



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 12:44 PM UTC

PDB ID : 3B5U / pdb_00003b5u
EMDB ID : EMD-1088
Title : Actin filament model from extended form of acromsomal bundle in the Limulus sperm
Authors : Cong, Y.; Topf, M.; Sali, A.; Matsudaira, P.; Dougherty, M.; Chiu, W.; Schmid, M.F.
Deposited on : 2007-10-26
Resolution : 9.50 Å(reported)
Based on initial model : ?

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:

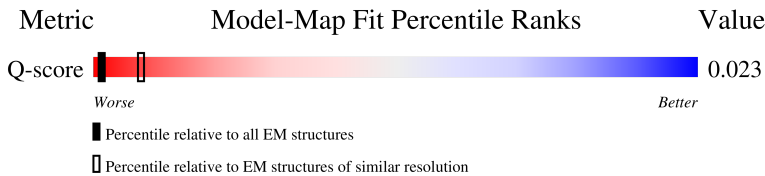
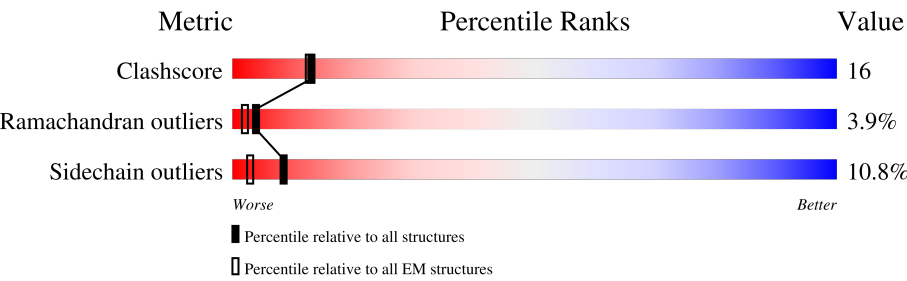
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 9.50 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	234 (9.00 - 10.00)

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	377	 93% 52% 38% 7% ..
1	B	377	 89% 51% 38% 8% ..
1	C	377	 88% 61% 30% 8% ..
1	D	377	 92% 51% 38% 7% ..

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Mol	Chain	Length	Quality of chain
1	E	377	91% 56%31%11% ..
1	F	377	90% 55%33%9% ..
1	G	377	93% 60%32%7% ..
1	H	377	97% 62%32%6% ..
1	I	377	98% 55%38%6% ..
1	J	377	95% 56%31%10% ..
1	K	377	96% 55%33%9% ..
1	L	377	95% 51%37%9% ..
1	M	377	92% 56%33%8% ..
1	N	377	92% 53%37%8% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 41062 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.

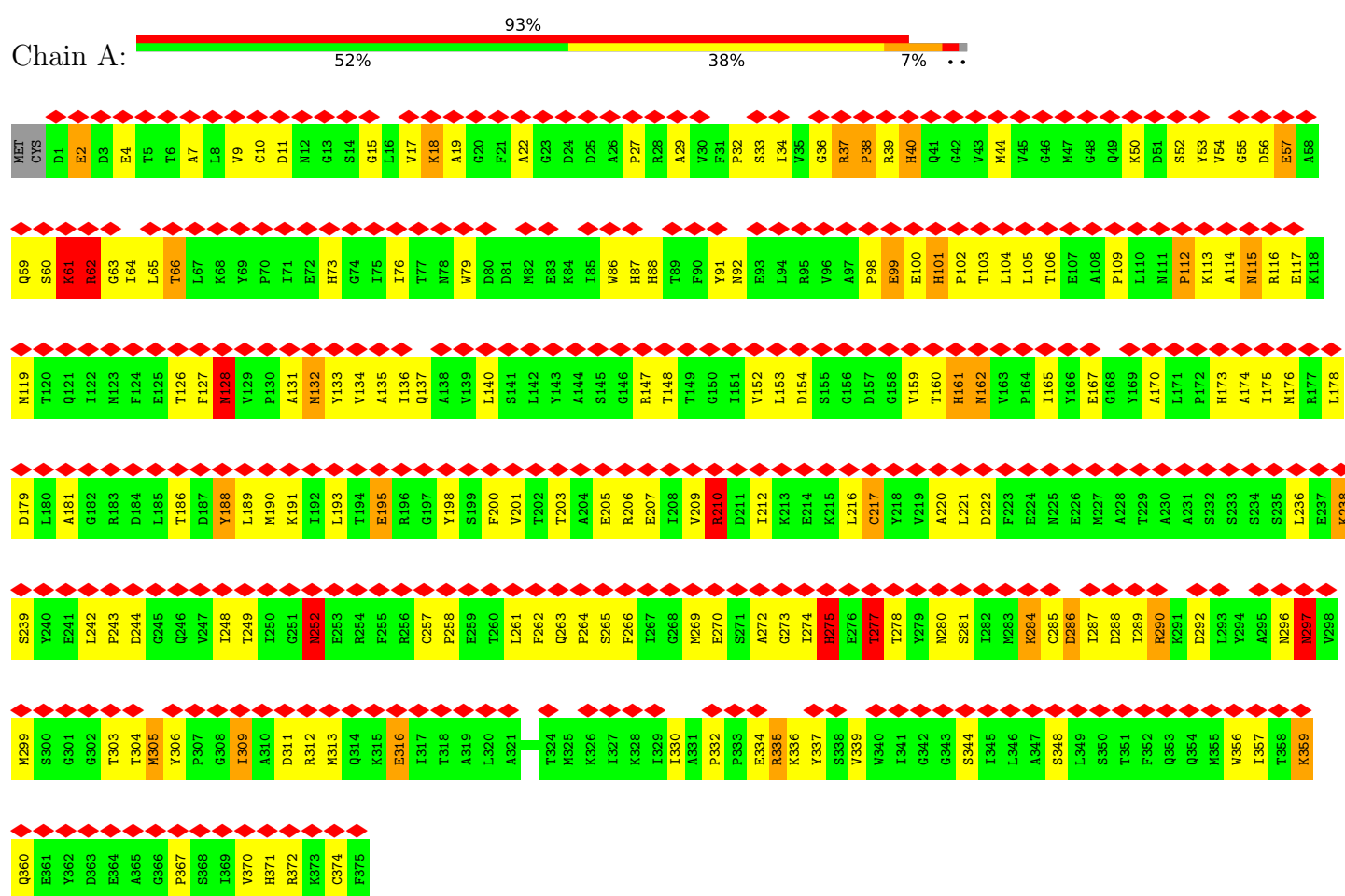
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	B	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	C	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	F	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	G	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	H	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	I	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	J	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	K	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	L	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	M	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	N	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		

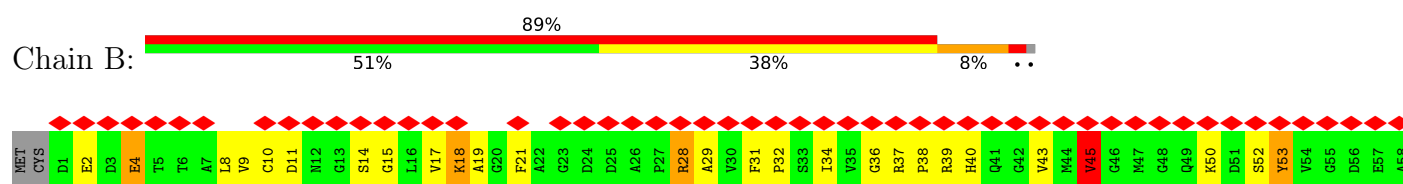
3 Residue-property plots

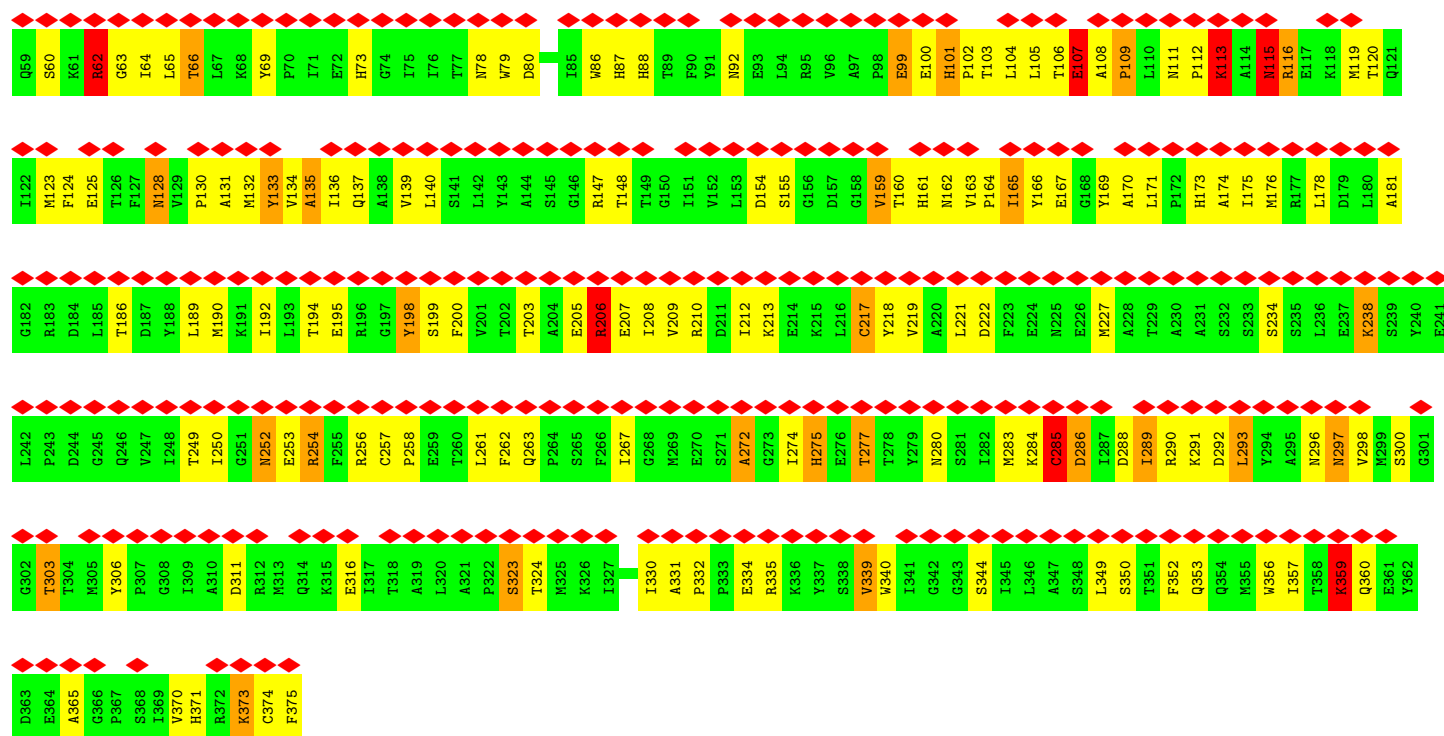
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

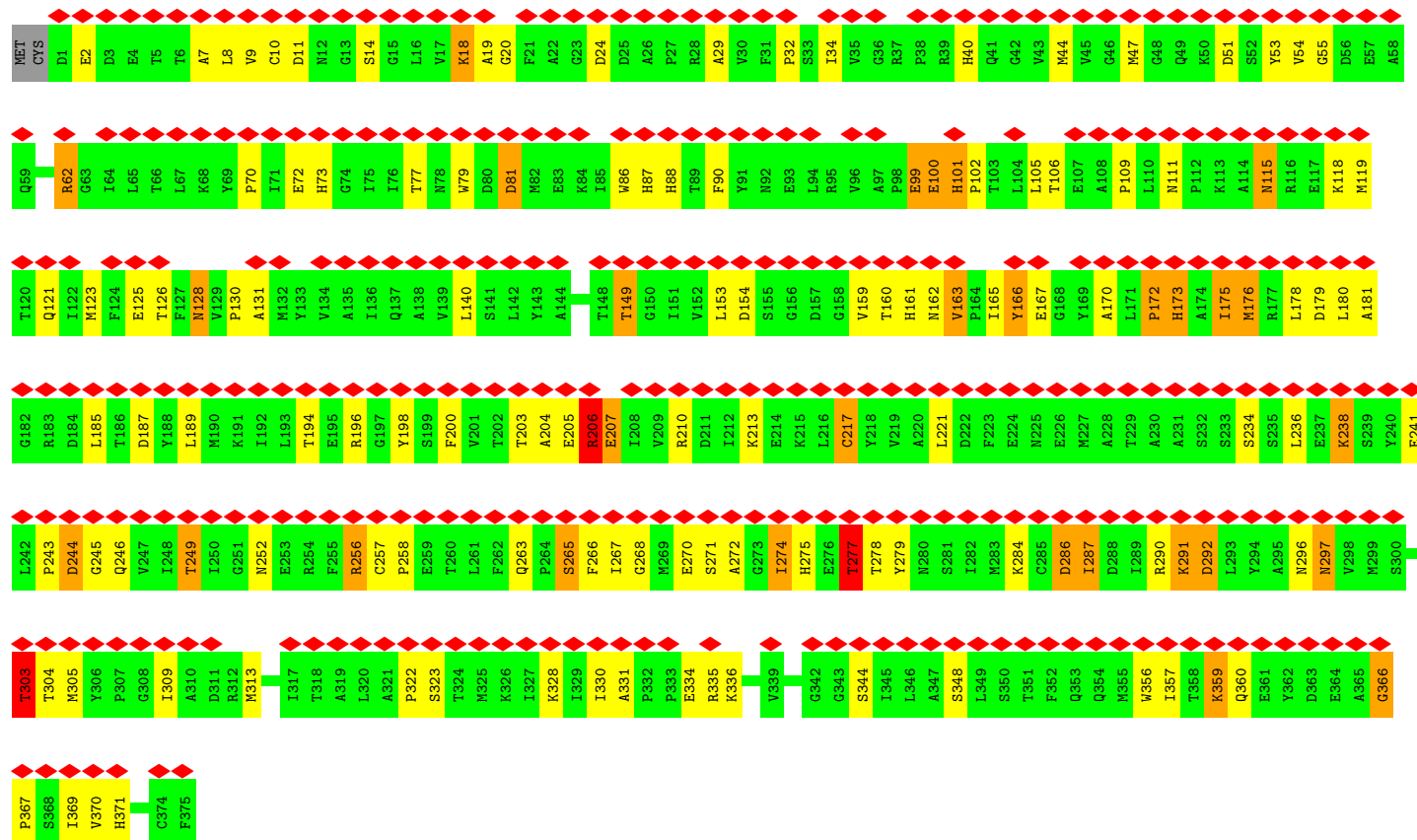
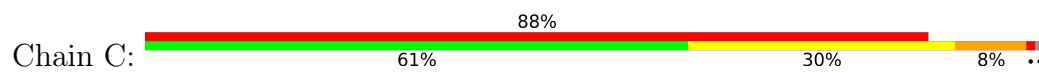


- Molecule 1: Actin, alpha skeletal muscle

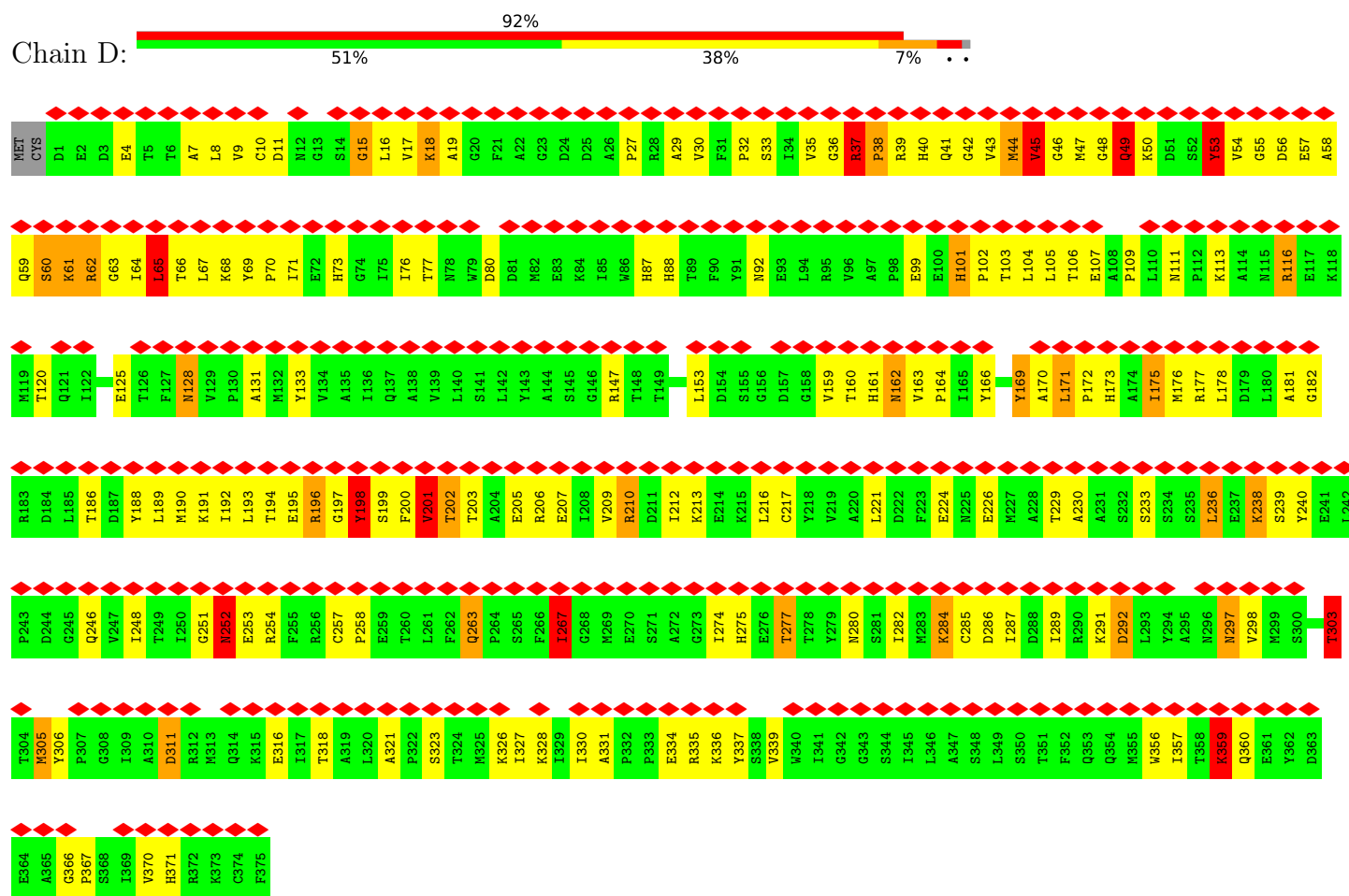




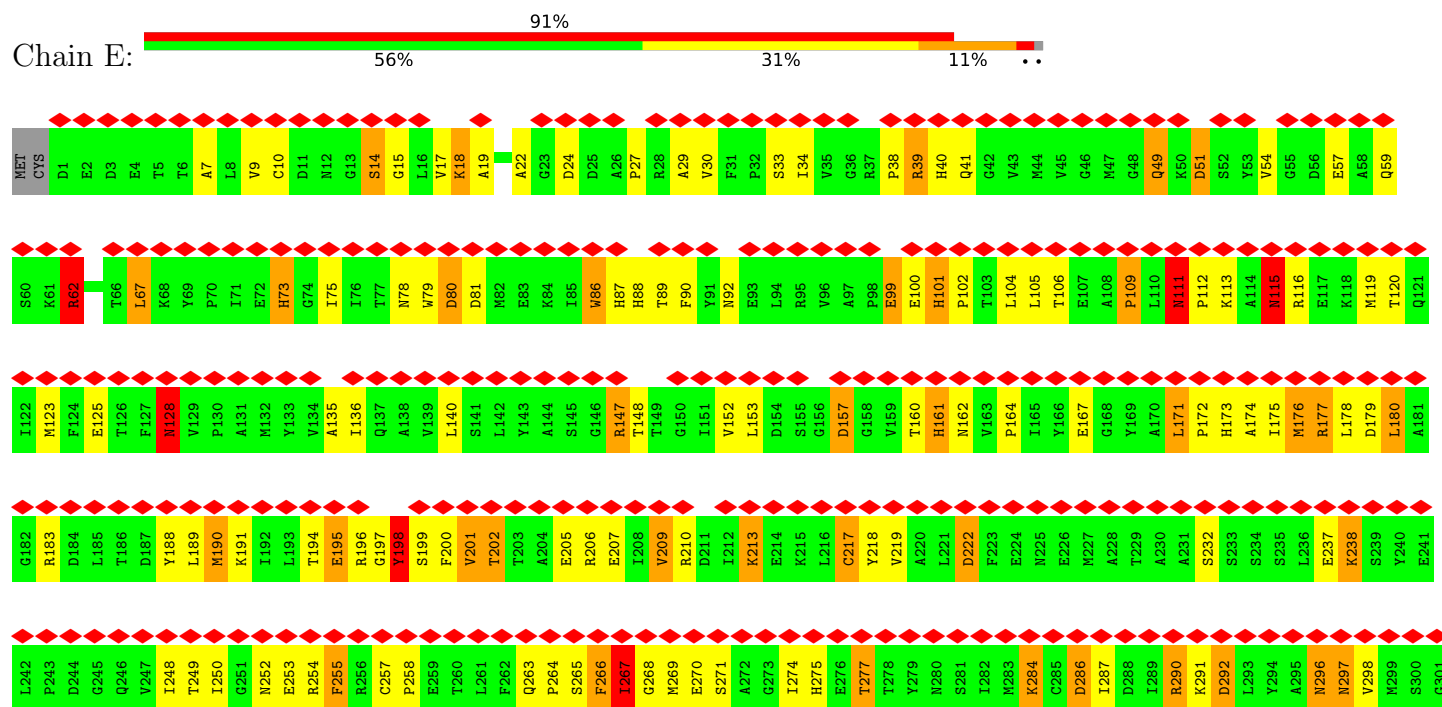
• Molecule 1: Actin, alpha skeletal muscle



• Molecule 1: Actin, alpha skeletal muscle

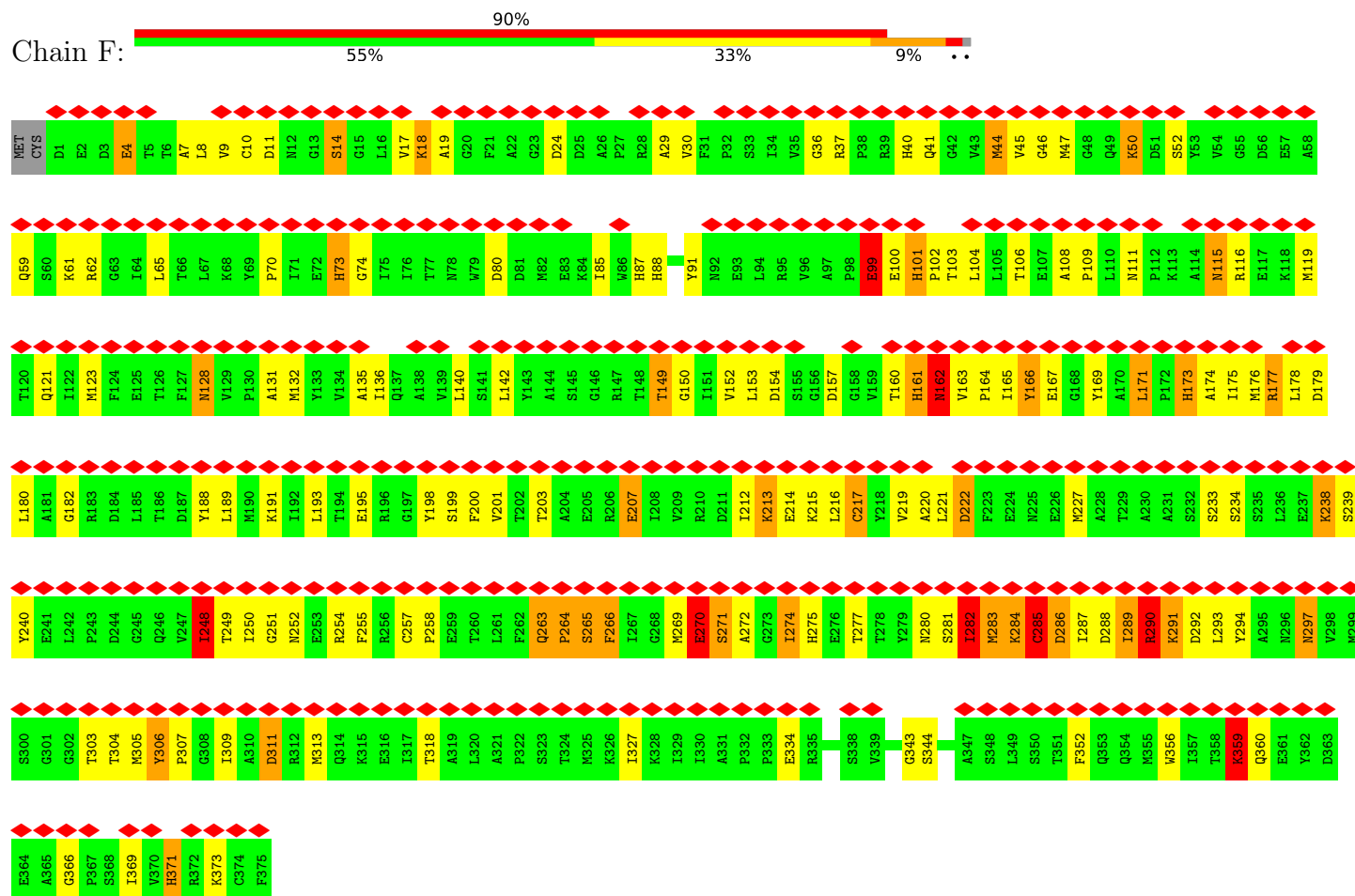


• Molecule 1: Actin, alpha skeletal muscle

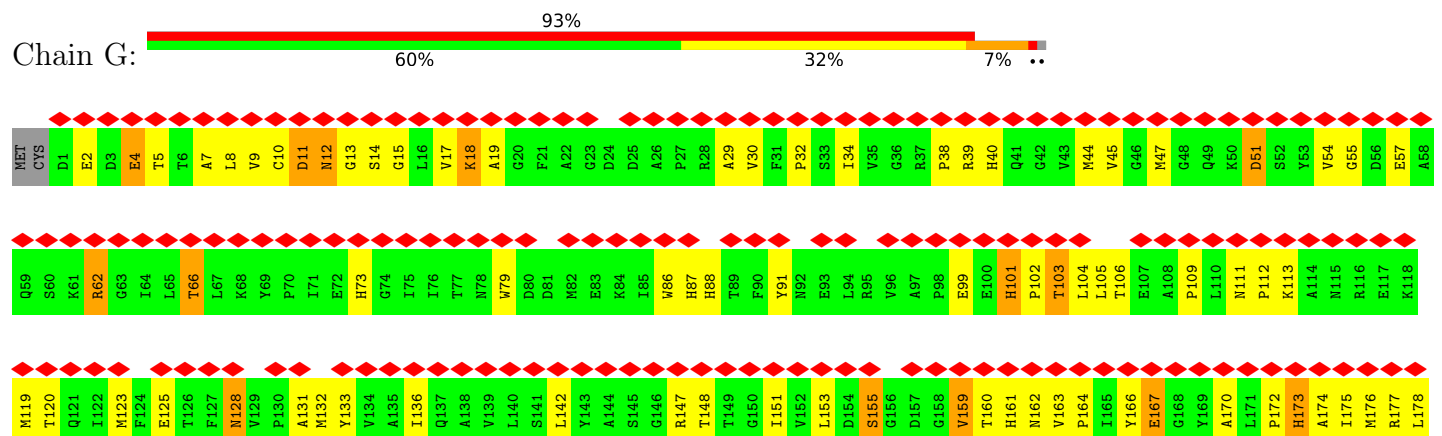


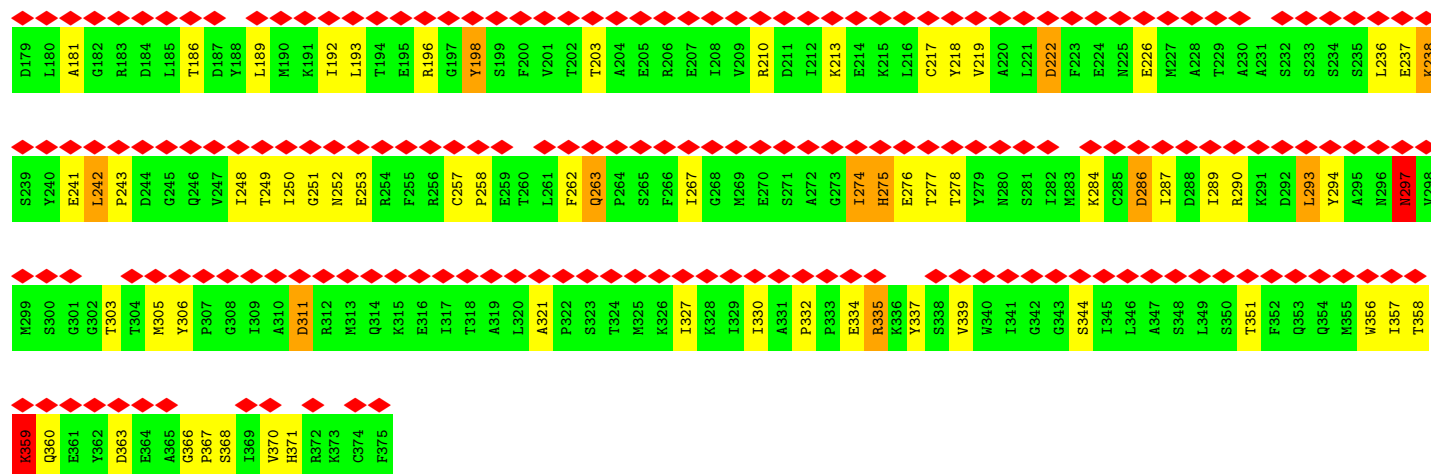


• Molecule 1: Actin, alpha skeletal muscle

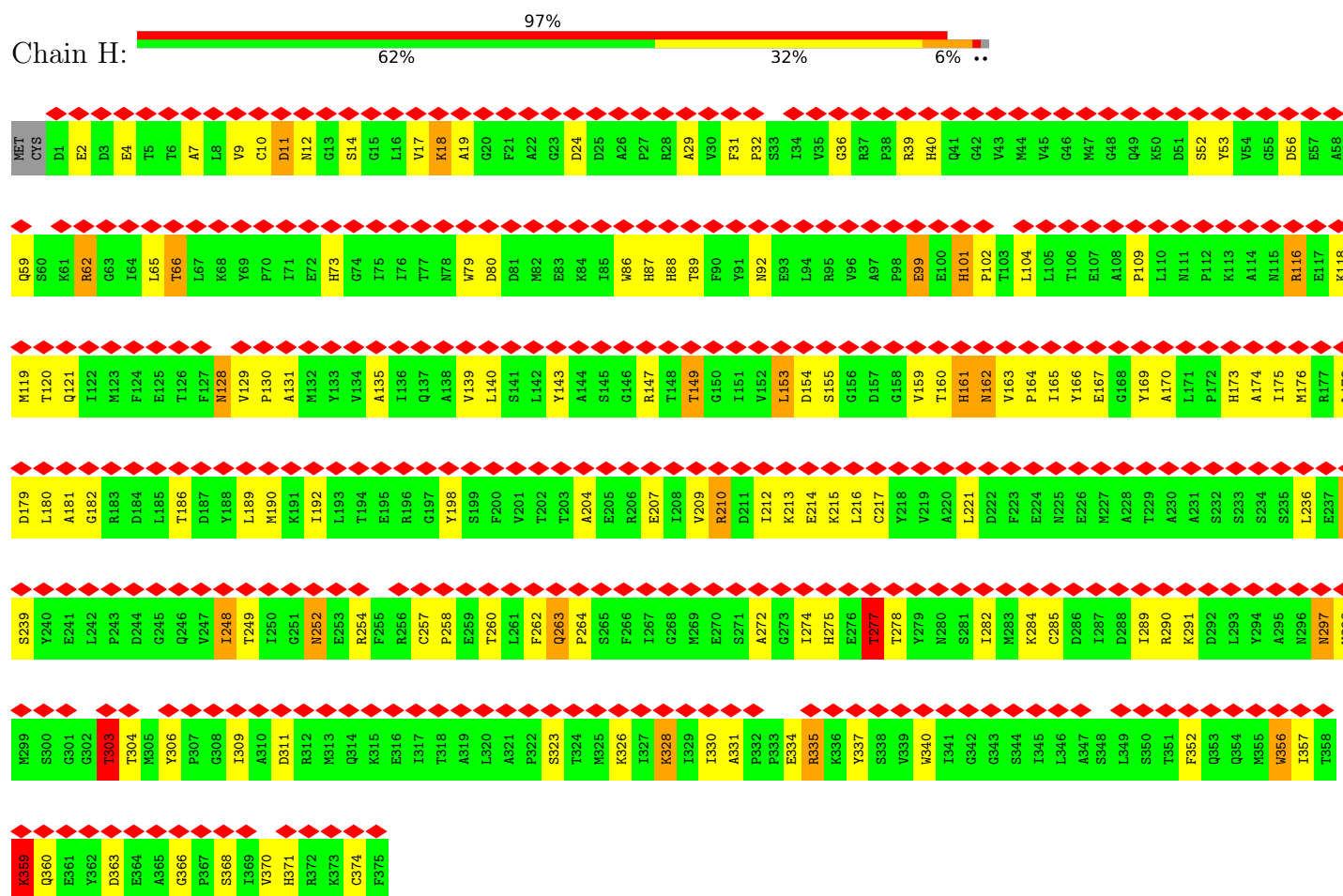


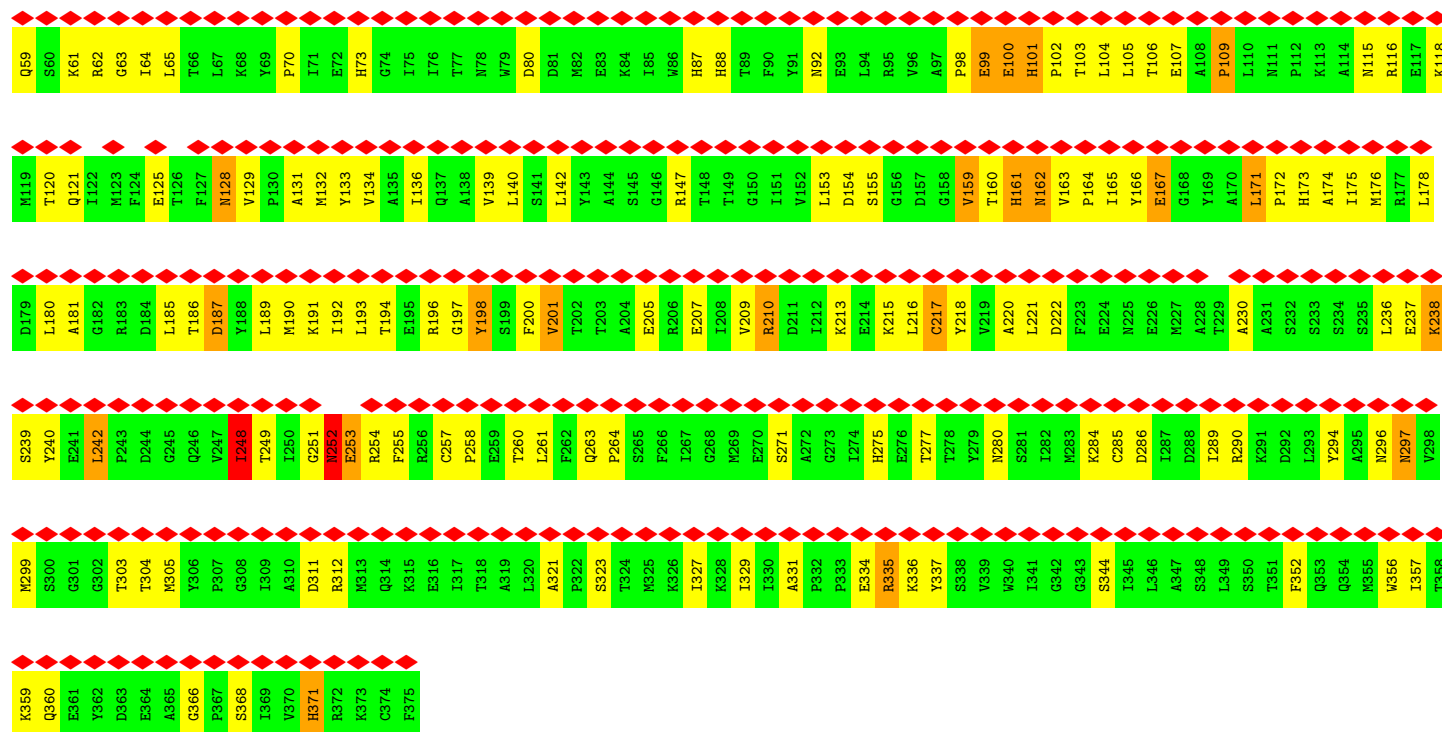
• Molecule 1: Actin, alpha skeletal muscle



