Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 03:26 pm GMT

PDB ID	:	2WVW
EMDB ID	:	EMD-1655
Title	:	Cryo-EM structure of the RbcL-RbcX complex
Authors	:	Liu, C.; Young, A.L.; Starling-Windhof, A.; Bracher, A.; Saschenbrecker, S.; Rao, B.V.; Rao, K.V.; Berninghausen, O.; Mielke, T.; Hartl, F.U.; Beckmann, R.; Hayer-Hartl, M.
Deposited on	:	2009-10-20
Resolution	:	9.00 Å(reported)
Based on initial model	:	3HYB

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:

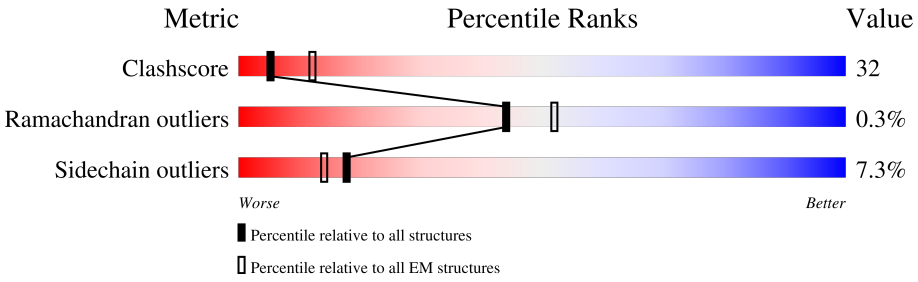
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 9.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	472	55% 72% 22%
1	B	472	54% 71% 23%
1	C	472	53% 72% 22%
1	D	472	54% 71% 22%
1	E	472	54% 72% 22%
1	F	472	54% 71% 22%
1	G	472	54% 71% 22%
1	H	472	53% 71% 23%

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Mol	Chain	Length	Quality of chain
2	I	155	68% 47% 18% 32%
2	J	155	67% 48% 15% 5% 32%
2	K	155	68% 48% 17% 32%
2	L	155	67% 48% 15% 5% 32%
2	M	155	68% 47% 18% 32%
2	N	155	67% 48% 15% 5% 32%
2	O	155	68% 46% 19% 32%
2	P	155	67% 48% 15% 5% 32%
2	Q	155	68% 46% 19% 32%
2	R	155	67% 48% 14% 5% 32%
2	S	155	68% 46% 19% 32%
2	T	155	67% 48% 15% 5% 32%
2	U	155	68% 46% 19% 32%
2	V	155	67% 48% 15% 5% 32%
2	W	155	68% 47% 18% 32%
2	X	155	67% 48% 15% 5% 32%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 42856 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 RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		
1	B	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		
1	C	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		
1	D	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		
1	E	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		
1	F	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		
1	G	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		
1	H	467	Total	C	N	O	S	0	0
			3653	2324	638	673	18		

- Molecule 2 is a protein called RBCX PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	J	105	Total	C	N	O	S	4	0
			870	555	151	160	4		
2	K	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	L	105	Total	C	N	O	S	4	0
			870	555	151	160	4		
2	M	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	N	105	Total	C	N	O	S	4	0
			870	555	151	160	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	P	105	Total	C	N	O	S	4	0
			870	555	151	160	4		
2	Q	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	R	105	Total	C	N	O	S	4	0
			870	555	151	160	4		
2	S	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	T	105	Total	C	N	O	S	4	0
			870	555	151	160	4		
2	U	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	V	105	Total	C	N	O	S	4	0
			870	555	151	160	4		
2	W	105	Total	C	N	O	S	3	0
			834	532	141	157	4		
2	X	105	Total	C	N	O	S	4	0
			870	555	151	160	4		

3 Residue-property plots (i)

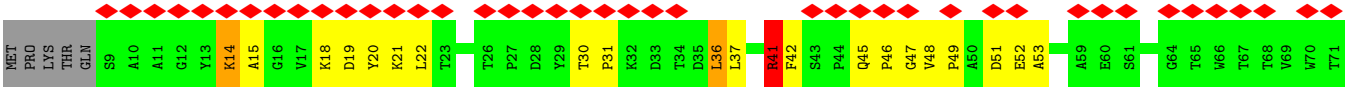
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

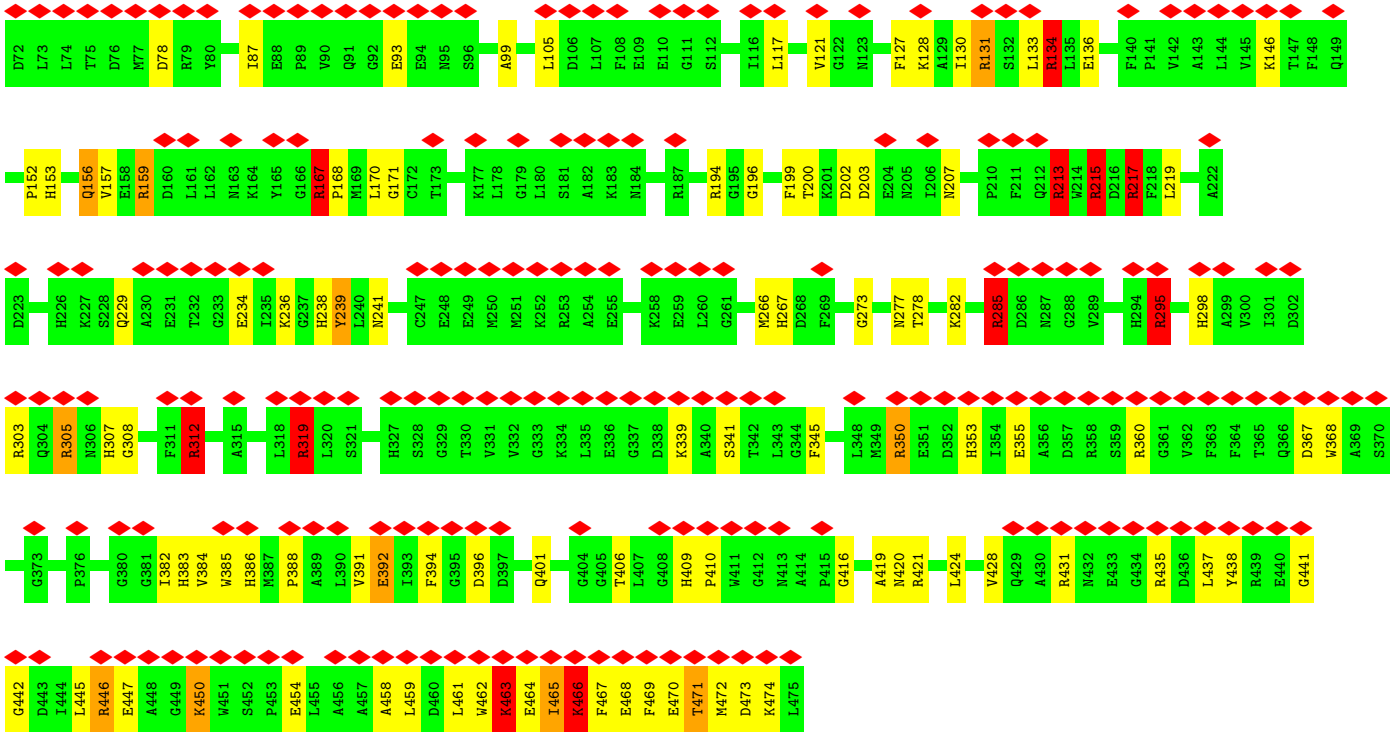
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain A:

• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

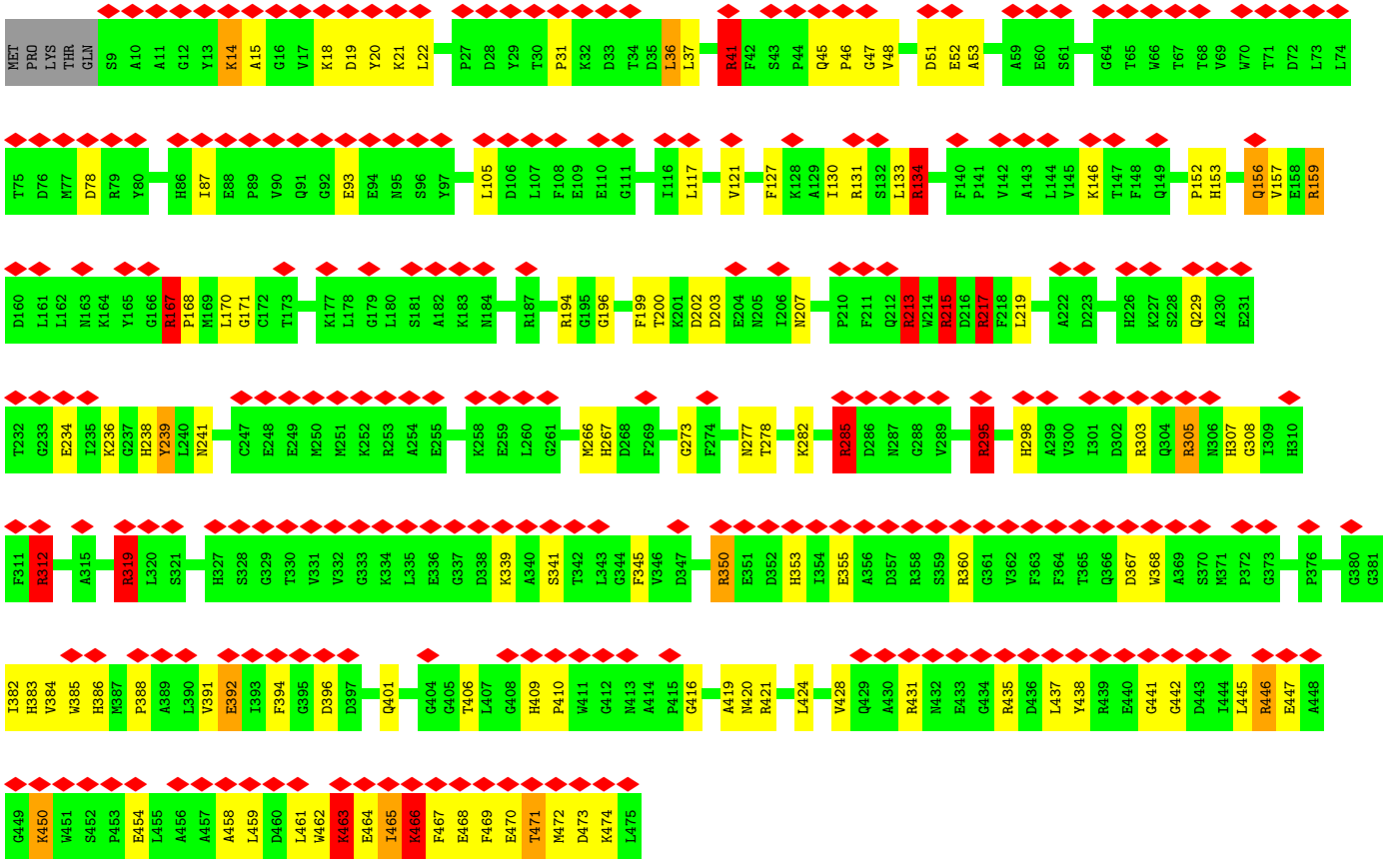
Chain B:





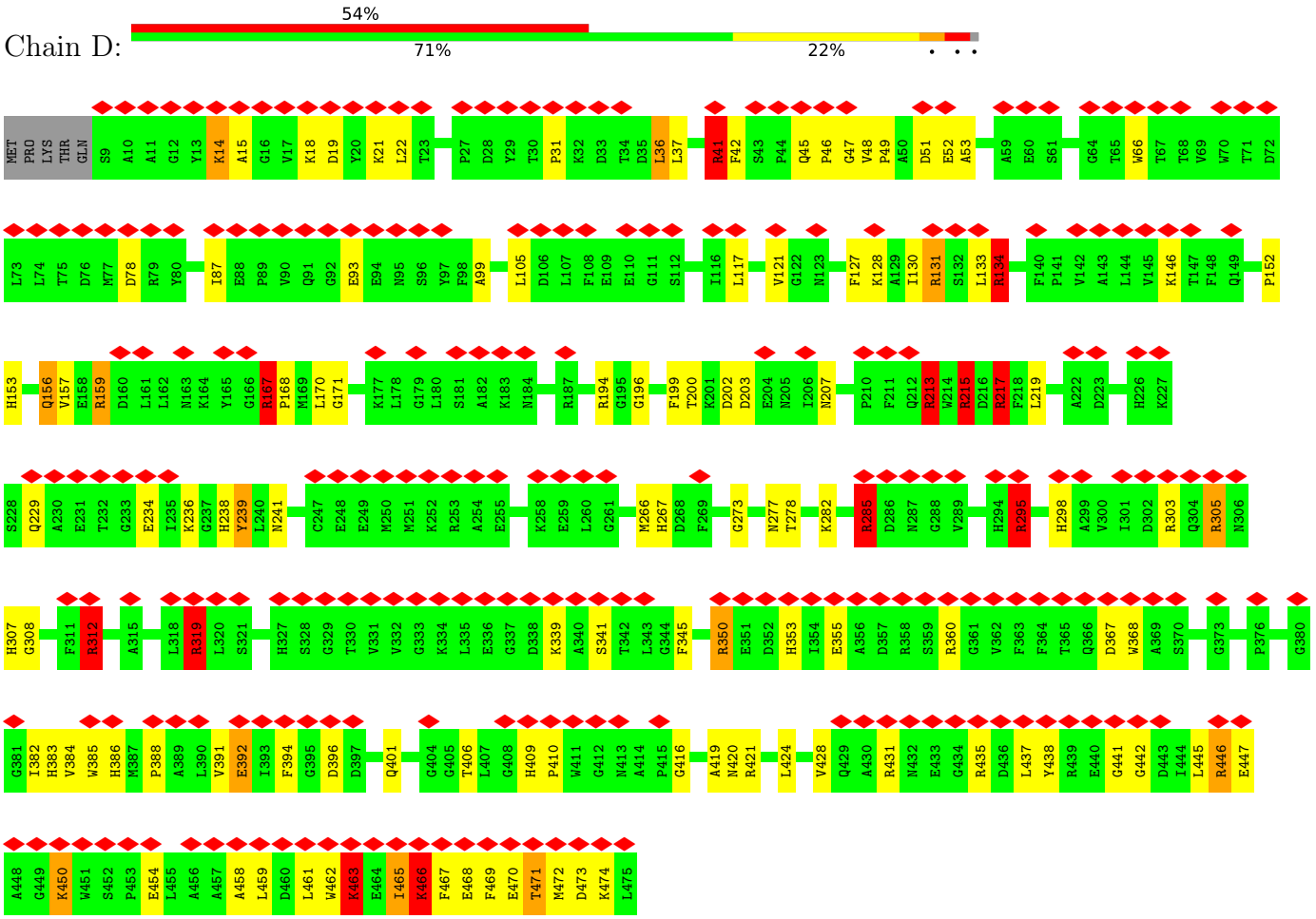
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain C:



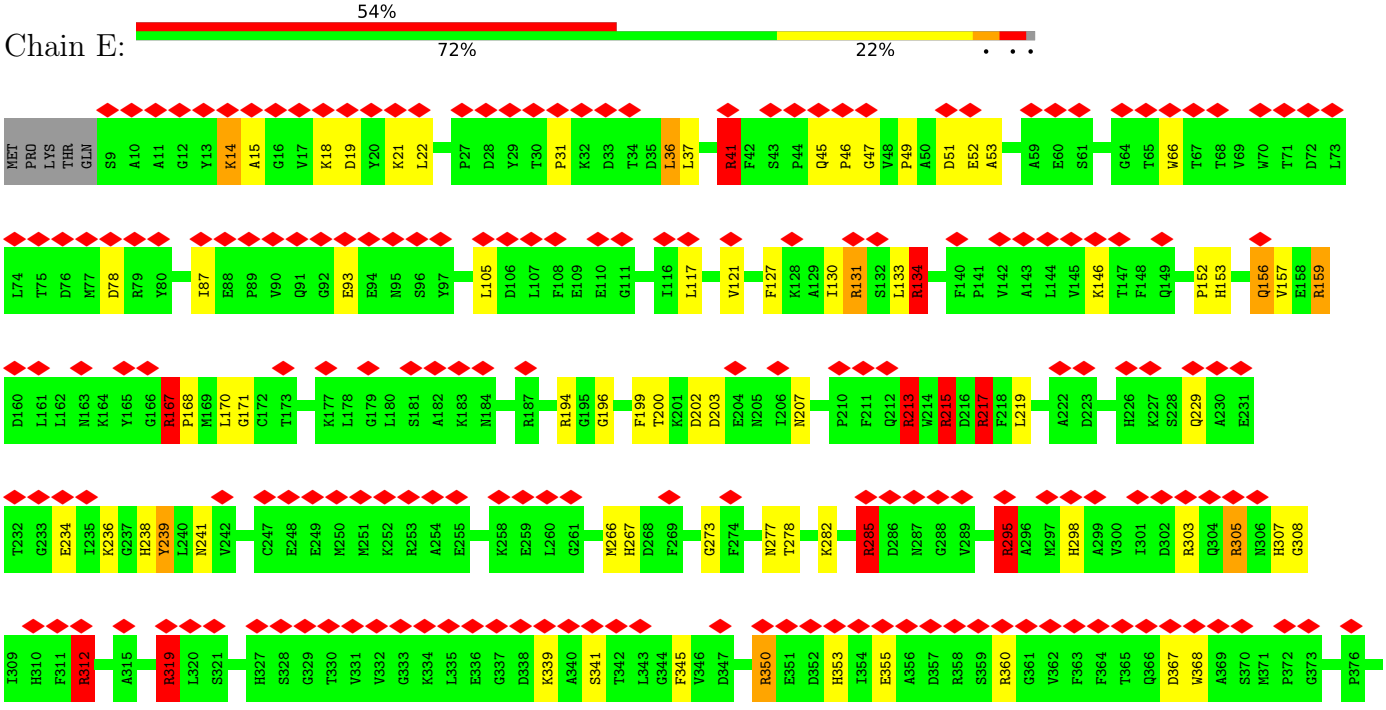
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

