



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:12 AM UTC

PDB ID : 3B63 / pdb_00003b63
EMDB ID : EMD-1088
Title : Actin filament model in the 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 models : 1YVN, 1ESV, 1T44, 1HIV, 1NWK, 1YAG, 1HLU, 1ATN, 1MDU

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:

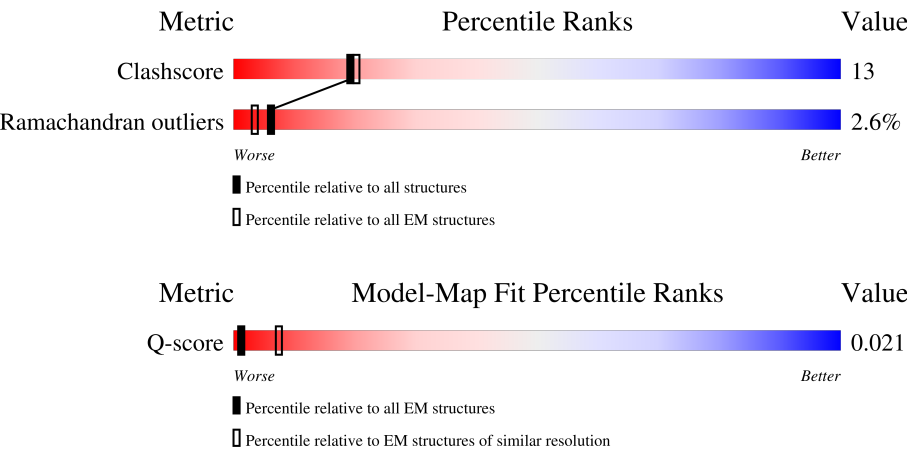
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 MICROSCOPY

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	-
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	365	92% 67%31%
1	G	365	93% 68%30%
2	B	364	90% 59%34%6%
3	C	365	90% 67%31%
3	I	365	99% 62%34%

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Mol	Chain	Length	Quality of chain
4	D	357	92% 61%32%8%
5	E	365	92% 58%37%5%
5	H	365	97% 61%34%. .
5	J	365	97% 62%32%6% .
5	K	365	96% 64%32%. .
5	N	365	93% 56%38%5%
6	F	357	90% 56%38%5% .
7	L	365	95% 60%35%5%
7	M	365	92% 63%31%5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 39685 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	365	Total	C	N	O	S	0	0
			2843	1800	480	545	18		
1	G	365	Total	C	N	O	S	0	0
			2843	1800	480	545	18		

- Molecule 2 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	364	Total	C	N	O	S	0	0
			2835	1796	474	545	20		

- Molecule 3 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	365	Total	C	N	O	S	0	0
			2842	1801	479	544	18		
3	I	365	Total	C	N	O	S	0	0
			2842	1801	479	544	18		

- Molecule 4 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	357	Total	C	N	O	S	0	0
			2791	1768	467	536	20		

- Molecule 5 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		
5	H	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		
5	K	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		
5	N	365	Total	C	N	O	S	0	0
			2845	1802	477	546	20		

- Molecule 6 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	357	Total	C	N	O	S	0	0
			2788	1767	467	534	20		

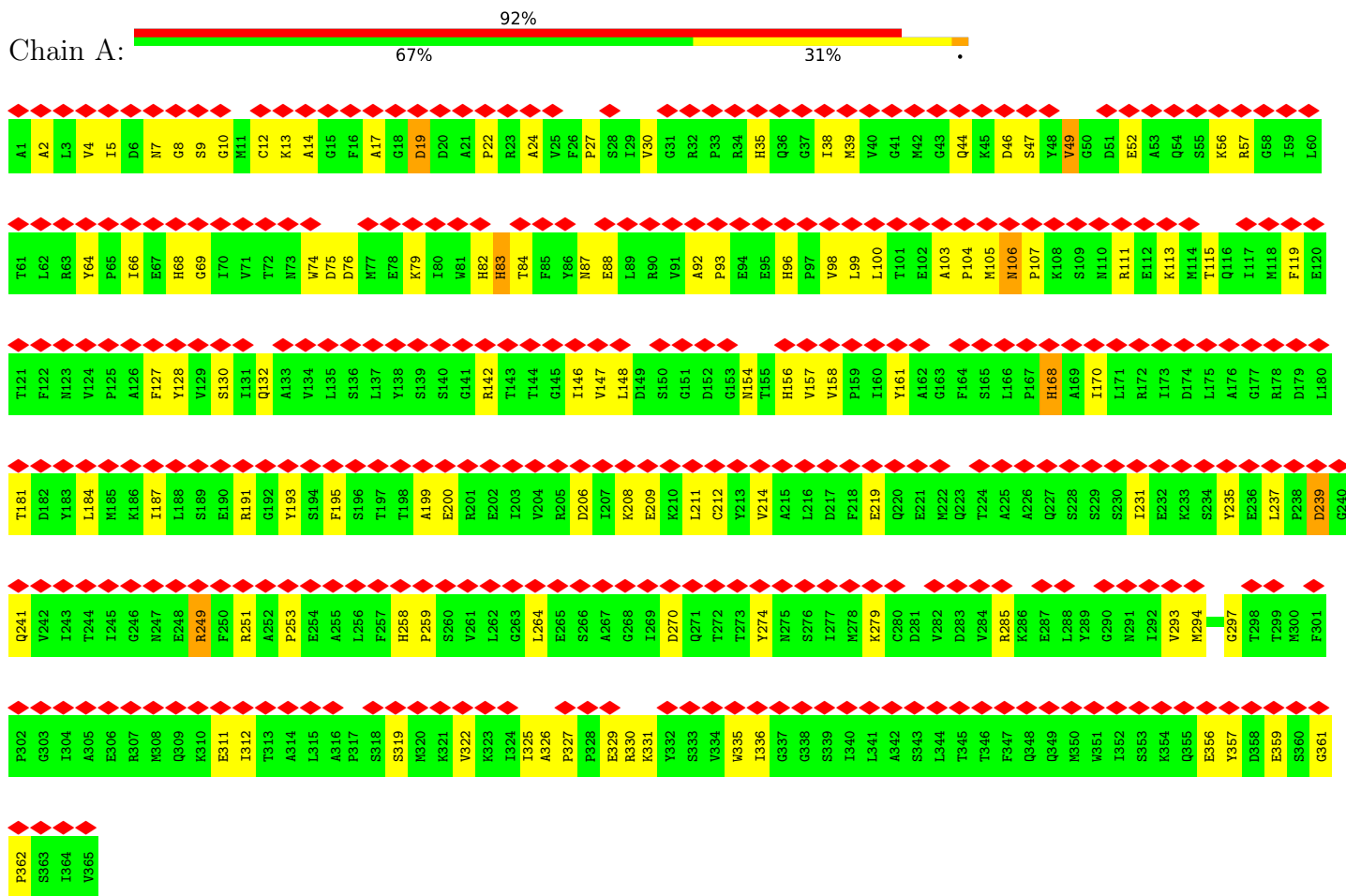
- Molecule 7 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	365	Total	C	N	O	S	0	0
			2838	1797	475	545	21		
7	M	365	Total	C	N	O	S	0	0
			2838	1797	475	545	21		

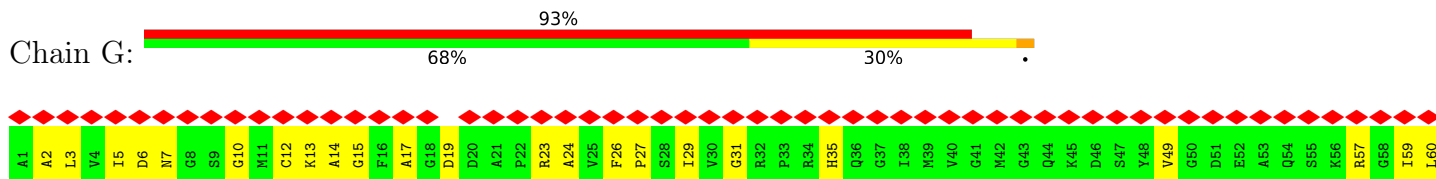
3 Residue-property plots

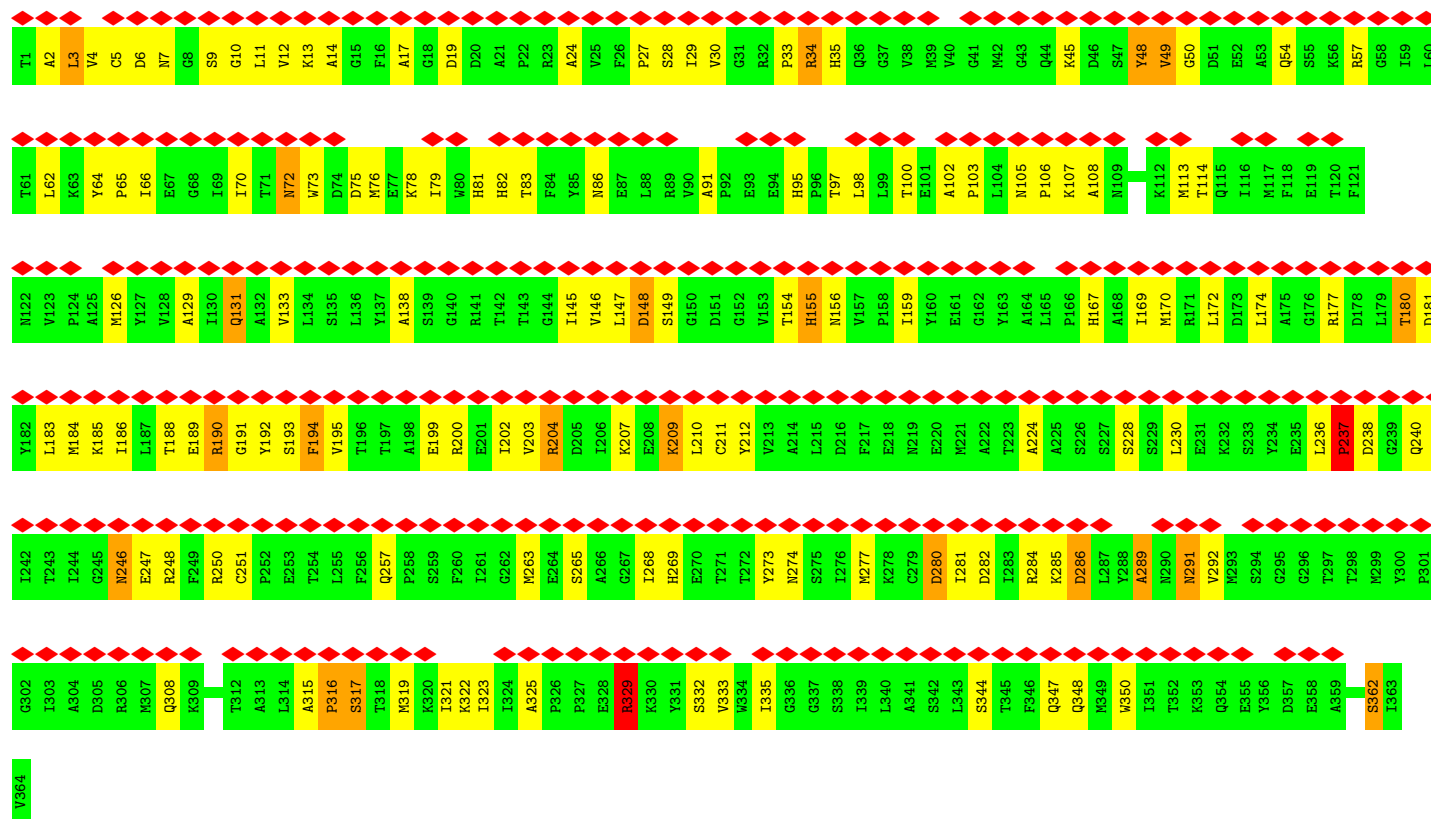
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

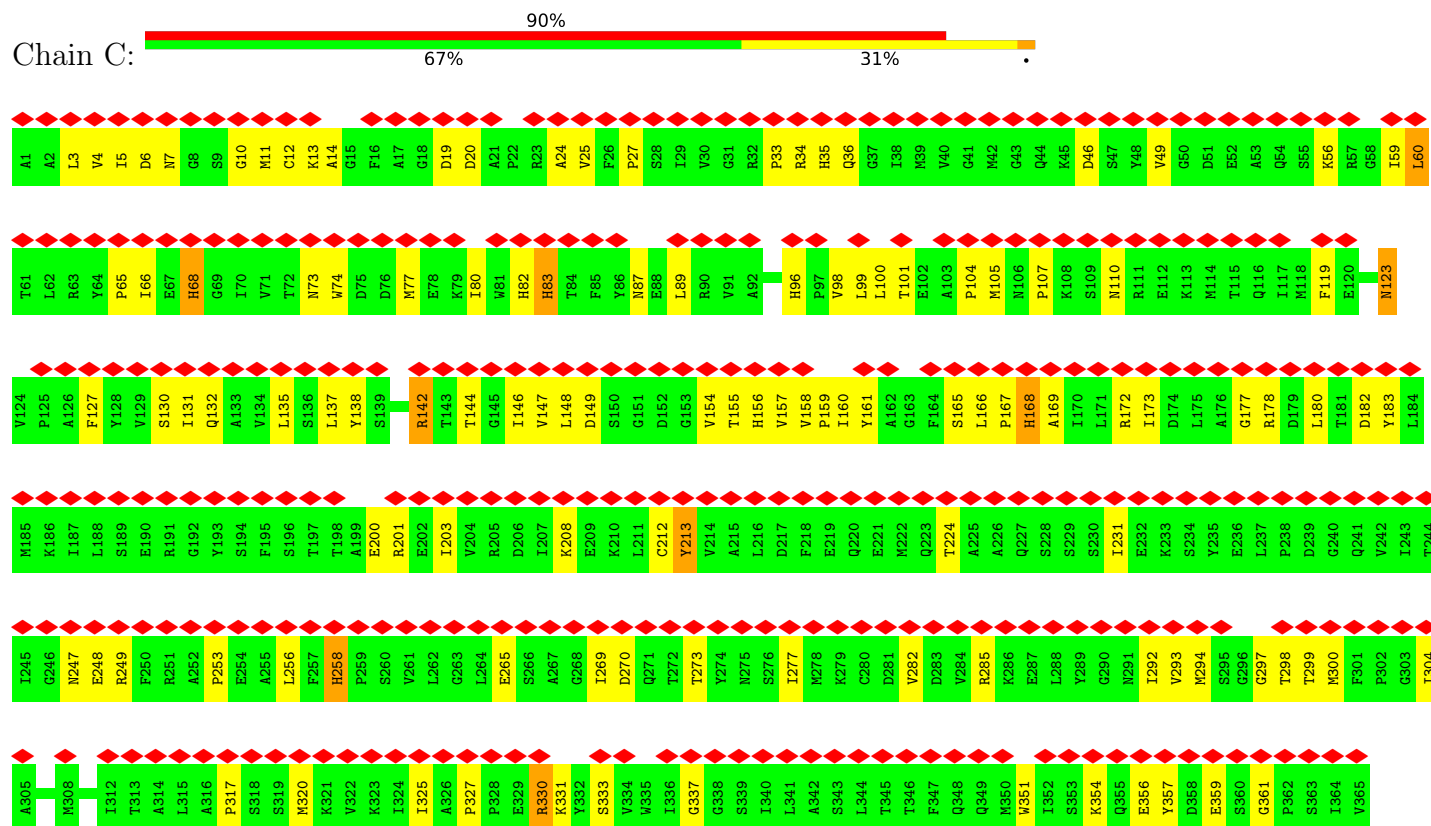


• Molecule 1: Actin

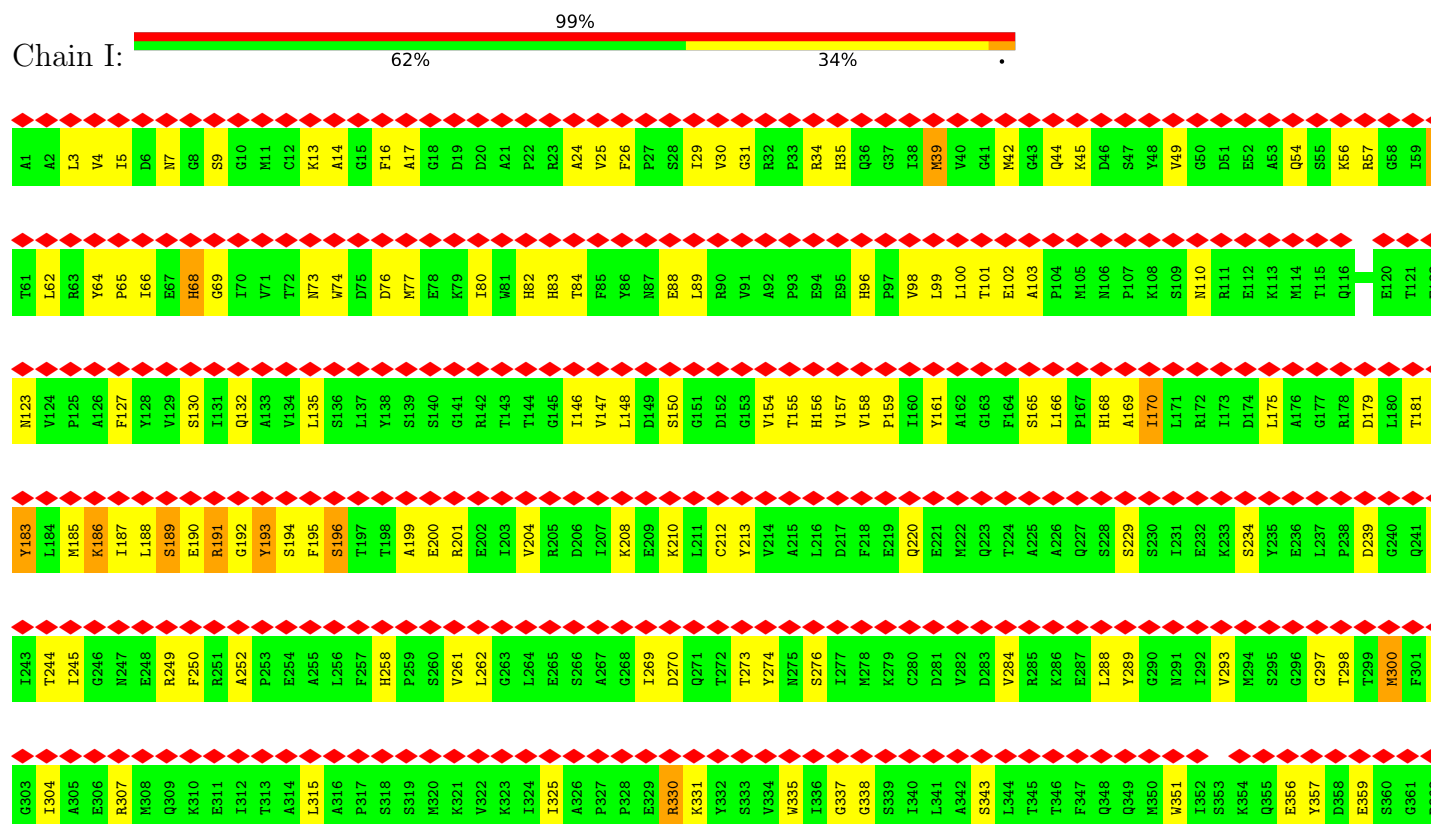




● Molecule 3: Actin

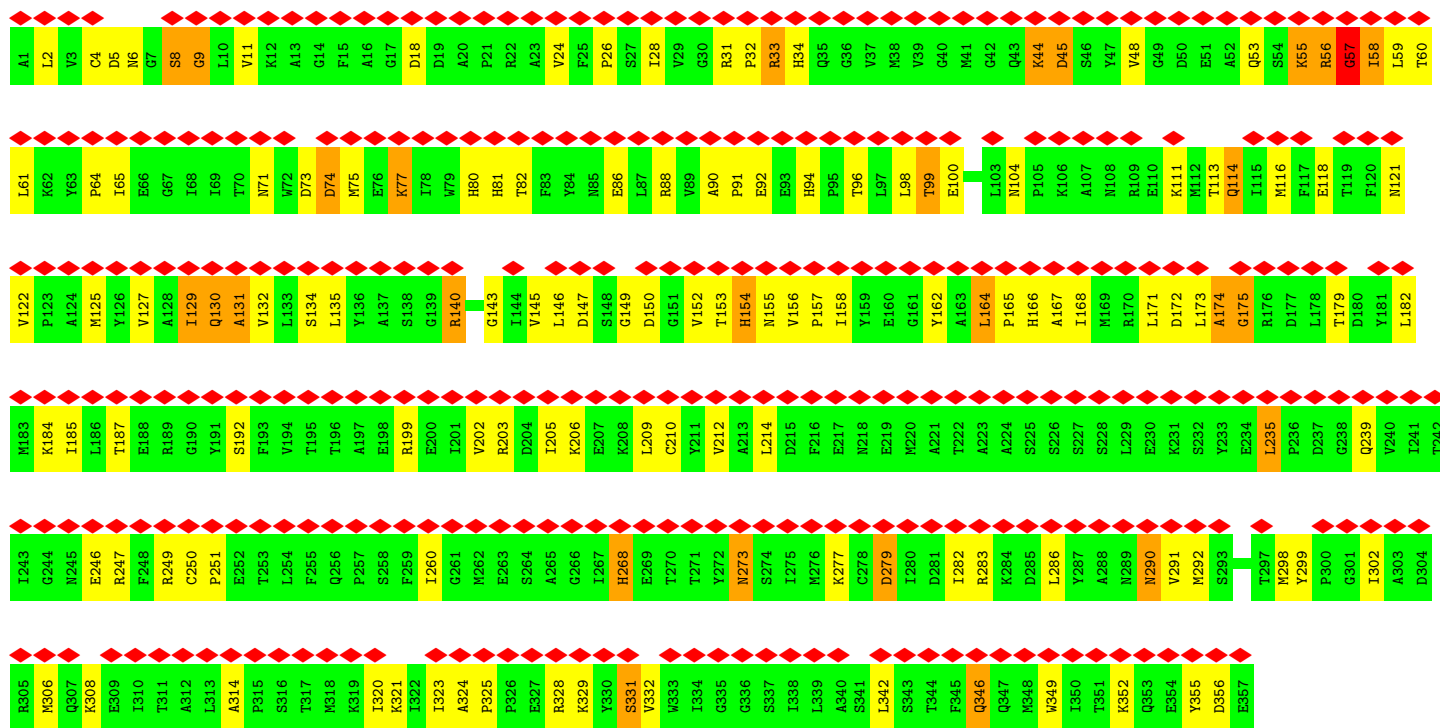
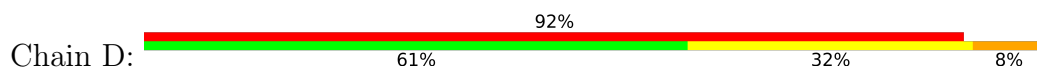