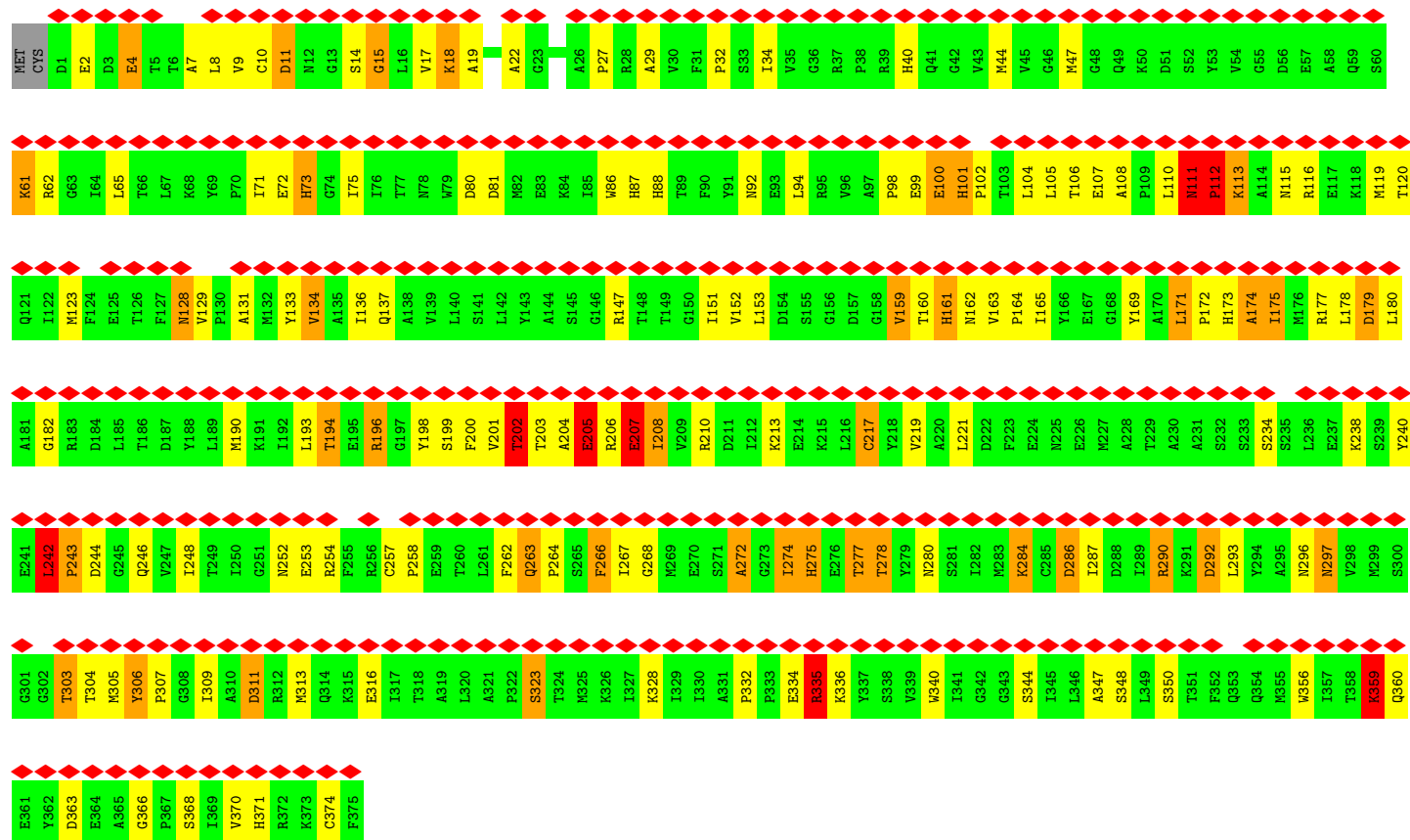


- Molecule 1: Actin, alpha skeletal muscle

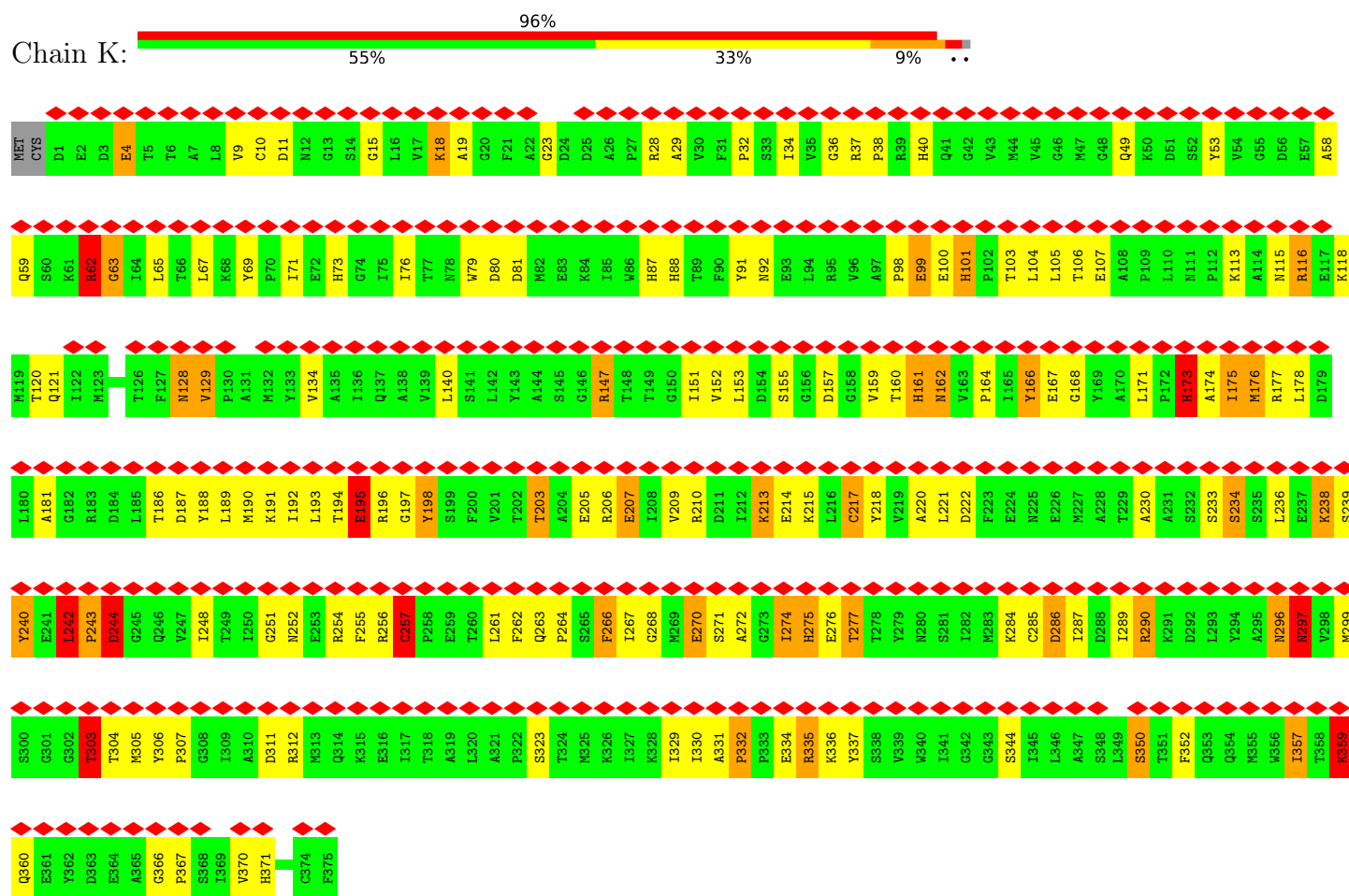




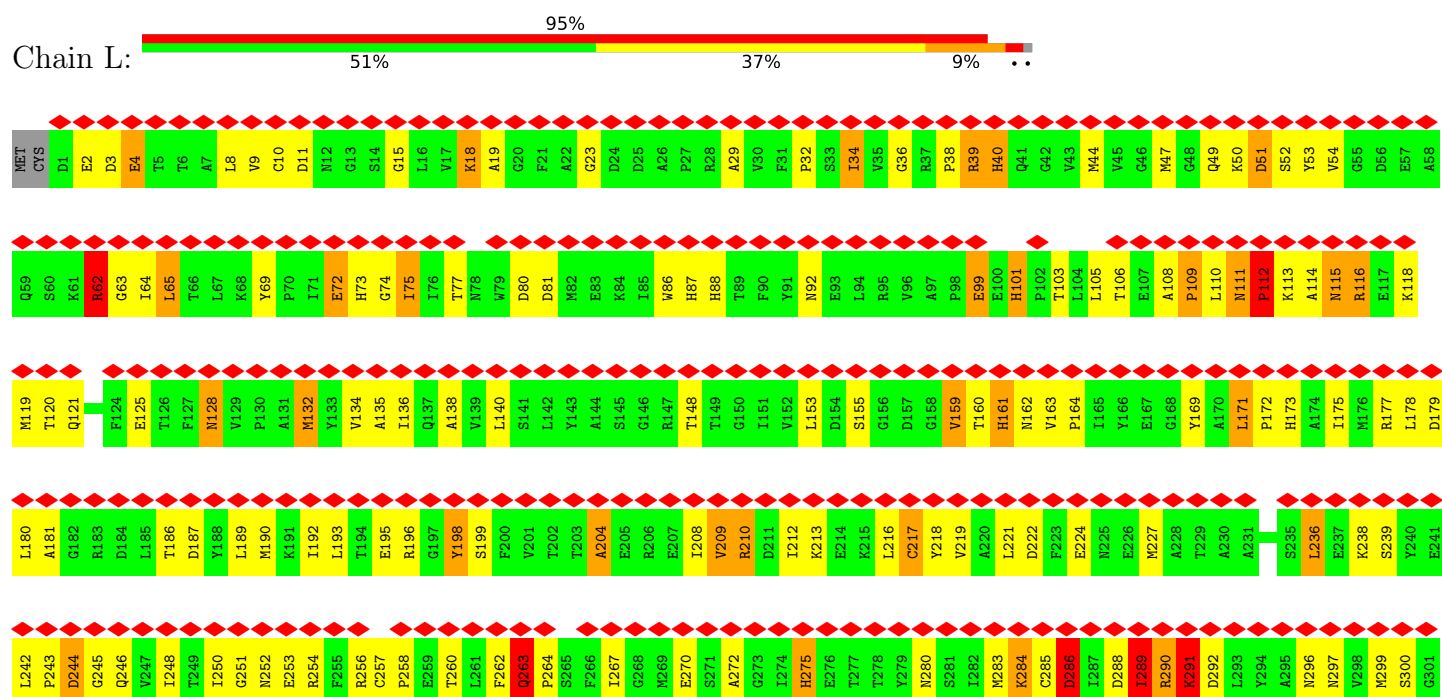
• Molecule 1: Actin, alpha skeletal muscle



• Molecule 1: Actin, alpha skeletal muscle

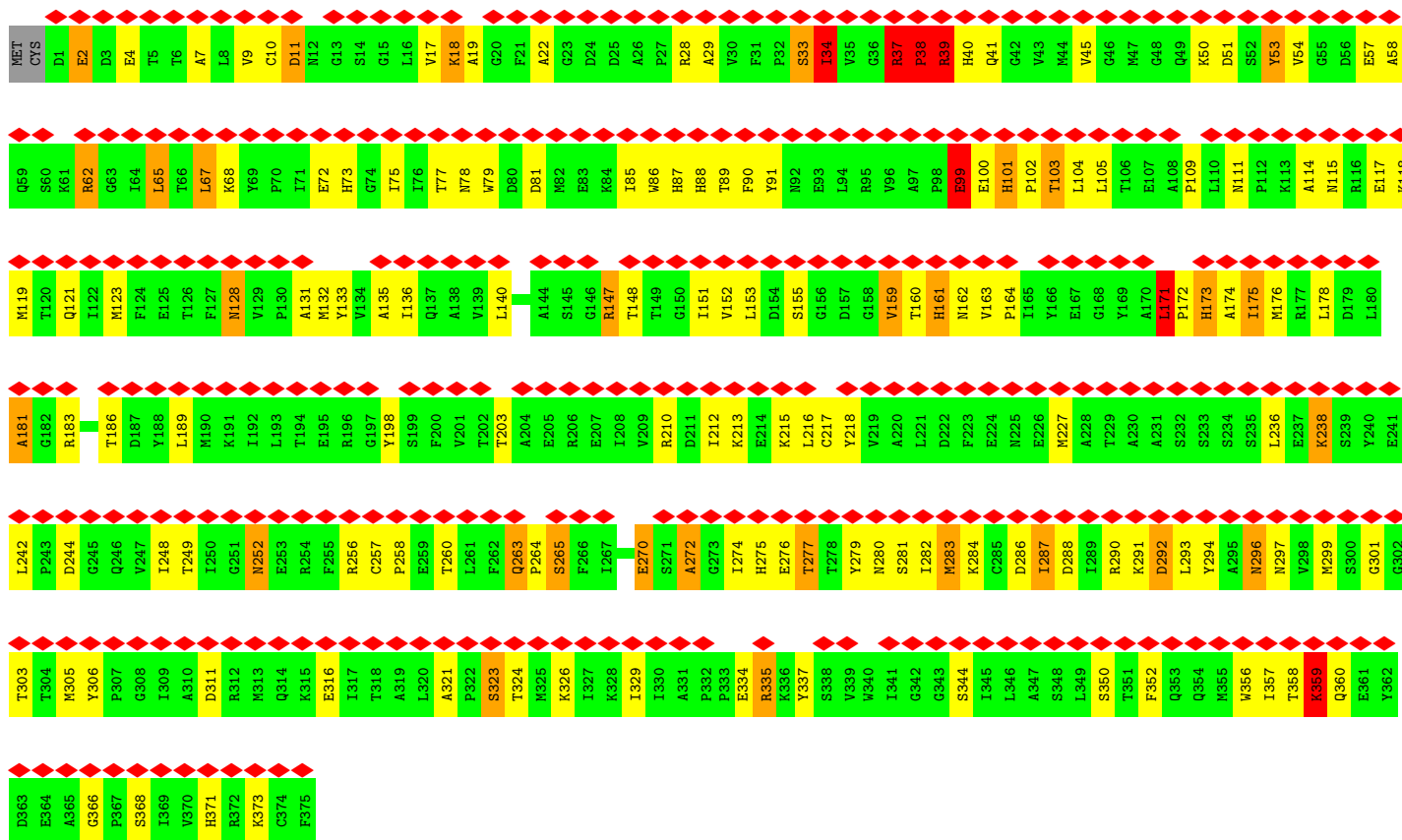
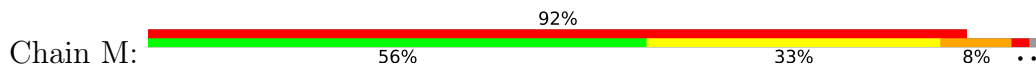


• Molecule 1: Actin, alpha skeletal muscle

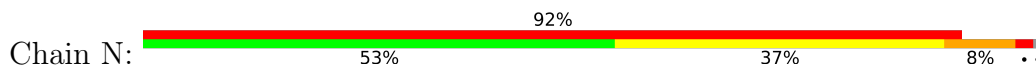




• Molecule 1: Actin, alpha skeletal muscle



• Molecule 1: Actin, alpha skeletal muscle





4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, a =Not provided Å, b =Not provided Å, c =Not provided Å, α =Not provided°, β =Not provided°, γ =Not provided°, space group=Not provided	Depositor
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	Not provided	
Microscope	JEOL 4000EX	Depositor
Voltage (kV)	400	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	40000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	977.199	Depositor
Minimum map value	-974.403	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	215.097	Depositor
Recommended contour level	430	Depositor
Map size (Å)	255.99936, 148.00015, 765.7977	wwPDB
Map dimensions	576, 192, 112	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33333, 1.32143, 1.32951	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	0.85	14/2996 (0.5%)	1.65	39/4058 (1.0%)
1	B	0.84	13/2996 (0.4%)	1.66	49/4058 (1.2%)
1	C	0.77	9/2996 (0.3%)	1.60	38/4058 (0.9%)
1	D	0.80	9/2996 (0.3%)	1.72	60/4058 (1.5%)
1	E	0.80	11/2996 (0.4%)	1.71	58/4058 (1.4%)
1	F	0.78	10/2996 (0.3%)	1.68	45/4058 (1.1%)
1	G	0.78	10/2996 (0.3%)	1.61	43/4058 (1.1%)
1	H	0.81	10/2996 (0.3%)	1.64	54/4058 (1.3%)
1	I	0.81	10/2996 (0.3%)	1.60	48/4058 (1.2%)
1	J	1.29	17/2996 (0.6%)	1.63	57/4058 (1.4%)
1	K	2.72	14/2996 (0.5%)	1.75	62/4058 (1.5%)
1	L	1.43	16/2996 (0.5%)	1.75	61/4058 (1.5%)
1	M	0.85	10/2996 (0.3%)	1.72	54/4058 (1.3%)
1	N	0.84	10/2996 (0.3%)	1.70	57/4058 (1.4%)
All	All	1.14	163/41944 (0.4%)	1.67	725/56812 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	11
1	C	0	7
1	D	0	11
1	E	0	10
1	F	0	8
1	G	0	3
1	H	0	6
1	I	0	9
1	J	0	8
1	K	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	13
1	M	0	7
1	N	0	10
All	All	0	123

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	173	HIS	CB-CG	117.88	3.15	1.50
1	K	195	GLU	CB-CG	77.40	3.84	1.52
1	L	112	PRO	CA-CB	42.33	2.13	1.53
1	L	112	PRO	N-CD	28.98	1.88	1.47
1	L	112	PRO	N-CA	28.57	1.83	1.47
1	J	266	PHE	CG-CD2	27.25	1.96	1.38
1	J	266	PHE	CG-CD1	26.78	1.95	1.38
1	L	112	PRO	CG-CD	21.09	2.22	1.50
1	J	266	PHE	CE2-CZ	18.98	1.95	1.38
1	J	266	PHE	CD2-CE2	18.95	1.95	1.38
1	J	266	PHE	CE1-CZ	18.88	1.95	1.38
1	J	266	PHE	CD1-CE1	18.44	1.94	1.38
1	L	112	PRO	CB-CG	12.65	2.12	1.49
1	K	173	HIS	CG-CD2	8.31	1.45	1.35
1	K	173	HIS	CD2-NE2	-7.53	1.29	1.37
1	L	88	HIS	CD2-NE2	-7.40	1.29	1.37
1	B	73	HIS	CD2-NE2	-7.40	1.29	1.37
1	A	33	SER	C-N	7.39	1.44	1.33
1	A	73	HIS	CD2-NE2	-7.38	1.29	1.37
1	L	173	HIS	CD2-NE2	-7.36	1.29	1.37
1	E	173	HIS	CD2-NE2	-7.33	1.29	1.37
1	A	371	HIS	CD2-NE2	-7.32	1.29	1.37
1	B	173	HIS	CD2-NE2	-7.32	1.29	1.37
1	M	73	HIS	CD2-NE2	-7.23	1.29	1.37
1	H	101	HIS	CD2-NE2	-7.14	1.29	1.37
1	E	101	HIS	CD2-NE2	-7.09	1.30	1.37
1	K	40	HIS	CD2-NE2	-7.05	1.30	1.37
1	L	371	HIS	CD2-NE2	-7.03	1.30	1.37
1	G	40	HIS	CD2-NE2	-7.01	1.30	1.37
1	F	101	HIS	CD2-NE2	-7.00	1.30	1.37
1	L	101	HIS	CD2-NE2	-6.96	1.30	1.37
1	J	371	HIS	CD2-NE2	-6.93	1.30	1.37
1	L	87	HIS	CD2-NE2	-6.91	1.30	1.37
1	C	101	HIS	CD2-NE2	-6.87	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	101	HIS	CD2-NE2	-6.84	1.30	1.37
1	K	371	HIS	CD2-NE2	-6.81	1.30	1.37
1	D	73	HIS	CD2-NE2	-6.80	1.30	1.37
1	A	101	HIS	CD2-NE2	-6.79	1.30	1.37
1	D	40	HIS	CD2-NE2	-6.78	1.30	1.37
1	L	73	HIS	CD2-NE2	-6.75	1.30	1.37
1	J	88	HIS	CD2-NE2	-6.74	1.30	1.37
1	N	101	HIS	CD2-NE2	-6.72	1.30	1.37
1	N	371	HIS	CD2-NE2	-6.72	1.30	1.37
1	M	161	HIS	CD2-NE2	-6.71	1.30	1.37
1	A	87	HIS	CD2-NE2	-6.71	1.30	1.37
1	K	161	HIS	CD2-NE2	-6.71	1.30	1.37
1	M	40	HIS	CD2-NE2	-6.71	1.30	1.37
1	G	88	HIS	CD2-NE2	-6.71	1.30	1.37
1	B	87	HIS	CD2-NE2	-6.69	1.30	1.37
1	N	73	HIS	CD2-NE2	-6.68	1.30	1.37
1	H	88	HIS	CD2-NE2	-6.68	1.30	1.37
1	F	173	HIS	CD2-NE2	-6.64	1.30	1.37
1	F	161	HIS	CD2-NE2	-6.64	1.30	1.37
1	E	88	HIS	CD2-NE2	-6.63	1.30	1.37
1	G	275	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	161	HIS	CD2-NE2	-6.61	1.30	1.37
1	H	275	HIS	CD2-NE2	-6.59	1.30	1.37
1	B	275	HIS	CD2-NE2	-6.57	1.30	1.37
1	G	101	HIS	CD2-NE2	-6.55	1.30	1.37
1	C	73	HIS	CD2-NE2	-6.55	1.30	1.37
1	B	52	SER	C-N	-6.54	1.25	1.33
1	M	101	HIS	CD2-NE2	-6.54	1.30	1.37
1	F	371	HIS	CD2-NE2	-6.54	1.30	1.37
1	E	371	HIS	CD2-NE2	-6.53	1.30	1.37
1	K	87	HIS	CD2-NE2	-6.53	1.30	1.37
1	I	73	HIS	CD2-NE2	-6.53	1.30	1.37
1	H	73	HIS	CD2-NE2	-6.52	1.30	1.37
1	C	40	HIS	CD2-NE2	-6.52	1.30	1.37
1	J	40	HIS	CD2-NE2	-6.51	1.30	1.37
1	H	87	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	40	HIS	CD2-NE2	-6.49	1.30	1.37
1	F	87	HIS	CD2-NE2	-6.49	1.30	1.37
1	F	88	HIS	CD2-NE2	-6.48	1.30	1.37
1	H	40	HIS	CD2-NE2	-6.47	1.30	1.37
1	D	371	HIS	CD2-NE2	-6.45	1.30	1.37
1	I	88	HIS	CD2-NE2	-6.44	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	161	HIS	CD2-NE2	-6.44	1.30	1.37
1	K	88	HIS	CD2-NE2	-6.44	1.30	1.37
1	G	73	HIS	CD2-NE2	-6.42	1.30	1.37
1	D	101	HIS	CD2-NE2	-6.42	1.30	1.37
1	M	371	HIS	CD2-NE2	-6.40	1.30	1.37
1	J	87	HIS	CD2-NE2	-6.40	1.30	1.37
1	M	88	HIS	CD2-NE2	-6.40	1.30	1.37
1	E	73	HIS	CD2-NE2	-6.39	1.30	1.37
1	I	87	HIS	CD2-NE2	-6.38	1.30	1.37
1	G	371	HIS	CD2-NE2	-6.35	1.30	1.37
1	C	275	HIS	CD2-NE2	-6.35	1.30	1.37
1	E	40	HIS	CD2-NE2	-6.34	1.30	1.37
1	B	101	HIS	CD2-NE2	-6.32	1.30	1.37
1	E	87	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	88	HIS	CD2-NE2	-6.32	1.30	1.37
1	I	101	HIS	CD2-NE2	-6.32	1.30	1.37
1	I	371	HIS	CD2-NE2	-6.32	1.30	1.37
1	N	275	HIS	CD2-NE2	-6.32	1.30	1.37
1	B	371	HIS	CD2-NE2	-6.30	1.30	1.37
1	C	161	HIS	CD2-NE2	-6.30	1.30	1.37
1	D	161	HIS	CD2-NE2	-6.30	1.30	1.37
1	M	87	HIS	CD2-NE2	-6.30	1.30	1.37
1	C	88	HIS	CD2-NE2	-6.30	1.30	1.37
1	F	40	HIS	CD2-NE2	-6.28	1.30	1.37
1	J	73	HIS	CD2-NE2	-6.27	1.30	1.37
1	G	161	HIS	CD2-NE2	-6.27	1.30	1.37
1	B	40	HIS	CD2-NE2	-6.25	1.30	1.37
1	H	173	HIS	CD2-NE2	-6.25	1.30	1.37
1	F	275	HIS	CD2-NE2	-6.24	1.30	1.37
1	C	173	HIS	CD2-NE2	-6.24	1.30	1.37
1	I	275	HIS	CD2-NE2	-6.20	1.31	1.37
1	D	275	HIS	CD2-NE2	-6.19	1.31	1.37
1	N	173	HIS	CD2-NE2	-6.19	1.31	1.37
1	E	161	HIS	CD2-NE2	-6.17	1.31	1.37
1	N	88	HIS	CD2-NE2	-6.15	1.31	1.37
1	N	87	HIS	CD2-NE2	-6.13	1.31	1.37
1	L	40	HIS	CD2-NE2	-6.11	1.31	1.37
1	M	173	HIS	CD2-NE2	-6.09	1.31	1.37
1	N	40	HIS	CD2-NE2	-6.09	1.31	1.37
1	F	73	HIS	CD2-NE2	-6.09	1.31	1.37
1	B	161	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	173	HIS	CD2-NE2	-6.06	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	87	HIS	CD2-NE2	-6.06	1.31	1.37
1	C	87	HIS	CD2-NE2	-6.03	1.31	1.37
1	G	87	HIS	CD2-NE2	-6.03	1.31	1.37
1	H	161	HIS	CD2-NE2	-6.02	1.31	1.37
1	D	173	HIS	CD2-NE2	-5.99	1.31	1.37
1	I	40	HIS	CD2-NE2	-5.98	1.31	1.37
1	B	88	HIS	CD2-NE2	-5.97	1.31	1.37
1	D	88	HIS	CD2-NE2	-5.97	1.31	1.37
1	I	161	HIS	CD2-NE2	-5.96	1.31	1.37
1	K	73	HIS	CD2-NE2	-5.95	1.31	1.37
1	I	173	HIS	CD2-NE2	-5.93	1.31	1.37
1	H	371	HIS	CD2-NE2	-5.91	1.31	1.37
1	K	101	HIS	CD2-NE2	-5.91	1.31	1.37
1	E	275	HIS	CD2-NE2	-5.87	1.31	1.37
1	C	371	HIS	CD2-NE2	-5.82	1.31	1.37
1	J	161	HIS	CG-ND1	-5.80	1.31	1.38
1	A	275	HIS	CD2-NE2	-5.76	1.31	1.37
1	N	161	HIS	CD2-NE2	-5.75	1.31	1.37
1	K	195	GLU	CA-CB	5.75	1.63	1.53
1	M	275	HIS	CD2-NE2	-5.74	1.31	1.37
1	K	275	HIS	CD2-NE2	-5.70	1.31	1.37
1	L	161	HIS	CD2-NE2	-5.68	1.31	1.37
1	L	275	HIS	CD2-NE2	-5.67	1.31	1.37
1	G	173	HIS	CD2-NE2	-5.64	1.31	1.37
1	A	54	VAL	C-N	5.64	1.41	1.33
1	J	173	HIS	CD2-NE2	-5.63	1.31	1.37
1	F	173	HIS	CG-ND1	-5.54	1.32	1.38
1	H	88	HIS	CG-ND1	-5.52	1.32	1.38
1	G	173	HIS	CG-ND1	-5.38	1.32	1.38
1	B	371	HIS	CG-ND1	-5.33	1.32	1.38
1	N	73	HIS	CG-ND1	-5.33	1.32	1.38
1	L	88	HIS	CG-ND1	-5.32	1.32	1.38
1	I	161	HIS	CG-ND1	-5.31	1.32	1.38
1	K	173	HIS	CA-CB	5.27	1.62	1.53
1	E	101	HIS	CG-ND1	-5.24	1.32	1.38
1	L	40	HIS	CG-ND1	-5.20	1.32	1.38
1	A	88	HIS	CG-ND1	-5.16	1.32	1.38
1	B	88	HIS	CG-ND1	-5.14	1.32	1.38
1	A	73	HIS	CG-ND1	-5.12	1.32	1.38
1	J	275	HIS	CD2-NE2	-5.10	1.32	1.37
1	M	173	HIS	CG-ND1	-5.10	1.32	1.38
1	B	161	HIS	CG-ND1	-5.07	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	40	HIS	CG-ND1	-5.06	1.32	1.38
1	E	161	HIS	CG-ND1	-5.06	1.32	1.38
1	A	161	HIS	CG-ND1	-5.01	1.32	1.38