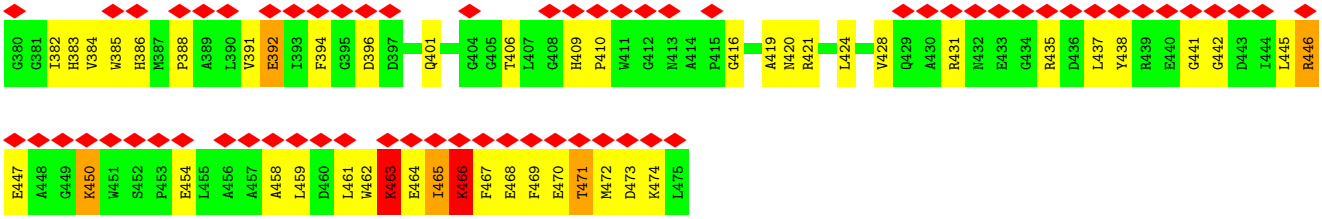
Chain D:



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

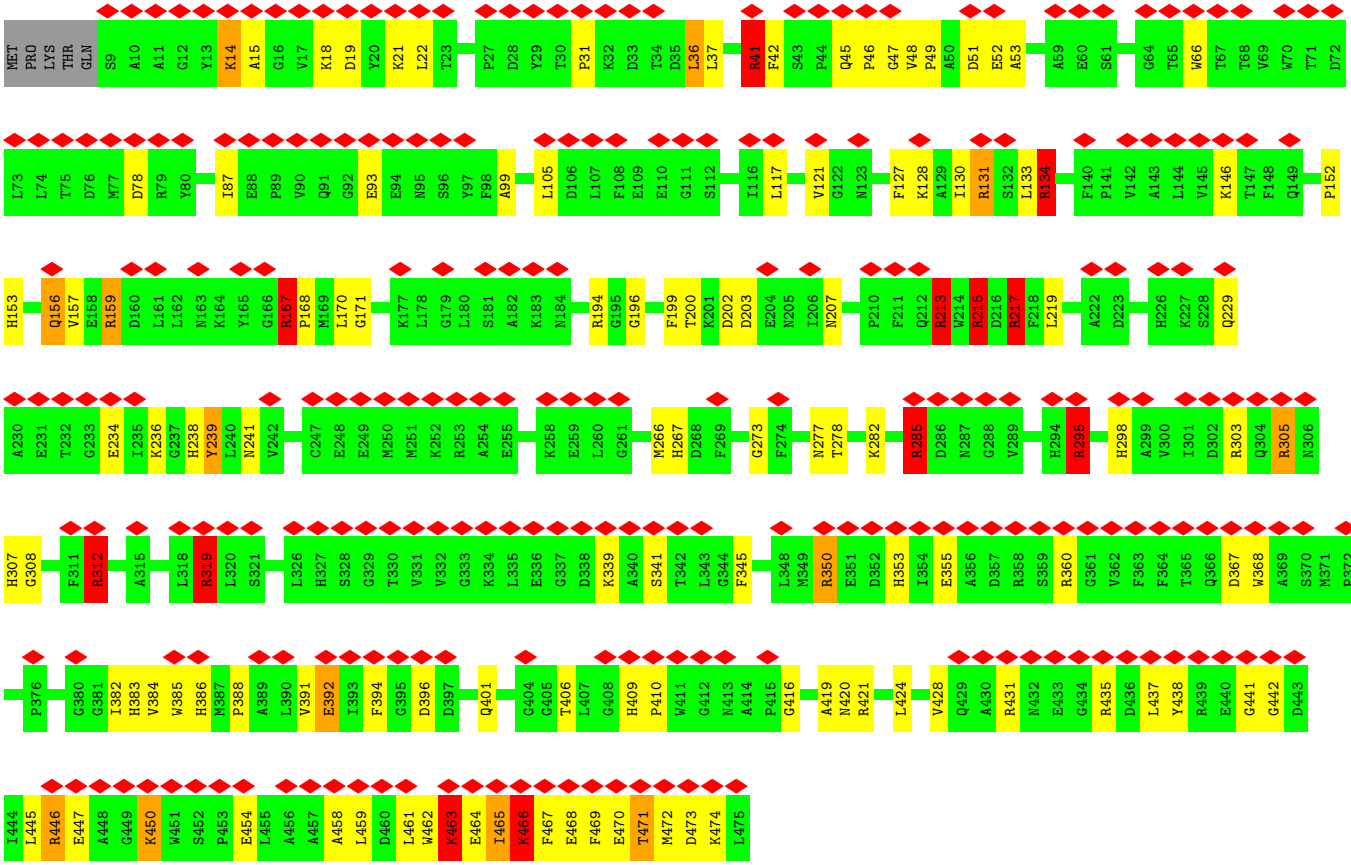
Chain E:





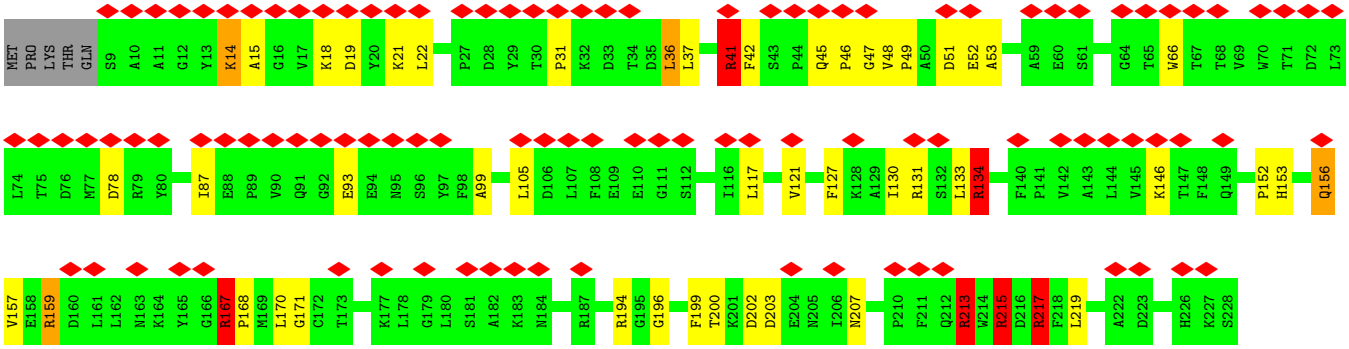
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

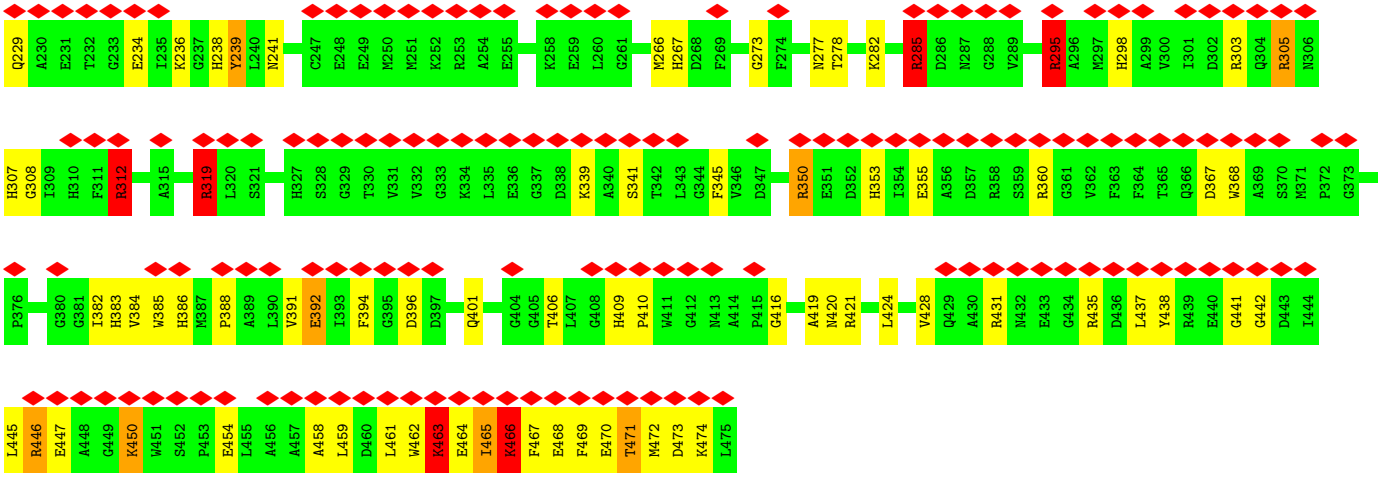
Chain F:



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

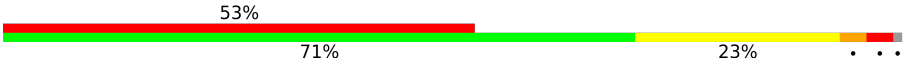
Chain G:

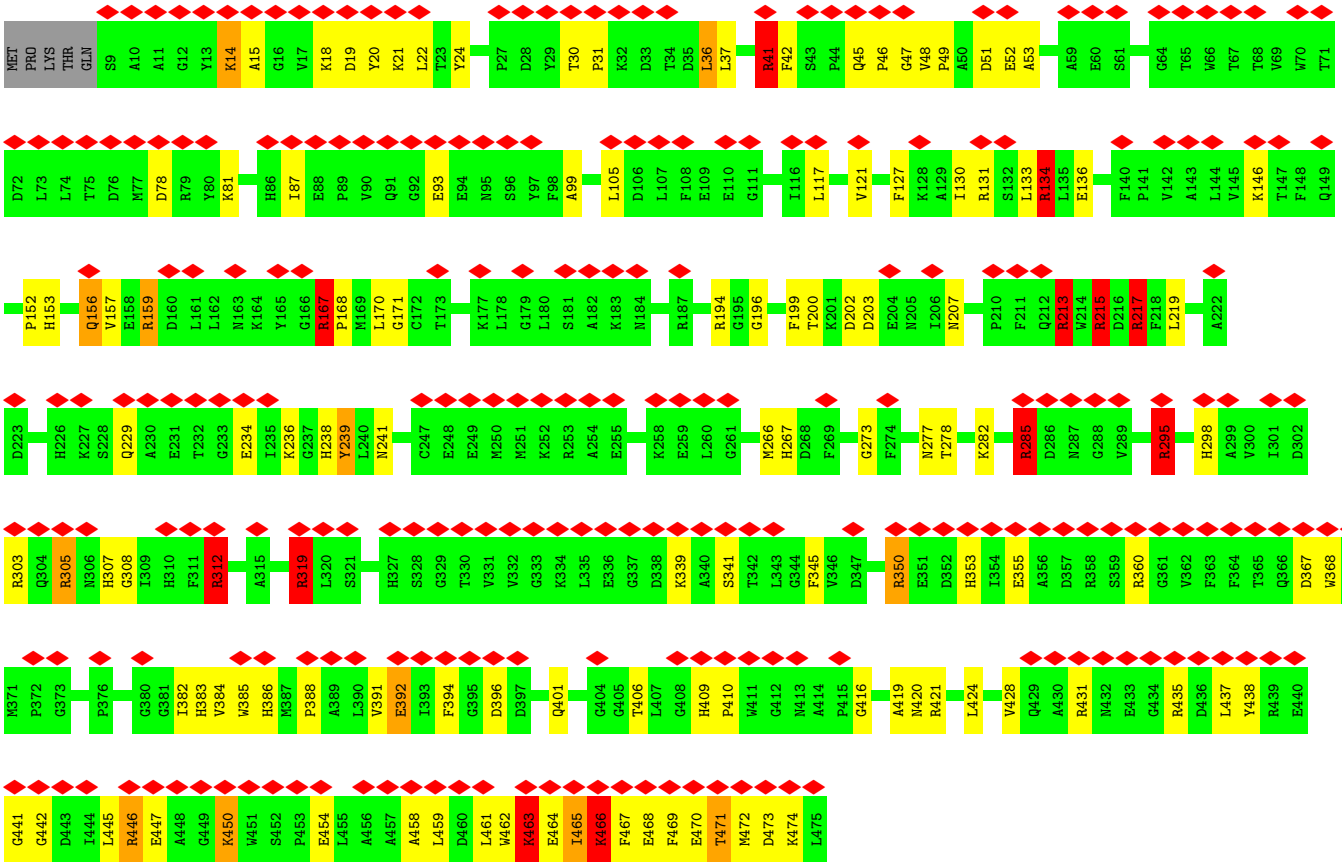




- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

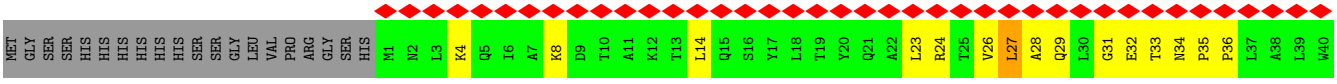
Chain H:

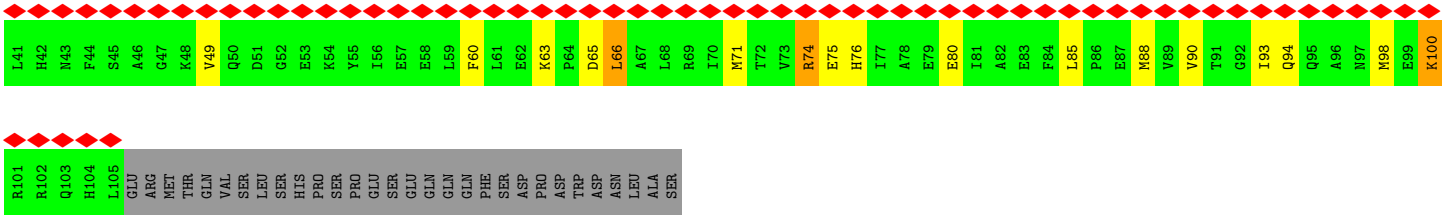




- Molecule 2: RBCX PROTEIN

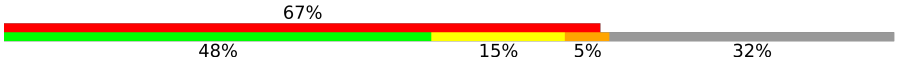
Chain I:

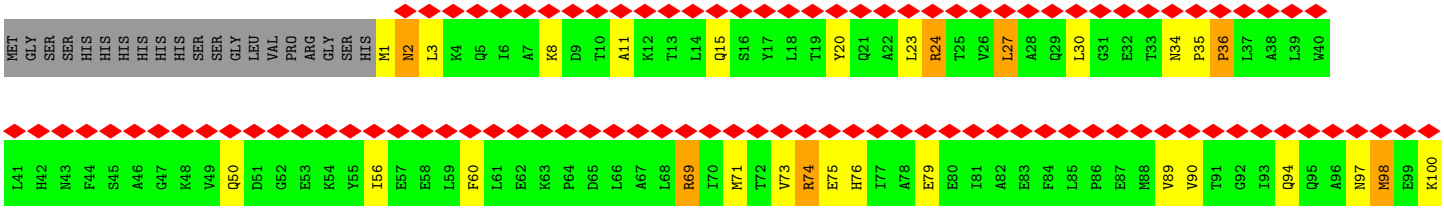




• Molecule 2: RBCX PROTEIN

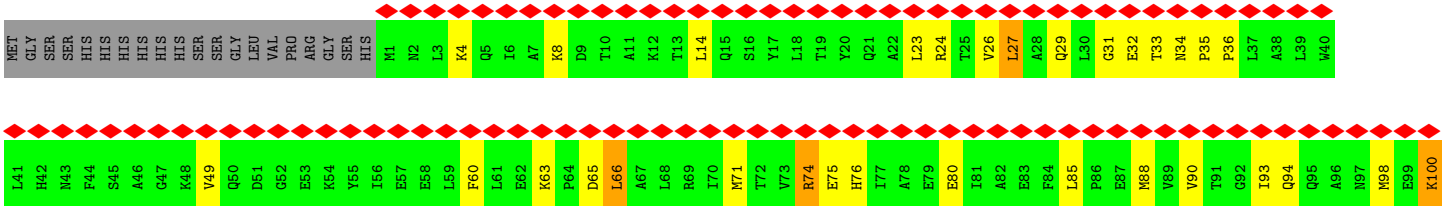
Chain J:





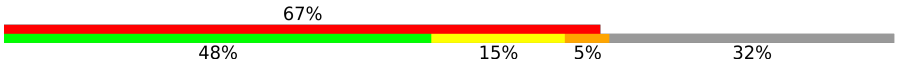
• Molecule 2: RBCX PROTEIN

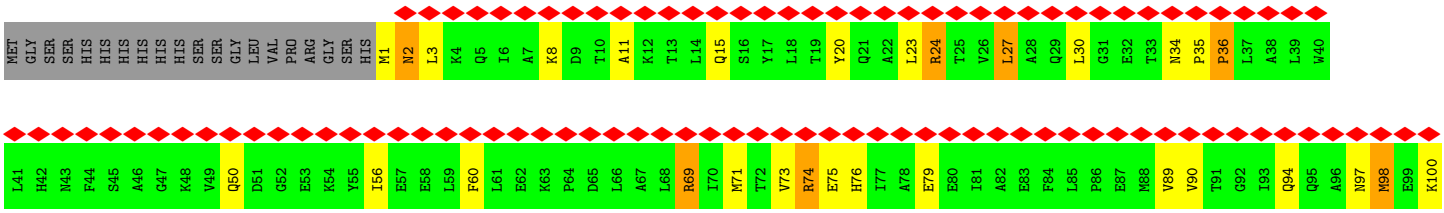
Chain K:



• Molecule 2: RBCX PROTEIN

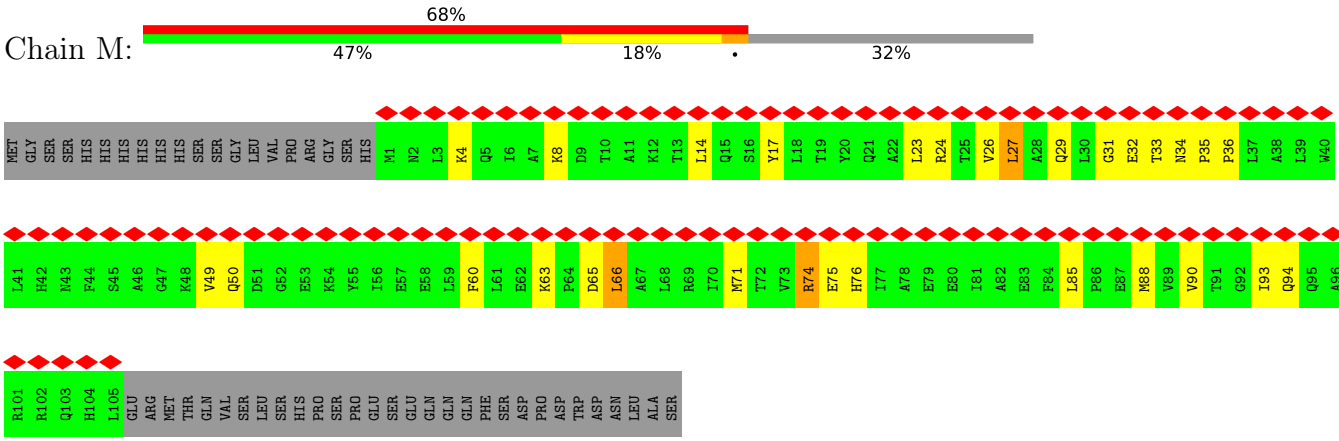
Chain L:





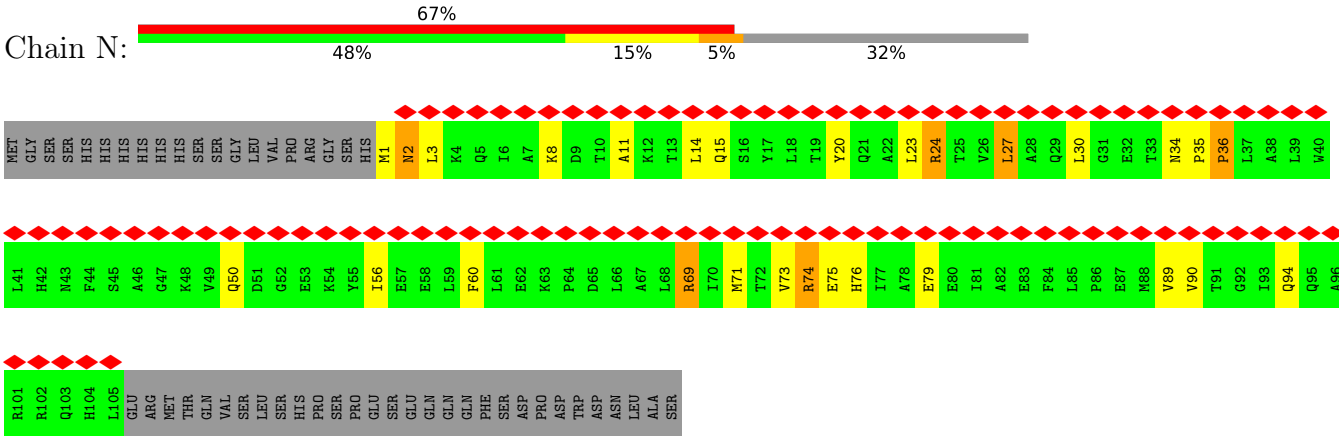
• Molecule 2: RBCX PROTEIN

Chain M:



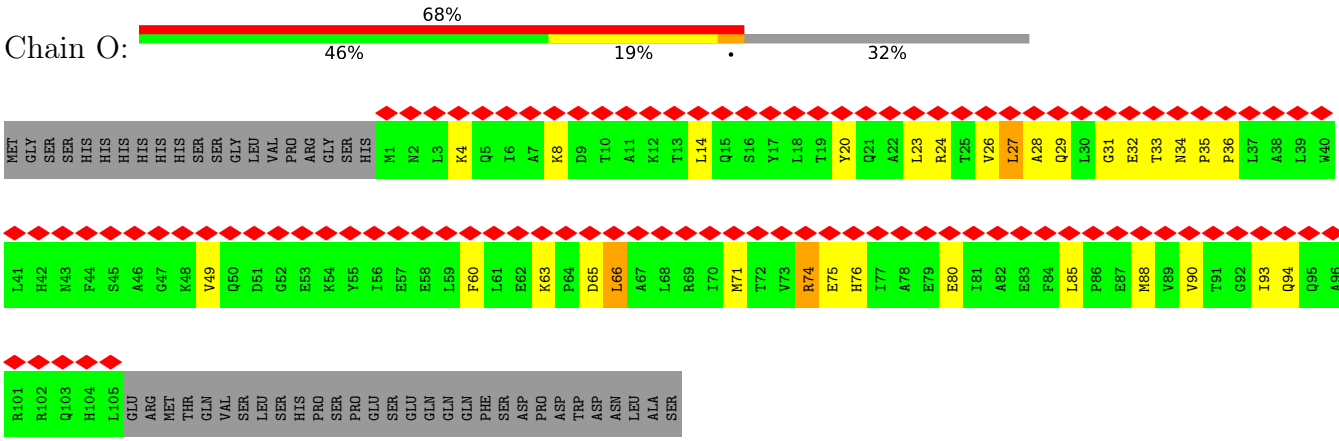
• Molecule 2: RBCX PROTEIN

Chain N:



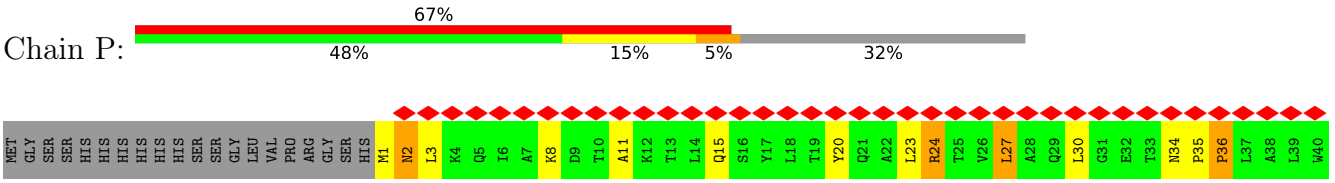
• Molecule 2: RBCX PROTEIN

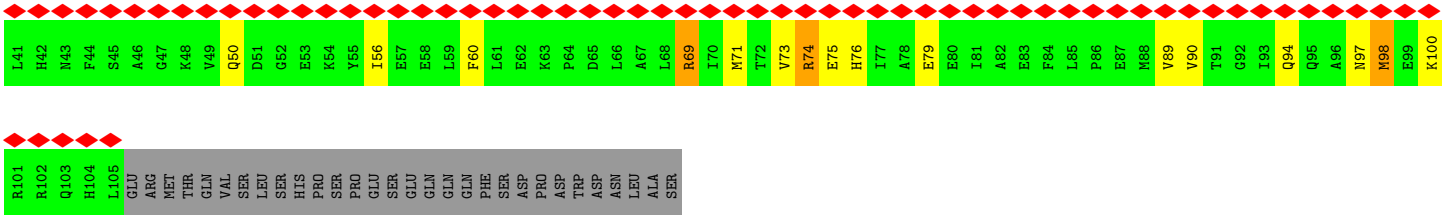
Chain O:



• Molecule 2: RBCX PROTEIN

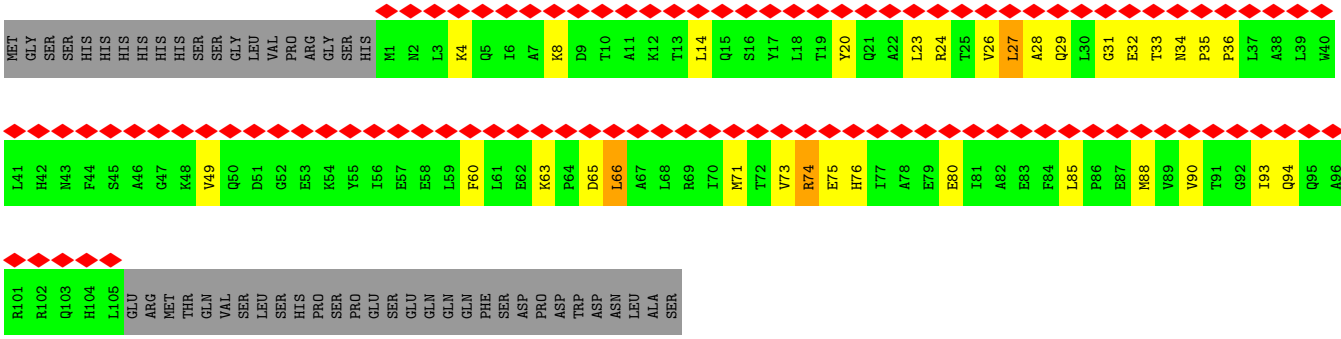
Chain P:





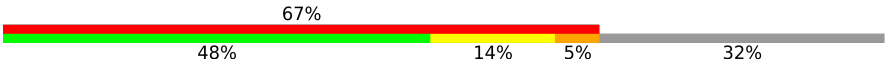
- Molecule 2: RBCX PROTEIN

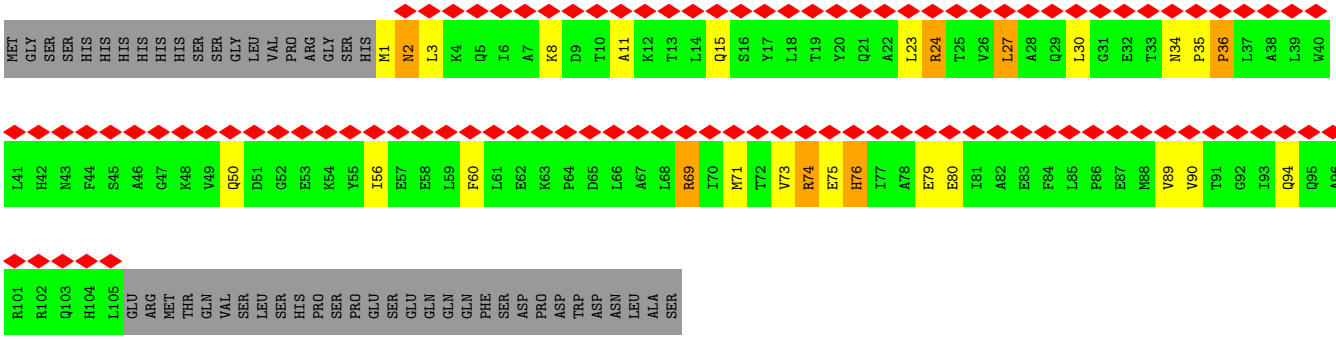
Chain Q:



- Molecule 2: RBCX PROTEIN

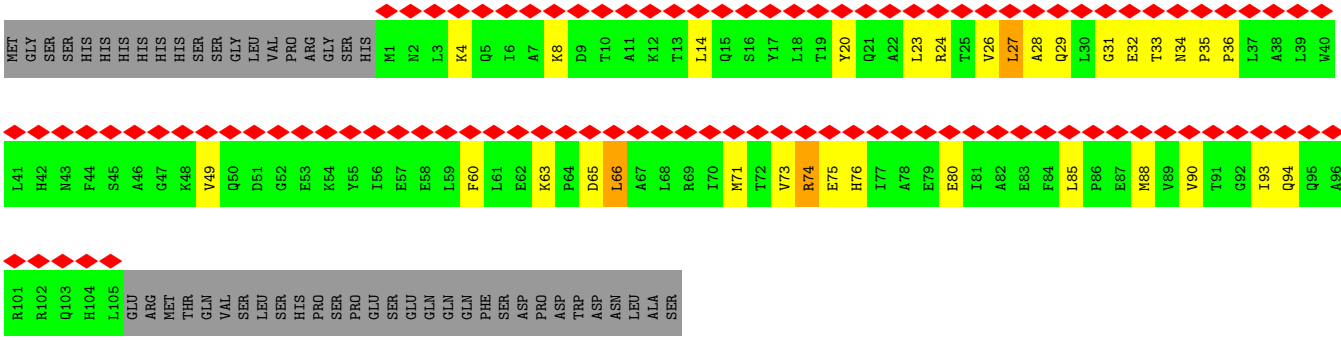
Chain R:





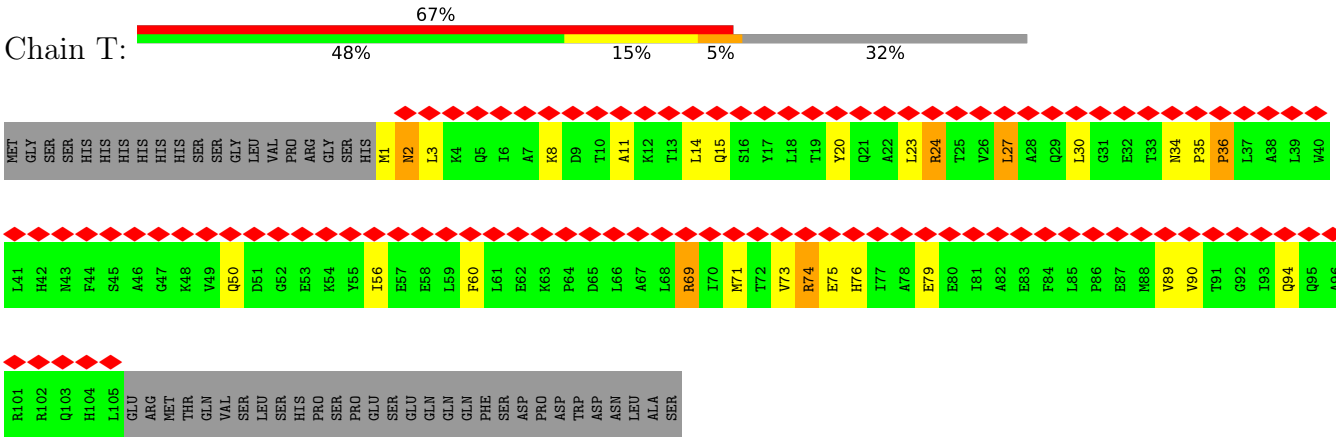
- Molecule 2: RBCX PROTEIN

Chain S:



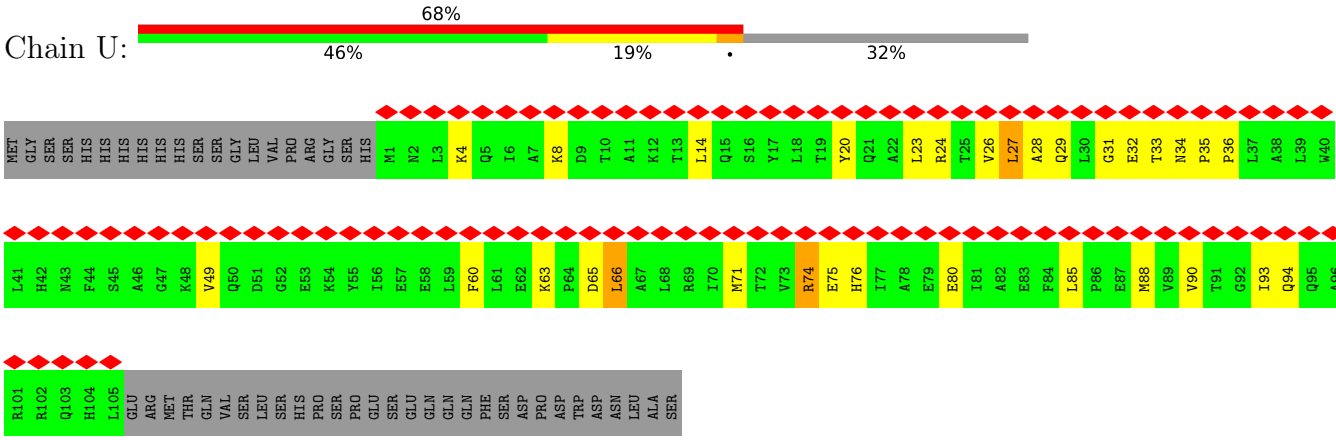
• Molecule 2: RBCX PROTEIN

Chain T:



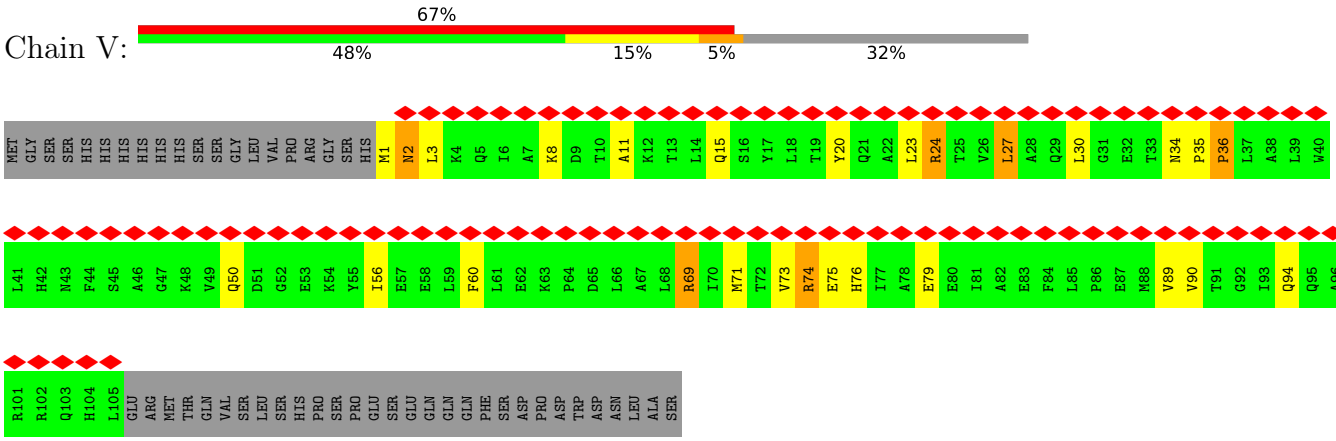
• Molecule 2: RBCX PROTEIN

Chain U:



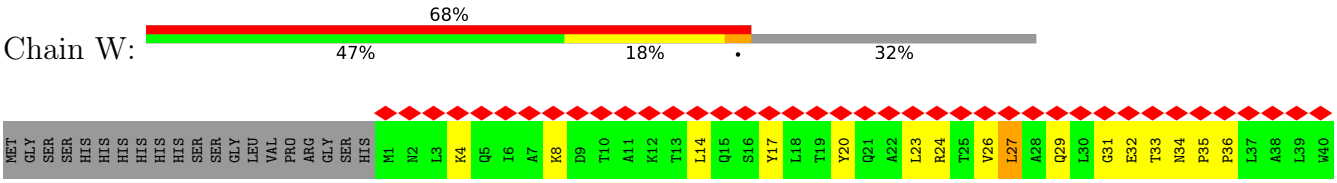
• Molecule 2: RBCX PROTEIN

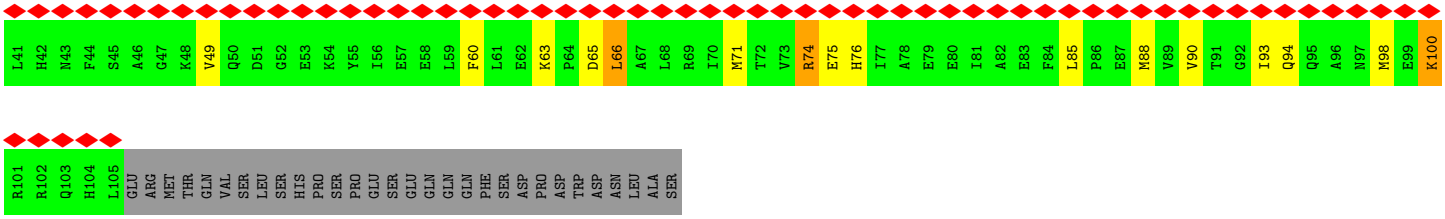
Chain V:



• Molecule 2: RBCX PROTEIN

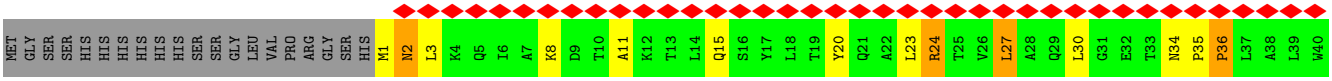
Chain W:

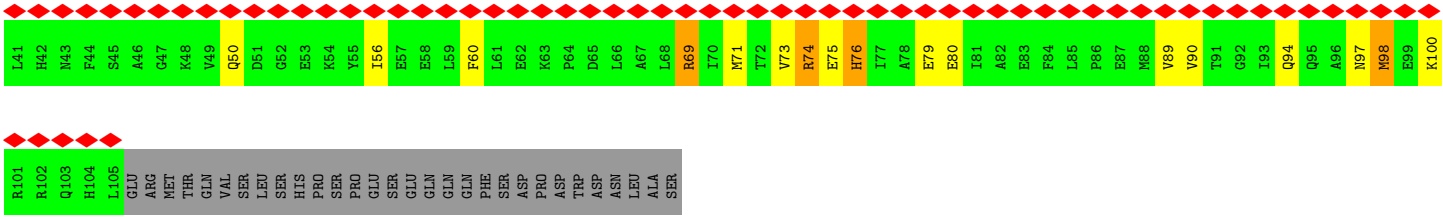




• Molecule 2: RBCX PROTEIN

Chain X:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11104	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	38900	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	10.756	Depositor
Minimum map value	-13.709	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.6	Depositor
Map size (Å)	286.88, 286.88, 286.88	wwPDB
Map dimensions	176, 176, 176	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	1.63, 1.63, 1.63	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	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
1	B	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
1	C	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
1	D	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
1	E	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
1	F	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
1	G	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
1	H	0.55	3/3738 (0.1%)	1.00	18/5049 (0.4%)
2	I	0.59	0/847	0.66	0/1148
2	J	0.76	5/884 (0.6%)	0.69	0/1194
2	K	0.59	0/847	0.66	0/1148
2	L	0.76	5/884 (0.6%)	0.69	0/1194
2	M	0.59	0/847	0.66	0/1148
2	N	0.76	5/884 (0.6%)	0.69	0/1194
2	O	0.59	0/847	0.66	0/1148
2	P	0.76	5/884 (0.6%)	0.69	0/1194
2	Q	0.59	0/847	0.66	0/1148
2	R	0.76	5/884 (0.6%)	0.69	0/1194
2	S	0.59	0/847	0.66	0/1148
2	T	0.76	5/884 (0.6%)	0.69	0/1194
2	U	0.59	0/847	0.66	0/1148
2	V	0.76	5/884 (0.6%)	0.69	0/1194
2	W	0.59	0/847	0.66	0/1148
2	X	0.76	5/884 (0.6%)	0.69	0/1194
All	All	0.60	64/43752 (0.1%)	0.91	144/59128 (0.2%)

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	20

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	20
1	C	0	20
1	D	0	20
1	E	0	20
1	F	0	20
1	G	0	20
1	H	0	20
2	J	0	1
2	L	0	1
2	N	0	1
2	P	0	1
2	R	0	1
2	T	0	1
2	V	0	1
2	X	0	1
All	All	0	168

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	471	THR	C-N	20.46	1.81	1.34
1	G	471	THR	C-N	20.45	1.81	1.34
1	F	471	THR	C-N	20.45	1.81	1.34
1	A	471	THR	C-N	20.43	1.81	1.34
1	E	471	THR	C-N	20.43	1.81	1.34
1	H	471	THR	C-N	20.43	1.81	1.34
1	B	471	THR	C-N	20.41	1.80	1.34
1	C	471	THR	C-N	20.40	1.80	1.34
1	F	466	LYS	C-N	-12.37	1.05	1.34
1	B	466	LYS	C-N	-12.36	1.05	1.34
1	H	466	LYS	C-N	-12.35	1.05	1.34
1	A	466	LYS	C-N	-12.34	1.05	1.34
1	G	466	LYS	C-N	-12.32	1.05	1.34
1	E	466	LYS	C-N	-12.32	1.05	1.34
1	D	466	LYS	C-N	-12.32	1.05	1.34
1	C	466	LYS	C-N	-12.31	1.05	1.34
1	H	465	ILE	C-N	-10.80	1.09	1.34
1	C	465	ILE	C-N	-10.79	1.09	1.34
1	B	465	ILE	C-N	-10.79	1.09	1.34
1	D	465	ILE	C-N	-10.78	1.09	1.34
1	G	465	ILE	C-N	-10.78	1.09	1.34
1	F	465	ILE	C-N	-10.77	1.09	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	465	ILE	C-N	-10.77	1.09	1.34
1	E	465	ILE	C-N	-10.76	1.09	1.34
2	J	36	PRO	C-N	8.32	1.53	1.34
2	L	36	PRO	C-N	8.32	1.53	1.34
2	N	36	PRO	C-N	8.32	1.53	1.34
2	P	36	PRO	C-N	8.32	1.53	1.34
2	R	36	PRO	C-N	8.32	1.53	1.34
2	T	36	PRO	C-N	8.32	1.53	1.34
2	V	36	PRO	C-N	8.32	1.53	1.34
2	X	36	PRO	C-N	8.32	1.53	1.34
2	J	34	ASN	CG-ND2	6.35	1.48	1.32
2	L	34	ASN	CG-ND2	6.35	1.48	1.32
2	N	34	ASN	CG-ND2	6.35	1.48	1.32
2	P	34	ASN	CG-ND2	6.35	1.48	1.32
2	R	34	ASN	CG-ND2	6.35	1.48	1.32
2	T	34	ASN	CG-ND2	6.35	1.48	1.32
2	V	34	ASN	CG-ND2	6.35	1.48	1.32
2	X	34	ASN	CG-ND2	6.35	1.48	1.32
2	J	34	ASN	CG-OD1	5.58	1.36	1.24
2	J	35	PRO	N-CD	5.58	1.55	1.47
2	L	34	ASN	CG-OD1	5.58	1.36	1.24
2	L	35	PRO	N-CD	5.58	1.55	1.47
2	N	34	ASN	CG-OD1	5.58	1.36	1.24
2	N	35	PRO	N-CD	5.58	1.55	1.47
2	P	34	ASN	CG-OD1	5.58	1.36	1.24
2	P	35	PRO	N-CD	5.58	1.55	1.47
2	R	34	ASN	CG-OD1	5.58	1.36	1.24
2	R	35	PRO	N-CD	5.58	1.55	1.47
2	T	34	ASN	CG-OD1	5.58	1.36	1.24
2	T	35	PRO	N-CD	5.58	1.55	1.47
2	V	34	ASN	CG-OD1	5.58	1.36	1.24
2	V	35	PRO	N-CD	5.58	1.55	1.47
2	X	34	ASN	CG-OD1	5.58	1.36	1.24
2	X	35	PRO	N-CD	5.58	1.55	1.47
2	J	34	ASN	C-O	5.37	1.33	1.23
2	L	34	ASN	C-O	5.37	1.33	1.23
2	N	34	ASN	C-O	5.37	1.33	1.23
2	P	34	ASN	C-O	5.37	1.33	1.23
2	R	34	ASN	C-O	5.37	1.33	1.23
2	T	34	ASN	C-O	5.37	1.33	1.23
2	V	34	ASN	C-O	5.37	1.33	1.23
2	X	34	ASN	C-O	5.37	1.33	1.23

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	463	LYS	O-C-N	-34.97	66.75	122.70
1	F	463	LYS	O-C-N	-34.96	66.77	122.70
1	H	463	LYS	O-C-N	-34.96	66.77	122.70
1	B	463	LYS	O-C-N	-34.95	66.79	122.70
1	E	463	LYS	O-C-N	-34.95	66.79	122.70
1	A	463	LYS	O-C-N	-34.94	66.79	122.70
1	G	463	LYS	O-C-N	-34.94	66.79	122.70
1	D	463	LYS	O-C-N	-34.94	66.80	122.70
1	D	463	LYS	CA-C-N	22.71	167.16	117.20
1	E	463	LYS	CA-C-N	22.71	167.16	117.20
1	H	463	LYS	CA-C-N	22.71	167.16	117.20
1	A	463	LYS	CA-C-N	22.68	167.10	117.20
1	C	463	LYS	CA-C-N	22.68	167.10	117.20
1	F	463	LYS	CA-C-N	22.68	167.09	117.20
1	G	463	LYS	CA-C-N	22.67	167.08	117.20
1	B	463	LYS	CA-C-N	22.67	167.07	117.20
1	H	466	LYS	O-C-N	-22.55	86.63	122.70
1	C	466	LYS	O-C-N	-22.54	86.64	122.70
1	B	466	LYS	O-C-N	-22.53	86.65	122.70
1	G	466	LYS	O-C-N	-22.53	86.66	122.70
1	A	466	LYS	O-C-N	-22.52	86.67	122.70
1	D	466	LYS	O-C-N	-22.51	86.69	122.70
1	E	466	LYS	O-C-N	-22.51	86.69	122.70
1	F	466	LYS	O-C-N	-22.51	86.69	122.70
1	H	466	LYS	CA-C-N	16.02	152.45	117.20
1	A	466	LYS	CA-C-N	16.00	152.40	117.20
1	F	466	LYS	CA-C-N	16.00	152.39	117.20
1	B	466	LYS	CA-C-N	15.99	152.38	117.20
1	G	466	LYS	CA-C-N	15.99	152.37	117.20
1	C	466	LYS	CA-C-N	15.98	152.37	117.20
1	E	466	LYS	CA-C-N	15.98	152.36	117.20
1	D	466	LYS	CA-C-N	15.98	152.35	117.20
1	H	471	THR	O-C-N	12.46	142.63	122.70
1	C	471	THR	O-C-N	12.45	142.61	122.70
1	E	471	THR	O-C-N	12.45	142.61	122.70
1	D	471	THR	O-C-N	12.44	142.60	122.70
1	B	471	THR	O-C-N	12.44	142.60	122.70
1	A	471	THR	O-C-N	12.43	142.59	122.70
1	F	471	THR	O-C-N	12.41	142.56	122.70
1	G	471	THR	O-C-N	12.41	142.56	122.70
1	G	465	ILE	O-C-N	-12.18	103.21	122.70
1	E	465	ILE	O-C-N	-12.17	103.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	465	ILE	O-C-N	-12.16	103.24	122.70
1	A	465	ILE	O-C-N	-12.15	103.26	122.70
1	D	465	ILE	O-C-N	-12.15	103.26	122.70
1	F	465	ILE	O-C-N	-12.15	103.27	122.70
1	H	465	ILE	O-C-N	-12.14	103.27	122.70
1	B	465	ILE	O-C-N	-12.14	103.28	122.70
1	H	471	THR	CA-C-N	-9.46	96.39	117.20
1	E	471	THR	CA-C-N	-9.45	96.42	117.20
1	A	471	THR	CA-C-N	-9.45	96.42	117.20
1	G	471	THR	CA-C-N	-9.45	96.42	117.20
1	F	471	THR	CA-C-N	-9.44	96.43	117.20
1	D	471	THR	CA-C-N	-9.44	96.44	117.20
1	B	471	THR	CA-C-N	-9.43	96.45	117.20
1	C	471	THR	CA-C-N	-9.43	96.46	117.20
1	G	463	LYS	C-N-CA	8.29	142.44	121.70
1	E	463	LYS	C-N-CA	8.29	142.43	121.70
1	A	463	LYS	C-N-CA	8.29	142.43	121.70
1	B	463	LYS	C-N-CA	8.29	142.43	121.70
1	D	463	LYS	C-N-CA	8.29	142.42	121.70
1	C	463	LYS	C-N-CA	8.29	142.41	121.70
1	F	463	LYS	C-N-CA	8.28	142.39	121.70
1	H	463	LYS	C-N-CA	8.27	142.37	121.70
1	E	465	ILE	CA-C-N	8.13	135.09	117.20
1	B	465	ILE	CA-C-N	8.13	135.08	117.20
1	C	465	ILE	CA-C-N	8.12	135.06	117.20
1	F	465	ILE	CA-C-N	8.12	135.06	117.20
1	H	465	ILE	CA-C-N	8.12	135.06	117.20
1	A	465	ILE	CA-C-N	8.11	135.05	117.20
1	G	465	ILE	CA-C-N	8.11	135.04	117.20
1	D	465	ILE	CA-C-N	8.11	135.03	117.20
1	E	285	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	C	159	ARG	NE-CZ-NH1	-8.09	116.26	120.30
1	E	159	ARG	NE-CZ-NH1	-8.08	116.26	120.30
1	H	285	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	285	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	F	285	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	C	285	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	H	159	ARG	NE-CZ-NH1	-8.07	116.26	120.30
1	D	159	ARG	NE-CZ-NH1	-8.07	116.27	120.30
1	D	285	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	A	159	ARG	NE-CZ-NH1	-8.06	116.27	120.30
1	G	285	ARG	NE-CZ-NH2	-8.04	116.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	159	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	F	159	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	G	159	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	B	285	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	D	312	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	E	312	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	G	217	ARG	NE-CZ-NH1	-7.93	116.34	120.30
1	H	312	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	B	217	ARG	NE-CZ-NH1	-7.91	116.34	120.30
1	B	312	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	G	312	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	217	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	H	217	ARG	NE-CZ-NH1	-7.87	116.36	120.30
1	C	312	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	312	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	E	217	ARG	NE-CZ-NH1	-7.85	116.38	120.30
1	F	217	ARG	NE-CZ-NH1	-7.84	116.38	120.30
1	F	312	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	217	ARG	NE-CZ-NH1	-7.83	116.39	120.30
1	D	217	ARG	NE-CZ-NH1	-7.76	116.42	120.30
1	G	36	LEU	CA-CB-CG	6.67	130.63	115.30
1	B	36	LEU	CA-CB-CG	6.65	130.60	115.30
1	F	36	LEU	CA-CB-CG	6.65	130.59	115.30
1	A	36	LEU	CA-CB-CG	6.64	130.57	115.30
1	D	36	LEU	CA-CB-CG	6.63	130.56	115.30
1	H	36	LEU	CA-CB-CG	6.63	130.56	115.30
1	C	36	LEU	CA-CB-CG	6.63	130.55	115.30
1	E	36	LEU	CA-CB-CG	6.63	130.55	115.30
1	H	215	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	F	215	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	C	215	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	B	215	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	215	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	E	215	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	D	215	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	G	215	ARG	NE-CZ-NH1	-5.47	117.57	120.30
1	B	134	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	C	134	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	H	213	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	H	134	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	C	213	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	213	ARG	NE-CZ-NH2	-5.19	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	134	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	G	134	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	D	134	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	E	213	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	D	213	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	213	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	G	41	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	E	134	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	F	134	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	G	213	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	41	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	F	213	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	C	41	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	D	41	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	E	41	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	F	41	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	41	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	H	41	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (168) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Sidechain
1	A	134	ARG	Sidechain
1	A	159	ARG	Sidechain
1	A	167	ARG	Sidechain
1	A	194	ARG	Sidechain
1	A	213	ARG	Sidechain
1	A	215	ARG	Sidechain
1	A	217	ARG	Sidechain
1	A	285	ARG	Sidechain
1	A	295	ARG	Sidechain
1	A	305	ARG	Sidechain
1	A	312	ARG	Sidechain
1	A	319	ARG	Sidechain
1	A	350	ARG	Sidechain
1	A	360	ARG	Sidechain
1	A	41	ARG	Sidechain
1	A	446	ARG	Sidechain
1	A	463	LYS	Mainchain,Peptide
1	A	466	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	131	ARG	Sidechain
1	B	134	ARG	Sidechain
1	B	159	ARG	Sidechain
1	B	167	ARG	Sidechain
1	B	194	ARG	Sidechain
1	B	213	ARG	Sidechain
1	B	215	ARG	Sidechain
1	B	217	ARG	Sidechain
1	B	285	ARG	Sidechain
1	B	295	ARG	Sidechain
1	B	305	ARG	Sidechain
1	B	312	ARG	Sidechain
1	B	319	ARG	Sidechain
1	B	350	ARG	Sidechain
1	B	360	ARG	Sidechain
1	B	41	ARG	Sidechain
1	B	446	ARG	Sidechain
1	B	463	LYS	Mainchain,Peptide
1	B	466	LYS	Peptide
1	C	131	ARG	Sidechain
1	C	134	ARG	Sidechain
1	C	159	ARG	Sidechain
1	C	167	ARG	Sidechain
1	C	194	ARG	Sidechain
1	C	213	ARG	Sidechain
1	C	215	ARG	Sidechain
1	C	217	ARG	Sidechain
1	C	285	ARG	Sidechain
1	C	295	ARG	Sidechain
1	C	305	ARG	Sidechain
1	C	312	ARG	Sidechain
1	C	319	ARG	Sidechain
1	C	350	ARG	Sidechain
1	C	360	ARG	Sidechain
1	C	41	ARG	Sidechain
1	C	446	ARG	Sidechain
1	C	463	LYS	Mainchain,Peptide
1	C	466	LYS	Peptide
1	D	131	ARG	Sidechain
1	D	134	ARG	Sidechain
1	D	159	ARG	Sidechain
1	D	167	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	194	ARG	Sidechain
1	D	213	ARG	Sidechain
1	D	215	ARG	Sidechain
1	D	217	ARG	Sidechain
1	D	285	ARG	Sidechain
1	D	295	ARG	Sidechain
1	D	305	ARG	Sidechain
1	D	312	ARG	Sidechain
1	D	319	ARG	Sidechain
1	D	350	ARG	Sidechain
1	D	360	ARG	Sidechain
1	D	41	ARG	Sidechain
1	D	446	ARG	Sidechain
1	D	463	LYS	Mainchain,Peptide
1	D	466	LYS	Peptide
1	E	131	ARG	Sidechain
1	E	134	ARG	Sidechain
1	E	159	ARG	Sidechain
1	E	167	ARG	Sidechain
1	E	194	ARG	Sidechain
1	E	213	ARG	Sidechain
1	E	215	ARG	Sidechain
1	E	217	ARG	Sidechain
1	E	285	ARG	Sidechain
1	E	295	ARG	Sidechain
1	E	305	ARG	Sidechain
1	E	312	ARG	Sidechain
1	E	319	ARG	Sidechain
1	E	350	ARG	Sidechain
1	E	360	ARG	Sidechain
1	E	41	ARG	Sidechain
1	E	446	ARG	Sidechain
1	E	463	LYS	Mainchain,Peptide
1	E	466	LYS	Peptide
1	F	131	ARG	Sidechain
1	F	134	ARG	Sidechain
1	F	159	ARG	Sidechain
1	F	167	ARG	Sidechain
1	F	194	ARG	Sidechain
1	F	213	ARG	Sidechain
1	F	215	ARG	Sidechain
1	F	217	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	285	ARG	Sidechain
1	F	295	ARG	Sidechain
1	F	305	ARG	Sidechain
1	F	312	ARG	Sidechain
1	F	319	ARG	Sidechain
1	F	350	ARG	Sidechain
1	F	360	ARG	Sidechain
1	F	41	ARG	Sidechain
1	F	446	ARG	Sidechain
1	F	463	LYS	Mainchain,Peptide
1	F	466	LYS	Peptide
1	G	131	ARG	Sidechain
1	G	134	ARG	Sidechain
1	G	159	ARG	Sidechain
1	G	167	ARG	Sidechain
1	G	194	ARG	Sidechain
1	G	213	ARG	Sidechain
1	G	215	ARG	Sidechain
1	G	217	ARG	Sidechain
1	G	285	ARG	Sidechain
1	G	295	ARG	Sidechain
1	G	305	ARG	Sidechain
1	G	312	ARG	Sidechain
1	G	319	ARG	Sidechain
1	G	350	ARG	Sidechain
1	G	360	ARG	Sidechain
1	G	41	ARG	Sidechain
1	G	446	ARG	Sidechain
1	G	463	LYS	Mainchain,Peptide
1	G	466	LYS	Peptide
1	H	131	ARG	Sidechain
1	H	134	ARG	Sidechain
1	H	159	ARG	Sidechain
1	H	167	ARG	Sidechain
1	H	194	ARG	Sidechain
1	H	213	ARG	Sidechain
1	H	215	ARG	Sidechain
1	H	217	ARG	Sidechain
1	H	285	ARG	Sidechain
1	H	295	ARG	Sidechain
1	H	305	ARG	Sidechain
1	H	312	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	H	319	ARG	Sidechain
1	H	350	ARG	Sidechain
1	H	360	ARG	Sidechain
1	H	41	ARG	Sidechain
1	H	446	ARG	Sidechain
1	H	463	LYS	Mainchain,Peptide
1	H	466	LYS	Peptide
2	J	36	PRO	Mainchain
2	L	36	PRO	Mainchain
2	N	36	PRO	Mainchain
2	P	36	PRO	Mainchain
2	R	36	PRO	Mainchain
2	T	36	PRO	Mainchain
2	V	36	PRO	Mainchain
2	X	36	PRO	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3653	0	3547	317	0
1	B	3653	0	3546	322	0
1	C	3653	0	3547	286	0
1	D	3653	0	3548	332	0
1	E	3653	0	3548	334	0
1	F	3653	0	3547	313	0
1	G	3653	0	3547	312	0
1	H	3653	0	3547	296	0
2	I	834	0	820	110	0
2	J	870	0	880	43	0
2	K	834	0	821	140	0
2	L	870	0	880	40	0
2	M	834	0	822	95	0
2	N	870	0	880	41	0
2	O	834	0	820	139	0
2	P	870	0	880	46	0
2	Q	834	0	821	120	0
2	R	870	0	880	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	834	0	820	120	0
2	T	870	0	880	54	0
2	U	834	0	820	118	0
2	V	870	0	880	49	0
2	W	834	0	822	101	0
2	X	870	0	880	38	0
All	All	42856	0	41983	2709	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 32.