● Molecule 3: Actin

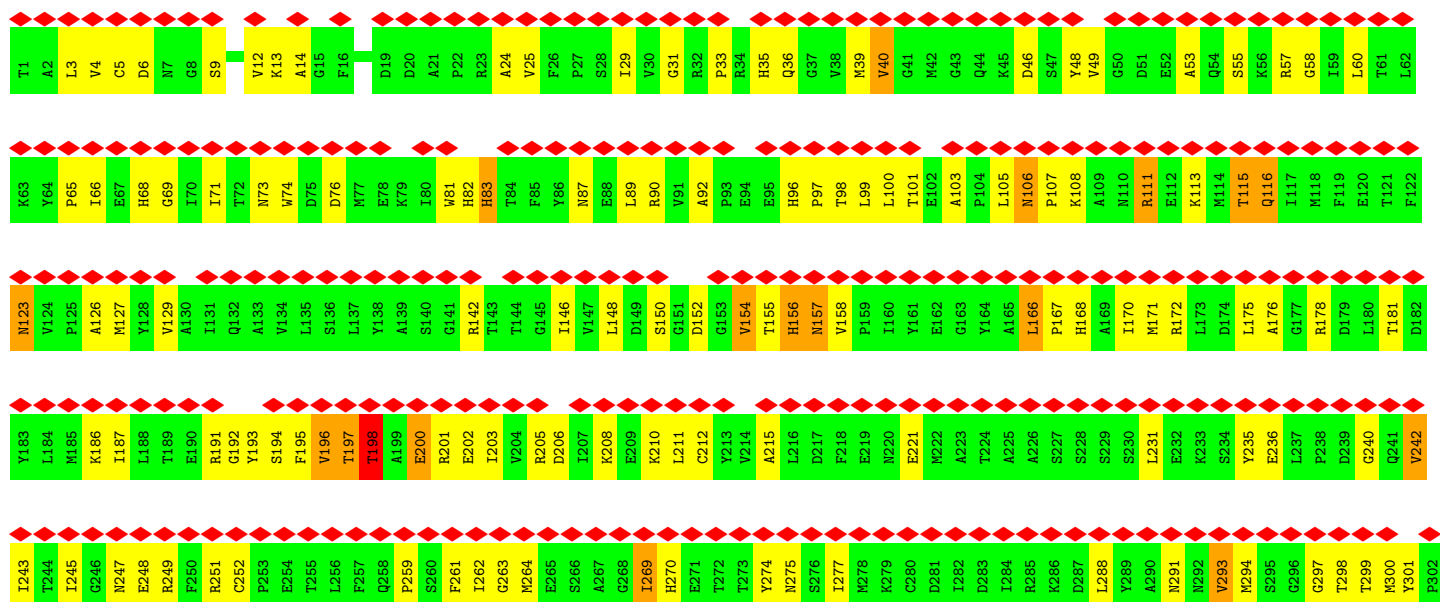


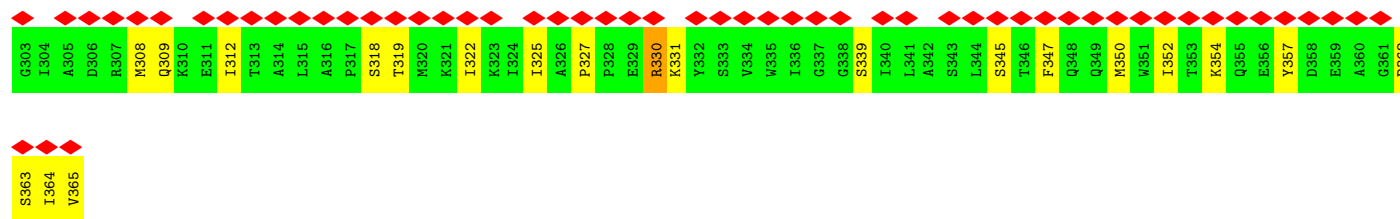


• Molecule 4: Actin

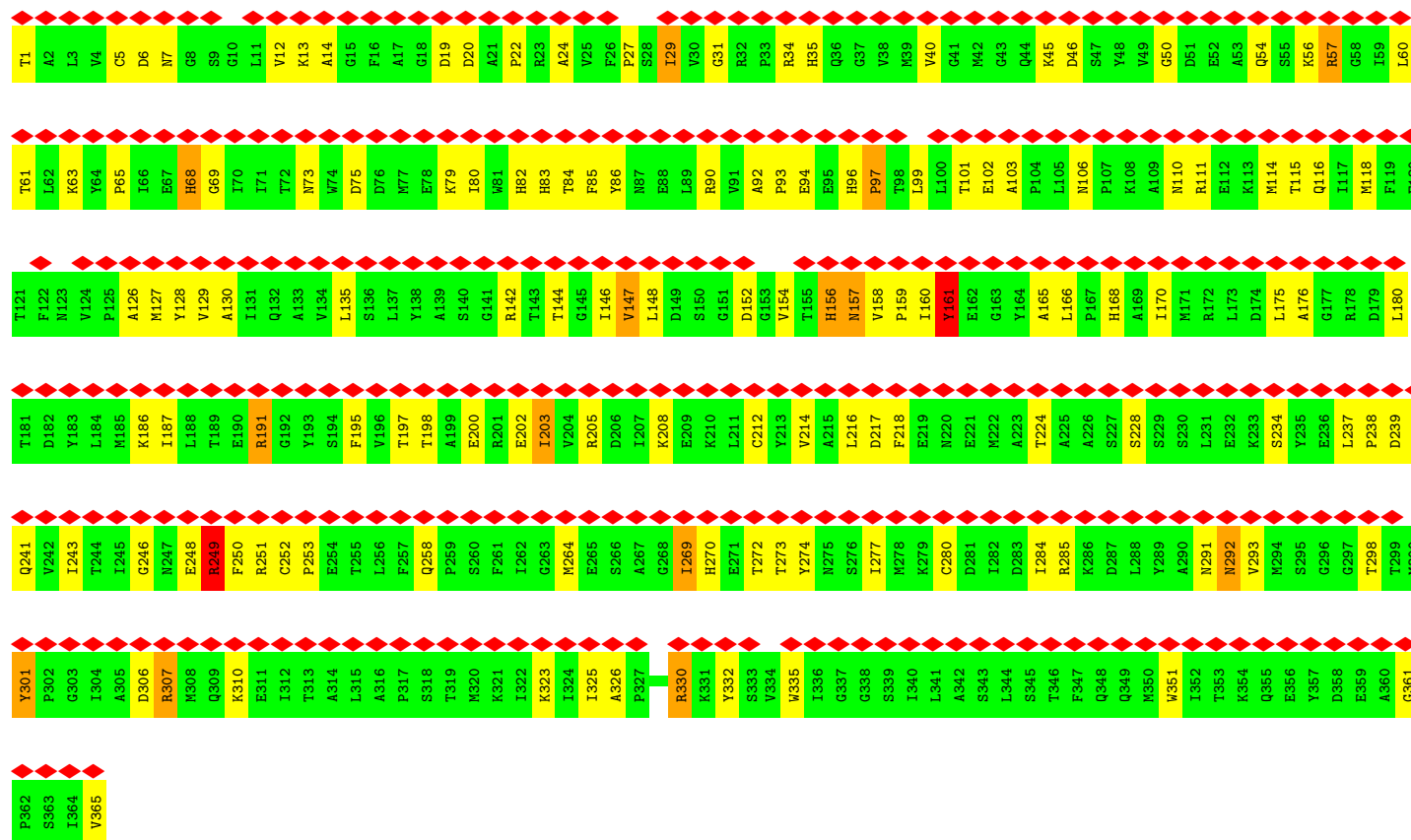


• Molecule 5: Actin





• Molecule 5: Actin

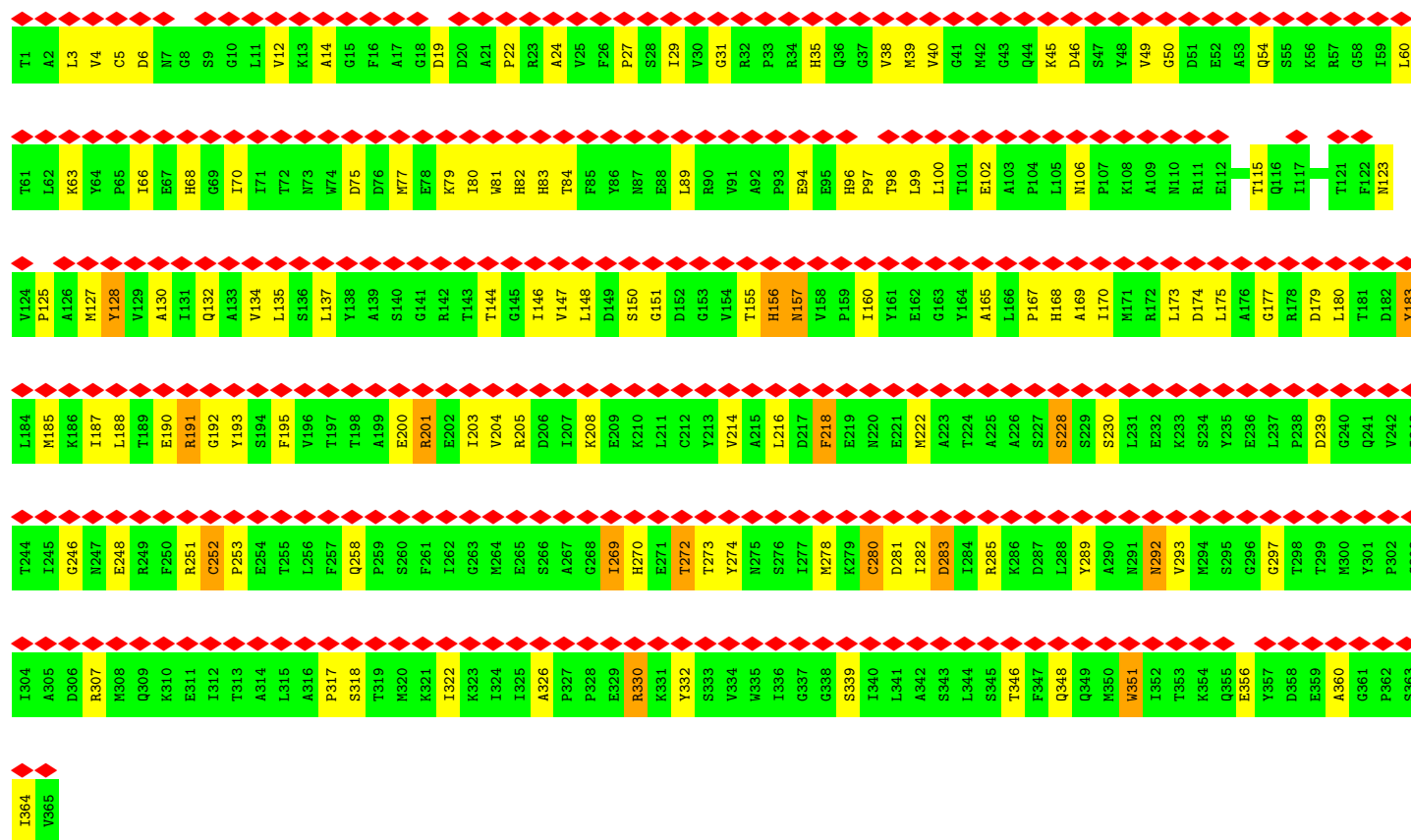


• Molecule 5: Actin



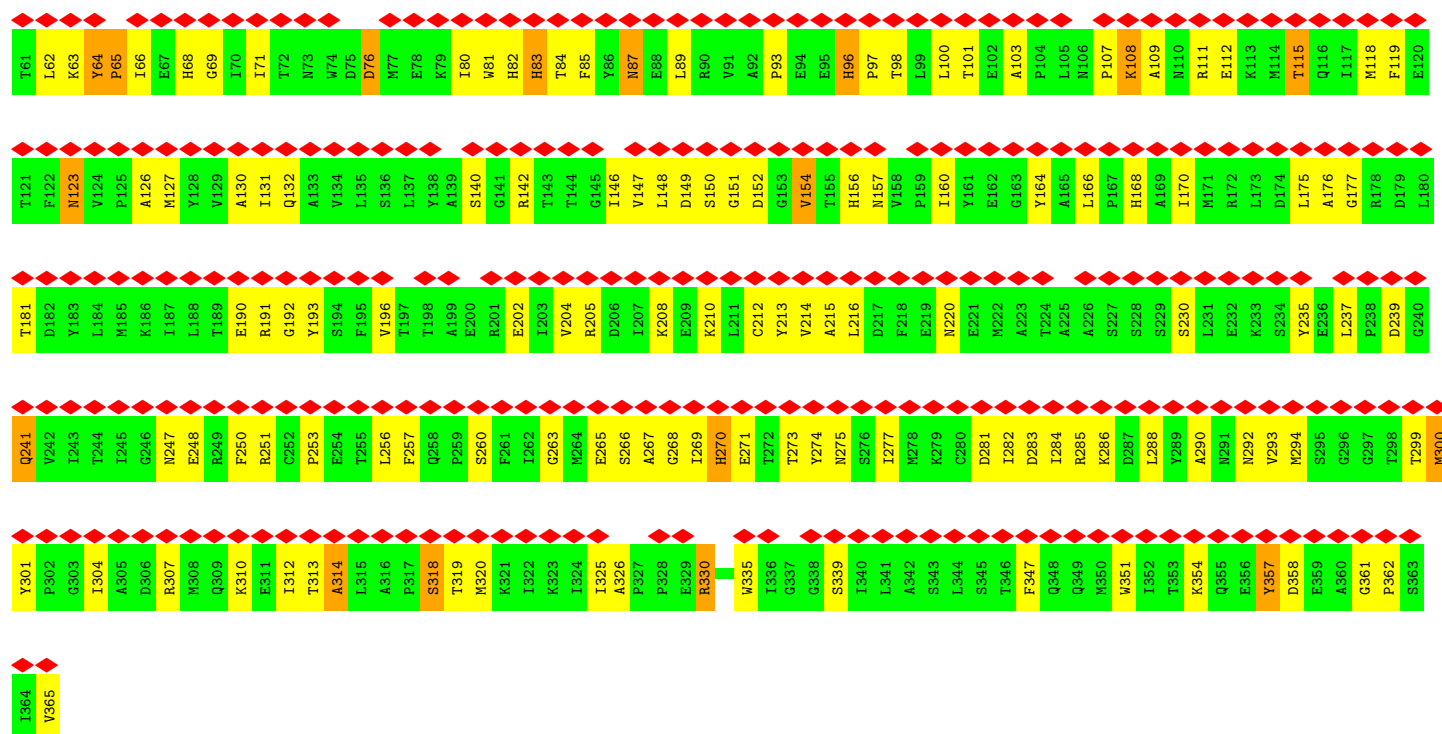


• Molecule 5: Actin

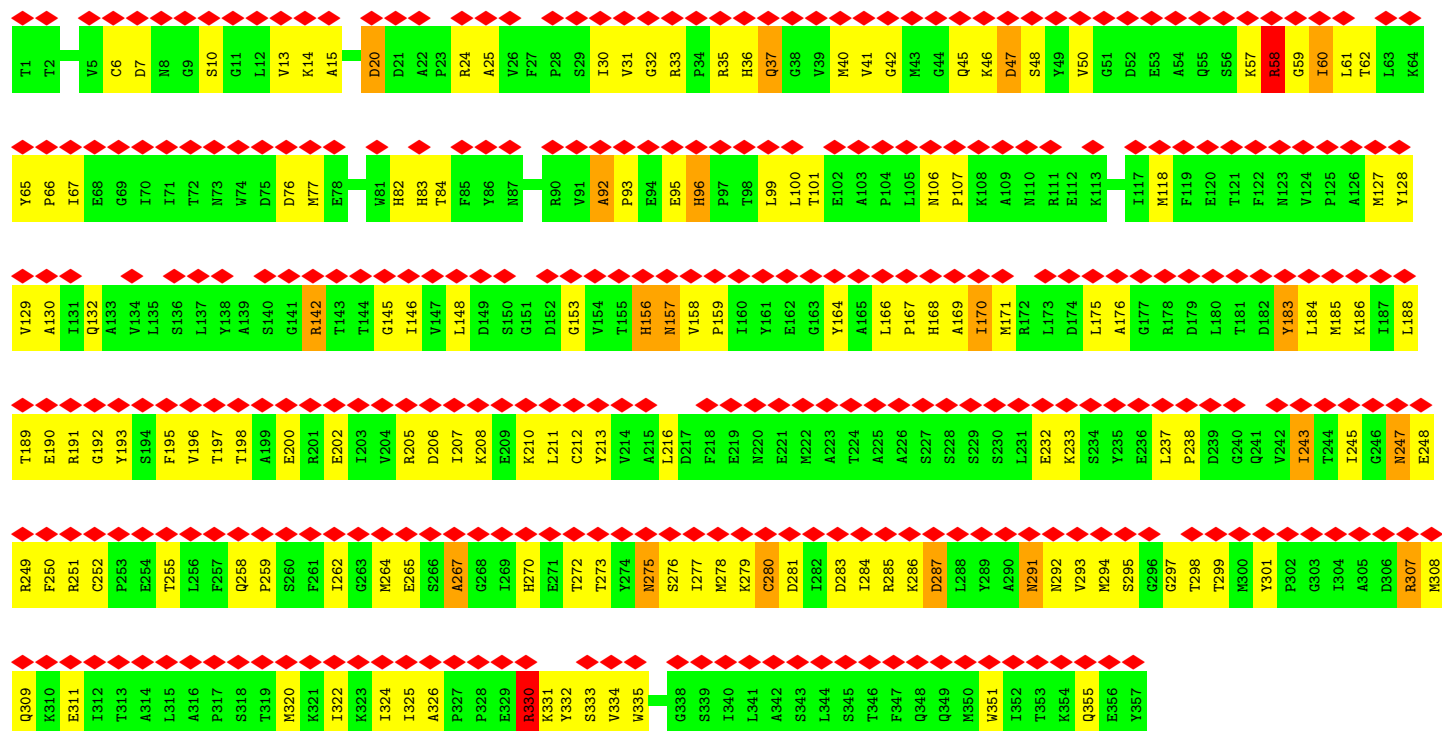


• Molecule 5: Actin



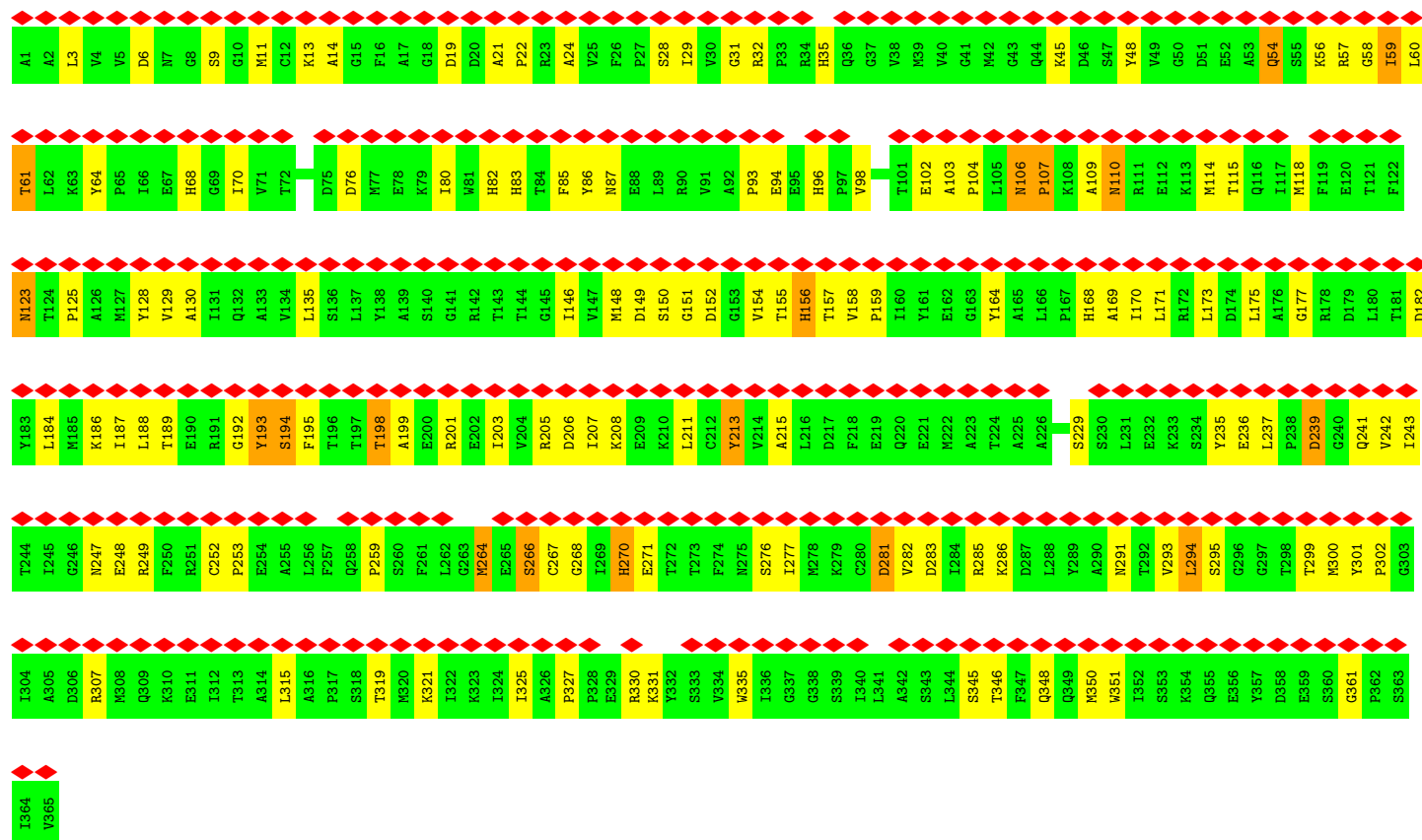


• Molecule 6: Actin



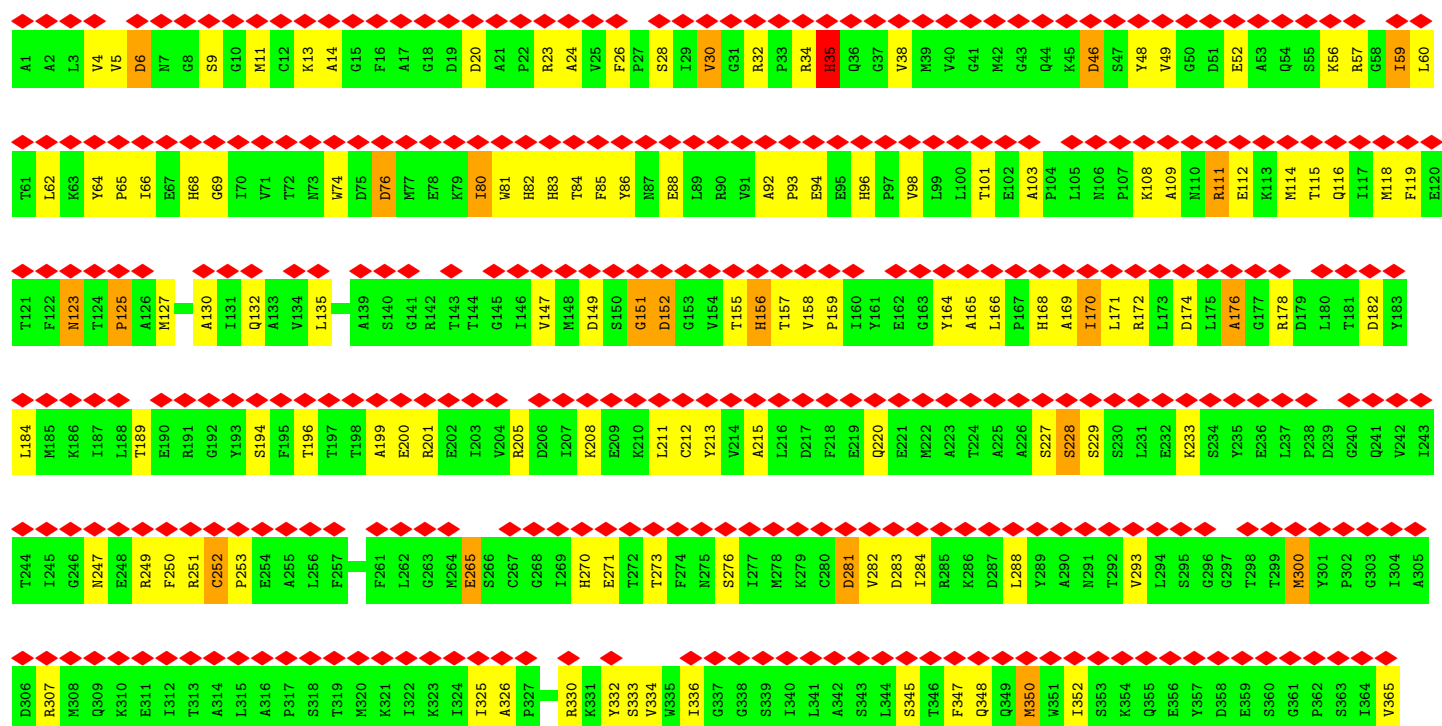
• Molecule 7: Actin





• Molecule 7: Actin

Chain M:



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	Not provided	
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	0.76	8/2904 (0.3%)	1.56	36/3931 (0.9%)
1	G	0.76	8/2904 (0.3%)	1.53	39/3931 (1.0%)
2	B	0.75	8/2895 (0.3%)	1.65	59/3923 (1.5%)
3	C	0.75	8/2903 (0.3%)	1.56	31/3930 (0.8%)
3	I	0.74	8/2903 (0.3%)	1.59	41/3930 (1.0%)
4	D	0.75	7/2850 (0.2%)	1.63	45/3860 (1.2%)
5	E	0.77	9/2906 (0.3%)	1.63	45/3938 (1.1%)
5	H	0.75	8/2906 (0.3%)	1.61	44/3938 (1.1%)
5	J	0.77	9/2906 (0.3%)	1.65	59/3938 (1.5%)
5	K	0.77	10/2906 (0.3%)	1.62	35/3938 (0.9%)
5	N	0.76	9/2906 (0.3%)	1.60	44/3938 (1.1%)
6	F	0.75	7/2847 (0.2%)	1.62	36/3857 (0.9%)
7	L	0.77	8/2899 (0.3%)	1.69	47/3927 (1.2%)
7	M	0.77	9/2899 (0.3%)	1.63	44/3927 (1.1%)
All	All	0.76	116/40534 (0.3%)	1.61	605/54906 (1.1%)

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	12
1	G	0	7
2	B	0	9
3	C	0	6
3	I	0	9
4	D	0	5
5	E	0	8
5	H	0	7
5	J	0	6
5	K	0	9
5	N	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	7
7	L	0	5
7	M	0	6
All	All	0	104

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	166	HIS	CD2-NE2	-7.16	1.29	1.37
1	G	168	HIS	CD2-NE2	-7.12	1.30	1.37
5	H	68	HIS	CD2-NE2	-7.04	1.30	1.37
5	E	168	HIS	CD2-NE2	-6.99	1.30	1.37
5	E	270	HIS	CD2-NE2	-6.99	1.30	1.37
3	I	168	HIS	CD2-NE2	-6.97	1.30	1.37
1	A	68	HIS	CD2-NE2	-6.91	1.30	1.37
5	E	82	HIS	CD2-NE2	-6.89	1.30	1.37
5	J	96	HIS	CD2-NE2	-6.89	1.30	1.37
5	J	168	HIS	CD2-NE2	-6.89	1.30	1.37
7	M	96	HIS	CD2-NE2	-6.86	1.30	1.37
5	K	68	HIS	CD2-NE2	-6.85	1.30	1.37
6	F	96	HIS	CD2-NE2	-6.83	1.30	1.37
5	N	96	HIS	CD2-NE2	-6.82	1.30	1.37
7	M	68	HIS	CD2-NE2	-6.82	1.30	1.37
6	F	168	HIS	CD2-NE2	-6.81	1.30	1.37
5	J	270	HIS	CD2-NE2	-6.81	1.30	1.37
2	B	269	HIS	CD2-NE2	-6.79	1.30	1.37
3	C	168	HIS	CD2-NE2	-6.76	1.30	1.37
5	N	83	HIS	CD2-NE2	-6.74	1.30	1.37
4	D	80	HIS	CD2-NE2	-6.72	1.30	1.37
1	G	96	HIS	CD2-NE2	-6.72	1.30	1.37
1	A	168	HIS	CD2-NE2	-6.71	1.30	1.37
6	F	270	HIS	CD2-NE2	-6.71	1.30	1.37
7	L	168	HIS	CD2-NE2	-6.69	1.30	1.37
5	N	156	HIS	CD2-NE2	-6.66	1.30	1.37
1	G	68	HIS	CD2-NE2	-6.64	1.30	1.37
7	L	270	HIS	CD2-NE2	-6.64	1.30	1.37
4	D	154	HIS	CD2-NE2	-6.64	1.30	1.37
3	I	68	HIS	CD2-NE2	-6.63	1.30	1.37
1	A	96	HIS	CD2-NE2	-6.61	1.30	1.37
5	E	83	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	82	HIS	CD2-NE2	-6.59	1.30	1.37
2	B	167	HIS	CD2-NE2	-6.59	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	270	HIS	CD2-NE2	-6.58	1.30	1.37
7	L	96	HIS	CD2-NE2	-6.57	1.30	1.37
1	G	156	HIS	CD2-NE2	-6.57	1.30	1.37
5	N	35	HIS	CD2-NE2	-6.56	1.30	1.37
7	M	168	HIS	CD2-NE2	-6.55	1.30	1.37
7	L	156	HIS	CD2-NE2	-6.54	1.30	1.37
4	D	268	HIS	CD2-NE2	-6.53	1.30	1.37
3	I	83	HIS	CD2-NE2	-6.52	1.30	1.37
3	C	258	HIS	CD2-NE2	-6.51	1.30	1.37
5	E	35	HIS	CD2-NE2	-6.51	1.30	1.37
7	M	82	HIS	CD2-NE2	-6.50	1.30	1.37
5	N	168	HIS	CD2-NE2	-6.49	1.30	1.37
5	K	168	HIS	CD2-NE2	-6.49	1.30	1.37
3	C	35	HIS	CD2-NE2	-6.49	1.30	1.37
5	J	35	HIS	CD2-NE2	-6.47	1.30	1.37
5	N	68	HIS	CD2-NE2	-6.47	1.30	1.37
3	C	68	HIS	CD2-NE2	-6.47	1.30	1.37
7	M	83	HIS	CD2-NE2	-6.46	1.30	1.37
5	H	82	HIS	CD2-NE2	-6.46	1.30	1.37
6	F	83	HIS	CD2-NE2	-6.46	1.30	1.37
2	B	95	HIS	CD2-NE2	-6.44	1.30	1.37
5	H	83	HIS	CD2-NE2	-6.44	1.30	1.37
3	C	83	HIS	CD2-NE2	-6.43	1.30	1.37
5	K	156	HIS	CD2-NE2	-6.43	1.30	1.37
5	J	83	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	83	HIS	CD2-NE2	-6.41	1.30	1.37
2	B	81	HIS	CD2-NE2	-6.41	1.30	1.37
7	L	83	HIS	CD2-NE2	-6.39	1.30	1.37
5	J	68	HIS	CD2-NE2	-6.38	1.30	1.37
3	I	96	HIS	CD2-NE2	-6.38	1.30	1.37
2	B	35	HIS	CD2-NE2	-6.38	1.30	1.37
5	K	83	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	258	HIS	CD2-NE2	-6.35	1.30	1.37
1	G	35	HIS	CD2-NE2	-6.35	1.30	1.37
4	D	34	HIS	CD2-NE2	-6.33	1.30	1.37
2	B	155	HIS	CD2-NE2	-6.33	1.30	1.37
3	I	258	HIS	CD2-NE2	-6.33	1.30	1.37
5	K	82	HIS	CD2-NE2	-6.33	1.30	1.37
5	J	82	HIS	CD2-NE2	-6.32	1.30	1.37
2	B	82	HIS	CD2-NE2	-6.31	1.30	1.37
6	F	36	HIS	CD2-NE2	-6.30	1.30	1.37
1	G	83	HIS	CD2-NE2	-6.30	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	35	HIS	CD2-NE2	-6.30	1.30	1.37
5	N	270	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	35	HIS	CD2-NE2	-6.29	1.30	1.37
1	G	258	HIS	CD2-NE2	-6.27	1.30	1.37
5	E	68	HIS	CD2-NE2	-6.26	1.30	1.37
6	F	82	HIS	CD2-NE2	-6.26	1.30	1.37
3	I	82	HIS	CD2-NE2	-6.24	1.30	1.37
5	K	270	HIS	CD2-NE2	-6.24	1.30	1.37
7	M	156	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	156	HIS	CD2-NE2	-6.23	1.31	1.37
4	D	81	HIS	CD2-NE2	-6.21	1.31	1.37
5	K	96	HIS	CD2-NE2	-6.21	1.31	1.37
4	D	94	HIS	CD2-NE2	-6.21	1.31	1.37
5	H	96	HIS	CD2-NE2	-6.21	1.31	1.37
1	G	82	HIS	CD2-NE2	-6.18	1.31	1.37
7	M	35	HIS	CD2-NE2	-6.18	1.31	1.37
3	C	96	HIS	CD2-NE2	-6.17	1.31	1.37
5	H	35	HIS	CD2-NE2	-6.16	1.31	1.37
7	L	35	HIS	CD2-NE2	-6.15	1.31	1.37
5	H	270	HIS	CD2-NE2	-6.15	1.31	1.37
5	H	156	HIS	CD2-NE2	-6.15	1.31	1.37
5	N	82	HIS	CD2-NE2	-6.12	1.31	1.37
5	J	156	HIS	CD2-NE2	-6.11	1.31	1.37
7	L	68	HIS	CD2-NE2	-6.10	1.31	1.37
3	I	156	HIS	CD2-NE2	-6.10	1.31	1.37
3	I	35	HIS	CD2-NE2	-6.05	1.31	1.37
7	L	82	HIS	CD2-NE2	-6.02	1.31	1.37
3	C	156	HIS	CD2-NE2	-5.99	1.31	1.37
5	E	96	HIS	CD2-NE2	-5.94	1.31	1.37
5	H	168	HIS	CD2-NE2	-5.88	1.31	1.37
5	E	156	HIS	CD2-NE2	-5.85	1.31	1.37
6	F	156	HIS	CD2-NE2	-5.84	1.31	1.37
3	C	82	HIS	CD2-NE2	-5.66	1.31	1.37
5	K	270	HIS	CG-ND1	-5.42	1.32	1.38
5	E	270	HIS	CG-ND1	-5.21	1.32	1.38
7	M	270	HIS	CG-ND1	-5.19	1.32	1.38
5	N	156	HIS	CG-ND1	-5.14	1.32	1.38
5	J	96	HIS	CG-ND1	-5.12	1.32	1.38
2	B	155	HIS	CG-ND1	-5.07	1.32	1.38
5	K	83	HIS	CG-ND1	-5.05	1.32	1.38