All (725) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	173	HIS	CA-CB-CG	28.18	141.98	113.80
1	K	173	HIS	ND1-CG-CD2	-13.01	93.09	106.10
1	M	306	TYR	N-CA-C	11.58	122.92	109.60
1	K	195	GLU	CB-CG-CD	11.42	132.01	112.60
1	F	285	CYS	CA-C-N	10.82	136.16	120.90
1	F	285	CYS	C-N-CA	10.82	136.16	120.90
1	M	34	ILE	CB-CA-C	-10.13	102.22	111.74
1	K	195	GLU	CA-CB-CG	10.04	134.18	114.10
1	D	128	ASN	CA-CB-CG	9.91	122.51	112.60
1	A	62	ARG	N-CA-C	9.71	123.54	112.57
1	N	275	HIS	CB-CG-CD2	-9.69	118.61	131.20
1	N	24	ASP	CA-CB-CG	9.68	122.28	112.60
1	G	128	ASN	CA-CB-CG	9.65	122.25	112.60
1	L	244	ASP	O-C-N	-9.49	112.49	121.79
1	K	128	ASN	CA-CB-CG	9.44	122.04	112.60
1	L	112	PRO	N-CA-C	9.40	131.83	112.47
1	E	306	TYR	N-CA-C	9.38	121.56	109.64
1	L	112	PRO	CA-N-CD	9.37	125.11	112.00
1	K	4	GLU	N-CA-C	9.33	122.44	111.71
1	D	297	ASN	OD1-CG-ND2	-9.29	113.31	122.60
1	J	128	ASN	CA-CB-CG	9.13	121.73	112.60
1	E	252	ASN	OD1-CG-ND2	-9.09	113.51	122.60
1	N	297	ASN	OD1-CG-ND2	-8.97	113.63	122.60
1	K	244	ASP	CA-CB-CG	8.89	121.49	112.60
1	M	128	ASN	CA-CB-CG	8.77	121.37	112.60
1	K	287	ILE	N-CA-C	8.68	118.69	110.53
1	K	297	ASN	CA-CB-CG	8.66	121.26	112.60
1	B	306	TYR	N-CA-C	8.66	120.22	109.57
1	K	242	LEU	N-CA-C	-8.60	98.81	109.65
1	G	173	HIS	CA-CB-CG	8.60	122.39	113.80
1	H	275	HIS	CB-CG-CD2	-8.54	120.10	131.20
1	I	128	ASN	CA-CB-CG	8.54	121.14	112.60
1	K	81	ASP	CA-CB-CG	8.54	121.14	112.60
1	D	202	THR	N-CA-CB	8.46	121.76	110.25
1	E	286	ASP	N-CA-C	8.44	121.67	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	275	HIS	CA-CB-CG	8.43	122.23	113.80
1	H	371	HIS	CB-CG-CD2	-8.43	120.24	131.20
1	L	128	ASN	CA-CB-CG	8.38	120.98	112.60
1	G	120	THR	CA-CB-OG1	-8.27	97.20	109.60
1	D	4	GLU	N-CA-C	8.23	121.17	111.71
1	F	101	HIS	CB-CG-CD2	-8.16	120.59	131.20
1	J	297	ASN	OD1-CG-ND2	-8.14	114.46	122.60
1	I	125	GLU	N-CA-C	8.09	120.10	111.28
1	G	275	HIS	CB-CG-CD2	-8.08	120.69	131.20
1	A	128	ASN	N-CA-C	8.00	122.39	112.47
1	A	62	ARG	O-C-N	-7.97	111.91	122.19
1	H	4	GLU	N-CA-C	7.96	120.66	111.11
1	D	80	ASP	CA-CB-CG	7.94	120.54	112.60
1	L	323	SER	N-CA-C	7.94	122.07	112.38
1	N	322	PRO	N-CA-C	7.93	128.80	112.47
1	A	217	CYS	N-CA-C	7.89	120.77	110.43
1	L	244	ASP	CA-CB-CG	7.89	120.49	112.60
1	E	80	ASP	CA-CB-CG	7.84	120.44	112.60
1	H	275	HIS	CA-CB-CG	7.83	121.63	113.80
1	F	306	TYR	N-CA-C	7.83	119.19	109.57
1	M	297	ASN	CA-CB-CG	7.82	120.42	112.60
1	F	297	ASN	OD1-CG-ND2	-7.79	114.81	122.60
1	I	297	ASN	CA-CB-CG	7.79	120.39	112.60
1	F	80	ASP	CA-CB-CG	7.77	120.37	112.60
1	E	177	ARG	NE-CZ-NH2	7.76	126.18	119.20
1	J	111	ASN	O-C-N	-7.74	112.41	121.32
1	H	128	ASN	CA-CB-CG	7.74	120.33	112.60
1	H	306	TYR	N-CA-C	7.73	119.08	109.57
1	H	120	THR	CA-CB-OG1	-7.73	98.01	109.60
1	F	371	HIS	CB-CG-CD2	-7.72	121.17	131.20
1	G	306	TYR	N-CA-C	7.69	120.56	109.48
1	J	371	HIS	CB-CG-CD2	-7.63	121.28	131.20
1	I	297	ASN	OD1-CG-ND2	-7.61	114.99	122.60
1	K	217	CYS	N-CA-C	7.54	120.01	109.15
1	H	277	THR	N-CA-CB	-7.53	97.77	110.49
1	E	198	TYR	N-CA-C	7.52	120.51	109.69
1	B	272	ALA	N-CA-C	7.51	121.76	110.64
1	A	371	HIS	CA-CB-CG	-7.50	106.30	113.80
1	B	128	ASN	CA-CB-CG	7.47	120.07	112.60
1	A	297	ASN	OD1-CG-ND2	-7.47	115.13	122.60
1	G	311	ASP	CA-CB-CG	7.46	120.06	112.60
1	E	173	HIS	CB-CG-CD2	-7.42	121.55	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	296	ASN	CA-CB-CG	7.42	120.02	112.60
1	E	111	ASN	CA-CB-CG	7.41	120.01	112.60
1	D	128	ASN	OD1-CG-ND2	-7.40	115.20	122.60
1	A	275	HIS	CA-CB-CG	7.35	121.15	113.80
1	E	371	HIS	CB-CG-CD2	-7.30	121.72	131.20
1	M	78	ASN	OD1-CG-ND2	-7.28	115.32	122.60
1	L	171	LEU	CA-C-N	7.27	126.98	119.56
1	L	171	LEU	C-N-CA	7.27	126.98	119.56
1	L	101	HIS	CB-CG-CD2	-7.26	121.76	131.20
1	L	297	ASN	OD1-CG-ND2	-7.26	115.34	122.60
1	B	217	CYS	N-CA-C	7.25	119.67	110.24
1	H	298	VAL	O-C-N	-7.21	115.41	123.20
1	L	4	GLU	N-CA-C	7.20	119.20	111.36
1	A	128	ASN	CA-CB-CG	7.19	119.79	112.60
1	B	206	ARG	N-CA-C	7.17	120.01	111.33
1	A	371	HIS	CB-CG-CD2	-7.16	121.90	131.20
1	I	275	HIS	CB-CG-CD2	-7.15	121.90	131.20
1	K	40	HIS	CB-CG-CD2	-7.14	121.92	131.20
1	M	217	CYS	N-CA-C	7.13	119.51	110.24
1	B	198	TYR	N-CA-C	7.12	120.53	107.99
1	N	101	HIS	CB-CG-CD2	-7.12	121.94	131.20
1	I	371	HIS	CB-CG-CD2	-7.08	122.00	131.20
1	A	101	HIS	CB-CG-CD2	-7.07	122.01	131.20
1	L	120	THR	CA-CB-OG1	-7.07	99.00	109.60
1	J	275	HIS	CB-CG-CD2	-7.07	122.01	131.20
1	C	128	ASN	CA-CB-CG	7.06	119.66	112.60
1	J	207	GLU	N-CA-C	7.06	120.78	111.75
1	D	280	ASN	CA-CB-CG	7.05	119.65	112.60
1	L	290	ARG	N-CA-C	-7.05	103.68	111.36
1	H	371	HIS	CB-CG-ND1	7.04	133.26	122.70
1	I	120	THR	CA-CB-OG1	-7.04	99.05	109.60
1	C	234	SER	N-CA-C	7.01	118.38	108.00
1	I	101	HIS	CB-CG-CD2	-7.00	122.10	131.20
1	L	303	THR	CB-CA-C	6.99	122.47	110.94
1	J	242	LEU	O-C-N	-6.98	113.29	121.32
1	K	296	ASN	OD1-CG-ND2	-6.98	115.62	122.60
1	D	45	VAL	N-CA-C	-6.95	98.38	108.11
1	N	275	HIS	CB-CG-ND1	6.95	133.12	122.70
1	N	371	HIS	CB-CG-CD2	-6.92	122.20	131.20
1	N	322	PRO	CA-N-CD	-6.90	102.35	112.00
1	G	275	HIS	CA-CB-CG	6.89	120.69	113.80
1	J	111	ASN	CA-CB-CG	6.89	119.49	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	ASN	OD1-CG-ND2	-6.87	115.73	122.60
1	K	73	HIS	CA-CB-CG	6.87	120.67	113.80
1	L	81	ASP	CA-CB-CG	6.87	119.47	112.60
1	G	40	HIS	CB-CG-CD2	-6.86	122.28	131.20
1	C	297	ASN	OD1-CG-ND2	-6.86	115.74	122.60
1	G	321	ALA	N-CA-C	6.86	119.37	109.84
1	N	66	THR	N-CA-C	6.86	119.60	108.63
1	H	101	HIS	CB-CG-CD2	-6.84	122.30	131.20
1	K	173	HIS	CG-CD2-NE2	6.84	114.04	107.20
1	J	323	SER	N-CA-C	6.83	119.60	111.33
1	D	321	ALA	N-CA-C	6.83	118.50	109.83
1	M	371	HIS	CB-CG-CD2	-6.82	122.33	131.20
1	E	111	ASN	OD1-CG-ND2	-6.82	115.78	122.60
1	H	311	ASP	CA-CB-CG	6.79	119.39	112.60
1	M	321	ALA	N-CA-C	6.78	118.34	109.93
1	B	101	HIS	CB-CG-CD2	-6.77	122.40	131.20
1	H	275	HIS	CB-CG-ND1	6.76	132.84	122.70
1	L	275	HIS	CB-CG-CD2	-6.75	122.42	131.20
1	E	217	CYS	N-CA-C	6.75	120.09	109.96
1	C	101	HIS	CB-CG-CD2	-6.74	122.43	131.20
1	E	286	ASP	CA-CB-CG	6.73	119.33	112.60
1	E	128	ASN	CA-CB-CG	6.72	119.32	112.60
1	K	120	THR	CA-CB-OG1	-6.72	99.52	109.60
1	N	128	ASN	CA-CB-CG	6.72	119.32	112.60
1	E	201	VAL	N-CA-C	6.70	118.23	108.58
1	K	80	ASP	CA-CB-CG	6.70	119.30	112.60
1	B	173	HIS	CB-CG-CD2	-6.69	122.50	131.20
1	J	297	ASN	CB-CG-ND2	6.68	126.43	116.40
1	N	278	THR	CA-CB-OG1	-6.68	99.57	109.60
1	F	271	SER	N-CA-C	6.66	116.84	108.45
1	G	363	ASP	CA-CB-CG	6.66	119.26	112.60
1	N	321	ALA	CA-C-N	6.65	128.15	119.84
1	N	321	ALA	C-N-CA	6.65	128.15	119.84
1	A	59	GLN	OE1-CD-NE2	-6.65	115.95	122.60
1	F	24	ASP	CA-CB-CG	6.64	119.24	112.60
1	G	128	ASN	OD1-CG-ND2	-6.63	115.97	122.60
1	F	305	MET	N-CA-C	6.63	121.11	112.89
1	A	162	ASN	OD1-CG-ND2	-6.61	115.99	122.60
1	C	286	ASP	CA-CB-CG	6.61	119.21	112.60
1	D	27	PRO	N-CA-C	6.61	121.60	111.15
1	A	128	ASN	OD1-CG-ND2	-6.60	116.00	122.60
1	N	277	THR	CA-CB-CG2	6.59	121.70	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	297	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	B	275	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	H	24	ASP	CA-CB-CG	6.56	119.16	112.60
1	L	198	TYR	N-CA-C	6.56	118.80	110.33
1	B	125	GLU	N-CA-C	6.53	119.22	111.71
1	D	37	ARG	CA-C-N	6.53	128.00	119.84
1	D	37	ARG	C-N-CA	6.53	128.00	119.84
1	L	297	ASN	CB-CG-ND2	6.53	126.19	116.40
1	H	128	ASN	N-CA-C	6.52	120.55	111.74
1	A	306	TYR	N-CA-C	6.52	117.92	109.64
1	I	92	ASN	CA-CB-CG	6.52	119.12	112.60
1	D	297	ASN	CB-CG-ND2	6.51	126.17	116.40
1	B	286	ASP	CA-CB-CG	6.51	119.11	112.60
1	L	72	GLU	O-C-N	6.51	130.61	123.13
1	H	80	ASP	CA-CB-CG	6.48	119.08	112.60
1	E	237	GLU	N-CA-C	6.48	124.61	110.80
1	N	80	ASP	CA-CB-CG	6.48	119.08	112.60
1	D	125	GLU	N-CA-C	6.48	118.42	111.36
1	J	81	ASP	CA-CB-CG	6.47	119.07	112.60
1	L	371	HIS	CB-CG-CD2	-6.46	122.80	131.20
1	M	265	SER	N-CA-C	6.46	118.92	108.32
1	A	305	MET	N-CA-C	6.45	120.98	113.18
1	N	297	ASN	CA-CB-CG	6.44	119.04	112.60
1	C	81	ASP	CA-CB-CG	6.43	119.03	112.60
1	E	275	HIS	CA-CB-CG	6.42	120.22	113.80
1	B	92	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	M	311	ASP	CA-CB-CG	6.41	119.01	112.60
1	N	125	GLU	N-CA-C	6.41	119.95	111.75
1	B	115	ASN	CA-CB-CG	6.40	119.00	112.60
1	G	286	ASP	CA-CB-CG	6.40	119.00	112.60
1	H	272	ALA	N-CA-C	6.40	119.76	110.42
1	I	198	TYR	N-CA-C	6.39	119.86	110.59
1	I	80	ASP	CA-CB-CG	6.39	118.99	112.60
1	C	187	ASP	CA-CB-CG	6.37	118.97	112.60
1	H	366	GLY	CA-C-N	6.37	126.59	119.32
1	H	366	GLY	C-N-CA	6.37	126.59	119.32
1	G	101	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	H	297	ASN	CA-CB-CG	6.36	118.96	112.60
1	K	303	THR	CB-CA-C	6.36	121.31	111.02
1	C	179	ASP	CA-CB-CG	6.35	118.95	112.60
1	H	356	TRP	CG-CD2-CE3	6.35	140.25	133.90
1	G	371	HIS	CB-CG-CD2	-6.34	122.95	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	275	HIS	CB-CG-ND1	6.34	132.21	122.70
1	I	311	ASP	CA-CB-CG	6.33	118.93	112.60
1	K	23	GLY	N-CA-C	-6.33	106.81	113.58
1	J	280	ASN	CB-CG-ND2	6.33	125.89	116.40
1	A	311	ASP	CA-CB-CG	6.33	118.92	112.60
1	B	62	ARG	N-CA-C	6.32	124.26	110.80
1	J	92	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	A	265	SER	N-CA-C	6.31	124.24	110.80
1	K	371	HIS	CB-CG-CD2	-6.30	123.00	131.20
1	L	291	LYS	N-CA-C	6.30	124.22	110.80
1	E	73	HIS	CB-CG-CD2	-6.30	123.01	131.20
1	K	266	PHE	CA-CB-CG	6.29	120.09	113.80
1	L	363	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	76	ILE	N-CA-C	6.28	117.84	108.54
1	D	128	ASN	CB-CG-ND2	6.27	125.81	116.40
1	E	100	GLU	N-CA-CB	-6.27	101.19	110.53
1	J	198	TYR	N-CA-C	6.26	119.43	110.10
1	L	173	HIS	CB-CG-CD2	-6.26	123.06	131.20
1	K	162	ASN	CA-CB-CG	6.26	118.86	112.60
1	F	207	GLU	N-CA-C	6.25	120.37	112.87
1	I	73	HIS	CB-CG-CD2	-6.25	123.07	131.20
1	K	101	HIS	CB-CG-CD2	-6.25	123.07	131.20
1	L	115	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	N	37	ARG	O-C-N	-6.24	117.45	121.88
1	L	115	ASN	CB-CG-ND2	6.23	125.75	116.40
1	L	217	CYS	N-CA-C	6.23	119.07	110.35
1	C	275	HIS	CB-CG-CD2	-6.21	123.12	131.20
1	F	101	HIS	CB-CG-ND1	6.21	132.02	122.70
1	M	296	ASN	CA-CB-CG	6.21	118.81	112.60
1	A	56	ASP	N-CA-C	6.20	117.73	110.97
1	F	135	ALA	N-CA-C	6.20	118.52	108.34
1	K	198	TYR	N-CA-C	6.20	119.62	109.76
1	D	40	HIS	CB-CG-CD2	-6.20	123.14	131.20
1	L	73	HIS	CB-CG-CD2	-6.19	123.15	131.20
1	I	154	ASP	CA-CB-CG	6.19	118.79	112.60
1	M	34	ILE	N-CA-CB	6.19	118.01	109.84
1	L	23	GLY	N-CA-C	-6.17	106.98	113.58
1	C	217	CYS	N-CA-C	6.17	118.94	110.24
1	G	128	ASN	CB-CG-ND2	6.17	125.65	116.40
1	L	289	ILE	CA-C-O	6.17	128.49	120.78
1	C	163	VAL	CA-C-O	-6.17	116.73	119.94
1	N	116	ARG	NE-CZ-NH2	6.16	124.74	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	101	HIS	CB-CG-CD2	-6.16	123.20	131.20
1	A	275	HIS	CB-CG-CD2	-6.15	123.20	131.20
1	H	73	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	A	277	THR	CA-CB-CG2	6.13	120.93	110.50
1	M	198	TYR	N-CA-C	6.13	118.83	110.55
1	D	252	ASN	CB-CG-ND2	6.13	125.60	116.40
1	M	79	TRP	N-CA-C	6.12	120.82	113.23
1	N	161	HIS	CB-CG-CD2	-6.12	123.24	131.20
1	I	167	GLU	CB-CG-CD	6.12	123.00	112.60
1	D	173	HIS	CA-CB-CG	6.11	119.91	113.80
1	G	12	ASN	CA-CB-CG	6.11	118.71	112.60
1	A	38	PRO	N-CA-C	6.10	120.07	110.50
1	H	277	THR	CA-CB-CG2	6.09	120.86	110.50
1	C	73	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	L	111	ASN	CA-C-N	-6.08	112.25	119.84
1	L	111	ASN	C-N-CA	-6.08	112.25	119.84
1	E	296	ASN	CA-CB-CG	6.07	118.67	112.60
1	L	208	ILE	N-CA-C	6.06	120.62	111.89
1	L	135	ALA	N-CA-C	6.06	118.28	109.07
1	J	27	PRO	N-CA-C	6.06	120.59	111.14
1	J	208	ILE	CB-CA-C	6.05	118.71	111.20
1	J	217	CYS	N-CA-C	6.05	118.97	109.96
1	I	277	THR	CA-CB-OG1	-6.04	100.53	109.60
1	D	56	ASP	CA-CB-CG	-6.04	106.56	112.60
1	M	101	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	F	282	ILE	O-C-N	-6.04	115.03	122.57
1	E	352	PHE	N-CA-C	6.03	120.11	112.87
1	E	366	GLY	CA-C-N	6.03	126.20	119.32
1	E	366	GLY	C-N-CA	6.03	126.20	119.32
1	F	263	GLN	N-CA-C	6.03	121.05	108.39
1	I	115	ASN	OD1-CG-ND2	-6.02	116.58	122.60
1	B	277	THR	CA-CB-OG1	-6.02	100.57	109.60
1	N	286	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	80	ASP	CA-CB-CG	6.02	118.62	112.60
1	H	179	ASP	CA-CB-CG	6.02	118.62	112.60
1	J	303	THR	CB-CA-C	6.01	120.86	110.94
1	N	311	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	73	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	K	303	THR	CA-CB-CG2	6.00	120.71	110.50
1	C	40	HIS	CB-CG-CD2	-5.99	123.41	131.20
1	M	173	HIS	CA-CB-CG	5.98	119.78	113.80
1	B	289	ILE	N-CA-C	5.98	118.75	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	278	THR	CA-CB-OG1	-5.98	100.63	109.60
1	M	54	VAL	N-CA-C	5.97	116.47	107.75
1	C	115	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	B	286	ASP	N-CA-C	5.97	119.31	110.48
1	B	297	ASN	CA-CB-CG	5.96	118.56	112.60
1	H	11	ASP	N-CA-C	5.96	117.73	109.15
1	H	356	TRP	CB-CG-CD1	-5.96	117.96	126.90
1	H	217	CYS	N-CA-C	5.96	118.64	110.24
1	K	266	PHE	N-CA-C	-5.95	98.12	110.80
1	H	56	ASP	N-CA-C	5.94	118.52	111.33
1	F	115	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	J	277	THR	CA-CB-CG2	5.93	120.59	110.50
1	I	70	PRO	N-CA-C	5.93	121.66	113.65
1	N	111	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	N	92	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	D	198	TYR	O-C-N	-5.91	113.54	123.00
1	K	234	SER	N-CA-C	5.91	123.39	110.80
1	B	356	TRP	CG-CD2-CE3	5.90	139.80	133.90
1	N	303	THR	CA-CB-CG2	5.90	120.53	110.50
1	C	303	THR	CB-CA-C	5.90	121.16	110.72
1	D	49	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	D	50	LYS	N-CA-C	5.90	119.21	110.48
1	E	24	ASP	CA-CB-CG	5.90	118.50	112.60
1	K	275	HIS	CB-CG-CD2	-5.89	123.54	131.20
1	F	286	ASP	CA-CB-CG	5.89	118.49	112.60
1	D	371	HIS	CB-CG-CD2	-5.88	123.56	131.20
1	L	72	GLU	CA-C-O	5.88	127.01	120.43
1	N	171	LEU	CA-C-N	5.88	125.08	118.97
1	N	171	LEU	C-N-CA	5.88	125.08	118.97
1	D	275	HIS	CB-CG-CD2	-5.87	123.56	131.20
1	J	356	TRP	CG-CD2-CE3	5.87	139.77	133.90
1	D	267	ILE	N-CA-C	5.87	121.55	109.34
1	B	78	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	N	303	THR	CA-CB-OG1	-5.86	100.81	109.60
1	E	115	ASN	CA-CB-CG	5.86	118.46	112.60
1	M	352	PHE	N-CA-C	5.86	119.61	112.23
1	E	87	HIS	CB-CG-CD2	-5.85	123.59	131.20
1	H	303	THR	CB-CA-C	5.85	121.08	110.72
1	M	34	ILE	CA-C-O	-5.85	116.74	120.66
1	E	173	HIS	CB-CG-ND1	5.85	131.48	122.70
1	D	101	HIS	CB-CG-CD2	-5.85	123.60	131.20
1	K	255	PHE	CA-C-O	5.84	125.22	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	278	THR	CA-CB-CG2	5.84	120.42	110.50
1	C	246	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	J	4	GLU	N-CA-C	5.83	117.71	111.36
1	L	172	PRO	N-CA-C	5.82	121.41	113.84
1	J	61	LYS	N-CA-C	5.82	119.45	112.93
1	F	162	ASN	CA-CB-CG	5.82	118.42	112.60
1	J	253	GLU	N-CA-C	-5.81	107.99	114.62
1	C	24	ASP	CA-CB-CG	5.81	118.41	112.60
1	I	352	PHE	N-CA-C	5.80	119.46	112.38
1	L	92	ASN	CA-CB-CG	5.80	118.40	112.60
1	H	303	THR	CA-CB-CG2	5.80	120.36	110.50
1	A	92	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	K	350	SER	N-CA-C	5.79	123.14	110.80
1	F	14	SER	N-CA-C	5.78	123.11	110.80
1	L	366	GLY	CA-C-N	5.78	125.91	119.32
1	L	366	GLY	C-N-CA	5.78	125.91	119.32
1	D	311	ASP	CA-CB-CG	5.78	118.38	112.60
1	F	352	PHE	N-CA-C	5.78	120.17	113.18
1	J	335	ARG	N-CA-C	5.78	123.10	110.80
1	D	275	HIS	CA-CB-CG	5.77	119.57	113.80
1	A	201	VAL	N-CA-C	5.76	117.14	111.67
1	H	12	ASN	CA-CB-CG	5.76	118.36	112.60
1	D	73	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	J	297	ASN	CA-CB-CG	5.75	118.35	112.60
1	M	39	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	D	62	ARG	N-CA-C	5.75	119.91	107.49
1	B	303	THR	CA-CB-CG2	5.75	120.27	110.50
1	E	125	GLU	N-CA-C	5.74	119.10	111.75
1	H	198	TYR	N-CA-C	5.74	117.47	110.41
1	D	171	LEU	CA-C-N	5.74	126.13	119.47
1	D	171	LEU	C-N-CA	5.74	126.13	119.47
1	B	356	TRP	CE2-CD2-CG	-5.72	100.34	107.20
1	G	275	HIS	CB-CG-ND1	5.72	131.28	122.70
1	A	286	ASP	CA-CB-CG	5.72	118.32	112.60
1	D	38	PRO	N-CA-C	5.71	124.24	112.47
1	F	366	GLY	CA-C-N	5.71	126.98	119.84
1	F	366	GLY	C-N-CA	5.71	126.98	119.84
1	J	371	HIS	CB-CG-ND1	5.71	131.27	122.70
1	E	254	ARG	N-CA-C	5.70	119.34	112.38
1	K	275	HIS	CA-CB-CG	5.70	119.50	113.80
1	K	366	GLY	CA-C-N	5.70	125.82	119.32
1	K	366	GLY	C-N-CA	5.70	125.82	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	106	THR	CA-CB-OG1	-5.69	101.06	109.60
1	I	297	ASN	CB-CG-ND2	5.69	124.94	116.40
1	I	28	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	K	331	ALA	CA-C-N	5.67	123.80	119.66
1	K	331	ALA	C-N-CA	5.67	123.80	119.66
1	G	222	ASP	N-CA-CB	5.66	120.06	110.49
1	N	135	ALA	N-CA-C	5.66	117.67	109.07
1	K	332	PRO	N-CA-C	5.66	115.90	110.47
1	A	54	VAL	O-C-N	5.66	129.05	123.00
1	F	263	GLN	OE1-CD-NE2	-5.65	116.95	122.60
1	F	371	HIS	CB-CG-ND1	5.65	131.17	122.70
1	D	92	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	J	87	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	D	356	TRP	CG-CD2-CE3	5.64	139.54	133.90
1	E	205	GLU	N-CA-C	5.63	119.77	113.01
1	B	4	GLU	N-CA-C	5.63	122.80	110.80
1	C	173	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	H	275	HIS	N-CA-C	5.63	117.28	111.03
1	C	125	GLU	N-CA-C	5.62	118.34	111.82
1	I	366	GLY	CA-C-N	5.62	125.99	119.47
1	I	366	GLY	C-N-CA	5.62	125.99	119.47
1	L	289	ILE	CB-CA-C	5.62	120.50	111.29
1	B	92	ASN	CA-CB-CG	5.62	118.22	112.60
1	F	161	HIS	CA-CB-CG	5.62	119.42	113.80
1	F	41	GLN	OE1-CD-NE2	-5.61	116.99	122.60
1	L	87	HIS	CB-CG-CD2	-5.61	123.90	131.20
1	B	165	ILE	N-CA-C	5.61	114.89	106.42
1	B	356	TRP	CB-CG-CD1	-5.61	118.49	126.90
1	J	210	ARG	CA-CB-CG	5.61	125.32	114.10
1	M	358	THR	N-CA-C	5.61	118.71	109.85
1	N	294	TYR	N-CA-C	5.60	118.91	111.75
1	E	371	HIS	CB-CG-ND1	5.59	131.09	122.70
1	N	371	HIS	CB-CG-ND1	5.58	131.07	122.70
1	K	28	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	D	277	THR	CA-CB-CG2	5.58	119.98	110.50
1	B	353	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	E	323	SER	N-CA-C	5.58	119.34	112.54
1	J	128	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	E	33	SER	N-CA-C	-5.57	101.86	109.71
1	N	322	PRO	N-CA-CB	-5.56	97.41	103.25
1	J	111	ASN	CA-C-N	5.56	126.79	119.84
1	J	111	ASN	C-N-CA	5.56	126.79	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	277	THR	CA-CB-OG1	-5.56	101.27	109.60
1	E	252	ASN	CB-CG-ND2	5.55	124.73	116.40
1	F	161	HIS	CB-CG-CD2	-5.55	123.98	131.20
1	C	303	THR	CA-CB-CG2	5.55	119.94	110.50
1	H	356	TRP	CE2-CD2-CG	-5.55	100.54	107.20
1	M	37	ARG	O-C-N	-5.54	114.94	121.32
1	G	297	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	K	115	ASN	N-CA-C	-5.54	105.31	112.68
1	M	277	THR	CA-CB-OG1	-5.54	101.28	109.60
1	M	81	ASP	CA-CB-CG	5.54	118.14	112.60
1	E	92	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	M	79	TRP	CE2-CD2-CG	-5.53	100.57	107.20
1	M	277	THR	N-CA-C	5.52	118.01	111.33
1	N	79	TRP	CE2-CD2-CG	-5.52	100.58	107.20
1	A	206	ARG	N-CA-C	5.52	120.02	113.12
1	E	177	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	J	72	GLU	CA-C-O	5.52	127.21	120.92
1	E	202	THR	N-CA-C	5.51	122.55	110.80
1	J	277	THR	N-CA-CB	-5.51	102.01	110.12
1	K	297	ASN	OD1-CG-ND2	-5.51	117.08	122.60
1	I	162	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	M	275	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	H	92	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	M	210	ARG	CA-CB-CG	5.50	125.10	114.10
1	D	252	ASN	CA-CB-CG	5.50	118.10	112.60
1	E	222	ASP	N-CA-CB	5.50	119.78	110.49
1	F	297	ASN	CB-CG-ND2	5.49	124.63	116.40
1	L	325	MET	N-CA-C	5.49	122.49	110.80
1	B	135	ALA	N-CA-C	5.49	117.52	109.24
1	F	128	ASN	CA-CB-CG	5.49	118.08	112.60
1	L	356	TRP	CG-CD2-CE3	5.49	139.39	133.90
1	H	154	ASP	CA-CB-CG	5.48	118.08	112.60
1	E	39	ARG	N-CA-C	-5.48	106.48	112.72
1	M	371	HIS	CB-CG-ND1	5.48	130.92	122.70
1	I	171	LEU	CA-C-N	5.46	124.92	119.24
1	I	171	LEU	C-N-CA	5.46	124.92	119.24
1	K	244	ASP	N-CA-CB	-5.46	100.19	110.07
1	N	79	TRP	CG-CD2-CE3	5.46	139.36	133.90
1	G	356	TRP	CG-CD2-CE3	5.46	139.36	133.90
1	N	75	ILE	N-CA-C	-5.46	99.89	107.80
1	I	128	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	H	254	ARG	N-CA-C	5.45	119.42	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	331	ALA	CA-C-N	5.45	125.99	120.38
1	H	331	ALA	C-N-CA	5.45	125.99	120.38
1	B	254	ARG	N-CA-C	5.44	122.39	110.80
1	K	62	ARG	CA-CB-CG	5.44	124.98	114.10
1	K	157	ASP	CA-CB-CG	5.44	118.04	112.60
1	N	128	ASN	CB-CG-ND2	5.44	124.56	116.40
1	D	202	THR	CA-CB-CG2	5.44	119.75	110.50
1	K	59	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	D	173	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	D	303	THR	CA-CB-CG2	5.44	119.74	110.50
1	B	45	VAL	N-CA-C	5.44	120.65	109.34
1	J	72	GLU	N-CA-C	5.43	118.19	110.10
1	L	69	TYR	CA-C-N	5.43	125.14	119.82
1	L	69	TYR	C-N-CA	5.43	125.14	119.82
1	A	179	ASP	CA-CB-CG	5.43	118.03	112.60
1	D	356	TRP	CB-CG-CD1	-5.43	118.76	126.90
1	J	11	ASP	N-CA-C	5.43	116.97	109.15
1	M	11	ASP	CA-CB-CG	5.43	118.03	112.60
1	H	59	GLN	OE1-CD-NE2	-5.42	117.17	122.60
1	K	257	CYS	CA-C-O	-5.42	114.14	119.13
1	I	217	CYS	N-CA-C	5.42	118.33	110.42
1	M	4	GLU	N-CA-C	5.42	117.63	111.02
1	D	356	TRP	CE2-CD2-CG	-5.42	100.70	107.20
1	F	87	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	B	79	TRP	CG-CD2-CE3	5.40	139.30	133.90
1	L	34	ILE	N-CA-C	-5.40	100.28	108.17
1	M	305	MET	N-CA-C	5.40	119.49	113.01
1	N	330	ILE	N-CA-C	-5.40	99.30	107.73
1	D	177	ARG	NE-CZ-NH1	-5.40	116.10	121.50
1	J	194	THR	N-CA-CB	5.40	118.65	110.28
1	N	62	ARG	N-CA-C	5.40	122.30	110.80
1	N	46	GLY	N-CA-C	5.39	123.67	115.63
1	E	297	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	F	47	MET	N-CA-C	-5.39	99.31	110.80
1	I	275	HIS	CA-CB-CG	5.39	119.19	113.80
1	N	56	ASP	N-CA-C	5.39	117.85	111.33
1	C	62	ARG	CB-CG-CD	-5.38	98.91	111.30
1	I	128	ASN	N-CA-C	5.38	118.82	111.39
1	J	202	THR	N-CA-C	5.38	118.48	110.52
1	K	371	HIS	CB-CG-ND1	5.37	130.76	122.70
1	D	331	ALA	CA-C-N	5.37	125.91	120.38
1	D	331	ALA	C-N-CA	5.37	125.91	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	321	ALA	N-CA-C	5.37	117.49	110.08
1	J	111	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	N	297	ASN	CB-CG-ND2	5.36	124.44	116.40
1	A	173	HIS	CA-CB-CG	5.35	119.15	113.80
1	F	311	ASP	CA-CB-CG	5.35	117.95	112.60
1	G	277	THR	CA-CB-OG1	-5.35	101.57	109.60
1	I	323	SER	N-CA-C	5.35	117.86	111.71
1	B	275	HIS	CA-CB-CG	5.35	119.15	113.80
1	K	257	CYS	O-C-N	-5.35	116.58	120.27
1	M	350	SER	N-CA-C	5.35	117.80	111.33
1	E	81	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	79	TRP	CE2-CD2-CG	-5.34	100.79	107.20
1	G	366	GLY	CA-C-N	5.34	125.41	119.32
1	G	366	GLY	C-N-CA	5.34	125.41	119.32
1	D	201	VAL	N-CA-C	5.34	120.45	109.34
1	F	73	HIS	CA-CB-CG	-5.34	108.46	113.80
1	K	270	GLU	N-CA-C	5.34	122.17	110.80
1	F	275	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	K	297	ASN	CB-CG-ND2	5.33	124.40	116.40
1	L	372	ARG	N-CA-C	5.33	119.26	112.34
1	J	128	ASN	N-CA-C	5.33	118.78	111.54
1	D	275	HIS	N-CA-C	5.32	119.29	111.04
1	L	356	TRP	CE2-CD2-CG	-5.32	100.81	107.20
1	I	356	TRP	CB-CG-CD1	-5.31	118.93	126.90
1	N	296	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	I	356	TRP	CG-CD2-CE3	5.31	139.21	133.90
1	N	320	LEU	N-CA-C	5.31	116.92	111.03
1	G	241	GLU	N-CA-C	5.30	118.23	109.85
1	G	335	ARG	NE-CZ-NH1	-5.30	116.19	121.50
1	F	4	GLU	N-CA-C	5.30	122.09	110.80
1	M	99	GLU	N-CA-C	5.30	119.23	112.87
1	M	33	SER	CA-C-N	5.30	127.27	121.97
1	M	33	SER	C-N-CA	5.30	127.27	121.97
1	C	367	PRO	N-CA-C	5.29	121.63	113.75
1	H	101	HIS	CB-CG-ND1	5.29	130.63	122.70
1	E	78	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	L	125	GLU	N-CA-C	5.29	118.99	112.54
1	C	356	TRP	CG-CD2-CE3	5.29	139.19	133.90
1	F	215	LYS	N-CA-C	5.29	119.48	112.72
1	G	128	ASN	N-CA-C	5.28	118.87	111.90
1	N	120	THR	CA-CB-OG1	-5.28	101.68	109.60
1	E	135	ALA	N-CA-C	5.28	118.05	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	275	HIS	CB-CG-ND1	5.27	130.61	122.70
1	K	49	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	A	40	HIS	CB-CG-CD2	-5.27	124.34	131.20
1	A	356	TRP	CE2-CD2-CG	-5.27	100.88	107.20
1	C	111	ASN	CA-C-N	5.27	125.21	119.78
1	C	111	ASN	C-N-CA	5.27	125.21	119.78
1	A	297	ASN	CA-CB-CG	5.27	117.87	112.60
1	I	371	HIS	CB-CG-ND1	5.26	130.60	122.70
1	L	62	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	G	358	THR	N-CA-C	5.26	117.41	109.41
1	M	274	ILE	N-CA-C	5.26	120.27	109.34
1	G	73	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	G	356	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	H	79	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	N	128	ASN	N-CA-C	5.25	121.97	110.80
1	G	356	TRP	CB-CG-CD1	-5.25	119.03	126.90
1	N	128	ASN	OD1-CG-ND2	-5.25	117.36	122.60
1	D	306	TYR	N-CA-C	5.24	116.30	109.64
1	D	162	ASN	CB-CA-C	-5.24	102.59	110.24
1	B	107	GLU	N-CA-C	5.24	117.03	109.07
1	E	267	ILE	N-CA-C	5.24	120.23	109.34
1	G	11	ASP	N-CA-C	5.23	117.00	108.63
1	J	94	LEU	N-CA-C	5.23	119.29	113.01
1	A	27	PRO	N-CA-C	5.23	119.29	111.14
1	E	255	PHE	CA-C-O	5.22	124.56	118.97
1	N	298	VAL	O-C-N	-5.22	117.56	123.20
1	D	41	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	M	28	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	J	350	SER	N-CA-C	5.21	121.90	110.80
1	I	215	LYS	N-CA-C	5.21	116.64	111.07
1	K	303	THR	CA-CB-OG1	-5.21	101.78	109.60
1	A	79	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	E	100	GLU	CA-CB-CG	5.20	124.50	114.10
1	F	157	ASP	CA-CB-CG	5.20	117.80	112.60
1	M	78	ASN	CB-CG-ND2	5.20	124.20	116.40
1	F	99	GLU	N-CA-C	5.20	119.38	113.19
1	C	356	TRP	CE2-CD2-CG	-5.20	100.97	107.20
1	I	167	GLU	N-CA-C	5.20	118.56	111.39
1	G	367	PRO	N-CA-C	5.19	121.49	113.75
1	M	183	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	J	311	ASP	CA-CB-CG	5.19	117.79	112.60
1	M	280	ASN	OD1-CG-ND2	-5.19	117.41	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	115	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	K	296	ASN	CB-CG-ND2	5.18	124.17	116.40
1	G	125	GLU	N-CA-C	5.18	117.67	111.71
1	J	277	THR	CB-CA-C	5.18	119.39	110.79
1	C	272	ALA	N-CA-C	5.18	117.60	110.35
1	M	356	TRP	CE2-CD2-CG	-5.17	100.99	107.20
1	I	11	ASP	N-CA-C	5.17	116.60	109.15
1	H	352	PHE	N-CA-C	5.17	118.69	112.38
1	M	79	TRP	CG-CD2-CE3	5.17	139.07	133.90
1	E	367	PRO	N-CA-C	5.17	121.45	113.75
1	M	335	ARG	N-CA-C	5.16	121.80	110.80
1	E	331	ALA	CA-C-N	5.16	125.69	120.38
1	E	331	ALA	C-N-CA	5.16	125.69	120.38
1	G	62	ARG	N-CA-C	5.16	117.57	111.33
1	C	277	THR	N-CA-CB	-5.16	101.83	110.39
1	C	331	ALA	CA-C-N	5.16	125.69	120.38
1	C	331	ALA	C-N-CA	5.16	125.69	120.38
1	F	198	TYR	N-CA-C	5.16	117.51	110.55
1	D	111	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	G	40	HIS	N-CA-C	5.15	116.81	108.26
1	L	114	ALA	N-CA-C	5.15	117.56	111.33
1	L	159	VAL	N-CA-C	5.15	115.15	108.35
1	C	72	GLU	N-CA-C	5.15	117.64	109.96
1	L	303	THR	CA-CB-CG2	5.15	119.25	110.50
1	E	356	TRP	CG-CD2-CE3	5.15	139.05	133.90
1	G	371	HIS	CB-CG-ND1	5.14	130.42	122.70
1	M	171	LEU	CA-C-N	5.14	126.27	119.84
1	M	171	LEU	C-N-CA	5.14	126.27	119.84
1	F	177	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	M	85	ILE	CA-C-O	-5.14	115.79	121.29
1	B	323	SER	N-CA-C	5.14	121.75	110.80
1	D	303	THR	CB-CA-C	5.14	119.88	110.11
1	G	62	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	E	356	TRP	CE2-CD2-CG	-5.14	101.04	107.20
1	I	4	GLU	N-CA-C	5.13	119.84	111.37
1	J	303	THR	CA-CB-CG2	5.13	119.23	110.50
1	N	285	CYS	CA-C-N	5.13	128.16	120.87
1	N	285	CYS	C-N-CA	5.13	128.16	120.87
1	B	331	ALA	CA-C-N	5.13	123.41	119.66
1	B	331	ALA	C-N-CA	5.13	123.41	119.66
1	A	128	ASN	CB-CG-ND2	5.13	124.09	116.40
1	L	263	GLN	N-CA-C	5.13	121.15	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	323	SER	N-CA-C	5.13	121.72	110.80
1	M	356	TRP	CG-CD2-CE3	5.13	139.03	133.90
1	A	101	HIS	CB-CG-ND1	5.13	130.39	122.70
1	B	298	VAL	O-C-N	-5.13	116.85	122.69
1	D	366	GLY	CA-C-N	5.13	125.42	119.47
1	D	366	GLY	C-N-CA	5.13	125.42	119.47
1	E	79	TRP	CE2-CD2-CG	-5.13	101.05	107.20
1	E	88	HIS	CB-CG-CD2	-5.13	124.54	131.20
1	N	39	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	H	129	VAL	CA-C-N	5.12	124.44	118.85
1	H	129	VAL	C-N-CA	5.12	124.44	118.85
1	H	162	ASN	CA-CB-CG	5.12	117.72	112.60
1	L	116	ARG	CA-C-N	5.12	127.10	120.44
1	L	116	ARG	C-N-CA	5.12	127.10	120.44
1	G	167	GLU	N-CA-C	5.12	118.46	111.39
1	F	248	ILE	CB-CA-C	5.12	118.18	111.53
1	B	296	ASN	CA-CB-CG	5.11	117.71	112.60
1	M	301	GLY	CA-C-O	5.11	125.54	122.22
1	N	275	HIS	N-CA-C	5.11	121.69	110.80
1	K	177	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	G	40	HIS	CB-CG-ND1	5.10	130.36	122.70
1	E	101	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	H	86	TRP	CE2-CD2-CG	-5.10	101.08	107.20
1	L	286	ASP	CA-CB-CG	5.10	117.70	112.60
1	K	367	PRO	N-CA-C	5.10	121.34	113.75
1	C	271	SER	N-CA-C	5.09	117.70	107.41
1	L	210	ARG	CA-CB-CG	5.09	124.29	114.10
1	A	309	ILE	N-CA-C	5.09	115.86	110.72
1	I	107	GLU	N-CA-C	5.09	116.73	109.14
1	J	340	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	I	331	ALA	CA-C-N	5.09	125.62	120.38
1	I	331	ALA	C-N-CA	5.09	125.62	120.38
1	L	236	LEU	N-CA-C	5.09	121.64	110.80
1	M	294	TYR	N-CA-C	5.08	116.82	111.28
1	C	62	ARG	CA-CB-CG	5.08	124.26	114.10
1	H	252	ASN	CA-C-O	5.08	127.78	120.51
1	J	86	TRP	CE2-CD2-CG	-5.08	101.10	107.20
1	N	72	GLU	N-CA-C	5.08	117.53	109.96
1	H	153	LEU	N-CA-C	-5.08	100.13	108.41
1	G	305	MET	N-CA-C	5.08	119.19	113.15
1	D	53	TYR	CA-CB-CG	5.08	123.04	113.90
1	F	290	ARG	N-CA-CB	5.08	119.07	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	H	149	THR	CA-CB-OG1	-5.07	101.99	109.60
1	H	278	THR	CA-CB-OG1	-5.07	101.99	109.60
1	J	363	ASP	CA-CB-CG	5.07	117.67	112.60
1	K	92	ASN	CA-CB-CG	5.07	117.67	112.60
1	L	101	HIS	CB-CG-ND1	5.07	130.31	122.70
1	K	129	VAL	CA-C-N	5.07	124.86	119.28
1	K	129	VAL	C-N-CA	5.07	124.86	119.28
1	B	69	TYR	CA-C-N	5.07	124.73	119.56
1	B	69	TYR	C-N-CA	5.07	124.73	119.56
1	E	49	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	L	187	ASP	CA-CB-CG	5.07	117.67	112.60
1	L	272	ALA	N-CA-C	5.07	118.14	110.64
1	H	340	TRP	CE2-CD2-CG	-5.06	101.12	107.20
1	N	352	PHE	N-CA-C	5.06	118.95	112.87
1	I	230	ALA	N-CA-C	5.06	117.46	111.33
1	N	207	GLU	N-CA-C	5.06	117.19	111.11
1	E	27	PRO	N-CA-C	5.06	119.03	111.14
1	A	277	THR	N-CA-CB	-5.06	102.47	110.06
1	B	371	HIS	CB-CG-CD2	-5.05	124.63	131.20
1	J	174	ALA	O-C-N	5.05	129.54	122.36
1	C	185	LEU	N-CA-C	5.05	117.68	111.82
1	B	28	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	B	40	HIS	CB-CG-CD2	-5.05	124.64	131.20
1	G	286	ASP	N-CA-CB	-5.05	101.96	110.49
1	H	363	ASP	CA-CB-CG	5.05	117.65	112.60
1	K	352	PHE	N-CA-C	5.05	118.70	112.54
1	C	366	GLY	CA-C-N	5.05	125.07	119.32
1	C	366	GLY	C-N-CA	5.05	125.07	119.32
1	K	79	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	J	356	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	J	280	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	B	350	SER	N-CA-C	5.04	117.43	111.33
1	C	79	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	E	297	ASN	CB-CG-ND2	5.04	123.96	116.40
1	B	340	TRP	CE2-CD2-CG	-5.03	101.16	107.20
1	E	86	TRP	CE2-CD2-CG	-5.03	101.16	107.20
1	B	365	ALA	N-CA-C	5.03	121.15	113.61
1	J	159	VAL	N-CA-C	5.03	114.50	108.06
1	F	217	CYS	N-CA-C	5.03	117.34	110.55
1	G	155	SER	O-C-N	5.03	129.05	122.87
1	I	40	HIS	CB-CG-CD2	-5.03	124.66	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	305	MET	N-CA-C	5.03	119.39	113.16
1	J	366	GLY	CA-C-N	5.03	125.05	119.32
1	J	366	GLY	C-N-CA	5.03	125.05	119.32
1	B	280	ASN	N-CA-C	5.02	119.04	113.01
1	I	56	ASP	N-CA-C	5.02	116.75	111.28
1	F	356	TRP	CE2-CD2-CG	-5.02	101.18	107.20
1	G	79	TRP	CE2-CD2-CG	-5.02	101.18	107.20
1	K	69	TYR	CA-C-N	5.02	124.68	119.56
1	K	69	TYR	C-N-CA	5.02	124.68	119.56
1	M	366	GLY	CA-C-N	5.02	126.11	119.84
1	M	366	GLY	C-N-CA	5.02	126.11	119.84
1	K	38	PRO	N-CA-C	5.02	118.96	111.14
1	E	59	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	I	248	ILE	CB-CA-C	5.01	116.65	111.09
1	J	128	ASN	CB-CG-ND2	5.01	123.91	116.40
1	D	367	PRO	N-CA-C	5.00	121.07	113.81
1	F	282	ILE	CB-CA-C	5.00	119.50	111.29
1	D	246	GLN	OE1-CD-NE2	-5.00	117.60	122.60