All (2709) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ARG:CG	1:D:428:VAL:HG22	1.22	1.65
1:H:167:ARG:CG	1:H:428:VAL:HG22	1.21	1.64
1:G:167:ARG:CG	1:G:428:VAL:HG22	1.22	1.64
1:C:47:GLY:HA3	2:N:1:MET:SD	1.34	1.63
1:E:22:LEU:CD2	2:K:33:THR:CA	1.77	1.63
1:B:167:ARG:CG	1:B:428:VAL:HG22	1.21	1.62
1:G:46:PRO:HA	2:I:76:HIS:CE1	1.32	1.61
1:A:465:ILE:HD12	2:W:24:ARG:CB	1.30	1.60
1:E:391:VAL:HG11	1:E:437:LEU:CD1	1.12	1.60
1:F:391:VAL:HG11	1:F:437:LEU:CD1	1.12	1.59
1:E:46:PRO:HB3	2:K:76:HIS:CD2	1.36	1.59
1:D:46:PRO:CB	2:O:80:GLU:CG	1.82	1.58
1:B:391:VAL:HG11	1:B:437:LEU:CD1	1.12	1.57
1:C:391:VAL:HG11	1:C:437:LEU:CD1	1.12	1.57
1:H:391:VAL:HG11	1:H:437:LEU:CD1	1.12	1.56
1:A:391:VAL:HG11	1:A:437:LEU:CD1	1.12	1.56
1:B:465:ILE:HD12	2:M:24:ARG:CB	1.22	1.56
1:D:52:GLU:CG	2:O:29[B]:GLN:HE22	1.17	1.56
1:E:46:PRO:HA	2:K:76:HIS:CE1	1.10	1.56
1:E:22:LEU:CD2	2:K:33:THR:HA	1.25	1.55
1:B:52:GLU:CB	2:Q:29[B]:GLN:HE22	1.09	1.55
1:F:167:ARG:CG	1:F:428:VAL:HG22	1.22	1.55
1:C:167:ARG:CG	1:C:428:VAL:HG22	1.21	1.55
1:F:52:GLU:CG	2:U:29[B]:GLN:HE22	1.15	1.55
1:H:52:GLU:CG	2:W:29[B]:GLN:HE22	1.13	1.54
1:E:167:ARG:CG	1:E:428:VAL:HG22	1.21	1.54
1:G:21:LYS:NZ	2:I:33:THR:CG2	1.70	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:391:VAL:HG11	1:G:437:LEU:CD1	1.12	1.54
1:A:167:ARG:CG	1:A:428:VAL:HG22	1.21	1.53
1:D:465:ILE:CD1	2:K:24:ARG:HB3	1.32	1.53
1:B:52:GLU:CG	2:Q:29[B]:GLN:HE22	1.19	1.53
1:D:46:PRO:HG3	2:O:80:GLU:CB	1.39	1.53
1:D:391:VAL:HG11	1:D:437:LEU:CD1	1.12	1.53
1:F:465:ILE:CD1	2:I:24:ARG:HB3	1.36	1.53
1:E:22:LEU:HD21	2:K:33:THR:CA	1.31	1.52
1:B:467:PHE:HA	1:B:468:GLU:N	1.19	1.51
1:A:465:ILE:CD1	2:W:24:ARG:HB3	1.04	1.51
1:A:52:GLU:CG	2:S:29[B]:GLN:NE2	1.72	1.51
1:H:467:PHE:HA	1:H:468:GLU:N	1.19	1.51
1:H:170:LEU:HD12	1:H:424:LEU:CD2	1.41	1.51
1:C:52:GLU:CG	2:M:29[B]:GLN:HE22	1.19	1.50
1:E:465:ILE:CD1	2:O:24:ARG:HB3	1.38	1.50
1:B:170:LEU:HD12	1:B:424:LEU:CD2	1.41	1.50
1:G:52:GLU:CG	2:I:29[B]:GLN:HE22	1.24	1.50
1:G:170:LEU:HD12	1:G:424:LEU:CD2	1.41	1.50
1:D:170:LEU:HD12	1:D:424:LEU:CD2	1.41	1.50
1:B:21:LYS:NZ	2:Q:33:THR:CG2	1.70	1.50
1:E:170:LEU:HD12	1:E:424:LEU:CD2	1.41	1.50
1:E:22:LEU:HD21	2:K:33:THR:C	1.12	1.50
1:F:21:LYS:NZ	2:U:33:THR:CG2	1.75	1.50
1:D:46:PRO:CD	2:O:80:GLU:CD	1.79	1.49
1:G:465:ILE:CD1	2:U:24:ARG:HB3	1.37	1.49
1:F:52:GLU:HG2	2:U:29[B]:GLN:NE2	1.21	1.49
1:F:170:LEU:HD12	1:F:424:LEU:CD2	1.41	1.49
1:C:170:LEU:HD12	1:C:424:LEU:CD2	1.41	1.49
1:G:46:PRO:HA	2:I:76:HIS:NE2	1.20	1.49
1:A:170:LEU:HD12	1:A:424:LEU:CD2	1.41	1.48
1:F:46:PRO:HA	2:U:76:HIS:CE1	1.46	1.48
1:A:21:LYS:NZ	2:S:33:THR:CG2	1.76	1.47
1:A:21:LYS:HZ3	2:S:33:THR:CB	1.26	1.46
1:C:467:PHE:HA	1:C:468:GLU:N	1.19	1.46
1:D:46:PRO:HA	2:O:76:HIS:CE1	1.48	1.46
1:E:46:PRO:CB	2:K:76:HIS:CD2	1.94	1.46
1:H:21:LYS:NZ	2:W:33:THR:HG21	1.24	1.46
1:A:21:LYS:HG3	2:S:33:THR:CG2	1.41	1.46
1:C:52:GLU:HG2	2:M:29[B]:GLN:NE2	1.21	1.46
1:A:467:PHE:HA	1:A:468:GLU:N	1.19	1.46
1:F:467:PHE:HA	1:F:468:GLU:N	1.19	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:LYS:NZ	2:O:33:THR:CG2	1.76	1.46
1:D:46:PRO:HA	2:O:76:HIS:NE2	1.28	1.46
1:G:467:PHE:HA	1:G:468:GLU:N	1.19	1.46
1:D:52:GLU:HG2	2:O:29[B]:GLN:NE2	1.24	1.45
1:A:21:LYS:NZ	2:S:33:THR:HG21	1.29	1.45
1:E:170:LEU:HD11	1:E:424:LEU:CB	1.47	1.45
1:E:467:PHE:HA	1:E:468:GLU:N	1.19	1.45
1:H:18:LYS:CB	2:W:32:GLU:HA	1.46	1.45
1:B:21:LYS:NZ	2:Q:33:THR:CB	1.76	1.45
1:C:21:LYS:NZ	2:M:33:THR:HG21	1.32	1.45
1:D:21:LYS:NZ	2:O:33:THR:HG21	1.14	1.45
1:F:170:LEU:HD11	1:F:424:LEU:CB	1.47	1.45
1:D:467:PHE:HA	1:D:468:GLU:N	1.19	1.44
1:D:472:MET:CB	1:D:473:ASP:N	1.79	1.44
1:G:472:MET:CB	1:G:473:ASP:N	1.79	1.44
1:C:170:LEU:HD11	1:C:424:LEU:CB	1.47	1.44
1:C:391:VAL:CG1	1:C:437:LEU:CD1	1.94	1.44
1:E:170:LEU:CD1	1:E:424:LEU:HB2	1.47	1.44
1:E:391:VAL:CG1	1:E:437:LEU:CD1	1.94	1.44
1:F:170:LEU:CD1	1:F:424:LEU:HB2	1.47	1.44
1:A:170:LEU:CD1	1:A:424:LEU:HB2	1.47	1.44
1:C:170:LEU:CD1	1:C:424:LEU:HB2	1.47	1.44
1:D:46:PRO:CG	2:O:80:GLU:CD	1.85	1.44
1:A:170:LEU:HD11	1:A:424:LEU:CB	1.47	1.43
1:A:391:VAL:CG1	1:A:437:LEU:CD1	1.94	1.43
1:F:391:VAL:CG1	1:F:437:LEU:CD1	1.94	1.43
1:B:170:LEU:HD11	1:B:424:LEU:CB	1.47	1.43
1:H:391:VAL:CG1	1:H:437:LEU:CD1	1.94	1.43
1:D:46:PRO:CB	2:O:80:GLU:HG3	1.42	1.43
1:F:52:GLU:CB	2:U:29[B]:GLN:HE22	1.28	1.43
1:D:391:VAL:CG1	1:D:437:LEU:CD1	1.94	1.43
1:E:21:LYS:NZ	2:K:33:THR:CG2	1.80	1.43
1:F:472:MET:CB	1:F:473:ASP:N	1.79	1.43
1:G:391:VAL:CG1	1:G:437:LEU:CD1	1.94	1.43
1:B:391:VAL:CG1	1:B:437:LEU:CD1	1.94	1.42
1:E:52:GLU:CG	2:K:29[B]:GLN:HE22	1.28	1.42
1:H:170:LEU:HD11	1:H:424:LEU:CB	1.47	1.42
1:A:52:GLU:CB	2:S:29[B]:GLN:NE2	1.79	1.42
1:A:21:LYS:CG	2:S:33:THR:CG2	1.95	1.42
1:A:52:GLU:HG2	2:S:29[B]:GLN:CD	1.38	1.42
1:B:52:GLU:HG2	2:Q:29[B]:GLN:CD	1.39	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:GLU:HG2	2:K:29[B]:GLN:NE2	1.26	1.42
1:H:472:MET:CB	1:H:473:ASP:N	1.79	1.42
1:E:472:MET:CB	1:E:473:ASP:N	1.79	1.42
1:G:170:LEU:CD1	1:G:424:LEU:HB2	1.47	1.42
1:B:472:MET:CB	1:B:473:ASP:N	1.79	1.42
1:H:47:GLY:N	2:W:76:HIS:ND1	1.61	1.42
1:D:170:LEU:CD1	1:D:424:LEU:HB2	1.47	1.41
1:F:21:LYS:NZ	2:U:33:THR:HG21	1.20	1.41
1:E:21:LYS:HZ2	2:K:33:THR:CG2	1.34	1.41
1:B:52:GLU:HG2	2:Q:29[B]:GLN:NE2	1.25	1.41
1:C:472:MET:CB	1:C:473:ASP:N	1.79	1.41
1:A:472:MET:CB	1:A:473:ASP:N	1.79	1.41
1:B:21:LYS:CE	2:Q:33:THR:HG21	1.51	1.41
1:G:170:LEU:HD11	1:G:424:LEU:CB	1.47	1.40
1:D:170:LEU:HD11	1:D:424:LEU:CB	1.47	1.40
1:H:170:LEU:CD1	1:H:424:LEU:HB2	1.47	1.40
1:E:46:PRO:HA	2:K:76:HIS:NE2	1.18	1.40
1:E:21:LYS:NZ	2:K:33:THR:HG21	1.21	1.40
1:B:21:LYS:HG3	2:Q:33:THR:CG2	1.49	1.39
1:B:170:LEU:CD1	1:B:424:LEU:HB2	1.47	1.39
1:A:52:GLU:HG2	2:S:29[B]:GLN:NE2	1.22	1.39
1:A:167:ARG:HG3	1:A:428:VAL:CG2	0.91	1.39
1:C:167:ARG:HG3	1:C:428:VAL:CG2	0.91	1.39
1:G:52:GLU:HG2	2:I:29[B]:GLN:NE2	1.29	1.39
1:B:21:LYS:CG	2:Q:33:THR:CG2	1.99	1.39
1:D:52:GLU:CB	2:O:29[B]:GLN:HE22	1.33	1.39
1:F:46:PRO:HA	2:U:76:HIS:NE2	1.34	1.39
1:H:52:GLU:HG2	2:W:29[B]:GLN:NE2	1.19	1.39
1:E:167:ARG:HG3	1:E:428:VAL:CG2	0.91	1.38
1:F:167:ARG:HG3	1:F:428:VAL:CG2	0.91	1.38
1:B:167:ARG:HG3	1:B:428:VAL:CG2	0.91	1.38
1:H:167:ARG:HG3	1:H:428:VAL:CG2	0.91	1.38
1:B:52:GLU:CG	2:Q:29[B]:GLN:NE2	1.79	1.38
1:G:46:PRO:HB3	2:I:76:HIS:CD2	1.58	1.38
1:B:465:ILE:CD1	2:M:24:ARG:HB3	0.93	1.38
1:D:46:PRO:HD3	2:O:80:GLU:CD	1.33	1.38
1:E:46:PRO:CA	2:K:76:HIS:CE1	2.03	1.37
1:D:167:ARG:HG3	1:D:428:VAL:CG2	0.91	1.37
1:G:167:ARG:HG3	1:G:428:VAL:CG2	0.91	1.37
1:E:46:PRO:CA	2:K:76:HIS:NE2	1.88	1.37
1:E:22:LEU:CD2	2:K:33:THR:O	1.69	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:LYS:NZ	2:I:33:THR:HG21	1.07	1.35
1:G:46:PRO:CD	2:I:80:GLU:OE1	1.67	1.35
1:F:45:GLN:OE1	2:V:3:LEU:CD1	1.73	1.35
1:C:471:THR:C	1:C:472:MET:N	1.81	1.35
1:D:46:PRO:HA	2:O:76:HIS:CD2	1.61	1.35
1:D:46:PRO:CD	2:O:80:GLU:OE1	1.65	1.34
1:G:471:THR:C	1:G:472:MET:N	1.81	1.34
1:A:471:THR:C	1:A:472:MET:N	1.81	1.34
1:B:21:LYS:NZ	2:Q:33:THR:HG21	1.25	1.34
1:B:52:GLU:CB	2:Q:29[B]:GLN:NE2	1.86	1.34
1:B:471:THR:C	1:B:472:MET:N	1.81	1.34
1:D:45:GLN:OE1	2:P:3:LEU:HD12	1.20	1.34
1:D:471:THR:C	1:D:472:MET:N	1.81	1.34
1:C:467:PHE:CA	1:C:468:GLU:N	1.91	1.34
1:H:471:THR:C	1:H:472:MET:N	1.81	1.34
1:A:467:PHE:CA	1:A:468:GLU:N	1.91	1.34
1:E:471:THR:C	1:E:472:MET:N	1.81	1.33
1:F:471:THR:C	1:F:472:MET:N	1.81	1.33
1:F:467:PHE:CA	1:F:468:GLU:N	1.91	1.33
1:H:20:TYR:N	2:W:32:GLU:OE1	1.60	1.33
1:E:467:PHE:CA	1:E:468:GLU:N	1.91	1.33
1:G:46:PRO:CB	2:I:76:HIS:CD2	2.12	1.33
1:D:45:GLN:OE1	2:P:3:LEU:CD1	1.77	1.33
1:A:473:ASP:OD2	2:X:24:ARG:NE	1.58	1.33
1:F:21:LYS:NZ	2:U:33:THR:CB	1.89	1.33
1:F:46:PRO:HA	2:U:76:HIS:CD2	1.63	1.33
1:B:467:PHE:CA	1:B:468:GLU:N	1.91	1.32
1:E:167:ARG:CG	1:E:428:VAL:CG2	1.86	1.32
1:A:21:LYS:CE	2:S:33:THR:HG21	1.57	1.31
1:A:167:ARG:CG	1:A:428:VAL:CG2	1.86	1.31
1:C:167:ARG:CG	1:C:428:VAL:CG2	1.86	1.31
1:H:465:ILE:CD1	2:S:24:ARG:HB3	1.60	1.31
1:A:21:LYS:HZ3	2:S:33:THR:CG2	1.31	1.31
1:C:47:GLY:CA	2:N:1:MET:SD	2.11	1.31
1:F:167:ARG:CG	1:F:428:VAL:CG2	1.86	1.31
1:G:46:PRO:HA	2:I:76:HIS:CD2	1.64	1.31
1:E:21:LYS:NZ	2:K:33:THR:CB	1.94	1.31
1:G:19:ASP:OD1	2:I:29[B]:GLN:CA	1.68	1.31
1:H:467:PHE:CA	1:H:468:GLU:N	1.91	1.31
1:H:21:LYS:HZ2	2:W:33:THR:CG2	1.42	1.31
1:D:467:PHE:CA	1:D:468:GLU:N	1.91	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:467:PHE:CA	1:G:468:GLU:N	1.91	1.30
1:A:21:LYS:NZ	2:S:33:THR:CB	1.83	1.30
1:E:46:PRO:CA	2:K:76:HIS:CD2	2.13	1.30
1:D:46:PRO:CD	2:O:80:GLU:CG	2.06	1.29
1:F:465:ILE:HD12	2:I:24:ARG:CB	1.62	1.29
1:G:21:LYS:NZ	2:I:33:THR:CB	1.93	1.29
1:B:170:LEU:CG	1:B:424:LEU:HD13	1.61	1.29
1:E:170:LEU:CG	1:E:424:LEU:HD13	1.61	1.29
1:E:22:LEU:CG	2:K:33:THR:HA	0.91	1.29
1:G:46:PRO:CA	2:I:76:HIS:CD2	2.16	1.29
1:A:46:PRO:HA	2:S:76:HIS:CD2	1.65	1.28
1:A:170:LEU:CG	1:A:424:LEU:HD13	1.61	1.28
1:C:170:LEU:CG	1:C:424:LEU:HD13	1.61	1.28
1:D:170:LEU:CG	1:D:424:LEU:HD13	1.61	1.28
1:F:170:LEU:CG	1:F:424:LEU:HD13	1.61	1.28
1:H:170:LEU:CG	1:H:424:LEU:HD13	1.61	1.28
1:G:170:LEU:CG	1:G:424:LEU:HD13	1.61	1.28