All (605) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	285	ARG	N-CA-C	11.03	122.87	111.07
5	E	197	THR	N-CA-C	10.19	124.82	108.41
2	B	246	ASN	OD1-CG-ND2	-9.67	112.93	122.60
2	B	194	PHE	N-CA-C	9.37	124.27	111.90
1	G	75	ASP	CA-CB-CG	9.30	121.91	112.60
7	L	194	SER	N-CA-C	9.22	130.44	110.80
5	J	330	ARG	N-CA-C	8.97	124.00	112.34
5	K	174	ASP	CA-CB-CG	8.91	121.51	112.60
2	B	286	ASP	CA-CB-CG	8.63	121.23	112.60
5	J	109	ALA	N-CA-C	8.59	121.72	111.33
5	N	247	ASN	CA-CB-CG	8.57	121.17	112.60
3	C	270	ASP	CA-CB-CG	8.54	121.14	112.60
7	L	198	THR	O-C-N	-8.39	111.31	122.22
2	B	106	PRO	N-CA-C	8.33	124.25	111.34
5	N	154	VAL	O-C-N	8.32	130.21	122.97
5	J	168	HIS	CB-CG-CD2	-8.30	120.41	131.20
5	E	157	ASN	OD1-CG-ND2	-8.00	114.60	122.60
1	A	87	ASN	OD1-CG-ND2	-7.93	114.67	122.60
5	J	6	ASP	CA-CB-CG	7.80	120.41	112.60
4	D	80	HIS	CB-CG-CD2	-7.79	121.08	131.20
7	L	264	MET	N-CA-C	7.78	121.67	110.24
4	D	166	HIS	CB-CG-CD2	-7.77	121.10	131.20
2	B	114	THR	CA-CB-OG1	-7.75	97.98	109.60
7	M	20	ASP	N-CA-C	7.72	120.38	111.11
6	F	281	ASP	CA-CB-CG	7.65	120.25	112.60
3	I	39	MET	N-CA-C	7.65	120.04	109.18
2	B	33	PRO	N-CA-C	7.60	122.43	110.50
1	A	319	SER	N-CA-C	7.59	120.44	111.71
5	H	292	ASN	OD1-CG-ND2	-7.59	115.01	122.60
4	D	131	ALA	N-CA-C	7.58	119.18	111.07
2	B	329	ARG	N-CA-C	7.55	126.88	110.80
7	L	54	GLN	OE1-CD-NE2	-7.51	115.09	122.60
7	M	281	ASP	CA-CB-CG	7.48	120.08	112.60
7	L	206	ASP	CA-CB-CG	7.47	120.07	112.60
3	C	87	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	A	68	HIS	CB-CG-CD2	-7.43	121.54	131.20
7	M	68	HIS	CB-CG-CD2	-7.43	121.54	131.20
5	J	239	ASP	CA-CB-CG	7.40	120.00	112.60
6	F	292	ASN	CA-CB-CG	7.40	120.00	112.60
5	E	269	ILE	N-CA-C	7.38	119.03	110.62
5	H	68	HIS	CB-CG-CD2	-7.38	121.61	131.20
1	A	330	ARG	N-CA-C	7.36	121.70	112.87
5	K	157	ASN	OD1-CG-ND2	-7.36	115.24	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	265	GLU	CA-CB-CG	7.32	128.74	114.10
5	N	7	ASN	OD1-CG-ND2	-7.30	115.30	122.60
3	C	273	THR	CA-CB-OG1	-7.30	98.65	109.60
5	N	115	THR	CA-CB-OG1	-7.30	98.65	109.60
5	K	258	GLN	OE1-CD-NE2	-7.29	115.31	122.60
7	M	156	HIS	CB-CG-CD2	-7.29	121.73	131.20
3	I	110	ASN	OD1-CG-ND2	-7.25	115.35	122.60
7	M	26	PHE	N-CA-C	7.24	117.45	108.11
4	D	290	ASN	CA-CB-CG	7.22	119.82	112.60
5	J	157	ASN	CA-CB-CG	7.22	119.82	112.60
3	I	83	HIS	CB-CG-CD2	-7.18	121.86	131.20
2	B	86	ASN	OD1-CG-ND2	-7.16	115.44	122.60
5	E	154	VAL	CB-CA-C	-7.15	105.02	111.74
6	F	96	HIS	CB-CG-CD2	-7.15	121.90	131.20
1	G	87	ASN	OD1-CG-ND2	-7.14	115.46	122.60
5	E	157	ASN	CA-CB-CG	7.14	119.74	112.60
5	K	272	THR	CA-CB-OG1	-7.13	98.91	109.60
1	A	239	ASP	CA-CB-CG	7.11	119.71	112.60
4	D	32	PRO	N-CA-C	7.11	122.41	111.11
5	E	115	THR	CA-CB-OG1	-7.10	98.95	109.60
5	N	318	SER	N-CA-C	7.10	125.92	110.80
5	N	149	ASP	CA-CB-CG	7.09	119.69	112.60
7	M	168	HIS	CB-CG-CD2	-7.09	121.98	131.20
5	K	330	ARG	N-CA-C	7.08	125.87	110.80
1	A	75	ASP	CA-CB-CG	7.07	119.67	112.60
5	E	152	ASP	CA-CB-CG	7.06	119.66	112.60
1	G	132	GLN	OE1-CD-NE2	-7.05	115.55	122.60
7	M	229	SER	N-CA-C	7.05	121.46	112.86
5	J	168	HIS	CA-CB-CG	7.04	120.83	113.80
6	F	130	ALA	N-CA-C	7.03	120.78	108.75
3	C	258	HIS	CA-C-N	7.03	127.62	119.47
3	C	258	HIS	C-N-CA	7.03	127.62	119.47
5	N	11	LEU	N-CA-C	7.02	119.85	108.41
1	G	19	ASP	CA-CB-CG	7.02	119.62	112.60
5	N	123	ASN	OD1-CG-ND2	-7.01	115.59	122.60
5	K	180	LEU	CA-C-O	-7.01	113.12	120.55
5	E	36	GLN	OE1-CD-NE2	-7.01	115.59	122.60
3	C	168	HIS	CB-CG-CD2	-6.97	122.14	131.20
5	N	168	HIS	CB-CG-CD2	-6.96	122.15	131.20
5	J	70	ILE	N-CA-CB	6.95	118.30	110.72
5	H	326	ALA	CA-C-N	6.94	124.66	119.66
5	H	326	ALA	C-N-CA	6.94	124.66	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	283	ASP	N-CA-C	6.93	118.83	111.28
3	I	210	LYS	N-CA-C	6.91	118.89	111.36
5	E	197	THR	CA-CB-OG1	-6.90	99.25	109.60
5	E	293	VAL	N-CA-C	6.87	117.76	107.80
5	H	306	ASP	CA-CB-CG	6.85	119.45	112.60
5	J	247	ASN	OD1-CG-ND2	-6.85	115.75	122.60
3	C	73	ASN	OD1-CG-ND2	-6.85	115.75	122.60
2	B	347	GLN	OE1-CD-NE2	-6.84	115.75	122.60
7	M	194	SER	N-CA-C	6.83	120.81	111.39
1	G	96	HIS	N-CA-C	6.79	121.56	108.45
6	F	270	HIS	CA-CB-CG	6.79	120.58	113.80
5	E	330	ARG	N-CA-C	6.78	125.24	110.80
6	F	168	HIS	CB-CG-CD2	-6.76	122.41	131.20
3	C	65	PRO	N-CA-C	6.75	122.30	114.20
7	M	76	ASP	CA-CB-CG	6.73	119.33	112.60
5	N	96	HIS	CB-CG-CD2	-6.73	122.45	131.20
5	K	281	ASP	CA-CB-CG	6.72	119.32	112.60
7	M	96	HIS	CB-CG-CD2	-6.71	122.47	131.20
5	J	70	ILE	CB-CA-C	-6.71	102.59	110.91
5	H	301	TYR	N-CA-C	6.71	117.82	109.57
5	H	68	HIS	CB-CG-ND1	6.71	132.76	122.70
5	N	52	GLU	CA-CB-CG	6.69	127.49	114.10
7	L	107	PRO	O-C-N	-6.69	113.61	122.64
3	I	330	ARG	N-CA-C	6.68	121.03	112.34
5	E	301	TYR	N-CA-C	6.68	118.12	109.64
5	N	196	VAL	N-CA-C	6.67	116.89	111.62
2	B	280	ASP	N-CA-C	6.65	124.97	110.80
1	G	168	HIS	CA-CB-CG	6.63	120.44	113.80
5	N	76	ASP	CA-CB-CG	6.63	119.23	112.60
7	L	87	ASN	CA-CB-CG	6.63	119.23	112.60
5	H	273	THR	CA-CB-OG1	-6.62	99.66	109.60
5	J	301	TYR	N-CA-C	6.62	119.02	109.48
5	H	330	ARG	N-CA-C	6.59	124.84	110.80
7	L	294	LEU	N-CA-C	6.58	120.76	110.17
7	L	76	ASP	CA-CB-CG	6.57	119.17	112.60
6	F	287	ASP	CA-CB-CG	6.56	119.16	112.60
4	D	279	ASP	CA-CB-CG	6.56	119.16	112.60
5	K	168	HIS	CB-CG-CD2	-6.56	122.67	131.20
5	K	19	ASP	CA-CB-CG	6.56	119.16	112.60
5	J	168	HIS	CB-CG-ND1	6.54	132.51	122.70
5	H	161	TYR	CA-CB-CG	6.53	125.66	113.90
6	F	92	ALA	CA-C-N	6.53	126.03	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	92	ALA	C-N-CA	6.53	126.03	119.24
1	G	156	HIS	CB-CG-CD2	-6.53	122.71	131.20
5	E	82	HIS	CB-CG-CD2	-6.50	122.75	131.20
5	J	104	PRO	N-CA-C	6.48	125.82	112.47
1	G	74	TRP	N-CA-C	6.46	120.26	112.38
5	E	198	THR	N-CA-C	6.46	124.56	110.80
2	B	180	THR	CA-CB-OG1	-6.46	99.92	109.60
3	I	168	HIS	CB-CG-CD2	-6.46	122.81	131.20
5	E	168	HIS	CB-CG-CD2	-6.45	122.81	131.20
5	H	157	ASN	OD1-CG-ND2	-6.45	116.15	122.60
7	L	361	GLY	CA-C-N	6.44	125.93	119.24
7	L	361	GLY	C-N-CA	6.44	125.93	119.24
5	H	94	GLU	N-CA-C	6.43	120.23	112.38
5	E	197	THR	CA-CB-CG2	6.42	121.42	110.50
7	L	110	ASN	CA-CB-CG	6.42	119.02	112.60
5	E	46	ASP	CA-CB-CG	6.42	119.02	112.60
5	K	68	HIS	CB-CG-CD2	-6.40	122.87	131.20
5	N	57	ARG	N-CA-C	6.40	124.43	110.80
5	E	166	LEU	CA-C-N	6.39	125.89	119.24
5	E	166	LEU	C-N-CA	6.39	125.89	119.24
7	M	30	VAL	N-CA-C	-6.38	98.28	107.78
4	D	273	ASN	OD1-CG-ND2	-6.36	116.24	122.60
5	H	19	ASP	CA-CB-CG	6.36	118.96	112.60
7	M	82	HIS	CB-CG-CD2	-6.36	122.93	131.20
7	L	285	ARG	CA-C-O	-6.34	114.16	120.82
5	N	301	TYR	N-CA-C	6.34	118.65	109.84
5	J	205	ARG	O-C-N	6.32	129.41	122.20
5	J	73	ASN	OD1-CG-ND2	-6.31	116.29	122.60
5	J	68	HIS	CB-CG-CD2	-6.30	123.00	131.20
7	L	156	HIS	CB-CG-CD2	-6.30	123.01	131.20
5	N	241	GLN	OE1-CD-NE2	-6.30	116.30	122.60
5	H	54	GLN	OE1-CD-NE2	-6.29	116.31	122.60
5	E	106	ASN	N-CA-C	6.28	117.29	109.57
3	I	155	THR	N-CA-CB	-6.27	100.70	110.55
4	D	6	ASN	CA-CB-CG	6.26	118.86	112.60
6	F	157	ASN	OD1-CG-ND2	-6.25	116.35	122.60
7	L	61	THR	N-CA-C	-6.24	98.55	108.73
3	I	130	SER	N-CA-C	6.24	119.67	109.06
5	H	310	LYS	N-CA-C	6.24	118.16	111.36
4	D	114	GLN	N-CA-C	6.23	117.95	111.03
1	A	156	HIS	CA-CB-CG	6.22	120.02	113.80
4	D	6	ASN	OD1-CG-ND2	-6.22	116.38	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	243	ILE	N-CA-CB	6.20	117.89	110.95
6	F	267	ALA	N-CA-C	6.19	119.59	110.30
1	A	168	HIS	CB-CG-CD2	-6.17	123.17	131.20
7	M	228	SER	N-CA-C	6.17	123.94	110.80
6	F	65	TYR	CA-C-N	6.17	125.86	119.82
6	F	65	TYR	C-N-CA	6.17	125.86	119.82
7	L	83	HIS	CB-CG-CD2	-6.16	123.19	131.20
7	L	68	HIS	CB-CG-CD2	-6.16	123.19	131.20
7	M	348	GLN	OE1-CD-NE2	-6.16	116.44	122.60
4	D	73	ASP	CA-CB-CG	6.14	118.75	112.60
7	M	300	MET	N-CA-C	6.14	120.50	113.19
1	G	247	ASN	OD1-CG-ND2	-6.13	116.47	122.60
5	K	273	THR	CA-CB-OG1	-6.13	100.41	109.60
5	H	198	THR	N-CA-C	6.12	118.46	111.11
5	N	130	ALA	N-CA-C	6.11	119.45	109.06
1	A	96	HIS	N-CA-C	6.11	120.24	108.45
1	A	130	SER	N-CA-C	6.11	119.44	109.24
5	K	156	HIS	CB-CG-CD2	-6.09	123.28	131.20
3	C	247	ASN	CA-CB-CG	6.09	118.69	112.60
3	C	156	HIS	CA-CB-CG	6.09	119.89	113.80
6	F	83	HIS	CB-CG-CD2	-6.08	123.29	131.20
4	D	114	GLN	OE1-CD-NE2	-6.08	116.52	122.60
1	A	270	ASP	CA-CB-CG	6.08	118.68	112.60
2	B	204	ARG	NE-CZ-NH2	-6.07	113.74	119.20
7	L	96	HIS	CB-CG-CD2	-6.07	123.31	131.20
5	J	51	ASP	N-CA-C	6.07	117.69	111.14
7	M	333	SER	N-CA-C	6.06	118.67	111.33
1	G	281	ASP	CA-CB-CG	6.06	118.66	112.60
1	G	83	HIS	CA-CB-CG	6.05	119.85	113.80
5	K	326	ALA	CA-C-N	6.05	124.01	119.66
5	K	326	ALA	C-N-CA	6.05	124.01	119.66
4	D	8	SER	N-CA-C	6.03	123.64	110.80
6	F	157	ASN	CA-CB-CG	6.03	118.62	112.60
3	C	330	ARG	N-CA-C	6.02	120.23	113.01
7	M	326	ALA	CA-C-N	6.02	123.99	119.66
7	M	326	ALA	C-N-CA	6.02	123.99	119.66
5	K	269	ILE	N-CA-CB	-6.01	104.31	110.62
6	F	330	ARG	N-CA-C	5.99	123.57	110.80
3	I	304	ILE	N-CA-C	5.99	116.73	110.62
5	J	191	ARG	CA-CB-CG	5.99	126.08	114.10
2	B	167	HIS	CB-CG-CD2	-5.97	123.44	131.20
5	H	20	ASP	N-CA-C	5.96	117.78	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	83	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	G	68	HIS	CB-CG-CD2	-5.95	123.47	131.20
5	K	157	ASN	CB-CG-ND2	5.95	125.32	116.40
5	J	270	HIS	CA-CB-CG	5.95	119.75	113.80
5	K	292	ASN	OD1-CG-ND2	-5.95	116.66	122.60
1	G	149	ASP	CA-CB-CG	5.94	118.54	112.60
1	G	212	CYS	N-CA-C	5.94	117.72	110.41
2	B	148	ASP	CA-CB-CG	5.94	118.54	112.60
5	K	123	ASN	CA-CB-CG	5.94	118.54	112.60
7	L	9	SER	N-CA-C	5.94	118.51	111.33
2	B	95	HIS	CB-CG-CD2	-5.93	123.49	131.20
2	B	82	HIS	CB-CG-CD2	-5.92	123.50	131.20
1	G	106	ASN	CA-C-N	5.92	125.90	120.03
1	G	106	ASN	C-N-CA	5.92	125.90	120.03
5	N	123	ASN	CB-CG-ND2	5.92	125.29	116.40
1	A	82	HIS	CB-CG-CD2	-5.92	123.51	131.20
4	D	325	PRO	O-C-N	-5.92	118.59	121.31
4	D	346	GLN	N-CA-C	5.90	123.38	110.80
5	N	300	MET	N-CA-C	5.90	120.09	113.01
1	A	19	ASP	CA-CB-CG	5.90	118.50	112.60
4	D	77	LYS	CA-CB-CG	-5.90	102.30	114.10
5	H	258	GLN	CA-C-N	5.89	125.59	119.82
5	H	258	GLN	C-N-CA	5.89	125.59	119.82
4	D	166	HIS	CB-CG-ND1	5.89	131.53	122.70
5	J	70	ILE	CA-CB-CG1	5.86	120.37	110.40
5	J	247	ASN	CB-CG-ND2	5.86	125.19	116.40
4	D	44	LYS	N-CA-C	-5.86	104.58	110.97
4	D	104	ASN	CA-CB-CG	5.85	118.45	112.60
7	L	168	HIS	CB-CG-CD2	-5.85	123.60	131.20
7	M	152	ASP	CA-CB-CG	5.85	118.45	112.60
4	D	155	ASN	OD1-CG-ND2	-5.84	116.76	122.60
3	C	258	HIS	CB-CG-CD2	-5.84	123.61	131.20
5	E	300	MET	N-CA-C	5.84	117.65	111.28
3	I	220	GLN	OE1-CD-NE2	-5.83	116.77	122.60
4	D	331	SER	N-CA-C	5.82	123.20	110.80
7	L	195	PHE	N-CA-C	5.82	117.63	111.28
3	C	19	ASP	CA-CB-CG	5.82	118.42	112.60
3	I	101	THR	N-CA-C	5.82	118.33	109.95
3	C	130	SER	N-CA-C	5.82	118.95	109.06
4	D	129	ILE	N-CA-C	5.82	116.78	108.93
6	F	291	ASN	CA-CB-CG	5.82	118.42	112.60
7	L	54	GLN	CG-CD-NE2	5.82	125.13	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	319	THR	N-CA-C	5.82	117.62	111.28
5	N	131	ILE	N-CA-C	5.82	115.91	108.12
5	K	82	HIS	CB-CG-CD2	-5.81	123.64	131.20
5	J	344	LEU	N-CA-C	5.81	118.19	108.96
3	C	35	HIS	CB-CG-CD2	-5.80	123.66	131.20
5	J	309	GLN	OE1-CD-NE2	-5.79	116.81	122.60
5	N	93	PRO	CA-C-N	5.79	128.35	120.54
5	N	93	PRO	C-N-CA	5.79	128.35	120.54
6	F	247	ASN	N-CA-C	5.79	117.59	111.28
5	J	166	LEU	CA-C-N	5.79	125.49	119.82
5	J	166	LEU	C-N-CA	5.79	125.49	119.82
2	B	325	ALA	CA-C-N	5.78	123.83	119.66
2	B	325	ALA	C-N-CA	5.78	123.83	119.66
7	M	92	ALA	CA-C-N	5.78	125.49	119.82
7	M	92	ALA	C-N-CA	5.78	125.49	119.82
1	A	361	GLY	CA-C-N	5.78	125.46	119.56
1	A	361	GLY	C-N-CA	5.78	125.46	119.56
1	A	154	ASN	CA-CB-CG	5.78	118.38	112.60
7	L	281	ASP	CA-CB-CG	5.77	118.37	112.60
5	N	87	ASN	OD1-CG-ND2	-5.77	116.83	122.60
3	C	83	HIS	CB-CG-CD2	-5.77	123.70	131.20
5	K	96	HIS	CB-CG-CD2	-5.76	123.71	131.20
7	L	115	THR	CA-CB-OG1	-5.73	101.00	109.60
5	E	116	GLN	CA-CB-CG	5.73	125.56	114.10
3	I	132	GLN	N-CA-C	5.73	117.98	111.11
4	D	80	HIS	CB-CG-ND1	5.72	131.29	122.70
4	D	45	ASP	N-CA-C	5.72	117.98	111.11
5	J	201	ARG	CA-CB-CG	5.72	125.54	114.10
2	B	246	ASN	CB-CG-ND2	5.72	124.98	116.40
4	D	94	HIS	CB-CG-CD2	-5.71	123.77	131.20
4	D	18	ASP	CA-CB-CG	5.71	118.31	112.60
5	N	361	GLY	CA-C-N	5.71	125.56	119.28
5	N	361	GLY	C-N-CA	5.71	125.56	119.28
4	D	57	GLY	O-C-N	-5.71	116.75	123.09
5	E	33	PRO	N-CA-C	5.71	120.04	111.14
7	M	271	GLU	N-CA-C	5.71	118.71	111.69
3	I	60	LEU	N-CA-C	5.70	118.90	110.46
7	L	83	HIS	CB-CG-ND1	5.70	131.26	122.70
4	D	71	ASN	OD1-CG-ND2	-5.70	116.90	122.60
6	F	37	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	A	22	PRO	N-CA-C	5.69	120.17	110.95
2	B	291	ASN	OD1-CG-ND2	-5.67	116.93	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	151	GLY	O-C-N	5.67	125.03	121.85
1	G	84	THR	CA-CB-OG1	-5.67	101.10	109.60
5	H	272	THR	CA-CB-OG1	-5.66	101.11	109.60
2	B	257	GLN	CA-C-N	5.66	125.33	119.56
2	B	257	GLN	C-N-CA	5.66	125.33	119.56
2	B	237	PRO	N-CA-C	5.65	124.12	112.47
7	M	83	HIS	CB-CG-CD2	-5.65	123.85	131.20
2	B	7	ASN	CA-CB-CG	5.65	118.25	112.60
5	N	283	ASP	CA-CB-CG	5.65	118.25	112.60
2	B	105	ASN	CA-C-N	5.64	125.96	119.92
2	B	105	ASN	C-N-CA	5.64	125.96	119.92
7	L	247	ASN	CA-C-N	5.64	129.29	120.82
7	L	247	ASN	C-N-CA	5.64	129.29	120.82
1	G	95	GLU	CA-CB-CG	5.63	125.37	114.10
1	G	344	LEU	N-CA-C	5.63	117.27	109.15
2	B	246	ASN	CA-CB-CG	5.63	118.23	112.60
6	F	142	ARG	N-CA-C	5.63	118.65	109.24
3	I	273	THR	CA-CB-OG1	-5.63	101.15	109.60
3	I	83	HIS	CB-CG-ND1	5.63	131.14	122.70
4	D	71	ASN	CA-CB-CG	5.62	118.22	112.60
5	E	187	ILE	N-CA-C	5.62	118.11	111.09
5	J	20	ASP	CA-CB-CG	5.62	118.22	112.60
4	D	140	ARG	N-CA-C	5.61	117.72	109.24
7	M	270	HIS	N-CA-C	5.61	117.08	111.07
5	J	173	LEU	N-CA-C	-5.61	98.38	108.48
4	D	164	LEU	CA-C-N	5.61	125.07	119.24
4	D	164	LEU	C-N-CA	5.61	125.07	119.24
5	H	203	ILE	N-CA-C	5.59	116.33	110.62
7	M	166	LEU	CA-C-N	5.59	125.96	119.47
7	M	166	LEU	C-N-CA	5.59	125.96	119.47
7	M	68	HIS	CB-CG-ND1	5.59	131.08	122.70
5	E	157	ASN	CB-CG-ND2	5.58	124.77	116.40
4	D	55	LYS	N-CA-C	5.58	120.58	113.55
5	E	101	THR	N-CA-C	5.58	118.49	109.40
5	K	272	THR	CA-CB-CG2	5.58	119.98	110.50
5	H	35	HIS	CB-CG-CD2	-5.57	123.96	131.20
5	K	280	CYS	N-CA-C	5.57	117.73	110.43
1	A	68	HIS	CB-CG-ND1	5.57	131.05	122.70
5	K	283	ASP	CA-CB-CG	5.57	118.17	112.60
5	J	96	HIS	N-CA-C	5.55	119.17	108.45
5	K	258	GLN	CG-CD-NE2	5.55	124.73	116.40
5	J	35	HIS	CB-CG-CD2	-5.55	123.98	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	156	HIS	CB-CG-ND1	5.54	131.00	122.70
2	B	348	GLN	OE1-CD-NE2	-5.53	117.07	122.60
7	L	106	ASN	CA-CB-CG	5.53	118.13	112.60
4	D	154	HIS	CB-CG-CD2	-5.53	124.02	131.20
6	F	58	ARG	N-CA-C	5.51	122.54	110.80
5	H	180	LEU	N-CA-C	5.51	116.97	111.07
2	B	83	THR	N-CA-C	5.51	117.99	111.33
3	C	156	HIS	CB-CG-CD2	-5.50	124.04	131.20
3	I	166	LEU	CA-C-N	5.50	125.60	119.32
3	I	166	LEU	C-N-CA	5.50	125.60	119.32
2	B	291	ASN	CB-CG-ND2	5.50	124.66	116.40
1	G	35	HIS	CB-CG-CD2	-5.50	124.05	131.20
5	H	118	MET	N-CA-C	5.50	117.73	111.02
7	L	35	HIS	CB-CG-CD2	-5.50	124.06	131.20
5	N	52	GLU	CB-CA-C	-5.49	102.26	110.88
7	L	270	HIS	CB-CG-CD2	-5.49	124.06	131.20
2	B	269	HIS	CB-CG-CD2	-5.48	124.08	131.20
7	M	288	LEU	N-CA-C	-5.47	104.72	111.40
6	F	326	ALA	CA-C-N	5.47	123.66	119.66
6	F	326	ALA	C-N-CA	5.47	123.66	119.66
5	J	123	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	A	46	ASP	N-CA-C	5.47	119.45	112.34
3	I	258	HIS	CB-CG-CD2	-5.47	124.09	131.20
7	L	267	CYS	N-CA-C	-5.47	103.31	110.53
5	N	168	HIS	CB-CG-ND1	5.47	130.90	122.70
1	A	326	ALA	CA-C-N	5.47	126.01	120.38
1	A	326	ALA	C-N-CA	5.47	126.01	120.38
7	L	247	ASN	CA-CB-CG	5.46	118.06	112.60
5	J	258	GLN	CA-C-N	5.46	125.08	119.56
5	J	258	GLN	C-N-CA	5.46	125.08	119.56
5	N	132	GLN	N-CA-C	5.46	122.43	110.80
3	C	300	MET	N-CA-C	5.45	119.77	113.18
5	J	335	TRP	CE2-CD2-CG	-5.45	100.66	107.20
5	E	123	ASN	CA-CB-CG	5.45	118.05	112.60
3	I	289	TYR	N-CA-C	5.44	117.92	111.33
4	D	99	THR	CA-CB-OG1	-5.43	101.45	109.60
3	C	74	TRP	CE2-CD2-CG	-5.43	100.68	107.20
5	H	110	ASN	OD1-CG-ND2	-5.43	117.17	122.60
5	J	304	ILE	N-CA-C	5.43	116.81	110.62
5	H	96	HIS	CB-CG-CD2	-5.42	124.15	131.20
7	M	273	THR	CA-CB-OG1	-5.42	101.46	109.60
3	I	181	THR	CA-CB-OG1	-5.42	101.47	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	81	HIS	CB-CG-CD2	-5.42	124.16	131.20
5	E	318	SER	N-CA-C	5.41	117.88	111.33
5	J	96	HIS	CB-CG-CD2	-5.41	124.17	131.20
5	H	307	ARG	NE-CZ-NH2	5.41	124.07	119.20
5	E	35	HIS	CB-CG-CD2	-5.40	124.18	131.20
5	E	298	THR	CA-CB-OG1	-5.39	101.51	109.60
4	D	74	ASP	CA-CB-CG	5.39	117.99	112.60
5	N	35	HIS	CB-CG-CD2	-5.39	124.20	131.20
5	J	320	MET	N-CA-C	5.39	117.91	111.71
5	N	83	HIS	CB-CG-ND1	5.38	130.77	122.70
5	E	309	GLN	OE1-CD-NE2	-5.37	117.23	122.60
5	N	239	ASP	CA-CB-CG	5.37	117.97	112.60
3	I	96	HIS	CB-CG-CD2	-5.37	124.22	131.20
7	M	116	GLN	OE1-CD-NE2	-5.36	117.24	122.60
5	J	293	VAL	O-C-N	-5.36	117.25	122.93
1	G	351	TRP	CG-CD2-CE3	5.36	139.26	133.90
3	I	82	HIS	CB-CG-CD2	-5.35	124.24	131.20
5	K	218	PHE	N-CA-C	5.35	117.11	111.28
5	N	220	ASN	OD1-CG-ND2	-5.35	117.25	122.60
5	E	275	ASN	CA-CB-CG	5.35	117.95	112.60
3	C	168	HIS	CB-CG-ND1	5.35	130.72	122.70
3	C	361	GLY	CA-C-N	5.34	125.01	119.56
3	C	361	GLY	C-N-CA	5.34	125.01	119.56
2	B	362	SER	N-CA-C	5.34	122.18	110.80
5	J	326	ALA	CA-C-N	5.34	125.88	120.38
5	J	326	ALA	C-N-CA	5.34	125.88	120.38
4	D	346	GLN	OE1-CD-NE2	-5.34	117.26	122.60
1	G	270	ASP	CA-CB-CG	5.34	117.94	112.60
2	B	72	ASN	N-CA-C	5.33	118.31	109.46
6	F	168	HIS	CB-CG-ND1	5.33	130.70	122.70
2	B	54	GLN	OE1-CD-NE2	-5.33	117.27	122.60
5	J	57	ARG	N-CA-C	5.33	118.57	111.75
7	L	229	SER	N-CA-C	5.33	122.15	110.80
5	K	351	TRP	CE2-CD2-CG	-5.33	100.80	107.20
7	M	125	PRO	N-CA-C	-5.33	106.26	113.40
5	N	266	SER	N-CA-C	5.33	117.41	110.43
2	B	129	ALA	N-CA-C	5.32	118.11	108.69
5	K	278	MET	CA-C-O	-5.31	115.42	121.00
5	H	147	VAL	N-CA-C	5.31	115.23	107.37
5	N	108	LYS	N-CA-C	5.31	116.76	110.97
3	I	155	THR	CB-CA-C	5.31	118.89	110.19
4	D	53	GLN	OE1-CD-NE2	-5.30	117.30	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	123	ASN	OD1-CG-ND2	-5.30	117.30	122.60
4	D	179	THR	CA-CB-OG1	-5.30	101.66	109.60
1	G	82	HIS	CB-CG-CD2	-5.29	124.32	131.20
5	N	319	THR	CA-C-O	5.29	124.72	118.90
3	C	83	HIS	CA-CB-CG	5.29	119.09	113.80
4	D	130	GLN	CB-CG-CD	5.29	121.59	112.60
5	K	318	SER	N-CA-C	5.28	120.38	113.30
5	K	351	TRP	CG-CD2-CE3	5.28	139.18	133.90
5	H	224	THR	CA-CB-OG1	-5.28	101.68	109.60
1	A	83	HIS	CA-CB-CG	5.28	119.08	113.80
2	B	240	GLN	OE1-CD-NE2	-5.28	117.32	122.60
5	N	83	HIS	CB-CG-CD2	-5.27	124.35	131.20
3	I	73	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	A	327	PRO	N-CA-C	5.26	117.12	110.70
2	B	3	LEU	N-CA-C	-5.26	101.18	109.50
3	I	74	TRP	CE2-CD2-CG	-5.26	100.88	107.20
5	J	106	ASN	N-CA-C	5.26	117.23	110.39
5	J	345	SER	N-CA-C	5.26	117.01	111.28
3	C	351	TRP	CE2-CD2-CG	-5.26	100.89	107.20
7	M	345	SER	N-CA-C	5.25	119.17	112.87
3	C	224	THR	CA-CB-OG1	-5.25	101.73	109.60
3	I	26	PHE	N-CA-C	5.25	114.33	108.25
1	G	156	HIS	CB-CG-ND1	5.24	130.57	122.70
7	M	252	CYS	CA-C-O	-5.24	113.59	118.73
5	N	330	ARG	N-CA-C	5.24	121.97	110.80
1	A	49	VAL	N-CA-C	5.24	116.27	108.46
6	F	335	TRP	CG-CD2-CE3	5.24	139.14	133.90
3	I	102	GLU	N-CA-C	5.24	117.21	108.99
3	I	315	LEU	N-CA-C	5.23	117.89	111.82
7	L	193	TYR	N-CA-C	5.23	117.08	109.71
2	B	86	ASN	CB-CG-ND2	5.22	124.24	116.40
1	G	361	GLY	CA-C-N	5.22	124.84	119.56
1	G	361	GLY	C-N-CA	5.22	124.84	119.56
5	E	74	TRP	CE2-CD2-CG	-5.22	100.93	107.20
5	J	255	THR	N-CA-C	5.22	118.43	111.75
5	J	333	SER	N-CA-C	5.22	117.64	111.33
5	J	7	ASN	CA-CB-CG	5.22	117.82	112.60
7	M	46	ASP	CA-CB-CG	5.22	117.82	112.60
5	N	210	LYS	N-CA-C	5.22	117.77	111.40
1	A	258	HIS	CB-CG-CD2	-5.21	124.42	131.20
2	B	180	THR	CA-CB-CG2	5.21	119.36	110.50
5	E	73	ASN	OD1-CG-ND2	-5.21	117.39	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	80	ILE	N-CA-CB	5.21	116.64	110.55
5	N	166	LEU	CA-C-N	5.21	124.83	119.05
5	N	166	LEU	C-N-CA	5.21	124.83	119.05
2	B	19	ASP	CA-CB-CG	5.21	117.81	112.60
2	B	265	SER	N-CA-C	5.20	117.00	110.24
7	M	74	TRP	CE2-CD2-CG	-5.20	100.95	107.20
1	G	83	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	G	316	ALA	CA-C-N	5.20	125.19	119.89
1	G	316	ALA	C-N-CA	5.20	125.19	119.89
5	J	237	LEU	CA-C-N	5.20	126.34	119.84
5	J	237	LEU	C-N-CA	5.20	126.34	119.84
2	B	72	ASN	OD1-CG-ND2	-5.20	117.40	122.60
5	J	287	ASP	CA-CB-CG	5.20	117.80	112.60
7	M	176	ALA	CA-C-N	5.20	125.86	119.99
7	M	176	ALA	C-N-CA	5.20	125.86	119.99
1	G	311	GLU	CB-CG-CD	5.20	121.44	112.60
3	C	60	LEU	N-CA-C	5.19	117.77	110.14
2	B	91	ALA	CA-C-N	5.19	125.23	119.32
2	B	91	ALA	C-N-CA	5.19	125.23	119.32
3	I	351	TRP	CE2-CD2-CG	-5.19	100.97	107.20
7	M	220	GLN	OE1-CD-NE2	-5.19	117.41	122.60
5	H	361	GLY	CA-C-N	5.18	125.48	119.47
5	H	361	GLY	C-N-CA	5.18	125.48	119.47
5	H	156	HIS	CB-CG-CD2	-5.18	124.46	131.20
5	J	103	ALA	CA-C-N	5.18	126.32	119.84
5	J	103	ALA	C-N-CA	5.18	126.32	119.84
3	C	351	TRP	CB-CG-CD1	-5.18	119.13	126.90
2	B	344	SER	N-CA-C	5.17	117.59	111.33
5	E	92	ALA	CA-C-N	5.17	125.22	119.32
5	E	92	ALA	C-N-CA	5.17	125.22	119.32
2	B	73	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	G	241	GLN	N-CA-C	5.17	117.97	109.76
5	H	1	THR	CA-CB-OG1	-5.16	101.86	109.60
5	K	228	SER	N-CA-C	5.16	121.79	110.80
2	B	268	ILE	N-CA-C	5.16	115.77	110.36
3	C	123	ASN	OD1-CG-ND2	-5.15	117.45	122.60
7	L	87	ASN	OD1-CG-ND2	-5.15	117.45	122.60
5	E	327	PRO	CA-C-N	5.15	124.32	118.97
5	E	327	PRO	C-N-CA	5.15	124.32	118.97
3	I	101	THR	CA-CB-OG1	-5.14	101.88	109.60
3	I	300	MET	N-CA-C	5.14	119.27	112.89
5	J	311	GLU	N-CA-C	5.13	116.57	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	201	ARG	CA-CB-CG	5.13	124.37	114.10
4	D	71	ASN	CB-CG-ND2	5.13	124.10	116.40
3	I	7	ASN	OD1-CG-ND2	-5.13	117.47	122.60
3	I	363	SER	N-CA-C	5.13	119.03	112.87
7	L	152	ASP	CA-CB-CG	5.13	117.73	112.60
6	F	298	THR	CA-CB-OG1	-5.13	101.91	109.60
6	F	335	TRP	CE2-CD2-CG	-5.13	101.05	107.20
3	I	189	SER	N-CA-C	5.13	116.95	111.36
5	J	205	ARG	CA-C-N	5.13	129.27	120.71
5	J	205	ARG	C-N-CA	5.13	129.27	120.71
7	M	96	HIS	CA-C-N	5.13	125.06	119.78
7	M	96	HIS	C-N-CA	5.13	125.06	119.78
2	B	131	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	G	130	SER	N-CA-C	5.12	116.86	109.07
5	N	351	TRP	CE2-CD2-CG	-5.12	101.05	107.20
2	B	108	ALA	N-CA-C	5.12	116.86	111.28
6	F	258	GLN	CA-C-N	5.12	124.73	119.56
6	F	258	GLN	C-N-CA	5.12	124.73	119.56
2	B	315	ALA	N-CA-C	5.11	117.91	109.58
1	A	74	TRP	CG-CD2-CE3	5.11	139.01	133.90
7	L	54	GLN	N-CA-C	5.11	116.53	111.07
2	B	49	VAL	N-CA-C	5.10	115.81	107.24
2	B	350	TRP	CE2-CD2-CG	-5.10	101.08	107.20
4	D	31	ARG	CA-C-N	5.10	125.09	119.89
4	D	31	ARG	C-N-CA	5.10	125.09	119.89
5	H	116	GLN	OE1-CD-NE2	-5.10	117.50	122.60
6	F	60	ILE	CA-C-O	5.10	123.57	119.29
1	A	311	GLU	CA-C-O	-5.09	115.47	120.82
5	K	258	GLN	O-C-N	-5.09	116.81	121.34
1	A	74	TRP	N-CA-C	5.09	119.12	113.01
6	F	333	SER	N-CA-C	5.09	118.27	111.75
7	L	266	SER	CA-C-O	5.09	126.49	120.89
5	N	81	TRP	CE2-CD2-CG	-5.09	101.09	107.20
7	L	319	THR	N-CA-CB	-5.09	102.62	110.25
7	M	6	ASP	CA-CB-CG	5.09	117.69	112.60
5	E	106	ASN	CA-C-N	5.09	125.00	119.76
5	E	106	ASN	C-N-CA	5.09	125.00	119.76
3	I	34	ARG	N-CA-C	5.08	118.58	112.38
6	F	82	HIS	CB-CG-CD2	-5.08	124.59	131.20
5	H	351	TRP	CE2-CD2-CG	-5.08	101.10	107.20
5	J	106	ASN	OD1-CG-ND2	-5.08	117.52	122.60
7	L	22	PRO	N-CA-C	5.08	118.85	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	TRP	CE2-CD2-CG	-5.07	101.11	107.20
5	K	68	HIS	CB-CG-ND1	5.07	130.31	122.70
3	I	156	HIS	CA-CB-CG	5.07	118.87	113.80
3	C	74	TRP	CG-CD2-CE3	5.07	138.97	133.90
5	K	94	GLU	N-CA-C	5.07	118.95	112.87
5	J	44	GLN	OE1-CD-NE2	-5.06	117.54	122.60
5	H	7	ASN	CA-CB-CG	5.06	117.66	112.60
5	H	97	PRO	CA-C-O	-5.06	115.57	121.34
5	E	40	VAL	N-CA-C	5.06	114.90	108.12
1	G	258	HIS	CA-C-N	5.06	124.84	119.28
1	G	258	HIS	C-N-CA	5.06	124.84	119.28
5	H	186	LYS	CA-CB-CG	5.06	124.21	114.10
3	C	20	ASP	CA-CB-CG	5.06	117.66	112.60
6	F	20	ASP	CA-CB-CG	5.05	117.65	112.60
5	J	74	TRP	CE2-CD2-CG	-5.05	101.14	107.20
5	E	81	TRP	CE2-CD2-CG	-5.05	101.14	107.20
5	H	152	ASP	CA-CB-CG	5.05	117.65	112.60
2	B	209	LYS	CA-CB-CG	5.05	124.19	114.10
2	B	289	ALA	N-CA-C	5.05	119.44	113.28
1	A	219	GLU	N-CA-C	5.04	116.59	111.14
5	H	29	ILE	N-CA-C	-5.04	100.99	108.45
5	E	247	ASN	CA-CB-CG	5.04	117.64	112.60
5	H	130	ALA	N-CA-C	5.04	117.63	109.06
3	I	270	ASP	CA-CB-CG	5.04	117.64	112.60
5	N	335	TRP	CE2-CD2-CG	-5.04	101.15	107.20
6	F	351	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	G	103	ALA	CA-C-N	5.04	125.04	119.90
1	G	103	ALA	C-N-CA	5.04	125.04	119.90
1	A	362	PRO	N-CA-C	5.04	120.39	113.84
4	D	235	LEU	CA-C-N	5.04	125.06	119.32
4	D	235	LEU	C-N-CA	5.04	125.06	119.32
5	H	298	THR	CA-CB-OG1	-5.04	102.05	109.60
5	J	236	GLU	CB-CG-CD	5.04	121.16	112.60
1	G	351	TRP	CE2-CD2-CG	-5.03	101.16	107.20
7	L	21	ALA	CA-C-N	5.03	125.26	119.83
7	L	21	ALA	C-N-CA	5.03	125.26	119.83
1	A	106	ASN	CA-C-N	5.03	124.94	119.76
1	A	106	ASN	C-N-CA	5.03	124.94	119.76
2	B	75	ASP	CA-CB-CG	5.03	117.63	112.60
2	B	204	ARG	O-C-N	5.03	127.52	122.09
3	C	46	ASP	N-CA-C	5.03	118.67	112.54
3	I	168	HIS	CB-CG-ND1	5.03	130.24	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	32	ARG	CA-C-N	5.03	124.94	119.76
7	L	32	ARG	C-N-CA	5.03	124.94	119.76
2	B	54	GLN	CG-CD-NE2	5.02	123.94	116.40
6	F	275	ASN	CA-CB-CG	5.02	117.62	112.60
5	H	22	PRO	N-CA-C	5.02	119.08	111.15
3	I	335	TRP	CE2-CD2-CG	-5.02	101.17	107.20
1	A	258	HIS	CA-C-N	5.02	124.68	119.56
1	A	258	HIS	C-N-CA	5.02	124.68	119.56
1	G	74	TRP	CE2-CD2-CG	-5.02	101.18	107.20
3	I	156	HIS	CB-CG-CD2	-5.02	124.68	131.20
5	H	335	TRP	CE2-CD2-CG	-5.01	101.19	107.20
7	L	103	ALA	N-CA-C	5.01	117.42	110.20
1	A	83	HIS	CB-CG-CD2	-5.01	124.69	131.20
5	J	177	GLY	N-CA-C	5.00	118.69	112.64
2	B	317	SER	N-CA-C	5.00	121.45	110.80
5	K	22	PRO	N-CA-C	5.00	118.94	111.14