There are no chirality outliers.

All (123) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	TYR	Sidechain
1	A	210	ARG	Sidechain
1	A	269	MET	Peptide
1	A	290	ARG	Sidechain
1	A	337	TYR	Sidechain
1	A	37	ARG	Sidechain
1	A	62	ARG	Sidechain
1	A	91	TYR	Sidechain
1	B	116	ARG	Sidechain
1	B	133	TYR	Sidechain
1	B	147	ARG	Sidechain
1	B	169	TYR	Sidechain
1	B	206	ARG	Sidechain
1	B	272	ALA	Peptide
1	B	28	ARG	Sidechain
1	B	285	CYS	Peptide
1	B	37	ARG	Sidechain
1	B	53	TYR	Sidechain
1	B	62	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	166	TYR	Sidechain
1	C	206	ARG	Sidechain
1	C	256	ARG	Sidechain
1	C	279	TYR	Sidechain
1	C	290	ARG	Sidechain
1	C	303	THR	Peptide
1	C	53	TYR	Sidechain
1	D	116	ARG	Sidechain
1	D	169	TYR	Sidechain
1	D	196	ARG	Sidechain
1	D	198	TYR	Sidechain
1	D	206	ARG	Sidechain
1	D	233	SER	Peptide
1	D	337	TYR	Sidechain
1	D	37	ARG	Sidechain
1	D	53	TYR	Sidechain
1	D	60	SER	Peptide
1	D	65	LEU	Peptide
1	E	111	ASN	Peptide
1	E	147	ARG	Sidechain
1	E	188	TYR	Sidechain
1	E	198	TYR	Sidechain
1	E	232	SER	Peptide
1	E	290	ARG	Sidechain
1	E	337	TYR	Sidechain
1	E	362	TYR	Sidechain
1	E	39	ARG	Sidechain
1	E	62	ARG	Sidechain
1	F	233	SER	Peptide
1	F	240	TYR	Sidechain
1	F	280	ASN	Peptide
1	F	281	SER	Peptide
1	F	282	ILE	Peptide
1	F	37	ARG	Sidechain
1	F	44	MET	Peptide
1	F	91	TYR	Sidechain
1	G	198	TYR	Sidechain
1	G	337	TYR	Sidechain
1	G	91	TYR	Sidechain
1	H	116	ARG	Sidechain
1	H	143	TYR	Sidechain
1	H	147	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	H	335	ARG	Sidechain
1	H	337	TYR	Sidechain
1	H	62	ARG	Sidechain
1	I	116	ARG	Sidechain
1	I	147	ARG	Sidechain
1	I	166	TYR	Sidechain
1	I	197	GLY	Peptide
1	I	252	ASN	Peptide
1	I	335	ARG	Sidechain
1	I	337	TYR	Sidechain
1	I	37	ARG	Sidechain
1	I	53	TYR	Sidechain
1	J	111	ASN	Peptide
1	J	196	ARG	Sidechain
1	J	202	THR	Peptide
1	J	205	GLU	Peptide
1	J	206	ARG	Sidechain
1	J	272	ALA	Peptide
1	J	290	ARG	Sidechain
1	J	306	TYR	Sidechain
1	K	116	ARG	Sidechain
1	K	147	ARG	Sidechain
1	K	166	TYR	Sidechain
1	K	206	ARG	Sidechain
1	K	218	TYR	Sidechain
1	K	240	TYR	Sidechain
1	K	290	ARG	Sidechain
1	K	303	THR	Peptide
1	K	337	TYR	Sidechain
1	K	37	ARG	Sidechain
1	K	53	TYR	Sidechain
1	K	91	TYR	Sidechain
1	L	116	ARG	Sidechain
1	L	169	TYR	Sidechain
1	L	179	ASP	Peptide
1	L	239	SER	Peptide
1	L	284	LYS	Peptide
1	L	289	ILE	Peptide
1	L	303	THR	Peptide
1	L	322	PRO	Peptide
1	L	337	TYR	Sidechain
1	L	39	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	L	53	TYR	Sidechain
1	L	62	ARG	Sidechain
1	L	65	LEU	Peptide
1	M	147	ARG	Sidechain
1	M	272	ALA	Peptide
1	M	337	TYR	Sidechain
1	M	39	ARG	Sidechain
1	M	53	TYR	Sidechain
1	M	62	ARG	Sidechain
1	M	91	TYR	Sidechain
1	N	143	TYR	Sidechain
1	N	147	ARG	Sidechain
1	N	196	ARG	Sidechain
1	N	254	ARG	Sidechain
1	N	275	HIS	Sidechain
1	N	306	TYR	Sidechain
1	N	37	ARG	Sidechain
1	N	53	TYR	Sidechain
1	N	62	ARG	Sidechain
1	N	91	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2933	0	2894	114	0
1	B	2933	0	2894	117	0
1	C	2933	0	2894	101	0
1	D	2933	0	2894	245	0
1	E	2933	0	2894	113	0
1	F	2933	0	2894	273	0
1	G	2933	0	2894	69	0
1	H	2933	0	2894	86	0
1	I	2933	0	2894	79	0
1	J	2933	0	2894	104	0
1	K	2933	0	2894	126	0
1	L	2933	0	2894	116	0
1	M	2933	0	2894	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	2933	0	2894	82	0
All	All	41062	0	40516	1341	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 16.