1:F:46:PRO:CD	2:U:80:GLU:OE1	1.74	1.27
1:A:52:GLU:CD	2:S:29[B]:GLN:OE1	1.69	1.27
1:D:46:PRO:HG3	2:O:80:GLU:CD	1.43	1.27
1:F:21:LYS:CE	2:U:33:THR:HG21	1.63	1.27
1:G:46:PRO:CA	2:I:76:HIS:NE2	1.98	1.27
1:G:52:GLU:CB	2:I:29[B]:GLN:HE22	1.47	1.26
1:B:21:LYS:NZ	2:Q:33:THR:OG1	1.67	1.26
1:F:45:GLN:OE1	2:V:3:LEU:HD12	1.18	1.26
1:F:46:PRO:HB3	2:U:76:HIS:CD2	1.68	1.26
1:D:170:LEU:CD1	1:D:424:LEU:CB	2.09	1.25
1:D:46:PRO:CD	2:O:80:GLU:HG3	1.64	1.25
1:D:409:HIS:CG	1:D:416:GLY:HA2	1.71	1.25
1:G:21:LYS:CE	2:I:33:THR:HG21	1.66	1.25
1:G:409:HIS:CG	1:G:416:GLY:HA2	1.71	1.25
1:H:170:LEU:CD1	1:H:424:LEU:CB	2.09	1.25
1:A:21:LYS:NZ	2:S:33:THR:OG1	1.66	1.25
1:B:46:PRO:HA	2:Q:76:HIS:CE1	1.69	1.25
1:D:465:ILE:HD12	2:K:24:ARG:CB	1.65	1.25
1:G:170:LEU:CD1	1:G:424:LEU:CB	2.09	1.25
1:A:409:HIS:CG	1:A:416:GLY:HA2	1.71	1.25
1:C:18:LYS:CB	2:M:32:GLU:HA	1.39	1.25
1:C:409:HIS:CG	1:C:416:GLY:HA2	1.71	1.25
1:E:465:ILE:HD12	2:O:24:ARG:CB	1.65	1.25
1:F:21:LYS:HZ2	2:U:33:THR:CB	1.45	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PRO:HA	2:S:76:HIS:CE1	1.71	1.24
1:G:45:GLN:OE1	2:J:3:LEU:HD12	1.36	1.24
1:B:465:ILE:CG1	2:M:24:ARG:HB3	1.67	1.24
1:C:465:ILE:CD1	2:Q:24:ARG:HB3	1.64	1.24
1:B:21:LYS:CG	2:Q:33:THR:HG22	1.62	1.24
1:F:21:LYS:CG	2:U:33:THR:CG2	2.16	1.24
1:G:465:ILE:HD12	2:U:24:ARG:CB	1.65	1.24
1:E:409:HIS:CG	1:E:416:GLY:HA2	1.71	1.24
1:F:52:GLU:HG2	2:U:29[B]:GLN:CD	1.55	1.24
1:F:409:HIS:CG	1:F:416:GLY:HA2	1.71	1.24
1:E:46:PRO:HA	2:K:76:HIS:CD2	1.71	1.24
1:F:473:ASP:OD2	2:J:24:ARG:CD	1.86	1.24
1:B:473:ASP:OD2	2:N:24:ARG:NE	1.71	1.23
1:B:409:HIS:CG	1:B:416:GLY:HA2	1.71	1.23
1:C:170:LEU:CD1	1:C:424:LEU:CB	2.09	1.23
1:D:21:LYS:NZ	2:O:33:THR:CB	1.99	1.23
1:F:21:LYS:HG3	2:U:33:THR:CG2	1.65	1.23
1:C:409:HIS:CB	1:C:416:GLY:HA2	1.67	1.23
1:D:46:PRO:HB3	2:O:76:HIS:CD2	1.73	1.23
1:H:409:HIS:CG	1:H:416:GLY:HA2	1.71	1.23
1:A:409:HIS:CB	1:A:416:GLY:HA2	1.67	1.23
1:F:46:PRO:CA	2:U:76:HIS:CD2	2.21	1.23
1:H:21:LYS:NZ	2:W:33:THR:CG2	1.97	1.23
1:G:409:HIS:CB	1:G:416:GLY:HA2	1.67	1.22
1:B:409:HIS:CB	1:B:416:GLY:HA2	1.67	1.22
1:D:46:PRO:CA	2:O:76:HIS:CD2	2.20	1.22
1:D:385:TRP:CD1	1:D:463:LYS:HA	1.75	1.22
1:F:385:TRP:CD1	1:F:463:LYS:HA	1.75	1.22
1:G:385:TRP:CD1	1:G:463:LYS:HA	1.75	1.22
1:D:409:HIS:CB	1:D:416:GLY:HA2	1.67	1.22
1:E:22:LEU:CD2	2:K:33:THR:C	1.92	1.22
1:E:385:TRP:CD1	1:E:463:LYS:HA	1.75	1.22
1:H:409:HIS:CB	1:H:416:GLY:HA2	1.67	1.22
1:A:170:LEU:CD1	1:A:424:LEU:CB	2.09	1.22
1:D:170:LEU:CD1	1:D:424:LEU:HD22	1.70	1.22
1:E:47:GLY:N	2:K:76:HIS:ND1	1.88	1.22
1:F:46:PRO:CB	2:U:76:HIS:CD2	2.23	1.22
1:F:391:VAL:CG1	1:F:437:LEU:HD13	1.60	1.22
1:G:170:LEU:CD1	1:G:424:LEU:HD22	1.70	1.22
1:G:473:ASP:OD2	2:V:24:ARG:CD	1.85	1.22
1:H:170:LEU:CD1	1:H:424:LEU:HD22	1.70	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:LEU:CD1	1:B:424:LEU:HD22	1.70	1.22
1:F:170:LEU:CD1	1:F:424:LEU:HD22	1.70	1.22
1:H:385:TRP:CD1	1:H:463:LYS:HA	1.75	1.22
1:B:52:GLU:CD	2:Q:29[B]:GLN:OE1	1.78	1.21
1:E:170:LEU:CD1	1:E:424:LEU:HD22	1.70	1.21
1:B:385:TRP:CD1	1:B:463:LYS:HA	1.75	1.21
1:E:473:ASP:OD2	2:P:24:ARG:CD	1.87	1.21
1:E:391:VAL:CG1	1:E:437:LEU:HD13	1.60	1.21
1:B:46:PRO:HA	2:Q:76:HIS:CD2	1.74	1.21
1:F:409:HIS:CB	1:F:416:GLY:HA2	1.67	1.21
1:A:46:PRO:CD	2:S:80:GLU:OE1	1.85	1.21
1:E:409:HIS:CB	1:E:416:GLY:HA2	1.67	1.21
1:A:385:TRP:CD1	1:A:463:LYS:HA	1.75	1.20
1:A:391:VAL:CG1	1:A:437:LEU:HD13	1.60	1.20
1:C:20:TYR:N	2:M:32:GLU:OE1	1.75	1.20
1:E:170:LEU:CD1	1:E:424:LEU:CB	2.09	1.20
1:C:170:LEU:CD1	1:C:424:LEU:HD22	1.70	1.20
1:D:472:MET:HB2	1:D:473:ASP:N	0.88	1.20
1:G:472:MET:HB2	1:G:473:ASP:N	0.88	1.20
1:F:170:LEU:CD1	1:F:424:LEU:CB	2.09	1.20
1:F:472:MET:HB2	1:F:473:ASP:N	0.88	1.20
1:A:465:ILE:CD1	2:W:24:ARG:CB	1.96	1.20
1:C:385:TRP:CD1	1:C:463:LYS:HA	1.75	1.20
1:E:472:MET:HB2	1:E:473:ASP:N	0.88	1.20
1:G:45:GLN:OE1	2:J:3:LEU:CD1	1.90	1.20
1:H:167:ARG:CG	1:H:428:VAL:CG2	1.86	1.20
1:A:170:LEU:CD1	1:A:424:LEU:HD22	1.70	1.20
1:E:19:ASP:OD1	2:K:29[B]:GLN:CA	1.75	1.20
1:C:391:VAL:CG1	1:C:437:LEU:HD13	1.60	1.19
1:C:472:MET:HB2	1:C:473:ASP:N	0.88	1.19
1:D:21:LYS:CE	2:O:33:THR:HG21	1.70	1.19
1:B:472:MET:HB2	1:B:473:ASP:N	0.88	1.19
1:H:18:LYS:HB3	2:W:32:GLU:CA	1.73	1.19
1:H:472:MET:HB2	1:H:473:ASP:N	0.88	1.19
1:A:472:MET:HB2	1:A:473:ASP:N	0.88	1.19
1:D:46:PRO:CB	2:O:76:HIS:CD2	2.25	1.19
1:D:52:GLU:CG	2:O:29[B]:GLN:NE2	1.87	1.19
1:B:167:ARG:CG	1:B:428:VAL:CG2	1.86	1.19
1:A:470:GLU:CG	1:A:471:THR:N	2.06	1.18
1:C:21:LYS:NZ	2:M:33:THR:CG2	2.06	1.18
1:D:391:VAL:CG1	1:D:437:LEU:HD13	1.60	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:PRO:CA	2:I:76:HIS:CE1	2.24	1.18
1:G:391:VAL:CG1	1:G:437:LEU:HD13	1.60	1.18
1:B:21:LYS:CG	2:Q:33:THR:HG21	1.68	1.18
1:C:18:LYS:HB3	2:M:32:GLU:CA	1.73	1.18
1:D:470:GLU:CG	1:D:471:THR:N	2.06	1.18
1:F:52:GLU:CG	2:U:29[B]:GLN:NE2	1.84	1.18
1:H:470:GLU:CG	1:H:471:THR:N	2.06	1.18
1:B:167:ARG:CB	1:B:428:VAL:HG22	1.74	1.18
1:B:470:GLU:CG	1:B:471:THR:N	2.06	1.18
1:C:470:GLU:CG	1:C:471:THR:N	2.06	1.18
1:G:167:ARG:CG	1:G:428:VAL:CG2	1.86	1.18
1:G:470:GLU:CG	1:G:471:THR:N	2.06	1.18
1:A:167:ARG:CB	1:A:428:VAL:HG22	1.74	1.18
1:C:167:ARG:CB	1:C:428:VAL:HG22	1.74	1.18
1:E:21:LYS:CE	2:K:33:THR:HG21	1.74	1.18
1:H:167:ARG:CB	1:H:428:VAL:HG22	1.74	1.18
1:B:465:ILE:CD1	2:M:24:ARG:CB	1.88	1.17
1:E:470:GLU:CG	1:E:471:THR:N	2.06	1.17
1:A:46:PRO:HA	2:S:76:HIS:NE2	1.57	1.17
1:A:170:LEU:CD1	1:A:424:LEU:CG	2.23	1.17
1:D:170:LEU:CD1	1:D:424:LEU:CG	2.23	1.17
1:E:22:LEU:HD21	2:K:33:THR:O	1.24	1.17
1:F:470:GLU:CG	1:F:471:THR:N	2.06	1.17
1:G:170:LEU:CD1	1:G:424:LEU:CG	2.23	1.17
1:B:391:VAL:CG1	1:B:437:LEU:HD13	1.60	1.17
1:C:170:LEU:CD1	1:C:424:LEU:CG	2.23	1.17
1:E:170:LEU:HG	1:E:424:LEU:HD13	1.17	1.17
1:F:170:LEU:HG	1:F:424:LEU:HD13	1.17	1.17
1:D:46:PRO:CB	2:O:80:GLU:HG2	1.55	1.16
1:D:167:ARG:CG	1:D:428:VAL:CG2	1.86	1.16
1:G:167:ARG:CB	1:G:428:VAL:HG22	1.74	1.16
1:H:391:VAL:CG1	1:H:437:LEU:HD13	1.60	1.16
1:A:170:LEU:HG	1:A:424:LEU:HD13	1.17	1.16
1:E:170:LEU:CD1	1:E:424:LEU:CG	2.23	1.16
1:F:170:LEU:CD1	1:F:424:LEU:CG	2.23	1.16
1:D:167:ARG:CB	1:D:428:VAL:HG22	1.74	1.16
1:E:167:ARG:CB	1:E:428:VAL:HG22	1.74	1.16
1:G:391:VAL:CG1	1:G:437:LEU:HD12	1.65	1.16
1:A:21:LYS:CG	2:S:33:THR:HG21	1.62	1.15
1:B:170:LEU:CD1	1:B:424:LEU:CB	2.09	1.15
1:B:170:LEU:CD1	1:B:424:LEU:CG	2.23	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LEU:HG	1:C:424:LEU:HD13	1.17	1.15
1:D:45:GLN:CD	2:P:3:LEU:HD12	1.64	1.15
1:F:21:LYS:HZ2	2:U:33:THR:CG2	1.47	1.15
1:D:391:VAL:CG1	1:D:437:LEU:HD12	1.65	1.15
1:F:167:ARG:CB	1:F:428:VAL:HG22	1.74	1.15
1:A:409:HIS:HB3	1:A:416:GLY:CA	1.77	1.15
1:D:52:GLU:HG2	2:O:29[B]:GLN:CD	1.65	1.15
1:A:21:LYS:CG	2:S:33:THR:HG22	1.64	1.15
1:C:409:HIS:HB3	1:C:416:GLY:CA	1.77	1.15
1:F:45:GLN:CD	2:V:3:LEU:HD12	1.65	1.15
1:H:170:LEU:CD1	1:H:424:LEU:CG	2.23	1.15
2:K:14:LEU:HD23	2:L:89[A]:VAL:HG21	1.28	1.15
2:U:14:LEU:HD23	2:V:89[A]:VAL:HG21	1.28	1.15
1:A:21:LYS:CD	2:S:33:THR:HG21	1.77	1.14
1:G:21:LYS:HG3	2:I:33:THR:HG22	1.23	1.14
1:D:46:PRO:CA	2:O:76:HIS:NE2	2.10	1.14
1:E:46:PRO:HA	2:K:76:HIS:ND1	1.59	1.14
1:E:409:HIS:HB3	1:E:416:GLY:CA	1.77	1.14
1:F:409:HIS:HB3	1:F:416:GLY:CA	1.77	1.14
1:G:47:GLY:N	2:I:76:HIS:ND1	1.95	1.14
1:B:409:HIS:HB3	1:B:416:GLY:CA	1.77	1.14
1:C:391:VAL:CG1	1:C:437:LEU:HD12	1.65	1.14
1:A:46:PRO:HA	2:S:76:HIS:CG	1.82	1.14
1:A:391:VAL:CG1	1:A:437:LEU:HD12	1.65	1.14
1:E:18:LYS:HB3	2:K:32:GLU:HA	1.17	1.14
1:G:473:ASP:OD2	2:V:24:ARG:NE	1.80	1.14
1:D:18:LYS:CB	2:O:32:GLU:HA	1.70	1.14
1:D:21:LYS:HG3	2:O:33:THR:CG2	1.75	1.14
1:G:465:ILE:CD1	2:U:24:ARG:CB	2.22	1.14
1:H:409:HIS:HB3	1:H:416:GLY:CA	1.77	1.14
1:A:46:PRO:CA	2:S:76:HIS:CD2	2.31	1.13
1:G:170:LEU:HG	1:G:424:LEU:HD13	1.17	1.13
1:A:409:HIS:CB	1:A:416:GLY:CA	2.27	1.13
1:C:409:HIS:CB	1:C:416:GLY:CA	2.27	1.13
1:E:46:PRO:CD	2:K:80:GLU:OE1	1.83	1.13
1:E:409:HIS:CB	1:E:416:GLY:CA	2.27	1.13
1:F:409:HIS:CB	1:F:416:GLY:CA	2.27	1.13
1:F:473:ASP:OD2	2:J:24:ARG:NE	1.80	1.13
1:D:21:LYS:HZ3	2:O:33:THR:CB	1.57	1.13
1:E:45:GLN:OE1	2:L:3:LEU:HD12	1.48	1.13
1:E:473:ASP:OD2	2:P:24:ARG:HD3	1.47	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PRO:CD	2:S:29[A]:GLN:NE2	2.11	1.13
1:B:409:HIS:CB	1:B:416:GLY:CA	2.27	1.13
1:C:19:ASP:CB	2:M:33:THR:HG23	1.79	1.13
1:E:391:VAL:CG1	1:E:437:LEU:HD12	1.65	1.13
1:F:391:VAL:CG1	1:F:437:LEU:HD12	1.65	1.13
1:H:19:ASP:C	2:W:32:GLU:OE1	1.86	1.13
1:D:21:LYS:HZ2	2:O:33:THR:CG2	1.46	1.12
1:D:170:LEU:HG	1:D:424:LEU:HD13	1.17	1.12
1:D:409:HIS:HB3	1:D:416:GLY:CA	1.77	1.13
1:G:409:HIS:HB3	1:G:416:GLY:CA	1.77	1.12
1:H:47:GLY:N	2:W:76:HIS:CG	2.17	1.12
1:E:19:ASP:OD1	2:K:29[A]:GLN:HA	1.33	1.12
1:E:45:GLN:OE1	2:L:3:LEU:CD1	1.97	1.12
1:H:409:HIS:CB	1:H:416:GLY:CA	2.27	1.12
1:D:465:ILE:CG1	2:K:24:ARG:HB3	1.79	1.12
1:B:21:LYS:CD	2:Q:33:THR:HG21	1.79	1.12
1:G:409:HIS:CB	1:G:416:GLY:CA	2.27	1.12
1:D:409:HIS:CB	1:D:416:GLY:CA	2.27	1.12
1:E:465:ILE:CD1	2:O:24:ARG:CB	2.24	1.11
1:A:52:GLU:CG	2:S:29[B]:GLN:CD	2.10	1.11
1:B:49:PRO:CD	2:Q:29[A]:GLN:NE2	2.12	1.11
