C-N	6.50	129.29	120.38
2	I	455	GLU	C-N-CA	6.50	129.29	120.38
1	K	315	LYS	O-C-N	-6.50	112.77	122.39
1	K	30	ASP	CA-C-N	6.50	129.72	120.49
1	K	30	ASP	C-N-CA	6.50	129.72	120.49
2	F	534	MET	N-CA-CB	6.49	121.46	110.49
1	D	30	ASP	CA-C-N	6.48	129.70	120.49
1	D	30	ASP	C-N-CA	6.48	129.70	120.49
2	E	417	VAL	CA-C-N	6.47	129.25	120.38
2	E	417	VAL	C-N-CA	6.47	129.25	120.38
1	K	303	GLN	CA-C-N	6.47	129.79	120.79
1	K	303	GLN	C-N-CA	6.47	129.79	120.79
1	D	315	LYS	O-C-N	-6.47	112.82	122.39
2	E	492	ASP	CA-C-O	-6.47	111.26	120.51
1	G	44	LYS	N-CA-C	6.46	118.86	111.11
2	I	487	ASN	O-C-N	-6.46	114.00	122.59
2	J	492	ASP	CA-C-O	-6.46	111.28	120.51
1	D	318	ARG	N-CA-CB	6.44	121.83	110.37
2	J	417	VAL	CA-C-N	6.44	129.20	120.38
2	J	417	VAL	C-N-CA	6.44	129.20	120.38
2	I	467	ARG	CA-CB-CG	-6.44	101.22	114.10
1	A	44	LYS	N-CA-C	6.43	118.83	111.11
2	I	387	GLU	CA-C-N	6.43	129.59	120.53
2	I	387	GLU	C-N-CA	6.43	129.59	120.53
2	B	655	LEU	CA-C-N	6.42	129.18	120.38
2	B	655	LEU	C-N-CA	6.42	129.18	120.38
2	I	655	LEU	CA-C-N	6.42	129.18	120.38
2	I	655	LEU	C-N-CA	6.42	129.18	120.38
2	B	487	ASN	O-C-N	-6.42	114.05	122.59
1	K	318	ARG	N-CA-CB	6.42	121.80	110.37
2	B	467	ARG	CA-CB-CG	-6.42	101.26	114.10
2	H	533	ILE	O-C-N	-6.42	115.23	121.90
2	C	533	ILE	O-C-N	-6.41	115.24	121.90
2	J	362	ILE	N-CA-CB	6.38	118.30	110.64
2	B	387	GLU	CA-C-N	6.38	129.52	120.53
2	B	387	GLU	C-N-CA	6.38	129.52	120.53
2	E	362	ILE	N-CA-CB	6.38	118.30	110.64
1	A	67	ARG	NE-CZ-NH2	6.37	124.93	119.20
1	G	67	ARG	NE-CZ-NH2	6.36	124.93	119.20
1	A	299	LYS	CA-C-N	6.36	128.80	120.28
1	A	299	LYS	C-N-CA	6.36	128.80	120.28
1	G	299	LYS	CA-C-N	6.36	128.80	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	299	LYS	C-N-CA	6.36	128.80	120.28
2	B	368	GLU	CA-C-N	6.35	132.19	122.23
2	B	368	GLU	C-N-CA	6.35	132.19	122.23
2	J	335	GLN	CA-C-N	6.34	128.78	120.28
2	J	335	GLN	C-N-CA	6.34	128.78	120.28
2	E	481	ILE	CA-C-N	6.33	129.06	120.38
2	E	481	ILE	C-N-CA	6.33	129.06	120.38
2	I	368	GLU	CA-C-N	6.33	132.17	122.23
2	I	368	GLU	C-N-CA	6.33	132.17	122.23
2	H	520	VAL	CA-C-N	6.32	129.40	120.42
2	H	520	VAL	C-N-CA	6.32	129.40	120.42
1	D	89	LYS	CA-C-N	6.32	131.83	122.86
1	D	89	LYS	C-N-CA	6.32	131.83	122.86
2	J	481	ILE	CA-C-N	6.32	129.03	120.38
2	J	481	ILE	C-N-CA	6.32	129.03	120.38
2	C	520	VAL	CA-C-N	6.31	129.38	120.42
2	C	520	VAL	C-N-CA	6.31	129.38	120.42
2	E	335	GLN	CA-C-N	6.31	128.74	120.28
2	E	335	GLN	C-N-CA	6.31	128.74	120.28
1	K	89	LYS	CA-C-N	6.31	131.82	122.86
1	K	89	LYS	C-N-CA	6.31	131.82	122.86
1	A	741	ILE	CA-CB-CG1	-6.31	99.68	110.40
2	E	485	TYR	CG-CD2-CE2	-6.30	111.75	121.20
1	G	741	ILE	CA-CB-CG1	-6.30	99.69	110.40
2	J	485	TYR	CG-CD2-CE2	-6.30	111.75	121.20
2	E	384	LEU	CA-C-N	6.29	129.34	120.28
2	E	384	LEU	C-N-CA	6.29	129.34	120.28
1	G	272	MET	CA-C-N	6.29	132.21	121.39
1	G	272	MET	C-N-CA	6.29	132.21	121.39
1	A	272	MET	CA-C-N	6.29	132.21	121.39
1	A	272	MET	C-N-CA	6.29	132.21	121.39
2	J	384	LEU	CA-C-N	6.27	129.31	120.28
2	J	384	LEU	C-N-CA	6.27	129.31	120.28
2	L	563	TYR	N-CA-C	6.26	118.07	108.42
2	I	449	TYR	O-C-N	6.25	126.74	121.31
2	I	415	LYS	CA-C-N	6.23	131.12	120.71
2	I	415	LYS	C-N-CA	6.23	131.12	120.71
2	B	415	LYS	CA-C-N	6.23	131.11	120.71
2	B	415	LYS	C-N-CA	6.23	131.11	120.71
2	F	563	TYR	N-CA-C	6.23	118.01	108.42
2	E	700	GLU	N-CA-C	6.22	118.87	111.71
2	C	584	HIS	CA-CB-CG	6.20	120.00	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	700	GLU	N-CA-C	6.20	118.84	111.71
2	J	451	ARG	N-CA-CB	6.19	119.93	110.39
2	H	584	HIS	CA-CB-CG	6.18	119.98	113.80
2	E	679	ASP	CA-C-N	6.18	129.06	120.29
2	E	679	ASP	C-N-CA	6.18	129.06	120.29
2	E	451	ARG	N-CA-CB	6.17	119.90	110.39
2	B	449	TYR	O-C-N	6.17	126.67	121.31
2	J	679	ASP	CA-C-N	6.17	129.04	120.29
2	J	679	ASP	C-N-CA	6.17	129.04	120.29
1	A	120	ILE	N-CA-C	-6.16	99.00	107.99
2	B	673	VAL	O-C-N	-6.15	115.49	121.83
1	D	89	LYS	N-CA-CB	6.15	121.44	110.80
1	G	120	ILE	N-CA-C	-6.15	99.01	107.99
1	K	89	LYS	N-CA-CB	6.15	121.44	110.80
2	I	673	VAL	O-C-N	-6.14	115.50	121.83
2	B	467	ARG	NH1-CZ-NH2	-6.14	111.32	119.30
1	D	89	LYS	CA-C-O	-6.13	113.51	120.32
2	I	467	ARG	NH1-CZ-NH2	-6.13	111.33	119.30
2	E	456	MET	CA-C-N	6.12	128.76	120.44
2	E	456	MET	C-N-CA	6.12	128.76	120.44
2	E	414	LYS	CA-C-O	-6.11	114.36	120.90
2	J	414	LYS	CA-C-O	-6.11	114.36	120.90
2	J	456	MET	CA-C-N	6.11	128.75	120.44
2	J	456	MET	C-N-CA	6.11	128.75	120.44
1	K	89	LYS	CA-C-O	-6.11	113.54	120.32
2	J	705	LEU	N-CA-C	6.11	117.63	110.97
2	E	705	LEU	N-CA-C	6.10	117.62	110.97
2	F	560	GLU	O-C-N	-6.06	115.83	122.38
2	I	463	HIS	CA-CB-CG	6.05	119.86	113.80
2	L	560	GLU	O-C-N	-6.05	115.85	122.38
2	C	564	MET	N-CA-C	-6.04	97.93	110.80
2	H	564	MET	N-CA-C	-6.04	97.94	110.80
1	G	87	LYS	CA-C-O	-6.01	111.91	120.51
1	A	87	LYS	CA-C-O	-6.01	111.92	120.51
2	H	584	HIS	N-CA-CB	6.00	120.21	110.42
2	C	584	HIS	N-CA-CB	6.00	120.20	110.42
2	J	673	VAL	CA-C-N	6.00	128.60	120.38
2	J	673	VAL	C-N-CA	6.00	128.60	120.38
2	B	463	HIS	CA-CB-CG	5.99	119.79	113.80
1	A	248	ILE	N-CA-C	5.99	116.17	110.42
2	E	673	VAL	CA-C-N	5.99	128.58	120.38
2	E	673	VAL	C-N-CA	5.99	128.58	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	455	GLU	O-C-N	-5.98	115.68	122.08
2	J	484	ALA	N-CA-CB	-5.98	101.29	110.44
2	I	676	THR	CA-CB-CG2	5.97	120.66	110.50
2	E	484	ALA	N-CA-CB	-5.97	101.31	110.44
2	L	560	GLU	N-CA-CB	5.96	119.58	110.39
2	C	564	MET	CA-C-N	5.96	130.95	122.72
2	C	564	MET	C-N-CA	5.96	130.95	122.72
2	F	560	GLU	N-CA-CB	5.96	119.57	110.39
2	B	676	THR	CA-CB-CG2	5.96	120.62	110.50
2	E	455	GLU	O-C-N	-5.95	115.71	122.08
1	D	300	LEU	CA-C-N	5.95	128.18	120.44
1	D	300	LEU	C-N-CA	5.95	128.18	120.44
2	I	361	ARG	CA-C-N	-5.95	113.62	120.88
2	I	361	ARG	C-N-CA	-5.95	113.62	120.88
1	K	300	LEU	CA-C-N	5.95	128.18	120.44
1	K	300	LEU	C-N-CA	5.95	128.18	120.44
2	B	707	SER	N-CA-CB	5.94	120.60	110.50
2	I	707	SER	N-CA-CB	5.94	120.59	110.50
2	H	564	MET	CA-C-N	5.94	130.91	122.72
2	H	564	MET	C-N-CA	5.94	130.91	122.72
1	D	304	LEU	CA-C-N	5.93	128.55	120.54
1	D	304	LEU	C-N-CA	5.93	128.55	120.54
1	K	304	LEU	CA-C-N	5.93	128.55	120.54
1	K	304	LEU	C-N-CA	5.93	128.55	120.54
2	B	361	ARG	CA-C-N	-5.93	113.65	120.88
2	B	361	ARG	C-N-CA	-5.93	113.65	120.88
2	B	417	VAL	CA-C-N	5.91	128.20	120.28
2	B	417	VAL	C-N-CA	5.91	128.20	120.28
2	E	409	PHE	CA-C-N	5.91	128.12	120.44
2	E	409	PHE	C-N-CA	5.91	128.12	120.44
2	J	409	PHE	CA-C-N	5.90	128.11	120.44
2	J	409	PHE	C-N-CA	5.90	128.11	120.44
2	I	417	VAL	CA-C-N	5.89	128.18	120.28
2	I	417	VAL	C-N-CA	5.89	128.18	120.28
2	J	372	PHE	CA-C-N	5.88	128.48	120.54
2	J	372	PHE	C-N-CA	5.88	128.48	120.54
2	J	456	MET	CB-CG-SD	-5.88	95.06	112.70
2	B	485	TYR	CG-CD2-CE2	-5.88	112.39	121.20
2	J	694	LYS	CA-C-N	5.88	128.96	120.79
2	J	694	LYS	C-N-CA	5.88	128.96	120.79
2	E	456	MET	CB-CG-SD	-5.87	95.08	112.70
2	B	461	THR	CA-C-O	-5.87	114.66	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	694	LYS	CA-C-N	5.87	128.94	120.79
2	E	694	LYS	C-N-CA	5.87	128.94	120.79
2	E	372	PHE	CA-C-N	5.86	128.45	120.54
2	E	372	PHE	C-N-CA	5.86	128.45	120.54
2	I	485	TYR	CG-CD2-CE2	-5.86	112.42	121.20
2	I	461	THR	CA-C-O	-5.85	114.67	120.82
1	G	131	ASN	CA-C-N	5.85	133.38	122.74
1	G	131	ASN	C-N-CA	5.85	133.38	122.74
1	A	131	ASN	CA-C-N	5.84	133.38	122.74
1	A	131	ASN	C-N-CA	5.84	133.38	122.74
2	E	698	PHE	CA-C-N	5.84	132.79	121.63
2	E	698	PHE	C-N-CA	5.84	132.79	121.63
2	J	698	PHE	CA-C-N	5.84	132.78	121.63
2	J	698	PHE	C-N-CA	5.84	132.78	121.63
1	G	244	GLY	O-C-N	-5.83	114.46	122.68
2	E	386	ARG	CA-C-N	5.83	128.36	120.38
2	E	386	ARG	C-N-CA	5.83	128.36	120.38
1	A	244	GLY	O-C-N	-5.82	114.48	122.68
1	G	67	ARG	NE-CZ-NH1	-5.82	115.69	121.50
2	J	386	ARG	CA-C-N	5.81	128.35	120.38
2	J	386	ARG	C-N-CA	5.81	128.35	120.38
2	I	414	LYS	CA-C-N	5.79	130.40	120.72
2	I	414	LYS	C-N-CA	5.79	130.40	120.72
1	D	285	LEU	CA-C-N	5.79	128.31	120.38
1	D	285	LEU	C-N-CA	5.79	128.31	120.38
1	A	67	ARG	NE-CZ-NH1	-5.79	115.72	121.50
2	E	450	PRO	CB-CG-CD	-5.79	87.59	106.10
2	H	575	VAL	N-CA-CB	5.78	118.14	111.90
2	B	414	LYS	CA-C-N	5.78	130.37	120.72
2	B	414	LYS	C-N-CA	5.78	130.37	120.72
2	J	450	PRO	CB-CG-CD	-5.78	87.61	106.10
2	H	575	VAL	CA-C-N	5.77	132.57	121.54
2	H	575	VAL	C-N-CA	5.77	132.57	121.54
2	E	671	ALA	CA-C-O	5.77	127.07	120.90
2	C	575	VAL	CA-C-N	5.77	132.56	121.54
2	C	575	VAL	C-N-CA	5.77	132.56	121.54
1	K	285	LEU	CA-C-N	5.77	128.28	120.38
1	K	285	LEU	C-N-CA	5.77	128.28	120.38
2	J	671	ALA	CA-C-O	5.75	127.06	120.90
1	K	279	LYS	CA-C-N	5.75	127.80	120.56
1	K	279	LYS	C-N-CA	5.75	127.80	120.56
2	I	461	THR	CA-C-N	5.75	127.98	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	461	THR	C-N-CA	5.75	127.98	120.28
2	C	575	VAL	N-CA-CB	5.74	118.10	111.90
1	G	190	ALA	CA-C-N	5.74	129.78	120.60
1	G	190	ALA	C-N-CA	5.74	129.78	120.60
1	A	190	ALA	CA-C-N	5.74	129.78	120.60
1	A	190	ALA	C-N-CA	5.74	129.78	120.60
1	G	170	LEU	CA-C-N	5.73	129.65	122.43
1	G	170	LEU	C-N-CA	5.73	129.65	122.43
2	C	576	GLU	O-C-N	-5.73	114.97	122.59
1	A	89	LYS	N-CA-CB	5.73	118.01	109.19
2	B	461	THR	CA-C-N	5.73	127.96	120.28
2	B	461	THR	C-N-CA	5.73	127.96	120.28
2	E	489	ASN	OD1-CG-ND2	-5.72	116.88	122.60
2	J	455	GLU	CA-C-O	5.72	127.37	121.07
1	A	170	LEU	CA-C-N	5.72	129.64	122.43
1	A	170	LEU	C-N-CA	5.72	129.64	122.43
1	G	89	LYS	N-CA-CB	5.72	118.00	109.19
1	D	312	GLU	O-C-N	-5.72	116.14	122.09
1	D	282	ASN	CA-C-N	5.72	127.94	120.28
1	D	282	ASN	C-N-CA	5.72	127.94	120.28
1	K	312	GLU	O-C-N	-5.71	116.15	122.09
1	K	282	ASN	CA-C-N	5.71	127.94	120.28
1	K	282	ASN	C-N-CA	5.71	127.94	120.28
2	J	672	ILE	N-CA-CB	-5.71	100.89	110.65
1	D	279	LYS	CA-C-N	5.71	127.75	120.56
1	D	279	LYS	C-N-CA	5.71	127.75	120.56
1	A	244	GLY	CA-C-O	5.71	128.44	119.31
2	E	672	ILE	N-CA-CB	-5.71	100.89	110.65
2	E	455	GLU	CA-C-O	5.70	127.34	121.07
2	J	480	ASP	CA-C-N	5.70	132.23	121.97
2	J	480	ASP	C-N-CA	5.70	132.23	121.97
1	G	244	GLY	CA-C-O	5.70	128.42	119.31
2	E	480	ASP	CA-C-N	5.68	132.20	121.97
2	E	480	ASP	C-N-CA	5.68	132.20	121.97
2	J	453	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	G	169	CYS	CA-C-N	5.68	129.96	121.72
1	G	169	CYS	C-N-CA	5.68	129.96	121.72
2	H	576	GLU	O-C-N	-5.68	115.04	122.59
2	I	414	LYS	CB-CG-CD	5.67	124.35	111.30
2	F	573	ARG	NE-CZ-NH1	-5.67	115.83	121.50
2	I	697	ILE	CA-C-N	5.67	128.15	120.38
2	I	697	ILE	C-N-CA	5.67	128.15	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	236	ASN	N-CA-C	5.67	118.20	110.55
2	E	472	LYS	CA-C-N	5.67	127.87	120.28
2	E	472	LYS	C-N-CA	5.67	127.87	120.28
1	A	169	CYS	CA-C-N	5.66	129.93	121.72
1	A	169	CYS	C-N-CA	5.66	129.93	121.72
2	J	472	LYS	CA-C-N	5.66	127.87	120.28
2	J	472	LYS	C-N-CA	5.66	127.87	120.28
2	L	573	ARG	NE-CZ-NH1	-5.66	115.84	121.50
2	E	453	ARG	NE-CZ-NH2	5.66	124.29	119.20
2	F	530	ASN	N-CA-C	5.66	119.95	112.25
2	J	489	ASN	OD1-CG-ND2	-5.66	116.94	122.60
2	E	331	GLN	CA-C-N	5.65	127.85	120.28
2	E	331	GLN	C-N-CA	5.65	127.85	120.28
2	B	695	GLU	CA-C-N	5.65	132.32	121.54
2	B	695	GLU	C-N-CA	5.65	132.32	121.54
2	B	492	ASP	N-CA-CB	5.65	120.03	110.49
1	D	236	ASN	N-CA-C	5.65	118.17	110.55
2	E	450	PRO	CA-CB-CG	-5.64	93.78	104.50
2	I	492	ASP	N-CA-CB	5.64	120.03	110.49
2	J	450	PRO	CA-CB-CG	-5.64	93.78	104.50
2	B	414	LYS	CB-CG-CD	5.64	124.27	111.30
1	D	38	GLY	CA-C-O	-5.64	116.08	121.49
2	C	528	ILE	CA-C-N	5.64	128.88	120.31
2	C	528	ILE	C-N-CA	5.64	128.88	120.31
2	L	530	ASN	N-CA-C	5.64	119.92	112.25
2	B	696	PHE	CA-C-N	5.63	128.18	120.46
2	B	696	PHE	C-N-CA	5.63	128.18	120.46
2	L	627	PRO	CA-C-N	5.63	129.13	123.04
2	L	627	PRO	C-N-CA	5.63	129.13	123.04
1	K	38	GLY	CA-C-O	-5.63	116.08	121.49
2	B	697	ILE	CA-C-N	5.63	128.10	120.38
2	B	697	ILE	C-N-CA	5.63	128.10	120.38
2	E	338	VAL	O-C-N	-5.63	114.35	122.12
1	D	92	THR	N-CA-C	-5.63	107.05	114.31
2	J	338	VAL	O-C-N	-5.63	114.35	122.12
2	F	627	PRO	CA-C-N	5.63	129.12	123.04
2	F	627	PRO	C-N-CA	5.63	129.12	123.04
1	G	741	ILE	CA-CB-CG2	5.62	120.06	110.50
2	J	331	GLN	CA-C-N	5.62	127.82	120.28
2	J	331	GLN	C-N-CA	5.62	127.82	120.28
2	H	528	ILE	CA-C-N	5.62	128.85	120.31
2	H	528	ILE	C-N-CA	5.62	128.85	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	695	GLU	CA-C-N	5.62	132.28	121.54
2	I	695	GLU	C-N-CA	5.62	132.28	121.54
2	I	696	PHE	CA-C-N	5.62	128.16	120.46
2	I	696	PHE	C-N-CA	5.62	128.16	120.46
1	A	741	ILE	CA-CB-CG2	5.62	120.05	110.50
1	K	92	THR	N-CA-C	-5.61	107.07	114.31
2	L	612	GLU	CA-C-N	5.61	128.14	120.46
2	L	612	GLU	C-N-CA	5.61	128.14	120.46
2	I	478	LEU	CA-C-N	5.59	127.61	120.56
2	I	478	LEU	C-N-CA	5.59	127.61	120.56
2	F	568	ASP	N-CA-C	5.58	118.28	109.96
1	A	80	TYR	CA-C-N	5.57	131.72	121.85
1	A	80	TYR	C-N-CA	5.57	131.72	121.85
2	B	371	PRO	CA-C-N	5.57	128.02	120.38
2	B	371	PRO	C-N-CA	5.57	128.02	120.38
2	F	612	GLU	CA-C-N	5.57	128.10	120.46
2	F	612	GLU	C-N-CA	5.57	128.10	120.46
1	K	166	LYS	N-CA-CB	5.57	118.42	109.28
2	C	629	ARG	NE-CZ-NH1	-5.57	115.93	121.50
2	B	478	LEU	CA-C-N	5.57	127.57	120.56
2	B	478	LEU	C-N-CA	5.57	127.57	120.56
2	I	488	THR	N-CA-CB	-5.57	103.47	111.54
1	K	734	ALA	CA-C-N	5.56	127.74	120.28
1	K	734	ALA	C-N-CA	5.56	127.74	120.28
2	B	490	HIS	CG-ND1-CE1	5.56	118.75	109.30
2	C	568	ASP	N-CA-C	5.56	118.64	110.30
2	I	490	HIS	CG-ND1-CE1	5.56	118.75	109.30
1	D	166	LYS	N-CA-CB	5.56	118.39	109.28
1	D	171	ILE	CB-CG1-CD1	5.56	125.47	113.80
1	D	159	MET	CB-CG-SD	5.56	129.37	112.70
1	K	171	ILE	CB-CG1-CD1	5.56	125.47	113.80
1	K	159	MET	CB-CG-SD	5.55	129.37	112.70
2	I	468	GLU	N-CA-C	-5.55	104.86	111.69
2	J	493	PHE	N-CA-C	5.55	117.85	110.53
2	I	371	PRO	CA-C-N	5.54	127.98	120.38
2	I	371	PRO	C-N-CA	5.54	127.98	120.38
2	L	568	ASP	N-CA-C	5.54	118.22	109.96
1	G	80	TYR	CA-C-N	5.54	131.66	121.85
1	G	80	TYR	C-N-CA	5.54	131.66	121.85
2	I	483	LEU	CA-C-O	-5.54	112.79	119.49
2	E	493	PHE	N-CA-C	5.54	117.84	110.53
2	B	468	GLU	N-CA-C	-5.53	104.88	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	488	THR	N-CA-CB	-5.53	103.52	111.54
2	J	489	ASN	CB-CA-C	5.53	120.78	109.55
1	D	734	ALA	CA-C-N	5.53	127.69	120.28
1	D	734	ALA	C-N-CA	5.53	127.69	120.28
2	E	672	ILE	CG1-CB-CG2	5.53	127.30	110.70
2	E	489	ASN	CB-CA-C	5.53	120.78	109.55
2	H	575	VAL	CA-C-O	-5.53	113.42	120.89
2	J	672	ILE	CG1-CB-CG2	5.53	127.28	110.70
2	J	449	TYR	N-CA-CB	-5.52	100.54	110.37
2	H	568	ASP	N-CA-C	5.52	118.58	110.30
2	J	700	GLU	N-CA-CB	5.52	118.72	110.22
2	C	575	VAL	CA-C-O	-5.52	113.44	120.89
2	E	700	GLU	N-CA-CB	5.51	118.71	110.22
2	B	483	LEU	CA-C-O	-5.51	112.82	119.49
1	D	102	GLU	CA-C-N	5.51	127.66	120.28
1	D	102	GLU	C-N-CA	5.51	127.66	120.28
2	H	629	ARG	NE-CZ-NH1	-5.51	115.99	121.50
2	E	449	TYR	N-CA-CB	-5.50	100.57	110.37
2	I	379	PHE	N-CA-C	5.50	117.42	109.07
2	B	379	PHE	N-CA-C	5.49	117.42	109.07
2	J	377	MET	CA-C-N	5.49	131.57	121.85
2	J	377	MET	C-N-CA	5.49	131.57	121.85
2	H	621	LEU	CA-C-N	5.49	128.18	120.28
2	H	621	LEU	C-N-CA	5.49	128.18	120.28
2	C	621	LEU	CA-C-N	5.48	128.18	120.28
2	C	621	LEU	C-N-CA	5.48	128.18	120.28
1	K	102	GLU	CA-C-N	5.48	127.63	120.28
1	K	102	GLU	C-N-CA	5.48	127.63	120.28
2	C	564	MET	CA-C-O	5.47	128.34	120.51
2	E	377	MET	CA-C-N	5.47	131.54	121.85
2	E	377	MET	C-N-CA	5.47	131.54	121.85
1	K	254	ALA	CA-C-N	5.47	127.88	120.38
1	K	254	ALA	C-N-CA	5.47	127.88	120.38
2	E	489	ASN	CB-CG-ND2	5.46	124.59	116.40
2	H	563	TYR	CA-C-N	5.46	131.98	121.54
2	H	563	TYR	C-N-CA	5.46	131.98	121.54
1	G	106	ASP	CA-C-N	5.46	129.01	120.82
1	G	106	ASP	C-N-CA	5.46	129.01	120.82
1	A	270	ASP	O-C-N	-5.46	114.93	122.46
2	H	564	MET	CA-C-O	5.45	128.31	120.51
2	B	344	ILE	N-CA-CB	5.45	116.81	110.65
2	C	563	TYR	CA-C-N	5.45	131.94	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	563	TYR	C-N-CA	5.45	131.94	121.54
1	G	270	ASP	O-C-N	-5.45	114.94	122.46
1	D	254	ALA	CA-C-N	5.44	127.84	120.38
1	D	254	ALA	C-N-CA	5.44	127.84	120.38
1	A	106	ASP	CA-C-N	5.44	128.99	120.82
1	A	106	ASP	C-N-CA	5.44	128.99	120.82
2	I	675	LYS	CA-CB-CG	5.44	124.98	114.10
2	B	675	LYS	CA-CB-CG	5.44	124.98	114.10
2	C	584	HIS	CB-CA-C	5.44	119.00	110.19
2	J	489	ASN	CB-CG-ND2	5.44	124.56	116.40
2	I	344	ILE	N-CA-CB	5.44	116.80	110.65
1	G	248	ILE	N-CA-C	5.43	116.16	110.62
2	J	671	ALA	O-C-N	-5.42	116.45	122.09
2	B	459	ILE	CA-C-O	-5.42	114.62	120.47
2	I	449	TYR	CA-CB-CG	5.42	123.65	113.90
2	B	449	TYR	CA-CB-CG	5.42	123.65	113.90
2	E	671	ALA	O-C-N	-5.42	116.46	122.09
2	J	454	GLU	CB-CG-CD	5.42	121.81	112.60
1	A	85	HIS	CA-C-N	5.41	132.21	123.33
1	A	85	HIS	C-N-CA	5.41	132.21	123.33
2	E	452	LEU	CA-CB-CG	5.41	135.25	116.30
2	H	584	HIS	CB-CA-C	5.41	118.96	110.19
2	J	445	LYS	CA-CB-CG	5.41	124.92	114.10
1	D	276	TYR	CA-C-N	5.41	127.53	120.28
1	D	276	TYR	C-N-CA	5.41	127.53	120.28
2	E	454	GLU	CB-CG-CD	5.41	121.79	112.60
2	F	621	LEU	CA-C-N	5.41	128.07	120.28
2	F	621	LEU	C-N-CA	5.41	128.07	120.28
1	A	736	LYS	CA-C-N	5.41	127.47	120.44
1	A	736	LYS	C-N-CA	5.41	127.47	120.44
2	B	700	GLU	O-C-N	-5.41	115.90	122.22
2	E	445	LYS	CA-CB-CG	5.41	124.91	114.10
1	D	95	GLU	CA-C-N	5.40	127.52	120.28
1	D	95	GLU	C-N-CA	5.40	127.52	120.28
2	J	452	LEU	CA-CB-CG	5.40	135.21	116.30
2	L	576	GLU	CA-C-N	5.40	131.85	121.54
2	L	576	GLU	C-N-CA	5.40	131.85	121.54
2	B	673	VAL	CA-C-N	5.39	127.82	120.54
2	B	673	VAL	C-N-CA	5.39	127.82	120.54
2	I	700	GLU	O-C-N	-5.39	115.91	122.22
1	G	85	HIS	CA-C-N	5.39	132.17	123.33
1	G	85	HIS	C-N-CA	5.39	132.17	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	621	LEU	CA-C-N	5.39	128.05	120.28
2	L	621	LEU	C-N-CA	5.39	128.05	120.28
2	H	575	VAL	N-CA-C	5.39	115.02	107.37
2	H	593	GLN	N-CA-C	5.39	116.47	108.60
1	K	276	TYR	CA-C-N	5.39	127.50	120.28
1	K	276	TYR	C-N-CA	5.39	127.50	120.28
2	F	576	GLU	CA-C-N	5.39	131.83	121.54
2	F	576	GLU	C-N-CA	5.39	131.83	121.54
1	K	95	GLU	CA-C-N	5.39	127.50	120.28
1	K	95	GLU	C-N-CA	5.39	127.50	120.28
2	I	673	VAL	CA-C-N	5.38	127.81	120.54
2	I	673	VAL	C-N-CA	5.38	127.81	120.54
2	C	593	GLN	N-CA-C	5.38	116.45	108.60
1	G	736	LYS	CA-C-N	5.38	127.43	120.44
1	G	736	LYS	C-N-CA	5.38	127.43	120.44
2	I	459	ILE	CA-C-O	-5.38	114.66	120.47
2	B	415	LYS	N-CA-C	5.37	119.10	112.54
2	C	575	VAL	N-CA-C	5.37	115.00	107.37
2	B	674	ASN	CA-C-N	5.37	129.73	121.19
2	B	674	ASN	C-N-CA	5.37	129.73	121.19
2	I	415	LYS	N-CA-C	5.37	119.09	112.54
2	I	674	ASN	CA-C-N	5.37	129.73	121.19
2	I	674	ASN	C-N-CA	5.37	129.73	121.19
1	A	113	LYS	N-CA-C	5.37	119.78	113.23
2	E	369	ARG	N-CA-C	-5.36	107.40	114.31
2	L	604	GLU	CA-CB-CG	5.36	124.81	114.10
1	K	123	ARG	CB-CG-CD	5.35	123.60	111.30
2	J	371	PRO	CA-C-N	5.34	127.70	120.38
2	J	371	PRO	C-N-CA	5.34	127.70	120.38
1	K	173	ALA	CA-C-N	5.34	129.26	122.37
1	K	173	ALA	C-N-CA	5.34	129.26	122.37
2	E	371	PRO	CA-C-N	5.34	127.70	120.38
2	E	371	PRO	C-N-CA	5.34	127.70	120.38
2	J	369	ARG	N-CA-C	-5.34	107.42	114.31
1	A	123	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	D	726	ASP	O-C-N	-5.33	114.47	123.00
2	E	451	ARG	N-CA-C	5.33	120.91	110.56
2	F	604	GLU	CA-CB-CG	5.33	124.77	114.10
2	J	655	LEU	CA-C-N	5.33	127.69	120.38
2	J	655	LEU	C-N-CA	5.33	127.69	120.38
2	J	451	ARG	N-CA-C	5.33	120.90	110.56
1	D	123	ARG	CB-CG-CD	5.33	123.56	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	ALA	CA-C-N	5.33	129.25	122.37
1	D	173	ALA	C-N-CA	5.33	129.25	122.37
1	G	113	LYS	N-CA-C	5.33	119.73	113.23
2	I	338	VAL	CA-CB-CG1	5.32	119.45	110.40
2	F	577	LYS	O-C-N	-5.32	115.52	122.59
1	A	85	HIS	O-C-N	-5.32	114.52	122.39
2	B	338	VAL	CA-CB-CG1	5.31	119.43	110.40
2	J	674	ASN	O-C-N	-5.31	116.49	122.12
1	K	726	ASP	O-C-N	-5.31	114.50	123.00
2	L	577	LYS	O-C-N	-5.31	115.53	122.59
1	A	266	ARG	N-CA-C	5.31	117.98	111.82
1	G	123	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	G	266	ARG	N-CA-C	5.31	117.98	111.82
2	E	670	MET	O-C-N	-5.30	116.51	122.03
2	B	672	ILE	CB-CG1-CD1	-5.30	102.67	113.80
2	E	655	LEU	CA-C-N	5.30	127.64	120.38
2	E	655	LEU	C-N-CA	5.30	127.64	120.38
1	K	196	GLN	N-CA-C	5.30	117.74	111.33
1	D	196	GLN	N-CA-C	5.29	117.73	111.33
2	E	674	ASN	O-C-N	-5.29	116.51	122.12
1	G	85	HIS	O-C-N	-5.29	114.56	122.39
1	D	60	GLY	O-C-N	-5.29	117.26	123.55
1	K	124	VAL	CA-C-N	5.29	129.38	121.72
1	K	124	VAL	C-N-CA	5.29	129.38	121.72
1	D	105	THR	CA-C-N	5.28	127.36	120.28
1	D	105	THR	C-N-CA	5.28	127.36	120.28
2	I	672	ILE	CB-CG1-CD1	-5.28	102.70	113.80
2	J	670	MET	O-C-N	-5.28	116.53	122.03
1	D	124	VAL	CA-C-N	5.28	129.37	121.72
1	D	124	VAL	C-N-CA	5.28	129.37	121.72
2	E	368	GLU	CA-C-N	5.28	130.52	122.24
2	E	368	GLU	C-N-CA	5.28	130.52	122.24
1	K	299	LYS	CA-CB-CG	5.27	124.65	114.10
2	J	368	GLU	CA-C-N	5.27	130.51	122.24
2	J	368	GLU	C-N-CA	5.27	130.51	122.24
2	J	494	ILE	CA-CB-CG2	5.27	119.46	110.50
1	K	105	THR	CA-C-N	5.27	127.34	120.28
1	K	105	THR	C-N-CA	5.27	127.34	120.28
1	K	60	GLY	O-C-N	-5.26	117.29	123.55
1	D	299	LYS	CA-CB-CG	5.26	124.62	114.10
1	G	242	ILE	CA-C-N	5.26	127.28	120.44
1	G	242	ILE	C-N-CA	5.26	127.28	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	494	ILE	CA-CB-CG2	5.26	119.44	110.50
2	B	468	GLU	CA-C-N	5.25	125.81	119.98
2	B	468	GLU	C-N-CA	5.25	125.81	119.98
2	B	487	ASN	CA-C-N	-5.25	112.95	122.50
2	B	487	ASN	C-N-CA	-5.25	112.95	122.50
2	L	529	ASN	CB-CA-C	5.25	119.50	110.79
2	I	696	PHE	O-C-N	-5.25	115.61	122.59
2	B	696	PHE	O-C-N	-5.24	115.62	122.59
2	J	487	ASN	OD1-CG-ND2	5.24	127.84	122.60
1	K	247	ASP	N-CA-C	5.24	117.44	110.53
2	I	487	ASN	CA-C-N	-5.24	112.97	122.50
2	I	487	ASN	C-N-CA	-5.24	112.97	122.50
1	D	247	ASP	N-CA-C	5.23	117.44	110.53
2	I	468	GLU	CA-C-N	5.23	125.79	119.98
2	I	468	GLU	C-N-CA	5.23	125.79	119.98
1	K	81	ALA	O-C-N	-5.23	117.28	123.25
1	D	727	GLU	CA-C-N	5.23	127.60	120.54
1	D	727	GLU	C-N-CA	5.23	127.60	120.54
1	D	81	ALA	O-C-N	-5.23	117.29	123.25
1	A	242	ILE	CA-C-N	5.22	127.23	120.44
1	A	242	ILE	C-N-CA	5.22	127.23	120.44
2	J	666	VAL	CA-C-N	5.22	127.53	120.38
2	J	666	VAL	C-N-CA	5.22	127.53	120.38
1	K	727	GLU	CA-C-N	5.22	127.59	120.54
1	K	727	GLU	C-N-CA	5.22	127.59	120.54
2	E	700	GLU	CA-C-O	5.22	126.00	120.10
2	E	487	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	K	310	GLU	CA-C-N	5.21	127.61	120.46
1	K	310	GLU	C-N-CA	5.21	127.61	120.46
2	L	614	ASP	N-CA-C	5.21	116.96	111.28
2	F	529	ASN	CB-CA-C	5.21	119.44	110.79
2	L	556	ASP	CA-C-N	5.21	130.25	121.14
2	L	556	ASP	C-N-CA	5.21	130.25	121.14
2	F	614	ASP	N-CA-C	5.20	116.95	111.28
2	J	700	GLU	CA-C-O	5.20	125.97	120.10
2	E	666	VAL	CA-C-N	5.20	127.50	120.38
2	E	666	VAL	C-N-CA	5.20	127.50	120.38
2	L	575	VAL	CG1-CB-CG2	5.19	122.22	110.80
1	D	310	GLU	CA-C-N	5.19	127.57	120.46
1	D	310	GLU	C-N-CA	5.19	127.57	120.46
2	F	556	ASP	CA-C-N	5.18	130.21	121.14
2	F	556	ASP	C-N-CA	5.18	130.21	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	575	VAL	CG1-CB-CG2	5.18	122.20	110.80
2	J	336	PHE	CA-C-N	5.18	127.47	120.38
2	J	336	PHE	C-N-CA	5.18	127.47	120.38
2	F	568	ASP	CA-C-O	5.17	126.65	120.70
1	K	249	THR	CA-C-N	5.17	127.47	120.38
1	K	249	THR	C-N-CA	5.17	127.47	120.38
1	D	249	THR	CA-C-N	5.16	127.45	120.38
1	D	249	THR	C-N-CA	5.16	127.45	120.38
2	I	678	ARG	NH1-CZ-NH2	-5.16	112.59	119.30
2	J	361	ARG	CA-C-N	-5.16	114.58	120.88
2	J	361	ARG	C-N-CA	-5.16	114.58	120.88
2	L	568	ASP	CA-C-O	5.16	126.63	120.70
2	E	336	PHE	CA-C-N	5.16	127.44	120.38
2	E	336	PHE	C-N-CA	5.16	127.44	120.38
2	E	412	ILE	CA-CB-CG1	5.16	119.17	110.40
2	I	365	ILE	N-CA-CB	5.16	116.03	110.62
2	E	361	ARG	CA-C-N	-5.15	114.59	120.88
2	E	361	ARG	C-N-CA	-5.15	114.59	120.88
2	J	412	ILE	CA-CB-CG1	5.15	119.16	110.40
2	E	685	ILE	CA-C-N	5.15	127.50	120.54
2	E	685	ILE	C-N-CA	5.15	127.50	120.54
2	I	495	GLY	CA-C-O	5.15	127.95	122.03
2	B	495	GLY	CA-C-O	5.15	127.95	122.03
2	J	685	ILE	CA-C-N	5.15	127.49	120.54
2	J	685	ILE	C-N-CA	5.15	127.49	120.54
1	G	92	THR	N-CA-C	-5.14	107.03	113.72
2	L	604	GLU	N-CA-CB	5.14	118.25	109.87
2	B	365	ILE	N-CA-CB	5.14	116.02	110.62
2	F	604	GLU	N-CA-CB	5.13	118.24	109.87
2	B	678	ARG	NH1-CZ-NH2	-5.13	112.63	119.30
1	G	87	LYS	O-C-N	5.13	129.41	122.59
1	K	303	GLN	CB-CG-CD	5.13	121.32	112.60
1	A	92	THR	N-CA-C	-5.13	107.05	113.72
1	D	164	VAL	N-CA-C	5.13	119.67	113.00
2	L	616	TRP	CA-C-N	5.13	127.15	120.28
2	L	616	TRP	C-N-CA	5.13	127.15	120.28
1	K	164	VAL	N-CA-C	5.13	119.67	113.00
1	D	303	GLN	CB-CG-CD	5.12	121.31	112.60
2	J	494	ILE	N-CA-CB	5.12	123.19	111.30
2	F	616	TRP	CA-C-N	5.12	127.14	120.28
2	F	616	TRP	C-N-CA	5.12	127.14	120.28
1	A	87	LYS	O-C-N	5.12	129.40	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	556	ASP	N-CA-C	5.12	119.28	113.19
2	E	494	ILE	N-CA-CB	5.12	123.17	111.30
1	D	155	GLN	N-CA-C	-5.11	105.78	111.36
2	F	593	GLN	N-CA-C	5.11	116.06	108.60
2	C	560	GLU	CA-C-O	-5.11	115.53	120.89
1	G	282	ASN	O-C-N	-5.11	116.71	122.12
2	H	560	GLU	CA-C-O	-5.10	115.53	120.89
1	K	155	GLN	N-CA-C	-5.10	105.80	111.36
2	E	693	THR	CB-CA-C	-5.10	102.33	110.79
2	F	556	ASP	N-CA-C	5.09	119.25	113.19
2	I	678	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	282	ASN	O-C-N	-5.09	116.72	122.12
1	A	102	GLU	CA-C-N	5.09	127.10	120.28
1	A	102	GLU	C-N-CA	5.09	127.10	120.28
2	J	693	THR	CB-CA-C	-5.09	102.34	110.79
2	E	420	ILE	CA-CB-CG2	5.09	119.15	110.50
2	L	593	GLN	N-CA-C	5.08	116.02	108.60
2	J	420	ILE	CA-CB-CG2	5.08	119.13	110.50
2	C	528	ILE	N-CA-CB	5.07	117.55	111.31
1	G	102	GLU	CA-C-N	5.07	127.08	120.28
1	G	102	GLU	C-N-CA	5.07	127.08	120.28
2	B	480	ASP	CA-C-N	5.07	131.10	121.97
2	B	480	ASP	C-N-CA	5.07	131.10	121.97
1	G	87	LYS	CB-CG-CD	5.07	122.96	111.30
1	A	87	LYS	CB-CG-CD	5.06	122.94	111.30
1	G	124	VAL	CA-C-N	5.06	129.58	122.09
1	G	124	VAL	C-N-CA	5.06	129.58	122.09
2	H	528	ILE	N-CA-CB	5.06	117.53	111.31
2	I	480	ASP	CA-C-N	5.06	131.08	121.97
2	I	480	ASP	C-N-CA	5.06	131.08	121.97
1	A	124	VAL	CA-C-N	5.05	129.57	122.09
1	A	124	VAL	C-N-CA	5.05	129.57	122.09
1	G	21	SER	CA-C-N	5.05	127.05	120.28
1	G	21	SER	C-N-CA	5.05	127.05	120.28
1	G	41	SER	CA-CB-OG	5.05	121.21	111.10
1	A	194	ASP	CA-C-N	5.05	125.33	119.47
1	A	194	ASP	C-N-CA	5.05	125.33	119.47
2	I	699	SER	CA-C-N	5.05	127.55	120.28
2	I	699	SER	C-N-CA	5.05	127.55	120.28
1	K	310	GLU	CA-C-O	5.05	125.90	120.55
1	A	21	SER	CA-C-N	5.05	127.04	120.28
1	A	21	SER	C-N-CA	5.05	127.04	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	SER	CA-CB-OG	5.04	121.19	111.10
2	C	630	VAL	CA-CB-CG1	-5.04	101.83	110.40
2	E	685	ILE	O-C-N	-5.04	116.27	122.57
2	H	630	VAL	CA-CB-CG1	-5.04	101.83	110.40
2	B	416	GLN	CA-C-N	5.04	127.58	120.42
2	B	416	GLN	C-N-CA	5.04	127.58	120.42
2	B	699	SER	CA-C-N	5.04	127.53	120.28
2	B	699	SER	C-N-CA	5.04	127.53	120.28
2	J	685	ILE	O-C-N	-5.04	116.27	122.57
2	J	485	TYR	CG-CD1-CE1	-5.04	113.65	121.20
2	B	678	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	D	310	GLU	CA-C-O	5.03	125.88	120.55
1	G	194	ASP	CA-C-N	5.03	125.30	119.47
1	G	194	ASP	C-N-CA	5.03	125.30	119.47
1	G	262	HIS	CA-C-N	5.02	124.80	119.28
1	G	262	HIS	C-N-CA	5.02	124.80	119.28
2	C	614	ASP	N-CA-C	5.01	116.74	111.28
2	E	485	TYR	CG-CD1-CE1	-5.01	113.69	121.20
2	E	449	TYR	CB-CG-CD2	-5.00	113.29	120.80
1	A	262	HIS	CA-C-N	5.00	124.78	119.28
1	A	262	HIS	C-N-CA	5.00	124.78	119.28
2	E	494	ILE	CB-CA-C	5.00	117.48	111.13
2	I	416	GLN	CA-C-N	5.00	127.52	120.42
2	I	416	GLN	C-N-CA	5.00	127.52	120.42