There are no chirality outliers.

All (104) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ARG	Sidechain
1	A	142	ARG	Sidechain
1	A	161	TYR	Sidechain
1	A	191	ARG	Sidechain
1	A	193	TYR	Sidechain
1	A	249	ARG	Sidechain
1	A	251	ARG	Sidechain
1	A	274	TYR	Sidechain
1	A	285	ARG	Sidechain
1	A	357	TYR	Sidechain
1	A	57	ARG	Sidechain
1	A	64	TYR	Sidechain
2	B	177	ARG	Sidechain
2	B	190	ARG	Sidechain
2	B	212	TYR	Sidechain
2	B	273	TYR	Sidechain
2	B	284	ARG	Sidechain
2	B	329	ARG	Sidechain
2	B	34	ARG	Sidechain
2	B	48	TYR	Sidechain
2	B	64	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	C	138	TYR	Sidechain
3	C	142	ARG	Peptide
3	C	161	TYR	Sidechain
3	C	183	TYR	Sidechain
3	C	213	TYR	Sidechain
3	C	357	TYR	Sidechain
4	D	140	ARG	Sidechain
4	D	199	ARG	Sidechain
4	D	33	ARG	Sidechain,Peptide
4	D	57	GLY	Peptide
5	E	111	ARG	Sidechain
5	E	193	TYR	Sidechain
5	E	196	VAL	Peptide
5	E	201	ARG	Sidechain
5	E	274	TYR	Sidechain
5	E	357	TYR	Sidechain
5	E	57	ARG	Sidechain
5	E	90	ARG	Sidechain
6	F	164	TYR	Sidechain
6	F	183	TYR	Sidechain
6	F	193	TYR	Sidechain
6	F	301	TYR	Sidechain
6	F	307	ARG	Sidechain
6	F	33	ARG	Sidechain
6	F	332	TYR	Sidechain
1	G	111	ARG	Sidechain
1	G	142	ARG	Sidechain
1	G	167	PRO	Peptide
1	G	193	TYR	Sidechain
1	G	251	ARG	Sidechain
1	G	274	TYR	Sidechain
1	G	64	TYR	Sidechain
5	H	161	TYR	Sidechain
5	H	191	ARG	Sidechain
5	H	205	ARG	Sidechain
5	H	249	ARG	Sidechain
5	H	274	TYR	Sidechain
5	H	332	TYR	Sidechain
5	H	57	ARG	Sidechain
3	I	161	TYR	Sidechain
3	I	183	TYR	Sidechain
3	I	186	LYS	Peptide

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Mol	Chain	Res	Type	Group
3	I	191	ARG	Sidechain
3	I	193	TYR	Sidechain
3	I	274	TYR	Sidechain
3	I	307	ARG	Sidechain
3	I	357	TYR	Sidechain
3	I	64	TYR	Sidechain
5	J	164	TYR	Sidechain
5	J	166	LEU	Peptide
5	J	191	ARG	Sidechain
5	J	281	ASP	Peptide
5	J	307	ARG	Sidechain
5	J	48	TYR	Sidechain
5	K	128	TYR	Sidechain
5	K	183	TYR	Sidechain
5	K	191	ARG	Sidechain
5	K	193	TYR	Sidechain
5	K	201	ARG	Sidechain
5	K	205	ARG	Sidechain
5	K	274	TYR	Sidechain
5	K	317	PRO	Peptide
5	K	332	TYR	Sidechain
7	L	128	TYR	Sidechain
7	L	164	TYR	Sidechain
7	L	213	TYR	Sidechain
7	L	64	TYR	Sidechain
7	L	86	TYR	Sidechain
7	M	111	ARG	Sidechain
7	M	164	TYR	Sidechain
7	M	213	TYR	Sidechain
7	M	227	SER	Peptide
7	M	64	TYR	Sidechain
7	M	86	TYR	Sidechain
5	N	190	GLU	Peptide
5	N	191	ARG	Sidechain
5	N	193	TYR	Sidechain
5	N	213	TYR	Sidechain
5	N	274	TYR	Sidechain
5	N	357	TYR	Sidechain
5	N	60	LEU	Peptide
5	N	64	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	2843	0	2818	54	0
1	G	2843	0	2818	60	0
2	B	2835	0	2813	83	0
3	C	2842	0	2821	72	0
3	I	2842	0	2821	80	0
4	D	2791	0	2766	81	0
5	E	2845	0	2820	78	0
5	H	2845	0	2820	68	0
5	J	2845	0	2820	84	0
5	K	2845	0	2820	72	0
5	N	2845	0	2820	88	0
6	F	2788	0	2770	110	0
7	L	2838	0	2812	80	0
7	M	2838	0	2812	70	0
All	All	39685	0	39351	1001	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 13.