All (1341) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:MET:CG	1:F:293:LEU:CD2	1.79	1.58
1:J:266:PHE:CZ	1:J:266:PHE:CE2	1.95	1.52
1:J:266:PHE:CD1	1:J:266:PHE:CE1	1.94	1.52
1:J:266:PHE:CD1	1:J:266:PHE:CG	1.95	1.52
1:J:266:PHE:CZ	1:J:266:PHE:CE1	1.95	1.51
1:J:266:PHE:CE2	1:J:266:PHE:CD2	1.95	1.51
1:D:44:MET:CG	1:F:293:LEU:HD21	1.06	1.50
1:J:266:PHE:CG	1:J:266:PHE:CD2	1.96	1.49
1:D:44:MET:SD	1:F:293:LEU:CD1	2.01	1.49
1:D:61:LYS:NZ	1:F:291:LYS:HD2	1.19	1.41
1:D:43:VAL:CB	1:F:166:TYR:HD1	1.34	1.39
1:L:112:PRO:N	1:L:112:PRO:CA	1.83	1.39
1:A:62:ARG:HH21	1:C:287:ILE:CD1	1.33	1.39
1:D:57:GLU:OE1	1:F:291:LYS:HE3	1.24	1.38
1:D:64:ILE:C	1:F:287:ILE:HD11	1.45	1.37
1:L:112:PRO:N	1:L:112:PRO:CD	1.88	1.35
1:A:62:ARG:NH2	1:C:287:ILE:HD11	1.37	1.34
1:D:65:LEU:N	1:F:287:ILE:HD11	1.39	1.33
1:B:64:ILE:CG2	1:C:267:ILE:HB	1.59	1.31
1:D:44:MET:HG3	1:F:293:LEU:CD2	1.45	1.31
1:D:61:LYS:NZ	1:F:291:LYS:CD	1.91	1.31
1:F:45:VAL:HG21	1:H:166:TYR:CE1	1.64	1.31
1:D:44:MET:SD	1:F:293:LEU:HD11	1.62	1.31
1:B:64:ILE:HG23	1:C:267:ILE:CB	1.63	1.26
1:L:112:PRO:CG	1:L:112:PRO:CB	2.12	1.25
1:L:112:PRO:CA	1:L:112:PRO:CB	2.13	1.25
1:A:62:ARG:HD2	1:C:287:ILE:CD1	1.68	1.23
1:D:43:VAL:HB	1:F:166:TYR:CD1	1.73	1.22
1:D:43:VAL:CB	1:F:166:TYR:CD1	2.25	1.18
1:D:65:LEU:N	1:F:287:ILE:CD1	2.06	1.18
1:L:112:PRO:CD	1:L:112:PRO:CG	2.22	1.18
1:F:45:VAL:CG2	1:H:166:TYR:CE1	2.24	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:MET:HG3	1:F:293:LEU:HD22	1.23	1.16
1:F:45:VAL:HA	1:H:167:GLU:CB	1.78	1.13
1:D:43:VAL:CG1	1:F:166:TYR:HD1	1.62	1.13
1:D:44:MET:SD	1:F:293:LEU:HD13	1.74	1.12
1:D:57:GLU:OE1	1:F:291:LYS:CE	1.97	1.12
1:F:45:VAL:HA	1:H:167:GLU:HB2	1.23	1.12
1:F:45:VAL:HG11	1:H:166:TYR:CE1	1.83	1.12
1:D:44:MET:HG2	1:F:293:LEU:CD2	1.56	1.11
1:D:65:LEU:HD23	1:F:287:ILE:HG13	1.22	1.10
1:B:50:LYS:HD3	1:B:53:TYR:OH	1.52	1.10
1:F:45:VAL:CG1	1:H:166:TYR:CE1	2.35	1.09
1:A:62:ARG:HD2	1:C:287:ILE:HD13	1.30	1.09
1:D:43:VAL:HG12	1:F:166:TYR:CD1	1.87	1.09
1:E:267:ILE:HD12	1:F:287:ILE:O	1.53	1.08
1:F:45:VAL:HG11	1:H:166:TYR:CZ	1.89	1.08
1:A:243:PRO:O	1:C:323:SER:N	1.86	1.08
1:D:43:VAL:HB	1:F:166:TYR:HD1	1.09	1.06
1:D:43:VAL:CG1	1:F:166:TYR:CD1	2.37	1.05
1:F:45:VAL:CG2	1:H:166:TYR:CD1	2.41	1.04
1:J:266:PHE:CZ	1:K:173:HIS:CG	2.46	1.02
1:J:266:PHE:CD1	1:K:173:HIS:CG	2.48	1.02
1:J:266:PHE:CE1	1:K:173:HIS:CG	2.47	1.02
1:D:57:GLU:CD	1:F:291:LYS:HE3	1.85	1.02
1:J:266:PHE:CE2	1:K:173:HIS:CG	2.47	1.02
1:J:266:PHE:CG	1:K:173:HIS:CG	2.48	1.01
1:J:266:PHE:CD2	1:K:173:HIS:CG	2.48	1.00
1:D:45:VAL:HA	1:F:165:ILE:O	1.63	0.99
1:E:112:PRO:HB2	1:E:115:ASN:HB3	1.44	0.99
1:F:45:VAL:HG21	1:H:166:TYR:CD1	1.97	0.99
1:F:45:VAL:CG1	1:H:166:TYR:CZ	2.50	0.95
1:D:64:ILE:HD11	1:F:286:ASP:HA	1.47	0.93
1:D:43:VAL:HG11	1:F:169:TYR:HD1	1.32	0.93
1:J:266:PHE:CD2	1:K:173:HIS:CB	2.52	0.92
1:D:64:ILE:HG13	1:F:287:ILE:HG12	1.49	0.92
1:D:45:VAL:HG13	1:F:165:ILE:HB	1.51	0.92
1:B:45:VAL:HG21	1:D:289:ILE:HD13	1.50	0.91
1:D:45:VAL:HG22	1:F:164:PRO:HA	1.52	0.91
1:F:45:VAL:HG11	1:H:166:TYR:OH	1.68	0.91
1:J:266:PHE:CG	1:K:173:HIS:CB	2.53	0.91
1:D:61:LYS:HZ2	1:F:291:LYS:CD	1.65	0.91
1:J:266:PHE:CE2	1:K:173:HIS:CB	2.54	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:266:PHE:CE1	1:K:173:HIS:CB	2.54	0.91
1:F:45:VAL:HG22	1:H:166:TYR:CD1	2.05	0.90
1:J:266:PHE:CZ	1:K:173:HIS:CB	2.55	0.90
1:D:61:LYS:HZ1	1:F:291:LYS:CD	1.76	0.89
1:F:45:VAL:HG21	1:H:166:TYR:HE1	1.12	0.89
1:J:266:PHE:CD2	1:K:173:HIS:HB2	2.06	0.89
1:J:266:PHE:CD1	1:K:173:HIS:CB	2.54	0.89
1:D:64:ILE:CA	1:F:287:ILE:HD11	2.02	0.89
1:D:64:ILE:C	1:F:287:ILE:CD1	2.42	0.88
1:K:192:ILE:HA	1:L:112:PRO:HG3	1.54	0.88
1:B:39:ARG:HD3	1:B:66:THR:HG23	1.55	0.87
1:B:45:VAL:HG13	1:D:171:LEU:HB2	1.56	0.87
1:D:45:VAL:HG11	1:F:142:LEU:HD13	1.56	0.87
1:D:64:ILE:CD1	1:F:286:ASP:HA	2.05	0.87
1:D:65:LEU:H	1:F:287:ILE:CD1	1.84	0.87
1:A:357:ILE:HG13	1:A:370:VAL:HG22	1.55	0.86
1:D:44:MET:CE	1:F:293:LEU:HD13	2.06	0.86
1:D:43:VAL:HA	1:F:166:TYR:CE1	2.10	0.86
1:D:44:MET:O	1:F:165:ILE:N	2.09	0.85
1:K:195:GLU:CB	1:L:112:PRO:N	2.39	0.85
1:E:267:ILE:HG23	1:F:290:ARG:HB2	1.59	0.85
1:B:63:GLY:HA3	1:C:267:ILE:HA	1.58	0.84
1:N:102:PRO:HB3	1:N:131:ALA:HB3	1.58	0.84
1:F:154:ASP:HB3	1:F:161:HIS:HB2	1.59	0.84
1:J:266:PHE:CD1	1:K:173:HIS:HB3	2.12	0.84
1:B:102:PRO:HB3	1:B:131:ALA:HB3	1.59	0.84
1:L:160:THR:HB	1:L:178:LEU:HB3	1.59	0.83
1:A:62:ARG:CD	1:C:287:ILE:CD1	2.54	0.83
1:A:62:ARG:HG3	1:C:286:ASP:HB2	1.58	0.83
1:D:44:MET:HB2	1:F:289:ILE:CG2	2.10	0.82
1:A:243:PRO:HB2	1:C:322:PRO:HB2	1.62	0.82
1:K:195:GLU:CG	1:L:112:PRO:N	2.43	0.82
1:A:102:PRO:HB3	1:A:131:ALA:HB3	1.62	0.81
1:A:257:CYS:SG	1:A:258:PRO:HD3	2.20	0.81
1:J:19:ALA:HB3	1:J:29:ALA:HB3	1.61	0.81
1:D:61:LYS:HZ3	1:F:291:LYS:HD2	1.40	0.81
1:K:195:GLU:CG	1:L:112:PRO:CA	2.59	0.81
1:C:160:THR:HB	1:C:178:LEU:HB2	1.62	0.81
1:K:195:GLU:CB	1:L:112:PRO:CD	2.59	0.81
1:B:63:GLY:H	1:C:268:GLY:H	1.25	0.81
1:A:62:ARG:HD2	1:C:287:ILE:HD11	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:MET:O	1:F:166:TYR:HD2	1.65	0.79
1:E:267:ILE:CD1	1:F:287:ILE:O	2.30	0.79
1:K:195:GLU:CG	1:L:112:PRO:CD	2.61	0.79
1:E:267:ILE:CG2	1:F:290:ARG:HB2	2.14	0.78
1:G:257:CYS:SG	1:G:258:PRO:HD3	2.24	0.78
1:H:164:PRO:HG3	1:H:174:ALA:HB3	1.64	0.78
1:L:19:ALA:HB3	1:L:29:ALA:HB3	1.65	0.78
1:D:64:ILE:N	1:F:287:ILE:HD13	1.99	0.77
1:N:36:GLY:HA2	1:N:66:THR:HB	1.64	0.77
1:D:64:ILE:N	1:F:287:ILE:CD1	2.48	0.77
1:D:65:LEU:H	1:F:287:ILE:HD12	1.49	0.77
1:D:44:MET:SD	1:F:293:LEU:CD2	2.71	0.77
1:K:195:GLU:CB	1:L:112:PRO:CA	2.62	0.77
1:D:47:MET:O	1:F:166:TYR:CD2	2.38	0.77
1:D:43:VAL:CA	1:F:166:TYR:CD1	2.69	0.76
1:F:45:VAL:HG13	1:H:167:GLU:HG2	1.68	0.76
1:M:160:THR:HB	1:M:178:LEU:HB2	1.68	0.76
1:E:206:ARG:HG3	1:F:264:PRO:HB2	1.68	0.75
1:D:44:MET:CG	1:F:293:LEU:HD22	1.90	0.75
1:B:63:GLY:N	1:C:268:GLY:H	1.84	0.75
1:A:38:PRO:HA	1:A:65:LEU:HA	1.67	0.75
1:B:45:VAL:HG22	1:D:171:LEU:HD12	1.68	0.75
1:D:57:GLU:CD	1:F:291:LYS:CE	2.54	0.75
1:A:62:ARG:NH2	1:C:287:ILE:CD1	2.18	0.75
1:A:62:ARG:HH21	1:C:287:ILE:HD11	0.61	0.75
1:B:257:CYS:SG	1:B:258:PRO:HD3	2.26	0.75
1:C:200:PHE:HB3	1:C:206:ARG:HG2	1.69	0.74
1:K:195:GLU:CG	1:L:112:PRO:CG	2.64	0.74
1:D:65:LEU:N	1:F:287:ILE:HD12	2.03	0.74
1:F:163:VAL:HG13	1:F:175:ILE:HG12	1.68	0.74
1:B:63:GLY:CA	1:C:267:ILE:HA	2.17	0.74
1:D:257:CYS:SG	1:D:258:PRO:HD3	2.28	0.74
1:H:257:CYS:SG	1:H:258:PRO:HD3	2.27	0.74
1:N:19:ALA:HB3	1:N:29:ALA:HB3	1.69	0.74
1:C:19:ALA:HB3	1:C:29:ALA:HB3	1.70	0.73
1:B:164:PRO:HG2	1:B:171:LEU:HB3	1.69	0.73
1:F:45:VAL:CA	1:H:167:GLU:HB2	2.12	0.73
1:G:267:ILE:CD1	1:H:169:TYR:OH	2.37	0.73
1:D:43:VAL:HA	1:F:166:TYR:CD1	2.23	0.73
1:K:195:GLU:CG	1:L:112:PRO:CB	2.67	0.73
1:K:195:GLU:CB	1:L:112:PRO:CG	2.66	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:195:GLU:CB	1:L:112:PRO:CB	2.67	0.73
1:A:62:ARG:CZ	1:C:287:ILE:HD11	2.17	0.73
1:F:195:GLU:HA	1:G:172:PRO:HB2	1.71	0.72
1:D:43:VAL:CA	1:F:166:TYR:HD1	2.02	0.72
1:F:36:GLY:HA3	1:F:65:LEU:HD13	1.71	0.72
1:B:160:THR:HB	1:B:178:LEU:HB3	1.71	0.72
1:H:357:ILE:HG13	1:H:370:VAL:HG22	1.71	0.72
1:D:64:ILE:HG13	1:F:287:ILE:CG1	2.20	0.72
1:L:357:ILE:HG13	1:L:370:VAL:HG22	1.72	0.72
1:C:257:CYS:SG	1:C:258:PRO:HD3	2.29	0.71
1:D:45:VAL:HB	1:F:150:GLY:H	1.55	0.71
1:D:61:LYS:HZ1	1:F:291:LYS:HB3	1.54	0.71
1:D:191:LYS:HE2	1:E:172:PRO:HG2	1.72	0.71
1:B:60:SER:O	1:D:287:ILE:HG21	1.91	0.71
1:B:163:VAL:HG22	1:B:175:ILE:HG23	1.72	0.71
1:D:47:MET:O	1:F:167:GLU:HG2	1.91	0.71
1:M:102:PRO:HB3	1:M:131:ALA:HB3	1.70	0.71
1:N:24:ASP:HB2	1:N:340:TRP:HH2	1.54	0.71
1:B:38:PRO:HA	1:B:65:LEU:HA	1.73	0.71
1:L:244:ASP:HB2	1:L:245:GLY:HA2	1.73	0.71
1:F:45:VAL:HG13	1:H:167:GLU:CG	2.20	0.71
1:I:257:CYS:SG	1:I:258:PRO:HD3	2.30	0.71
1:E:199:SER:HB2	1:F:179:ASP:HB2	1.72	0.70
1:J:266:PHE:CG	1:K:173:HIS:HB3	2.26	0.70
1:D:61:LYS:HZ2	1:F:291:LYS:HD2	0.77	0.70
1:D:65:LEU:CD2	1:F:287:ILE:HG21	2.21	0.70
1:E:183:ARG:HG3	1:F:270:GLU:HG2	1.73	0.70
1:A:174:ALA:HA	1:A:284:LYS:HE2	1.73	0.70
1:F:19:ALA:HB3	1:F:29:ALA:HB3	1.74	0.70
1:K:191:LYS:HE2	1:L:110:LEU:HD22	1.72	0.70
1:B:39:ARG:HD3	1:B:66:THR:CG2	2.22	0.70
1:D:61:LYS:NZ	1:F:291:LYS:HD3	2.00	0.69
1:L:204:ALA:HA	1:N:287:ILE:HD12	1.75	0.69
1:E:257:CYS:SG	1:E:258:PRO:HD3	2.32	0.69
1:N:164:PRO:HG3	1:N:174:ALA:HB3	1.73	0.69
1:L:190:MET:HA	1:L:209:VAL:HG11	1.74	0.69
1:D:61:LYS:NZ	1:F:291:LYS:HB3	2.06	0.69
1:N:265:SER:HA	1:N:270:GLU:HA	1.74	0.69
1:A:62:ARG:HG3	1:C:286:ASP:CB	2.22	0.69
1:L:111:ASN:C	1:L:112:PRO:CA	2.64	0.69
1:D:282:ILE:HA	1:D:285:CYS:SG	2.33	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:194:THR:HB	1:L:75:ILE:HG12	1.75	0.69
1:N:160:THR:HB	1:N:178:LEU:HB2	1.75	0.69
1:D:197:GLY:HA2	1:E:112:PRO:HA	1.72	0.68
1:H:285:CYS:HB3	1:H:289:ILE:HD11	1.76	0.68
1:J:180:LEU:HD11	1:J:264:PRO:HB3	1.73	0.68
1:K:264:PRO:HB2	1:K:271:SER:HB3	1.76	0.68
1:D:58:ALA:O	1:D:62:ARG:HB3	1.93	0.68
1:J:266:PHE:CD2	1:K:173:HIS:CD2	2.82	0.68
1:B:105:LEU:HD21	1:B:123:MET:HE2	1.76	0.68
1:F:213:LYS:HA	1:F:217:CYS:SG	2.34	0.68
1:D:45:VAL:HG13	1:F:165:ILE:CB	2.25	0.67
1:D:53:TYR:HB2	1:F:288:ASP:OD1	1.93	0.67
1:F:45:VAL:C	1:H:167:GLU:HG3	2.19	0.67
1:D:64:ILE:CA	1:F:287:ILE:CD1	2.70	0.67
1:F:163:VAL:HG22	1:F:175:ILE:HG23	1.76	0.67
1:D:65:LEU:HD23	1:F:287:ILE:CG1	2.14	0.67
1:F:45:VAL:HG11	1:H:166:TYR:HE1	1.54	0.67
1:J:160:THR:HB	1:J:178:LEU:HB2	1.76	0.67
1:D:49:GLN:N	1:F:166:TYR:CD2	2.62	0.67
1:D:44:MET:HB2	1:F:289:ILE:HG21	1.76	0.67
1:I:191:LYS:HE2	1:J:172:PRO:HB2	1.77	0.67
1:L:242:LEU:HB2	1:L:245:GLY:HA3	1.76	0.67
1:L:300:SER:HA	1:L:335:ARG:HB2	1.77	0.67
1:I:19:ALA:HB3	1:I:29:ALA:HB3	1.76	0.66
1:J:193:LEU:HA	1:J:196:ARG:HB3	1.77	0.66
1:L:36:GLY:HA3	1:L:65:LEU:HD13	1.77	0.66
1:L:257:CYS:SG	1:L:258:PRO:HD3	2.35	0.66
1:D:47:MET:C	1:F:167:GLU:HG2	2.21	0.66
1:M:9:VAL:HG21	1:M:344:SER:HA	1.78	0.66
1:D:43:VAL:HA	1:F:166:TYR:HE1	1.57	0.66
1:E:210:ARG:HB2	1:F:269:MET:SD	2.36	0.66
1:G:286:ASP:HB3	1:G:289:ILE:HG12	1.77	0.66
1:N:266:PHE:HB3	1:N:269:MET:SD	2.35	0.66
1:D:45:VAL:HG13	1:F:165:ILE:CD1	2.24	0.66
1:I:180:LEU:HD11	1:I:264:PRO:HB3	1.76	0.66
1:D:201:VAL:HB	1:E:177:ARG:HB3	1.76	0.66
1:B:64:ILE:HD13	1:C:267:ILE:HD12	1.76	0.66
1:F:45:VAL:HG13	1:H:166:TYR:CZ	2.31	0.66
1:N:106:THR:HG22	1:N:140:LEU:HD12	1.78	0.66
1:F:160:THR:HB	1:F:178:LEU:HB3	1.77	0.65
1:I:189:LEU:HA	1:I:192:ILE:HG12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:PRO:HB3	1:D:131:ALA:HB3	1.78	0.65
1:E:10:CYS:SG	1:E:89:THR:HG21	2.37	0.65
1:F:45:VAL:CG1	1:H:166:TYR:OH	2.39	0.65
1:A:285:CYS:HB3	1:A:289:ILE:HD11	1.79	0.65
1:E:116:ARG:NH2	1:E:374:CYS:SG	2.70	0.65
1:F:257:CYS:SG	1:F:258:PRO:HD3	2.37	0.65
1:G:7:ALA:HA	1:G:102:PRO:HG2	1.79	0.65
1:I:102:PRO:HB3	1:I:131:ALA:HB3	1.79	0.65
1:K:357:ILE:HG13	1:K:370:VAL:HG22	1.78	0.65
1:A:243:PRO:HB2	1:C:322:PRO:CB	2.27	0.65
1:F:46:GLY:H	1:H:167:GLU:HB3	1.62	0.64
1:J:174:ALA:HA	1:J:284:LYS:HZ3	1.60	0.64
1:F:45:VAL:CB	1:H:166:TYR:CE1	2.80	0.64
1:D:43:VAL:HG11	1:F:166:TYR:HB2	1.78	0.64
1:D:44:MET:HB2	1:F:289:ILE:HG22	1.79	0.64
1:D:213:LYS:HA	1:D:217:CYS:SG	2.37	0.64
1:K:244:ASP:HB3	1:M:287:ILE:O	1.98	0.64
1:B:213:LYS:HA	1:B:217:CYS:SG	2.38	0.64
1:D:65:LEU:HD21	1:F:287:ILE:HG21	1.79	0.64
1:N:257:CYS:SG	1:N:258:PRO:HD3	2.38	0.64
1:B:45:VAL:HB	1:D:166:TYR:HB3	1.79	0.64
1:D:57:GLU:OE2	1:F:291:LYS:CE	2.46	0.64
1:F:45:VAL:CA	1:H:167:GLU:CB	2.68	0.64
1:I:164:PRO:HG3	1:I:174:ALA:HB3	1.79	0.64
1:N:155:SER:HA	1:N:160:THR:HA	1.80	0.64
1:G:213:LYS:HA	1:G:217:CYS:SG	2.38	0.63
1:M:10:CYS:SG	1:M:89:THR:HG21	2.37	0.63
1:A:137:GLN:HG2	1:A:339:VAL:HG11	1.80	0.63
1:C:245:GLY:H	1:E:325:MET:HB2	1.63	0.63
1:C:267:ILE:HG21	1:D:284:LYS:HG3	1.80	0.63
1:J:266:PHE:CE1	1:K:173:HIS:ND1	2.66	0.63
1:K:160:THR:HB	1:K:178:LEU:HB2	1.80	0.63
1:E:357:ILE:HG21	1:E:370:VAL:HG22	1.79	0.63
1:M:257:CYS:SG	1:M:258:PRO:HD3	2.38	0.63
1:N:162:ASN:OD1	1:N:277:THR:HG23	1.99	0.63
1:B:109:PRO:HA	1:B:136:ILE:HG23	1.80	0.63
1:D:43:VAL:HG11	1:F:169:TYR:CD1	2.23	0.63
1:D:44:MET:HG2	1:F:293:LEU:HD21	0.64	0.63
1:K:164:PRO:HG2	1:K:171:LEU:HB2	1.81	0.63
1:L:289:ILE:HA	1:L:291:LYS:HG2	1.81	0.62
1:N:66:THR:HG22	1:N:68:LYS:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:THR:HB	1:E:178:LEU:HB2	1.81	0.62
1:N:357:ILE:HG13	1:N:370:VAL:HG22	1.81	0.62
1:G:9:VAL:HG21	1:G:344:SER:HA	1.80	0.62
1:N:200:PHE:HA	1:N:205:GLU:HB3	1.82	0.62
1:B:60:SER:OG	1:D:287:ILE:HD13	1.99	0.62
1:D:44:MET:O	1:F:165:ILE:C	2.42	0.62
1:D:48:GLY:C	1:F:166:TYR:CE2	2.78	0.62
1:D:197:GLY:HA2	1:E:113:LYS:H	1.64	0.62
1:E:62:ARG:HH21	1:E:62:ARG:HB2	1.65	0.62
1:D:45:VAL:CG1	1:F:165:ILE:CD1	2.78	0.62
1:B:227:MET:HE1	1:B:256:ARG:HD3	1.81	0.62
1:D:160:THR:HB	1:D:178:LEU:HB3	1.82	0.62
1:I:242:LEU:HD11	1:I:248:ILE:HD13	1.80	0.62
1:K:205:GLU:HG2	1:M:287:ILE:HG13	1.82	0.62
1:D:36:GLY:HA3	1:D:65:LEU:HD22	1.81	0.62
1:H:160:THR:HB	1:H:178:LEU:HB2	1.81	0.62
1:D:298:VAL:HG22	1:D:330:ILE:HB	1.82	0.62
1:B:63:GLY:HA3	1:C:268:GLY:N	2.15	0.62
1:A:10:CYS:HB3	1:A:105:LEU:HD23	1.80	0.61
1:A:153:LEU:HD21	1:A:274:ILE:HG23	1.81	0.61
1:C:178:LEU:HD11	1:C:277:THR:HG21	1.81	0.61
1:N:103:THR:O	1:N:132:MET:HA	2.00	0.61
1:C:328:LYS:HZ1	1:C:330:ILE:HG12	1.63	0.61
1:A:36:GLY:HA2	1:A:66:THR:O	2.00	0.61
1:D:61:LYS:HZ1	1:F:291:LYS:HD3	1.58	0.61
1:E:287:ILE:HD12	1:E:287:ILE:H	1.65	0.61
1:J:153:LEU:HA	1:J:161:HIS:O	2.00	0.61
1:N:189:LEU:HD13	1:N:257:CYS:SG	2.40	0.61
1:F:45:VAL:HA	1:H:167:GLU:HB3	1.78	0.61
1:F:45:VAL:CG2	1:H:166:TYR:HE1	1.83	0.61
1:F:46:GLY:N	1:H:167:GLU:HG3	2.15	0.61
1:I:63:GLY:HA3	1:J:268:GLY:H	1.66	0.61
1:J:105:LEU:HB2	1:J:134:VAL:HG12	1.82	0.61
1:D:65:LEU:CD2	1:F:287:ILE:HG13	2.14	0.61
1:F:248:ILE:HG23	1:F:250:ILE:HD11	1.81	0.61
1:D:43:VAL:CG1	1:F:169:TYR:HD1	2.08	0.61
1:J:266:PHE:CZ	1:K:173:HIS:ND1	2.68	0.61
1:E:265:SER:HB3	1:F:285:CYS:HA	1.81	0.61
1:F:45:VAL:HG13	1:H:166:TYR:CE1	2.33	0.60
1:L:189:LEU:HA	1:L:192:ILE:HG12	1.83	0.60
1:D:170:ALA:HB1	1:D:175:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:205:GLU:HA	1:L:288:ASP:HB2	1.82	0.60
1:M:34:ILE:HG21	1:M:67:LEU:HB3	1.83	0.60
1:C:203:THR:HG21	1:D:267:ILE:HG23	1.84	0.60
1:D:57:GLU:OE2	1:F:291:LYS:HD2	2.02	0.60
1:K:63:GLY:HA3	1:L:267:ILE:HA	1.83	0.60
1:C:9:VAL:HG21	1:C:344:SER:HA	1.83	0.60
1:J:266:PHE:HE1	1:K:171:LEU:HB3	1.66	0.60
1:L:305:MET:SD	1:L:336:LYS:HB3	2.42	0.60
1:E:189:LEU:HD13	1:E:257:CYS:SG	2.42	0.60
1:K:164:PRO:HG3	1:K:174:ALA:HB3	1.84	0.60
1:A:32:PRO:HB2	1:A:34:ILE:HG12	1.84	0.60
1:A:189:LEU:HD13	1:A:257:CYS:SG	2.42	0.60
1:D:120:THR:HG21	1:D:370:VAL:HG21	1.82	0.60
1:J:205:GLU:HB3	1:L:289:ILE:H	1.66	0.60
1:L:164:PRO:HG2	1:L:171:LEU:HB2	1.83	0.60
1:C:11:ASP:HB3	1:C:18:LYS:HB2	1.84	0.60
1:B:63:GLY:CA	1:C:268:GLY:H	2.14	0.60
1:G:170:ALA:O	1:G:172:PRO:HD3	2.01	0.60
1:I:9:VAL:HG21	1:I:344:SER:HA	1.84	0.60
1:K:32:PRO:HB2	1:K:34:ILE:HG12	1.83	0.60
1:M:282:ILE:HG12	1:M:293:LEU:HD23	1.83	0.60
1:A:160:THR:HB	1:A:178:LEU:HB3	1.84	0.60
1:K:10:CYS:HA	1:K:18:LYS:O	2.02	0.60
1:J:266:PHE:CE2	1:K:173:HIS:HB2	2.37	0.59
1:C:357:ILE:HG21	1:C:370:VAL:HG22	1.84	0.59
1:E:213:LYS:HA	1:E:217:CYS:SG	2.42	0.59
1:J:266:PHE:CG	1:K:173:HIS:CD2	2.90	0.59
1:L:155:SER:HA	1:L:160:THR:HA	1.84	0.59
1:H:190:MET:SD	1:H:209:VAL:HG21	2.42	0.59
1:J:266:PHE:CE1	1:K:171:LEU:HB3	2.37	0.59
1:D:44:MET:SD	1:F:293:LEU:CG	2.87	0.59
1:C:86:TRP:HH2	1:C:119:MET:HG2	1.68	0.59
1:D:44:MET:HE2	1:F:293:LEU:HD22	1.83	0.59
1:B:63:GLY:HA3	1:C:267:ILE:CA	2.31	0.59
1:C:328:LYS:NZ	1:C:330:ILE:HG12	2.18	0.59
1:E:207:GLU:HB3	1:F:269:MET:H	1.68	0.59
1:L:219:VAL:HG22	1:L:258:PRO:HB3	1.84	0.59
1:A:103:THR:O	1:A:132:MET:HA	2.03	0.59
1:A:203:THR:OG1	1:C:287:ILE:HG23	2.03	0.58
1:E:250:ILE:HG23	1:E:253:GLU:HB2	1.85	0.58
1:F:70:PRO:HG3	1:F:85:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:203:THR:HB	1:K:268:GLY:HA3	1.85	0.58
1:K:195:GLU:HG2	1:L:112:PRO:CG	2.33	0.58
1:D:47:MET:HA	1:F:167:GLU:OE2	2.03	0.58
1:G:102:PRO:HB3	1:G:131:ALA:HB3	1.84	0.58
1:K:153:LEU:HD21	1:K:274:ILE:HG23	1.85	0.58
1:A:53:TYR:CZ	1:A:61:LYS:CD	2.86	0.58
1:E:164:PRO:HG2	1:E:171:LEU:HB2	1.85	0.58
1:G:189:LEU:HD12	1:G:192:ILE:HD11	1.85	0.58
1:D:64:ILE:HG13	1:F:287:ILE:CD1	2.34	0.58
1:A:19:ALA:HB3	1:A:29:ALA:HB3	1.84	0.58
1:J:7:ALA:HA	1:J:102:PRO:HG2	1.86	0.58
1:E:10:CYS:HB3	1:E:105:LEU:HD23	1.85	0.58
1:I:153:LEU:HA	1:I:161:HIS:O	2.03	0.58
1:J:120:THR:HG21	1:J:370:VAL:HG21	1.86	0.58
1:J:219:VAL:HG21	1:J:309:ILE:HB	1.86	0.58
1:D:38:PRO:HB3	1:D:64:ILE:HD12	1.86	0.58
1:L:227:MET:HE1	1:L:256:ARG:HD3	1.86	0.58
1:A:53:TYR:CZ	1:A:61:LYS:HD2	2.39	0.58
1:I:240:TYR:HB3	1:I:248:ILE:HG22	1.85	0.58
1:C:205:GLU:N	1:E:287:ILE:HD13	2.19	0.57
1:I:286:ASP:O	1:I:290:ARG:HG3	2.04	0.57
1:C:207:GLU:O	1:C:210:ARG:HB2	2.04	0.57
1:G:109:PRO:HA	1:G:136:ILE:HG23	1.85	0.57
1:A:153:LEU:HA	1:A:161:HIS:O	2.05	0.57
1:J:213:LYS:HA	1:J:217:CYS:SG	2.45	0.57
1:L:213:LYS:HA	1:L:217:CYS:SG	2.43	0.57
1:B:194:THR:HG22	1:B:198:TYR:O	2.04	0.57
1:D:33:SER:O	1:D:70:PRO:HD2	2.04	0.57
1:D:61:LYS:HZ1	1:F:291:LYS:CB	2.16	0.57
1:I:164:PRO:HG2	1:I:171:LEU:HB2	1.85	0.57
1:A:243:PRO:O	1:C:322:PRO:C	2.47	0.57
1:I:98:PRO:HB2	1:I:129:VAL:HG12	1.87	0.57
1:E:19:ALA:HB3	1:E:29:ALA:HB3	1.85	0.57
1:G:160:THR:HB	1:G:178:LEU:HB3	1.86	0.57
1:M:151:ILE:HB	1:M:293:LEU:HG	1.86	0.57
1:A:165:ILE:HG12	1:A:170:ALA:HA	1.87	0.57
1:D:194:THR:HG22	1:D:198:TYR:H	1.70	0.57
1:F:9:VAL:HG21	1:F:344:SER:HA	1.85	0.57
1:K:62:ARG:HG3	1:K:67:LEU:HD11	1.87	0.57
1:K:195:GLU:HB3	1:L:112:PRO:N	2.19	0.57
1:B:165:ILE:HA	1:B:170:ALA:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:VAL:HG22	1:C:175:ILE:HG23	1.87	0.57
1:E:268:GLY:H	1:F:290:ARG:HE	1.51	0.57
1:K:195:GLU:HG3	1:L:112:PRO:CA	2.35	0.57
1:B:63:GLY:HA3	1:C:268:GLY:H	1.70	0.56
1:G:10:CYS:HA	1:G:18:LYS:O	2.04	0.56
1:A:9:VAL:HG21	1:A:344:SER:HA	1.86	0.56
1:A:37:ARG:O	1:A:66:THR:N	2.37	0.56
1:D:359:LYS:HD2	1:D:360:GLN:HB2	1.87	0.56
1:J:9:VAL:HG21	1:J:344:SER:HA	1.87	0.56
1:L:330:ILE:O	1:L:332:PRO:HD3	2.05	0.56
1:N:213:LYS:HA	1:N:217:CYS:SG	2.45	0.56
1:D:44:MET:CG	1:F:293:LEU:CG	2.77	0.56
1:K:153:LEU:HA	1:K:161:HIS:O	2.05	0.56
1:E:153:LEU:HA	1:E:161:HIS:O	2.06	0.56
1:G:142:LEU:HG	1:G:147:ARG:HB2	1.87	0.56
1:B:286:ASP:HB3	1:B:289:ILE:HD11	1.88	0.56
1:K:188:TYR:HE2	1:K:257:CYS:HA	1.71	0.56
1:L:75:ILE:HD11	1:L:177:ARG:HH22	1.70	0.56
1:N:135:ALA:HB3	1:N:140:LEU:HD11	1.88	0.56
1:A:98:PRO:HB2	1:A:127:PHE:O	2.06	0.56
1:A:152:VAL:O	1:A:162:ASN:HA	2.06	0.55
1:D:48:GLY:C	1:F:166:TYR:CD2	2.84	0.55
1:A:262:PHE:O	1:A:275:HIS:HE1	1.88	0.55
1:B:104:LEU:HG	1:B:133:TYR:HB3	1.89	0.55
1:J:359:LYS:HD2	1:J:360:GLN:HB2	1.87	0.55
1:K:286:ASP:O	1:K:290:ARG:HG3	2.07	0.55
1:A:252:ASN:H	1:A:252:ASN:ND2	2.04	0.55
1:E:190:MET:SD	1:F:272:ALA:HB3	2.47	0.55
1:G:148:THR:HB	1:G:167:GLU:HA	1.88	0.55
1:I:103:THR:O	1:I:132:MET:HA	2.06	0.55
1:K:213:LYS:HD3	1:K:214:GLU:HG3	1.89	0.55
1:L:369:ILE:HA	1:L:372:ARG:HB2	1.89	0.55
1:E:198:TYR:CZ	1:E:248:ILE:HA	2.41	0.55
1:G:242:LEU:HG	1:G:243:PRO:HD2	1.87	0.55
1:I:10:CYS:HB3	1:I:105:LEU:HD23	1.89	0.55
1:J:164:PRO:HG2	1:J:171:LEU:HB2	1.87	0.55
1:B:63:GLY:HA3	1:C:266:PHE:O	2.07	0.55
1:J:303:THR:HG23	1:J:306:TYR:HE2	1.72	0.55
1:G:44:MET:HB2	1:G:47:MET:HB2	1.89	0.55
1:H:359:LYS:HD2	1:H:360:GLN:HB2	1.86	0.55
1:L:280:ASN:HA	1:L:283:MET:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:SER:HA	1:B:335:ARG:HB2	1.88	0.55
1:C:244:ASP:HB3	1:E:287:ILE:HG23	1.88	0.55
1:F:7:ALA:HA	1:F:102:PRO:HG2	1.89	0.55
1:B:238:LYS:HE3	1:B:238:LYS:HA	1.88	0.55
1:H:162:ASN:OD1	1:H:277:THR:HG23	2.07	0.55
1:I:32:PRO:HB2	1:I:34:ILE:HG12	1.89	0.55
1:D:7:ALA:HA	1:D:102:PRO:HG2	1.89	0.55
1:D:46:GLY:HA2	1:F:149:THR:HG23	1.89	0.55
1:C:7:ALA:HA	1:C:102:PRO:HG2	1.88	0.54
1:D:45:VAL:HG11	1:F:142:LEU:CD1	2.34	0.54
1:F:188:TYR:HA	1:F:191:LYS:HD3	1.88	0.54
1:L:32:PRO:HB2	1:L:34:ILE:HG12	1.88	0.54
1:D:44:MET:CE	1:F:293:LEU:HD22	2.38	0.54
1:K:106:THR:HG22	1:K:140:LEU:HD12	1.89	0.54
1:L:64:ILE:HG13	1:L:65:LEU:HG	1.89	0.54
1:A:148:THR:HB	1:A:167:GLU:HA	1.90	0.54
1:D:357:ILE:HG21	1:D:370:VAL:HG22	1.88	0.54
1:E:153:LEU:HD21	1:E:274:ILE:HD12	1.89	0.54
1:I:190:MET:SD	1:I:209:VAL:HG21	2.48	0.54
1:J:98:PRO:HB2	1:J:129:VAL:HG12	1.88	0.54
1:M:103:THR:O	1:M:132:MET:HA	2.07	0.54
1:N:330:ILE:O	1:N:332:PRO:HD3	2.08	0.54
1:F:140:LEU:HD22	1:F:343:GLY:HA2	1.89	0.54
1:D:43:VAL:HG21	1:F:169:TYR:O	2.07	0.54
1:G:10:CYS:HB3	1:G:105:LEU:HD23	1.90	0.54
1:C:189:LEU:HD13	1:C:257:CYS:SG	2.48	0.54
1:D:61:LYS:HA	1:E:268:GLY:HA2	1.89	0.54
1:E:190:MET:HA	1:E:209:VAL:HG11	1.90	0.54
1:F:161:HIS:HA	1:F:176:MET:O	2.08	0.54
1:J:162:ASN:O	1:J:175:ILE:HA	2.07	0.54
1:K:162:ASN:OD1	1:K:277:THR:HG23	2.06	0.54
1:B:103:THR:O	1:B:132:MET:HA	2.07	0.54
1:D:62:ARG:O	1:E:270:GLU:HA	2.08	0.54
1:A:203:THR:OG1	1:C:287:ILE:CG2	2.56	0.54
1:A:304:THR:O	1:A:309:ILE:HG21	2.07	0.54
1:F:304:THR:O	1:F:309:ILE:HG21	2.07	0.54
1:K:330:ILE:O	1:K:332:PRO:HD3	2.08	0.54
1:N:98:PRO:HB2	1:N:127:PHE:O	2.08	0.54
1:N:190:MET:O	1:N:194:THR:HG23	2.08	0.54
1:D:44:MET:HG2	1:F:293:LEU:CG	2.32	0.54
1:D:203:THR:HG21	1:E:269:MET:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:THR:HA	1:E:309:ILE:HD13	1.90	0.54
1:H:162:ASN:O	1:H:175:ILE:HA	2.08	0.54
1:B:162:ASN:O	1:B:175:ILE:HA	2.08	0.54
1:D:57:GLU:OE2	1:F:291:LYS:HE3	2.04	0.54
1:M:109:PRO:HA	1:M:136:ILE:HG23	1.90	0.54
1:A:114:ALA:HA	1:A:117:GLU:HB2	1.88	0.53
1:C:305:MET:SD	1:C:336:LYS:HD3	2.49	0.53
1:G:359:LYS:HD2	1:G:360:GLN:HB2	1.89	0.53
1:A:299:MET:SD	1:A:313:MET:HG3	2.48	0.53
1:C:102:PRO:HB3	1:C:131:ALA:HB3	1.90	0.53
1:B:330:ILE:O	1:B:332:PRO:HD3	2.08	0.53
1:H:163:VAL:HG22	1:H:175:ILE:HG23	1.91	0.53
1:K:197:GLY:O	1:L:77:THR:HA	2.08	0.53
1:D:239:SER:HA	1:D:248:ILE:O	2.07	0.53
1:E:180:LEU:HD21	1:F:283:MET:HG2	1.90	0.53
1:F:359:LYS:HD2	1:F:360:GLN:HB2	1.90	0.53
1:M:90:PHE:HZ	1:M:123:MET:HE1	1.73	0.53
1:N:300:SER:HA	1:N:335:ARG:HB2	1.90	0.53
1:A:186:THR:HG21	1:A:210:ARG:HB3	1.91	0.53
1:D:43:VAL:HG22	1:F:171:LEU:HG	1.89	0.53
1:D:45:VAL:CA	1:F:165:ILE:O	2.49	0.53
1:K:19:ALA:HB3	1:K:29:ALA:HB3	1.91	0.53
1:D:188:TYR:HE2	1:D:257:CYS:HA	1.73	0.53
1:E:148:THR:HB	1:E:167:GLU:HA	1.89	0.53
1:G:163:VAL:HA	1:G:175:ILE:HG12	1.90	0.53
1:K:272:ALA:HB1	1:K:276:GLU:HB2	1.91	0.53
1:E:238:LYS:HE3	1:E:238:LYS:HA	1.90	0.53
1:E:266:PHE:CZ	1:F:282:ILE:HA	2.44	0.53
1:K:100:GLU:HG3	1:K:101:HIS:CD2	2.44	0.53
1:D:43:VAL:CG1	1:F:166:TYR:HB2	2.38	0.53
1:K:359:LYS:HD2	1:K:360:GLN:N	2.24	0.53
1:L:39:ARG:HE	1:M:263:GLN:HG2	1.73	0.53
1:I:216:LEU:HB3	1:I:254:ARG:HG3	1.91	0.53
1:A:7:ALA:HA	1:A:102:PRO:HG2	1.91	0.53
1:F:193:LEU:HB3	1:F:200:PHE:HE1	1.73	0.53
1:F:290:ARG:HD2	1:F:294:TYR:HE2	1.73	0.53
1:I:100:GLU:HG2	1:I:101:HIS:CD2	2.44	0.53
1:I:185:LEU:HD21	1:I:261:LEU:HB2	1.91	0.53
1:A:22:ALA:HB1	1:A:348:SER:HB2	1.91	0.52
1:B:359:LYS:HD2	1:B:360:GLN:N	2.24	0.52
1:D:359:LYS:HD2	1:D:360:GLN:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:VAL:CG1	1:F:142:LEU:HD13	2.35	0.52
1:J:15:GLY:O	1:J:32:PRO:HA	2.10	0.52
1:J:240:TYR:HB3	1:J:248:ILE:HG22	1.91	0.52
1:A:312:ARG:O	1:A:316:GLU:HB2	2.09	0.52
1:D:45:VAL:CG2	1:F:164:PRO:HA	2.32	0.52
1:K:305:MET:SD	1:K:336:LYS:HB3	2.49	0.52
1:L:9:VAL:HG21	1:L:344:SER:HA	1.92	0.52
1:M:7:ALA:HB3	1:M:22:ALA:HB2	1.92	0.52
1:D:45:VAL:HG22	1:F:165:ILE:H	1.73	0.52
1:D:57:GLU:OE1	1:F:291:LYS:HE2	2.02	0.52
1:D:153:LEU:HD21	1:D:274:ILE:HG23	1.91	0.52
1:I:200:PHE:HA	1:I:205:GLU:HB3	1.91	0.52
1:N:58:ALA:HB1	1:N:65:LEU:HD11	1.91	0.52
1:N:70:PRO:HG2	1:N:71:ILE:HG13	1.91	0.52
1:N:159:VAL:HA	1:N:178:LEU:O	2.10	0.52
1:E:164:PRO:HG3	1:E:174:ALA:HB3	1.90	0.52
1:H:39:ARG:HD3	1:H:66:THR:HG23	1.91	0.52
1:C:44:MET:HB2	1:C:47:MET:HB2	1.91	0.52
1:D:42:GLY:HA3	1:F:285:CYS:CB	2.40	0.52
1:F:359:LYS:HD2	1:F:360:GLN:N	2.24	0.52
1:G:162:ASN:O	1:G:175:ILE:HA	2.10	0.52
1:I:61:LYS:HE3	1:K:166:TYR:HE1	1.75	0.52
1:L:296:ASN:HA	1:L:330:ILE:HD11	1.91	0.52
1:C:296:ASN:HA	1:C:330:ILE:HD11	1.91	0.52
1:D:45:VAL:CG1	1:F:165:ILE:HD13	2.39	0.52
1:I:210:ARG:HB3	1:I:210:ARG:CZ	2.39	0.52
1:A:53:TYR:CE2	1:A:61:LYS:HD2	2.44	0.52
1:B:64:ILE:HG23	1:C:267:ILE:CG1	2.38	0.52
1:A:9:VAL:O	1:A:19:ALA:HA	2.10	0.52
1:F:238:LYS:HE3	1:F:238:LYS:HA	1.92	0.52
1:G:8:LEU:HG	1:G:101:HIS:HB3	1.92	0.52
1:G:106:THR:HG21	1:G:339:VAL:HG12	1.92	0.52
1:L:40:HIS:HE1	1:M:263:GLN:O	1.93	0.52
1:A:53:TYR:HD2	1:A:57:GLU:HB3	1.75	0.52
1:A:65:LEU:HB2	1:B:267:ILE:HD12	1.92	0.52
1:A:261:LEU:HG	1:A:274:ILE:HG13	1.92	0.52
1:C:213:LYS:HA	1:C:217:CYS:SG	2.50	0.52
1:C:265:SER:OG	1:C:270:GLU:HA	2.10	0.52
1:B:105:LEU:O	1:B:134:VAL:HA	2.10	0.51
1:D:19:ALA:HB3	1:D:29:ALA:HB3	1.91	0.51
1:I:162:ASN:O	1:I:175:ILE:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:359:LYS:HD2	1:K:360:GLN:HB2	1.91	0.51
1:N:355:MET:HA	1:N:373:LYS:HD3	1.92	0.51
1:A:53:TYR:CD2	1:A:57:GLU:HB3	2.45	0.51
1:A:104:LEU:HA	1:A:133:TYR:O	2.10	0.51
1:D:286:ASP:HB3	1:D:289:ILE:HG23	1.91	0.51
1:E:201:VAL:HG12	1:E:202:THR:HG23	1.93	0.51
1:K:15:GLY:O	1:K:32:PRO:HA	2.09	0.51
1:N:359:LYS:HD2	1:N:360:GLN:N	2.25	0.51
1:A:153:LEU:HD11	1:A:274:ILE:HD13	1.91	0.51
1:D:197:GLY:CA	1:E:112:PRO:HA	2.40	0.51
1:J:204:ALA:HA	1:J:207:GLU:HB2	1.92	0.51
1:D:45:VAL:HG22	1:F:165:ILE:N	2.26	0.51
1:I:194:THR:HB	1:J:110:LEU:HB3	1.93	0.51
1:A:136:ILE:HD12	1:A:136:ILE:H	1.75	0.51
1:C:162:ASN:OD1	1:C:277:THR:HG23	2.11	0.51
1:D:68:LYS:O	1:D:70:PRO:HD3	2.10	0.51
1:H:182:GLY:HA2	1:H:303:THR:OG1	2.11	0.51
1:H:359:LYS:HD2	1:H:360:GLN:N	2.26	0.51
1:K:192:ILE:HA	1:L:112:PRO:CG	2.34	0.51
1:B:349:LEU:HB3	1:B:352:PHE:HB2	1.91	0.51
1:D:238:LYS:HE3	1:D:238:LYS:HA	1.92	0.51
1:N:137:GLN:HG2	1:N:339:VAL:HG11	1.93	0.51
1:A:212:ILE:HG23	1:A:216:LEU:HD12	1.92	0.51
1:E:206:ARG:NH1	1:F:271:SER:O	2.43	0.51
1:N:294:TYR:HE1	1:N:321:ALA:HB1	1.75	0.51
1:D:45:VAL:HG13	1:F:165:ILE:HD12	1.92	0.51
1:F:191:LYS:HB3	1:G:173:HIS:HB2	1.93	0.51
1:H:11:ASP:O	1:H:17:VAL:HA	2.11	0.51
1:I:153:LEU:HD23	1:I:299:MET:HG2	1.92	0.51
1:I:160:THR:HB	1:I:178:LEU:HB3	1.93	0.51
1:A:359:LYS:HD2	1:A:360:GLN:HB2	1.92	0.51
1:D:45:VAL:CG1	1:F:165:ILE:HD12	2.40	0.51
1:D:49:GLN:HA	1:F:166:TYR:CZ	2.46	0.51
1:E:160:THR:O	1:E:177:ARG:HA	2.11	0.51
1:G:34:ILE:O	1:G:54:VAL:HA	2.11	0.51
1:I:163:VAL:HG22	1:I:175:ILE:HG23	1.93	0.51
1:L:359:LYS:HD2	1:L:360:GLN:HB2	1.93	0.51
1:B:357:ILE:HG13	1:B:370:VAL:HG22	1.93	0.51
1:C:153:LEU:HD22	1:C:313:MET:HE2	1.92	0.51
1:E:359:LYS:HD2	1:E:360:GLN:HB2	1.93	0.51
1:A:238:LYS:HE3	1:A:238:LYS:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:LYS:HZ3	1:C:292:ASP:CG	2.19	0.50
1:J:163:VAL:HG22	1:J:175:ILE:HG23	1.92	0.50
1:K:244:ASP:HB2	1:M:290:ARG:HB2	1.92	0.50
1:M:19:ALA:HB3	1:M:29:ALA:HB3	1.93	0.50
1:E:99:GLU:HB3	1:E:128:ASN:ND2	2.26	0.50
1:M:359:LYS:HD2	1:M:360:GLN:N	2.26	0.50
1:B:174:ALA:HB2	1:B:285:CYS:SG	2.51	0.50
1:L:322:PRO:O	1:L:325:MET:HG2	2.10	0.50
1:D:61:LYS:NZ	1:F:291:LYS:CG	2.72	0.50
1:D:182:GLY:HA2	1:D:303:THR:OG1	2.11	0.50
1:D:210:ARG:O	1:D:213:LYS:HB3	2.11	0.50
1:F:212:ILE:HG23	1:F:216:LEU:HD12	1.93	0.50
1:E:106:THR:HG22	1:E:140:LEU:HD12	1.93	0.50
1:E:359:LYS:HD2	1:E:360:GLN:N	2.27	0.50
1:H:210:ARG:HH11	1:H:210:ARG:HB2	1.77	0.50
1:I:139:VAL:HA	1:I:165:ILE:HD13	1.93	0.50
1:D:64:ILE:HG12	1:F:285:CYS:O	2.11	0.50
1:F:45:VAL:HG22	1:H:166:TYR:CE1	2.27	0.50
1:D:305:MET:SD	1:D:336:LYS:HB3	2.51	0.50
1:F:193:LEU:HG	1:F:250:ILE:HD12	1.93	0.50
1:I:299:MET:HE2	1:I:329:ILE:HG21	1.93	0.50
1:I:305:MET:SD	1:I:336:LYS:HB3	2.51	0.50
1:J:10:CYS:HA	1:J:18:LYS:O	2.12	0.50
1:J:100:GLU:HG2	1:J:101:HIS:CD2	2.46	0.50
1:J:332:PRO:HB2	1:J:335:ARG:HB3	1.92	0.50
1:K:162:ASN:HB2	1:K:176:MET:HB2	1.93	0.50
1:A:153:LEU:HD13	1:A:162:ASN:ND2	2.27	0.50
1:E:120:THR:HG21	1:E:370:VAL:HG21	1.94	0.50
1:F:174:ALA:HB2	1:F:284:LYS:HG2	1.93	0.50
1:G:267:ILE:HD13	1:H:169:TYR:OH	2.11	0.50
1:N:102:PRO:HD3	1:N:130:PRO:HG2	1.93	0.50
1:E:34:ILE:O	1:E:54:VAL:HA	2.12	0.50
1:G:166:TYR:HB2	1:G:289:ILE:HD13	1.94	0.50
1:M:37:ARG:HB3	1:M:38:PRO:CD	2.42	0.50
1:C:203:THR:HG22	1:C:206:ARG:NH2	2.27	0.49
1:G:151:ILE:HB	1:G:293:LEU:HG	1.94	0.49
1:L:292:ASP:HB3	1:L:296:ASN:HD22	1.76	0.49
1:L:312:ARG:HD2	1:L:315:LYS:HE3	1.94	0.49
1:E:213:LYS:HG3	1:E:306:TYR:OH	2.12	0.49
1:H:102:PRO:HB3	1:H:131:ALA:HB3	1.94	0.49
1:N:109:PRO:HA	1:N:136:ILE:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ASP:HB3	1:B:18:LYS:HB2	1.95	0.49
1:C:359:LYS:HD2	1:C:360:GLN:HB2	1.93	0.49
1:D:64:ILE:H	1:F:287:ILE:HD13	1.75	0.49
1:H:36:GLY:HA3	1:H:65:LEU:HD13	1.93	0.49
1:J:263:GLN:HE21	1:J:263:GLN:HA	1.76	0.49
1:K:193:LEU:HB3	1:K:198:TYR:HB2	1.93	0.49
1:L:10:CYS:HA	1:L:18:LYS:O	2.12	0.49
1:M:283:MET:SD	1:M:290:ARG:NH2	2.85	0.49
1:I:104:LEU:HA	1:I:133:TYR:O	2.12	0.49
1:J:243:PRO:HD2	1:L:291:LYS:HD3	1.95	0.49
1:M:39:ARG:HB2	1:N:265:SER:C	2.36	0.49
1:B:8:LEU:HA	1:B:21:PHE:HA	1.94	0.49
1:G:242:LEU:HD13	1:G:248:ILE:HD11	1.93	0.49
1:I:239:SER:HA	1:I:248:ILE:O	2.13	0.49
1:J:153:LEU:HD21	1:J:274:ILE:HD12	1.95	0.49
1:L:193:LEU:HG	1:L:250:ILE:HD11	1.94	0.49
1:L:212:ILE:HG23	1:L:216:LEU:HD12	1.95	0.49
1:L:242:LEU:HD11	1:L:248:ILE:HD13	1.93	0.49
1:N:7:ALA:HA	1:N:102:PRO:HG2	1.94	0.49
1:N:282:ILE:HG22	1:N:290:ARG:HD2	1.94	0.49
1:B:19:ALA:HB3	1:B:29:ALA:HB3	1.95	0.49
1:D:43:VAL:CG1	1:F:169:TYR:CD1	2.91	0.49
1:D:44:MET:CG	1:F:293:LEU:HD11	2.39	0.49
1:L:210:ARG:O	1:L:213:LYS:HB3	2.12	0.49
1:A:10:CYS:HA	1:A:18:LYS:O	2.12	0.49
1:A:117:GLU:HB3	1:A:367:PRO:HB3	1.94	0.49
1:B:15:GLY:O	1:B:32:PRO:HA	2.12	0.49
1:B:17:VAL:C	1:B:18:LYS:HE3	2.38	0.49
1:E:200:PHE:H	1:F:180:LEU:HD22	1.77	0.49