All (54) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	726	ASP	CA
2	B	339	ASP	CA
2	B	442	CYS	CA
2	B	489	ASN	CA
2	B	490	HIS	CA
2	B	707	SER	CA
2	C	534	MET	CA
2	C	560	GLU	CA
2	C	563	TYR	CA
2	C	630	VAL	CA
2	E	339	ASP	CA
2	E	442	CYS	CA
2	E	445	LYS	CA
2	E	452	LEU	CA

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Mol	Chain	Res	Type	Atom
2	E	454	GLU	CA
2	E	490	HIS	CA
2	E	491	GLU	CA
2	E	492	ASP	CA
2	E	494	ILE	CB
2	E	672	ILE	CB
2	F	529	ASN	CA
2	F	534	MET	CA
2	F	560	GLU	CA
2	F	574	ASP	CA
2	F	575	VAL	CA
2	F	581	SER	CA
2	F	627	PRO	CA
1	G	726	ASP	CA
2	H	534	MET	CA
2	H	560	GLU	CA
2	H	563	TYR	CA
2	H	630	VAL	CA
2	I	339	ASP	CA
2	I	442	CYS	CA
2	I	489	ASN	CA
2	I	490	HIS	CA
2	I	707	SER	CA
2	J	339	ASP	CA
2	J	442	CYS	CA
2	J	445	LYS	CA
2	J	452	LEU	CA
2	J	454	GLU	CA
2	J	490	HIS	CA
2	J	491	GLU	CA
2	J	492	ASP	CA
2	J	494	ILE	CB
2	J	672	ILE	CB
2	L	529	ASN	CA
2	L	534	MET	CA
2	L	560	GLU	CA
2	L	574	ASP	CA
2	L	575	VAL	CA
2	L	581	SER	CA
2	L	627	PRO	CA

All (240) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	THR	Mainchain
1	A	123	ARG	Sidechain
1	A	177	ALA	Mainchain
1	A	206	LYS	Mainchain
1	A	228	ARG	Sidechain
1	A	233	GLY	Mainchain
1	A	237	ARG	Sidechain
1	A	28	ASP	Mainchain
1	A	41	SER	Mainchain
1	A	50	ASN	Sidechain
1	A	727	GLU	Mainchain
2	B	336	PHE	Sidechain
2	B	337	ALA	Mainchain
2	B	339	ASP	Mainchain
2	B	340	PHE	Mainchain,Sidechain
2	B	341	GLU	Mainchain
2	B	358	GLY	Mainchain
2	B	361	ARG	Mainchain
2	B	362	ILE	Mainchain
2	B	371	PRO	Mainchain
2	B	391	ALA	Mainchain
2	B	409	PHE	Sidechain
2	B	414	LYS	Mainchain
2	B	440	ARG	Mainchain,Sidechain
2	B	441	GLN	Mainchain
2	B	461	THR	Peptide
2	B	467	ARG	Mainchain,Sidechain
2	B	470	ARG	Sidechain
2	B	483	LEU	Mainchain
2	B	485	TYR	Sidechain
2	B	486	MET	Peptide
2	B	487	ASN	Mainchain
2	B	488	THR	Mainchain,Peptide
2	B	490	HIS	Mainchain,Sidechain
2	B	491	GLU	Mainchain
2	B	492	ASP	Mainchain
2	B	654	GLN	Mainchain
2	B	669	TYR	Sidechain
2	B	678	ARG	Mainchain,Sidechain
2	B	696	PHE	Sidechain
2	B	698	PHE	Sidechain
2	B	699	SER	Mainchain
2	B	700	GLU	Mainchain

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Mol	Chain	Res	Type	Group
2	B	702	LEU	Peptide
2	B	706	TYR	Sidechain
2	C	532	GLY	Mainchain
2	C	564	MET	Mainchain
2	C	569	ASN	Mainchain
2	C	576	GLU	Mainchain
2	C	579	PHE	Sidechain
2	C	584	HIS	Sidechain
2	C	594	ARG	Sidechain
2	C	607	CYS	Mainchain
2	C	629	ARG	Sidechain
1	D	125	TYR	Sidechain
1	D	177	ALA	Mainchain
1	D	206	LYS	Mainchain
1	D	221	GLU	Mainchain
1	D	237	ARG	Sidechain
1	D	313	GLU	Mainchain
1	D	316	ASN	Mainchain
1	D	318	ARG	Mainchain,Sidechain
1	D	41	SER	Mainchain
1	D	43	GLY	Mainchain
1	D	50	ASN	Sidechain
1	D	62	GLY	Mainchain
1	D	82	GLU	Mainchain
2	E	339	ASP	Mainchain
2	E	340	PHE	Mainchain,Sidechain
2	E	358	GLY	Mainchain
2	E	361	ARG	Mainchain
2	E	370	PHE	Sidechain
2	E	371	PRO	Mainchain
2	E	378	GLU	Mainchain
2	E	381	GLU	Peptide
2	E	414	LYS	Mainchain
2	E	440	ARG	Sidechain
2	E	448	GLN	Mainchain
2	E	449	TYR	Mainchain,Sidechain
2	E	451	ARG	Sidechain
2	E	453	ARG	Mainchain
2	E	455	GLU	Sidechain
2	E	457	GLU	Sidechain
2	E	467	ARG	Mainchain
2	E	469	GLY	Mainchain

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Mol	Chain	Res	Type	Group
2	E	470	ARG	Sidechain
2	E	482	GLU	Mainchain
2	E	485	TYR	Sidechain
2	E	489	ASN	Mainchain,Peptide
2	E	490	HIS	Mainchain,Sidechain
2	E	491	GLU	Peptide
2	E	492	ASP	Peptide
2	E	494	ILE	Mainchain
2	E	653	PRO	Mainchain
2	E	654	GLN	Mainchain
2	E	670	MET	Mainchain
2	E	678	ARG	Mainchain
2	E	696	PHE	Sidechain
2	E	698	PHE	Sidechain
2	F	522	ARG	Sidechain
2	F	532	GLY	Mainchain
2	F	563	TYR	Mainchain,Sidechain
2	F	569	ASN	Mainchain,Sidechain
2	F	576	GLU	Mainchain
2	F	581	SER	Mainchain
2	F	594	ARG	Sidechain
2	F	607	CYS	Mainchain
1	G	105	THR	Mainchain
1	G	123	ARG	Sidechain
1	G	177	ALA	Mainchain
1	G	197	GLY	Mainchain
1	G	206	LYS	Mainchain
1	G	228	ARG	Sidechain
1	G	233	GLY	Mainchain
1	G	237	ARG	Sidechain
1	G	28	ASP	Mainchain
1	G	41	SER	Mainchain
1	G	50	ASN	Sidechain
1	G	727	GLU	Mainchain
2	H	532	GLY	Mainchain
2	H	564	MET	Mainchain
2	H	569	ASN	Mainchain
2	H	576	GLU	Mainchain
2	H	579	PHE	Sidechain
2	H	584	HIS	Sidechain
2	H	594	ARG	Sidechain
2	H	607	CYS	Mainchain

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Mol	Chain	Res	Type	Group
2	H	629	ARG	Sidechain
2	I	336	PHE	Sidechain
2	I	337	ALA	Mainchain
2	I	339	ASP	Mainchain
2	I	340	PHE	Mainchain,Sidechain
2	I	358	GLY	Mainchain
2	I	361	ARG	Mainchain
2	I	362	ILE	Mainchain
2	I	371	PRO	Mainchain
2	I	391	ALA	Mainchain
2	I	409	PHE	Sidechain
2	I	414	LYS	Mainchain
2	I	440	ARG	Mainchain,Sidechain
2	I	441	GLN	Mainchain
2	I	461	THR	Peptide
2	I	467	ARG	Mainchain,Sidechain
2	I	470	ARG	Sidechain
2	I	483	LEU	Mainchain
2	I	485	TYR	Sidechain
2	I	486	MET	Peptide
2	I	487	ASN	Mainchain
2	I	488	THR	Mainchain,Peptide
2	I	490	HIS	Mainchain,Sidechain
2	I	491	GLU	Mainchain
2	I	492	ASP	Mainchain
2	I	654	GLN	Mainchain
2	I	669	TYR	Sidechain
2	I	678	ARG	Mainchain,Sidechain
2	I	696	PHE	Sidechain
2	I	698	PHE	Sidechain
2	I	699	SER	Mainchain
2	I	700	GLU	Mainchain
2	I	702	LEU	Peptide
2	I	706	TYR	Sidechain
2	J	339	ASP	Mainchain
2	J	340	PHE	Mainchain,Sidechain
2	J	358	GLY	Mainchain
2	J	361	ARG	Mainchain
2	J	362	ILE	Mainchain
2	J	370	PHE	Sidechain
2	J	371	PRO	Mainchain
2	J	378	GLU	Mainchain

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Mol	Chain	Res	Type	Group
2	J	381	GLU	Peptide
2	J	414	LYS	Mainchain
2	J	440	ARG	Sidechain
2	J	448	GLN	Mainchain
2	J	449	TYR	Mainchain,Sidechain
2	J	451	ARG	Sidechain
2	J	453	ARG	Mainchain
2	J	455	GLU	Sidechain
2	J	457	GLU	Sidechain
2	J	467	ARG	Mainchain
2	J	469	GLY	Mainchain
2	J	470	ARG	Sidechain
2	J	485	TYR	Sidechain
2	J	489	ASN	Mainchain,Peptide
2	J	490	HIS	Mainchain,Sidechain
2	J	491	GLU	Peptide
2	J	492	ASP	Peptide
2	J	494	ILE	Mainchain
2	J	653	PRO	Mainchain
2	J	654	GLN	Mainchain
2	J	670	MET	Mainchain
2	J	678	ARG	Mainchain
2	J	696	PHE	Sidechain
2	J	698	PHE	Sidechain
1	K	125	TYR	Sidechain
1	K	177	ALA	Mainchain
1	K	206	LYS	Mainchain
1	K	221	GLU	Mainchain
1	K	237	ARG	Sidechain
1	K	313	GLU	Mainchain
1	K	316	ASN	Mainchain
1	K	318	ARG	Mainchain,Sidechain
1	K	41	SER	Mainchain
1	K	43	GLY	Mainchain
1	K	50	ASN	Sidechain
1	K	62	GLY	Mainchain
1	K	82	GLU	Mainchain
2	L	522	ARG	Sidechain
2	L	532	GLY	Mainchain
2	L	563	TYR	Mainchain,Sidechain
2	L	569	ASN	Mainchain,Sidechain
2	L	576	GLU	Mainchain

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Mol	Chain	Res	Type	Group
2	L	581	SER	Mainchain
2	L	594	ARG	Sidechain
2	L	607	CYS	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2567	0	2629	80	0
1	D	2643	0	2693	169	0
1	G	2567	0	2629	76	0
1	K	2643	0	2693	173	0
2	B	1728	0	1780	205	0
2	C	946	0	939	29	0
2	E	1728	0	1780	294	0
2	F	946	0	938	29	0
2	H	946	0	939	29	0
2	I	1728	0	1780	103	0
2	J	1728	0	1780	197	0
2	L	946	0	938	27	0
All	All	21116	0	21518	1106	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 26.