All (1001) 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)
5:E:198:THR:HA	6:F:265:GLU:HG3	1.51	0.91
5:E:248:GLU:HA	5:E:251:ARG:HB3	1.54	0.88
7:L:159:PRO:HG3	7:L:169:ALA:HB3	1.56	0.86
1:G:317:PRO:HG2	1:G:320:MET:HB2	1.58	0.85
7:L:259:PRO:HG2	7:L:266:SER:HB2	1.58	0.84
7:M:159:PRO:HG3	7:M:169:ALA:HB3	1.58	0.84
6:F:190:GLU:HG2	1:G:167:PRO:HB2	1.60	0.83
2:B:154:THR:HB	2:B:172:LEU:HB3	1.59	0.81
4:D:185:ILE:HD13	4:D:246:GLU:HB3	1.62	0.81
1:G:14:ALA:HB3	1:G:24:ALA:HB3	1.61	0.81
3:I:14:ALA:HB3	3:I:24:ALA:HB3	1.62	0.81
5:H:280:CYS:HB3	5:H:284:ILE:HD11	1.62	0.81
5:E:197:THR:HA	6:F:264:MET:HA	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:186:LYS:HZ1	6:F:272:THR:HG22	1.47	0.79
4:D:64:PRO:HB3	4:D:74:ASP:HB2	1.63	0.79
6:F:259:PRO:HB2	6:F:264:MET:HB2	1.64	0.79
3:I:84:THR:HA	3:I:88:GLU:HG2	1.64	0.78
5:H:200:GLU:HA	5:H:203:ILE:HB	1.65	0.78
6:F:66:PRO:HG3	6:F:76:ASP:HB3	1.64	0.77
4:D:157:PRO:HG3	4:D:167:ALA:HB3	1.68	0.76
5:H:159:PRO:HB2	5:H:166:LEU:HD12	1.65	0.76
3:I:195:PHE:HA	3:I:200:GLU:HB3	1.68	0.76
5:J:159:PRO:HG3	5:J:169:ALA:HB3	1.67	0.76
4:D:279:ASP:HB3	4:D:282:ILE:HG12	1.67	0.75
5:N:14:ALA:HB3	5:N:24:ALA:HB3	1.67	0.75
2:B:131:GLN:HG2	2:B:333:VAL:HG21	1.68	0.75
7:M:48:TYR:HB2	7:M:60:LEU:HD21	1.67	0.75
1:G:208:LYS:HA	1:G:212:CYS:SG	2.27	0.75
5:K:191:ARG:HA	7:L:109:ALA:HB3	1.68	0.75
6:F:132:GLN:HG2	6:F:334:VAL:HG11	1.69	0.75
5:K:222:MET:SD	5:K:251:ARG:HD3	2.26	0.74
4:D:57:GLY:HA2	6:F:283:ASP:HB2	1.68	0.74
5:N:215:ALA:HB2	5:N:250:PHE:HB2	1.70	0.74
5:N:6:ASP:HA	5:N:101:THR:HB	1.68	0.74
5:J:263:GLY:HA3	5:K:167:PRO:HD2	1.71	0.73
5:J:200:GLU:HG2	7:L:283:ASP:HB2	1.70	0.72
7:M:132:GLN:HG2	7:M:334:VAL:HG11	1.71	0.72
5:K:248:GLU:HA	5:K:251:ARG:HB2	1.70	0.72
5:J:240:GLY:HA3	7:L:286:LYS:HB3	1.72	0.72
1:A:297:GLY:HA2	1:A:331:LYS:HG2	1.72	0.72
2:B:65:PRO:HG2	2:B:79:ILE:HD12	1.71	0.72
7:L:14:ALA:HB3	7:L:24:ALA:HB3	1.71	0.72
4:D:5:ASP:HA	4:D:99:THR:OG1	1.90	0.71
1:A:239:ASP:HA	3:C:317:PRO:HB3	1.72	0.71
5:K:218:PHE:HD2	5:K:307:ARG:HH21	1.36	0.71
7:L:31:GLY:HA3	7:L:60:LEU:HD23	1.72	0.71
3:C:148:LEU:HD13	3:C:157:VAL:HG22	1.73	0.71
7:M:98:VAL:HG11	7:M:118:MET:HE3	1.72	0.70
3:C:208:LYS:HA	3:C:212:CYS:SG	2.32	0.70
3:I:297:GLY:HA2	3:I:331:LYS:HG2	1.74	0.70
1:A:184:LEU:HA	1:A:187:ILE:HG12	1.74	0.69
3:C:14:ALA:HB3	3:C:24:ALA:HB3	1.73	0.69
6:F:186:LYS:HD2	1:G:168:HIS:HA	1.72	0.69
2:B:194:PHE:HA	2:B:199:GLU:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LYS:HA	1:A:212:CYS:SG	2.33	0.69
3:C:159:PRO:HG3	3:C:169:ALA:HB3	1.75	0.69
5:E:196:VAL:HB	6:F:264:MET:SD	2.32	0.68
3:C:178:ARG:HB3	3:C:178:ARG:NH1	2.08	0.68
1:G:167:PRO:HA	1:G:170:ILE:HG13	1.73	0.68
5:H:14:ALA:HB3	5:H:24:ALA:HB3	1.75	0.68
7:M:252:CYS:SG	7:M:253:PRO:HD3	2.34	0.68
6:F:15:ALA:HB3	6:F:25:ALA:HB3	1.76	0.68
1:G:104:PRO:HG3	1:G:131:ILE:HG23	1.76	0.68
5:K:14:ALA:HB3	5:K:24:ALA:HB3	1.76	0.67
7:M:6:ASP:HB3	7:M:13:LYS:HB2	1.74	0.67
3:I:191:ARG:HG2	5:J:110:ASN:HB2	1.77	0.67
3:C:178:ARG:HB3	3:C:178:ARG:HH11	1.60	0.67
1:A:14:ALA:HB3	1:A:24:ALA:HB3	1.76	0.67
4:D:113:THR:HA	4:D:125:MET:SD	2.35	0.67
5:J:3:LEU:HB2	5:J:98:THR:HG22	1.77	0.66
6:F:273:THR:O	6:F:277:ILE:HG12	1.95	0.66
4:D:64:PRO:HG2	4:D:65:ILE:HG13	1.78	0.66
5:N:31:GLY:HA3	5:N:60:LEU:HD13	1.78	0.66
3:C:135:LEU:HB3	3:C:337:GLY:HA3	1.78	0.66
5:H:248:GLU:HA	5:H:251:ARG:HB2	1.77	0.65
7:L:327:PRO:HG2	7:L:330:ARG:HB3	1.77	0.65
1:A:214:VAL:HG22	1:A:253:PRO:HB3	1.78	0.65
1:A:148:LEU:HD13	1:A:157:VAL:HG22	1.77	0.65
5:K:200:GLU:HA	5:K:203:ILE:HG22	1.76	0.65
1:G:195:PHE:HA	1:G:200:GLU:HB3	1.78	0.65
3:I:175:LEU:HD13	3:I:262:LEU:HG	1.78	0.65
7:L:252:CYS:SG	7:L:253:PRO:HD3	2.36	0.65
5:N:214:VAL:HG22	5:N:253:PRO:HB2	1.78	0.65
5:N:10:GLY:O	5:N:27:PRO:HA	1.97	0.65
5:E:236:GLU:HG2	5:E:242:VAL:HG22	1.78	0.65
3:I:234:SER:HA	3:I:244:THR:HA	1.78	0.64
2:B:184:MET:HB2	2:B:203:VAL:HG11	1.78	0.64
6:F:175:LEU:HD11	6:F:255:THR:HG22	1.80	0.64
3:I:30:VAL:HG21	3:I:76:ASP:HB3	1.80	0.64
3:I:190:GLU:HB3	5:J:102:GLU:HB2	1.78	0.64
3:I:192:GLY:HA3	5:J:70:ILE:HG23	1.80	0.64
2:B:188:THR:HB	3:C:105:MET:HE3	1.79	0.64
7:L:150:SER:HA	7:L:154:VAL:O	1.97	0.64
7:M:14:ALA:HB3	7:M:24:ALA:HB3	1.79	0.64
5:H:208:LYS:HA	5:H:212:CYS:SG	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:247:ASN:HB3	7:M:251:ARG:HH21	1.62	0.64
1:A:237:LEU:HD12	1:A:241:GLN:HG3	1.78	0.63
2:B:191:GLY:HA3	3:C:107:PRO:HA	1.80	0.63
2:B:195:VAL:HG22	3:C:172:ARG:NH1	2.14	0.63
3:I:57:ARG:HG2	3:I:62:LEU:HD11	1.79	0.63
5:N:277:ILE:HG22	5:N:285:ARG:HG2	1.81	0.63
1:A:147:VAL:HA	1:A:293:VAL:O	1.98	0.63
5:H:68:HIS:HB3	5:H:154:VAL:HG13	1.79	0.63
5:E:48:TYR:HB3	5:E:53:ALA:HB2	1.80	0.63
3:I:159:PRO:HG3	3:I:169:ALA:HB3	1.80	0.63
7:L:148:MET:HA	7:L:156:HIS:O	1.98	0.63
2:B:147:LEU:HA	2:B:155:HIS:O	1.99	0.62
5:H:218:PHE:HD2	5:H:307:ARG:HH21	1.46	0.62
4:D:145:VAL:HA	4:D:291:VAL:O	1.99	0.62
7:M:98:VAL:O	7:M:127:MET:HA	1.99	0.62
5:N:115:THR:HA	5:N:127:MET:SD	2.40	0.62
5:K:137:LEU:HD22	5:K:160:ILE:HD13	1.81	0.62
5:H:127:MET:HE1	5:H:129:VAL:HG22	1.82	0.62
5:N:97:PRO:HB3	5:N:126:ALA:HB3	1.80	0.62
2:B:193:SER:HB3	3:C:172:ARG:NH2	2.14	0.62
3:C:66:ILE:HD11	3:C:77:MET:SD	2.39	0.62
6:F:237:LEU:HG	6:F:243:ILE:HD12	1.80	0.62
5:N:83:HIS:HA	5:N:87:ASN:HD22	1.66	0.61
3:C:327:PRO:HB2	3:C:330:ARG:HB3	1.82	0.61
5:E:9:SER:HA	5:E:66:ILE:HB	1.81	0.61
1:G:247:ASN:ND2	1:G:251:ARG:HH21	1.98	0.61
2:B:14:ALA:HB3	2:B:24:ALA:HB3	1.81	0.61
5:E:312:ILE:HB	5:E:322:ILE:HG13	1.81	0.61
5:J:127:MET:SD	5:J:129:VAL:HG23	2.40	0.61
1:A:10:GLY:O	1:A:27:PRO:HA	2.00	0.60
2:B:29:ILE:HD11	2:B:62:LEU:HB3	1.83	0.60
3:C:49:VAL:HG21	3:C:80:ILE:HA	1.83	0.60
3:I:183:TYR:HD2	3:I:252:ALA:HA	1.65	0.60
7:L:70:ILE:HG13	7:L:106:ASN:HD21	1.66	0.60
1:A:356:GLU:HA	1:A:359:GLU:HG2	1.83	0.60
5:E:297:GLY:HA2	5:E:331:LYS:HG3	1.84	0.60
2:B:34:ARG:HG2	2:B:34:ARG:HH21	1.66	0.60
5:J:146:ILE:HD11	5:J:157:ASN:HB3	1.83	0.60
7:M:147:VAL:O	7:M:157:THR:HA	2.02	0.60
5:N:277:ILE:HD12	5:N:288:LEU:HD23	1.82	0.60
3:I:186:LYS:HE2	5:J:167:PRO:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:277:ILE:HG22	6:F:285:ARG:HG2	1.83	0.60
7:L:104:PRO:HB2	7:L:156:HIS:CD2	2.37	0.60
5:E:14:ALA:HB3	5:E:24:ALA:HB3	1.84	0.60
5:E:195:PHE:HZ	5:E:243:ILE:HG12	1.67	0.60
6:F:32:GLY:O	6:F:48:SER:HA	2.02	0.60
5:N:281:ASP:O	5:N:285:ARG:HG3	2.02	0.60
6:F:171:MET:HG2	6:F:276:SER:HB3	1.84	0.59
3:I:190:GLU:HB2	5:J:106:ASN:CG	2.27	0.59
6:F:248:GLU:HA	6:F:251:ARG:HB3	1.83	0.59
5:J:6:ASP:HA	5:J:101:THR:HG22	1.84	0.59
3:I:148:LEU:HD13	3:I:157:VAL:HG22	1.83	0.59
3:I:39:MET:SD	5:K:346:THR:HB	2.43	0.59
3:I:245:ILE:HG22	3:I:249:ARG:HG3	1.84	0.59
5:J:99:LEU:HA	5:J:128:TYR:O	2.03	0.59
7:L:31:GLY:HA2	7:L:61:THR:O	2.03	0.59
5:J:131:ILE:HB	5:J:134:VAL:HB	1.84	0.59
7:L:300:MET:SD	7:L:331:LYS:HG3	2.43	0.59
2:B:190:ARG:NH2	2:B:246:ASN:HB3	2.18	0.59
5:J:330:ARG:HA	5:J:333:SER:OG	2.03	0.59
2:B:97:THR:O	2:B:126:MET:HA	2.03	0.58
3:I:188:LEU:HA	5:J:107:PRO:HG3	1.84	0.58
6:F:211:LEU:HD12	6:F:233:LYS:HB3	1.85	0.58
3:I:183:TYR:CD2	3:I:252:ALA:HA	2.38	0.58
5:K:4:VAL:HG21	5:K:339:SER:HA	1.85	0.58
5:N:256:LEU:HB3	5:N:269:ILE:HD12	1.84	0.58
7:L:6:ASP:HB3	7:L:13:LYS:HB2	1.84	0.58
7:M:62:LEU:HB2	5:N:265:GLU:HG2	1.84	0.58
1:G:97:PRO:HA	1:G:126:ALA:O	2.03	0.58
5:N:146:ILE:HD12	5:N:277:ILE:HD11	1.84	0.58
5:N:281:ASP:HB3	5:N:284:ILE:HG12	1.84	0.58
2:B:3:LEU:HB3	2:B:97:THR:HA	1.85	0.58
5:K:183:TYR:HE2	5:K:252:CYS:HA	1.68	0.57
5:K:66:ILE:HD11	5:K:77:MET:HE1	1.85	0.57
5:K:148:LEU:HA	5:K:156:HIS:O	2.03	0.57
5:J:147:VAL:HA	5:J:293:VAL:O	2.04	0.57
3:C:98:VAL:O	3:C:127:PHE:HA	2.04	0.57
6:F:6:CYS:HA	6:F:14:LYS:O	2.05	0.57
3:I:31:GLY:HA3	3:I:60:LEU:HD13	1.86	0.57
7:L:155:THR:OG1	7:L:173:LEU:HB3	2.05	0.57
7:M:184:LEU:HD13	7:M:252:CYS:SG	2.44	0.57
4:D:5:ASP:O	4:D:11:VAL:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:45:GLN:HE22	6:F:60:ILE:HB	1.70	0.57
5:N:140:SER:HB2	5:N:142:ARG:HH21	1.69	0.57
2:B:190:ARG:HH21	2:B:246:ASN:HB3	1.69	0.57
5:J:14:ALA:HB3	5:J:24:ALA:HB3	1.84	0.57
2:B:29:ILE:HG23	2:B:50:GLY:HA2	1.87	0.57
4:D:152:VAL:HG12	4:D:172:ASP:HA	1.85	0.57
5:E:113:LYS:HA	5:E:116:GLN:NE2	2.20	0.57
1:G:159:PRO:HG2	1:G:169:ALA:HB3	1.87	0.57
5:H:203:ILE:HD12	5:H:238:PRO:HD3	1.87	0.57
2:B:146:VAL:HA	2:B:292:VAL:O	2.05	0.56
4:D:203:ARG:O	4:D:206:LYS:HG2	2.05	0.56
5:H:148:LEU:HA	5:H:156:HIS:O	2.04	0.56
5:H:234:SER:HA	5:H:243:ILE:O	2.06	0.56
3:C:149:ASP:O	3:C:155:THR:HA	2.05	0.56
5:H:157:ASN:O	5:H:170:ILE:HA	2.05	0.56
5:K:102:GLU:HB2	5:K:106:ASN:ND2	2.18	0.56
5:J:6:ASP:O	5:J:12:VAL:HA	2.05	0.56
2:B:200:ARG:HA	2:B:203:VAL:HG12	1.87	0.56
5:E:158:VAL:HG22	5:E:170:ILE:HG23	1.88	0.56
7:L:158:VAL:HG22	7:L:170:ILE:HG23	1.88	0.56
1:A:7:ASN:HA	1:A:12:CYS:SG	2.46	0.56
2:B:30:VAL:HG12	2:B:49:VAL:HG23	1.87	0.56
5:K:98:THR:O	5:K:127:MET:HA	2.06	0.56
7:M:94:GLU:HA	7:M:123:ASN:O	2.06	0.56
6:F:37:GLN:OE1	6:F:37:GLN:HA	2.06	0.56
5:N:267:ALA:HB1	5:N:271:GLU:HB2	1.88	0.56
5:E:6:ASP:O	5:E:12:VAL:HA	2.06	0.55
5:H:65:PRO:HG2	5:H:80:ILE:HD11	1.89	0.55
3:C:33:PRO:HG2	3:C:36:GLN:HG2	1.88	0.55
4:D:9:GLY:O	4:D:26:PRO:HA	2.05	0.55
6:F:192:GLY:HA2	1:G:105:MET:HA	1.88	0.55
5:N:257:PHE:O	5:N:268:GLY:HA3	2.05	0.55
6:F:286:LYS:HD3	6:F:320:MET:HG3	1.87	0.55
7:L:293:VAL:HA	7:L:325:ILE:O	2.06	0.55
7:M:6:ASP:HA	7:M:101:THR:HG22	1.89	0.55
5:E:146:ILE:HB	5:E:288:LEU:HG	1.88	0.55
5:E:197:THR:OG1	6:F:264:MET:SD	2.64	0.55
7:L:188:LEU:HD23	7:L:193:TYR:HB2	1.89	0.55
7:L:192:GLY:O	7:M:109:ALA:HB2	2.06	0.55
2:B:174:LEU:HD12	2:B:263:MET:SD	2.46	0.55
7:M:293:VAL:HA	7:M:325:ILE:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:190:GLU:HG2	5:J:103:ALA:C	2.32	0.55
2:B:186:ILE:HA	2:B:189:GLU:HG2	1.89	0.55
4:D:153:THR:OG1	4:D:171:LEU:HB3	2.07	0.55
6:F:7:ASP:HA	6:F:101:THR:OG1	2.06	0.55
7:M:30:VAL:HG21	7:M:76:ASP:O	2.07	0.55
1:G:356:GLU:HA	1:G:359:GLU:HG2	1.89	0.55
6:F:148:LEU:HA	6:F:156:HIS:O	2.07	0.55
5:E:196:VAL:HG12	6:F:264:MET:HB3	1.88	0.54
5:E:3:LEU:HD22	5:E:89:LEU:HD13	1.89	0.54
5:E:40:VAL:HB	1:G:163:GLY:HA3	1.89	0.54
5:E:4:VAL:HG21	5:E:339:SER:HA	1.89	0.54
3:I:54:GLN:O	3:I:57:ARG:HG3	2.06	0.54
5:J:10:GLY:O	5:J:27:PRO:HA	2.07	0.54
7:M:157:THR:O	7:M:170:ILE:HA	2.08	0.54
5:E:148:LEU:HD22	5:E:308:MET:HE2	1.90	0.54
1:G:5:ILE:HB	1:G:100:LEU:HD23	1.89	0.54
5:H:31:GLY:HA3	5:H:60:LEU:HD13	1.88	0.54
5:H:146:ILE:O	5:H:292:ASN:HA	2.08	0.54
6:F:259:PRO:CB	6:F:264:MET:HB2	2.35	0.54
5:K:239:ASP:HB3	7:M:283:ASP:HA	1.90	0.54
5:N:152:ASP:HA	5:N:177:GLY:HA3	1.90	0.54
5:J:201:ARG:HG3	5:J:201:ARG:HH11	1.71	0.54
7:L:130:ALA:HB1	7:L:135:LEU:HD11	1.90	0.54
5:N:286:LYS:HD2	5:N:320:MET:HA	1.90	0.54
2:B:202:ILE:HD12	2:B:237:PRO:HD2	1.90	0.54
4:D:98:LEU:HD11	4:D:116:MET:SD	2.48	0.54
6:F:210:LYS:HB2	6:F:211:LEU:HD22	1.88	0.54
7:L:293:VAL:HG22	7:L:325:ILE:HB	1.90	0.54
6:F:146:ILE:HD11	6:F:157:ASN:HB3	1.88	0.54
3:I:44:GLN:HG3	3:I:45:LYS:HG3	1.88	0.54
3:I:175:LEU:HD12	3:I:179:ASP:HB2	1.89	0.54
3:I:300:MET:HA	3:I:330:ARG:NH2	2.23	0.54
5:K:146:ILE:O	5:K:292:ASN:HA	2.07	0.54
2:B:155:HIS:HA	2:B:170:MET:O	2.08	0.54
4:D:130:GLN:HG2	4:D:332:VAL:HG11	1.90	0.54
5:E:150:SER:HA	5:E:155:THR:HA	1.89	0.54
5:E:157:ASN:HB2	5:E:171:MET:HB2	1.90	0.54
5:E:200:GLU:HA	5:E:203:ILE:HB	1.89	0.54
1:G:146:ILE:HA	1:G:158:VAL:O	2.07	0.54
3:I:68:HIS:HA	3:I:154:VAL:HB	1.89	0.54
5:J:208:LYS:HA	5:J:212:CYS:SG	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:151:GLY:O	7:M:176:ALA:HB1	2.08	0.54
4:D:156:VAL:HG22	4:D:168:ILE:HG23	1.91	0.53
3:I:148:LEU:HD21	3:I:269:ILE:HB	1.90	0.53
2:B:4:VAL:HG12	2:B:98:LEU:HB3	1.90	0.53
5:N:4:VAL:HG21	5:N:339:SER:HA	1.90	0.53
2:B:207:LYS:HA	2:B:211:CYS:SG	2.48	0.53
5:E:293:VAL:HG22	5:E:325:ILE:HB	1.91	0.53
7:L:186:LYS:O	7:L:189:THR:HG22	2.09	0.53
2:B:6:ASP:O	2:B:12:VAL:HA	2.09	0.53
5:H:27:PRO:HB2	5:H:29:ILE:HG12	1.90	0.53
1:A:30:VAL:HB	1:A:76:ASP:OD2	2.09	0.53
1:A:84:THR:HA	1:A:88:GLU:HB2	1.91	0.53
3:I:356:GLU:HA	3:I:359:GLU:HG2	1.90	0.53
5:K:102:GLU:HB2	5:K:106:ASN:HD22	1.74	0.53
5:J:148:LEU:HA	5:J:156:HIS:O	2.08	0.53
7:M:52:GLU:O	7:M:56:LYS:HG2	2.09	0.53
5:H:86:TYR:O	5:H:90:ARG:HA	2.08	0.53
3:I:3:LEU:HD22	3:I:89:LEU:HD13	1.91	0.53
5:K:188:LEU:HA	5:K:191:ARG:HB2	1.91	0.53
5:N:146:ILE:O	5:N:292:ASN:HA	2.09	0.53
3:C:180:LEU:HB3	3:C:208:LYS:HD2	1.91	0.53
7:L:58:GLY:O	7:M:265:GLU:HB2	2.09	0.53
7:L:205:ARG:O	7:L:208:LYS:HB3	2.09	0.53
3:C:142:ARG:HG2	3:C:144:THR:O	2.09	0.53
6:F:208:LYS:HA	6:F:212:CYS:SG	2.49	0.53
5:E:69:GLY:O	5:E:103:ALA:HB2	2.08	0.52
6:F:95:GLU:HB2	6:F:96:HIS:ND1	2.24	0.52
7:M:59:ILE:HG23	7:M:60:LEU:HD13	1.91	0.52
4:D:91:PRO:O	4:D:122:VAL:HA	2.10	0.52
4:D:210:CYS:HB3	4:D:251:PRO:HD3	1.90	0.52
4:D:214:LEU:O	4:D:308:LYS:HE2	2.08	0.52
5:H:69:GLY:O	5:H:103:ALA:HB2	2.09	0.52
5:K:289:TYR:O	5:K:322:ILE:HA	2.10	0.52
7:L:294:LEU:HD23	7:L:299:THR:HB	1.89	0.52
5:N:27:PRO:O	5:N:50:GLY:HA2	2.10	0.52
2:B:308:GLN:HG3	2:B:321:ILE:HG21	1.91	0.52
3:C:5:ILE:HB	3:C:100:LEU:HD23	1.91	0.52
4:D:57:GLY:CA	6:F:283:ASP:HB2	2.37	0.52
5:J:27:PRO:O	5:J:50:GLY:HA2	2.09	0.52
7:L:184:LEU:HD13	7:L:252:CYS:SG	2.49	0.52
7:L:236:GLU:HG3	7:L:242:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ARG:NH1	3:C:258:HIS:HB3	2.25	0.52
4:D:28:ILE:O	4:D:48:VAL:HA	2.09	0.52
1:G:180:LEU:HD21	1:G:256:LEU:HG	1.90	0.52
3:I:98:VAL:O	3:I:127:PHE:HA	2.09	0.52
7:L:70:ILE:HG13	7:L:106:ASN:ND2	2.24	0.52
5:N:98:THR:O	5:N:127:MET:HA	2.08	0.52
5:E:108:LYS:HA	5:E:111:ARG:HG2	1.92	0.52
6:F:67:ILE:HG13	6:F:77:MET:SD	2.50	0.52
5:H:45:LYS:HD3	5:H:46:ASP:H	1.74	0.52
3:I:4:VAL:HG11	3:I:338:GLY:HA3	1.90	0.52
5:J:197:THR:OG1	5:J:200:GLU:HG3	2.09	0.52
5:K:75:ASP:CG	5:K:79:LYS:HZ1	2.18	0.52
7:L:270:HIS:HD2	7:L:315:LEU:HD11	1.74	0.52
7:M:189:THR:HG21	5:N:107:PRO:HB3	1.91	0.52
1:A:113:LYS:NZ	1:A:113:LYS:HA	2.25	0.52
3:I:49:VAL:HG21	3:I:80:ILE:HA	1.91	0.52
7:M:211:LEU:O	7:M:249:ARG:HD2	2.10	0.52
1:G:2:ALA:HB3	1:G:17:ALA:HB2	1.92	0.52
1:G:92:ALA:O	1:G:95:GLU:HB3	2.10	0.52
3:I:147:VAL:O	3:I:157:VAL:HA	2.10	0.52
5:J:312:ILE:HG22	5:J:322:ILE:HD13	1.91	0.52
2:B:209:LYS:HB2	2:B:210:LEU:HD22	1.92	0.52
3:C:294:MET:O	3:C:327:PRO:HD2	2.09	0.52
5:J:3:LEU:HA	5:J:15:GLY:O	2.10	0.52
5:J:4:VAL:O	5:J:14:ALA:HA	2.10	0.52
5:N:7:ASN:HA	5:N:12:VAL:HA	1.91	0.52
2:B:5:CYS:HA	2:B:13:LYS:O	2.09	0.52
3:C:297:GLY:HA2	3:C:331:LYS:HG2	1.91	0.52
5:K:5:CYS:O	5:K:100:LEU:HA	2.10	0.52
1:G:98:VAL:O	1:G:127:PHE:HA	2.10	0.51
7:L:235:TYR:O	7:L:243:ILE:HG12	2.10	0.51
7:M:11:MET:O	7:M:13:LYS:NZ	2.43	0.51
5:J:160:ILE:HA	5:J:165:ALA:HA	1.92	0.51
7:L:149:ASP:HB3	7:L:156:HIS:HB2	1.92	0.51
4:D:111:LYS:HA	4:D:114:GLN:HG3	1.92	0.51
5:H:148:LEU:HD11	5:H:269:ILE:HG23	1.92	0.51
7:M:208:LYS:HA	7:M:212:CYS:SG	2.50	0.51
5:N:5:CYS:HB3	5:N:100:LEU:HD23	1.92	0.51
4:D:33:ARG:HG2	4:D:58:ILE:HA	1.93	0.51
6:F:46:LYS:HZ1	6:F:61:LEU:HD21	1.75	0.51
3:I:192:GLY:O	5:J:70:ILE:HD12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:155:THR:HG23	7:L:175:LEU:O	2.10	0.51
3:I:3:LEU:HA	3:I:16:PHE:HA	1.92	0.51
2:B:183:LEU:HD23	2:B:203:VAL:HG22	1.92	0.51
2:B:274:ASN:HA	2:B:277:MET:HB2	1.92	0.51
4:D:246:GLU:HG3	4:D:249:ARG:HH11	1.76	0.51
5:E:347:PHE:HA	5:E:350:MET:HB2	1.93	0.51
7:L:187:ILE:HG22	7:L:248:GLU:HG3	1.92	0.51
2:B:180:THR:OG1	2:B:204:ARG:HA	2.11	0.51
5:E:98:THR:O	5:E:127:MET:HA	2.10	0.51
5:H:187:ILE:HD11	5:H:252:CYS:HB2	1.93	0.51
5:N:248:GLU:HA	5:N:251:ARG:HB2	1.92	0.51
3:C:107:PRO:HB2	3:C:110:ASN:HB2	1.92	0.51
4:D:135:LEU:HD11	4:D:158:ILE:HG13	1.93	0.51
3:I:190:GLU:HG3	5:J:105:LEU:C	2.36	0.51
7:M:34:ARG:HD2	5:N:260:SER:O	2.11	0.51
5:E:97:PRO:HB3	5:E:126:ALA:HB3	1.93	0.51
6:F:42:GLY:C	5:H:161:TYR:HB3	2.35	0.51
6:F:189:THR:O	1:G:105:MET:HG3	2.11	0.51
6:F:207:ILE:HG23	6:F:211:LEU:HD23	1.93	0.51
3:I:186:LYS:NZ	3:I:261:VAL:O	2.44	0.51
5:J:361:GLY:O	5:J:364:ILE:HG13	2.10	0.51
5:E:181:THR:HG22	5:E:208:LYS:HE2	1.92	0.50
6:F:293:VAL:HA	6:F:325:ILE:O	2.11	0.50
3:I:4:VAL:O	3:I:14:ALA:HA	2.11	0.50
3:I:135:LEU:HB3	3:I:337:GLY:HA3	1.93	0.50
7:L:48:TYR:HB2	7:L:60:LEU:HD21	1.93	0.50
2:B:183:LEU:HD22	2:B:207:LYS:HB2	1.93	0.50
5:E:261:PHE:HD1	6:F:279:LYS:HE2	1.77	0.50
6:F:14:LYS:N	6:F:14:LYS:HD2	2.26	0.50
6:F:233:LYS:HB2	6:F:249:ARG:HD2	1.93	0.50
5:J:7:ASN:HA	5:J:12:VAL:HG22	1.92	0.50
5:J:188:LEU:HA	5:J:191:ARG:HB3	1.93	0.50
7:M:211:LEU:HD23	7:M:233:LYS:HB3	1.94	0.50
5:K:31:GLY:HA3	5:K:60:LEU:HD13	1.94	0.50
5:N:3:LEU:HB2	5:N:98:THR:HA	1.93	0.50
1:A:5:ILE:HB	1:A:100:LEU:HD23	1.92	0.50
3:C:104:PRO:HD3	3:C:132:GLN:HB2	1.93	0.50
3:C:146:ILE:O	3:C:292:ILE:HA	2.12	0.50
4:D:153:THR:HG23	4:D:173:LEU:O	2.11	0.50
4:D:210:CYS:HA	4:D:247:ARG:O	2.11	0.50
5:E:175:LEU:HD13	5:E:262:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:29:ILE:HD11	7:L:54:GLN:HG2	1.93	0.50
7:L:268:GLY:HA3	7:L:270:HIS:CE1	2.47	0.50
3:C:5:ILE:HA	3:C:13:LYS:O	2.12	0.50
5:K:165:ALA:HB1	5:K:170:ILE:HD11	1.92	0.50
7:M:281:ASP:HB3	7:M:284:ILE:HG12	1.92	0.50
5:N:66:ILE:HG12	5:N:71:ILE:HG12	1.93	0.50
5:N:294:MET:SD	5:N:326:ALA:HB2	2.52	0.50
1:A:5:ILE:HA	1:A:13:LYS:O	2.11	0.50
3:I:208:LYS:HA	3:I:212:CYS:SG	2.51	0.50
7:L:94:GLU:HA	7:L:123:ASN:O	2.12	0.50
7:L:345:SER:O	7:L:348:GLN:HB2	2.11	0.50
7:M:34:ARG:O	7:M:35:HIS:HB2	2.12	0.50
1:A:4:VAL:O	1:A:14:ALA:HA	2.12	0.50
2:B:185:LYS:HD2	3:C:168:HIS:HB3	1.94	0.50
4:D:132:VAL:HG22	4:D:158:ILE:HD12	1.94	0.50
1:G:150:SER:HA	1:G:155:THR:HA	1.92	0.50
1:A:98:VAL:O	1:A:127:PHE:HA	2.12	0.49
2:B:289:ALA:O	2:B:322:LYS:NZ	2.42	0.49
6:F:186:LYS:O	6:F:190:GLU:HG3	2.12	0.49
5:J:104:PRO:HG2	5:J:158:VAL:HG21	1.94	0.49
5:J:240:GLY:HA2	7:L:286:LYS:NZ	2.27	0.49
7:M:93:PRO:O	7:M:125:PRO:HD3	2.12	0.49
7:M:215:ALA:O	7:M:307:ARG:HD3	2.12	0.49
1:A:206:ASP:HA	1:A:209:GLU:HB2	1.93	0.49
3:C:148:LEU:HD21	3:C:269:ILE:HB	1.94	0.49
5:E:83:HIS:HA	5:E:87:ASN:HB2	1.93	0.49
5:N:202:GLU:HA	5:N:205:ARG:HG2	1.92	0.49
1:A:9:SER:HA	1:A:66:ILE:HB	1.94	0.49
1:A:157:VAL:O	1:A:170:ILE:HA	2.12	0.49
5:E:9:SER:HB3	5:E:178:ARG:NH2	2.27	0.49
1:G:66:ILE:HG12	1:G:71:VAL:HG22	1.92	0.49
5:N:299:THR:O	5:N:304:ILE:HG21	2.12	0.49
3:I:186:LYS:NZ	3:I:262:LEU:HA	2.27	0.49
5:K:66:ILE:HA	5:K:70:ILE:O	2.12	0.49
7:M:205:ARG:O	7:M:208:LYS:HB3	2.12	0.49
5:N:4:VAL:O	5:N:14:ALA:HA	2.12	0.49
5:N:175:LEU:HD11	5:N:256:LEU:HA	1.95	0.49
3:C:4:VAL:HA	3:C:99:LEU:O	2.11	0.49
4:D:298:MET:SD	4:D:329:LYS:HD2	2.53	0.49
6:F:184:LEU:HB2	6:F:252:CYS:SG	2.53	0.49
6:F:157:ASN:O	6:F:170:ILE:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:192:GLY:HA2	1:G:105:MET:CA	2.42	0.49
5:N:151:GLY:O	5:N:176:ALA:HB1	2.12	0.49
3:I:5:ILE:HB	3:I:100:LEU:HD23	1.95	0.49
1:A:2:ALA:HB3	1:A:17:ALA:HB2	1.95	0.49
2:B:156:ASN:O	2:B:169:ILE:HA	2.13	0.49
4:D:45:ASP:HA	4:D:77:LYS:HD3	1.95	0.49
4:D:235:LEU:HD12	4:D:239:GLN:HB2	1.94	0.49
1:G:247:ASN:HD21	1:G:251:ARG:NH2	2.11	0.49
5:J:317:PRO:O	5:J:320:MET:HB2	2.12	0.49
7:L:28:SER:HB3	7:L:80:ILE:HD13	1.94	0.49
2:B:10:GLY:O	2:B:27:PRO:HA	2.13	0.49
5:H:240:GLY:HA3	5:J:317:PRO:HB3	1.94	0.49
5:K:185:MET:HA	5:K:204:VAL:HG21	1.95	0.49
7:L:85:PHE:HZ	7:L:118:MET:HE1	1.78	0.49
2:B:107:LYS:N	2:B:107:LYS:HD3	2.28	0.49
3:C:177:GLY:O	3:C:208:LYS:NZ	2.44	0.49
5:H:214:VAL:HG23	5:H:301:TYR:HB3	1.95	0.49
7:L:11:MET:O	7:L:13:LYS:NZ	2.46	0.49
7:L:93:PRO:O	7:L:125:PRO:HD3	2.12	0.49
5:N:118:MET:HB3	5:N:127:MET:SD	2.53	0.49
2:B:210:LEU:HB3	2:B:248:ARG:HD2	1.94	0.48
4:D:182:LEU:HD12	4:D:185:ILE:HD11	1.95	0.48
6:F:211:LEU:HG	6:F:245:ILE:HD11	1.95	0.48
5:K:27:PRO:HB2	5:K:29:ILE:HD11	1.95	0.48
5:J:189:THR:HG22	5:J:194:SER:HA	1.94	0.48
2:B:45:LYS:HB2	2:B:48:TYR:CE1	2.48	0.48
2:B:247:GLU:HA	2:B:250:ARG:HB3	1.94	0.48
5:E:5:CYS:HA	5:E:13:LYS:O	2.13	0.48
3:C:146:ILE:HG21	3:C:277:ILE:HD11	1.94	0.48
6:F:206:ASP:O	6:F:210:LYS:HG2	2.13	0.48
1:G:7:ASN:HD21	1:G:100:LEU:HD22	1.79	0.48
3:I:150:SER:HB3	3:I:298:THR:HB	1.95	0.48
5:K:187:ILE:HD11	5:K:252:CYS:HB2	1.95	0.48
5:N:107:PRO:O	5:N:111:ARG:HG3	2.13	0.48
7:L:19:ASP:HB2	7:L:335:TRP:CH2	2.48	0.48
5:N:119:PHE:O	5:N:123:ASN:HA	2.14	0.48
3:C:56:LYS:HD3	3:C:59:ILE:HD11	1.96	0.48
3:C:155:THR:O	3:C:172:ARG:HA	2.13	0.48
4:D:98:LEU:O	4:D:127:VAL:HA	2.13	0.48
7:L:239:ASP:HA	5:N:313:THR:HG23	1.95	0.48
7:M:112:GLU:HA	7:M:365:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:HD11	1:A:235:TYR:HB2	1.96	0.48
2:B:186:ILE:O	2:B:189:GLU:HG2	2.14	0.48
7:L:348:GLN:NE2	7:L:351:TRP:HE1	2.11	0.48
5:E:146:ILE:HD11	5:E:157:ASN:HB3	1.95	0.48
3:I:239:ASP:HB3	5:K:285:ARG:HE	1.79	0.48
5:E:4:VAL:HG13	5:E:99:LEU:HD22	1.95	0.48
3:I:191:ARG:NH2	5:J:109:ALA:HB3	2.29	0.48
5:J:146:ILE:HA	5:J:158:VAL:O	2.14	0.48
5:J:155:THR:HG21	5:J:269:ILE:HD11	1.96	0.48
7:M:84:THR:HA	7:M:88:GLU:HB2	1.96	0.48
2:B:236:LEU:HG	2:B:238:ASP:OD1	2.14	0.48
1:G:214:VAL:HG22	1:G:253:PRO:HB3	1.95	0.48
1:A:49:VAL:HB	1:A:83:HIS:CD2	2.49	0.47
3:C:330:ARG:HA	3:C:333:SER:OG	2.14	0.47
6:F:297:GLY:HA2	6:F:331:LYS:HG2	1.96	0.47
7:L:110:ASN:O	7:L:114:MET:HB2	2.14	0.47
7:L:301:TYR:HA	7:L:302:PRO:HD3	1.76	0.47
7:M:101:THR:HA	7:M:130:ALA:O	2.14	0.47
7:M:347:PHE:HA	7:M:350:MET:HB3	1.95	0.47
1:A:38:ILE:HG13	1:A:39:MET:HG3	1.96	0.47
2:B:9:SER:HB3	2:B:66:ILE:O	2.14	0.47
5:J:6:ASP:HB3	5:J:13:LYS:HD3	1.95	0.47
1:A:104:PRO:HD3	1:A:132:GLN:HB2	1.96	0.47
3:C:104:PRO:HA	3:C:131:ILE:HG23	1.96	0.47
6:F:41:VAL:HB	5:H:280:CYS:HA	1.95	0.47
1:G:10:GLY:O	1:G:27:PRO:HA	2.14	0.47
3:I:158:VAL:HG22	3:I:170:ILE:HG23	1.97	0.47
4:D:260:ILE:HD13	4:D:260:ILE:H	1.79	0.47
4:D:268:HIS:HA	4:D:306:MET:HE1	1.95	0.47
3:I:188:LEU:HD23	5:J:107:PRO:HG3	1.96	0.47
5:N:29:ILE:HG21	5:N:62:LEU:HB3	1.94	0.47
1:G:312:ILE:HD13	1:G:315:LEU:HD12	1.97	0.47
5:H:6:ASP:O	5:H:12:VAL:HA	2.14	0.47
5:H:34:ARG:HD3	5:H:61:THR:HG23	1.95	0.47
3:I:158:VAL:HG13	3:I:170:ILE:HG12	1.96	0.47
5:K:3:LEU:HD22	5:K:89:LEU:HD13	1.96	0.47
7:L:156:HIS:HA	7:L:171:LEU:O	2.15	0.47
7:M:32:ARG:HD2	7:M:46:ASP:O	2.15	0.47
7:M:130:ALA:HB3	7:M:135:LEU:HD11	1.97	0.47
5:N:208:LYS:HA	5:N:212:CYS:SG	2.54	0.47
1:A:147:VAL:O	1:A:157:VAL:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:65:PRO:HG2	7:M:80:ILE:HD11	1.96	0.47
5:N:216:LEU:O	5:N:310:LYS:NZ	2.43	0.47
1:A:47:SER:OG	1:A:79:LYS:HG2	2.15	0.47