1:B:465:ILE:CG1	2:M:24:ARG:CB	2.25	1.11
1:B:46:PRO:HA	2:Q:76:HIS:CG	1.85	1.11
1:B:46:PRO:HB3	2:Q:76:HIS:CD2	1.85	1.11
1:H:473:ASP:OD2	2:T:24:ARG:CD	1.98	1.11
1:B:46:PRO:HA	2:Q:76:HIS:NE2	1.63	1.11
1:A:465:ILE:HD11	2:W:24:ARG:HB3	1.30	1.10
1:B:46:PRO:CD	2:Q:80:GLU:OE1	1.92	1.10
1:D:21:LYS:HZ3	2:O:33:THR:CG2	1.48	1.10
1:D:46:PRO:HD3	2:O:80:GLU:OE1	1.21	1.10
1:E:21:LYS:HZ2	2:K:33:THR:CB	1.55	1.10
1:H:391:VAL:CG1	1:H:437:LEU:HD12	1.65	1.10
1:B:18:LYS:HB3	2:Q:32:GLU:HA	1.15	1.10
1:B:391:VAL:CG1	1:B:437:LEU:HD12	1.65	1.10
1:A:473:ASP:OD2	2:X:24:ARG:CD	1.98	1.10
2:I:14:LEU:HD23	2:J:89[A]:VAL:HG21	1.28	1.10
1:D:21:LYS:HG3	2:O:33:THR:HG22	1.15	1.10
2:O:14:LEU:HD23	2:P:89[A]:VAL:HG21	1.28	1.10
1:A:46:PRO:HB3	2:S:76:HIS:CD2	1.87	1.09
1:F:473:ASP:OD2	2:J:24:ARG:HD3	1.43	1.09
1:D:52:GLU:CB	2:O:29[B]:GLN:NE2	2.10	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:LYS:CB	2:K:32:GLU:HA	1.70	1.09
1:C:21:LYS:HZ2	2:M:33:THR:CG2	1.64	1.09
1:F:21:LYS:CG	2:U:33:THR:HG22	1.79	1.09
1:F:52:GLU:CB	2:U:29[B]:GLN:NE2	2.04	1.09
2:M:14:LEU:HD23	2:N:89[A]:VAL:HG21	1.28	1.09
2:S:14:LEU:HD23	2:T:89[A]:VAL:HG21	1.28	1.09
1:D:21:LYS:CG	2:O:33:THR:CG2	2.29	1.09
1:E:473:ASP:OD2	2:P:24:ARG:NE	1.84	1.09
1:A:52:GLU:CG	2:S:29[B]:GLN:OE1	2.01	1.08
1:B:170:LEU:HG	1:B:424:LEU:HD13	1.17	1.08
1:D:465:ILE:CD1	2:K:24:ARG:CB	2.24	1.08
1:G:473:ASP:OD2	2:V:24:ARG:HD3	1.47	1.08
1:F:21:LYS:NZ	2:U:33:THR:OG1	1.85	1.08
1:F:46:PRO:CA	2:U:76:HIS:NE2	2.13	1.08
1:F:465:ILE:CD1	2:I:24:ARG:CB	2.26	1.08
2:Q:14:LEU:HD23	2:R:89[A]:VAL:HG21	1.28	1.08
1:D:170:LEU:CD1	1:D:424:LEU:HD13	1.84	1.08
1:F:46:PRO:HA	2:U:76:HIS:CG	1.88	1.08
1:F:52:GLU:CD	2:U:29[B]:GLN:OE1	1.92	1.08
1:D:46:PRO:HB3	2:O:80:GLU:HG2	1.30	1.07
1:G:170:LEU:CD1	1:G:424:LEU:HD13	1.84	1.07
2:W:14:LEU:HD23	2:X:89[A]:VAL:HG21	1.28	1.07
1:B:167:ARG:HG3	1:B:428:VAL:HG21	1.10	1.07
1:C:470:GLU:HG2	1:C:471:THR:N	1.65	1.07
1:F:170:LEU:CD1	1:F:424:LEU:HD13	1.84	1.07
1:H:52:GLU:CB	2:W:29[B]:GLN:HE22	1.66	1.07
1:H:167:ARG:HG3	1:H:428:VAL:HG21	1.10	1.07
1:H:470:GLU:HG2	1:H:471:THR:N	1.65	1.07
1:A:170:LEU:CD1	1:A:424:LEU:HD13	1.84	1.07
1:B:52:GLU:CG	2:Q:29[B]:GLN:OE1	2.02	1.07
1:B:170:LEU:CD1	1:B:424:LEU:HD13	1.84	1.07
1:E:170:LEU:CD1	1:E:424:LEU:HD13	1.84	1.07
1:E:465:ILE:HD12	2:O:24:ARG:HB3	1.10	1.07
1:H:473:ASP:OD2	2:T:24:ARG:HD3	1.52	1.07
1:C:170:LEU:CD1	1:C:424:LEU:HD13	1.84	1.07
1:E:470:GLU:HG2	1:E:471:THR:N	1.65	1.07
1:F:167:ARG:HG3	1:F:428:VAL:HG21	1.10	1.07
1:F:470:GLU:HG2	1:F:471:THR:N	1.65	1.07
1:G:465:ILE:HD12	2:U:24:ARG:HB3	1.13	1.07
1:H:170:LEU:CD1	1:H:424:LEU:HD13	1.84	1.07
1:A:167:ARG:HG3	1:A:428:VAL:HG21	1.11	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:LEU:HD22	2:K:33:THR:O	1.53	1.07
1:H:170:LEU:HG	1:H:424:LEU:HD13	1.17	1.06
1:D:46:PRO:CG	2:O:80:GLU:CB	2.08	1.06
1:G:470:GLU:HG2	1:G:471:THR:N	1.65	1.06
1:C:167:ARG:HG3	1:C:428:VAL:HG21	1.11	1.06
1:E:196:GLY:CA	1:E:421:ARG:HH11	1.67	1.06
1:F:21:LYS:HZ1	2:U:33:THR:CG2	1.47	1.06
1:F:196:GLY:CA	1:F:421:ARG:HH11	1.67	1.06
1:H:20:TYR:N	2:W:32:GLU:CD	2.07	1.06
1:A:45:GLN:C	2:T:1:MET:CE	2.22	1.06
1:D:470:GLU:HG2	1:D:471:THR:N	1.65	1.06
1:E:167:ARG:HG3	1:E:428:VAL:HG21	1.11	1.06
1:F:18:LYS:CB	2:U:32:GLU:HA	1.76	1.06
1:F:46:PRO:CA	2:U:76:HIS:CE1	2.38	1.06
1:G:52:GLU:HG2	2:I:29[B]:GLN:CD	1.74	1.06
1:A:470:GLU:HG2	1:A:471:THR:N	1.65	1.06
1:B:470:GLU:HG2	1:B:471:THR:N	1.65	1.06
1:G:465:ILE:HD11	2:U:24:ARG:HB3	1.37	1.06
1:B:46:PRO:CA	2:Q:76:HIS:CD2	2.38	1.05
1:D:196:GLY:CA	1:D:421:ARG:HH11	1.67	1.05
1:A:465:ILE:CG1	2:W:24:ARG:HB3	1.85	1.05
1:G:167:ARG:HG3	1:G:428:VAL:HG21	1.10	1.05
1:G:196:GLY:CA	1:G:421:ARG:HH11	1.67	1.05
1:H:18:LYS:CA	2:W:32:GLU:HA	1.85	1.05
1:C:170:LEU:HD12	1:C:424:LEU:CG	1.85	1.05
1:G:18:LYS:CB	2:I:32:GLU:HA	1.76	1.05
1:G:52:GLU:CG	2:I:29[B]:GLN:NE2	1.98	1.05
1:G:18:LYS:HB3	2:I:32:GLU:HA	1.06	1.05
1:B:45:GLN:C	2:R:1:MET:CE	2.20	1.05
1:B:196:GLY:CA	1:B:421:ARG:HH11	1.67	1.05
1:D:391:VAL:HG11	1:D:437:LEU:HD12	1.25	1.05
1:A:170:LEU:HD12	1:A:424:LEU:CG	1.85	1.04
1:A:196:GLY:CA	1:A:421:ARG:HH11	1.67	1.04
1:A:465:ILE:HD12	2:W:24:ARG:CG	1.86	1.04
1:B:170:LEU:CD1	1:B:424:LEU:CD2	2.29	1.04
1:D:167:ARG:HG3	1:D:428:VAL:HG21	1.10	1.04
1:E:52:GLU:CB	2:K:29[B]:GLN:HE22	1.68	1.04
1:H:196:GLY:CA	1:H:421:ARG:HH11	1.67	1.04
1:D:47:GLY:N	2:O:76:HIS:ND1	2.03	1.04
1:F:170:LEU:CD1	1:F:424:LEU:CD2	2.29	1.04
1:A:18:LYS:HB3	2:S:32:GLU:HA	1.08	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:GLY:CA	1:C:421:ARG:HH11	1.67	1.04
1:E:46:PRO:HA	2:K:76:HIS:CG	1.91	1.04
1:A:388:PRO:HB3	1:A:441:GLY:CA	1.88	1.04
1:C:19:ASP:C	2:M:32:GLU:OE1	1.96	1.04
1:G:391:VAL:HG11	1:G:437:LEU:HD12	1.25	1.04
1:C:388:PRO:HB3	1:C:441:GLY:CA	1.88	1.04
1:E:170:LEU:CD1	1:E:424:LEU:CD2	2.29	1.04
1:C:388:PRO:CB	1:C:441:GLY:HA3	1.87	1.03
1:E:465:ILE:HD11	2:O:24:ARG:HB3	1.40	1.03
1:G:19:ASP:OD1	2:I:29[A]:GLN:HA	1.23	1.03
1:G:45:GLN:CD	2:J:3:LEU:HD12	1.78	1.03
1:A:388:PRO:CB	1:A:441:GLY:HA3	1.87	1.03
1:B:388:PRO:CB	1:B:441:GLY:HA3	1.87	1.03
1:C:473:ASP:OD2	2:R:24:ARG:HD3	1.59	1.03
1:D:46:PRO:HA	2:O:76:HIS:CG	1.93	1.03
1:E:22:LEU:CG	2:K:33:THR:CA	1.79	1.03
1:E:52:GLU:HG2	2:K:29[B]:GLN:CD	1.78	1.03
1:H:388:PRO:CB	1:H:441:GLY:HA3	1.87	1.03
1:E:170:LEU:HD12	1:E:424:LEU:CG	1.85	1.03
1:E:388:PRO:CB	1:E:441:GLY:HA3	1.87	1.03
1:F:388:PRO:HB3	1:F:441:GLY:CA	1.88	1.03
1:F:388:PRO:CB	1:F:441:GLY:HA3	1.87	1.03
1:H:465:ILE:HD12	2:S:24:ARG:CB	1.89	1.03
1:A:46:PRO:CB	2:S:76:HIS:CD2	2.42	1.02
1:D:52:GLU:CD	2:O:29[B]:GLN:OE1	1.97	1.02
1:E:388:PRO:HB3	1:E:441:GLY:CA	1.88	1.02
1:F:21:LYS:CG	2:U:33:THR:HG21	1.81	1.02
1:G:46:PRO:HA	2:I:76:HIS:CG	1.94	1.02
1:G:388:PRO:HB3	1:G:441:GLY:CA	1.88	1.02
1:D:46:PRO:CA	2:O:76:HIS:CE1	2.40	1.02
1:D:388:PRO:HB3	1:D:441:GLY:CA	1.88	1.02
1:F:170:LEU:HD12	1:F:424:LEU:CG	1.85	1.02
1:G:21:LYS:HG3	2:I:33:THR:CG2	1.88	1.02
1:G:409:HIS:HB3	1:G:416:GLY:HA3	1.38	1.02
1:B:465:ILE:HD11	2:M:24:ARG:HB3	1.36	1.02
1:E:46:PRO:CA	2:K:76:HIS:CG	2.40	1.02
1:G:388:PRO:CB	1:G:441:GLY:HA3	1.87	1.02
1:D:388:PRO:CB	1:D:441:GLY:HA3	1.87	1.01
1:G:170:LEU:HD12	1:G:424:LEU:CG	1.85	1.01
1:H:45:GLN:OE1	2:X:3:LEU:CD1	2.08	1.01
1:B:388:PRO:HB3	1:B:441:GLY:CA	1.88	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:HD12	1:D:424:LEU:CG	1.85	1.01
1:G:391:VAL:HG11	1:G:437:LEU:CG	1.90	1.01
1:H:388:PRO:HB3	1:H:441:GLY:CA	1.88	1.01
1:D:46:PRO:CG	2:O:80:GLU:HG2	1.57	1.01
1:D:391:VAL:HG11	1:D:437:LEU:CG	1.90	1.01
1:D:409:HIS:HB3	1:D:416:GLY:HA3	1.38	1.01
1:G:21:LYS:CG	2:I:33:THR:CG2	2.37	1.01
1:G:465:ILE:HD12	2:U:24:ARG:CG	1.88	1.01
1:A:18:LYS:CB	2:S:32:GLU:HA	1.88	1.01
1:A:52:GLU:HB2	2:S:29[B]:GLN:NE2	1.73	1.01
1:D:473:ASP:OD2	2:L:24:ARG:HD3	1.61	1.01
1:E:21:LYS:HG3	2:K:33:THR:HG22	1.39	1.01
1:E:22:LEU:HG	2:K:33:THR:CA	1.59	1.01
1:E:46:PRO:HD3	2:K:80:GLU:OE1	1.54	1.01
1:H:21:LYS:NZ	2:W:33:THR:CB	2.24	1.01
1:A:170:LEU:CD1	1:A:424:LEU:CD2	2.29	1.01
1:A:170:LEU:HD11	1:A:424:LEU:CG	1.89	1.01
1:C:19:ASP:HB2	2:M:33:THR:HG23	1.39	1.01
1:C:170:LEU:CD1	1:C:424:LEU:CD2	2.29	1.01
1:E:170:LEU:HD11	1:E:424:LEU:CG	1.89	1.01
1:F:170:LEU:HD11	1:F:424:LEU:CG	1.89	1.01
1:F:47:GLY:N	2:U:76:HIS:ND1	2.08	1.00
1:G:46:PRO:HA	2:I:76:HIS:ND1	1.76	1.00
1:A:391:VAL:HG11	1:A:437:LEU:CG	1.90	1.00
1:B:52:GLU:HB3	2:Q:29[B]:GLN:HE22	1.23	1.00
1:D:465:ILE:HD12	2:K:24:ARG:HB3	1.03	1.00
1:E:21:LYS:HZ1	2:K:33:THR:CG2	1.67	1.00
1:H:409:HIS:HB3	1:H:416:GLY:HA3	1.38	1.00
1:A:409:HIS:HB3	1:A:416:GLY:HA3	1.38	1.00
1:B:170:LEU:CD1	1:B:424:LEU:CD1	2.40	1.00
1:C:170:LEU:HD11	1:C:424:LEU:CG	1.89	1.00
1:E:391:VAL:HG11	1:E:437:LEU:CG	1.90	1.00
1:H:465:ILE:HD12	2:S:24:ARG:HB3	1.41	1.00
1:F:18:LYS:HB3	2:U:32:GLU:HA	1.02	1.00
1:F:391:VAL:HG11	1:F:437:LEU:CG	1.90	1.00
1:H:170:LEU:CD1	1:H:424:LEU:CD1	2.40	1.00
1:C:170:LEU:CD1	1:C:424:LEU:CD1	2.40	1.00
1:C:391:VAL:HG11	1:C:437:LEU:CG	1.90	1.00
1:H:391:VAL:HG11	1:H:437:LEU:CG	1.90	1.00
1:A:170:LEU:CD1	1:A:424:LEU:CD1	2.40	1.00
1:E:409:HIS:HB3	1:E:416:GLY:HA3	1.38	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:HIS:HB3	1:B:416:GLY:HA3	1.38	0.99
1:D:170:LEU:HD11	1:D:424:LEU:CG	1.89	0.99
1:D:383:HIS:CE1	1:D:462:TRP:O	2.16	0.99
1:G:383:HIS:CE1	1:G:462:TRP:O	2.16	0.99
1:B:391:VAL:HG11	1:B:437:LEU:CG	1.90	0.99
1:C:409:HIS:HB3	1:C:416:GLY:HA3	1.38	0.99
1:F:409:HIS:HB3	1:F:416:GLY:HA3	1.38	0.99
1:E:19:ASP:CB	2:K:33:THR:HG23	1.92	0.99
1:B:46:PRO:CB	2:Q:76:HIS:CD2	2.44	0.99
1:F:21:LYS:HG3	2:U:33:THR:HG22	1.03	0.99
1:G:170:LEU:HD11	1:G:424:LEU:CG	1.89	0.99
1:D:19:ASP:OD1	2:O:29[A]:GLN:HA	1.15	0.99
1:F:46:PRO:HA	2:U:76:HIS:ND1	1.77	0.99
1:A:383:HIS:CE1	1:A:462:TRP:O	2.16	0.99
1:C:196:GLY:HA2	1:C:421:ARG:NH1	1.44	0.99
1:D:170:LEU:CD1	1:D:424:LEU:CD1	2.40	0.99
1:H:18:LYS:CA	2:W:32:GLU:CA	2.40	0.99
1:E:383:HIS:CE1	1:E:462:TRP:O	2.16	0.98
1:F:383:HIS:CE1	1:F:462:TRP:O	2.16	0.98
1:H:19:ASP:CB	2:W:33:THR:HG23	1.91	0.98
1:C:383:HIS:CE1	1:C:462:TRP:O	2.16	0.98
1:D:18:LYS:HB3	2:O:32:GLU:CA	1.92	0.98
1:E:465:ILE:HD12	2:O:24:ARG:CG	1.90	0.98
1:H:170:LEU:HD12	1:H:424:LEU:CG	1.85	0.98