All (1106) 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)
2:J:491:GLU:CB	2:J:491:GLU:CA	1.74	1.58
2:E:491:GLU:CB	2:E:491:GLU:CA	1.74	1.57
2:B:338:VAL:HG13	2:E:687:HIS:CE1	1.40	1.54
2:B:463:HIS:HE1	2:E:334:GLN:CD	1.19	1.46
2:J:453:ARG:HG2	1:K:318:ARG:N	1.17	1.44
1:D:318:ARG:N	2:E:453:ARG:HG2	1.17	1.44
2:J:455:GLU:N	1:K:318:ARG:NH2	1.64	1.41
1:D:318:ARG:NH2	2:E:455:GLU:N	1.64	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:463:HIS:CE1	2:E:334:GLN:NE2	1.91	1.39
2:B:698:PHE:CG	2:E:695:GLU:HG3	1.55	1.38
1:D:318:ARG:CA	2:E:453:ARG:HG2	1.56	1.35
2:J:453:ARG:HG2	1:K:318:ARG:CA	1.56	1.35
2:B:707:SER:CA	2:E:704:ASN:HD21	1.31	1.34
2:B:703:ALA:CB	2:E:700:GLU:HA	1.55	1.33
2:J:449:TYR:CG	1:K:316:ASN:N	1.68	1.30
2:B:707:SER:C	2:E:704:ASN:HD21	1.38	1.29
1:D:318:ARG:N	2:E:453:ARG:CG	1.94	1.28
2:J:454:GLU:H	1:K:318:ARG:CB	1.46	1.28
2:J:453:ARG:CG	1:K:318:ARG:N	1.94	1.28
1:D:318:ARG:CB	2:E:454:GLU:H	1.46	1.28
2:B:463:HIS:CE1	2:E:334:GLN:CD	2.08	1.27
1:D:316:ASN:N	2:E:449:TYR:CG	1.68	1.27
2:J:454:GLU:N	1:K:318:ARG:HB2	1.48	1.26
1:D:318:ARG:HB2	2:E:454:GLU:N	1.48	1.26
2:B:338:VAL:CG1	2:E:687:HIS:CE1	2.19	1.25
2:B:330:LEU:HD21	2:E:466:GLU:OE1	1.30	1.24
2:B:463:HIS:CE1	2:E:334:GLN:OE1	1.96	1.18
2:B:463:HIS:HE1	2:E:334:GLN:OE1	1.23	1.17
2:J:449:TYR:CD1	1:K:316:ASN:N	2.12	1.17
1:D:316:ASN:N	2:E:449:TYR:CD1	2.12	1.17
2:B:467:ARG:HH21	2:E:334:GLN:HG2	1.06	1.16
2:B:330:LEU:HD11	2:E:466:GLU:HB3	1.26	1.15
2:B:342:LYS:CE	2:I:392:ILE:O	1.95	1.15
1:D:317:PHE:HB3	2:E:453:ARG:HD2	1.17	1.14
2:J:455:GLU:N	1:K:318:ARG:CZ	2.10	1.13
1:D:318:ARG:CZ	2:E:455:GLU:N	2.10	1.13
2:E:491:GLU:CB	2:E:491:GLU:C	2.21	1.13
2:J:491:GLU:CB	2:J:491:GLU:C	2.21	1.13
2:B:703:ALA:HB2	2:E:700:GLU:HA	1.17	1.12
2:J:453:ARG:HD2	1:K:317:PHE:HB3	1.17	1.11
2:B:330:LEU:HD13	2:E:467:ARG:NH1	1.67	1.10
2:B:698:PHE:CB	2:E:695:GLU:HG3	1.81	1.10
2:B:463:HIS:CE1	2:E:334:GLN:HE22	1.54	1.10
2:J:453:ARG:HB3	1:K:317:PHE:CA	1.83	1.09
2:B:330:LEU:HD11	2:E:466:GLU:CB	1.83	1.08
1:D:317:PHE:CA	2:E:453:ARG:HB3	1.83	1.07
2:B:706:TYR:CE2	2:E:700:GLU:OE1	2.08	1.07
1:D:317:PHE:CE1	2:E:443:THR:O	2.08	1.06
2:J:443:THR:O	1:K:317:PHE:CE1	2.08	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:698:PHE:CD1	2:E:695:GLU:HG3	1.90	1.06
2:B:330:LEU:CD1	2:E:466:GLU:HB3	1.84	1.06
2:B:702:LEU:HB2	2:E:700:GLU:CD	1.80	1.05
2:B:698:PHE:HB3	2:E:695:GLU:HB3	1.32	1.04
1:D:222:ASN:O	1:K:319:PRO:HB2	1.58	1.03
1:D:316:ASN:HB2	2:E:449:TYR:CE1	1.93	1.02
2:J:449:TYR:CE1	1:K:316:ASN:HB2	1.93	1.02
1:D:318:ARG:HB2	2:E:454:GLU:H	0.96	1.01
2:B:704:ASN:OD1	2:E:704:ASN:HA	1.61	1.01
2:J:454:GLU:H	1:K:318:ARG:HB2	0.96	1.00
2:B:698:PHE:HB3	2:E:695:GLU:CB	1.91	0.99
2:B:330:LEU:CD1	2:E:467:ARG:HH12	1.74	0.98
1:D:314:TYR:OH	2:E:450:PRO:CB	2.03	0.98
1:D:318:ARG:NH2	2:E:455:GLU:CA	2.26	0.98
1:D:314:TYR:OH	2:E:450:PRO:HB2	1.61	0.97
2:B:330:LEU:HD13	2:E:467:ARG:HH12	0.82	0.97
2:J:450:PRO:HB2	1:K:314:TYR:OH	1.61	0.97
1:D:318:ARG:HB2	2:E:453:ARG:C	1.88	0.97
2:J:455:GLU:CA	1:K:318:ARG:NH2	2.26	0.97
2:J:450:PRO:CB	1:K:314:TYR:OH	2.03	0.96
2:J:453:ARG:CG	1:K:317:PHE:C	2.37	0.96
2:J:453:ARG:C	1:K:318:ARG:HB2	1.88	0.96
1:D:317:PHE:C	2:E:453:ARG:CG	2.37	0.96
2:J:453:ARG:HB3	1:K:317:PHE:C	1.91	0.96
2:B:702:LEU:HB2	2:E:700:GLU:OE2	1.66	0.96
2:J:328:ALA:HB2	1:K:316:ASN:CG	1.91	0.96
1:D:316:ASN:CG	2:E:328:ALA:HB2	1.91	0.95
2:B:707:SER:CA	2:E:704:ASN:ND2	2.02	0.95
1:D:317:PHE:C	2:E:453:ARG:HB3	1.91	0.95
2:B:330:LEU:HD11	2:E:466:GLU:CG	1.96	0.95
2:B:707:SER:C	2:E:704:ASN:ND2	2.19	0.94
2:B:467:ARG:NH2	2:E:334:GLN:HG2	1.81	0.94
2:B:703:ALA:CB	2:E:700:GLU:CA	2.45	0.94
2:B:330:LEU:CD2	2:E:466:GLU:OE1	2.16	0.94
2:J:471:THR:HG21	2:J:689:MET:HG2	1.50	0.93
2:E:471:THR:HG21	2:E:689:MET:HG2	1.50	0.92
2:B:414:LYS:HD2	2:B:483:LEU:HB3	1.52	0.92
2:I:414:LYS:HD2	2:I:483:LEU:HB3	1.52	0.92
1:G:12:LEU:HB3	1:G:745:ILE:HG12	1.52	0.92
1:D:317:PHE:HA	2:E:453:ARG:HB3	1.51	0.92
1:A:12:LEU:HB3	1:A:745:ILE:HG12	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HB2	1:A:235:VAL:HG22	1.52	0.91
2:B:463:HIS:ND1	2:E:334:GLN:NE2	2.19	0.91
2:B:695:GLU:OE1	2:E:694:LYS:NZ	2.03	0.91
2:J:453:ARG:HB3	1:K:317:PHE:HA	1.51	0.91
1:G:207:LEU:HB2	1:G:235:VAL:HG22	1.52	0.90
2:B:342:LYS:NZ	2:I:392:ILE:O	2.04	0.90
2:J:453:ARG:CB	1:K:318:ARG:N	2.35	0.90
2:J:453:ARG:CA	1:K:318:ARG:HB2	2.01	0.89
1:D:317:PHE:C	2:E:453:ARG:CB	2.45	0.89
1:D:318:ARG:N	2:E:453:ARG:CB	2.35	0.89
2:J:453:ARG:CB	1:K:317:PHE:C	2.45	0.89
1:D:318:ARG:HB2	2:E:453:ARG:CA	2.01	0.89
2:B:707:SER:N	2:E:704:ASN:ND2	2.20	0.89
2:B:703:ALA:HB1	2:E:700:GLU:HA	1.55	0.88
1:G:67:ARG:HD3	1:G:105:THR:HA	1.54	0.87
2:B:698:PHE:CB	2:E:695:GLU:CG	2.53	0.87
1:A:67:ARG:HD3	1:A:105:THR:HA	1.54	0.87
2:B:338:VAL:HG13	2:E:687:HIS:HE1	1.08	0.86
2:B:698:PHE:HB3	2:E:695:GLU:CG	2.05	0.86
1:D:316:ASN:CA	2:E:449:TYR:CD1	2.58	0.86
2:J:454:GLU:H	1:K:318:ARG:HB3	1.40	0.86
2:J:452:LEU:O	1:K:318:ARG:NE	2.09	0.86
2:J:449:TYR:CD1	1:K:316:ASN:CA	2.58	0.86
1:D:235:VAL:HB	1:D:255:GLU:HA	1.57	0.86
2:F:561:LYS:HD2	2:F:564:MET:HB2	1.58	0.86
2:L:561:LYS:HD2	2:L:564:MET:HB2	1.58	0.86
1:D:318:ARG:NE	2:E:452:LEU:O	2.08	0.86
1:K:235:VAL:HB	1:K:255:GLU:HA	1.57	0.86
2:B:345:GLU:HA	2:B:345:GLU:OE1	1.76	0.85
2:I:345:GLU:HA	2:I:345:GLU:OE1	1.76	0.85
1:K:9:LEU:HD11	1:K:289:ILE:HD12	1.55	0.85
1:D:9:LEU:HD11	1:D:289:ILE:HD12	1.55	0.85
1:D:34:ILE:HD13	1:D:170:LEU:HD23	1.58	0.85
1:K:34:ILE:HD13	1:K:170:LEU:HD23	1.58	0.85
1:D:318:ARG:HB3	2:E:454:GLU:H	1.40	0.84
1:A:31:LEU:HG	1:A:285:LEU:HD22	1.58	0.84
1:G:31:LEU:HG	1:G:285:LEU:HD22	1.58	0.84
2:B:700:GLU:HB3	2:E:699:SER:HB2	1.60	0.84
2:B:330:LEU:O	2:E:470:ARG:NH2	2.11	0.84
1:D:317:PHE:C	2:E:453:ARG:HG2	2.00	0.83
2:B:672:ILE:HD11	2:J:489:ASN:HA	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:391:ALA:HB1	2:I:408:ALA:HB1	1.59	0.83
2:J:451:ARG:O	1:K:318:ARG:HD3	1.79	0.83
1:D:137:LEU:HB3	1:D:160:LEU:HD22	1.61	0.82
1:K:137:LEU:HB3	1:K:160:LEU:HD22	1.61	0.82
1:D:170:LEU:HD21	1:D:281:LEU:HD22	1.60	0.82
1:D:318:ARG:HD3	2:E:451:ARG:O	1.79	0.82
2:B:391:ALA:HB1	2:B:408:ALA:HB1	1.59	0.82
2:E:489:ASN:HA	2:I:672:ILE:HD11	1.61	0.82
1:K:170:LEU:HD21	1:K:281:LEU:HD22	1.60	0.81
2:B:342:LYS:HE2	2:I:392:ILE:O	1.80	0.81
2:B:695:GLU:CD	2:E:694:LYS:NZ	2.39	0.81
2:J:345:GLU:OE1	2:J:345:GLU:HA	1.81	0.80
1:D:317:PHE:CD1	2:E:443:THR:O	2.34	0.80
1:D:318:ARG:CZ	2:E:454:GLU:CA	2.60	0.80
2:J:454:GLU:CA	1:K:318:ARG:CZ	2.60	0.80
2:J:443:THR:O	1:K:317:PHE:CD1	2.34	0.79
1:D:318:ARG:CB	2:E:454:GLU:N	2.23	0.79
2:E:421:ARG:HG2	2:E:479:ILE:HD13	1.62	0.79
2:J:454:GLU:N	1:K:318:ARG:CB	2.23	0.79
2:E:345:GLU:OE1	2:E:345:GLU:HA	1.81	0.79
2:B:698:PHE:HB3	2:E:695:GLU:HG3	1.64	0.79
2:B:698:PHE:CD1	2:E:695:GLU:CG	2.67	0.78
1:D:317:PHE:CE2	2:E:445:LYS:HA	2.19	0.78
1:D:318:ARG:NH2	2:E:455:GLU:HB2	1.98	0.78
2:J:421:ARG:HG2	2:J:479:ILE:HD13	1.62	0.78
2:J:445:LYS:HA	1:K:317:PHE:CE2	2.19	0.78
1:D:222:ASN:O	1:K:319:PRO:CB	2.32	0.78
2:J:422:GLU:HB3	2:J:423:PRO:HD3	1.64	0.78
2:B:698:PHE:CD2	2:E:695:GLU:HG3	2.18	0.78
2:J:455:GLU:HB2	1:K:318:ARG:NH2	1.98	0.78
1:G:59:ARG:HB3	1:G:242:ILE:HG23	1.67	0.77
1:D:16:LEU:HD23	1:D:29:LEU:HD11	1.66	0.77
2:E:422:GLU:HB3	2:E:423:PRO:HD3	1.64	0.77
1:A:206:LYS:HE2	1:A:238:SER:HA	1.66	0.77
2:B:346:GLY:HA3	2:I:654:GLN:H	1.49	0.77
2:B:491:GLU:HG3	2:J:494:ILE:HB	1.66	0.77
1:A:59:ARG:HB3	1:A:242:ILE:HG23	1.67	0.76
2:E:407:MET:HE2	2:I:474:GLN:HG2	1.67	0.76
2:B:474:GLN:HG2	2:J:407:MET:HE2	1.67	0.76
2:B:698:PHE:CG	2:E:695:GLU:CG	2.52	0.76
1:G:206:LYS:HE2	1:G:238:SER:HA	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:16:LEU:HD23	1:K:29:LEU:HD11	1.65	0.76
2:B:422:GLU:HB3	2:B:423:PRO:HD3	1.68	0.76
2:I:422:GLU:HB3	2:I:423:PRO:HD3	1.68	0.76
1:D:317:PHE:CB	2:E:453:ARG:HD2	2.09	0.75
1:K:40:GLN:HB2	1:K:141:THR:HG22	1.68	0.75
2:J:453:ARG:CG	1:K:318:ARG:CA	2.52	0.75
2:J:455:GLU:CB	1:K:318:ARG:NH2	2.49	0.75
2:B:707:SER:N	2:E:704:ASN:HD21	1.81	0.75
2:E:494:ILE:HB	2:I:491:GLU:HG3	1.66	0.75
1:A:191:LYS:HA	1:A:195:PRO:HA	1.69	0.75
1:G:191:LYS:HA	1:G:195:PRO:HA	1.69	0.74
1:A:27:ALA:HB1	1:A:296:LEU:HD12	1.68	0.74
1:D:40:GLN:HB2	1:D:141:THR:HG22	1.68	0.74
2:I:702:LEU:H	2:I:702:LEU:CD2	1.99	0.74
1:D:318:ARG:NH2	2:E:455:GLU:CB	2.49	0.74
1:G:27:ALA:HB1	1:G:296:LEU:HD12	1.68	0.74
2:L:573:ARG:HD2	2:L:575:VAL:HG12	1.70	0.74
2:J:453:ARG:HD2	1:K:317:PHE:CB	2.09	0.74
1:D:317:PHE:CD1	2:E:444:LYS:HA	2.23	0.73
2:B:374:LEU:HD13	2:B:423:PRO:HB2	1.71	0.73
2:B:702:LEU:H	2:B:702:LEU:CD2	1.99	0.73
2:B:699:SER:HB2	2:E:696:PHE:HA	1.69	0.73
2:I:374:LEU:HD13	2:I:423:PRO:HB2	1.71	0.73
1:K:161:MET:HA	1:K:164:VAL:HG22	1.69	0.73
1:D:161:MET:HA	1:D:164:VAL:HG22	1.69	0.73
2:J:444:LYS:HA	1:K:317:PHE:CD1	2.23	0.73
1:D:317:PHE:C	2:E:453:ARG:CD	2.62	0.72
2:J:453:ARG:CD	1:K:317:PHE:C	2.62	0.72
2:B:695:GLU:HG3	2:E:698:PHE:CE1	2.24	0.72
1:A:83:PHE:HZ	1:A:97:VAL:HG13	1.55	0.72
2:B:702:LEU:CB	2:E:700:GLU:OE2	2.38	0.72
1:G:83:PHE:HZ	1:G:97:VAL:HG13	1.55	0.72
2:F:573:ARG:HD2	2:F:575:VAL:HG12	1.70	0.71
2:B:330:LEU:HD11	2:E:466:GLU:HG2	1.71	0.71
1:D:81:ALA:HB1	1:D:122:LEU:HD11	1.72	0.71
1:K:81:ALA:HB1	1:K:122:LEU:HD11	1.72	0.71
2:J:450:PRO:HD2	1:K:314:TYR:CE2	2.13	0.71
2:B:346:GLY:C	2:I:654:GLN:HB3	2.16	0.71
1:G:48:LEU:HG	1:G:134:LEU:HD23	1.72	0.71
2:J:444:LYS:HA	1:K:317:PHE:CG	2.26	0.70
1:G:140:MET:HE2	1:G:160:LEU:HD21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:PHE:HB2	1:D:86:CYS:HB2	1.72	0.70
1:D:314:TYR:CE2	2:E:450:PRO:HD2	2.13	0.70
1:D:317:PHE:CG	2:E:444:LYS:HA	2.26	0.70
2:E:688:LEU:N	2:E:688:LEU:HD23	2.07	0.70
2:J:453:ARG:CD	1:K:317:PHE:O	2.40	0.70
1:A:48:LEU:HG	1:A:134:LEU:HD23	1.72	0.70
1:A:140:MET:HE2	1:A:160:LEU:HD21	1.73	0.70
2:B:703:ALA:HB1	2:E:700:GLU:CA	2.19	0.70
2:E:702:LEU:HD23	2:E:702:LEU:H	1.55	0.70
2:B:692:ASN:C	2:B:692:ASN:HD22	2.00	0.70
1:D:318:ARG:CZ	2:E:454:GLU:C	2.64	0.70
2:J:688:LEU:N	2:J:688:LEU:HD23	2.07	0.70
2:J:453:ARG:CD	1:K:317:PHE:HB3	2.11	0.70
2:J:454:GLU:C	1:K:318:ARG:CZ	2.64	0.70
2:J:702:LEU:HD23	2:J:702:LEU:H	1.55	0.70
2:I:687:HIS:CD2	2:I:688:LEU:CD2	2.75	0.69
2:I:692:ASN:C	2:I:692:ASN:HD22	2.00	0.69
1:K:83:PHE:HB2	1:K:86:CYS:HB2	1.72	0.69
2:L:518:ILE:HG13	2:L:519:LEU:H	1.57	0.69
1:D:317:PHE:CB	2:E:453:ARG:HB3	2.22	0.69
2:I:688:LEU:N	2:I:688:LEU:HD23	2.07	0.69
1:K:36:VAL:HG22	1:K:48:LEU:HD22	1.74	0.69
2:B:330:LEU:HD21	2:E:466:GLU:CD	2.14	0.69
2:B:346:GLY:HA3	2:I:654:GLN:N	2.06	0.69
1:D:36:VAL:HG22	1:D:48:LEU:HD22	1.74	0.69
1:D:316:ASN:CG	2:E:328:ALA:CB	2.66	0.69
1:D:317:PHE:O	2:E:453:ARG:CD	2.40	0.69
2:B:338:VAL:CG1	2:E:687:HIS:NE2	2.55	0.69
2:B:687:HIS:CD2	2:B:688:LEU:CD2	2.75	0.69
2:J:453:ARG:HB3	1:K:317:PHE:CB	2.22	0.69
1:A:29:LEU:HD23	1:A:289:ILE:HG12	1.74	0.69
2:J:687:HIS:CD2	2:J:688:LEU:CD2	2.75	0.69
1:A:57:LEU:HD22	1:A:136:ASP:HB2	1.74	0.69
1:G:29:LEU:HD23	1:G:289:ILE:HG12	1.74	0.69
2:B:698:PHE:HE1	2:E:692:ASN:HA	1.57	0.69
2:B:699:SER:OG	2:E:695:GLU:O	2.10	0.69
2:I:687:HIS:CD2	2:I:688:LEU:HD21	2.27	0.69
2:J:328:ALA:CB	1:K:316:ASN:CG	2.66	0.69
2:J:692:ASN:C	2:J:692:ASN:HD22	2.00	0.69
2:B:687:HIS:CD2	2:B:688:LEU:HD21	2.28	0.69
2:E:412:ILE:HG21	2:E:666:VAL:HG11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:HD13	1:A:745:ILE:HA	1.75	0.69
2:E:687:HIS:CD2	2:E:688:LEU:CD2	2.75	0.69
2:B:688:LEU:HD23	2:B:688:LEU:N	2.07	0.68
2:B:692:ASN:HA	2:E:341:GLU:OE2	1.93	0.68
1:G:57:LEU:HD22	1:G:136:ASP:HB2	1.74	0.68
1:G:12:LEU:HD13	1:G:745:ILE:HA	1.75	0.68
2:J:412:ILE:HG21	2:J:666:VAL:HG11	1.74	0.68
2:E:687:HIS:CD2	2:E:688:LEU:HD21	2.28	0.68
2:J:687:HIS:CD2	2:J:688:LEU:HD21	2.28	0.68
2:I:452:LEU:HD13	2:I:452:LEU:C	2.19	0.68
1:K:85:HIS:HE1	1:K:120:ILE:HG23	1.59	0.68
2:F:518:ILE:HG13	2:F:519:LEU:H	1.57	0.68
1:D:66:ARG:HG2	1:D:115:ILE:HG22	1.75	0.68
2:B:452:LEU:HD13	2:B:452:LEU:C	2.19	0.68
2:E:692:ASN:C	2:E:692:ASN:HD22	2.00	0.68
2:H:565:LEU:HD11	2:H:596:VAL:HG22	1.76	0.67
1:K:303:GLN:HG2	1:K:735:LEU:HD11	1.76	0.67
2:C:565:LEU:HD11	2:C:596:VAL:HG22	1.76	0.67
1:K:66:ARG:HG2	1:K:115:ILE:HG22	1.76	0.67
1:D:303:GLN:HG2	1:D:735:LEU:HD11	1.76	0.67
2:B:695:GLU:HA	2:E:695:GLU:OE1	1.94	0.67
1:D:318:ARG:CA	2:E:453:ARG:CG	2.52	0.67
2:J:449:TYR:CE1	1:K:316:ASN:CB	2.76	0.67
2:C:518:ILE:HG13	2:C:519:LEU:H	1.59	0.67
2:E:491:GLU:C	2:E:491:GLU:CG	2.68	0.67
2:J:428:VAL:HG13	2:J:689:MET:HE3	1.76	0.67
2:B:338:VAL:CG1	2:E:687:HIS:HE1	1.83	0.67
2:E:428:VAL:HG13	2:E:689:MET:HE3	1.76	0.67
2:B:421:ARG:HD3	2:B:476:MET:HE1	1.76	0.66
2:I:421:ARG:HD3	2:I:476:MET:HE1	1.76	0.66
2:H:518:ILE:HG13	2:H:519:LEU:H	1.59	0.66
2:J:491:GLU:C	2:J:491:GLU:CG	2.68	0.66
2:B:341:GLU:OE1	2:E:691:ASN:ND2	2.27	0.66
1:D:60:GLY:H	1:D:64:VAL:HG13	1.60	0.66
2:C:522:ARG:HH12	2:C:615:SER:HB2	1.61	0.66
1:K:60:GLY:H	1:K:64:VAL:HG13	1.61	0.66
1:D:85:HIS:HE1	1:D:120:ILE:HG23	1.59	0.66
2:B:341:GLU:HG3	2:B:698:PHE:HE2	1.61	0.66
1:D:317:PHE:HB3	2:E:453:ARG:CD	2.11	0.66
2:H:522:ARG:HH12	2:H:615:SER:HB2	1.61	0.66
2:I:341:GLU:HG3	2:I:698:PHE:HE2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:445:LYS:HA	1:K:317:PHE:HE2	1.62	0.65
2:B:706:TYR:HE2	2:E:700:GLU:OE1	1.78	0.65
1:D:17:GLN:HG3	1:D:29:LEU:HD12	1.77	0.65
1:K:17:GLN:HG3	1:K:29:LEU:HD12	1.77	0.65
2:B:699:SER:CB	2:E:696:PHE:HA	2.26	0.65
2:C:578:GLY:HA3	2:C:585:ILE:HD12	1.78	0.65
2:J:690:ILE:HG22	2:J:691:ASN:N	2.11	0.64
2:H:578:GLY:HA3	2:H:585:ILE:HD12	1.78	0.64
1:K:98:ARG:HH22	1:K:245:LYS:HD2	1.63	0.64
1:A:56:PHE:HB3	1:A:94:PHE:HB3	1.78	0.64
2:B:338:VAL:HG11	2:E:687:HIS:NE2	2.12	0.64
2:B:342:LYS:HE3	2:I:392:ILE:O	1.93	0.64
1:D:316:ASN:CB	2:E:449:TYR:CE1	2.77	0.64
2:E:690:ILE:HG22	2:E:691:ASN:N	2.11	0.64
2:J:410:GLU:HG3	2:J:486:MET:HE1	1.78	0.64
2:J:448:GLN:HB3	1:K:313:GLU:HB2	1.80	0.64
2:L:574:ASP:H	2:L:630:VAL:HB	1.62	0.64
2:B:702:LEU:HG	2:E:700:GLU:OE2	1.98	0.64
1:D:98:ARG:HH22	1:D:245:LYS:HD2	1.63	0.64
1:D:313:GLU:HB2	2:E:448:GLN:HB3	1.79	0.64
2:E:435:LEU:HD11	2:E:693:THR:HB	1.79	0.64
1:G:56:PHE:HB3	1:G:94:PHE:HB3	1.78	0.64
2:B:703:ALA:HA	2:E:700:GLU:HB3	1.79	0.64
1:G:176:PRO:HB3	1:G:206:LYS:HD2	1.80	0.63
1:D:317:PHE:HE2	2:E:445:LYS:HA	1.62	0.63
2:F:574:ASP:H	2:F:630:VAL:HB	1.62	0.63
1:G:217:ARG:HG3	1:G:265:TYR:HE1	1.62	0.63
2:E:410:GLU:HG3	2:E:486:MET:HE1	1.78	0.63
2:B:690:ILE:HG22	2:B:691:ASN:N	2.14	0.63
2:J:435:LEU:HD11	2:J:693:THR:HB	1.79	0.63
1:A:217:ARG:HG3	1:A:265:TYR:HE1	1.62	0.62
1:D:20:PHE:HB3	1:D:27:ALA:HA	1.80	0.62
1:K:20:PHE:HB3	1:K:27:ALA:HA	1.80	0.62
2:B:680:LEU:HD21	2:J:406:ASP:HB3	1.81	0.62
2:I:690:ILE:HG22	2:I:691:ASN:N	2.14	0.62
1:A:161:MET:HA	1:A:164:VAL:HG22	1.82	0.62
1:G:161:MET:HA	1:G:164:VAL:HG22	1.82	0.62
2:J:681:MET:HB2	2:J:682:PRO:HD3	1.81	0.62
2:E:406:ASP:HB3	2:I:680:LEU:HD21	1.81	0.62
2:J:495:GLY:HA2	2:J:664:ASN:HB3	1.81	0.62
1:A:176:PRO:HB3	1:A:206:LYS:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:495:GLY:HA2	2:E:664:ASN:HB3	1.81	0.61
2:E:681:MET:HB2	2:E:682:PRO:HD3	1.81	0.61
1:D:318:ARG:N	2:E:453:ARG:CA	2.63	0.61
2:B:681:MET:HB2	2:B:682:PRO:HD3	1.83	0.61
2:B:698:PHE:CE1	2:E:692:ASN:HA	2.36	0.61
2:B:703:ALA:CA	2:E:700:GLU:HA	2.29	0.61
2:I:681:MET:HB2	2:I:682:PRO:HD3	1.83	0.61
1:G:209:LEU:HD11	1:G:238:SER:HB3	1.83	0.61
2:B:496:PHE:HA	2:B:660:GLU:HG3	1.83	0.61
2:I:496:PHE:HA	2:I:660:GLU:HG3	1.83	0.61
2:J:453:ARG:CA	1:K:318:ARG:N	2.63	0.61
1:K:256:ARG:HH12	1:K:269:ALA:HB1	1.65	0.61
2:C:567:VAL:HA	2:C:570:LEU:HD12	1.82	0.61
2:J:340:PHE:HE2	2:J:694:LYS:HA	1.65	0.61
1:D:10:ILE:HB	1:D:11:PRO:HD3	1.82	0.60
1:D:29:LEU:HD22	1:D:289:ILE:HG23	1.83	0.60
2:J:495:GLY:O	2:J:496:PHE:HB2	2.00	0.60
1:D:256:ARG:HH12	1:D:269:ALA:HB1	1.65	0.60
2:F:518:ILE:HG13	2:F:519:LEU:N	2.16	0.60
2:H:567:VAL:HA	2:H:570:LEU:HD12	1.82	0.60
1:D:318:ARG:CB	2:E:453:ARG:HG2	2.30	0.60
1:K:29:LEU:HD22	1:K:289:ILE:HG23	1.83	0.60
1:A:232:ILE:HG21	1:A:277:LEU:HA	1.82	0.60
2:E:340:PHE:HE2	2:E:694:LYS:HA	1.65	0.60
1:G:87:LYS:HE2	1:G:88:GLY:HA3	1.83	0.60
1:G:232:ILE:HG21	1:G:277:LEU:HA	1.82	0.60
2:L:518:ILE:HG13	2:L:519:LEU:N	2.16	0.60
1:A:87:LYS:HE2	1:A:88:GLY:HA3	1.83	0.60
2:B:706:TYR:CD2	2:E:700:GLU:OE1	2.55	0.60
2:E:495:GLY:O	2:E:496:PHE:HB2	2.00	0.60
1:A:23:ILE:HG22	1:A:25:GLN:HG2	1.83	0.60
1:K:290:ARG:HD3	1:K:745:ILE:HG22	1.84	0.60
1:A:209:LEU:HD11	1:A:238:SER:HB3	1.83	0.60
1:K:10:ILE:HB	1:K:11:PRO:HD3	1.82	0.60
2:L:565:LEU:HD21	2:L:570:LEU:HD21	1.83	0.60
2:C:518:ILE:HG13	2:C:519:LEU:N	2.16	0.59
2:E:660:GLU:HA	2:E:663:ARG:HH12	1.67	0.59
2:J:454:GLU:C	1:K:318:ARG:NH2	2.55	0.59