3:C:159:PRO:HG2	3:C:166:LEU:HB2	1.97	0.47
5:E:362:PRO:O	5:E:365:VAL:HG12	2.14	0.47
5:H:280:CYS:O	5:H:285:ARG:NH1	2.48	0.47
3:I:157:VAL:O	3:I:170:ILE:HA	2.15	0.47
3:I:284:VAL:O	3:I:288:LEU:HG	2.15	0.47
5:K:134:VAL:HG13	5:K:160:ILE:HG12	1.97	0.47
7:L:159:PRO:HD3	7:L:276:SER:HB3	1.96	0.47
5:N:181:THR:HG23	5:N:204:VAL:HG23	1.95	0.47
2:B:230:LEU:HB3	2:B:246:ASN:H	1.80	0.47
3:C:137:LEU:HD22	3:C:160:ILE:HG21	1.96	0.47
4:D:65:ILE:HD11	4:D:75:MET:SD	2.55	0.47
6:F:42:GLY:O	5:H:161:TYR:HB3	2.15	0.47
5:H:142:ARG:HD3	5:H:291:ASN:OD1	2.15	0.47
3:I:165:SER:HB2	3:I:170:ILE:HD11	1.97	0.47
5:K:147:VAL:HA	5:K:293:VAL:O	2.14	0.47
5:N:147:VAL:HA	5:N:293:VAL:O	2.15	0.47
1:A:113:LYS:HA	1:A:113:LYS:HZ3	1.79	0.47
3:C:182:ASP:CG	3:C:201:ARG:HH21	2.23	0.47
5:H:195:PHE:HA	5:H:200:GLU:HG3	1.97	0.47
7:M:158:VAL:HA	7:M:170:ILE:HG12	1.97	0.47
4:D:150:ASP:HA	4:D:175:GLY:HA3	1.97	0.47
6:F:309:GLN:HE22	6:F:322:ILE:HB	1.79	0.47
5:K:150:SER:HA	5:K:155:THR:HA	1.97	0.47
3:C:256:LEU:HD11	3:C:298:THR:HG22	1.96	0.46
6:F:213:TYR:O	6:F:250:PHE:HA	2.14	0.46
5:H:214:VAL:HG12	5:H:307:ARG:HG3	1.96	0.46
7:L:182:ASP:CG	7:L:201:ARG:HH21	2.23	0.46
7:M:172:ARG:HH12	7:M:174:ASP:CG	2.23	0.46
2:B:6:ASP:HB3	2:B:13:LYS:HD3	1.96	0.46
5:K:169:ALA:HB2	5:K:280:CYS:SG	2.55	0.46
7:L:286:LYS:HD2	7:L:321:LYS:H	1.79	0.46
7:M:62:LEU:O	5:N:265:GLU:HB3	2.15	0.46
5:E:49:VAL:HB	5:E:83:HIS:CD2	2.50	0.46
5:E:215:ALA:HB1	5:E:221:GLU:HG3	1.97	0.46
5:E:263:GLY:HA3	6:F:278:MET:HB3	1.97	0.46
5:H:216:LEU:HD23	5:H:216:LEU:H	1.80	0.46
3:I:5:ILE:HB	3:I:100:LEU:CD2	2.45	0.46
1:A:181:THR:OG1	1:A:208:LYS:NZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:SER:HA	2:B:335:ILE:HG12	1.97	0.46
3:C:299:THR:O	3:C:304:ILE:HG21	2.15	0.46
4:D:291:VAL:HG22	4:D:323:ILE:HB	1.97	0.46
1:G:105:MET:HE1	1:G:170:ILE:HD12	1.98	0.46
5:K:183:TYR:CE2	5:K:252:CYS:HA	2.47	0.46
5:K:282:ILE:HA	5:K:285:ARG:HG3	1.96	0.46
7:M:85:PHE:HZ	7:M:118:MET:HE1	1.81	0.46
1:A:168:HIS:O	1:A:279:LYS:NZ	2.49	0.46
2:B:291:ASN:O	2:B:323:ILE:HA	2.16	0.46
4:D:146:LEU:HD23	4:D:292:MET:HE3	1.97	0.46
4:D:246:GLU:HA	4:D:249:ARG:HD3	1.97	0.46
5:E:123:ASN:HD22	5:E:354:LYS:HD3	1.79	0.46
7:L:149:ASP:HA	7:L:295:SER:O	2.16	0.46
5:N:69:GLY:O	5:N:103:ALA:HB2	2.15	0.46
1:A:99:LEU:HD13	1:A:128:TYR:HB3	1.98	0.46
3:I:13:LYS:HG3	3:I:25:VAL:HG13	1.97	0.46
3:I:56:LYS:O	3:I:60:LEU:HG	2.16	0.46
3:I:66:ILE:HD11	3:I:77:MET:SD	2.56	0.46
7:L:146:ILE:HG21	7:L:277:ILE:HD11	1.98	0.46
5:N:109:ALA:HA	5:N:112:GLU:HG2	1.98	0.46
5:N:157:ASN:O	5:N:170:ILE:HA	2.15	0.46
5:N:286:LYS:HZ1	5:N:290:ALA:HB2	1.80	0.46
2:B:286:ASP:HB2	2:B:289:ALA:HB3	1.96	0.46
7:L:19:ASP:HB2	7:L:335:TRP:HH2	1.79	0.46
7:M:30:VAL:HG22	7:M:49:VAL:HG23	1.97	0.46
5:E:155:THR:HG21	5:E:269:ILE:HG22	1.98	0.46
6:F:175:LEU:HD12	6:F:264:MET:HG3	1.98	0.46
6:F:212:CYS:HA	6:F:249:ARG:O	2.16	0.46
5:J:224:THR:HA	5:J:227:SER:OG	2.16	0.46
5:N:52:GLU:HG3	5:N:83:HIS:HE1	1.80	0.46
1:A:5:ILE:HB	1:A:100:LEU:CD2	2.46	0.46
2:B:4:VAL:O	2:B:14:ALA:HA	2.16	0.46
2:B:11:LEU:HB2	2:B:13:LYS:HE3	1.98	0.46
5:E:210:LYS:HB2	5:E:211:LEU:HD22	1.97	0.46
5:N:54:GLN:OE1	5:N:57:ARG:HD2	2.16	0.46
2:B:12:VAL:HG23	2:B:28:SER:HB2	1.98	0.46
2:B:190:ARG:O	3:C:107:PRO:HA	2.16	0.46
4:D:58:ILE:HD12	6:F:284:ILE:H	1.81	0.46
5:E:100:LEU:O	5:E:129:VAL:HA	2.16	0.46
1:G:165:SER:O	1:G:167:PRO:HD3	2.15	0.46
5:K:348:GLN:HA	5:K:351:TRP:HD1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLY:HA3	1:A:103:ALA:HB2	1.98	0.45
5:E:39:MET:HA	1:G:164:PHE:HE1	1.81	0.45
6:F:46:LYS:NZ	6:F:61:LEU:HD21	2.31	0.45
5:K:185:MET:SD	5:K:195:PHE:HB2	2.56	0.45
7:L:215:ALA:O	7:L:307:ARG:HD3	2.16	0.45
7:M:4:VAL:O	7:M:14:ALA:HA	2.16	0.45
2:B:186:ILE:HG23	2:B:189:GLU:OE2	2.16	0.45
5:E:245:ILE:HG12	5:E:249:ARG:HG3	1.98	0.45
5:H:73:ASN:HD21	5:H:75:ASP:HB3	1.81	0.45
5:N:148:LEU:O	5:N:294:MET:HA	2.16	0.45
1:A:199:ALA:HB3	3:C:282:VAL:HB	1.98	0.45
3:C:147:VAL:HG22	3:C:293:VAL:HB	1.98	0.45
4:D:2:LEU:HB2	4:D:96:THR:HA	1.96	0.45
5:E:123:ASN:ND2	5:E:354:LYS:HD3	2.30	0.45
5:E:240:GLY:HA3	1:G:317:PRO:HB3	1.98	0.45
6:F:291:ASN:HA	6:F:325:ILE:HD13	1.99	0.45
2:B:188:THR:O	3:C:105:MET:HB3	2.16	0.45
3:C:356:GLU:HA	3:C:359:GLU:HG2	1.98	0.45
1:G:299:THR:HA	1:G:304:ILE:HD13	1.98	0.45
5:H:323:LYS:HE3	5:H:325:ILE:HG13	1.99	0.45
3:I:69:GLY:HA3	3:I:103:ALA:HB2	1.99	0.45
5:J:169:ALA:HB1	5:J:276:SER:HB2	1.97	0.45
5:K:195:PHE:HD1	5:K:200:GLU:HB3	1.81	0.45
7:L:213:TYR:O	7:L:253:PRO:HG2	2.15	0.45
7:M:81:TRP:CH2	7:M:114:MET:HG3	2.51	0.45
5:E:156:HIS:NE2	5:E:172:ARG:HG3	2.31	0.45
5:H:101:THR:HG22	5:H:135:LEU:HD12	1.99	0.45
5:H:158:VAL:HG22	5:H:170:ILE:HG12	1.98	0.45
5:H:237:LEU:HD22	5:H:241:GLN:HB3	1.98	0.45
7:L:203:ILE:O	7:L:207:ILE:HG13	2.17	0.45
7:L:259:PRO:CG	7:L:266:SER:HB2	2.39	0.45
4:D:33:ARG:NH2	4:D:60:THR:OG1	2.49	0.45
6:F:66:PRO:CG	6:F:76:ASP:HB3	2.42	0.45
5:H:56:LYS:O	5:H:60:LEU:HG	2.16	0.45
5:J:98:THR:O	5:J:127:MET:HA	2.16	0.45
5:J:200:GLU:O	5:J:204:VAL:HG23	2.16	0.45
3:C:119:PHE:O	3:C:123:ASN:HA	2.17	0.45
4:D:114:GLN:HB2	4:D:118:GLU:OE2	2.17	0.45
4:D:156:VAL:HG13	4:D:168:ILE:HG12	1.97	0.45
3:I:9:SER:HA	3:I:66:ILE:HB	1.99	0.45
5:N:237:LEU:HD12	5:N:241:GLN:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:293:VAL:HA	5:N:325:ILE:O	2.17	0.45
2:B:282:ASP:O	2:B:285:LYS:HG2	2.17	0.45
2:B:286:ASP:HA	2:B:289:ALA:H	1.81	0.45
6:F:183:TYR:O	6:F:186:LYS:HG3	2.17	0.45
6:F:247:ASN:HA	6:F:250:PHE:CE2	2.51	0.45
3:I:199:ALA:HB1	5:K:283:ASP:H	1.82	0.45
7:L:3:LEU:HB2	7:L:98:VAL:HG23	1.97	0.45
7:M:23:ARG:HA	7:M:23:ARG:HD3	1.81	0.45
2:B:103:PRO:HD3	2:B:131:GLN:HB2	1.98	0.45
3:C:6:ASP:HA	3:C:101:THR:OG1	2.16	0.45
4:D:4:CYS:HB3	4:D:98:LEU:HD23	1.99	0.45
6:F:32:GLY:HA2	6:F:62:THR:O	2.16	0.45
7:M:165:ALA:HB1	7:M:170:ILE:HD11	1.97	0.45
4:D:212:VAL:HG23	4:D:299:TYR:HB3	1.99	0.45
5:H:175:LEU:HD23	5:H:264:MET:SD	2.57	0.45
5:J:171:MET:HE3	5:J:279:LYS:HE2	1.98	0.45
7:M:300:MET:HA	7:M:330:ARG:NH1	2.32	0.45
5:N:5:CYS:HA	5:N:13:LYS:O	2.17	0.45
5:N:300:MET:HA	5:N:330:ARG:HH11	1.82	0.45
3:C:14:ALA:HB1	3:C:89:LEU:HD11	1.99	0.44
1:G:231:ILE:O	1:G:249:ARG:NH1	2.50	0.44
5:J:83:HIS:O	5:J:87:ASN:HB2	2.16	0.44
5:K:4:VAL:HG13	5:K:99:LEU:HD22	1.99	0.44
2:B:224:ALA:HA	2:B:230:LEU:HG	1.98	0.44
2:B:329:ARG:HA	2:B:332:SER:OG	2.18	0.44
3:C:3:LEU:HD22	3:C:89:LEU:HD13	1.98	0.44
4:D:153:THR:HG1	4:D:171:LEU:HB3	1.82	0.44
6:F:10:SER:HA	6:F:67:ILE:O	2.17	0.44
5:H:147:VAL:HA	5:H:293:VAL:O	2.17	0.44
5:J:111:ARG:HH12	5:J:365:VAL:HG22	1.82	0.44
5:E:352:ILE:HG23	5:E:364:ILE:HD13	1.99	0.44
3:I:293:VAL:HA	3:I:325:ILE:O	2.17	0.44
7:L:198:THR:N	7:L:199:ALA:HA	2.31	0.44
7:M:152:ASP:O	7:M:178:ARG:HG3	2.17	0.44
7:M:182:ASP:CG	7:M:201:ARG:HH21	2.26	0.44
2:B:149:SER:HA	2:B:154:THR:HA	2.00	0.44
2:B:188:THR:HA	2:B:192:TYR:O	2.16	0.44
4:D:149:GLY:O	4:D:174:ALA:HB1	2.18	0.44
5:H:5:CYS:SG	5:H:84:THR:HG21	2.56	0.44
5:H:147:VAL:HG22	5:H:293:VAL:HB	1.99	0.44
3:I:213:TYR:O	3:I:250:PHE:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:63:LYS:NZ	5:N:64:TYR:O	2.51	0.44
1:A:146:ILE:HA	1:A:158:VAL:O	2.17	0.44
5:E:155:THR:O	5:E:172:ARG:HA	2.17	0.44
6:F:92:ALA:HA	6:F:93:PRO:HD3	1.89	0.44
5:K:214:VAL:HG22	5:K:253:PRO:HB3	2.00	0.44
7:L:56:LYS:O	7:L:59:ILE:HG22	2.17	0.44
7:M:5:VAL:HA	7:M:13:LYS:O	2.17	0.44
5:N:123:ASN:ND2	5:N:354:LYS:HE3	2.32	0.44
2:B:30:VAL:HG11	2:B:78:LYS:HB3	2.00	0.44
3:C:317:PRO:HB2	3:C:320:MET:HB2	2.00	0.44
4:D:273:ASN:O	4:D:277:LYS:HG2	2.17	0.44
6:F:40:MET:O	5:H:166:LEU:HD22	2.17	0.44
5:K:29:ILE:HG13	5:K:54:GLN:HE21	1.83	0.44
5:K:157:ASN:OD1	5:K:272:THR:HG22	2.18	0.44
5:K:177:GLY:O	5:K:208:LYS:NZ	2.51	0.44
7:L:199:ALA:HB3	5:N:282:ILE:HG21	1.99	0.44
3:C:146:ILE:HA	3:C:158:VAL:O	2.18	0.44
3:C:248:GLU:H	3:C:248:GLU:CD	2.26	0.44
5:E:31:GLY:HA3	5:E:60:LEU:HD12	2.00	0.44
5:H:27:PRO:O	5:H:50:GLY:HA2	2.18	0.44
7:L:211:LEU:O	7:L:249:ARG:HD2	2.17	0.44
7:M:9:SER:HA	7:M:66:ILE:HB	1.99	0.44
5:N:277:ILE:CG2	5:N:285:ARG:HG2	2.47	0.44
3:C:80:ILE:O	3:C:83:HIS:HB3	2.17	0.44
5:E:29:ILE:O	5:E:49:VAL:HA	2.18	0.44
5:E:157:ASN:O	5:E:170:ILE:HA	2.18	0.44
6:F:67:ILE:HD11	6:F:77:MET:HE1	2.00	0.44
6:F:202:GLU:HG3	6:F:205:ARG:HH12	1.82	0.44
6:F:308:MET:HA	6:F:311:GLU:HB2	2.00	0.44
6:F:309:GLN:NE2	6:F:322:ILE:HB	2.33	0.44
5:H:111:ARG:O	5:H:114:MET:HG2	2.17	0.44
3:I:4:VAL:HA	3:I:99:LEU:O	2.17	0.44
7:L:175:LEU:HD13	7:L:264:MET:SD	2.58	0.44
5:N:3:LEU:HA	5:N:15:GLY:O	2.17	0.44
4:D:292:MET:HE1	4:D:302:ILE:HG13	1.99	0.44
6:F:60:ILE:HG13	6:F:61:LEU:HG	2.00	0.44
6:F:99:LEU:HA	6:F:128:TYR:O	2.18	0.44
1:G:247:ASN:ND2	1:G:251:ARG:NH2	2.66	0.44
5:H:218:PHE:HE1	5:H:250:PHE:HB2	1.82	0.44
5:J:9:SER:HA	5:J:66:ILE:HB	1.99	0.44
7:M:6:ASP:N	7:M:13:LYS:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:PHE:HA	1:A:200:GLU:HB3	2.00	0.43
4:D:57:GLY:HA3	4:D:59:LEU:N	2.33	0.43
5:J:194:SER:O	7:L:282:VAL:HG11	2.18	0.43
7:L:149:ASP:O	7:L:155:THR:HA	2.18	0.43
7:L:299:THR:OG1	7:L:330:ARG:NH1	2.51	0.43
7:M:111:ARG:O	7:M:114:MET:HB3	2.17	0.43
4:D:100:GLU:O	4:D:129:ILE:HA	2.18	0.43
5:J:285:ARG:HA	5:J:288:LEU:HD22	2.00	0.43
5:K:130:ALA:HB3	5:K:135:LEU:HD11	2.00	0.43
5:K:151:GLY:HA2	5:K:297:GLY:H	1.83	0.43
5:N:270:HIS:CD2	5:N:271:GLU:HG3	2.53	0.43
5:E:208:LYS:HA	5:E:212:CYS:SG	2.58	0.43
5:E:294:MET:HB3	5:E:299:THR:HG21	2.00	0.43
5:K:45:LYS:HD3	5:K:46:ASP:H	1.84	0.43
7:L:291:ASN:HA	7:L:325:ILE:HD12	1.99	0.43
1:A:148:LEU:HD23	1:A:294:MET:SD	2.58	0.43
3:C:10:GLY:O	3:C:27:PRO:HA	2.19	0.43
3:C:68:HIS:HA	3:C:154:VAL:HB	2.00	0.43
4:D:4:CYS:SG	4:D:82:THR:HG21	2.58	0.43
4:D:205:ILE:HG23	4:D:209:LEU:HD23	2.00	0.43
5:E:65:PRO:HG3	5:E:76:ASP:HB3	2.00	0.43
6:F:100:LEU:O	6:F:129:VAL:HA	2.18	0.43
6:F:185:MET:HE2	6:F:195:PHE:HB2	2.01	0.43
3:I:194:SER:HA	5:J:172:ARG:NE	2.33	0.43
7:M:115:THR:HG23	7:M:127:MET:SD	2.59	0.43
7:M:119:PHE:HZ	7:M:352:ILE:O	2.01	0.43
5:N:357:TYR:HE1	5:N:362:PRO:HG3	1.82	0.43
4:D:45:ASP:CG	4:D:77:LYS:HG2	2.44	0.43
5:K:4:VAL:O	5:K:14:ALA:HA	2.17	0.43
5:K:252:CYS:HB3	5:K:253:PRO:HD3	1.99	0.43
2:B:102:ALA:HA	2:B:131:GLN:OE1	2.18	0.43
2:B:138:ALA:HB1	2:B:335:ILE:HG13	2.00	0.43
3:C:7:ASN:HD21	3:C:100:LEU:HD22	1.84	0.43
3:C:155:THR:HB	3:C:173:ILE:O	2.19	0.43
6:F:20:ASP:CG	6:F:24:ARG:HH12	2.27	0.43
1:G:247:ASN:HD21	1:G:251:ARG:HH21	1.66	0.43
5:J:273:THR:HG21	5:J:312:ILE:HD13	2.00	0.43
1:A:231:ILE:O	1:A:249:ARG:NH1	2.50	0.43
1:A:259:PRO:HB2	1:A:264:LEU:O	2.19	0.43
3:C:165:SER:O	3:C:167:PRO:HD3	2.18	0.43
4:D:184:LYS:O	4:D:187:THR:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:235:TYR:O	5:E:243:ILE:HG13	2.19	0.43
6:F:7:ASP:O	6:F:13:VAL:HA	2.19	0.43
6:F:35:ARG:HD3	6:F:59:GLY:O	2.19	0.43
6:F:100:LEU:HD21	6:F:118:MET:HE1	2.00	0.43
5:H:5:CYS:HA	5:H:13:LYS:O	2.19	0.43
7:M:149:ASP:O	7:M:155:THR:HA	2.19	0.43
7:M:169:ALA:HB1	7:M:276:SER:O	2.17	0.43
5:E:105:LEU:HD12	5:E:172:ARG:HD3	2.01	0.43
6:F:295:SER:HA	6:F:330:ARG:HB2	2.01	0.43
1:G:115:THR:HA	1:G:127:PHE:HE2	1.83	0.43
5:J:240:GLY:HA2	7:L:286:LYS:HZ3	1.83	0.43
5:K:5:CYS:HB3	5:K:100:LEU:HD23	2.00	0.43
5:K:155:THR:HB	5:K:173:LEU:HB3	2.00	0.43
7:M:69:GLY:HA3	7:M:103:ALA:HB2	2.00	0.43
5:N:7:ASN:ND2	5:N:12:VAL:HG13	2.34	0.43
2:B:145:ILE:HG23	2:B:291:ASN:ND2	2.34	0.43
3:C:11:MET:HE3	3:C:25:VAL:HG12	2.00	0.43
1:G:15:GLY:HA2	1:G:23:ARG:HB2	2.01	0.43
5:H:75:ASP:CG	5:H:79:LYS:HZ1	2.26	0.43
5:N:150:SER:HA	5:N:154:VAL:O	2.19	0.43
2:B:57:ARG:HE	2:B:62:LEU:HD11	1.83	0.43
2:B:148:ASP:O	2:B:154:THR:HA	2.19	0.43
2:B:181:ASP:CG	2:B:200:ARG:HH21	2.27	0.43
4:D:164:LEU:HA	4:D:165:PRO:HD2	1.83	0.43
4:D:290:ASN:O	4:D:323:ILE:N	2.52	0.43
6:F:142:ARG:HD3	6:F:291:ASN:OD1	2.18	0.43
6:F:216:LEU:HD12	6:F:307:ARG:HA	2.01	0.43
5:H:85:PHE:HB3	5:H:93:PRO:HD3	2.01	0.43
1:A:92:ALA:HA	1:A:93:PRO:HD2	1.89	0.42
5:E:142:ARG:NH1	5:E:291:ASN:OD1	2.51	0.42
6:F:157:ASN:OD1	6:F:272:THR:HB	2.19	0.42
6:F:166:LEU:HA	6:F:167:PRO:HD3	1.85	0.42
5:H:197:THR:HB	5:J:283:ASP:HB2	2.01	0.42
5:H:277:ILE:HG22	5:H:285:ARG:HD3	2.00	0.42
3:I:186:LYS:HB3	5:J:167:PRO:HB2	2.00	0.42
5:K:216:LEU:HD23	5:K:216:LEU:H	1.84	0.42
4:D:167:ALA:HB2	4:D:277:LYS:HB2	2.01	0.42
5:E:31:GLY:HA3	5:E:48:TYR:HB2	2.00	0.42
1:G:5:ILE:HA	1:G:13:LYS:O	2.19	0.42
1:G:31:GLY:HA3	1:G:60:LEU:HD13	2.01	0.42
5:H:97:PRO:HA	5:H:126:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:115:THR:HG21	5:H:365:VAL:HG21	2.00	0.42
5:J:100:LEU:O	5:J:129:VAL:HA	2.19	0.42
6:F:30:ILE:O	6:F:50:VAL:HA	2.19	0.42
1:G:175:LEU:HD11	1:G:256:LEU:HA	2.01	0.42
5:H:61:THR:O	5:H:63:LYS:NZ	2.52	0.42
5:K:115:THR:HG23	5:K:127:MET:SD	2.60	0.42
5:N:119:PHE:O	5:N:354:LYS:HE2	2.19	0.42
1:A:119:PHE:CZ	1:A:127:PHE:HB3	2.55	0.42
2:B:2:ALA:HB3	2:B:17:ALA:HB2	2.00	0.42
2:B:145:ILE:O	2:B:291:ASN:HA	2.19	0.42
3:C:144:THR:HA	3:C:160:ILE:O	2.20	0.42
3:C:282:VAL:HG22	3:C:285:ARG:NH1	2.34	0.42
4:D:86:GLU:O	4:D:88:ARG:NH1	2.52	0.42
6:F:40:MET:SD	6:F:41:VAL:N	2.92	0.42
6:F:106:ASN:HA	6:F:107:PRO:HD3	1.91	0.42
1:G:26:PHE:HE2	1:G:80:ILE:HG23	1.84	0.42
1:G:151:GLY:O	1:G:176:ALA:HB1	2.18	0.42
3:I:17:ALA:HB1	3:I:343:SER:OG	2.19	0.42
1:A:105:MET:HG3	1:A:170:ILE:HD12	2.01	0.42
2:B:289:ALA:O	2:B:322:LYS:HB3	2.20	0.42
3:C:6:ASP:O	3:C:12:CYS:HA	2.19	0.42
3:C:325:ILE:O	3:C:327:PRO:HD3	2.19	0.42
5:E:106:ASN:HA	5:E:107:PRO:HD3	1.81	0.42
5:E:154:VAL:HG21	5:E:156:HIS:CE1	2.54	0.42
5:E:231:LEU:O	5:E:249:ARG:NH1	2.52	0.42
6:F:31:VAL:HG22	6:F:50:VAL:HG22	2.02	0.42
6:F:145:GLY:HA2	6:F:287:ASP:O	2.19	0.42
1:A:99:LEU:HA	1:A:128:TYR:O	2.20	0.42
1:A:312:ILE:HB	1:A:322:VAL:HG11	2.01	0.42
5:E:97:PRO:HA	5:E:126:ALA:O	2.20	0.42
6:F:192:GLY:O	1:G:107:PRO:HG3	2.19	0.42
6:F:275:ASN:O	6:F:279:LYS:HB2	2.19	0.42
1:G:27:PRO:HB2	1:G:29:ILE:HG13	2.02	0.42
3:I:191:ARG:HD2	5:J:108:LYS:H	1.83	0.42
3:I:213:TYR:HB2	3:I:302:PRO:O	2.20	0.42
5:N:85:PHE:HD1	5:N:89:LEU:HD12	1.84	0.42
5:N:96:HIS:HA	5:N:97:PRO:HD2	1.92	0.42
5:N:108:LYS:HA	5:N:108:LYS:HD3	1.84	0.42
2:B:29:ILE:CG2	2:B:50:GLY:HA2	2.50	0.42
5:N:54:GLN:O	5:N:57:ARG:HG3	2.19	0.42
3:C:34:ARG:NH2	3:C:60:LEU:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:11:VAL:O	4:D:24:VAL:HA	2.20	0.42
5:J:258:GLN:HB3	5:J:260:SER:OG	2.20	0.42
5:K:144:THR:HA	5:K:160:ILE:O	2.19	0.42
5:E:146:ILE:HG21	5:E:277:ILE:HD11	2.01	0.42
6:F:188:LEU:HA	6:F:191:ARG:HD3	2.01	0.42
6:F:285:ARG:HH12	6:F:320:MET:HE3	1.85	0.42
3:I:179:ASP:HA	3:I:182:ASP:HB2	2.01	0.42
5:K:49:VAL:HG13	5:K:80:ILE:HG12	2.02	0.42
5:K:148:LEU:HD21	5:K:269:ILE:HG23	2.02	0.42
5:K:356:GLU:HB3	5:K:364:ILE:HG12	2.01	0.42
1:A:115:THR:HA	1:A:127:PHE:HE2	1.85	0.42
2:B:186:ILE:HD13	2:B:250:ARG:HD3	2.02	0.42
3:C:119:PHE:HB3	3:C:354:LYS:HE2	2.02	0.42
4:D:131:ALA:O	4:D:134:SER:HB2	2.20	0.42
4:D:158:ILE:HA	4:D:162:TYR:O	2.20	0.42
4:D:352:LYS:HE3	4:D:356:ASP:OD2	2.20	0.42
6:F:183:TYR:CD1	6:F:262:ILE:HG22	2.54	0.42
6:F:245:ILE:HB	6:F:248:GLU:HG2	2.02	0.42
1:G:6:ASP:O	1:G:12:CYS:HA	2.20	0.42
1:G:188:LEU:HD22	1:G:245:ILE:HD12	2.01	0.42
5:H:144:THR:OG1	5:H:161:TYR:HA	2.20	0.42
5:H:246:GLY:O	5:H:249:ARG:HB3	2.19	0.42
3:I:169:ALA:HB1	3:I:276:SER:HA	2.01	0.42
5:K:360:ALA:HB3	5:K:364:ILE:HB	2.01	0.42
7:L:110:ASN:O	7:L:114:MET:N	2.52	0.42
5:N:215:ALA:O	5:N:307:ARG:HD3	2.20	0.42
1:A:19:ASP:HB2	1:A:335:TRP:HH2	1.86	0.41
2:B:6:ASP:HA	2:B:100:THR:OG1	2.20	0.41
4:D:185:ILE:HD11	4:D:250:CYS:SG	2.60	0.41
4:D:314:ALA:HB3	4:D:320:ILE:HD11	2.01	0.41
5:E:115:THR:HA	5:E:127:MET:SD	2.60	0.41
5:E:259:PRO:HB3	5:E:264:MET:HB2	2.02	0.41
1:G:49:VAL:HB	1:G:83:HIS:CD2	2.55	0.41
1:G:146:ILE:HA	1:G:159:PRO:HA	2.02	0.41
5:J:247:ASN:OD1	5:J:251:ARG:NH1	2.53	0.41
5:K:157:ASN:O	5:K:170:ILE:HA	2.19	0.41
5:K:160:ILE:HA	5:K:165:ALA:HA	2.02	0.41
5:K:173:LEU:HG	5:K:175:LEU:HG	2.02	0.41
5:N:27:PRO:HB2	5:N:29:ILE:HD11	2.02	0.41
5:H:103:ALA:HB3	5:H:106:ASN:HB2	2.03	0.41
5:K:63:LYS:HB2	5:K:63:LYS:HE2	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:106:ASN:N	7:L:107:PRO:HD3	2.35	0.41
7:L:270:HIS:CD2	7:L:271:GLU:HG3	2.54	0.41
2:B:133:VAL:HA	2:B:159:ILE:HD13	2.02	0.41
2:B:316:PRO:O	2:B:319:MET:SD	2.79	0.41
5:H:214:VAL:HG22	5:H:253:PRO:HB3	2.02	0.41
5:K:190:GLU:HG2	7:L:110:ASN:HB2	2.02	0.41
4:D:90:ALA:HA	4:D:91:PRO:HD2	1.94	0.41
4:D:202:VAL:HA	4:D:205:ILE:HD12	2.01	0.41
4:D:324:ALA:HB1	4:D:328:ARG:HD3	2.02	0.41
5:E:158:VAL:HG13	5:E:170:ILE:HG12	2.03	0.41
6:F:159:PRO:HG3	6:F:280:CYS:SG	2.60	0.41
3:I:188:LEU:HA	5:J:107:PRO:CG	2.49	0.41
5:J:178:ARG:HG3	5:J:201:ARG:HH22	1.84	0.41
3:C:231:ILE:O	3:C:249:ARG:NH1	2.53	0.41
5:E:13:LYS:HG3	5:E:25:VAL:HG13	2.02	0.41
5:E:66:ILE:HG12	5:E:71:ILE:HG12	2.02	0.41
6:F:46:LYS:HE3	6:F:57:LYS:HE3	2.02	0.41
6:F:208:LYS:O	6:F:212:CYS:HB2	2.21	0.41
6:F:267:ALA:O	6:F:272:THR:HG23	2.21	0.41
1:G:94:GLU:O	1:G:125:PRO:HD3	2.21	0.41
5:H:239:ASP:HB2	5:J:320:MET:HE1	2.02	0.41
3:I:187:ILE:HA	5:J:105:LEU:HB3	2.02	0.41
5:J:232:GLU:HA	5:J:245:ILE:O	2.20	0.41
5:K:6:ASP:O	5:K:12:VAL:HA	2.20	0.41
5:K:200:GLU:CD	7:M:282:VAL:HG21	2.45	0.41
2:B:184:MET:HG3	2:B:194:PHE:O	2.19	0.41
3:C:212:CYS:HB3	3:C:253:PRO:HG3	2.02	0.41
4:D:92:GLU:HA	4:D:121:ASN:O	2.21	0.41
3:I:191:ARG:NH1	3:I:244:THR:O	2.52	0.41
5:N:65:PRO:HB3	5:N:76:ASP:CB	2.51	0.41
5:N:312:ILE:O	5:N:314:ALA:N	2.54	0.41
3:C:213:TYR:OH	3:C:231:ILE:HG23	2.21	0.41
4:D:55:LYS:NZ	6:F:283:ASP:OD1	2.47	0.41
4:D:147:ASP:O	4:D:154:HIS:N	2.53	0.41
4:D:182:LEU:HD13	4:D:250:CYS:SG	2.61	0.41
5:K:175:LEU:HA	5:K:179:ASP:CG	2.46	0.41
7:L:102:GLU:HB3	7:L:129:VAL:HG12	2.03	0.41
7:L:237:LEU:HG	7:L:241:GLN:O	2.21	0.41
1:G:135:LEU:O	1:G:337:GLY:HA3	2.21	0.41
5:H:57:ARG:HH22	5:H:202:GLU:CD	2.28	0.41
5:N:111:ARG:HH12	5:N:365:VAL:C	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:VAL:HA	1:A:325:ILE:O	2.21	0.41
3:C:5:ILE:HB	3:C:100:LEU:CD2	2.51	0.41
4:D:44:LYS:H	4:D:44:LYS:HD2	1.85	0.41
4:D:279:ASP:O	4:D:283:ARG:HG3	2.21	0.41
5:E:39:MET:HA	1:G:164:PHE:CE1	2.55	0.41
5:E:202:GLU:HA	5:E:205:ARG:HG2	2.03	0.41
6:F:118:MET:HB3	6:F:127:MET:SD	2.61	0.41
5:H:99:LEU:HG	5:H:128:TYR:HB3	2.03	0.41
3:I:193:TYR:HB3	3:I:195:PHE:CE2	2.55	0.41
5:J:9:SER:HB2	5:J:152:ASP:HB3	2.02	0.41
5:K:27:PRO:O	5:K:50:GLY:HA2	2.20	0.41
7:M:81:TRP:HH2	7:M:114:MET:HG3	1.86	0.41
7:M:159:PRO:HG3	7:M:169:ALA:CB	2.38	0.41
7:M:332:TYR:O	7:M:336:ILE:HG12	2.20	0.41
5:N:160:ILE:HA	5:N:164:TYR:O	2.21	0.41
5:N:354:LYS:NZ	5:N:358:ASP:OD1	2.52	0.41
3:C:200:GLU:HG2	3:C:203:ILE:HD12	2.02	0.41
6:F:308:MET:HB3	6:F:324:ILE:HG12	2.03	0.41
1:G:99:LEU:HA	1:G:128:TYR:O	2.21	0.41
5:J:317:PRO:HD2	5:J:320:MET:HE2	2.03	0.41
7:M:156:HIS:HA	7:M:171:LEU:O	2.21	0.41
5:N:2:ALA:O	5:N:16:PHE:HA	2.20	0.41
5:N:235:TYR:CE2	5:N:237:LEU:HD23	2.56	0.41
4:D:143:GLY:HA2	4:D:286:LEU:HA	2.01	0.40
6:F:158:VAL:HG12	6:F:170:ILE:HG23	2.03	0.40
6:F:294:MET:HB3	6:F:299:THR:HB	2.03	0.40
1:G:186:LYS:NZ	1:G:190:GLU:OE1	2.53	0.40
5:H:160:ILE:HG13	5:H:165:ALA:HA	2.03	0.40
3:I:146:ILE:HB	3:I:288:LEU:HD22	2.02	0.40
3:I:201:ARG:O	3:I:204:VAL:HG12	2.21	0.40
5:J:233:LYS:HD3	5:J:233:LYS:HA	1.95	0.40
5:N:6:ASP:HB3	5:N:13:LYS:HB2	2.02	0.40
5:N:97:PRO:HA	5:N:126:ALA:O	2.20	0.40
1:A:8:GLY:H	1:A:12:CYS:HA	1.86	0.40
2:B:72:ASN:O	2:B:76:MET:HB2	2.21	0.40
6:F:47:ASP:HB3	6:F:48:SER:H	1.69	0.40
6:F:190:GLU:CG	1:G:167:PRO:HB2	2.41	0.40
6:F:195:PHE:HD1	6:F:200:GLU:HB3	1.85	0.40
1:G:3:LEU:HD12	1:G:98:VAL:HG22	2.02	0.40
1:G:59:ILE:HD13	1:G:59:ILE:H	1.86	0.40
1:G:85:PHE:HZ	1:G:118:MET:HE1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:65:PRO:HG2	3:I:66:ILE:HG13	2.03	0.40
3:I:185:MET:HB2	3:I:204:VAL:HG11	2.03	0.40
5:J:12:VAL:HG23	5:J:28:SER:OG	2.21	0.40
5:J:301:TYR:HA	5:J:302:PRO:HD3	1.82	0.40
7:L:249:ARG:HD2	7:L:249:ARG:HH11	1.77	0.40
4:D:321:LYS:NZ	4:D:323:ILE:HD13	2.36	0.40
5:E:166:LEU:HA	5:E:167:PRO:HD3	1.87	0.40
6:F:40:MET:HG2	6:F:57:LYS:HD2	2.04	0.40
1:G:13:LYS:HB2	1:G:13:LYS:HE2	1.95	0.40
5:H:92:ALA:HA	5:H:93:PRO:HD2	1.90	0.40
5:H:102:GLU:HB2	5:H:106:ASN:ND2	2.37	0.40
3:I:196:SER:HB3	5:J:172:ARG:HB3	2.04	0.40
5:J:248:GLU:HA	5:J:251:ARG:HB2	2.03	0.40
5:J:269:ILE:HD13	5:J:269:ILE:HA	1.98	0.40
5:K:97:PRO:HG3	5:K:125:PRO:HG2	2.02	0.40
7:L:146:ILE:HD11	7:L:157:THR:HB	2.03	0.40
5:N:65:PRO:HG3	5:N:80:ILE:HD12	2.02	0.40
5:N:248:GLU:H	5:N:248:GLU:CD	2.29	0.40
5:N:275:ASN:HD22	5:N:275:ASN:HA	1.77	0.40
1:A:44:GLN:H	1:A:44:GLN:NE2	2.19	0.40
4:D:56:ARG:HB3	4:D:61:LEU:HD11	2.03	0.40
4:D:157:PRO:HG2	4:D:164:LEU:HB2	2.02	0.40
5:E:206:ASP:O	5:E:210:LYS:HG2	2.22	0.40
6:F:58:ARG:HD2	6:F:198:THR:HB	2.03	0.40
6:F:169:ALA:HA	6:F:279:LYS:HG2	2.03	0.40
5:H:166:LEU:O	5:H:170:ILE:HG13	2.21	0.40
3:I:189:SER:HB2	5:J:104:PRO:O	2.20	0.40
5:J:180:LEU:O	5:J:252:CYS:SG	2.79	0.40
5:J:183:TYR:HD2	5:J:252:CYS:HA	1.86	0.40
5:J:257:PHE:O	5:J:268:GLY:HA3	2.22	0.40
5:K:99:LEU:HG	5:K:128:TYR:HB3	2.04	0.40
5:K:165:ALA:O	5:K:167:PRO:HD3	2.22	0.40
7:M:215:ALA:HB2	7:M:250:PHE:HB2	2.04	0.40
5:N:273:THR:O	5:N:277:ILE:HG12	2.22	0.40
1:A:52:GLU:HG2	1:A:56:LYS:NZ	2.36	0.40
1:A:106:ASN:HA	1:A:107:PRO:HD3	1.90	0.40
1:A:329:GLU:HG3	1:A:336:ILE:HD12	2.03	0.40
2:B:70:ILE:HD11	2:B:113:MET:HE3	2.03	0.40
5:H:31:GLY:HA2	5:H:61:THR:O	2.22	0.40
3:I:29:ILE:O	3:I:49:VAL:HA	2.22	0.40
5:J:57:ARG:HG3	5:J:58:GLY:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:211:LEU:HB3	5:J:249:ARG:HD2	2.02	0.40
5:K:81:TRP:HA	5:K:84:THR:OG1	2.21	0.40
7:M:94:GLU:CD	7:M:94:GLU:H	2.30	0.40
7:M:330:ARG:HH11	7:M:330:ARG:HD2	1.76	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	G	363/365 (100%)	333 (92%)	25 (7%)	5 (1%)	9	40
2	B	314/364 (86%)	275 (88%)	29 (9%)	10 (3%)	3	21
3	C	293/365 (80%)	269 (92%)	23 (8%)	1 (0%)	36	72
3	I	363/365 (100%)	328 (90%)	30 (8%)	5 (1%)	9	40
4	D	355/357 (99%)	307 (86%)	36 (10%)	12 (3%)	3	21
5	E	363/365 (100%)	314 (86%)	36 (10%)	13 (4%)	2	20
5	H	363/365 (100%)	319 (88%)	36 (10%)	8 (2%)	5	29
5	J	363/365 (100%)	309 (85%)	44 (12%)	10 (3%)	4	24
5	K	363/365 (100%)	315 (87%)	38 (10%)	10 (3%)	4	24
5	N	363/365 (100%)	322 (89%)	32 (9%)	9 (2%)	4	26
6	F	355/357 (99%)	295 (83%)	47 (13%)	13 (4%)	2	20
7	L	363/365 (100%)	305 (84%)	48 (13%)	10 (3%)	4	24
7	M	363/365 (100%)	307 (85%)	42 (12%)	14 (4%)	2	19
All	All	4584/4728 (97%)	3998 (87%)	466 (10%)	120 (3%)	6	25