1:K:195:GLU:HB2	1:L:112:PRO:CB	2.42	0.49
1:E:109:PRO:HA	1:E:136:ILE:HG23	1.93	0.49
1:F:46:GLY:N	1:H:167:GLU:CG	2.76	0.49
1:G:278:THR:HG21	1:G:297:ASN:OD1	2.12	0.49
1:I:252:ASN:HA	1:I:255:PHE:HE2	1.76	0.49
1:L:106:THR:HG22	1:L:140:LEU:HD12	1.95	0.49
1:L:204:ALA:HB1	1:N:287:ILE:HG23	1.94	0.49
1:N:299:MET:O	1:N:332:PRO:HD2	2.13	0.49
1:A:86:TRP:HH2	1:A:119:MET:HG2	1.78	0.49
1:B:205:GLU:O	1:B:208:ILE:HG12	2.13	0.49
1:D:61:LYS:HZ3	1:F:291:LYS:CD	2.06	0.49
1:D:194:THR:HA	1:D:197:GLY:C	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:TYR:HB3	1:D:248:ILE:HB	1.94	0.49
1:J:102:PRO:HA	1:J:131:ALA:O	2.12	0.49
1:K:203:THR:O	1:K:207:GLU:HB2	2.12	0.49
1:A:264:PRO:HD3	1:A:273:GLY:HA3	1.95	0.49
1:E:22:ALA:HB1	1:E:348:SER:HB2	1.95	0.49
1:E:174:ALA:HA	1:E:284:LYS:HZ3	1.78	0.49
1:F:290:ARG:HD2	1:F:294:TYR:CE2	2.48	0.49
1:I:155:SER:HA	1:I:160:THR:HA	1.94	0.49
1:K:217:CYS:HA	1:K:254:ARG:O	2.13	0.49
1:C:8:LEU:HG	1:C:101:HIS:HB3	1.94	0.48
1:F:74:GLY:O	1:F:108:ALA:HB2	2.12	0.48
1:G:186:THR:HG21	1:G:210:ARG:HG2	1.94	0.48
1:M:238:LYS:HE3	1:M:238:LYS:HA	1.95	0.48
1:N:59:GLN:OE1	1:N:62:ARG:NH1	2.46	0.48
1:N:242:LEU:HD22	1:N:246:GLN:HB3	1.94	0.48
1:B:64:ILE:HG23	1:C:267:ILE:HB	0.69	0.48
1:C:153:LEU:HD21	1:C:274:ILE:HG23	1.96	0.48
1:F:10:CYS:HA	1:F:18:LYS:O	2.13	0.48
1:K:217:CYS:HG	1:K:257:CYS:HG	1.58	0.48
1:L:153:LEU:HA	1:L:161:HIS:O	2.13	0.48
1:M:114:ALA:HA	1:M:117:GLU:HB2	1.96	0.48
1:N:104:LEU:HG	1:N:133:TYR:HB3	1.94	0.48
1:N:140:LEU:O	1:N:342:GLY:HA3	2.13	0.48
1:B:60:SER:OG	1:D:287:ILE:CD1	2.61	0.48
1:B:137:GLN:HA	1:B:339:VAL:HG13	1.95	0.48
1:E:191:LYS:HA	1:E:194:THR:OG1	2.13	0.48
1:I:106:THR:HG22	1:I:140:LEU:HD12	1.95	0.48
1:I:189:LEU:HD13	1:I:257:CYS:SG	2.53	0.48
1:L:162:ASN:O	1:L:175:ILE:HA	2.13	0.48
1:L:299:MET:O	1:L:332:PRO:HD2	2.12	0.48
1:A:239:SER:HA	1:A:248:ILE:O	2.13	0.48
1:E:195:GLU:HA	1:F:177:ARG:HB3	1.96	0.48
1:B:43:VAL:HB	1:D:169:TYR:OH	2.13	0.48
1:D:106:THR:HG21	1:D:339:VAL:HG12	1.96	0.48
1:D:162:ASN:O	1:D:175:ILE:HA	2.14	0.48
1:G:32:PRO:HB2	1:G:34:ILE:HG12	1.94	0.48
1:K:162:ASN:O	1:K:175:ILE:HA	2.13	0.48
1:A:359:LYS:HD2	1:A:360:GLN:N	2.28	0.48
1:J:262:PHE:O	1:J:275:HIS:HE1	1.97	0.48
1:A:53:TYR:CZ	1:A:61:LYS:HD3	2.47	0.48
1:B:189:LEU:HD12	1:B:192:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:LYS:O	1:F:65:LEU:HG	2.14	0.48
1:F:119:MET:O	1:F:123:MET:HG2	2.13	0.48
1:G:12:ASN:HA	1:G:17:VAL:HG22	1.95	0.48
1:J:102:PRO:HB3	1:J:131:ALA:HB3	1.96	0.48
1:M:155:SER:HA	1:M:160:THR:HA	1.95	0.48
1:B:286:ASP:O	1:B:289:ILE:HG13	2.14	0.48
1:I:359:LYS:HD2	1:I:360:GLN:HB2	1.95	0.48
1:J:182:GLY:O	1:J:213:LYS:NZ	2.44	0.48
1:A:330:ILE:O	1:A:332:PRO:HD3	2.13	0.48
1:B:62:ARG:HG2	1:C:268:GLY:HA2	1.96	0.48
1:B:64:ILE:N	1:C:267:ILE:HA	2.29	0.48
1:D:45:VAL:HG11	1:F:165:ILE:HD13	1.95	0.48
1:E:191:LYS:O	1:F:176:MET:SD	2.72	0.48
1:I:238:LYS:O	1:I:249:THR:HA	2.14	0.48
1:J:10:CYS:HB3	1:J:105:LEU:HD23	1.96	0.48
1:J:205:GLU:HB2	1:L:286:ASP:HB3	1.96	0.48
1:L:39:ARG:NH2	1:M:264:PRO:HD2	2.29	0.48
1:M:164:PRO:HG3	1:M:174:ALA:HB3	1.96	0.48
1:G:267:ILE:HD11	1:H:169:TYR:OH	2.13	0.48
1:J:151:ILE:HD11	1:J:162:ASN:HB3	1.95	0.48
1:K:252:ASN:O	1:K:256:ARG:NH2	2.47	0.48
1:L:253:GLU:HA	1:L:256:ARG:HE	1.78	0.48
1:B:155:SER:HA	1:B:160:THR:HA	1.96	0.47
1:D:57:GLU:OE2	1:F:291:LYS:CD	2.61	0.47
1:D:164:PRO:HG3	1:D:285:CYS:SG	2.54	0.47
1:E:152:VAL:HA	1:E:298:VAL:HB	1.96	0.47
1:G:332:PRO:HB2	1:G:335:ARG:HB3	1.96	0.47
1:H:10:CYS:SG	1:H:89:THR:HG21	2.53	0.47
1:J:292:ASP:O	1:J:296:ASN:HB2	2.14	0.47
1:M:162:ASN:O	1:M:175:ILE:HA	2.14	0.47
1:N:152:VAL:O	1:N:162:ASN:HA	2.14	0.47
1:A:15:GLY:O	1:A:32:PRO:HA	2.14	0.47
1:B:11:ASP:O	1:B:17:VAL:HA	2.14	0.47
1:B:39:ARG:CD	1:B:66:THR:HG23	2.37	0.47
1:D:11:ASP:O	1:D:17:VAL:HA	2.14	0.47
1:D:45:VAL:CG1	1:F:142:LEU:CD1	2.92	0.47
1:D:197:GLY:HA3	1:D:198:TYR:HA	1.67	0.47
1:G:103:THR:O	1:G:132:MET:HA	2.13	0.47
1:H:116:ARG:HA	1:H:119:MET:HE3	1.96	0.47
1:J:44:MET:HB2	1:J:47:MET:HB2	1.97	0.47
1:K:152:VAL:O	1:K:162:ASN:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:188:TYR:HA	1:K:191:LYS:HD3	1.95	0.47
1:L:39:ARG:HH21	1:M:264:PRO:HD2	1.79	0.47
1:A:135:ALA:HB3	1:A:140:LEU:HD11	1.97	0.47
1:B:250:ILE:HG23	1:B:253:GLU:HB2	1.96	0.47
1:D:298:VAL:HA	1:D:330:ILE:O	2.14	0.47
1:I:105:LEU:O	1:I:134:VAL:HA	2.14	0.47
1:K:217:CYS:SG	1:K:257:CYS:SG	3.12	0.47
1:N:9:VAL:HG21	1:N:344:SER:HA	1.97	0.47
1:C:90:PHE:HZ	1:C:123:MET:HE1	1.79	0.47
1:D:15:GLY:O	1:D:32:PRO:HA	2.14	0.47
1:F:9:VAL:HG13	1:F:104:LEU:HD22	1.96	0.47
1:G:86:TRP:HH2	1:G:119:MET:HG3	1.79	0.47
1:K:11:ASP:HA	1:K:106:THR:OG1	2.15	0.47
1:K:198:TYR:CZ	1:K:248:ILE:HG13	2.48	0.47
1:L:359:LYS:HD2	1:L:360:GLN:N	2.28	0.47
1:E:62:ARG:HE	1:E:67:LEU:HD11	1.78	0.47
1:H:36:GLY:HA2	1:H:66:THR:O	2.15	0.47
1:H:99:GLU:HA	1:H:130:PRO:HD3	1.96	0.47
1:I:10:CYS:HA	1:I:18:LYS:O	2.15	0.47
1:I:118:LYS:NZ	1:I:121:GLN:OE1	2.47	0.47
1:J:8:LEU:HG	1:J:101:HIS:HB3	1.95	0.47
1:K:58:ALA:O	1:K:62:ARG:HB2	2.14	0.47
1:L:8:LEU:HG	1:L:101:HIS:HB3	1.96	0.47
1:M:152:VAL:O	1:M:162:ASN:HA	2.14	0.47
1:D:251:GLY:O	1:D:254:ARG:HG3	2.15	0.47
1:L:9:VAL:O	1:L:19:ALA:HA	2.15	0.47
1:A:286:ASP:O	1:A:290:ARG:HG3	2.15	0.47
1:D:64:ILE:CG1	1:F:286:ASP:HA	2.44	0.47
1:D:200:PHE:HZ	1:D:248:ILE:HG12	1.79	0.47
1:E:86:TRP:CH2	1:E:119:MET:HG3	2.50	0.47
1:E:287:ILE:HA	1:E:290:ARG:HB2	1.95	0.47
1:F:201:VAL:HG21	1:G:177:ARG:HD3	1.95	0.47
1:G:45:VAL:HG23	1:I:167:GLU:HB3	1.96	0.47
1:H:186:THR:OG1	1:H:213:LYS:HD2	2.14	0.47
1:I:109:PRO:HA	1:I:136:ILE:HG23	1.97	0.47
1:I:186:THR:HG23	1:I:213:LYS:HB2	1.94	0.47
1:I:252:ASN:OD1	1:J:113:LYS:NZ	2.47	0.47
1:L:63:GLY:O	1:M:270:GLU:HB2	2.15	0.47
1:L:304:THR:HA	1:L:309:ILE:HD13	1.95	0.47
1:M:265:SER:HA	1:M:270:GLU:CD	2.39	0.47
1:N:71:ILE:HA	1:N:76:ILE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:105:LEU:O	1:N:134:VAL:HA	2.15	0.47
1:D:62:ARG:HG3	1:D:67:LEU:HD21	1.95	0.47
1:B:60:SER:C	1:D:287:ILE:HG21	2.40	0.47
1:C:32:PRO:HG2	1:C:55:GLY:HA2	1.97	0.47
1:D:39:ARG:NH2	1:E:264:PRO:O	2.48	0.47
1:K:147:ARG:NH1	1:K:296:ASN:OD1	2.46	0.47
1:K:213:LYS:HA	1:K:217:CYS:SG	2.54	0.47
1:M:227:MET:HE1	1:M:256:ARG:HD3	1.96	0.47
1:A:62:ARG:CD	1:C:287:ILE:HD11	2.34	0.47
1:F:136:ILE:HD12	1:F:136:ILE:H	1.80	0.47
1:F:369:ILE:O	1:F:373:LYS:HB2	2.14	0.47
1:G:19:ALA:HB3	1:G:29:ALA:HB3	1.96	0.47
1:G:32:PRO:HG2	1:G:55:GLY:HA2	1.97	0.47
1:G:45:VAL:HG21	1:I:167:GLU:OE1	2.14	0.47
1:G:263:GLN:HE21	1:G:263:GLN:HA	1.79	0.47
1:J:203:THR:C	1:J:205:GLU:H	2.23	0.47
1:J:359:LYS:HD2	1:J:360:GLN:N	2.29	0.47
1:K:153:LEU:HD23	1:K:299:MET:HG2	1.96	0.47
1:K:239:SER:HA	1:K:248:ILE:O	2.15	0.47
1:L:192:ILE:HA	1:L:195:GLU:HB2	1.96	0.47
1:M:86:TRP:CH2	1:M:119:MET:HG3	2.49	0.47
1:A:162:ASN:OD1	1:A:277:THR:HG23	2.16	0.46
1:E:90:PHE:HZ	1:E:123:MET:HE1	1.79	0.46
1:F:142:LEU:HD22	1:F:165:ILE:HD13	1.97	0.46
1:F:153:LEU:HA	1:F:161:HIS:O	2.15	0.46
1:H:36:GLY:O	1:H:52:SER:HA	2.15	0.46
1:K:188:TYR:CE2	1:K:257:CYS:HA	2.50	0.46
1:K:242:LEU:HD22	1:K:242:LEU:H	1.80	0.46
1:K:242:LEU:O	1:K:244:ASP:N	2.48	0.46
1:A:147:ARG:NH1	1:A:296:ASN:OD1	2.48	0.46
1:A:198:TYR:OH	1:A:248:ILE:HA	2.14	0.46
1:B:148:THR:HB	1:B:167:GLU:HA	1.98	0.46
1:D:44:MET:HE2	1:F:293:LEU:HA	1.96	0.46
1:E:9:VAL:HA	1:E:104:LEU:O	2.15	0.46
1:H:328:LYS:HZ1	1:H:330:ILE:HG13	1.80	0.46
1:I:36:GLY:HA3	1:I:65:LEU:HD13	1.96	0.46
1:J:190:MET:HG3	1:J:200:PHE:CD1	2.50	0.46
1:E:105:LEU:HD11	1:E:123:MET:HE2	1.97	0.46
1:E:206:ARG:HB2	1:F:265:SER:HA	1.98	0.46
1:F:152:VAL:O	1:F:162:ASN:HA	2.16	0.46
1:L:109:PRO:HA	1:L:136:ILE:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:353:GLN:HA	1:L:356:TRP:CD1	2.50	0.46
1:M:37:ARG:HB3	1:M:38:PRO:HD2	1.97	0.46
1:M:105:LEU:HD11	1:M:123:MET:HE2	1.96	0.46
1:D:32:PRO:O	1:D:55:GLY:HA2	2.15	0.46
1:D:193:LEU:HB3	1:D:198:TYR:HB2	1.97	0.46
1:F:99:GLU:H	1:F:99:GLU:CD	2.23	0.46
1:F:102:PRO:HB3	1:F:131:ALA:HB3	1.97	0.46
1:G:155:SER:HA	1:G:160:THR:HA	1.96	0.46
1:H:153:LEU:HD12	1:H:161:HIS:O	2.14	0.46
1:I:359:LYS:HD2	1:I:360:GLN:N	2.30	0.46
1:L:11:ASP:HA	1:L:106:THR:OG1	2.15	0.46
1:C:119:MET:O	1:C:123:MET:HG2	2.15	0.46
1:E:266:PHE:CE1	1:F:282:ILE:HA	2.51	0.46
1:F:182:GLY:O	1:F:213:LYS:NZ	2.48	0.46
1:M:104:LEU:HA	1:M:133:TYR:O	2.16	0.46
1:D:65:LEU:HG	1:F:287:ILE:HG21	1.98	0.46
1:D:104:LEU:HG	1:D:133:TYR:HB3	1.97	0.46
1:H:139:VAL:HG22	1:H:170:ALA:HB2	1.97	0.46
1:J:219:VAL:HG22	1:J:258:PRO:HB3	1.97	0.46
1:B:283:MET:SD	1:B:290:ARG:NH2	2.89	0.46
1:C:162:ASN:HB2	1:C:176:MET:HB2	1.98	0.46
1:D:49:GLN:N	1:F:166:TYR:CE2	2.84	0.46
1:D:58:ALA:HB1	1:D:65:LEU:HD11	1.97	0.46
1:D:212:ILE:HG23	1:D:216:LEU:HD12	1.98	0.46
1:E:207:GLU:HB3	1:F:269:MET:N	2.31	0.46
1:F:11:ASP:HA	1:F:106:THR:OG1	2.16	0.46
1:G:330:ILE:O	1:G:332:PRO:HD3	2.15	0.46
1:L:186:THR:HG21	1:L:210:ARG:HG2	1.98	0.46
1:M:174:ALA:HB1	1:M:281:SER:O	2.15	0.46
1:B:209:VAL:HA	1:B:212:ILE:HD12	1.97	0.46
1:D:61:LYS:NZ	1:F:291:LYS:CB	2.76	0.46
1:G:196:ARG:NH2	1:G:249:THR:OG1	2.49	0.46
1:J:286:ASP:O	1:J:290:ARG:HG3	2.16	0.46
1:J:305:MET:SD	1:J:336:LYS:HB3	2.56	0.46
1:K:195:GLU:H	1:L:112:PRO:HD2	1.81	0.46
1:A:61:LYS:C	1:A:63:GLY:HA3	2.41	0.46
1:C:106:THR:HG22	1:C:140:LEU:HD12	1.98	0.46
1:E:267:ILE:HB	1:F:287:ILE:O	2.16	0.46
1:H:155:SER:HA	1:H:160:THR:HA	1.96	0.46
1:I:192:ILE:HB	1:I:253:GLU:HG3	1.97	0.46
1:B:63:GLY:C	1:C:267:ILE:HA	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:PHE:HE1	1:B:359:LYS:HA	1.80	0.46
1:B:286:ASP:O	1:B:290:ARG:HG2	2.15	0.46
1:C:162:ASN:O	1:C:175:ILE:HA	2.16	0.46
1:D:61:LYS:CE	1:F:291:LYS:HB3	2.46	0.46
1:E:268:GLY:H	1:F:290:ARG:NE	2.13	0.46
1:J:119:MET:O	1:J:123:MET:HG2	2.16	0.46
1:B:359:LYS:HD2	1:B:360:GLN:HB2	1.98	0.45
1:D:197:GLY:HA2	1:E:113:LYS:N	2.31	0.45
1:G:359:LYS:HD2	1:G:360:GLN:N	2.31	0.45
1:I:220:ALA:O	1:I:312:ARG:HD3	2.15	0.45
1:K:9:VAL:HA	1:K:104:LEU:O	2.16	0.45
1:N:9:VAL:O	1:N:19:ALA:HA	2.16	0.45
1:N:210:ARG:CZ	1:N:210:ARG:HB3	2.46	0.45
1:A:100:GLU:HG3	1:A:101:HIS:CD2	2.51	0.45
1:B:36:GLY:HA2	1:B:66:THR:O	2.16	0.45
1:D:8:LEU:HG	1:D:101:HIS:HB3	1.98	0.45
1:D:186:THR:HG21	1:D:210:ARG:HG2	1.98	0.45
1:F:17:VAL:O	1:F:30:VAL:HA	2.16	0.45
1:F:189:LEU:HD13	1:F:257:CYS:SG	2.55	0.45
1:J:73:HIS:HB3	1:J:177:ARG:NH1	2.32	0.45
1:N:162:ASN:O	1:N:175:ILE:HA	2.16	0.45
1:J:303:THR:HG23	1:J:306:TYR:CE2	2.51	0.45
1:K:9:VAL:HG21	1:K:344:SER:HA	1.98	0.45
1:K:71:ILE:HA	1:K:76:ILE:HA	1.99	0.45
1:K:238:LYS:HE3	1:K:238:LYS:HA	1.98	0.45
1:M:7:ALA:HA	1:M:102:PRO:HG2	1.99	0.45
1:M:37:ARG:HG3	1:M:51:ASP:O	2.17	0.45
1:M:153:LEU:HA	1:M:161:HIS:O	2.17	0.45
1:N:62:ARG:HA	1:N:65:LEU:HB3	1.98	0.45
1:N:133:TYR:CE1	1:N:135:ALA:HB2	2.51	0.45
1:A:44:MET:HE3	1:A:64:ILE:HD13	1.97	0.45
1:B:108:ALA:HB3	1:B:111:ASN:HD22	1.81	0.45
1:H:238:LYS:HE3	1:H:238:LYS:HA	1.99	0.45
1:H:263:GLN:HE21	1:H:263:GLN:HA	1.81	0.45
1:J:11:ASP:HA	1:J:106:THR:OG1	2.16	0.45
1:M:11:ASP:O	1:M:17:VAL:HA	2.16	0.45
1:M:65:LEU:HG	1:N:269:MET:HA	1.98	0.45
1:N:324:THR:HB	1:N:325:MET:SD	2.57	0.45
1:B:102:PRO:HD3	1:B:130:PRO:HG2	1.98	0.45
1:B:111:ASN:OD1	1:B:115:ASN:HB3	2.16	0.45
1:B:163:VAL:HG13	1:B:175:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:GLN:HA	1:D:263:GLN:HE21	1.81	0.45
1:D:328:LYS:HZ1	1:D:330:ILE:HG13	1.80	0.45
1:E:62:ARG:HB2	1:E:62:ARG:NH2	2.30	0.45
1:F:227:MET:HB2	1:F:255:PHE:HE1	1.82	0.45
1:A:99:GLU:H	1:A:99:GLU:CD	2.25	0.45
1:C:118:LYS:NZ	1:C:121:GLN:OE1	2.48	0.45
1:D:65:LEU:CG	1:F:287:ILE:HG21	2.47	0.45
1:D:210:ARG:HB3	1:D:210:ARG:CZ	2.46	0.45
1:I:64:ILE:HG13	1:I:65:LEU:HG	1.98	0.45
1:M:135:ALA:HB3	1:M:140:LEU:HD11	1.99	0.45
1:A:105:LEU:O	1:A:134:VAL:HA	2.17	0.45
1:B:154:ASP:O	1:B:160:THR:HA	2.16	0.45
1:L:118:LYS:NZ	1:L:121:GLN:OE1	2.48	0.45
1:N:38:PRO:HB2	1:N:40:HIS:O	2.17	0.45
1:A:11:ASP:O	1:A:17:VAL:HA	2.17	0.45
1:A:305:MET:SD	1:A:336:LYS:HB3	2.57	0.45
1:B:136:ILE:HB	1:B:139:VAL:HG23	1.99	0.45
1:B:200:PHE:O	1:B:206:ARG:HG3	2.16	0.45
1:C:165:ILE:HA	1:C:170:ALA:HA	1.99	0.45
1:D:42:GLY:HA3	1:F:285:CYS:HB2	1.98	0.45
1:F:219:VAL:HG21	1:F:309:ILE:HB	1.98	0.45
1:I:7:ALA:HA	1:I:102:PRO:HG2	1.98	0.45
1:K:105:LEU:O	1:K:134:VAL:HA	2.17	0.45
1:K:240:TYR:O	1:K:248:ILE:HG22	2.16	0.45
1:C:100:GLU:HG2	1:C:101:HIS:CD2	2.52	0.45
1:E:7:ALA:HA	1:E:102:PRO:HG2	1.98	0.45
1:L:180:LEU:HD21	1:L:264:PRO:HB3	1.99	0.45
1:L:198:TYR:OH	1:L:248:ILE:HA	2.17	0.45
1:N:162:ASN:OD1	1:N:176:MET:HB3	2.16	0.45
1:E:9:VAL:O	1:E:19:ALA:HA	2.17	0.45
1:I:294:TYR:O	1:I:327:ILE:HA	2.15	0.45
1:K:99:GLU:H	1:K:99:GLU:CD	2.25	0.45
1:K:243:PRO:HB3	1:M:291:LYS:HE3	1.98	0.45
1:L:262:PHE:O	1:L:275:HIS:HE1	1.99	0.45
1:A:113:LYS:O	1:A:116:ARG:HB3	2.17	0.44
1:A:220:ALA:O	1:A:312:ARG:NH2	2.49	0.44
1:B:101:HIS:HA	1:B:102:PRO:HD2	1.85	0.44
1:D:17:VAL:HG23	1:D:33:SER:OG	2.18	0.44
1:D:47:MET:HA	1:F:167:GLU:CD	2.43	0.44
1:F:153:LEU:HD21	1:F:274:ILE:HG23	1.99	0.44
1:I:8:LEU:HG	1:I:101:HIS:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:193:LEU:O	1:L:196:ARG:HB3	2.17	0.44
1:M:118:LYS:NZ	1:M:121:GLN:OE1	2.48	0.44
1:B:104:LEU:HA	1:B:133:TYR:O	2.17	0.44
1:C:10:CYS:HB3	1:C:105:LEU:HD23	1.99	0.44
1:D:188:TYR:CE2	1:D:257:CYS:HA	2.51	0.44
1:F:59:GLN:O	1:F:62:ARG:HD2	2.17	0.44
1:K:243:PRO:O	1:M:291:LYS:HG2	2.16	0.44
1:M:163:VAL:HG22	1:M:175:ILE:HG23	2.00	0.44
1:M:171:LEU:HA	1:M:172:PRO:HD3	1.71	0.44
1:N:230:ALA:HB1	1:N:252:ASN:HD22	1.82	0.44
1:J:104:LEU:HG	1:J:133:TYR:HB3	1.99	0.44
1:K:243:PRO:HB2	1:M:288:ASP:O	2.17	0.44
1:L:10:CYS:HB3	1:L:105:LEU:HD23	2.00	0.44
1:D:10:CYS:HB3	1:D:105:LEU:HD23	1.99	0.44
1:D:17:VAL:C	1:D:18:LYS:HE3	2.43	0.44
1:D:44:MET:O	1:F:165:ILE:O	2.35	0.44
1:M:147:ARG:NH1	1:M:296:ASN:OD1	2.51	0.44
1:N:321:ALA:HA	1:N:322:PRO:HD2	1.67	0.44
1:B:120:THR:HA	1:B:132:MET:HE3	2.00	0.44
1:C:196:ARG:NH2	1:C:249:THR:OG1	2.51	0.44
1:D:35:VAL:HG22	1:D:54:VAL:HG22	1.98	0.44
1:E:312:ARG:HD2	1:E:315:LYS:HE3	1.99	0.44
1:F:45:VAL:CG1	1:H:167:GLU:HG3	2.47	0.44
1:F:282:ILE:HG22	1:F:283:MET:N	2.33	0.44
1:M:162:ASN:HB2	1:M:176:MET:HB3	1.97	0.44
1:A:193:LEU:HB3	1:A:200:PHE:HE1	1.82	0.44
1:D:37:ARG:HA	1:D:38:PRO:HD2	1.80	0.44
1:D:63:GLY:H	1:E:267:ILE:HA	1.82	0.44
1:E:38:PRO:HD2	1:E:51:ASP:O	2.17	0.44
1:H:212:ILE:HG23	1:H:216:LEU:HD12	1.99	0.44
1:K:186:THR:HG21	1:K:210:ARG:HG2	2.00	0.44
1:L:111:ASN:OD1	1:L:115:ASN:HB3	2.18	0.44
1:A:244:ASP:HA	1:C:323:SER:HB2	1.99	0.44
1:D:44:MET:SD	1:D:45:VAL:HG23	2.58	0.44
1:F:219:VAL:HG22	1:F:258:PRO:CB	2.47	0.44
1:I:194:THR:HG22	1:I:198:TYR:O	2.18	0.44
1:J:219:VAL:HG22	1:J:258:PRO:CB	2.48	0.44
1:A:154:ASP:O	1:A:160:THR:HA	2.18	0.44
1:B:135:ALA:HB3	1:B:140:LEU:HD11	1.98	0.44
1:C:163:VAL:HG13	1:C:175:ILE:HG12	2.00	0.44
1:C:366:GLY:O	1:C:369:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:ILE:HD12	1:E:287:ILE:N	2.30	0.44
1:F:103:THR:O	1:F:132:MET:HA	2.18	0.44
1:G:105:LEU:HD11	1:G:123:MET:HE2	1.99	0.44
1:H:53:TYR:CD1	1:H:65:LEU:HD21	2.53	0.44
1:J:112:PRO:HG2	1:J:116:ARG:HB2	2.00	0.44
1:L:217:CYS:O	1:L:307:PRO:HD2	2.18	0.44
1:A:191:LYS:HZ3	1:A:195:GLU:CD	2.25	0.44
1:B:10:CYS:HA	1:B:18:LYS:O	2.18	0.44
1:B:176:MET:HE2	1:B:277:THR:HG23	2.00	0.44
1:D:49:GLN:HA	1:F:166:TYR:CE2	2.53	0.44
1:D:147:ARG:CZ	1:D:330:ILE:HG12	2.48	0.44
1:D:202:THR:H	1:D:205:GLU:HB2	1.82	0.44
1:D:230:ALA:HB1	1:D:252:ASN:HB3	1.99	0.44
1:E:219:VAL:HG22	1:E:258:PRO:HB2	1.99	0.44
1:F:45:VAL:CB	1:H:166:TYR:HE1	2.26	0.44
1:F:50:LYS:NZ	1:F:52:SER:O	2.49	0.44
1:H:155:SER:HB3	1:H:304:THR:HG23	1.99	0.44
1:K:193:LEU:O	1:K:196:ARG:HB3	2.17	0.44
1:C:359:LYS:HD2	1:C:360:GLN:N	2.33	0.43
1:D:171:LEU:HA	1:D:172:PRO:HD2	1.83	0.43
1:H:262:PHE:HE2	1:H:309:ILE:HG13	1.82	0.43
1:I:45:VAL:HB	1:K:168:GLY:HA3	2.00	0.43
1:K:256:ARG:HD3	1:L:113:LYS:NZ	2.33	0.43
1:N:86:TRP:CH2	1:N:119:MET:HG3	2.53	0.43
1:N:124:PHE:HE1	1:N:359:LYS:HA	1.83	0.43
1:B:132:MET:HB2	1:B:132:MET:HE2	1.89	0.43
1:H:7:ALA:HA	1:H:102:PRO:HG2	2.00	0.43
1:H:9:VAL:HG13	1:H:104:LEU:HD22	2.00	0.43
1:H:53:TYR:HD1	1:H:65:LEU:HD21	1.83	0.43
1:H:118:LYS:NZ	1:H:121:GLN:OE1	2.49	0.43
1:K:189:LEU:HD12	1:K:192:ILE:HG13	2.00	0.43
1:K:220:ALA:O	1:K:312:ARG:HD3	2.18	0.43
1:L:105:LEU:O	1:L:134:VAL:HA	2.17	0.43
1:M:359:LYS:HD2	1:M:360:GLN:H	1.83	0.43
1:B:9:VAL:HG21	1:B:344:SER:HA	2.00	0.43
1:B:86:TRP:HH2	1:B:119:MET:HG2	1.82	0.43
1:D:163:VAL:HA	1:D:175:ILE:HG12	2.00	0.43
1:F:73:HIS:HB3	1:F:177:ARG:NH1	2.33	0.43
1:J:22:ALA:HB2	1:J:347:ALA:HB3	1.99	0.43
1:B:119:MET:O	1:B:123:MET:HG2	2.17	0.43
1:D:318:THR:HA	1:D:327:ILE:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:GLN:HA	1:E:49:GLN:OE1	2.19	0.43
1:E:206:ARG:HD2	1:F:271:SER:C	2.42	0.43
1:H:282:ILE:HG22	1:H:290:ARG:HG2	2.00	0.43
1:I:11:ASP:OD1	1:I:18:LYS:NZ	2.51	0.43
1:K:306:TYR:HA	1:K:307:PRO:HD3	1.86	0.43
1:L:74:GLY:O	1:L:108:ALA:HB2	2.18	0.43
1:N:290:ARG:HH11	1:N:290:ARG:HD3	1.67	0.43
1:D:194:THR:HA	1:D:197:GLY:O	2.18	0.43
1:G:164:PRO:HG3	1:G:174:ALA:HB3	2.01	0.43
1:I:11:ASP:HA	1:I:106:THR:OG1	2.18	0.43
1:K:62:ARG:HG2	1:L:270:GLU:HB2	2.00	0.43
1:L:39:ARG:CZ	1:M:272:ALA:HA	2.48	0.43
1:L:248:ILE:HG23	1:L:250:ILE:HG12	1.99	0.43
1:N:101:HIS:HA	1:N:102:PRO:HD2	1.81	0.43
1:C:238:LYS:HE3	1:C:238:LYS:HA	1.99	0.43
1:I:104:LEU:HG	1:I:133:TYR:HB3	2.00	0.43
1:N:299:MET:HG3	1:N:329:ILE:HG21	2.00	0.43
1:C:170:ALA:O	1:C:172:PRO:HD3	2.19	0.43
1:C:210:ARG:CZ	1:C:210:ARG:HB3	2.48	0.43
1:F:116:ARG:HE	1:F:371:HIS:HA	1.83	0.43
1:G:198:TYR:CZ	1:G:248:ILE:HA	2.54	0.43
1:I:44:MET:HE3	1:K:167:GLU:HB2	2.00	0.43
1:J:165:ILE:HA	1:J:169:TYR:O	2.19	0.43
1:L:44:MET:HB2	1:L:47:MET:HB2	2.01	0.43
1:B:111:ASN:HA	1:B:112:PRO:HD3	1.83	0.43
1:B:186:THR:HG21	1:B:210:ARG:HG2	2.01	0.43
1:B:210:ARG:O	1:B:213:LYS:HB3	2.19	0.43
1:D:57:GLU:HB3	1:F:288:ASP:OD1	2.18	0.43
1:F:239:SER:HA	1:F:248:ILE:O	2.18	0.43
1:F:306:TYR:HA	1:F:307:PRO:HD3	1.90	0.43
1:G:13:GLY:O	1:G:15:GLY:N	2.50	0.43
1:G:111:ASN:HA	1:G:112:PRO:HD3	1.86	0.43
1:G:193:LEU:O	1:G:198:TYR:HB2	2.18	0.43
1:G:357:ILE:HG21	1:G:370:VAL:HG22	2.00	0.43
1:M:357:ILE:CD1	1:M:373:LYS:HD2	2.48	0.43
1:D:42:GLY:HA2	1:F:171:LEU:HD11	2.01	0.43
1:D:199:SER:HB3	1:E:75:ILE:HG12	2.00	0.43
1:E:17:VAL:O	1:E:30:VAL:HA	2.18	0.43
1:E:196:ARG:O	1:F:177:ARG:NH2	2.52	0.43
1:G:172:PRO:HA	1:G:175:ILE:HD12	1.99	0.43
1:M:100:GLU:HG3	1:M:101:HIS:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:212:ILE:HG23	1:M:216:LEU:HD12	2.01	0.43
1:N:147:ARG:CZ	1:N:330:ILE:HG12	2.48	0.43
1:B:107:GLU:CD	1:B:116:ARG:NH1	2.77	0.43
1:B:108:ALA:HA	1:B:109:PRO:HD3	1.91	0.43
1:B:290:ARG:HA	1:B:293:LEU:HB2	2.00	0.43
1:D:202:THR:HA	1:E:179:ASP:OD1	2.19	0.43
1:M:58:ALA:HB1	1:M:65:LEU:HD11	2.01	0.43
1:N:151:ILE:O	1:N:297:ASN:HA	2.19	0.43
1:A:53:TYR:CD1	1:A:65:LEU:HD21	2.54	0.42
1:A:61:LYS:O	1:A:63:GLY:HA3	2.19	0.42
1:B:262:PHE:O	1:B:275:HIS:HE1	2.02	0.42
1:C:194:THR:HG22	1:C:198:TYR:O	2.19	0.42
1:D:71:ILE:HA	1:D:76:ILE:HA	2.01	0.42
1:D:189:LEU:HD13	1:D:257:CYS:SG	2.59	0.42
1:F:220:ALA:HB1	1:F:222:ASP:O	2.19	0.42
1:G:104:LEU:HA	1:G:133:TYR:O	2.19	0.42
1:I:99:GLU:HA	1:I:129:VAL:HA	2.01	0.42
1:I:196:ARG:HH22	1:I:237:GLU:CD	2.27	0.42
1:K:118:LYS:NZ	1:K:121:GLN:OE1	2.49	0.42
1:K:285:CYS:HB3	1:K:289:ILE:HD11	2.00	0.42
1:M:252:ASN:ND2	1:M:252:ASN:H	2.17	0.42
1:N:269:MET:SD	1:N:269:MET:N	2.92	0.42
1:A:278:THR:HG21	1:A:297:ASN:OD1	2.18	0.42
1:B:136:ILE:H	1:B:136:ILE:HD12	1.83	0.42
1:B:357:ILE:HD13	1:B:373:LYS:HD3	2.01	0.42
1:E:305:MET:HA	1:E:335:ARG:NH1	2.34	0.42
1:G:262:PHE:O	1:G:275:HIS:HE1	2.02	0.42
1:K:195:GLU:HG2	1:L:112:PRO:HG3	2.00	0.42
1:N:113:LYS:O	1:N:116:ARG:HB3	2.19	0.42
1:A:190:MET:HB2	1:A:209:VAL:HG11	2.01	0.42
1:A:217:CYS:SG	1:A:257:CYS:SG	3.15	0.42
1:C:149:THR:HA	1:C:165:ILE:O	2.19	0.42
1:E:10:CYS:HA	1:E:18:LYS:O	2.19	0.42
1:F:45:VAL:CG1	1:H:167:GLU:CG	2.93	0.42
1:K:262:PHE:O	1:K:275:HIS:HE1	2.01	0.42
1:L:163:VAL:HG22	1:L:175:ILE:HG23	2.01	0.42
1:L:283:MET:SD	1:L:290:ARG:NH2	2.92	0.42
1:M:189:LEU:HD13	1:M:257:CYS:SG	2.59	0.42
1:A:36:GLY:CA	1:A:66:THR:O	2.67	0.42
1:B:31:PHE:HA	1:B:32:PRO:HD2	1.87	0.42
1:D:107:GLU:CD	1:D:116:ARG:HH11	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:LYS:HZ2	1:D:292:ASP:CG	2.28	0.42
1:G:11:ASP:HA	1:G:106:THR:OG1	2.19	0.42
1:J:147:ARG:NH1	1:J:296:ASN:OD1	2.53	0.42
1:K:299:MET:HE2	1:K:329:ILE:HG21	2.01	0.42
1:A:50:LYS:HD3	1:A:53:TYR:CZ	2.54	0.42
1:G:294:TYR:O	1:G:327:ILE:HA	2.19	0.42
1:J:32:PRO:HB2	1:J:34:ILE:HG12	2.01	0.42
1:J:61:LYS:O	1:J:65:LEU:HG	2.20	0.42
1:M:290:ARG:HA	1:M:293:LEU:HB2	2.01	0.42
1:B:111:ASN:HD21	1:B:115:ASN:ND2	2.18	0.42
1:D:59:GLN:O	1:D:62:ARG:HD2	2.19	0.42
1:D:236:LEU:O	1:D:251:GLY:HA2	2.20	0.42
1:E:147:ARG:NH1	1:E:296:ASN:OD1	2.52	0.42
1:E:180:LEU:HG	1:E:264:PRO:HB3	2.02	0.42
1:I:186:THR:O	1:I:189:LEU:HB3	2.20	0.42
1:K:36:GLY:HA3	1:K:65:LEU:HD13	2.02	0.42
1:L:286:ASP:O	1:L:290:ARG:NH1	2.53	0.42
1:C:154:ASP:O	1:C:160:THR:HA	2.20	0.42
1:E:313:MET:O	1:E:317:ILE:HG12	2.20	0.42
1:J:217:CYS:HA	1:J:254:ARG:O	2.20	0.42
1:L:103:THR:H	1:L:132:MET:HA	1.84	0.42
1:M:10:CYS:HA	1:M:18:LYS:O	2.20	0.42
1:N:163:VAL:HG22	1:N:175:ILE:HG23	2.02	0.42
1:A:11:ASP:HA	1:A:106:THR:OG1	2.19	0.42
1:A:161:HIS:HA	1:A:176:MET:O	2.19	0.42
1:B:11:ASP:HA	1:B:106:THR:OG1	2.19	0.42
1:D:46:GLY:O	1:F:167:GLU:OE2	2.38	0.42
1:D:164:PRO:HG2	1:D:171:LEU:HB3	2.02	0.42
1:E:197:GLY:HA2	1:F:177:ARG:NH1	2.34	0.42
1:E:306:TYR:HA	1:E:307:PRO:HD3	1.92	0.42
1:F:45:VAL:CG2	1:H:166:TYR:HD1	2.16	0.42
1:F:219:VAL:HG22	1:F:258:PRO:HB3	2.02	0.42
1:G:11:ASP:HB3	1:G:18:LYS:HD2	2.01	0.42
1:H:204:ALA:HB3	1:J:287:ILE:HB	2.01	0.42
1:I:142:LEU:HD22	1:I:165:ILE:HB	2.02	0.42
1:J:9:VAL:HA	1:J:104:LEU:O	2.20	0.42
1:J:328:LYS:HB3	1:J:328:LYS:HE3	1.83	0.42
1:K:107:GLU:CD	1:K:116:ARG:HH11	2.27	0.42
1:N:304:THR:O	1:N:309:ILE:HG21	2.19	0.42
1:A:102:PRO:HA	1:A:131:ALA:O	2.19	0.42
1:A:305:MET:HA	1:A:335:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:VAL:O	1:B:374:CYS:SG	2.78	0.42
1:B:162:ASN:OD1	1:B:277:THR:HG22	2.20	0.42
1:C:101:HIS:O	1:C:130:PRO:HD2	2.20	0.42
1:D:44:MET:SD	1:F:293:LEU:HD22	2.52	0.42
1:E:291:LYS:HZ2	1:E:292:ASP:CG	2.26	0.42
1:F:102:PRO:HA	1:F:131:ALA:O	2.20	0.42
1:F:289:ILE:O	1:F:291:LYS:HD3	2.20	0.42
1:H:135:ALA:HB3	1:H:140:LEU:HD11	2.02	0.42
1:L:138:ALA:HB2	1:L:163:VAL:HG21	2.02	0.42
1:A:39:ARG:NH1	1:B:267:ILE:HG22	2.34	0.42
1:D:43:VAL:HG22	1:F:171:LEU:CB	2.50	0.42
1:I:187:ASP:O	1:I:190:MET:HB3	2.20	0.42
1:I:213:LYS:HA	1:I:217:CYS:SG	2.59	0.42
1:K:299:MET:HB3	1:K:304:THR:HG21	2.00	0.42
1:L:86:TRP:CH2	1:L:119:MET:HG3	2.55	0.42
1:N:11:ASP:HA	1:N:106:THR:OG1	2.19	0.42
1:A:162:ASN:O	1:A:175:ILE:HA	2.19	0.41
1:B:290:ARG:HA	1:B:293:LEU:HD12	2.02	0.41
1:C:70:PRO:HB3	1:C:81:ASP:HB2	2.02	0.41
1:D:61:LYS:HZ1	1:F:291:LYS:CG	2.32	0.41
1:F:318:THR:HA	1:F:327:ILE:HD13	2.02	0.41
1:J:304:THR:O	1:J:309:ILE:HG21	2.19	0.41
1:K:230:ALA:HB1	1:K:252:ASN:HD22	1.84	0.41
1:N:62:ARG:HH22	1:N:207:GLU:CD	2.27	0.41
1:A:36:GLY:O	1:A:52:SER:HA	2.20	0.41
1:A:98:PRO:HG2	1:A:128:ASN:HD21	1.85	0.41
1:C:213:LYS:O	1:C:217:CYS:HB2	2.20	0.41
1:F:8:LEU:HG	1:F:101:HIS:HB3	2.02	0.41
1:G:153:LEU:HD21	1:G:274:ILE:HD12	2.02	0.41
1:I:285:CYS:HB3	1:I:289:ILE:HD11	2.01	0.41
1:J:107:GLU:OE1	1:J:112:PRO:HG3	2.21	0.41
1:K:264:PRO:HD2	1:K:271:SER:O	2.20	0.41
1:N:153:LEU:HD21	1:N:274:ILE:HG23	2.02	0.41
1:D:189:LEU:HD12	1:D:192:ILE:HD11	2.02	0.41
1:D:196:ARG:HA	1:E:113:LYS:HD2	2.02	0.41
1:G:4:GLU:HG2	1:G:5:THR:HG23	2.02	0.41
1:I:171:LEU:HA	1:I:172:PRO:HD2	1.93	0.41
1:M:186:THR:OG1	1:M:213:LYS:HD2	2.19	0.41
1:N:322:PRO:O	1:N:327:ILE:HD11	2.20	0.41
1:D:17:VAL:O	1:D:30:VAL:HA	2.21	0.41
1:D:45:VAL:HG11	1:F:165:ILE:CD1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:GLU:CD	1:E:99:GLU:H	2.28	0.41
1:F:274:ILE:HG22	1:F:313:MET:SD	2.60	0.41
1:G:39:ARG:HD3	1:G:66:THR:HG23	2.01	0.41
1:J:306:TYR:HA	1:J:307:PRO:HD3	1.96	0.41
1:L:242:LEU:H	1:L:245:GLY:HA3	1.84	0.41
1:F:160:THR:O	1:F:177:ARG:HA	2.21	0.41
1:H:180:LEU:HD11	1:H:264:PRO:HB3	2.03	0.41
1:I:264:PRO:HB2	1:I:271:SER:HB3	2.03	0.41
1:J:10:CYS:HA	1:J:19:ALA:HA	2.01	0.41
1:B:9:VAL:O	1:B:19:ALA:HA	2.20	0.41
1:B:116:ARG:HH12	1:B:375:PHE:HD2	1.68	0.41
1:C:34:ILE:O	1:C:54:VAL:HA	2.21	0.41
1:D:190:MET:HB2	1:D:209:VAL:HG11	2.03	0.41
1:F:11:ASP:OD1	1:F:18:LYS:NZ	2.51	0.41
1:F:269:MET:O	1:F:270:GLU:HB2	2.21	0.41
1:G:237:GLU:O	1:G:238:LYS:NZ	2.51	0.41
1:H:163:VAL:HA	1:H:175:ILE:HG12	2.02	0.41
1:H:239:SER:HA	1:H:248:ILE:O	2.21	0.41
1:K:98:PRO:O	1:K:129:VAL:HA	2.21	0.41
1:L:253:GLU:HG3	1:L:256:ARG:HH21	1.85	0.41
1:M:160:THR:OG1	1:M:181:ALA:HB2	2.20	0.41
1:N:71:ILE:HG23	1:N:76:ILE:HG12	2.01	0.41
1:N:274:ILE:HG22	1:N:313:MET:SD	2.61	0.41
1:N:362:TYR:OH	1:N:367:PRO:HG3	2.21	0.41
1:A:38:PRO:HB2	1:A:40:HIS:O	2.21	0.41
1:B:113:LYS:O	1:B:116:ARG:HB3	2.21	0.41
1:B:203:THR:HG21	1:C:268:GLY:O	2.20	0.41
1:D:10:CYS:HA	1:D:18:LYS:O	2.20	0.41
1:D:359:LYS:NZ	1:D:360:GLN:OE1	2.54	0.41
1:E:62:ARG:NH2	1:F:266:PHE:O	2.52	0.41
1:E:190:MET:CA	1:E:209:VAL:HG11	2.51	0.41
1:F:11:ASP:O	1:F:17:VAL:HA	2.21	0.41
1:H:101:HIS:O	1:H:130:PRO:HD2	2.20	0.41
1:J:152:VAL:O	1:J:162:ASN:HA	2.19	0.41
1:K:190:MET:HA	1:K:209:VAL:HG11	2.02	0.41
1:A:200:PHE:HA	1:A:205:GLU:HB3	2.03	0.41
1:B:8:LEU:HG	1:B:101:HIS:HB3	2.03	0.41
1:B:10:CYS:HB3	1:B:105:LEU:HD23	2.01	0.41
1:E:101:HIS:HA	1:E:102:PRO:HD2	1.96	0.41
1:N:113:LYS:HB2	1:N:113:LYS:HE3	1.94	0.41
1:B:289:ILE:HA	1:B:292:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:ASN:OD1	1:E:277:THR:HG23	2.21	0.41
1:E:191:LYS:HD2	1:F:176:MET:HG2	2.02	0.41
1:F:213:LYS:HD3	1:F:214:GLU:HG3	2.02	0.41
1:G:17:VAL:O	1:G:30:VAL:HA	2.20	0.41
1:G:196:ARG:HE	1:G:249:THR:HG23	1.86	0.41
1:G:287:ILE:HA	1:G:290:ARG:HG3	2.03	0.41
1:H:149:THR:HA	1:H:165:ILE:O	2.21	0.41
1:H:189:LEU:HD12	1:H:192:ILE:HD11	2.03	0.41
1:I:201:VAL:HG21	1:J:179:ASP:OD2	2.21	0.41
1:J:202:THR:HG21	1:L:285:CYS:HA	2.03	0.41
1:M:99:GLU:H	1:M:99:GLU:CD	2.28	0.41
1:M:359:LYS:HD2	1:M:360:GLN:HB2	2.02	0.41
1:N:304:THR:HA	1:N:309:ILE:HD13	2.02	0.41
1:A:186:THR:O	1:A:189:LEU:HB3	2.21	0.41
1:A:281:SER:HA	1:A:284:LYS:NZ	2.36	0.41
1:C:101:HIS:HA	1:C:102:PRO:HD2	1.86	0.41
1:C:305:MET:SD	1:C:336:LYS:HB3	2.61	0.41
1:D:39:ARG:NH2	1:E:271:SER:O	2.54	0.41
1:E:162:ASN:O	1:E:175:ILE:HA	2.20	0.41
1:E:218:TYR:O	1:E:255:PHE:HA	2.21	0.41
1:E:219:VAL:HG22	1:E:258:PRO:CB	2.51	0.41
1:F:46:GLY:N	1:H:167:GLU:HB3	2.32	0.41
1:G:159:VAL:HA	1:G:178:LEU:O	2.20	0.41
1:I:17:VAL:O	1:I:30:VAL:HA	2.21	0.41
1:N:118:LYS:NZ	1:N:121:GLN:OE1	2.48	0.41
1:A:188:TYR:CE2	1:A:257:CYS:HA	2.56	0.40
1:C:304:THR:HA	1:C:309:ILE:HD13	2.03	0.40
1:D:45:VAL:CA	1:F:165:ILE:H	2.34	0.40
1:F:108:ALA:O	1:F:111:ASN:HB2	2.21	0.40
1:G:38:PRO:HD2	1:G:51:ASP:O	2.21	0.40
1:I:9:VAL:O	1:I:19:ALA:HA	2.22	0.40
1:I:210:ARG:O	1:I:213:LYS:HB3	2.21	0.40
1:J:248:ILE:HD12	1:J:248:ILE:HA	1.97	0.40
1:K:155:SER:HA	1:K:160:THR:HA	2.03	0.40
1:L:34:ILE:O	1:L:54:VAL:HA	2.22	0.40
1:M:291:LYS:HG3	1:M:292:ASP:H	1.85	0.40
1:N:294:TYR:O	1:N:327:ILE:HA	2.21	0.40
1:A:112:PRO:O	1:A:115:ASN:HB3	2.21	0.40
1:A:137:GLN:HG2	1:A:339:VAL:CG1	2.48	0.40
1:B:32:PRO:HB2	1:B:34:ILE:HG12	2.03	0.40
1:D:9:VAL:O	1:D:19:ALA:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:CYS:HA	1:D:254:ARG:O	2.21	0.40
1:J:108:ALA:O	1:J:111:ASN:HB2	2.22	0.40
1:M:53:TYR:HB2	1:N:268:GLY:HA2	2.03	0.40
1:N:14:SER:O	1:N:183:ARG:NH2	2.53	0.40
1:N:79:TRP:HA	1:N:82:MET:HB2	2.02	0.40
1:A:44:MET:SD	1:C:166:TYR:HD1	2.45	0.40
1:B:99:GLU:C	1:B:130:PRO:HD3	2.47	0.40
1:B:190:MET:HA	1:B:209:VAL:HG11	2.04	0.40
1:C:8:LEU:HA	1:C:20:GLY:O	2.22	0.40
1:F:100:GLU:HG3	1:F:101:HIS:CD2	2.55	0.40
1:I:11:ASP:HB3	1:I:18:LYS:HB2	2.03	0.40
1:J:17:VAL:C	1:J:18:LYS:HE3	2.46	0.40
1:M:10:CYS:HB3	1:M:105:LEU:HD23	2.04	0.40
1:M:299:MET:HE2	1:M:329:ILE:HG21	2.03	0.40
1:C:99:GLU:C	1:C:130:PRO:HD3	2.47	0.40
1:E:161:HIS:HA	1:E:176:MET:O	2.20	0.40
1:F:284:LYS:C	1:F:285:CYS:SG	3.05	0.40
1:I:155:SER:HB3	1:I:304:THR:HG23	2.03	0.40
1:L:50:LYS:NZ	1:L:52:SER:O	2.51	0.40
1:L:99:GLU:CD	1:L:99:GLU:H	2.30	0.40
1:M:33:SER:O	1:M:34:ILE:HG23	2.22	0.40
1:C:243:PRO:O	1:E:291:LYS:HB3	2.21	0.40
1:D:46:GLY:HA2	1:F:149:THR:HA	2.04	0.40
1:D:182:GLY:O	1:D:213:LYS:NZ	2.50	0.40
1:D:198:TYR:CE2	1:D:248:ILE:HG23	2.57	0.40
1:D:202:THR:N	1:D:205:GLU:HB2	2.37	0.40
1:F:101:HIS:HA	1:F:102:PRO:HD2	1.85	0.40
1:H:10:CYS:HA	1:H:18:LYS:O	2.22	0.40
1:H:19:ALA:HB3	1:H:29:ALA:HB3	2.04	0.40
1:H:31:PHE:HA	1:H:32:PRO:HD2	1.92	0.40
1:I:132:MET:HG3	1:I:357:ILE:HB	2.03	0.40
1:K:151:ILE:O	1:K:297:ASN:HA	2.22	0.40
1:K:171:LEU:O	1:K:175:ILE:HG13	2.22	0.40
1:K:332:PRO:HB2	1:K:335:ARG:HB3	2.03	0.40
1:L:38:PRO:HD2	1:L:51:ASP:O	2.21	0.40
1:L:193:LEU:HD21	1:L:212:ILE:HD13	2.03	0.40
1:M:75:ILE:HG23	1:M:111:ASN:ND2	2.36	0.40
1:M:279:TYR:O	1:M:283:MET:HB2	2.21	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	373/377 (99%)	297 (80%)	63 (17%)	13 (4%)	3	20
1	B	373/377 (99%)	298 (80%)	58 (16%)	17 (5%)	2	17
1	C	373/377 (99%)	310 (83%)	55 (15%)	8 (2%)	5	30
1	D	373/377 (99%)	310 (83%)	49 (13%)	14 (4%)	2	19
1	E	373/377 (99%)	303 (81%)	56 (15%)	14 (4%)	2	19
1	F	373/377 (99%)	291 (78%)	62 (17%)	20 (5%)	1	15
1	G	373/377 (99%)	315 (84%)	46 (12%)	12 (3%)	3	21
1	H	373/377 (99%)	308 (83%)	55 (15%)	10 (3%)	4	25
1	I	373/377 (99%)	318 (85%)	45 (12%)	10 (3%)	4	25
1	J	373/377 (99%)	308 (83%)	48 (13%)	17 (5%)	2	17
1	K	373/377 (99%)	323 (87%)	33 (9%)	17 (5%)	2	17
1	L	373/377 (99%)	311 (83%)	44 (12%)	18 (5%)	2	16
1	M	373/377 (99%)	300 (80%)	54 (14%)	19 (5%)	1	15
1	N	373/377 (99%)	307 (82%)	51 (14%)	15 (4%)	2	18
All	All	5222/5278 (99%)	4299 (82%)	719 (14%)	204 (4%)	4	19