2:F:565:LEU:HD21	2:F:570:LEU:HD21	1.84	0.59
2:H:518:ILE:HG13	2:H:519:LEU:N	2.16	0.59
2:B:333:VAL:HG12	2:B:333:VAL:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:374:LEU:HD13	2:J:423:PRO:HB2	1.83	0.59
1:G:23:ILE:HG22	1:G:25:GLN:HG2	1.83	0.59
2:I:333:VAL:HG12	2:I:333:VAL:O	2.01	0.59
2:L:573:ARG:HA	2:L:630:VAL:HA	1.85	0.59
2:C:607:CYS:HB2	2:C:613:VAL:HG23	1.85	0.59
1:D:300:LEU:HB2	1:D:739:LEU:HD21	1.85	0.59
2:F:573:ARG:HA	2:F:630:VAL:HA	1.85	0.59
2:B:695:GLU:CD	2:E:694:LYS:HZ1	2.08	0.59
2:E:491:GLU:CA	2:E:491:GLU:CG	2.67	0.59
2:B:703:ALA:HA	2:E:700:GLU:CB	2.32	0.59
1:G:94:PHE:HZ	1:G:124:VAL:HG11	1.68	0.59
2:C:579:PHE:CD1	2:C:579:PHE:N	2.70	0.59
2:E:374:LEU:HD13	2:E:423:PRO:HB2	1.83	0.58
2:H:607:CYS:HB2	2:H:613:VAL:HG23	1.84	0.58
2:J:660:GLU:HA	2:J:663:ARG:HH12	1.67	0.58
2:J:450:PRO:HD3	1:K:314:TYR:O	2.03	0.58
1:A:70:VAL:HG23	1:A:119:PRO:HB3	1.85	0.58
2:B:388:ILE:HD12	2:B:412:ILE:HD12	1.86	0.58
2:B:495:GLY:O	2:B:496:PHE:HB2	2.04	0.58
2:J:491:GLU:OE1	2:J:492:ASP:N	2.37	0.58
1:D:290:ARG:HD3	1:D:745:ILE:HG22	1.84	0.58
1:D:314:TYR:O	2:E:450:PRO:HD3	2.03	0.58
1:G:70:VAL:HG23	1:G:119:PRO:HB3	1.85	0.58
2:I:495:GLY:O	2:I:496:PHE:HB2	2.04	0.58
2:J:333:VAL:HG12	2:J:333:VAL:O	2.03	0.58
1:A:94:PHE:HZ	1:A:124:VAL:HG11	1.68	0.58
2:B:695:GLU:CD	2:E:694:LYS:HZ2	1.95	0.58
2:B:702:LEU:CD2	2:B:702:LEU:N	2.67	0.58
2:E:491:GLU:OE1	2:E:492:ASP:N	2.37	0.58
2:I:388:ILE:HD12	2:I:412:ILE:HD12	1.86	0.58
2:I:428:VAL:HG11	2:I:472:LYS:HG3	1.86	0.58
1:K:43:GLY:HA3	1:K:236:ASN:HD22	1.68	0.58
2:J:344:ILE:HD12	2:J:694:LYS:HG3	1.86	0.58
2:E:702:LEU:N	2:E:702:LEU:CD2	2.67	0.58
2:J:702:LEU:N	2:J:702:LEU:CD2	2.67	0.57
1:K:300:LEU:HB2	1:K:739:LEU:HD21	1.85	0.57
1:D:43:GLY:HA3	1:D:236:ASN:HD22	1.68	0.57
2:J:450:PRO:CD	1:K:314:TYR:O	2.53	0.57
2:B:340:PHE:O	2:B:341:GLU:C	2.43	0.57
2:B:428:VAL:HG11	2:B:472:LYS:HG3	1.86	0.57
1:D:314:TYR:O	2:E:450:PRO:CD	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:333:VAL:HG12	2:E:333:VAL:O	2.02	0.57
2:J:471:THR:HG22	2:J:688:LEU:HB2	1.87	0.57
2:E:471:THR:HG22	2:E:688:LEU:HB2	1.87	0.57
2:F:579:PHE:N	2:F:579:PHE:HD1	2.02	0.57
1:G:235:VAL:HB	1:G:255:GLU:HB2	1.87	0.57
2:H:583:LYS:HD2	2:H:606:ALA:HB1	1.87	0.57
1:K:87:LYS:HD3	1:K:87:LYS:H	1.70	0.57
2:B:388:ILE:HG12	2:B:666:VAL:HG21	1.87	0.57
2:B:670:MET:HE2	2:B:670:MET:HA	1.85	0.57
2:E:344:ILE:HD12	2:E:694:LYS:HG3	1.86	0.57
2:J:491:GLU:CA	2:J:491:GLU:CG	2.67	0.57
1:A:69:LEU:HD13	1:A:101:ILE:HG12	1.86	0.56
1:D:241:ASP:HB3	1:D:246:LYS:HD2	1.85	0.56
1:D:316:ASN:N	2:E:449:TYR:CB	2.58	0.56
1:D:317:PHE:CG	2:E:444:LYS:CA	2.87	0.56
2:F:579:PHE:N	2:F:579:PHE:CD1	2.72	0.56
1:A:13:VAL:HG11	1:A:289:ILE:HD13	1.87	0.56
2:B:688:LEU:O	2:B:689:MET:C	2.45	0.56
2:E:392:ILE:HG13	2:E:393:LYS:HG2	1.88	0.56
1:G:13:VAL:HG11	1:G:289:ILE:HD13	1.87	0.56
2:I:340:PHE:O	2:I:341:GLU:C	2.43	0.56
2:I:388:ILE:HG12	2:I:666:VAL:HG21	1.87	0.56
2:I:392:ILE:HG13	2:I:393:LYS:HG2	1.86	0.56
2:I:670:MET:HE2	2:I:670:MET:HA	1.85	0.56
2:I:688:LEU:O	2:I:689:MET:C	2.45	0.56
2:J:392:ILE:HG13	2:J:393:LYS:HG2	1.88	0.56
2:J:453:ARG:HG2	1:K:318:ARG:CB	2.29	0.56
1:D:157:ARG:HH22	1:D:188:LYS:HD3	1.71	0.56
2:E:489:ASN:N	2:E:489:ASN:OD1	2.38	0.56
2:J:702:LEU:H	2:J:702:LEU:CD2	2.18	0.56
1:K:241:ASP:HB3	1:K:246:LYS:HD2	1.86	0.56
1:K:252:LEU:HD21	1:K:274:THR:HB	1.88	0.56
2:C:583:LYS:HD2	2:C:606:ALA:HB1	1.87	0.56
1:K:157:ARG:HH22	1:K:188:LYS:HD3	1.71	0.56
2:L:579:PHE:CD1	2:L:579:PHE:N	2.72	0.56
2:B:345:GLU:OE1	2:B:345:GLU:CA	2.52	0.56
2:B:687:HIS:CG	2:B:688:LEU:HD23	2.41	0.56
1:G:69:LEU:HD13	1:G:101:ILE:HG12	1.86	0.56
2:B:392:ILE:HG13	2:B:393:LYS:HG2	1.86	0.56
2:E:491:GLU:OE1	2:E:492:ASP:HA	2.06	0.56
2:J:470:ARG:HG3	2:J:470:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:579:PHE:N	2:L:579:PHE:HD1	2.02	0.56
2:C:571:LYS:HD3	2:C:591:THR:HG21	1.87	0.56
2:E:340:PHE:O	2:E:341:GLU:C	2.48	0.56
2:I:470:ARG:HG3	2:I:470:ARG:HH11	1.71	0.56
2:J:489:ASN:N	2:J:489:ASN:OD1	2.38	0.56
1:A:235:VAL:HB	1:A:255:GLU:HB2	1.87	0.55
2:E:470:ARG:HG3	2:E:470:ARG:HH11	1.71	0.55
2:I:687:HIS:CG	2:I:688:LEU:HD23	2.41	0.55
1:G:15:ARG:HG3	1:G:15:ARG:HH11	1.71	0.55
1:G:66:ARG:HB2	1:G:105:THR:HG21	1.88	0.55
2:H:579:PHE:N	2:H:579:PHE:CD1	2.70	0.55
1:A:66:ARG:HB2	1:A:105:THR:HG21	1.88	0.55
2:B:495:GLY:HA2	2:B:664:ASN:HB2	1.89	0.55
1:D:87:LYS:HD3	1:D:87:LYS:H	1.70	0.55
2:H:571:LYS:HD3	2:H:591:THR:HG21	1.87	0.55
1:K:218:ASP:HB3	1:K:224:LEU:HB2	1.88	0.55
1:D:56:PHE:HA	1:D:98:ARG:HB2	1.89	0.55
2:I:491:GLU:OE2	2:I:492:ASP:N	2.39	0.55
2:J:340:PHE:O	2:J:341:GLU:C	2.48	0.55
1:D:65:THR:HB	1:D:138:PRO:HA	1.88	0.55
2:I:495:GLY:HA2	2:I:664:ASN:HB2	1.89	0.55
1:K:56:PHE:HA	1:K:98:ARG:HB2	1.89	0.55
2:L:562:LYS:O	2:L:563:TYR:HB2	2.07	0.55
2:B:491:GLU:OE2	2:B:492:ASP:N	2.39	0.55
2:I:702:LEU:CD2	2:I:702:LEU:N	2.67	0.55
1:K:65:THR:HB	1:K:138:PRO:HA	1.88	0.55
2:C:579:PHE:N	2:C:579:PHE:HD1	2.03	0.55
1:D:229:ARG:HD2	1:D:280:VAL:HG22	1.89	0.55
1:D:252:LEU:HD21	1:D:274:THR:HB	1.88	0.55
1:D:318:ARG:CD	2:E:452:LEU:O	2.54	0.55
1:K:229:ARG:HD2	1:K:280:VAL:HG22	1.89	0.55
1:D:6:MET:HE3	1:D:282:ASN:HB3	1.89	0.55
2:I:345:GLU:OE1	2:I:345:GLU:CA	2.52	0.55
1:D:317:PHE:O	2:E:453:ARG:HD3	2.07	0.54
2:J:452:LEU:O	1:K:318:ARG:CD	2.54	0.54
2:J:491:GLU:OE1	2:J:492:ASP:HA	2.06	0.54
2:E:388:ILE:HD11	2:E:666:VAL:HG11	1.89	0.54
1:G:271:ARG:O	1:G:272:MET:HE2	2.08	0.54
2:J:388:ILE:HD11	2:J:666:VAL:HG11	1.89	0.54
2:J:688:LEU:O	2:J:689:MET:C	2.46	0.54
1:K:6:MET:HE3	1:K:282:ASN:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ASP:HB3	1:D:224:LEU:HB2	1.89	0.54
2:E:409:PHE:HE2	2:E:486:MET:HB3	1.72	0.54
2:H:579:PHE:N	2:H:579:PHE:HD1	2.03	0.54
2:J:453:ARG:HD3	1:K:317:PHE:O	2.07	0.54
1:K:57:LEU:HD22	1:K:136:ASP:HB2	1.89	0.54
2:E:702:LEU:H	2:E:702:LEU:CD2	2.18	0.54
2:J:362:ILE:CG2	2:J:363:ASN:N	2.70	0.54
2:J:409:PHE:HE2	2:J:486:MET:HB3	1.72	0.54
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.71	0.54
2:B:470:ARG:HH11	2:B:470:ARG:HG3	1.71	0.54
1:D:57:LEU:HD22	1:D:136:ASP:HB2	1.89	0.54
2:F:562:LYS:O	2:F:563:TYR:HB2	2.07	0.54
2:L:570:LEU:HD13	2:L:588:LEU:HD13	1.90	0.54
2:E:688:LEU:O	2:E:689:MET:C	2.46	0.54
2:F:570:LEU:HD13	2:F:588:LEU:HD13	1.90	0.54
1:A:271:ARG:O	1:A:272:MET:HE2	2.08	0.53
2:B:695:GLU:HG3	2:E:698:PHE:CZ	2.43	0.53
2:E:687:HIS:CG	2:E:688:LEU:HD23	2.42	0.53
1:G:274:THR:HB	1:G:275:PRO:HD3	1.90	0.53
2:J:453:ARG:HG2	1:K:318:ARG:C	2.31	0.53
2:J:687:HIS:CG	2:J:688:LEU:HD23	2.42	0.53
2:E:362:ILE:CG2	2:E:363:ASN:N	2.70	0.53
1:A:274:THR:HB	1:A:275:PRO:HD3	1.90	0.53
2:B:346:GLY:HA3	2:I:654:GLN:CB	2.39	0.53
2:B:703:ALA:HB1	2:E:700:GLU:C	2.33	0.53
2:E:436:ILE:HG13	2:E:464:ILE:HG21	1.90	0.53
2:B:362:ILE:CG2	2:B:363:ASN:N	2.72	0.53
2:H:577:LYS:HE3	2:H:577:LYS:H	1.73	0.53
2:I:702:LEU:H	2:I:702:LEU:HD22	1.74	0.53
1:K:36:VAL:HG13	1:K:48:LEU:HD13	1.91	0.53
2:C:577:LYS:HE3	2:C:577:LYS:H	1.73	0.53
1:D:36:VAL:HG13	1:D:48:LEU:HD13	1.91	0.53
1:D:117:PRO:HB2	1:D:159:MET:HE1	1.89	0.53
1:K:307:ILE:HB	1:K:728:MET:HG3	1.91	0.53
2:B:702:LEU:H	2:B:702:LEU:HD22	1.74	0.53
2:J:491:GLU:CB	2:J:491:GLU:O	2.55	0.53
2:B:485:TYR:HB3	2:J:485:TYR:CE2	2.44	0.53
2:E:485:TYR:CE2	2:I:485:TYR:HB3	2.44	0.53
2:I:362:ILE:CG2	2:I:363:ASN:N	2.72	0.53
2:J:436:ILE:HG13	2:J:464:ILE:HG21	1.90	0.53
2:B:409:PHE:CE2	2:B:486:MET:HE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:361:ARG:O	2:I:362:ILE:C	2.52	0.52
2:J:370:PHE:CE1	2:J:427:CYS:HB2	2.44	0.52
2:J:370:PHE:N	2:J:371:PRO:HD2	2.24	0.52
1:A:33:GLN:HB2	1:A:133:THR:HB	1.90	0.52
2:C:574:ASP:H	2:C:630:VAL:HG21	1.74	0.52
2:I:702:LEU:N	2:I:702:LEU:HD22	2.24	0.52
2:I:459:ILE:HD13	2:I:704:ASN:HB3	1.90	0.52
2:J:417:VAL:HG21	2:J:482:GLU:HB2	1.90	0.52
1:K:117:PRO:HB2	1:K:159:MET:HE1	1.89	0.52
2:L:577:LYS:HE3	2:L:577:LYS:H	1.74	0.52
1:D:318:ARG:HB2	2:E:453:ARG:N	2.24	0.52
2:H:574:ASP:H	2:H:630:VAL:HG21	1.74	0.52
2:J:451:ARG:O	1:K:318:ARG:CD	2.55	0.52
2:B:459:ILE:HD13	2:B:704:ASN:HB3	1.90	0.52
1:D:318:ARG:CD	2:E:451:ARG:O	2.55	0.52
2:J:453:ARG:N	1:K:318:ARG:HB2	2.24	0.52
1:G:33:GLN:HB2	1:G:133:THR:HB	1.90	0.52
2:B:361:ARG:O	2:B:362:ILE:C	2.52	0.52
2:E:370:PHE:N	2:E:371:PRO:HD2	2.24	0.52
2:B:702:LEU:N	2:B:702:LEU:HD22	2.24	0.52
2:E:370:PHE:CE1	2:E:427:CYS:HB2	2.44	0.52
2:E:490:HIS:CD2	2:I:490:HIS:HA	2.45	0.52
2:E:417:VAL:HG21	2:E:482:GLU:HB2	1.90	0.52
2:F:577:LYS:HE3	2:F:577:LYS:H	1.75	0.52
1:G:31:LEU:HD21	1:G:130:LEU:HD12	1.92	0.52
2:J:452:LEU:C	1:K:318:ARG:CD	2.83	0.52
2:J:453:ARG:CA	1:K:318:ARG:CB	2.84	0.52
2:B:346:GLY:CA	2:I:654:GLN:HB3	2.39	0.51
2:B:384:LEU:HD22	2:B:670:MET:HG2	1.92	0.51
2:B:707:SER:C	2:E:458:ARG:HH22	2.18	0.51
2:E:371:PRO:HA	2:E:374:LEU:HD23	1.92	0.51
2:J:371:PRO:HA	2:J:374:LEU:HD23	1.92	0.51
1:K:232:ILE:HD11	1:K:276:TYR:HD2	1.75	0.51
1:A:31:LEU:HD21	1:A:130:LEU:HD12	1.92	0.51
2:I:409:PHE:CE2	2:I:486:MET:HE3	2.45	0.51
2:J:361:ARG:O	2:J:362:ILE:C	2.51	0.51
2:J:445:LYS:CA	1:K:317:PHE:CE2	2.93	0.51
2:B:490:HIS:HA	2:J:490:HIS:CD2	2.45	0.51
1:D:307:ILE:HB	1:D:728:MET:HG3	1.91	0.51
2:J:453:ARG:HG2	1:K:318:ARG:O	2.11	0.51
2:C:545:LEU:HD13	2:C:550:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:587:ALA:HB1	2:C:602:GLN:HB2	1.93	0.51
1:D:232:ILE:HD11	1:D:276:TYR:HD2	1.76	0.51
2:I:337:ALA:HB1	2:I:698:PHE:CD1	2.46	0.51
2:L:579:PHE:HD1	2:L:579:PHE:H	1.59	0.51
2:B:337:ALA:HB1	2:B:698:PHE:CD1	2.46	0.51
1:D:318:ARG:CD	2:E:452:LEU:C	2.83	0.51
1:G:300:LEU:HB3	1:G:735:LEU:HD22	1.92	0.51
1:K:66:ARG:O	1:K:67:ARG:HG3	2.11	0.51
1:K:74:VAL:HG21	1:K:123:ARG:HH21	1.76	0.51
1:K:221:GLU:HG2	1:K:268:LEU:HD11	1.92	0.51
2:H:587:ALA:HB1	2:H:602:GLN:HB2	1.93	0.51
2:I:384:LEU:HD22	2:I:670:MET:HG2	1.92	0.51
1:A:83:PHE:HB2	1:A:86:CYS:HB2	1.94	0.50
2:B:491:GLU:O	2:B:491:GLU:HG2	2.10	0.50
1:D:318:ARG:O	2:E:453:ARG:HG2	2.11	0.50
2:E:361:ARG:O	2:E:362:ILE:C	2.51	0.50
1:G:83:PHE:HB2	1:G:86:CYS:HB2	1.94	0.50
2:H:545:LEU:HD13	2:H:550:LEU:HD13	1.93	0.50
2:I:369:ARG:C	2:I:369:ARG:CD	2.84	0.50
2:J:450:PRO:HB2	1:K:314:TYR:HH	1.75	0.50
1:A:300:LEU:HB3	1:A:735:LEU:HD22	1.92	0.50
2:E:478:LEU:HA	2:E:481:ILE:HD12	1.94	0.50
2:I:329:LEU:HD23	2:I:706:TYR:CE1	2.47	0.50
2:I:491:GLU:O	2:I:491:GLU:HG2	2.10	0.50
2:L:545:LEU:HD13	2:L:550:LEU:HD13	1.94	0.50
2:C:526:LEU:HB2	2:C:543:PHE:CE1	2.46	0.50
1:D:66:ARG:O	1:D:67:ARG:HG3	2.11	0.50
2:H:526:LEU:HB2	2:H:543:PHE:CE1	2.46	0.50
2:B:329:LEU:HD23	2:B:706:TYR:CE1	2.47	0.50
2:B:369:ARG:CD	2:B:369:ARG:C	2.84	0.50
2:E:369:ARG:C	2:E:369:ARG:CD	2.85	0.50
2:J:369:ARG:C	2:J:369:ARG:CD	2.85	0.50
2:B:700:GLU:N	2:E:699:SER:OG	2.44	0.50
2:E:345:GLU:OE1	2:E:345:GLU:CA	2.57	0.50
2:L:596:VAL:HG11	2:L:603:LEU:HB2	1.93	0.50
1:D:221:GLU:HG2	1:D:268:LEU:HD11	1.92	0.50
1:D:317:PHE:CE2	2:E:445:LYS:CA	2.93	0.50
2:E:387:GLU:HB2	2:E:412:ILE:HG23	1.94	0.50
2:E:491:GLU:C	2:E:491:GLU:CD	2.80	0.50
2:F:545:LEU:HD13	2:F:550:LEU:HD13	1.94	0.50
2:F:579:PHE:HD1	2:F:579:PHE:H	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:491:GLU:C	2:J:491:GLU:CD	2.80	0.50
2:B:707:SER:H	2:E:704:ASN:ND2	2.07	0.50
1:D:318:ARG:HD3	2:E:452:LEU:C	2.37	0.50
2:J:340:PHE:CE2	2:J:694:LYS:HA	2.45	0.50
2:J:452:LEU:C	1:K:318:ARG:HD3	2.37	0.50
2:J:478:LEU:HA	2:J:481:ILE:HD12	1.94	0.50
1:K:303:GLN:HE21	1:K:735:LEU:HD21	1.77	0.50
2:C:553:TYR:CG	2:C:558:GLU:HG2	2.47	0.49
1:D:74:VAL:HG21	1:D:123:ARG:HH21	1.76	0.49
2:J:345:GLU:OE1	2:J:345:GLU:CA	2.57	0.49
2:J:453:ARG:N	1:K:318:ARG:N	2.60	0.49
2:F:596:VAL:HG11	2:F:603:LEU:HB2	1.93	0.49
2:J:387:GLU:HB2	2:J:412:ILE:HG23	1.94	0.49
2:J:417:VAL:HG12	2:J:670:MET:HE1	1.94	0.49
2:E:417:VAL:HG12	2:E:670:MET:HE1	1.94	0.49
2:J:362:ILE:HG23	2:J:363:ASN:N	2.27	0.49
1:D:303:GLN:HE21	1:D:735:LEU:HD21	1.77	0.49
2:B:334:GLN:NE2	2:E:692:ASN:HD21	2.11	0.49
2:C:579:PHE:HD1	2:C:579:PHE:H	1.59	0.49
2:E:370:PHE:CE2	2:E:374:LEU:HD21	2.48	0.49
1:G:37:VAL:HG22	1:G:171:ILE:HG23	1.94	0.49
2:H:553:TYR:CG	2:H:558:GLU:HG2	2.47	0.49
2:B:467:ARG:HE	2:E:334:GLN:HG3	1.77	0.49
1:D:318:ARG:N	2:E:453:ARG:N	2.60	0.49
1:K:135:VAL:HG12	1:K:137:LEU:HG	1.94	0.49
1:A:83:PHE:CZ	1:A:97:VAL:HG13	2.43	0.49
1:D:318:ARG:C	2:E:453:ARG:HG2	2.31	0.49
2:F:525:TRP:HB3	2:F:540:GLU:HG2	1.95	0.49
2:I:384:LEU:HD11	2:I:412:ILE:HG22	1.94	0.49
1:A:217:ARG:HD2	1:A:264:SER:HB3	1.94	0.49
1:D:135:VAL:HG12	1:D:137:LEU:HG	1.94	0.49
2:L:525:TRP:HB3	2:L:540:GLU:HG2	1.95	0.49
2:J:328:ALA:HB2	1:K:316:ASN:ND2	2.27	0.49
2:E:676:THR:HG22	2:E:680:LEU:HD22	1.93	0.49
2:J:332:MET:SD	1:K:317:PHE:CE2	3.06	0.49
1:A:37:VAL:HG22	1:A:171:ILE:HG23	1.94	0.48
1:A:40:GLN:O	1:A:41:SER:HB3	2.13	0.48
1:D:229:ARG:HG3	1:D:280:VAL:CG1	2.43	0.48
2:E:692:ASN:C	2:E:692:ASN:ND2	2.70	0.48
2:I:377:MET:HG3	2:I:422:GLU:HG2	1.95	0.48
2:B:341:GLU:CD	2:E:691:ASN:HD22	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:PHE:CE2	2:E:332:MET:SD	3.06	0.48
2:E:491:GLU:CB	2:E:491:GLU:O	2.55	0.48
1:G:217:ARG:HD2	1:G:264:SER:HB3	1.94	0.48
2:H:579:PHE:HD1	2:H:579:PHE:H	1.59	0.48
2:I:672:ILE:C	2:I:672:ILE:HD12	2.38	0.48
2:J:370:PHE:CE2	2:J:374:LEU:HD21	2.48	0.48
2:J:676:THR:HG22	2:J:680:LEU:HD22	1.93	0.48
2:B:461:THR:HB	2:B:465:ARG:HE	1.79	0.48
2:I:370:PHE:N	2:I:371:PRO:HD2	2.28	0.48
2:B:370:PHE:N	2:B:371:PRO:HD2	2.28	0.48
2:B:672:ILE:C	2:B:672:ILE:HD12	2.38	0.48
2:E:340:PHE:CE2	2:E:694:LYS:HA	2.45	0.48
2:J:370:PHE:CZ	2:J:374:LEU:HD21	2.49	0.48
1:A:33:GLN:CB	1:A:133:THR:HB	2.43	0.48
2:B:377:MET:HG3	2:B:422:GLU:HG2	1.95	0.48
1:D:221:GLU:CG	1:D:268:LEU:HD11	2.44	0.48
2:B:384:LEU:HD11	2:B:412:ILE:HG22	1.94	0.48
1:G:33:GLN:CB	1:G:133:THR:HB	2.43	0.48
1:K:229:ARG:HG3	1:K:280:VAL:CG1	2.43	0.48
2:B:362:ILE:HG23	2:B:363:ASN:N	2.29	0.48
2:E:362:ILE:HG23	2:E:363:ASN:N	2.27	0.48
2:E:370:PHE:CZ	2:E:374:LEU:HD21	2.49	0.48
1:G:40:GLN:O	1:G:41:SER:HB3	2.13	0.48
1:K:221:GLU:CG	1:K:268:LEU:HD11	2.44	0.48
2:B:371:PRO:HA	2:B:374:LEU:HD23	1.96	0.48
1:D:318:ARG:N	2:E:453:ARG:H	2.11	0.48
2:I:428:VAL:HG13	2:I:689:MET:HE1	1.96	0.48
2:I:461:THR:HB	2:I:465:ARG:HE	1.78	0.48
2:B:370:PHE:CE1	2:B:427:CYS:HB2	2.49	0.48
2:B:428:VAL:HG13	2:B:689:MET:HE1	1.96	0.48
2:I:362:ILE:HG23	2:I:363:ASN:N	2.29	0.48
2:B:687:HIS:HD2	2:B:688:LEU:HD21	1.77	0.47
2:J:449:TYR:CB	1:K:316:ASN:N	2.58	0.47
2:B:485:TYR:CD1	2:J:481:ILE:HG21	2.49	0.47
1:G:173:ALA:HB1	1:G:187:LEU:HD23	1.97	0.47
2:J:384:LEU:HD22	2:J:670:MET:HB2	1.96	0.47
1:A:173:ALA:HB1	1:A:187:LEU:HD23	1.96	0.47
1:D:318:ARG:NH2	2:E:454:GLU:C	2.56	0.47
2:J:453:ARG:H	1:K:318:ARG:N	2.11	0.47
1:A:9:LEU:HG	1:A:286:THR:HG23	1.95	0.47
2:B:380:ASP:OD1	2:B:380:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:699:SER:HG	2:E:695:GLU:C	2.17	0.47
1:D:12:LEU:HG	1:D:745:ILE:HG12	1.96	0.47
1:D:42:ALA:HB1	1:D:174:VAL:HB	1.97	0.47
2:E:702:LEU:HD23	2:E:702:LEU:N	2.25	0.47
1:G:9:LEU:HG	1:G:286:THR:HG23	1.95	0.47
1:K:12:LEU:HG	1:K:745:ILE:HG12	1.96	0.47
1:K:201:ILE:HD12	1:K:277:LEU:HD12	1.95	0.47
1:D:201:ILE:HD12	1:D:277:LEU:HD12	1.95	0.47
2:E:384:LEU:HD11	2:E:412:ILE:HG22	1.96	0.47
2:E:481:ILE:HG21	2:I:485:TYR:CD1	2.49	0.47
2:H:567:VAL:HA	2:H:570:LEU:CD1	2.45	0.47
2:J:384:LEU:HD11	2:J:412:ILE:HG22	1.96	0.47
2:J:687:HIS:C	2:J:688:LEU:HD23	2.39	0.47
2:B:346:GLY:HA3	2:I:654:GLN:HB3	1.96	0.47
2:B:707:SER:N	2:E:704:ASN:CG	2.69	0.47
2:C:567:VAL:HA	2:C:570:LEU:CD1	2.45	0.47
2:E:384:LEU:HD22	2:E:670:MET:HB2	1.97	0.47
2:I:374:LEU:HD13	2:I:423:PRO:CB	2.44	0.47
2:I:452:LEU:HD13	2:I:452:LEU:O	2.15	0.47
1:K:42:ALA:HB1	1:K:174:VAL:HB	1.97	0.47
1:K:60:GLY:N	1:K:64:VAL:HG13	2.30	0.47
2:B:414:LYS:HB3	2:B:483:LEU:HD23	1.97	0.47
1:D:317:PHE:O	2:E:453:ARG:CG	2.60	0.47
2:I:702:LEU:H	2:I:702:LEU:HD23	1.76	0.47
2:J:444:LYS:CA	1:K:317:PHE:CG	2.87	0.47
2:B:374:LEU:HD13	2:B:423:PRO:CB	2.44	0.47
1:D:67:ARG:HH21	1:D:120:ILE:HG12	1.80	0.47
2:I:380:ASP:N	2:I:380:ASP:OD1	2.48	0.47
2:I:687:HIS:HD2	2:I:688:LEU:HD21	1.77	0.47
1:K:67:ARG:HH21	1:K:120:ILE:HG12	1.80	0.47
2:B:452:LEU:HD13	2:B:452:LEU:O	2.15	0.47
2:I:452:LEU:HD11	2:I:456:MET:HE3	1.97	0.47
2:L:589:PHE:CE2	2:L:591:THR:HG22	2.50	0.47
1:A:205:THR:HG22	1:A:236:ASN:HD22	1.81	0.46
2:E:687:HIS:C	2:E:688:LEU:HD23	2.39	0.46
1:G:205:THR:HG22	1:G:236:ASN:HD22	1.81	0.46
2:I:370:PHE:CE1	2:I:427:CYS:HB2	2.49	0.46
1:D:318:ARG:CB	2:E:453:ARG:CA	2.84	0.46
2:E:460:VAL:HA	2:E:696:PHE:CE1	2.50	0.46
2:F:589:PHE:CE2	2:F:591:THR:HG22	2.50	0.46
2:F:600:TYR:O	2:F:601:ARG:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:600:TYR:O	2:H:601:ARG:HB2	2.15	0.46
1:K:16:LEU:HD11	1:K:20:PHE:HE1	1.80	0.46