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	280	ASP
2	B	329	ARG
2	B	362	SER
3	C	265	GLU
4	D	8	SER
4	D	175	GLY
4	D	346	GLN
5	E	198	THR
5	E	345	SER
6	F	58	ARG
6	F	197	THR
6	F	330	ARG
1	G	168	HIS
5	J	104	PRO
5	J	107	PRO
5	J	166	LEU
5	J	241	GLN
5	K	132	GLN
5	K	330	ARG
7	L	57	ARG
7	L	59	ILE
7	L	123	ASN
7	L	177	GLY
7	L	194	SER
7	L	239	ASP
7	M	35	HIS
7	M	57	ARG
7	M	59	ILE
7	M	196	THR
7	M	199	ALA
5	N	57	ARG
5	N	314	ALA
5	N	318	SER
2	B	317	SER
4	D	56	ARG
4	D	58	ILE
4	D	174	ALA
4	D	192	SER
4	D	331	SER
4	D	355	TYR
5	E	58	GLY
5	E	191	ARG
5	E	200	GLU

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Mol	Chain	Res	Type
5	E	330	ARG
5	E	363	SER
6	F	232	GLU
6	F	280	CYS
1	G	57	ARG
5	H	40	VAL
5	H	191	ARG
5	H	228	SER
5	H	330	ARG
5	J	45	LYS
5	J	230	SER
5	K	38	VAL
5	K	228	SER
7	M	123	ASN
7	M	350	MET
5	N	84	THR
5	N	192	GLY
5	N	230	SER
4	D	9	GLY
5	E	55	SER
5	E	194	SER
6	F	84	THR
6	F	355	GLN
1	G	229	SER
5	J	105	LEU
5	J	242	VAL
7	L	281	ASP
7	M	108	LYS
7	M	151	GLY
7	M	200	GLU
5	N	263	GLY
5	N	347	PHE
2	B	237	PRO
4	D	349	TRP
5	E	252	CYS
6	F	47	ASP
5	H	176	ALA
3	I	42	MET
3	I	196	SER
3	I	229	SER
3	I	242	VAL
5	K	40	VAL