All (204) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	236	LEU
1	A	252	ASN
1	A	272	ALA
1	B	113	LYS
1	B	323	SER
1	C	236	LEU
1	D	49	GLN
1	D	61	LYS

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Mol	Chain	Res	Type
1	D	236	LEU
1	D	323	SER
1	E	111	ASN
1	E	128	ASN
1	E	222	ASP
1	E	263	GLN
1	E	266	PHE
1	E	359	LYS
1	F	14	SER
1	F	173	HIS
1	F	254	ARG
1	F	265	SER
1	F	270	GLU
1	F	282	ILE
1	F	289	ILE
1	G	14	SER
1	G	222	ASP
1	H	62	ARG
1	H	236	LEU
1	I	236	LEU
1	J	112	PRO
1	J	137	GLN
1	J	175	ILE
1	J	242	LEU
1	J	335	ARG
1	K	234	SER
1	K	267	ILE
1	K	270	GLU
1	K	350	SER
1	L	236	LEU
1	L	325	MET
1	M	2	GLU
1	M	37	ARG
1	M	173	HIS
1	M	236	LEU
1	M	263	GLN
1	N	47	MET
1	N	322	PRO
1	A	55	GLY
1	A	61	LYS
1	A	181	ALA
1	B	2	GLU

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Mol	Chain	Res	Type
1	B	4	GLU
1	B	14	SER
1	B	45	VAL
1	B	199	SER
1	B	252	ASN
1	B	254	ARG
1	C	181	ALA
1	D	69	TYR
1	D	113	LYS
1	D	267	ILE
1	D	335	ARG
1	E	14	SER
1	F	4	GLU
1	F	266	PHE
1	F	290	ARG
1	G	113	LYS
1	G	236	LEU
1	H	2	GLU
1	H	323	SER
1	I	253	GLU
1	J	14	SER
1	J	359	LYS
1	K	266	PHE
1	K	323	SER
1	K	335	ARG
1	L	62	ARG
1	L	204	ALA
1	L	291	LYS
1	L	359	LYS
1	M	41	GLN
1	M	67	LEU
1	M	68	LYS
1	M	323	SER
1	M	359	LYS
1	N	14	SER
1	N	128	ASN
1	N	267	ILE
1	A	2	GLU
1	A	335	ARG
1	A	374	CYS
1	B	181	ALA
1	C	204	ALA

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Mol	Chain	Res	Type
1	D	15	GLY
1	D	60	SER
1	E	73	HIS
1	E	157	ASP
1	F	44	MET
1	F	222	ASP
1	F	234	SER
1	F	359	LYS
1	G	359	LYS
1	H	181	ALA
1	H	359	LYS
1	I	2	GLU
1	I	335	ARG
1	J	272	ALA
1	K	181	ALA
1	K	236	LEU
1	K	359	LYS
1	L	2	GLU
1	L	49	GLN
1	L	112	PRO
1	L	222	ASP
1	L	254	ARG
1	L	286	ASP
1	M	270	GLU
1	M	283	MET
1	M	335	ARG
1	N	2	GLU
1	N	62	ARG
1	N	175	ILE
1	B	359	LYS
1	D	359	LYS
1	E	335	ARG
1	F	283	MET
1	F	285	CYS
1	G	2	GLU
1	G	4	GLU
1	G	181	ALA
1	G	242	LEU
1	H	14	SER
1	H	335	ARG
1	H	374	CYS
1	I	222	ASP

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Mol	Chain	Res	Type
1	J	234	SER
1	J	274	ILE
1	K	63	GLY
1	K	222	ASP
1	K	233	SER
1	K	243	PRO
1	L	15	GLY
1	L	181	ALA
1	L	246	GLN
1	M	242	LEU
1	N	181	ALA
1	N	222	ASP
1	N	251	GLY
1	N	270	GLU
1	A	222	ASP
1	B	234	SER
1	B	274	ILE
1	B	373	LYS
1	C	14	SER
1	C	274	ILE
1	C	335	ARG
1	D	253	GLU
1	E	62	ARG
1	F	264	PRO
1	G	253	GLU
1	H	274	ILE
1	I	14	SER
1	J	15	GLY
1	J	171	LEU
1	J	244	ASP
1	K	251	GLY
1	L	263	GLN
1	M	38	PRO
1	M	181	ALA
1	N	234	SER
1	A	372	ARG
1	B	222	ASP
1	C	62	ARG
1	D	181	ALA
1	E	171	LEU
1	F	109	PRO
1	F	251	GLY

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Mol	Chain	Res	Type
1	I	181	ALA
1	I	242	LEU
1	J	136	ILE
1	J	374	CYS
1	K	274	ILE
1	M	159	VAL
1	M	171	LEU
1	B	339	VAL
1	E	15	GLY
1	K	175	ILE
1	L	251	GLY
1	A	242	LEU
1	D	175	ILE
1	F	274	ILE
1	I	159	VAL
1	L	243	PRO
1	M	175	ILE
1	G	251	GLY
1	I	251	GLY
1	J	111	ASN
1	B	159	VAL
1	C	175	ILE
1	G	274	ILE
1	J	71	ILE
1	N	43	VAL
1	N	159	VAL
1	E	267	ILE

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	318/320 (99%)	282 (89%)	36 (11%)	5	19
1	B	318/320 (99%)	284 (89%)	34 (11%)	6	21
1	C	318/320 (99%)	279 (88%)	39 (12%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	318/320 (99%)	282 (89%)	36 (11%)	5	19
1	E	318/320 (99%)	287 (90%)	31 (10%)	8	24
1	F	318/320 (99%)	288 (91%)	30 (9%)	8	26
1	G	318/320 (99%)	290 (91%)	28 (9%)	9	28
1	H	318/320 (99%)	289 (91%)	29 (9%)	9	27
1	I	318/320 (99%)	288 (91%)	30 (9%)	8	26
1	J	318/320 (99%)	271 (85%)	47 (15%)	3	13
1	K	318/320 (99%)	286 (90%)	32 (10%)	7	23
1	L	318/320 (99%)	288 (91%)	30 (9%)	8	26
1	M	318/320 (99%)	280 (88%)	38 (12%)	5	18
1	N	318/320 (99%)	276 (87%)	42 (13%)	4	15
All	All	4452/4480 (99%)	3970 (89%)	482 (11%)	8	21

All (482) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	18	LYS
1	A	57	GLU
1	A	60	SER
1	A	61	LYS
1	A	66	THR
1	A	99	GLU
1	A	109	PRO
1	A	112	PRO
1	A	115	ASN
1	A	126	THR
1	A	128	ASN
1	A	132	MET
1	A	159	VAL
1	A	195	GLU
1	A	207	GLU
1	A	210	ARG
1	A	221	LEU
1	A	238	LYS
1	A	249	THR
1	A	252	ASN
1	A	263	GLN