2:B:452:LEU:HD11	2:B:456:MET:HE3	1.97	0.46
2:B:485:TYR:CD1	2:J:481:ILE:HD13	2.51	0.46
2:E:481:ILE:HD13	2:I:485:TYR:CD1	2.51	0.46
2:H:586:PHE:CD1	2:H:613:VAL:HG13	2.51	0.46
2:I:414:LYS:HB3	2:I:483:LEU:HD23	1.97	0.46
2:J:391:ALA:HB1	2:J:408:ALA:HA	1.96	0.46
2:B:703:ALA:CA	2:E:700:GLU:CA	2.92	0.46
2:E:391:ALA:HB1	2:E:408:ALA:HA	1.96	0.46
2:E:435:LEU:HD11	2:E:693:THR:CB	2.45	0.46
2:F:572:LEU:CD2	2:F:617:LYS:HE2	2.45	0.46
2:I:371:PRO:HA	2:I:374:LEU:HD23	1.96	0.46
2:C:600:TYR:O	2:C:601:ARG:HB2	2.16	0.46
2:E:489:ASN:HB2	2:I:669:TYR:CZ	2.51	0.46
2:B:669:TYR:CZ	2:J:489:ASN:HB2	2.51	0.46
2:B:702:LEU:H	2:B:702:LEU:HD23	1.76	0.46
2:C:586:PHE:CD1	2:C:613:VAL:HG13	2.50	0.46
1:D:39:GLY:N	1:D:186:ALA:HB2	2.31	0.46
1:D:316:ASN:ND2	2:E:328:ALA:HB2	2.27	0.46
2:J:455:GLU:N	1:K:318:ARG:NE	2.61	0.46
2:J:460:VAL:HA	2:J:696:PHE:CE1	2.50	0.46
1:A:170:LEU:HD22	1:A:201:ILE:CG1	2.46	0.46
2:B:692:ASN:CA	2:E:341:GLU:OE2	2.62	0.46
1:G:259:PHE:HB3	1:G:272:MET:HB3	1.98	0.46
1:K:12:LEU:CG	1:K:745:ILE:HG12	2.45	0.46
2:B:338:VAL:CB	2:E:687:HIS:HE1	2.29	0.46
2:B:687:HIS:C	2:B:688:LEU:HD23	2.40	0.46
2:E:406:ASP:OD1	2:E:407:MET:N	2.49	0.46
1:K:39:GLY:N	1:K:186:ALA:HB2	2.31	0.46
1:K:63:ILE:CD1	1:K:115:ILE:HG21	2.46	0.46
2:L:572:LEU:CD2	2:L:617:LYS:HE2	2.45	0.46
2:B:467:ARG:CZ	2:E:334:GLN:HG2	2.42	0.46
2:E:346:GLY:HA3	2:E:360:ALA:HB2	1.98	0.46
2:E:428:VAL:HG11	2:E:472:LYS:HG3	1.98	0.46
1:G:170:LEU:HD22	1:G:201:ILE:CG1	2.46	0.46
2:J:346:GLY:HA3	2:J:360:ALA:HB2	1.98	0.46
1:A:29:LEU:HD12	1:A:29:LEU:N	2.31	0.45
1:A:80:TYR:HB2	1:A:90:LYS:HB3	1.98	0.45
2:B:702:LEU:CG	2:E:700:GLU:OE2	2.64	0.45
1:D:63:ILE:CD1	1:D:115:ILE:HG21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:HD11	1:D:199:ARG:HB2	1.98	0.45
1:G:80:TYR:HB2	1:G:90:LYS:HB3	1.98	0.45
2:I:687:HIS:C	2:I:688:LEU:HD23	2.40	0.45
2:L:600:TYR:O	2:L:601:ARG:HB2	2.15	0.45
1:D:16:LEU:HD11	1:D:20:PHE:HE1	1.80	0.45
2:F:523:LYS:HE2	2:F:544:VAL:HG13	1.97	0.45
2:J:409:PHE:CE2	2:J:486:MET:HB3	2.51	0.45
1:D:20:PHE:CB	1:D:27:ALA:HA	2.46	0.45
2:I:452:LEU:C	2:I:452:LEU:CD1	2.88	0.45
1:K:20:PHE:CB	1:K:27:ALA:HA	2.47	0.45
2:B:452:LEU:C	2:B:452:LEU:CD1	2.88	0.45
1:G:309:LYS:NZ	1:G:309:LYS:HB3	2.31	0.45
2:I:413:VAL:HG12	2:I:670:MET:HE3	1.98	0.45
2:J:428:VAL:HG11	2:J:472:LYS:HG3	1.98	0.45
2:L:523:LYS:HE2	2:L:544:VAL:HG13	1.97	0.45
1:A:51:PHE:CD1	1:A:281:LEU:HD12	2.51	0.45
2:B:375:VAL:HG13	2:B:629:ARG:NH1	2.32	0.45
2:E:435:LEU:HD21	2:E:693:THR:HG21	1.99	0.45
2:E:684:THR:HG22	2:E:685:ILE:N	2.32	0.45
1:G:29:LEU:N	1:G:29:LEU:HD12	2.31	0.45
2:J:380:ASP:OD1	2:J:380:ASP:N	2.49	0.45
2:J:435:LEU:HD11	2:J:693:THR:CB	2.45	0.45
2:J:459:ILE:HD11	2:J:704:ASN:HD22	1.82	0.45
1:A:259:PHE:HB3	1:A:272:MET:HB3	1.98	0.45
2:B:346:GLY:C	2:I:654:GLN:CB	2.88	0.45
1:D:12:LEU:CG	1:D:745:ILE:HG12	2.45	0.45
1:D:318:ARG:HB3	2:E:454:GLU:HA	1.99	0.45
1:D:318:ARG:O	2:E:453:ARG:CG	2.65	0.45
2:E:384:LEU:HD22	2:E:670:MET:CG	2.46	0.45
2:E:459:ILE:HD11	2:E:704:ASN:HD22	1.82	0.45
1:G:51:PHE:CD1	1:G:281:LEU:HD12	2.51	0.45
2:E:380:ASP:OD1	2:E:380:ASP:N	2.49	0.45
2:F:571:LYS:HD3	2:F:591:THR:HG21	1.99	0.45
1:G:9:LEU:HD23	1:G:290:ARG:CZ	2.46	0.45
2:J:435:LEU:HD21	2:J:693:THR:HG21	1.99	0.45
1:K:290:ARG:HD3	1:K:745:ILE:CG2	2.46	0.45
2:B:413:VAL:HG12	2:B:670:MET:HE3	1.98	0.45
1:D:63:ILE:HD13	1:D:115:ILE:HG21	1.98	0.45
2:I:375:VAL:HG13	2:I:629:ARG:NH1	2.32	0.45
2:J:384:LEU:HD22	2:J:670:MET:CG	2.46	0.45
1:K:42:ALA:HB1	1:K:174:VAL:CG1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:170:LEU:HD11	1:K:199:ARG:HB2	1.98	0.45
1:A:9:LEU:HD23	1:A:290:ARG:CZ	2.46	0.45
1:A:309:LYS:NZ	1:A:309:LYS:HB3	2.31	0.45
1:D:317:PHE:HE2	2:E:332:MET:SD	2.40	0.45
2:J:406:ASP:OD1	2:J:407:MET:N	2.49	0.45
2:J:453:ARG:CG	1:K:318:ARG:O	2.65	0.45
2:J:687:HIS:HD2	2:J:688:LEU:HD21	1.79	0.45
1:K:55:ASP:HB3	1:K:98:ARG:HD3	1.98	0.45
2:B:684:THR:HG22	2:B:685:ILE:N	2.31	0.45
1:D:317:PHE:CZ	2:E:444:LYS:C	2.84	0.45
2:E:329:LEU:HD12	2:E:329:LEU:HA	1.87	0.45
2:E:373:GLU:HG2	2:E:426:LYS:HD3	1.99	0.45
2:E:409:PHE:CE2	2:E:486:MET:HB3	2.51	0.45
2:I:370:PHE:CZ	2:I:374:LEU:HD21	2.52	0.45
2:I:684:THR:HG22	2:I:685:ILE:N	2.31	0.45
2:J:454:GLU:HA	1:K:318:ARG:HB3	1.98	0.45
2:L:571:LYS:HD3	2:L:591:THR:HG21	1.99	0.45
2:C:613:VAL:HG12	2:C:617:LYS:HE2	1.98	0.44
1:D:9:LEU:HD22	1:D:286:THR:HA	1.99	0.44
1:D:12:LEU:HD23	1:D:745:ILE:HG23	1.99	0.44
1:D:55:ASP:HB3	1:D:98:ARG:HD3	1.98	0.44
1:D:307:ILE:CB	1:D:728:MET:HG3	2.47	0.44
1:D:313:GLU:HB2	2:E:448:GLN:CB	2.42	0.44
1:D:318:ARG:NE	2:E:455:GLU:N	2.61	0.44
1:G:176:PRO:CB	1:G:206:LYS:HD2	2.46	0.44
2:J:373:GLU:HG2	2:J:426:LYS:HD3	1.99	0.44
2:J:684:THR:HG22	2:J:685:ILE:N	2.32	0.44
1:K:303:GLN:NE2	1:K:735:LEU:HD21	2.32	0.44
1:K:307:ILE:CB	1:K:728:MET:HG3	2.47	0.44
2:C:572:LEU:HB2	2:C:625:VAL:HG12	2.00	0.44
1:G:46:SER:HA	1:G:237:ARG:HH21	1.82	0.44
1:A:209:LEU:HD11	1:A:238:SER:CB	2.47	0.44
2:B:698:PHE:HB2	2:E:695:GLU:OE1	2.18	0.44
1:D:290:ARG:HD3	1:D:745:ILE:CG2	2.46	0.44
2:E:340:PHE:CZ	2:E:439:VAL:HG12	2.53	0.44
2:J:340:PHE:CZ	2:J:439:VAL:HG12	2.53	0.44
1:K:9:LEU:HD22	1:K:286:THR:HA	2.00	0.44
1:K:12:LEU:HD23	1:K:745:ILE:HG23	1.99	0.44
2:B:370:PHE:CZ	2:B:374:LEU:HD21	2.52	0.44
2:B:664:ASN:HD22	2:B:664:ASN:HA	1.60	0.44
2:H:572:LEU:HB2	2:H:625:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:388:ILE:CG1	2:I:666:VAL:HG21	2.48	0.44
2:J:449:TYR:CD1	1:K:316:ASN:CB	3.00	0.44
2:B:388:ILE:CG1	2:B:666:VAL:HG21	2.48	0.44
1:G:31:LEU:CD2	1:G:130:LEU:HD12	2.48	0.44
2:H:613:VAL:HG12	2:H:617:LYS:HE2	1.98	0.44
1:K:63:ILE:HD13	1:K:115:ILE:HG21	1.98	0.44
1:D:12:LEU:HD23	1:D:745:ILE:HG12	2.00	0.44
1:D:177:ALA:HB1	1:D:210:MET:SD	2.58	0.44
2:E:687:HIS:HD2	2:E:688:LEU:HD21	1.79	0.44
1:G:299:LYS:HD3	1:G:299:LYS:C	2.43	0.44
2:J:391:ALA:HB1	2:J:408:ALA:CA	2.48	0.44
2:J:444:LYS:C	1:K:317:PHE:CZ	2.84	0.44
1:K:140:MET:SD	1:K:157:ARG:HG3	2.57	0.44
1:A:46:SER:HA	1:A:237:ARG:HH21	1.82	0.44
1:A:83:PHE:CZ	1:A:122:LEU:HD22	2.53	0.44
1:D:303:GLN:NE2	1:D:735:LEU:HD21	2.32	0.44
1:G:83:PHE:CZ	1:G:97:VAL:HG13	2.43	0.44
2:H:526:LEU:HB2	2:H:543:PHE:CD1	2.53	0.44
1:K:282:ASN:HD22	1:K:282:ASN:HA	1.66	0.44
1:A:98:ARG:HA	1:A:101:ILE:HD12	1.99	0.44
1:A:176:PRO:CB	1:A:206:LYS:HD2	2.46	0.44
1:A:299:LYS:HD3	1:A:299:LYS:C	2.43	0.44
1:D:42:ALA:HB1	1:D:174:VAL:CG1	2.47	0.44
1:D:87:LYS:H	1:D:87:LYS:HZ2	1.65	0.44
2:E:391:ALA:HB1	2:E:408:ALA:CA	2.48	0.44
2:J:453:ARG:CG	1:K:317:PHE:O	2.60	0.44
2:B:330:LEU:HA	2:E:467:ARG:HH22	1.82	0.44
1:D:140:MET:SD	1:D:157:ARG:HG3	2.57	0.44
1:G:209:LEU:HD11	1:G:238:SER:CB	2.47	0.44
2:I:494:ILE:HG22	2:I:495:GLY:N	2.33	0.44
1:K:87:LYS:HD3	1:K:87:LYS:N	2.33	0.44
2:B:341:GLU:CD	2:E:691:ASN:ND2	2.75	0.43
1:D:87:LYS:HD3	1:D:87:LYS:N	2.33	0.43
2:E:475:VAL:HG22	2:E:681:MET:SD	2.58	0.43
1:G:57:LEU:HA	1:G:58:PRO:HD3	1.90	0.43
2:J:332:MET:SD	1:K:317:PHE:HE2	2.40	0.43
2:J:453:ARG:CB	1:K:317:PHE:HA	2.35	0.43
2:J:475:VAL:HG22	2:J:681:MET:SD	2.58	0.43
2:L:572:LEU:HD22	2:L:617:LYS:HE2	2.01	0.43
1:A:234:VAL:CG1	1:A:277:LEU:HD22	2.48	0.43
2:B:707:SER:O	2:E:458:ARG:NH2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:688:LEU:N	2:E:688:LEU:CD2	2.77	0.43
2:E:697:ILE:HD13	2:E:697:ILE:O	2.18	0.43
2:F:572:LEU:HD22	2:F:617:LYS:HE2	2.00	0.43
1:G:83:PHE:CZ	1:G:122:LEU:HD22	2.53	0.43
2:I:435:LEU:HD21	2:I:693:THR:HG21	2.00	0.43
2:B:435:LEU:HD21	2:B:693:THR:HG21	2.00	0.43
1:G:56:PHE:CB	1:G:94:PHE:HB3	2.48	0.43
1:G:234:VAL:CG1	1:G:277:LEU:HD22	2.47	0.43
2:I:697:ILE:HD13	2:I:697:ILE:O	2.18	0.43
2:J:385:ARG:NH1	2:J:663:ARG:HD2	2.33	0.43
1:K:208:ASP:HB3	1:K:258:PHE:CD1	2.54	0.43
1:G:16:LEU:HD21	1:G:742:ILE:HG12	2.01	0.43
2:I:406:ASP:OD1	2:I:407:MET:N	2.51	0.43
2:B:338:VAL:CG2	2:E:687:HIS:CE1	3.01	0.43
2:C:526:LEU:HB2	2:C:543:PHE:CD1	2.53	0.43
2:J:450:PRO:HD3	1:K:314:TYR:CG	2.27	0.43
1:K:87:LYS:HZ3	1:K:87:LYS:HB2	1.83	0.43
1:A:232:ILE:CG1	1:A:280:VAL:HG21	2.48	0.43
1:D:208:ASP:HB3	1:D:258:PHE:CD1	2.54	0.43
1:K:12:LEU:HD23	1:K:745:ILE:HG12	2.00	0.43
1:A:16:LEU:HD21	1:A:742:ILE:HG12	2.01	0.43
2:B:406:ASP:OD1	2:B:407:MET:N	2.51	0.43
2:B:697:ILE:HD13	2:B:697:ILE:O	2.18	0.43
1:D:318:ARG:CZ	2:E:454:GLU:CB	2.97	0.43
1:G:98:ARG:HA	1:G:101:ILE:HD12	1.99	0.43
1:K:157:ARG:NH2	1:K:188:LYS:HD3	2.33	0.43
1:A:31:LEU:CD2	1:A:130:LEU:HD12	2.48	0.43
2:B:406:ASP:HB3	2:J:680:LEU:HD11	2.01	0.43
2:B:494:ILE:HG22	2:B:495:GLY:N	2.33	0.43
1:D:316:ASN:CB	2:E:449:TYR:CD1	3.00	0.43
1:G:232:ILE:CG1	1:G:280:VAL:HG21	2.49	0.43
2:I:464:ILE:HD13	2:I:696:PHE:HD2	1.84	0.43
2:J:428:VAL:HG13	2:J:689:MET:CE	2.45	0.43
1:K:39:GLY:H	1:K:186:ALA:HB2	1.84	0.43
1:K:177:ALA:HB1	1:K:210:MET:SD	2.58	0.43
2:J:449:TYR:HB3	1:K:313:GLU:O	2.19	0.43
2:L:596:VAL:HG13	2:L:597:TYR:HD1	1.84	0.43
1:D:39:GLY:H	1:D:186:ALA:HB2	1.84	0.42
2:E:385:ARG:NH1	2:E:663:ARG:HD2	2.33	0.42
2:E:680:LEU:HD11	2:I:406:ASP:HB3	2.00	0.42
2:F:520:VAL:HG11	2:F:523:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:596:VAL:HG13	2:F:597:TYR:HD1	1.84	0.42
2:I:384:LEU:HD22	2:I:670:MET:CG	2.49	0.42
2:J:436:ILE:CD1	2:J:464:ILE:HG21	2.49	0.42
1:A:66:ARG:HB2	1:A:105:THR:CG2	2.48	0.42
2:E:428:VAL:HG13	2:E:689:MET:CE	2.45	0.42
2:E:436:ILE:CD1	2:E:464:ILE:HG21	2.49	0.42
1:G:63:ILE:HG21	1:G:148:GLN:HE22	1.84	0.42
2:J:454:GLU:CB	1:K:318:ARG:CZ	2.97	0.42
2:L:520:VAL:HG11	2:L:523:LYS:HG3	2.01	0.42
1:A:9:LEU:CD1	1:A:286:THR:HG23	2.49	0.42
2:B:695:GLU:OE2	2:E:694:LYS:NZ	2.37	0.42
1:D:313:GLU:O	2:E:449:TYR:HB3	2.19	0.42
2:J:697:ILE:HD13	2:J:697:ILE:O	2.18	0.42
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.91	0.42
1:G:9:LEU:CD1	1:G:286:THR:HG23	2.49	0.42
1:K:67:ARG:NH2	1:K:120:ILE:HG12	2.33	0.42
1:A:56:PHE:CB	1:A:94:PHE:HB3	2.48	0.42
2:B:341:GLU:OE2	2:E:691:ASN:CB	2.68	0.42
2:B:464:ILE:HD13	2:B:696:PHE:HD2	1.84	0.42
1:D:60:GLY:N	1:D:64:VAL:HG13	2.30	0.42
2:E:370:PHE:CD1	2:E:427:CYS:HB2	2.55	0.42
2:J:449:TYR:CE1	1:K:316:ASN:N	2.82	0.42
2:J:687:HIS:CD2	2:J:688:LEU:HD23	2.54	0.42
1:A:63:ILE:HG21	1:A:148:GLN:HE22	1.84	0.42
1:D:67:ARG:NH2	1:D:120:ILE:HG12	2.33	0.42
1:D:316:ASN:HB2	2:E:449:TYR:CD1	2.49	0.42
1:G:66:ARG:HB2	1:G:105:THR:CG2	2.48	0.42
1:G:167:GLU:O	1:G:168:ASN:HB2	2.19	0.42
2:I:388:ILE:HD12	2:I:388:ILE:N	2.35	0.42
2:J:485:TYR:CZ	2:J:487:ASN:HB3	2.55	0.42
1:A:67:ARG:HH22	1:A:107:ARG:HH21	1.67	0.42
2:C:526:LEU:HD13	2:C:605:LEU:HD22	2.01	0.42
1:D:78:THR:HB	1:D:80:TYR:CE1	2.54	0.42
2:I:489:ASN:N	2:I:489:ASN:OD1	2.51	0.42
1:K:81:ALA:HB1	1:K:122:LEU:CD1	2.47	0.42
2:L:539:LYS:NZ	2:L:554:LYS:HE2	2.34	0.42
1:A:167:GLU:O	1:A:168:ASN:HB2	2.19	0.42
2:B:654:GLN:HG2	2:B:654:GLN:O	2.20	0.42
2:B:687:HIS:CD2	2:B:688:LEU:HD23	2.53	0.42
2:H:526:LEU:HD13	2:H:605:LEU:HD22	2.01	0.42
2:I:628:GLU:O	2:I:628:GLU:CD	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:629:ARG:HA	2:J:629:ARG:HD2	1.81	0.42
2:J:664:ASN:HD22	2:J:664:ASN:HA	1.64	0.42
1:K:68:PRO:HD2	1:K:119:PRO:HA	2.01	0.42
2:B:680:LEU:HD12	2:B:680:LEU:HA	1.88	0.42
2:B:707:SER:H	2:E:704:ASN:CG	2.26	0.42
1:D:304:LEU:HD11	1:D:736:LYS:NZ	2.35	0.42
1:G:67:ARG:HH22	1:G:107:ARG:HH21	1.67	0.42
2:I:629:ARG:HA	2:I:629:ARG:HD2	1.83	0.42
1:K:78:THR:HB	1:K:80:TYR:CE1	2.54	0.42
2:B:672:ILE:HG13	2:B:673:VAL:N	2.35	0.41
2:E:494:ILE:HD12	2:E:494:ILE:HG21	1.91	0.41
1:G:170:LEU:HD22	1:G:201:ILE:HG12	2.02	0.41
2:J:370:PHE:CD1	2:J:427:CYS:HB2	2.55	0.41
2:J:453:ARG:N	1:K:318:ARG:CB	2.83	0.41
1:K:304:LEU:HD11	1:K:736:LYS:NZ	2.35	0.41
1:D:68:PRO:HD2	1:D:119:PRO:HA	2.01	0.41
1:D:157:ARG:NH2	1:D:188:LYS:HD3	2.33	0.41
2:E:672:ILE:CG2	2:I:489:ASN:HB2	2.50	0.41
2:I:654:GLN:O	2:I:654:GLN:HG2	2.20	0.41
2:I:681:MET:HE2	2:I:681:MET:HA	2.02	0.41
2:C:550:LEU:HD22	2:C:620:PHE:CE1	2.55	0.41
2:E:669:TYR:HA	2:E:672:ILE:HG13	2.02	0.41
2:E:681:MET:HE2	2:E:681:MET:HA	2.03	0.41
2:I:672:ILE:HG13	2:I:673:VAL:N	2.35	0.41
2:B:384:LEU:HD22	2:B:670:MET:CG	2.49	0.41
2:B:628:GLU:O	2:B:628:GLU:CD	2.63	0.41
2:C:607:CYS:HB3	2:C:612:GLU:HB3	2.03	0.41
1:D:113:LYS:HD2	1:D:113:LYS:N	2.36	0.41
2:J:669:TYR:HA	2:J:672:ILE:HG13	2.02	0.41
2:J:681:MET:HA	2:J:681:MET:HE2	2.03	0.41
1:K:262:HIS:CE1	1:K:264:SER:HB2	2.56	0.41
1:A:23:ILE:HG12	1:A:734:ALA:HB1	2.02	0.41
1:A:135:VAL:HG12	1:A:137:LEU:HG	2.02	0.41
1:A:170:LEU:HD22	1:A:201:ILE:HG12	2.02	0.41
2:B:388:ILE:HD12	2:B:388:ILE:N	2.35	0.41
2:B:489:ASN:N	2:B:489:ASN:OD1	2.51	0.41
1:D:316:ASN:N	2:E:449:TYR:CE1	2.82	0.41
2:B:681:MET:HE2	2:B:681:MET:HA	2.02	0.41
1:G:23:ILE:HG12	1:G:734:ALA:HB1	2.02	0.41
2:I:435:LEU:HD23	2:I:436:ILE:N	2.35	0.41
2:J:362:ILE:CG2	2:J:363:ASN:H	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:449:TYR:HA	2:J:450:PRO:HD3	1.81	0.41
1:K:262:HIS:HA	1:K:263:PRO:HD2	1.94	0.41
2:B:341:GLU:OE2	2:E:691:ASN:HB2	2.21	0.41
2:B:629:ARG:HA	2:B:629:ARG:HD2	1.83	0.41
1:D:262:HIS:CE1	1:D:264:SER:HB2	2.56	0.41
2:E:485:TYR:CZ	2:E:487:ASN:HB3	2.55	0.41
1:K:113:LYS:HD2	1:K:113:LYS:N	2.36	0.41
2:F:539:LYS:NZ	2:F:554:LYS:HE2	2.34	0.41
1:G:135:VAL:HG12	1:G:137:LEU:HG	2.02	0.41
2:H:550:LEU:HD22	2:H:620:PHE:CE1	2.55	0.41
2:J:444:LYS:CA	1:K:317:PHE:CD1	2.98	0.41
2:B:481:ILE:HG22	2:B:482:GLU:OE1	2.21	0.41
1:D:318:ARG:CB	2:E:453:ARG:N	2.83	0.41
2:E:445:LYS:NZ	2:E:445:LYS:HB3	2.36	0.41
2:H:535:LYS:O	2:H:535:LYS:HG2	2.21	0.41
2:I:370:PHE:HZ	2:I:681:MET:HG3	1.86	0.41
2:J:388:ILE:HD11	2:J:666:VAL:CG1	2.51	0.41
2:J:445:LYS:HB3	2:J:445:LYS:NZ	2.36	0.41
2:J:449:TYR:CD1	1:K:316:ASN:HB2	2.49	0.41
2:J:630:VAL:CG2	2:J:671:ALA:HB1	2.51	0.41
2:J:654:GLN:HG2	2:J:654:GLN:O	2.21	0.41
2:B:363:ASN:HD21	2:B:685:ILE:HG21	1.85	0.41
1:D:38:GLY:HA2	1:D:186:ALA:CB	2.51	0.41
1:G:63:ILE:HG21	1:G:148:GLN:NE2	2.36	0.41
2:H:607:CYS:HB3	2:H:612:GLU:HB3	2.02	0.41
2:B:489:ASN:HB2	2:J:672:ILE:CG2	2.50	0.40
2:C:535:LYS:O	2:C:535:LYS:HG2	2.21	0.40
1:D:13:VAL:HG13	1:D:29:LEU:HD13	2.02	0.40
2:E:629:ARG:HA	2:E:629:ARG:HD2	1.81	0.40
2:F:570:LEU:HD23	2:F:570:LEU:HA	1.92	0.40
2:J:370:PHE:CE2	2:J:681:MET:HB2	2.56	0.40
1:K:229:ARG:HG3	1:K:280:VAL:HG11	2.02	0.40
2:L:525:TRP:CE3	2:L:540:GLU:HG2	2.57	0.40
1:A:63:ILE:HG21	1:A:148:GLN:NE2	2.36	0.40
1:A:164:VAL:HG21	1:A:193:VAL:HG11	2.04	0.40
2:B:435:LEU:HD23	2:B:436:ILE:N	2.35	0.40
2:B:452:LEU:HD11	2:B:456:MET:CE	2.51	0.40
1:D:317:PHE:CD1	2:E:444:LYS:CA	2.98	0.40
2:E:370:PHE:CE2	2:E:681:MET:HB2	2.57	0.40
1:G:134:LEU:N	1:G:134:LEU:HD12	2.36	0.40
1:G:164:VAL:HG21	1:G:193:VAL:HG11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:ILE:HG21	1:G:728:MET:HB3	2.03	0.40
2:J:660:GLU:HA	2:J:663:ARG:NH1	2.35	0.40
1:K:6:MET:HE3	1:K:282:ASN:CB	2.51	0.40
2:L:624:GLY:HA2	2:L:626:TYR:CE1	2.56	0.40
1:A:307:ILE:HG21	1:A:728:MET:HB3	2.03	0.40
2:C:573:ARG:HB2	2:C:630:VAL:CG1	2.51	0.40
1:K:38:GLY:HA2	1:K:186:ALA:CB	2.51	0.40
1:A:59:ARG:HB3	1:A:242:ILE:CG2	2.45	0.40
1:A:138:PRO:HG2	1:A:159:MET:SD	2.62	0.40
1:A:231:TYR:C	1:A:232:ILE:HD12	2.47	0.40
1:A:301:GLN:HA	1:A:301:GLN:HE21	1.86	0.40
1:A:746:ASN:HD22	1:A:746:ASN:HA	1.78	0.40
1:D:221:GLU:HA	1:D:268:LEU:HD11	2.04	0.40
2:E:388:ILE:HD11	2:E:666:VAL:CG1	2.51	0.40
2:E:630:VAL:CG2	2:E:671:ALA:HB1	2.51	0.40
2:E:660:GLU:HA	2:E:663:ARG:NH1	2.35	0.40
2:E:664:ASN:HD22	2:E:664:ASN:HA	1.64	0.40
2:F:525:TRP:CE3	2:F:540:GLU:HG2	2.57	0.40
2:H:573:ARG:HB2	2:H:630:VAL:CG1	2.51	0.40
2:I:481:ILE:HG22	2:I:482:GLU:OE1	2.21	0.40
2:J:345:GLU:O	2:J:346:GLY:C	2.64	0.40
2:J:494:ILE:HD12	2:J:494:ILE:HG21	1.91	0.40
2:J:669:TYR:CD1	2:J:672:ILE:HD11	2.57	0.40
1:K:13:VAL:HG13	1:K:29:LEU:HD13	2.02	0.40
1:A:87:LYS:O	1:A:87:LYS:HG3	2.20	0.40
1:A:232:ILE:HG12	1:A:280:VAL:HG21	2.03	0.40
1:D:317:PHE:HB3	2:E:453:ARG:HB3	2.02	0.40
2:E:654:GLN:HG2	2:E:654:GLN:O	2.21	0.40
2:F:535:LYS:HG2	2:F:535:LYS:O	2.21	0.40
2:F:573:ARG:HD2	2:F:575:VAL:CG1	2.47	0.40
1:G:232:ILE:HG12	1:G:280:VAL:HG21	2.04	0.40
1:G:301:GLN:HA	1:G:301:GLN:HE21	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	325/864 (38%)	313 (96%)	10 (3%)	2 (1%)	21	59
1	D	333/864 (38%)	317 (95%)	14 (4%)	2 (1%)	21	59
1	G	325/864 (38%)	313 (96%)	10 (3%)	2 (1%)	21	59
1	K	333/864 (38%)	317 (95%)	14 (4%)	2 (1%)	21	59
2	B	196/864 (23%)	165 (84%)	22 (11%)	9 (5%)	2	17
2	C	111/864 (13%)	93 (84%)	13 (12%)	5 (4%)	2	17
2	E	196/864 (23%)	161 (82%)	27 (14%)	8 (4%)	2	18
2	F	111/864 (13%)	93 (84%)	12 (11%)	6 (5%)	1	15
2	H	111/864 (13%)	93 (84%)	13 (12%)	5 (4%)	2	17
2	I	196/864 (23%)	165 (84%)	22 (11%)	9 (5%)	2	17
2	J	196/864 (23%)	161 (82%)	27 (14%)	8 (4%)	2	18
2	L	111/864 (13%)	93 (84%)	12 (11%)	6 (5%)	1	15
All	All	2544/10368 (24%)	2284 (90%)	196 (8%)	64 (2%)	6	26