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Mol	Chain	Res	Type
5	K	230	SER
7	L	45	LYS
7	L	346	THR
7	L	350	MET
7	M	38	VAL
7	M	228	SER
4	D	342	LEU
5	E	176	ALA
6	F	176	ALA
6	F	238	PRO
5	H	217	ASP
5	H	249	ARG
5	J	252	CYS
5	K	39	MET
7	M	170	ILE
2	B	228	SER
2	B	251	CYS
2	B	281	ILE
2	B	316	PRO
5	H	269	ILE
5	K	192	GLY
7	M	28	SER
5	E	242	VAL
6	F	170	ILE
1	G	159	PRO
1	G	352	ILE
5	J	59	ILE
5	K	246	GLY
5	N	65	PRO
5	E	192	GLY
6	F	196	VAL
6	F	153	GLY
2	B	241	VAL
3	I	170	ILE
5	K	252	CYS

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

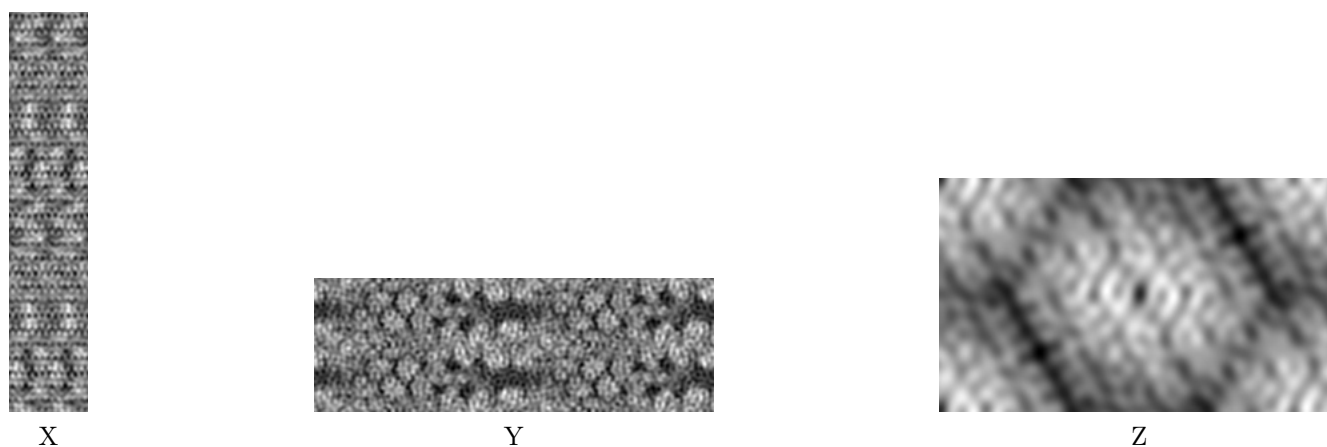
6 Map visualisation [i](#)

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](#)

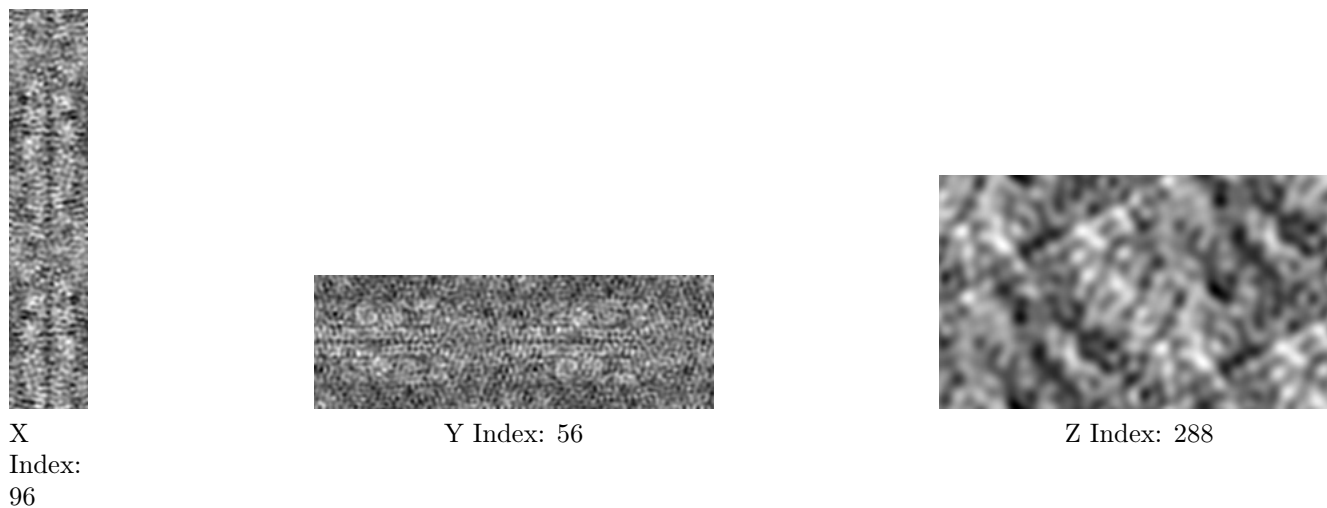
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



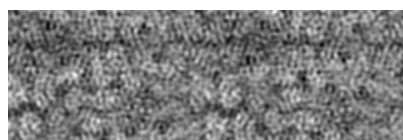
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X
Index:
123



Y Index: 84

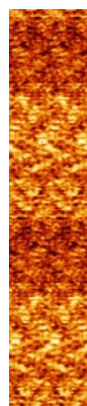


Z Index: 413

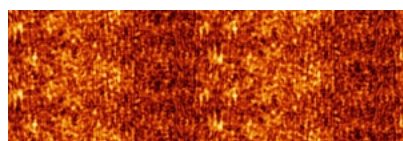
The images above show the largest variance slices of the map in three orthogonal directions.

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

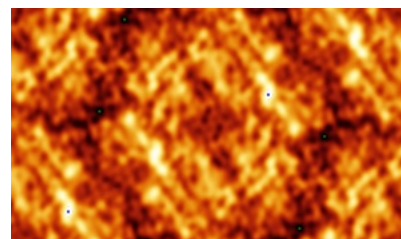
6.4.1 Primary map



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.

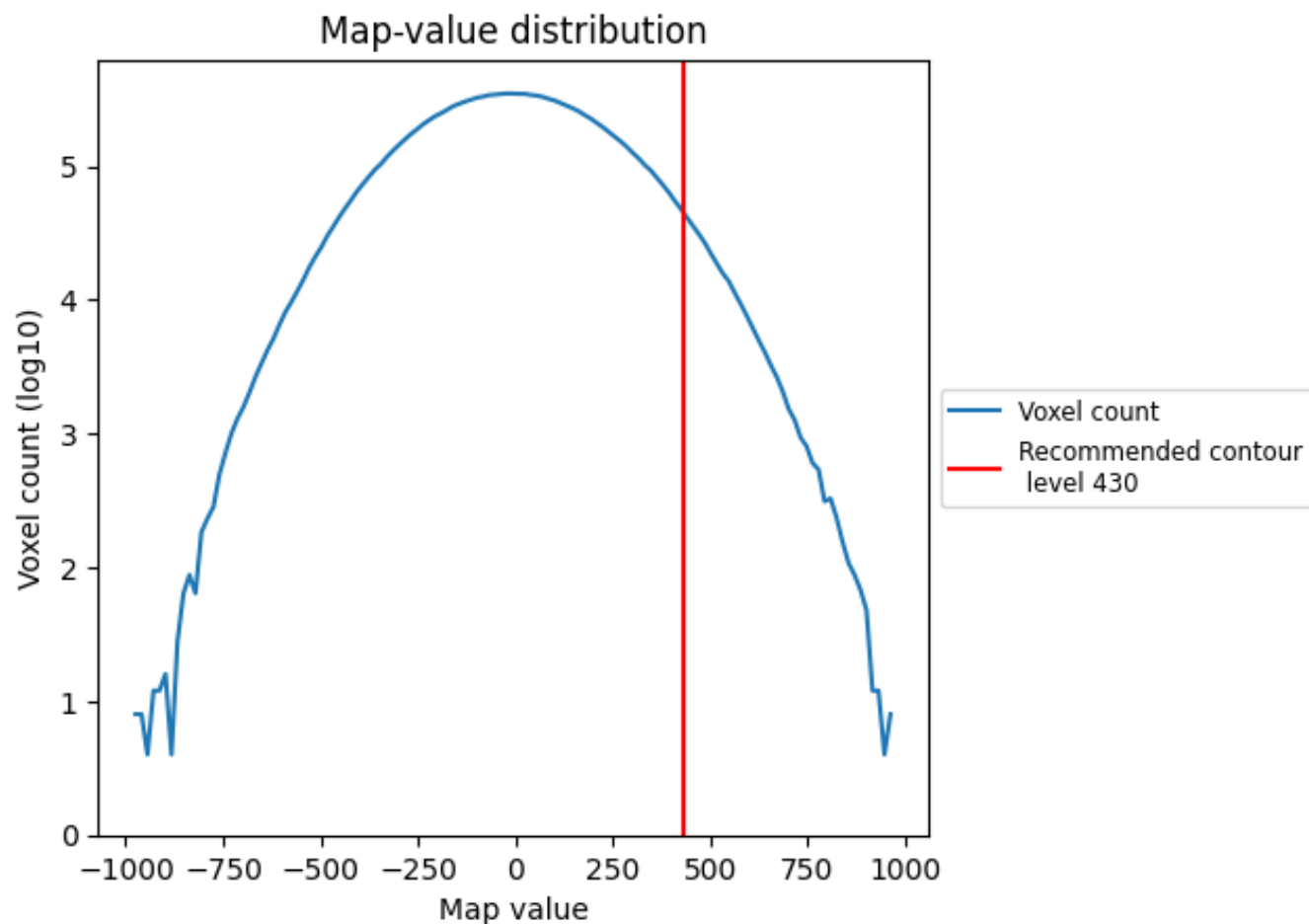
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

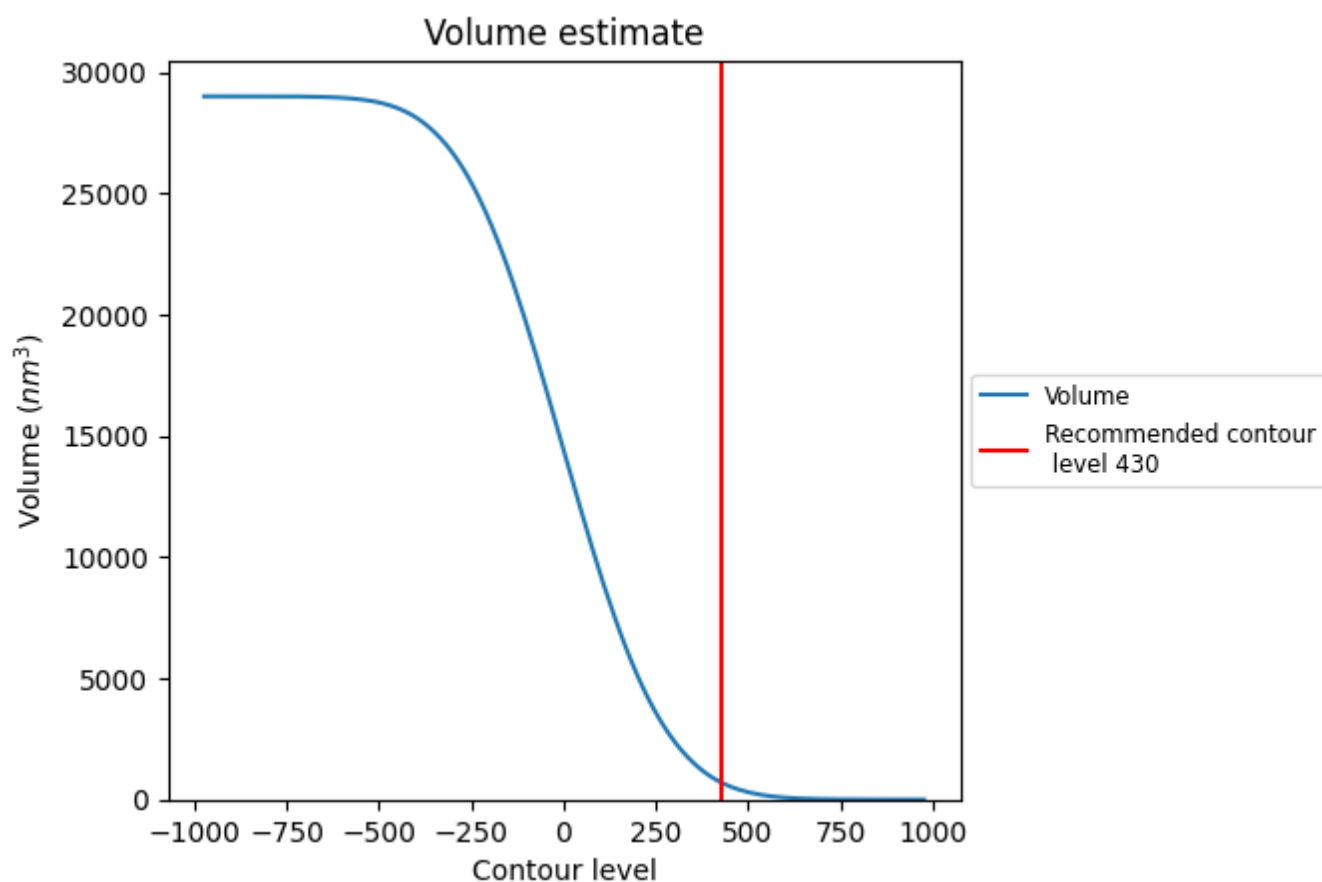
This section contains the results of statistical analysis of the map.

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.

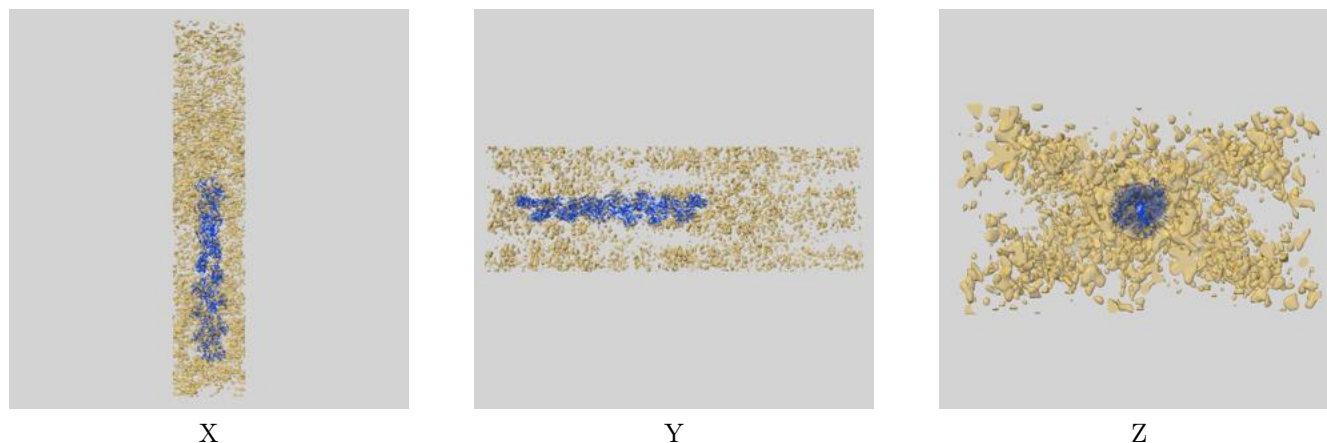
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

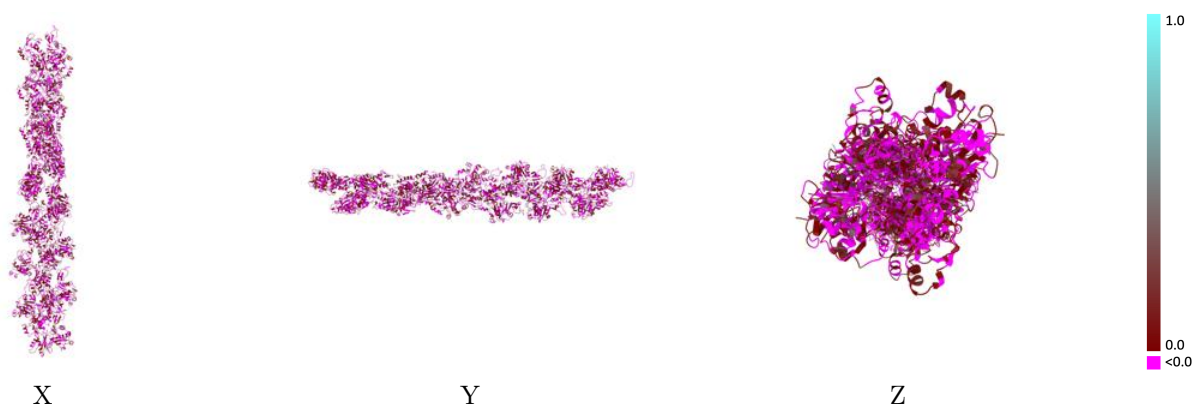
This section contains information regarding the fit between EMDB map EMD-1088 and PDB model 3B63. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



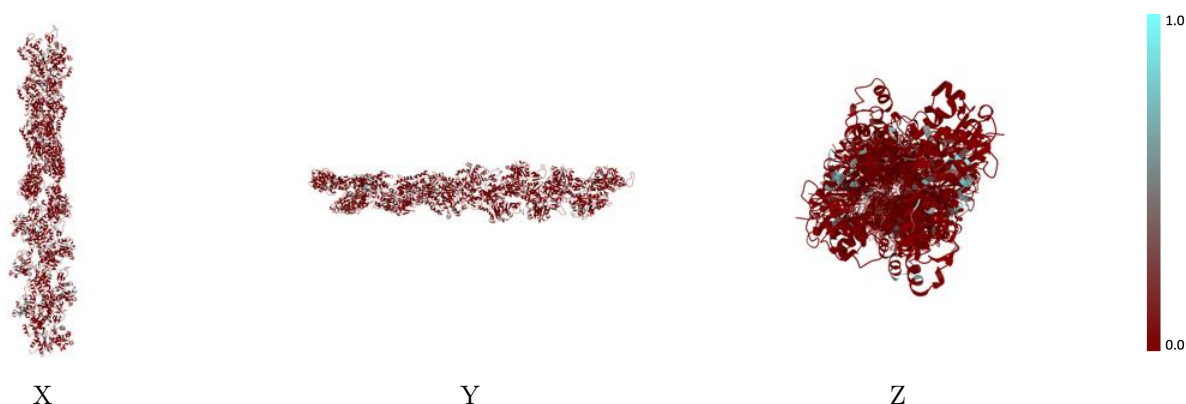
The images above show the 3D surface view of the map at the recommended contour level 430.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



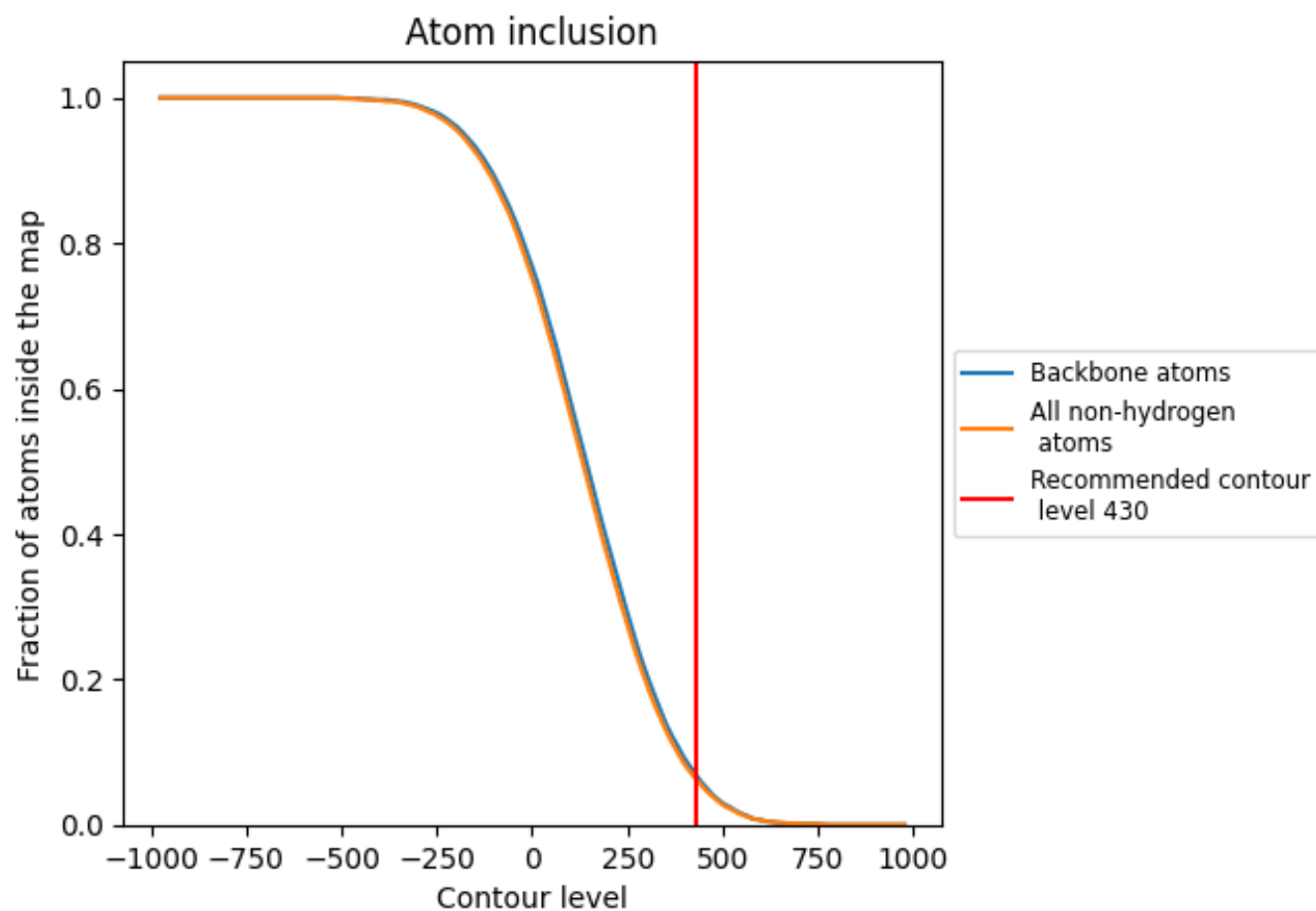
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.0630	0.0210
A	0.0670	0.0210
B	0.0970	0.0030
C	0.1090	0.0310
D	0.0810	0.0140
E	0.0780	0.0340
F	0.0810	0.0260
G	0.0640	0.0240
H	0.0340	0.0130
I	0.0130	0.0240
J	0.0300	0.0110
K	0.0330	0.0240
L	0.0560	0.0330
M	0.0740	0.0240
N	0.0700	0.0110

1.0

0.0

<0.0