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Mol	Chain	Res	Type
1	A	266	PHE
1	A	270	GLU
1	A	275	HIS
1	A	277	THR
1	A	280	ASN
1	A	284	LYS
1	A	287	ILE
1	A	288	ASP
1	A	292	ASP
1	A	297	ASN
1	A	303	THR
1	A	316	GLU
1	A	334	GLU
1	A	359	LYS
1	B	18	LYS
1	B	62	ARG
1	B	66	THR
1	B	99	GLU
1	B	100	GLU
1	B	107	GLU
1	B	109	PRO
1	B	113	LYS
1	B	115	ASN
1	B	128	ASN
1	B	159	VAL
1	B	166	TYR
1	B	195	GLU
1	B	207	GLU
1	B	218	TYR
1	B	219	VAL
1	B	221	LEU
1	B	238	LYS
1	B	249	THR
1	B	252	ASN
1	B	261	LEU
1	B	263	GLN
1	B	284	LYS
1	B	285	CYS
1	B	288	ASP
1	B	291	LYS
1	B	293	LEU
1	B	297	ASN

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Mol	Chain	Res	Type
1	B	303	THR
1	B	311	ASP
1	B	316	GLU
1	B	324	THR
1	B	334	GLU
1	B	359	LYS
1	C	2	GLU
1	C	18	LYS
1	C	51	ASP
1	C	77	THR
1	C	99	GLU
1	C	100	GLU
1	C	109	PRO
1	C	115	ASN
1	C	126	THR
1	C	128	ASN
1	C	149	THR
1	C	159	VAL
1	C	167	GLU
1	C	172	PRO
1	C	173	HIS
1	C	176	MET
1	C	180	LEU
1	C	206	ARG
1	C	207	GLU
1	C	221	LEU
1	C	238	LYS
1	C	241	GLU
1	C	244	ASP
1	C	249	THR
1	C	252	ASN
1	C	256	ARG
1	C	263	GLN
1	C	265	SER
1	C	277	THR
1	C	278	THR
1	C	284	LYS
1	C	287	ILE
1	C	291	LYS
1	C	292	ASP
1	C	297	ASN
1	C	303	THR

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Mol	Chain	Res	Type
1	C	334	GLU
1	C	348	SER
1	C	359	LYS
1	D	16	LEU
1	D	18	LYS
1	D	44	MET
1	D	45	VAL
1	D	53	TYR
1	D	65	LEU
1	D	66	THR
1	D	77	THR
1	D	99	GLU
1	D	103	THR
1	D	109	PRO
1	D	128	ASN
1	D	159	VAL
1	D	176	MET
1	D	195	GLU
1	D	201	VAL
1	D	207	GLU
1	D	210	ARG
1	D	221	LEU
1	D	224	GLU
1	D	226	GLU
1	D	229	THR
1	D	238	LYS
1	D	252	ASN
1	D	263	GLN
1	D	267	ILE
1	D	277	THR
1	D	284	LYS
1	D	292	ASP
1	D	297	ASN
1	D	303	THR
1	D	311	ASP
1	D	316	GLU
1	D	326	LYS
1	D	334	GLU
1	D	359	LYS
1	E	14	SER
1	E	18	LYS
1	E	51	ASP

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Mol	Chain	Res	Type
1	E	57	GLU
1	E	67	LEU
1	E	80	ASP
1	E	99	GLU
1	E	109	PRO
1	E	115	ASN
1	E	128	ASN
1	E	157	ASP
1	E	176	MET
1	E	180	LEU
1	E	190	MET
1	E	195	GLU
1	E	209	VAL
1	E	213	LYS
1	E	238	LYS
1	E	249	THR
1	E	267	ILE
1	E	277	THR
1	E	284	LYS
1	E	286	ASP
1	E	292	ASP
1	E	297	ASN
1	E	303	THR
1	E	313	MET
1	E	316	GLU
1	E	334	GLU
1	E	357	ILE
1	E	359	LYS
1	F	18	LYS
1	F	50	LYS
1	F	99	GLU
1	F	115	ASN
1	F	121	GLN
1	F	128	ASN
1	F	149	THR
1	F	162	ASN
1	F	166	TYR
1	F	171	LEU
1	F	199	SER
1	F	203	THR
1	F	207	GLU
1	F	213	LYS

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Mol	Chain	Res	Type
1	F	221	LEU
1	F	238	LYS
1	F	248	ILE
1	F	249	THR
1	F	252	ASN
1	F	263	GLN
1	F	270	GLU
1	F	277	THR
1	F	284	LYS
1	F	291	LYS
1	F	292	ASP
1	F	297	ASN
1	F	303	THR
1	F	311	ASP
1	F	334	GLU
1	F	359	LYS
1	G	18	LYS
1	G	51	ASP
1	G	57	GLU
1	G	62	ARG
1	G	66	THR
1	G	99	GLU
1	G	103	THR
1	G	128	ASN
1	G	159	VAL
1	G	176	MET
1	G	203	THR
1	G	218	TYR
1	G	219	VAL
1	G	226	GLU
1	G	238	LYS
1	G	250	ILE
1	G	252	ASN
1	G	263	GLN
1	G	276	GLU
1	G	284	LYS
1	G	293	LEU
1	G	297	ASN
1	G	303	THR
1	G	311	ASP
1	G	334	GLU
1	G	351	THR

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Mol	Chain	Res	Type
1	G	359	LYS
1	G	368	SER
1	H	18	LYS
1	H	66	THR
1	H	99	GLU
1	H	109	PRO
1	H	128	ASN
1	H	159	VAL
1	H	176	MET
1	H	207	GLU
1	H	210	ARG
1	H	214	GLU
1	H	215	LYS
1	H	221	LEU
1	H	238	LYS
1	H	248	ILE
1	H	249	THR
1	H	252	ASN
1	H	260	THR
1	H	263	GLN
1	H	277	THR
1	H	284	LYS
1	H	291	LYS
1	H	297	ASN
1	H	303	THR
1	H	326	LYS
1	H	328	LYS
1	H	334	GLU
1	H	356	TRP
1	H	359	LYS
1	H	368	SER
1	I	18	LYS
1	I	49	GLN
1	I	57	GLU
1	I	59	GLN
1	I	62	ARG
1	I	99	GLU
1	I	100	GLU
1	I	109	PRO
1	I	128	ASN
1	I	159	VAL
1	I	176	MET

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Mol	Chain	Res	Type
1	I	187	ASP
1	I	193	LEU
1	I	201	VAL
1	I	207	GLU
1	I	210	ARG
1	I	218	TYR
1	I	221	LEU
1	I	238	LYS
1	I	248	ILE
1	I	252	ASN
1	I	260	THR
1	I	263	GLN
1	I	280	ASN
1	I	284	LYS
1	I	297	ASN
1	I	303	THR
1	I	334	GLU
1	I	368	SER
1	I	371	HIS
1	J	2	GLU
1	J	4	GLU
1	J	18	LYS
1	J	62	ARG
1	J	75	ILE
1	J	80	ASP
1	J	99	GLU
1	J	100	GLU
1	J	111	ASN
1	J	112	PRO
1	J	113	LYS
1	J	115	ASN
1	J	128	ASN
1	J	134	VAL
1	J	159	VAL
1	J	179	ASP
1	J	194	THR
1	J	199	SER
1	J	201	VAL
1	J	202	THR
1	J	205	GLU
1	J	207	GLU
1	J	208	ILE

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Mol	Chain	Res	Type
1	J	221	LEU
1	J	238	LYS
1	J	242	LEU
1	J	243	PRO
1	J	246	GLN
1	J	252	ASN
1	J	257	CYS
1	J	263	GLN
1	J	267	ILE
1	J	277	THR
1	J	278	THR
1	J	284	LYS
1	J	286	ASP
1	J	292	ASP
1	J	293	LEU
1	J	297	ASN
1	J	311	ASP
1	J	313	MET
1	J	316	GLU
1	J	323	SER
1	J	334	GLU
1	J	348	SER
1	J	359	LYS
1	J	368	SER
1	K	4	GLU
1	K	18	LYS
1	K	62	ARG
1	K	99	GLU
1	K	103	THR
1	K	113	LYS
1	K	128	ASN
1	K	159	VAL
1	K	173	HIS
1	K	176	MET
1	K	187	ASP
1	K	195	GLU
1	K	203	THR
1	K	207	GLU
1	K	213	LYS
1	K	215	LYS
1	K	221	LEU
1	K	238	LYS

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Mol	Chain	Res	Type
1	K	242	LEU
1	K	244	ASP
1	K	257	CYS
1	K	261	LEU
1	K	263	GLN
1	K	277	THR
1	K	284	LYS
1	K	286	ASP
1	K	297	ASN
1	K	303	THR
1	K	311	ASP
1	K	334	GLU
1	K	357	ILE
1	K	359	LYS
1	L	3	ASP
1	L	4	GLU
1	L	18	LYS
1	L	51	ASP
1	L	72	GLU
1	L	75	ILE
1	L	80	ASP
1	L	99	GLU
1	L	109	PRO
1	L	128	ASN
1	L	132	MET
1	L	148	THR
1	L	159	VAL
1	L	199	SER
1	L	209	VAL
1	L	218	TYR
1	L	221	LEU
1	L	224	GLU
1	L	238	LYS
1	L	252	ASN
1	L	260	THR
1	L	263	GLN
1	L	284	LYS
1	L	289	ILE
1	L	303	THR
1	L	316	GLU
1	L	326	LYS
1	L	334	GLU

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Mol	Chain	Res	Type
1	L	348	SER
1	L	351	THR
1	M	2	GLU
1	M	18	LYS
1	M	34	ILE
1	M	38	PRO
1	M	45	VAL
1	M	50	LYS
1	M	57	GLU
1	M	62	ARG
1	M	65	LEU
1	M	72	GLU
1	M	77	THR
1	M	99	GLU
1	M	103	THR
1	M	128	ASN
1	M	148	THR
1	M	159	VAL
1	M	203	THR
1	M	215	LYS
1	M	218	TYR
1	M	238	LYS
1	M	244	ASP
1	M	248	ILE
1	M	249	THR
1	M	252	ASN
1	M	260	THR
1	M	276	GLU
1	M	277	THR
1	M	284	LYS
1	M	286	ASP
1	M	287	ILE
1	M	292	ASP
1	M	303	THR
1	M	316	GLU
1	M	324	THR
1	M	326	LYS
1	M	334	GLU
1	M	359	LYS
1	M	368	SER
1	N	4	GLU
1	N	14	SER

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Mol	Chain	Res	Type
1	N	18	LYS
1	N	40	HIS
1	N	43	VAL
1	N	44	MET
1	N	51	ASP
1	N	59	GLN
1	N	62	ARG
1	N	99	GLU
1	N	100	GLU
1	N	109	PRO
1	N	128	ASN
1	N	132	MET
1	N	148	THR
1	N	159	VAL
1	N	180	LEU
1	N	193	LEU
1	N	199	SER
1	N	210	ARG
1	N	221	LEU
1	N	238	LYS
1	N	250	ILE
1	N	252	ASN
1	N	263	GLN
1	N	266	PHE
1	N	271	SER
1	N	277	THR
1	N	278	THR
1	N	284	LYS
1	N	287	ILE
1	N	297	ASN
1	N	303	THR
1	N	311	ASP
1	N	313	MET
1	N	316	GLU
1	N	322	PRO
1	N	324	THR
1	N	326	LYS
1	N	334	GLU
1	N	359	LYS
1	N	368	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	115	ASN
1	A	280	ASN
1	B	49	GLN
1	B	115	ASN
1	B	161	HIS
1	B	162	ASN
1	B	263	GLN
1	C	353	GLN
1	D	41	GLN
1	D	111	ASN
1	D	115	ASN
1	D	161	HIS
1	D	173	HIS
1	D	263	GLN
1	E	128	ASN
1	E	371	HIS
1	F	111	ASN
1	F	263	GLN
1	F	280	ASN
1	G	115	ASN
1	G	263	GLN
1	G	296	ASN
1	H	111	ASN
1	H	115	ASN
1	H	173	HIS
1	H	263	GLN
1	H	354	GLN
1	I	40	HIS
1	I	41	GLN
1	I	162	ASN
1	I	263	GLN
1	J	128	ASN
1	J	173	HIS
1	J	263	GLN
1	J	353	GLN
1	K	128	ASN
1	K	263	GLN
1	K	353	GLN
1	L	162	ASN
1	L	297	ASN
1	L	371	HIS
1	M	115	ASN

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Mol	Chain	Res	Type
1	M	128	ASN
1	M	162	ASN
1	M	354	GLN
1	N	111	ASN
1	N	115	ASN
1	N	252	ASN
1	N	280	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

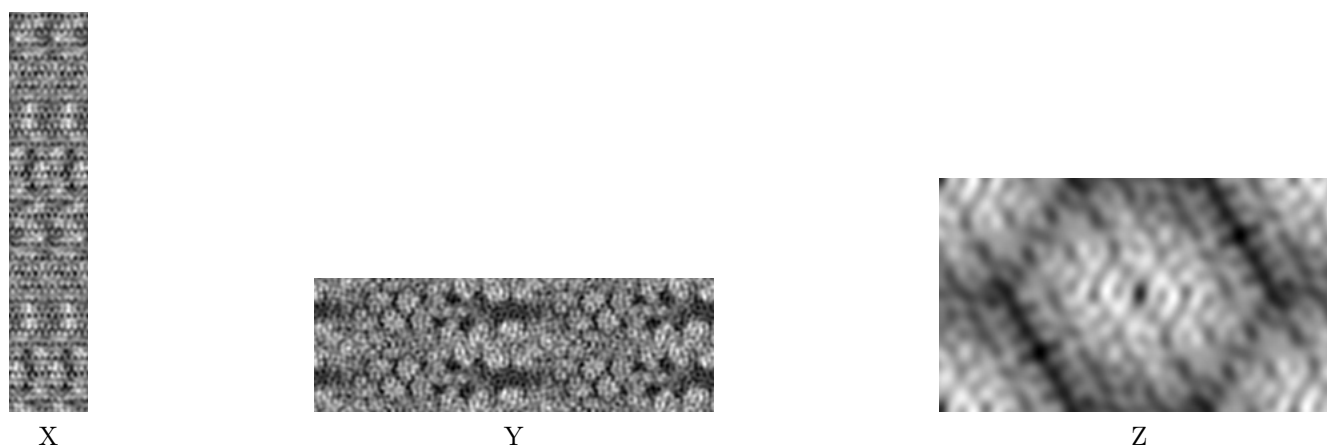
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1088. 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](#)

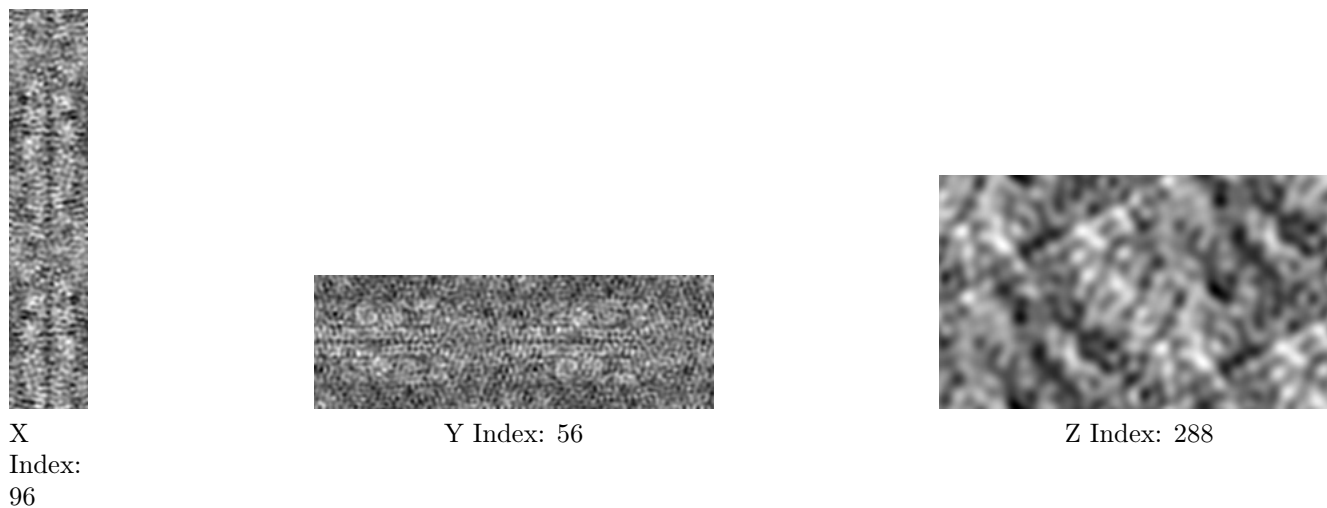
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



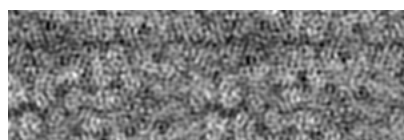
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X
Index:
123



Y Index: 84

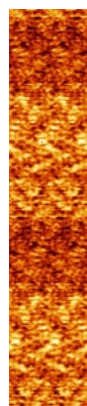


Z Index: 413

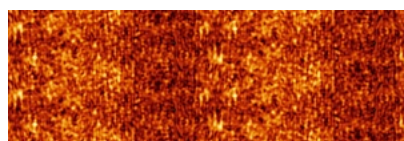
The images above show the largest variance slices of the map in three orthogonal directions.

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

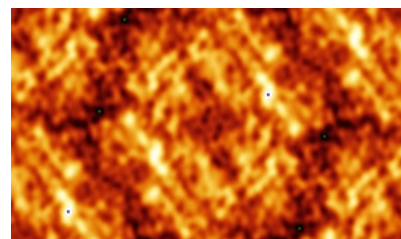
6.4.1 Primary map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 430.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

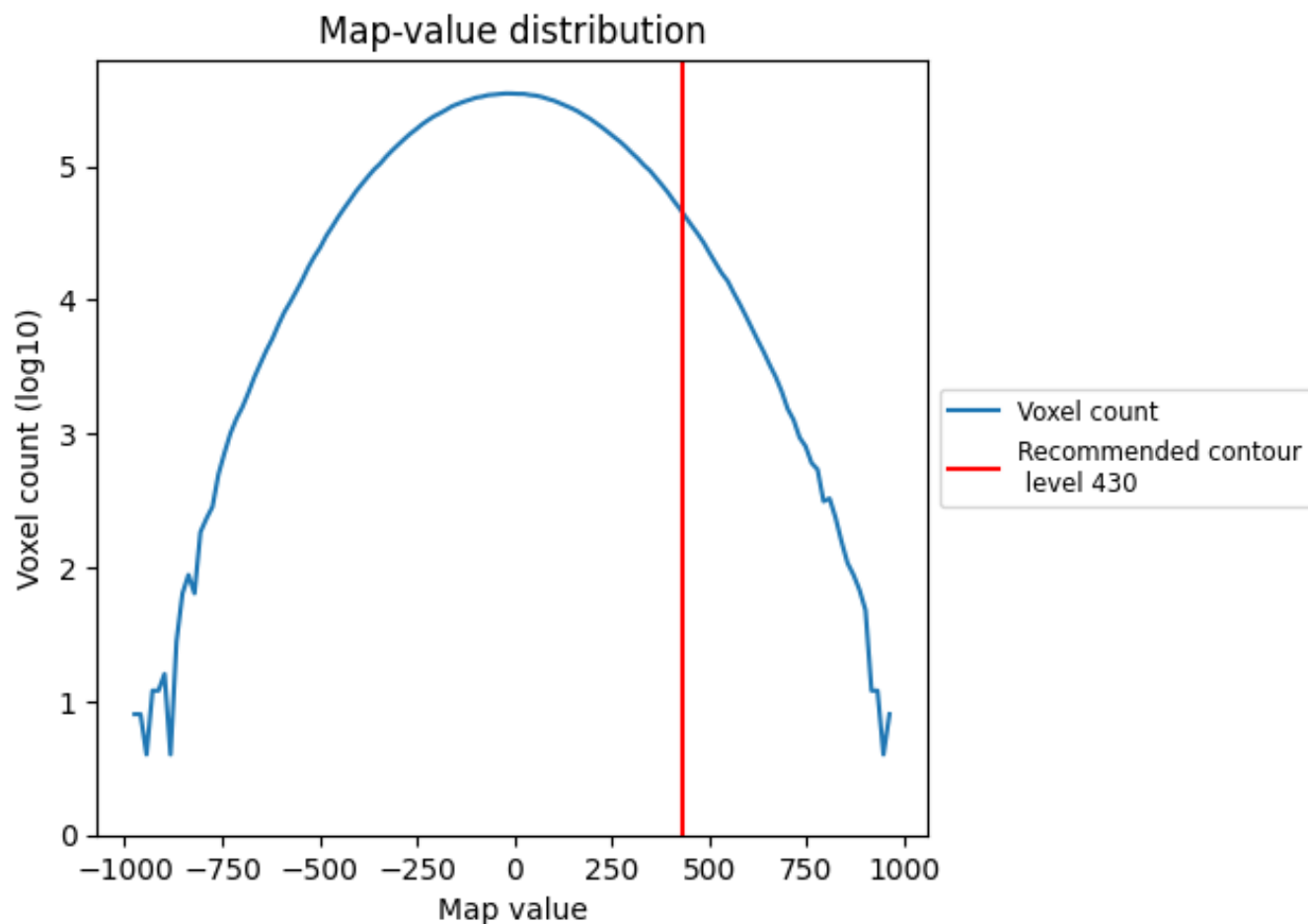
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

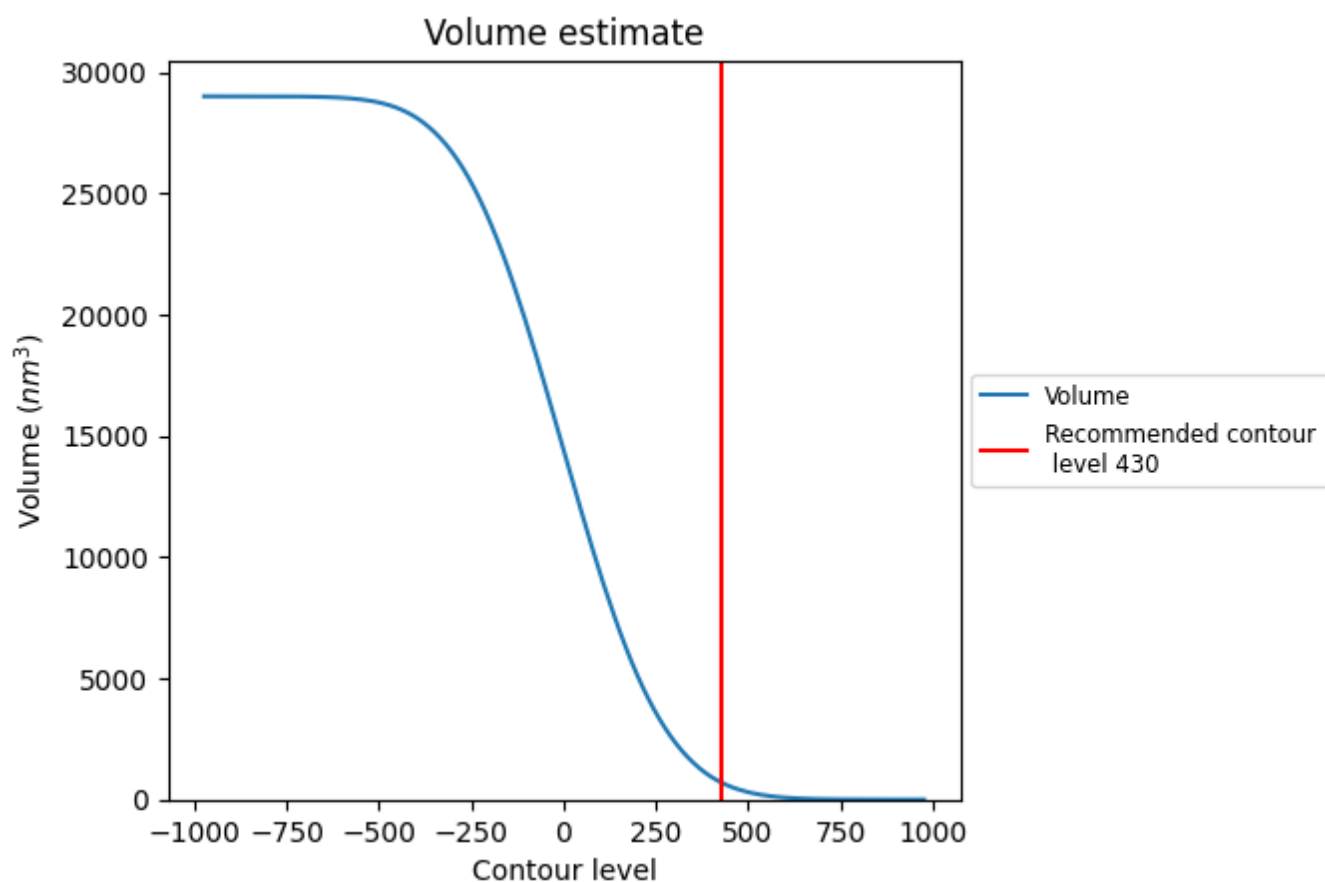
This section contains the results of statistical analysis of the map.

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 687 nm³; this corresponds to an approximate mass of 621 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

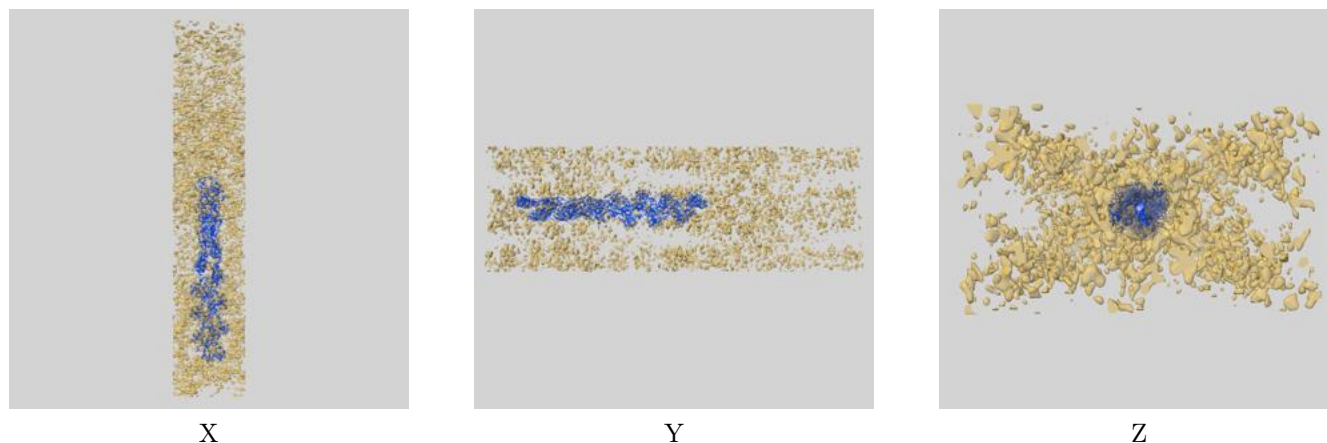
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

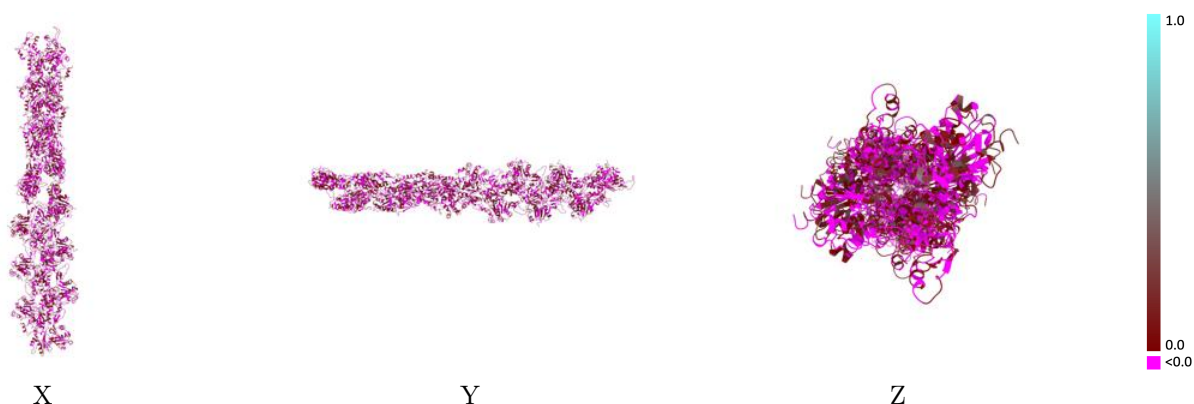
This section contains information regarding the fit between EMDB map EMD-1088 and PDB model 3B5U. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



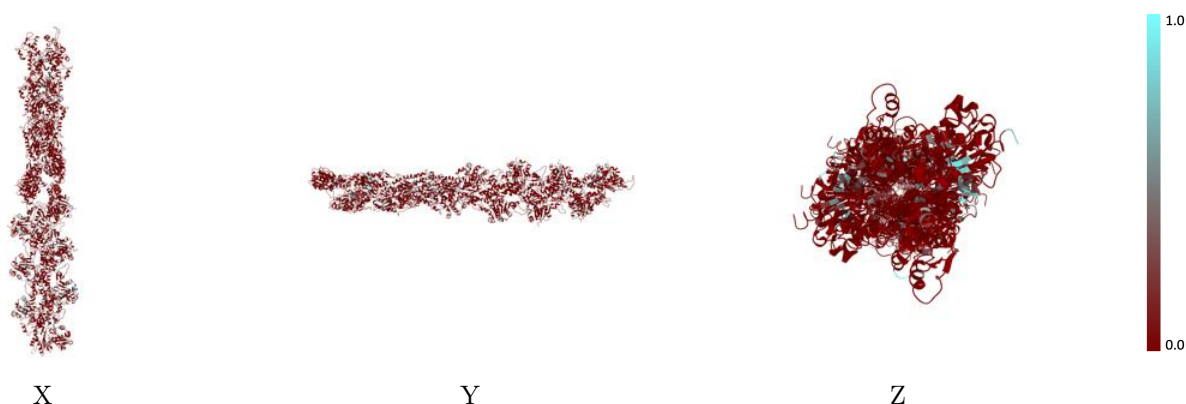
The images above show the 3D surface view of the map at the recommended contour level 430.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



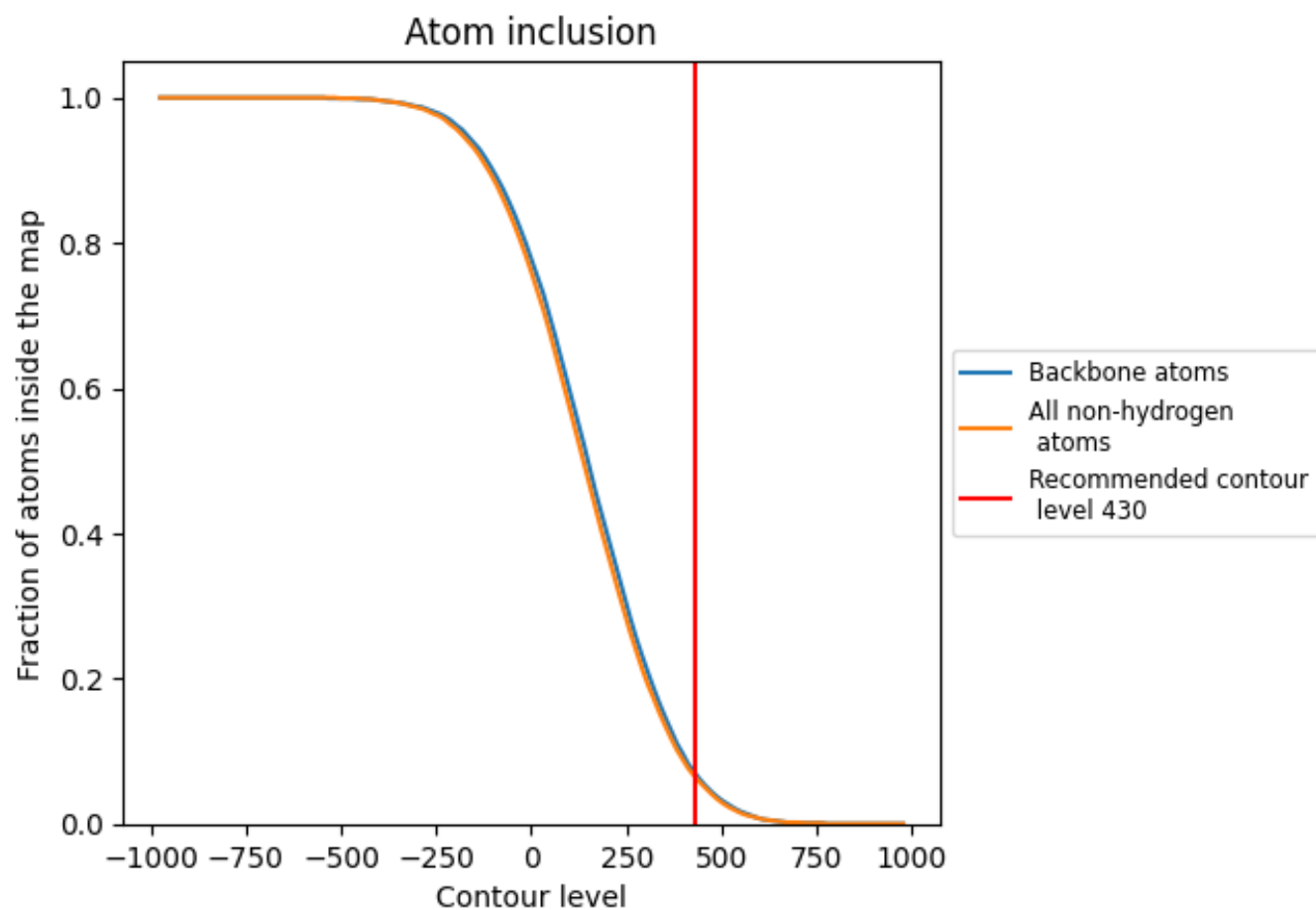
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (430).

9.4 Atom inclusion [i](#)



At the recommended contour level, 7% of all backbone atoms, 6% 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 (430) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0650	 0.0230
A	 0.0600	 0.0150
B	 0.0960	 0.0190
C	 0.1130	 0.0330
D	 0.0770	 0.0110
E	 0.0800	 0.0250
F	 0.0860	 0.0240
G	 0.0650	 0.0290
H	 0.0300	 0.0050
I	 0.0210	 0.0280
J	 0.0390	 0.0190
K	 0.0390	 0.0280
L	 0.0520	 0.0390
M	 0.0720	 0.0240
N	 0.0770	 0.0190