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	GLY
2	B	489	ASN
2	B	490	HIS
2	B	492	ASP
2	C	534	MET
2	C	576	GLU
2	E	449	TYR
2	E	450	PRO
2	E	490	HIS
2	E	492	ASP
2	F	534	MET
2	F	574	ASP
2	F	627	PRO
1	G	88	GLY
2	H	534	MET
2	H	576	GLU
2	I	489	ASN
2	I	490	HIS

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Mol	Chain	Res	Type
2	I	492	ASP
2	J	449	TYR
2	J	450	PRO
2	J	490	HIS
2	J	492	ASP
2	L	534	MET
2	L	574	ASP
2	L	627	PRO
2	B	414	LYS
2	B	487	ASN
2	B	690	ILE
2	C	577	LYS
2	E	454	GLU
2	F	576	GLU
2	H	577	LYS
2	I	414	LYS
2	I	487	ASN
2	I	690	ILE
2	L	576	GLU
2	B	696	PHE
1	D	79	GLU
2	E	452	LEU
2	I	696	PHE
2	J	452	LEU
2	J	454	GLU
1	K	79	GLU
2	B	689	MET
2	E	453	ARG
2	I	689	MET
2	J	453	ARG
2	C	563	TYR
2	E	689	MET
2	F	577	LYS
2	H	563	TYR
2	J	689	MET
2	L	577	LYS
1	A	87	LYS
1	D	41	SER
1	G	87	LYS
1	K	41	SER
2	B	412	ILE
2	F	575	VAL

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Mol	Chain	Res	Type
2	I	412	ILE
2	L	575	VAL
2	C	532	GLY
2	H	532	GLY

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	287/761 (38%)	272 (95%)	15 (5%)	21	42
1	D	295/761 (39%)	282 (96%)	13 (4%)	25	47
1	G	287/761 (38%)	272 (95%)	15 (5%)	21	42
1	K	295/761 (39%)	282 (96%)	13 (4%)	25	47
2	B	194/761 (26%)	150 (77%)	44 (23%)	1	6
2	C	102/761 (13%)	94 (92%)	8 (8%)	11	32
2	E	194/761 (26%)	153 (79%)	41 (21%)	1	6
2	F	102/761 (13%)	89 (87%)	13 (13%)	4	16
2	H	102/761 (13%)	94 (92%)	8 (8%)	11	32
2	I	194/761 (26%)	150 (77%)	44 (23%)	1	6
2	J	194/761 (26%)	153 (79%)	41 (21%)	1	6
2	L	102/761 (13%)	89 (87%)	13 (13%)	4	16
All	All	2348/9132 (26%)	2080 (89%)	268 (11%)	8	18

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	73	LEU
1	A	79	GLU
1	A	87	LYS
1	A	121	ASN
1	A	172	LEU

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Mol	Chain	Res	Type
1	A	175	SER
1	A	228	ARG
1	A	240	LYS
1	A	245	LYS
1	A	248	ILE
1	A	301	GLN
1	A	309	LYS
1	A	727	GLU
1	A	741	ILE
2	B	327	LYS
2	B	329	LEU
2	B	330	LEU
2	B	339	ASP
2	B	340	PHE
2	B	345	GLU
2	B	357	SER
2	B	368	GLU
2	B	369	ARG
2	B	380	ASP
2	B	388	ILE
2	B	428	VAL
2	B	435	LEU
2	B	438	THR
2	B	443	THR
2	B	445	LYS
2	B	449	TYR
2	B	451	ARG
2	B	468	GLU
2	B	482	GLU
2	B	489	ASN
2	B	490	HIS
2	B	491	GLU
2	B	492	ASP
2	B	493	PHE
2	B	494	ILE
2	B	628	GLU
2	B	664	ASN
2	B	667	ASP
2	B	672	ILE
2	B	676	THR
2	B	679	ASP
2	B	680	LEU

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Mol	Chain	Res	Type
2	B	682	PRO
2	B	684	THR
2	B	685	ILE
2	B	688	LEU
2	B	692	ASN
2	B	697	ILE
2	B	698	PHE
2	B	700	GLU
2	B	702	LEU
2	B	705	LEU
2	B	707	SER
2	C	534	MET
2	C	560	GLU
2	C	563	TYR
2	C	577	LYS
2	C	579	PHE
2	C	584	HIS
2	C	594	ARG
2	C	603	LEU
1	D	34	ILE
1	D	78	THR
1	D	87	LYS
1	D	99	LEU
1	D	123	ARG
1	D	159	MET
1	D	166	LYS
1	D	171	ILE
1	D	228	ARG
1	D	248	ILE
1	D	290	ARG
1	D	304	LEU
1	D	318	ARG
2	E	327	LYS
2	E	329	LEU
2	E	330	LEU
2	E	339	ASP
2	E	340	PHE
2	E	345	GLU
2	E	357	SER
2	E	368	GLU
2	E	369	ARG
2	E	380	ASP

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Mol	Chain	Res	Type
2	E	388	ILE
2	E	428	VAL
2	E	438	THR
2	E	443	THR
2	E	445	LYS
2	E	449	TYR
2	E	450	PRO
2	E	451	ARG
2	E	452	LEU
2	E	456	MET
2	E	464	ILE
2	E	468	GLU
2	E	482	GLU
2	E	486	MET
2	E	489	ASN
2	E	490	HIS
2	E	491	GLU
2	E	492	ASP
2	E	494	ILE
2	E	628	GLU
2	E	664	ASN
2	E	672	ILE
2	E	676	THR
2	E	679	ASP
2	E	680	LEU
2	E	682	PRO
2	E	688	LEU
2	E	692	ASN
2	E	697	ILE
2	E	698	PHE
2	E	702	LEU
2	F	529	ASN
2	F	534	MET
2	F	551	SER
2	F	558	GLU
2	F	560	GLU
2	F	569	ASN
2	F	573	ARG
2	F	575	VAL
2	F	577	LYS
2	F	579	PHE
2	F	594	ARG

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Mol	Chain	Res	Type
2	F	603	LEU
2	F	604	GLU
1	G	69	LEU
1	G	73	LEU
1	G	79	GLU
1	G	87	LYS
1	G	121	ASN
1	G	172	LEU
1	G	175	SER
1	G	228	ARG
1	G	240	LYS
1	G	245	LYS
1	G	248	ILE
1	G	301	GLN
1	G	309	LYS
1	G	727	GLU
1	G	741	ILE
2	H	534	MET
2	H	560	GLU
2	H	563	TYR
2	H	577	LYS
2	H	579	PHE
2	H	584	HIS
2	H	594	ARG
2	H	603	LEU
2	I	327	LYS
2	I	329	LEU
2	I	330	LEU
2	I	339	ASP
2	I	340	PHE
2	I	345	GLU
2	I	357	SER
2	I	368	GLU
2	I	369	ARG
2	I	380	ASP
2	I	388	ILE
2	I	428	VAL
2	I	435	LEU
2	I	438	THR
2	I	443	THR
2	I	445	LYS
2	I	449	TYR

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Mol	Chain	Res	Type
2	I	451	ARG
2	I	468	GLU
2	I	482	GLU
2	I	489	ASN
2	I	490	HIS
2	I	491	GLU
2	I	492	ASP
2	I	493	PHE
2	I	494	ILE
2	I	628	GLU
2	I	664	ASN
2	I	667	ASP
2	I	672	ILE
2	I	676	THR
2	I	679	ASP
2	I	680	LEU
2	I	682	PRO
2	I	684	THR
2	I	685	ILE
2	I	688	LEU
2	I	692	ASN
2	I	697	ILE
2	I	698	PHE
2	I	700	GLU
2	I	702	LEU
2	I	705	LEU
2	I	707	SER
2	J	327	LYS
2	J	329	LEU
2	J	330	LEU
2	J	339	ASP
2	J	340	PHE
2	J	345	GLU
2	J	357	SER
2	J	368	GLU
2	J	369	ARG
2	J	380	ASP
2	J	388	ILE
2	J	428	VAL
2	J	438	THR
2	J	443	THR
2	J	445	LYS

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Mol	Chain	Res	Type
2	J	449	TYR
2	J	450	PRO
2	J	451	ARG
2	J	452	LEU
2	J	456	MET
2	J	464	ILE
2	J	468	GLU
2	J	482	GLU
2	J	486	MET
2	J	489	ASN
2	J	490	HIS
2	J	491	GLU
2	J	492	ASP
2	J	494	ILE
2	J	628	GLU
2	J	664	ASN
2	J	672	ILE
2	J	676	THR
2	J	679	ASP
2	J	680	LEU
2	J	682	PRO
2	J	688	LEU
2	J	692	ASN
2	J	697	ILE
2	J	698	PHE
2	J	702	LEU
1	K	34	ILE
1	K	78	THR
1	K	87	LYS
1	K	99	LEU
1	K	123	ARG
1	K	159	MET
1	K	166	LYS
1	K	171	ILE
1	K	228	ARG
1	K	248	ILE
1	K	290	ARG
1	K	304	LEU
1	K	318	ARG
2	L	529	ASN
2	L	534	MET
2	L	551	SER

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Mol	Chain	Res	Type
2	L	558	GLU
2	L	560	GLU
2	L	569	ASN
2	L	573	ARG
2	L	575	VAL
2	L	577	LYS
2	L	579	PHE
2	L	594	ARG
2	L	603	LEU
2	L	604	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	155	GLN
1	A	168	ASN
1	A	236	ASN
1	A	301	GLN
1	A	744	ASN
1	A	746	ASN
2	B	334	GLN
2	B	335	GLN
2	B	363	ASN
2	B	367	HIS
2	B	463	HIS
2	B	658	GLN
2	B	664	ASN
2	B	687	HIS
2	B	692	ASN
2	C	529	ASN
2	C	602	GLN
1	D	25	GLN
1	D	26	ASN
1	D	33	GLN
1	D	72	GLN
1	D	85	HIS
1	D	131	ASN
1	D	148	GLN
1	D	155	GLN
1	D	236	ASN
1	D	239	GLN

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Mol	Chain	Res	Type
1	D	282	ASN
1	D	303	GLN
2	E	664	ASN
2	E	687	HIS
2	E	704	ASN
2	F	602	GLN
1	G	40	GLN
1	G	75	ASN
1	G	155	GLN
1	G	168	ASN
1	G	236	ASN
1	G	301	GLN
1	G	744	ASN
1	G	746	ASN
2	H	529	ASN
2	H	602	GLN
2	I	334	GLN
2	I	335	GLN
2	I	363	ASN
2	I	367	HIS
2	I	658	GLN
2	I	664	ASN
2	I	687	HIS
2	I	704	ASN
2	J	335	GLN
2	J	363	ASN
2	J	664	ASN
2	J	687	HIS
2	J	691	ASN
2	J	692	ASN
2	J	704	ASN
1	K	25	GLN
1	K	26	ASN
1	K	33	GLN
1	K	72	GLN
1	K	85	HIS
1	K	148	GLN
1	K	155	GLN
1	K	236	ASN
1	K	239	GLN
1	K	282	ASN
1	K	303	GLN

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Mol	Chain	Res	Type
2	L	602	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	K	1
2	B	1
2	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	316:ASN	C	317:PHE	N	1.18
1	K	316:ASN	C	317:PHE	N	1.18
1	B	489:ASN	C	490:HIS	N	1.17

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	489:ASN	C	490:HIS	N	1.17

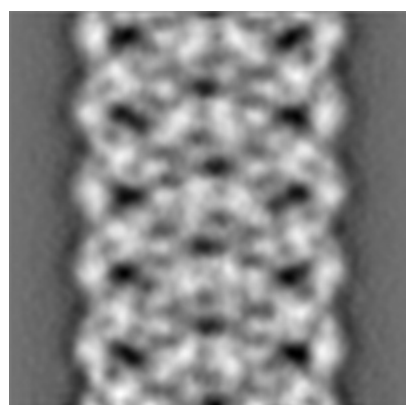
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2701. These allow visual inspection of the internal detail of the map and identification of artifacts.

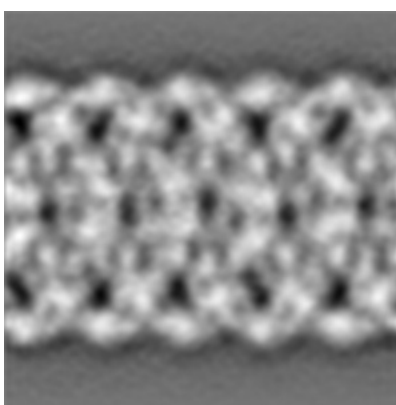
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

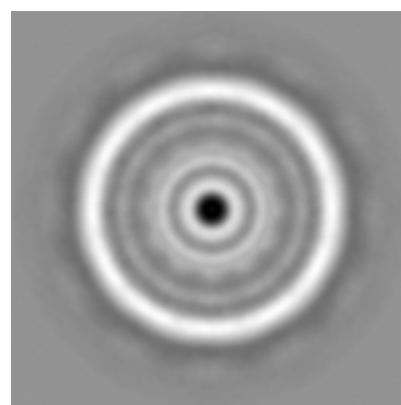
6.1.1 Primary map



X



Y

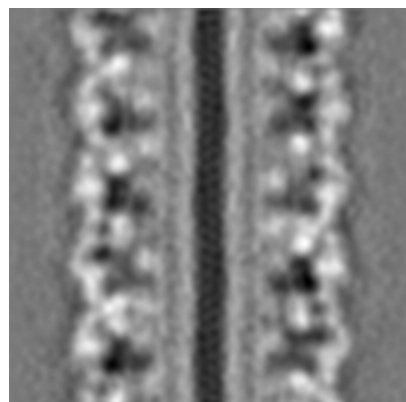


Z

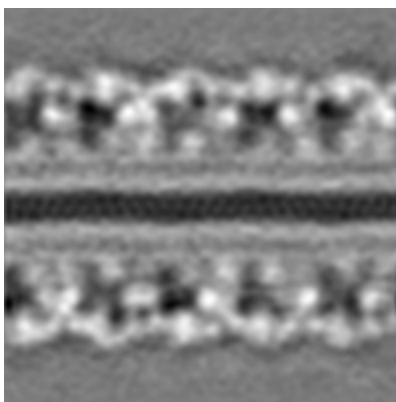
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 100



Y Index: 100

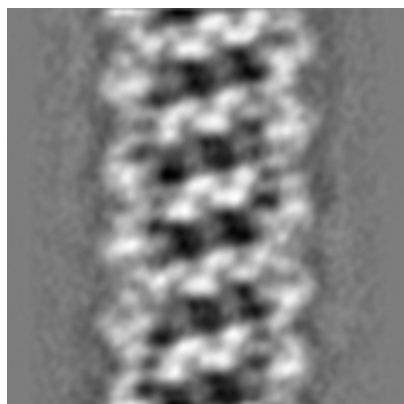


Z Index: 100

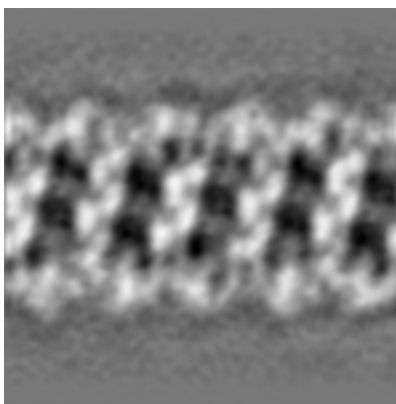
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 145



Y Index: 55

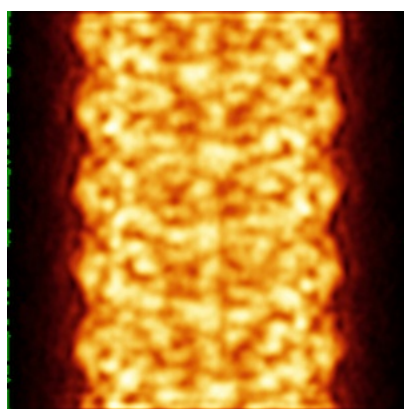


Z Index: 197

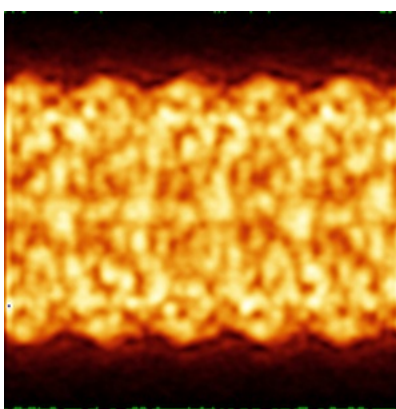
The images above show the largest variance slices of the map in three orthogonal directions.

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

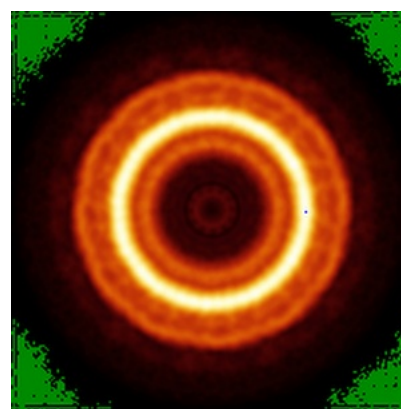
6.4.1 Primary map



X



Y

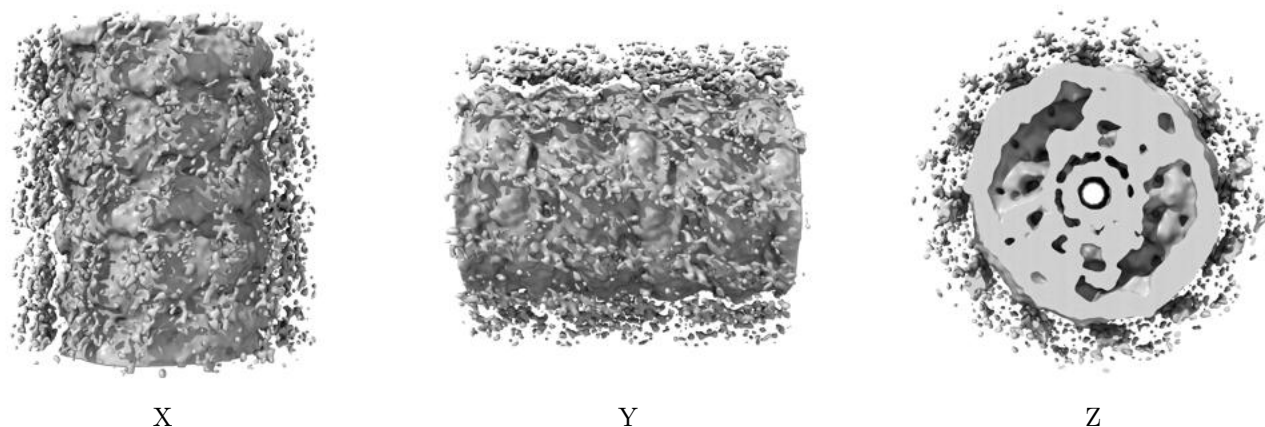


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

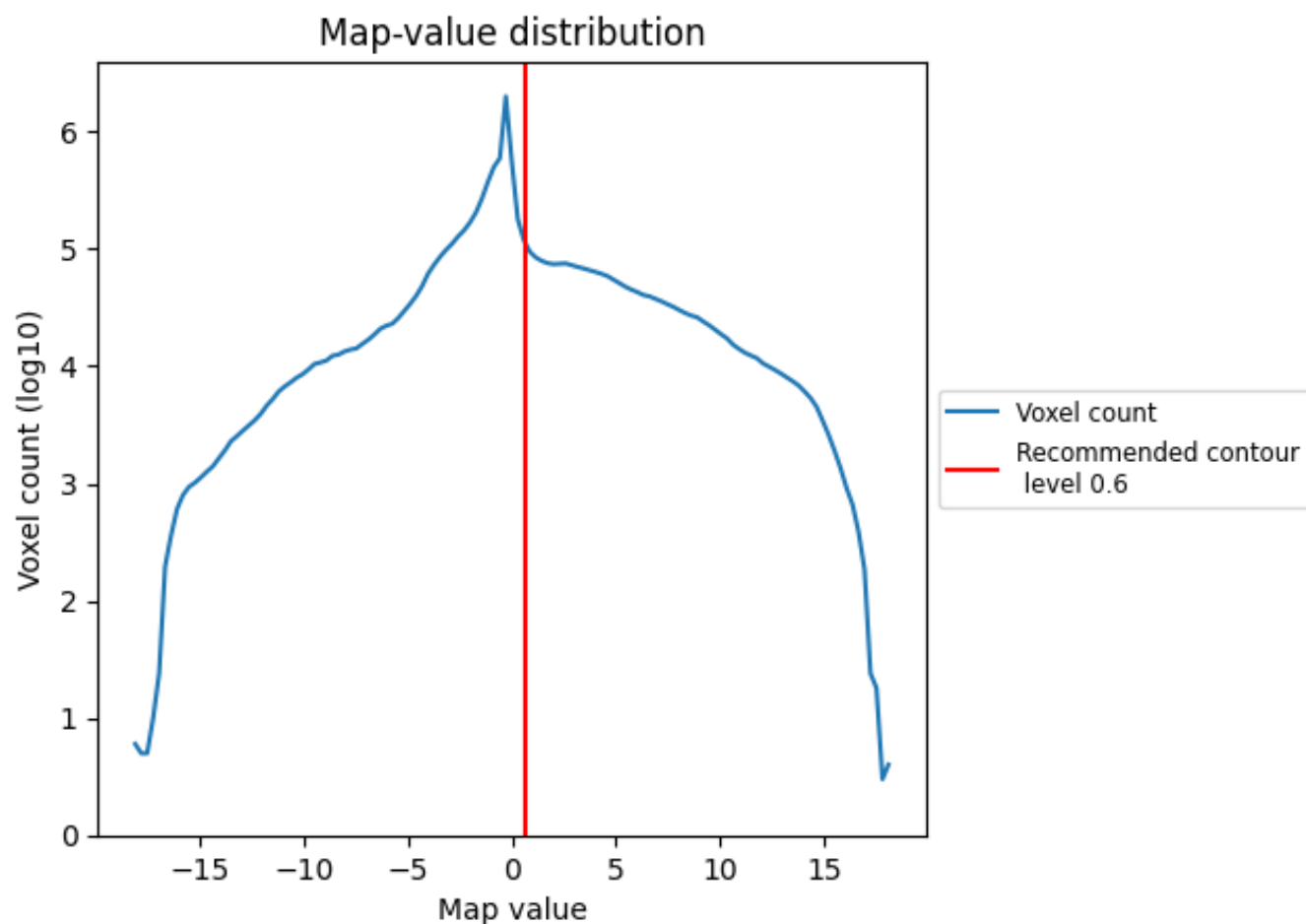
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

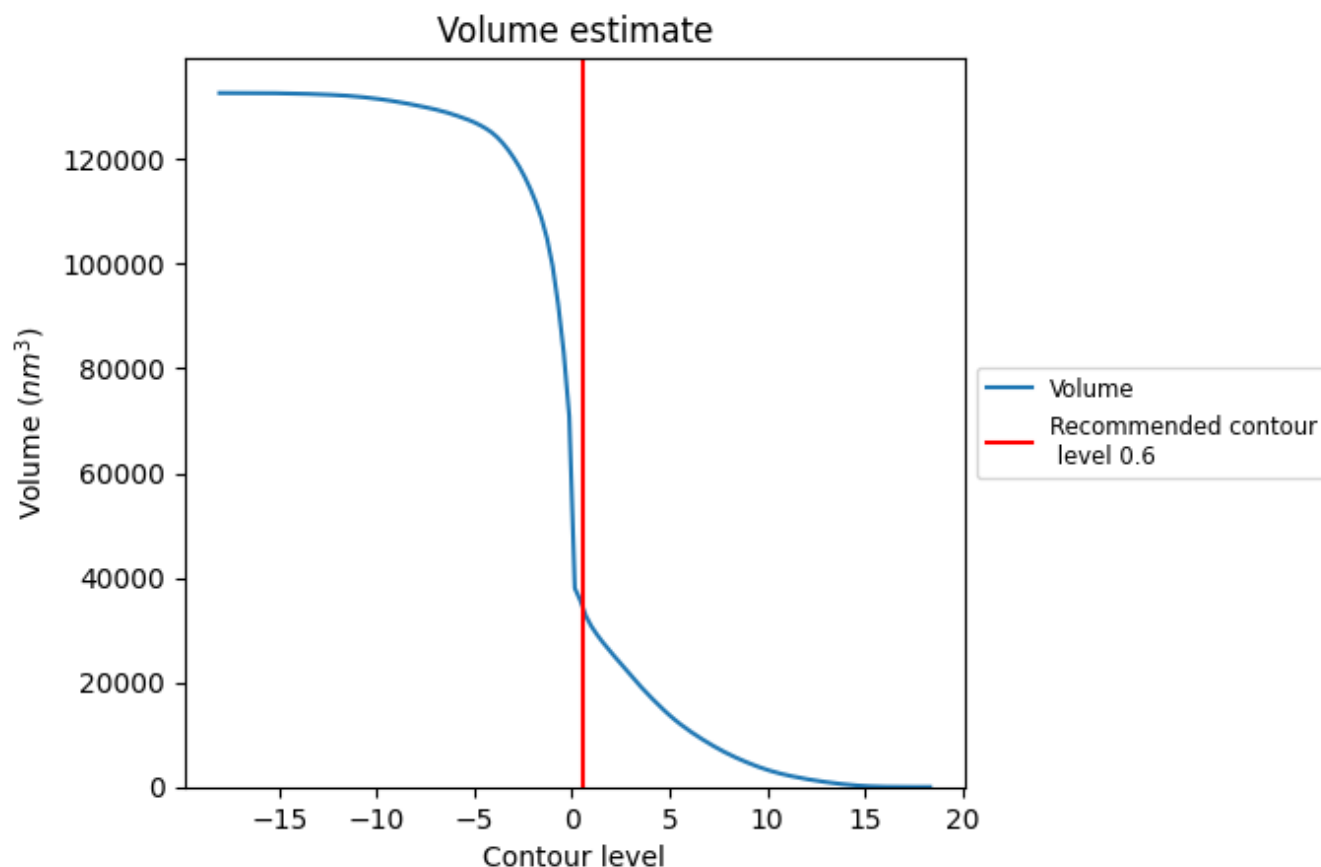
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

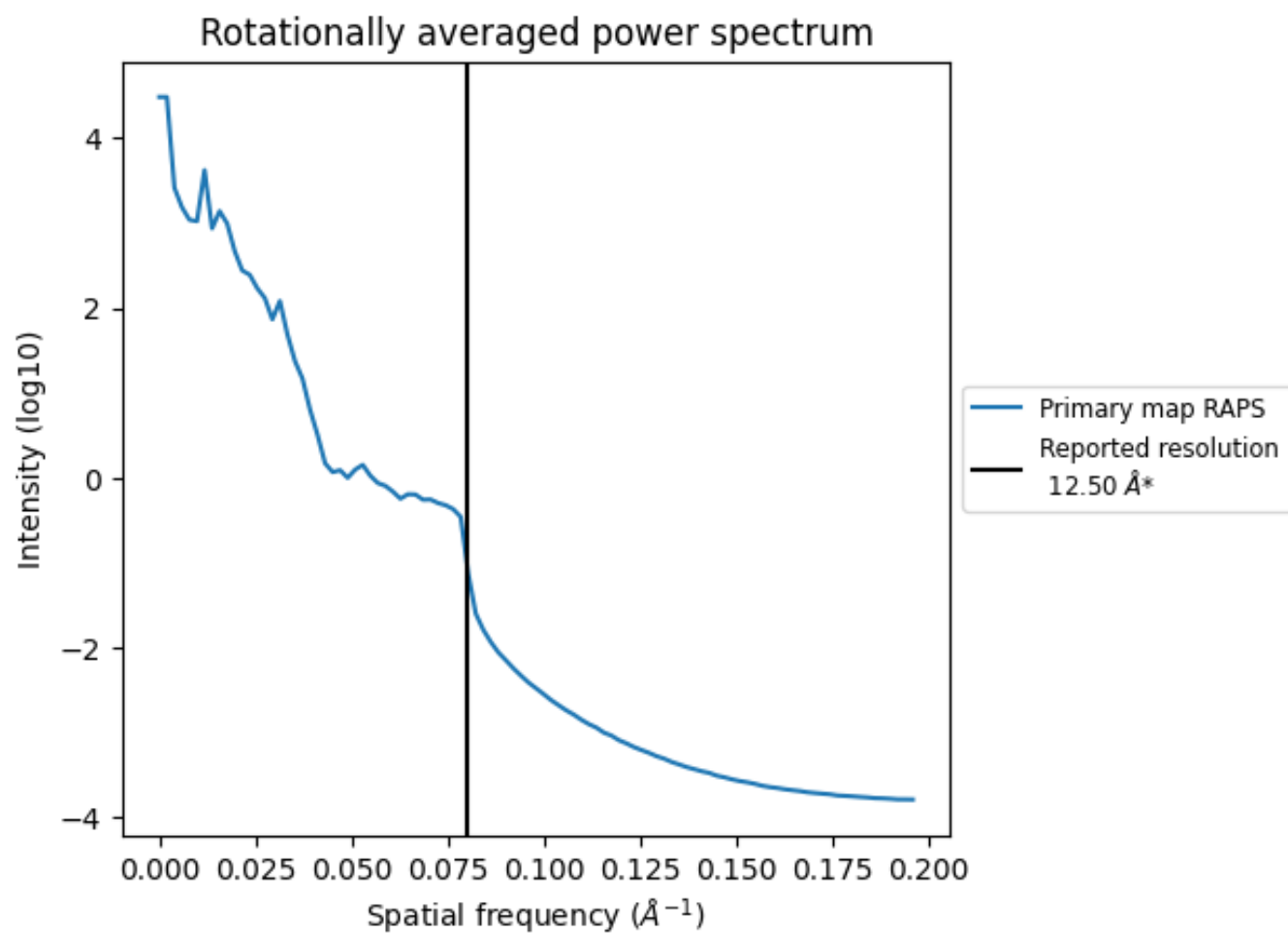
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 33840 nm^3 ; this corresponds to an approximate mass of 30569 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 0.080 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-2701 and PDB model 4UUK. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

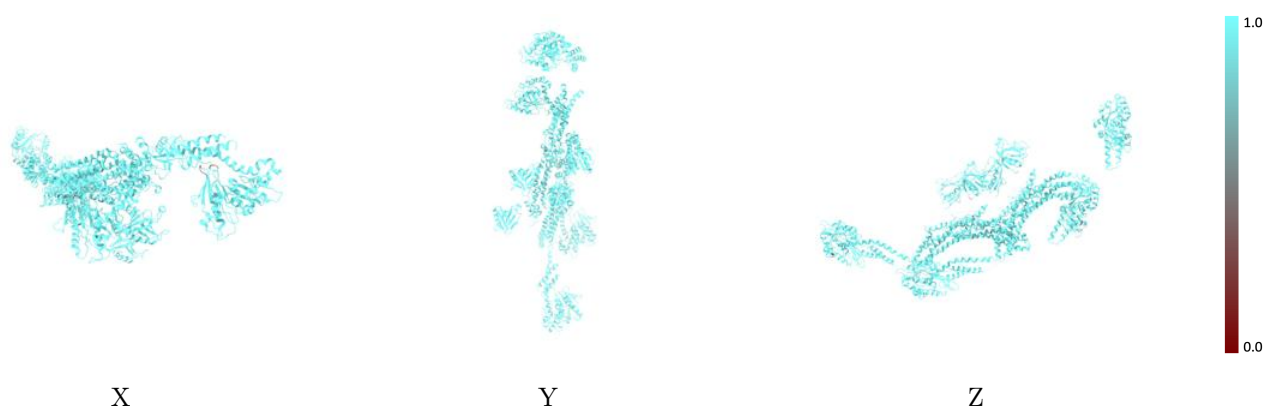
This section was not generated.

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



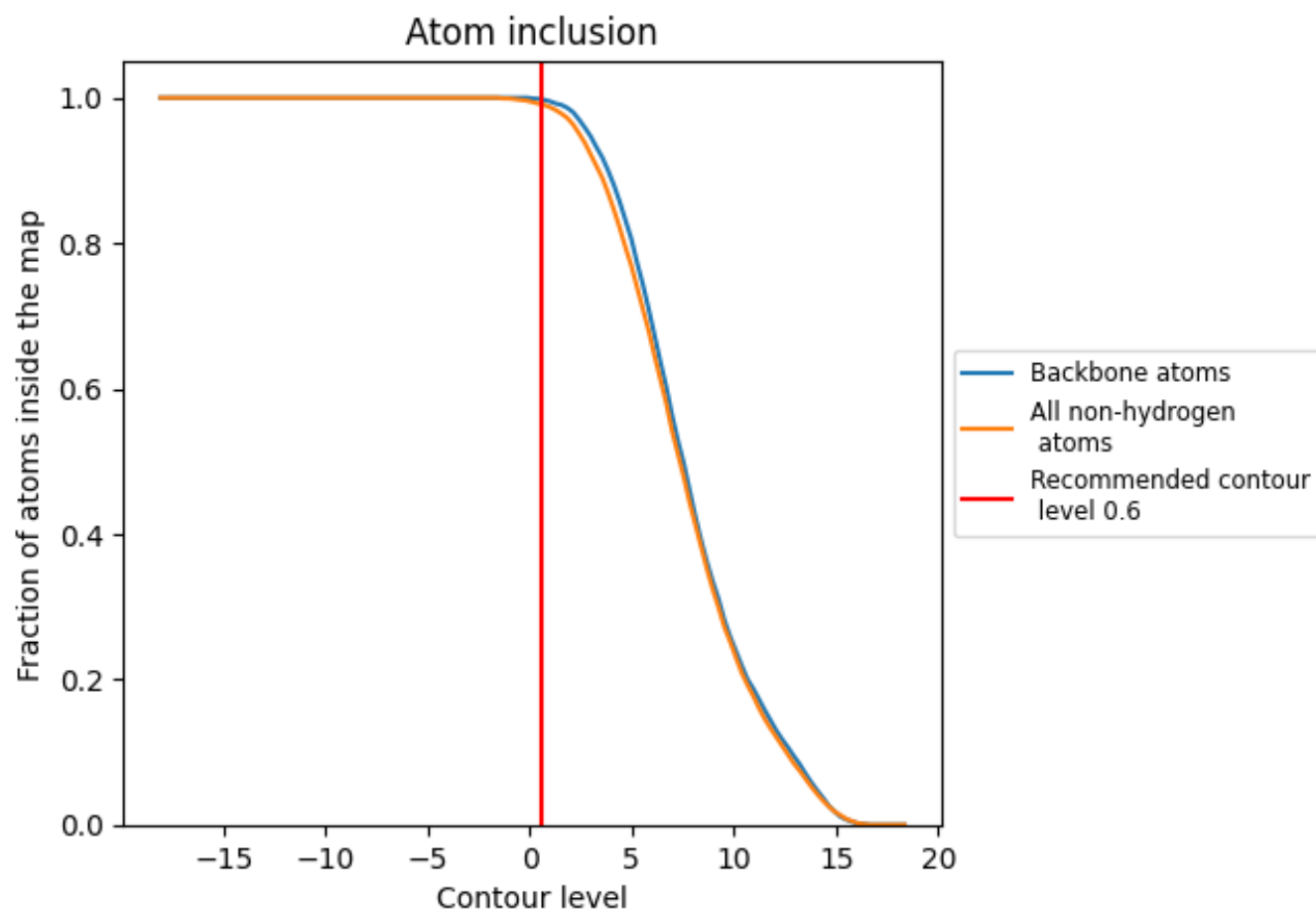
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9910	0.0570
A	0.9880	0.0550
B	0.9890	0.0420
C	0.9810	0.0730
D	0.9960	0.0570
E	0.9940	0.0620
F	0.9910	0.0590
G	0.9870	0.0550
H	0.9820	0.0730
I	0.9910	0.0410
J	0.9940	0.0640
K	0.9960	0.0570
L	0.9920	0.0570