1:H:383:HIS:CE1	1:H:462:TRP:O	2.16	0.98
1:H:466:LYS:O	2:S:20:TYR:OH	1.78	0.98
1:C:473:ASP:OD2	2:R:24:ARG:CD	2.11	0.98
1:G:46:PRO:HD2	2:I:80:GLU:OE1	1.59	0.98
1:G:170:LEU:CD1	1:G:424:LEU:CD1	2.40	0.98
1:H:465:ILE:CD1	2:S:24:ARG:CB	2.40	0.98
1:A:45:GLN:O	2:T:1:MET:CE	2.11	0.98
1:B:383:HIS:CE1	1:B:462:TRP:O	2.16	0.98
1:B:18:LYS:CB	2:Q:32:GLU:HA	1.90	0.98
1:B:170:LEU:HD12	1:B:424:LEU:CG	1.85	0.98
1:C:466:LYS:O	2:Q:20:TYR:OH	1.82	0.98
1:D:21:LYS:CG	2:O:33:THR:HG22	1.92	0.98
1:E:170:LEU:CD1	1:E:424:LEU:CD1	2.40	0.98
1:B:45:GLN:O	2:R:1:MET:HE2	1.64	0.98
1:D:170:LEU:HG	1:D:424:LEU:CD1	1.93	0.97
1:F:170:LEU:HG	1:F:424:LEU:CD1	1.93	0.97
1:A:49:PRO:HD3	2:S:29[A]:GLN:HE22	1.27	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:LEU:HD11	1:B:424:LEU:CG	1.89	0.97
1:E:170:LEU:HG	1:E:424:LEU:CD1	1.93	0.97
1:G:170:LEU:HG	1:G:424:LEU:CD1	1.93	0.97
1:B:170:LEU:HG	1:B:424:LEU:CD1	1.93	0.97
1:A:196:GLY:HA2	1:A:421:ARG:NH1	1.44	0.97
1:F:170:LEU:CD1	1:F:424:LEU:CD1	2.40	0.97
1:H:170:LEU:HG	1:H:424:LEU:CD1	1.93	0.97
1:C:19:ASP:C	2:M:32:GLU:CD	2.10	0.97
1:H:170:LEU:HD11	1:H:424:LEU:CG	1.89	0.97
1:B:45:GLN:O	2:R:1:MET:CE	2.13	0.97
1:D:46:PRO:HD2	2:O:80:GLU:OE1	1.61	0.97
1:F:465:ILE:HD12	2:I:24:ARG:HB3	0.99	0.97
1:A:21:LYS:HZ2	2:S:33:THR:CG2	1.69	0.97
1:G:392:GLU:CB	1:G:438:TYR:HD1	1.78	0.97
1:H:392:GLU:CB	1:H:438:TYR:HD1	1.78	0.97
1:A:21:LYS:HG2	2:S:33:THR:CG2	1.92	0.96
1:C:170:LEU:HG	1:C:424:LEU:CD1	1.93	0.96
1:C:465:ILE:HD12	2:Q:24:ARG:CB	1.95	0.96
1:H:465:ILE:HD11	2:S:24:ARG:HB3	1.46	0.96
1:B:49:PRO:HD3	2:Q:29[A]:GLN:NE2	1.76	0.96
1:D:392:GLU:CB	1:D:438:TYR:HD1	1.78	0.96
1:H:45:GLN:OE1	2:X:3:LEU:HD12	1.63	0.96
1:A:170:LEU:HG	1:A:424:LEU:CD1	1.93	0.96
1:C:388:PRO:HB3	1:C:441:GLY:HA3	0.97	0.96
1:B:46:PRO:HD2	2:R:3:LEU:HD11	1.48	0.96
1:A:388:PRO:HB3	1:A:441:GLY:HA3	0.97	0.96
1:G:52:GLU:CB	2:I:29[B]:GLN:NE2	2.25	0.96
1:B:21:LYS:HG2	2:Q:33:THR:CG2	1.91	0.96
1:B:196:GLY:HA2	1:B:421:ARG:HH11	1.13	0.96
1:H:196:GLY:HA2	1:H:421:ARG:HH11	1.13	0.96
1:A:45:GLN:O	2:T:1:MET:HE2	1.64	0.96
1:B:392:GLU:CB	1:B:438:TYR:HD1	1.78	0.96
1:G:21:LYS:CG	2:I:33:THR:HG22	1.95	0.96
1:A:465:ILE:CG1	2:W:24:ARG:CB	2.40	0.95
1:A:52:GLU:HG2	2:S:29[B]:GLN:OE1	1.64	0.95
1:F:15:ALA:CB	1:G:410:PRO:HA	1.96	0.95
1:G:46:PRO:CA	2:I:76:HIS:CG	2.50	0.95
1:C:18:LYS:HA	2:M:32:GLU:N	1.79	0.95
1:H:45:GLN:CD	2:X:3:LEU:HD12	1.86	0.95
1:C:392:GLU:HB2	1:C:438:TYR:HB2	1.47	0.95
1:D:18:LYS:HB3	2:O:32:GLU:HA	0.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196:GLY:HA2	1:H:421:ARG:NH1	1.44	0.95
1:B:392:GLU:HB2	1:B:438:TYR:HB2	1.47	0.95
1:D:46:PRO:HB3	2:O:76:HIS:HD2	1.30	0.95
1:G:392:GLU:HB2	1:G:438:TYR:HB2	1.47	0.95
1:A:52:GLU:HB3	2:S:29[B]:GLN:NE2	1.82	0.95
1:E:388:PRO:HB3	1:E:441:GLY:HA3	0.97	0.95
1:B:388:PRO:HB3	1:B:441:GLY:HA3	0.97	0.95
1:A:49:PRO:HD2	2:S:29[A]:GLN:NE2	1.79	0.94
1:A:392:GLU:HB2	1:A:438:TYR:HB2	1.47	0.94
1:B:52:GLU:HB2	2:Q:29[B]:GLN:NE2	1.81	0.94
1:D:21:LYS:NZ	2:O:33:THR:OG1	1.99	0.94
1:B:467:PHE:N	1:B:468:GLU:N	2.16	0.94
1:D:392:GLU:HB2	1:D:438:TYR:HB2	1.47	0.94
1:D:473:ASP:OD2	2:L:24:ARG:CD	2.15	0.94
1:E:392:GLU:HB2	1:E:438:TYR:HB2	1.47	0.94
1:F:388:PRO:HB3	1:F:441:GLY:HA3	0.97	0.94
1:F:392:GLU:HB2	1:F:438:TYR:HB2	1.47	0.94
1:G:46:PRO:HB3	2:I:76:HIS:HD2	1.19	0.94
1:H:388:PRO:HB3	1:H:441:GLY:HA3	0.97	0.94
1:H:392:GLU:HB2	1:H:438:TYR:HB2	1.47	0.94
1:B:465:ILE:HD12	2:M:24:ARG:CG	1.96	0.94
1:H:21:LYS:HG3	2:W:33:THR:HG22	1.49	0.94
1:H:467:PHE:N	1:H:468:GLU:N	2.16	0.94
1:D:196:GLY:HA2	1:D:421:ARG:HH11	1.13	0.94
1:D:19:ASP:OD1	2:O:29[A]:GLN:CA	1.73	0.94
2:R:24:ARG:HH11	2:R:24:ARG:HG3	1.33	0.94
1:B:52:GLU:HG2	2:Q:29[B]:GLN:OE1	1.59	0.94
1:B:196:GLY:HA2	1:B:421:ARG:NH1	1.44	0.94
1:C:465:ILE:HD12	2:Q:24:ARG:HB3	1.45	0.94
1:D:46:PRO:HG3	2:O:80:GLU:HG2	1.22	0.94
1:D:388:PRO:HB3	1:D:441:GLY:HA3	0.97	0.94
1:F:392:GLU:CB	1:F:438:TYR:HD1	1.78	0.94
1:H:465:ILE:HD12	2:S:24:ARG:CG	1.94	0.94
2:X:24:ARG:HH11	2:X:24:ARG:HG3	1.33	0.94
1:A:49:PRO:HD3	2:S:29[A]:GLN:NE2	1.80	0.94
1:A:196:GLY:HA2	1:A:421:ARG:HH11	1.13	0.94
1:B:49:PRO:HD3	2:Q:29[A]:GLN:HE22	1.27	0.94
1:C:196:GLY:HA2	1:C:421:ARG:HH11	1.13	0.94
1:G:196:GLY:HA2	1:G:421:ARG:HH11	1.13	0.94
1:G:467:PHE:N	1:G:468:GLU:N	2.16	0.94
1:D:467:PHE:N	1:D:468:GLU:N	2.16	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:PRO:HD2	2:Q:29[A]:GLN:NE2	1.81	0.93
1:E:392:GLU:CB	1:E:438:TYR:HD1	1.78	0.93
1:G:388:PRO:HB3	1:G:441:GLY:HA3	0.97	0.93
1:B:46:PRO:HA	2:Q:76:HIS:ND1	1.82	0.93
1:C:465:ILE:CD1	2:Q:24:ARG:CB	2.45	0.93
1:F:467:PHE:N	1:F:468:GLU:N	2.16	0.93
1:E:467:PHE:N	1:E:468:GLU:N	2.16	0.93
1:F:465:ILE:HD11	2:I:24:ARG:HB3	1.50	0.93
1:H:21:LYS:CE	2:W:33:THR:HG21	1.98	0.93
1:H:21:LYS:HZ2	2:W:33:THR:CB	1.79	0.92
1:E:196:GLY:HA2	1:E:421:ARG:NH1	1.44	0.92
1:E:472:MET:HB2	1:E:473:ASP:CA	1.99	0.92
1:F:410:PRO:HA	1:G:15:ALA:CB	1.99	0.92
1:F:472:MET:HB2	1:F:473:ASP:CA	1.99	0.92
1:A:46:PRO:HA	2:S:76:HIS:ND1	1.84	0.92
1:A:170:LEU:HD11	1:A:424:LEU:CD1	1.99	0.92
1:C:467:PHE:N	1:C:468:GLU:N	2.16	0.92
1:D:410:PRO:HA	1:E:15:ALA:CB	2.00	0.92
1:C:170:LEU:HD11	1:C:424:LEU:CD1	1.99	0.92
1:F:21:LYS:HZ2	2:U:33:THR:HB	1.32	0.92
1:C:52:GLU:CB	2:M:29[B]:GLN:HE22	1.82	0.92
1:G:196:GLY:HA2	1:G:421:ARG:NH1	1.44	0.92
1:H:52:GLU:HG2	2:W:29[B]:GLN:CD	1.89	0.92
1:A:467:PHE:N	1:A:468:GLU:N	2.16	0.92
1:B:170:LEU:HD11	1:B:424:LEU:CD1	1.99	0.92
2:P:24:ARG:HH11	2:P:24:ARG:HG3	1.33	0.92
2:V:24:ARG:HG3	2:V:24:ARG:HH11	1.33	0.92
1:A:21:LYS:HZ3	2:S:33:THR:HB	1.34	0.92
1:E:21:LYS:CG	2:K:33:THR:CG2	2.47	0.92
1:D:46:PRO:HA	2:O:76:HIS:ND1	1.85	0.92
1:D:196:GLY:HA2	1:D:421:ARG:NH1	1.44	0.92
2:J:24:ARG:HH11	2:J:24:ARG:HG3	1.33	0.92
1:C:21:LYS:NZ	2:M:33:THR:CB	2.32	0.91
1:C:392:GLU:CB	1:C:438:TYR:HD1	1.78	0.91
1:D:15:ALA:CB	1:E:410:PRO:HA	1.99	0.91
1:D:21:LYS:CG	2:O:33:THR:HG21	1.92	0.91
2:L:24:ARG:HH11	2:L:24:ARG:HG3	1.33	0.91
1:C:21:LYS:HZ2	2:M:33:THR:HG21	1.15	0.91
1:C:21:LYS:HZ1	2:M:33:THR:HG21	1.18	0.91
1:B:473:ASP:OD2	2:N:24:ARG:CD	2.17	0.91
1:D:170:LEU:HD11	1:D:424:LEU:CD1	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:GLY:HA2	1:F:421:ARG:NH1	1.44	0.91
1:H:170:LEU:HD11	1:H:424:LEU:CD1	1.99	0.91
1:C:45:GLN:OE1	2:N:3:LEU:CD1	2.18	0.91
1:H:470:GLU:HG3	1:H:471:THR:N	1.85	0.91
1:A:472:MET:HB2	1:A:473:ASP:CA	1.99	0.91
1:C:472:MET:HB2	1:C:473:ASP:CA	1.99	0.91
1:F:21:LYS:CD	2:U:33:THR:HG21	1.99	0.91
1:G:170:LEU:HD11	1:G:424:LEU:CD1	1.99	0.91
1:G:472:MET:HB2	1:G:473:ASP:CA	1.99	0.91
1:B:19:ASP:HB2	2:Q:33:THR:N	1.84	0.91
1:E:21:LYS:CG	2:K:33:THR:HG22	2.01	0.91
1:A:15:ALA:CB	1:H:410:PRO:HA	2.01	0.91
1:B:15:ALA:CB	1:C:410:PRO:HA	2.00	0.91
1:D:472:MET:HB2	1:D:473:ASP:CA	1.99	0.91
1:B:470:GLU:HG3	1:B:471:THR:N	1.85	0.91
1:F:170:LEU:HD11	1:F:424:LEU:CD1	1.99	0.91
1:A:392:GLU:CB	1:A:438:TYR:HD1	1.78	0.91
1:B:472:MET:HB2	1:B:473:ASP:CA	1.99	0.91
1:H:19:ASP:HB2	2:W:33:THR:HG23	1.51	0.91
1:B:52:GLU:CG	2:Q:29[B]:GLN:CD	2.15	0.90
1:B:410:PRO:HA	1:C:15:ALA:CB	2.01	0.90
1:E:196:GLY:HA2	1:E:421:ARG:HH11	1.13	0.90
1:F:46:PRO:HD3	2:U:80:GLU:OE1	1.30	0.90
1:F:196:GLY:HA2	1:F:421:ARG:HH11	1.13	0.90
1:H:21:LYS:HZ1	2:W:33:THR:HG21	1.31	0.90
1:E:45:GLN:CD	2:L:3:LEU:HD12	1.92	0.90
1:E:170:LEU:HD11	1:E:424:LEU:CD1	1.99	0.90
1:H:472:MET:HB2	1:H:473:ASP:CA	1.99	0.90
2:N:24:ARG:HG3	2:N:24:ARG:HH11	1.33	0.90
2:T:24:ARG:HH11	2:T:24:ARG:HG3	1.33	0.90
1:F:392:GLU:HB2	1:F:438:TYR:CB	2.01	0.90
1:A:19:ASP:OD1	2:S:28:ALA:O	1.86	0.90
1:E:392:GLU:HB2	1:E:438:TYR:CB	2.01	0.90
1:G:21:LYS:NZ	2:I:33:THR:OG1	2.04	0.90
1:A:473:ASP:OD2	2:X:24:ARG:HD3	1.70	0.90
1:C:19:ASP:HA	2:M:32:GLU:OE2	1.54	0.90
1:C:20:TYR:N	2:M:32:GLU:CD	2.25	0.90
1:E:22:LEU:HG	2:K:33:THR:HA	0.92	0.90
1:G:392:GLU:HB2	1:G:438:TYR:CB	2.01	0.90
1:D:392:GLU:HB2	1:D:438:TYR:CB	2.01	0.89
1:D:470:GLU:HG3	1:D:471:THR:N	1.85	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:392:GLU:HB2	1:H:438:TYR:CB	2.01	0.89
1:A:46:PRO:CA	2:S:76:HIS:CG	2.53	0.89
1:D:465:ILE:CG1	2:K:24:ARG:CB	2.47	0.89
1:F:52:GLU:CG	2:U:29[B]:GLN:CD	2.31	0.89
1:C:392:GLU:HB2	1:C:438:TYR:CB	2.01	0.89
1:G:470:GLU:HG3	1:G:471:THR:N	1.85	0.89
1:B:46:PRO:HD3	2:Q:80:GLU:OE1	1.34	0.89
1:B:392:GLU:HB2	1:B:438:TYR:CB	2.01	0.89
1:A:46:PRO:HD2	2:T:3:LEU:HD11	1.55	0.89
1:F:46:PRO:CA	2:U:76:HIS:CG	2.50	0.89
1:A:392:GLU:HB2	1:A:438:TYR:CB	2.01	0.89
1:F:46:PRO:HB3	2:U:76:HIS:HD2	1.28	0.89
1:C:465:ILE:HD11	2:Q:24:ARG:HB3	1.52	0.89
1:C:470:GLU:HG3	1:C:471:THR:N	1.85	0.89
1:E:19:ASP:HB2	2:K:33:THR:N	1.87	0.89
1:G:170:LEU:CG	1:G:424:LEU:CD1	2.50	0.89
1:H:47:GLY:N	2:W:76:HIS:CE1	2.38	0.89
1:B:19:ASP:OD1	2:Q:28:ALA:O	1.90	0.88
1:B:465:ILE:HG13	2:M:24:ARG:CB	2.03	0.88
1:C:18:LYS:HB3	2:M:32:GLU:HA	0.90	0.88
1:D:170:LEU:CG	1:D:424:LEU:CD1	2.50	0.88
1:F:46:PRO:HD2	2:U:80:GLU:OE1	1.69	0.88
1:G:46:PRO:HD3	2:I:80:GLU:OE1	1.33	0.88
1:E:46:PRO:HD2	2:K:80:GLU:OE1	1.70	0.88
1:G:18:LYS:HB3	2:I:32:GLU:CA	2.01	0.88
1:D:170:LEU:CD1	1:D:424:LEU:CD2	2.29	0.88
1:E:22:LEU:HD21	2:K:33:THR:CB	2.02	0.88
1:F:470:GLU:HG3	1:F:471:THR:N	1.85	0.88
1:E:52:GLU:HG2	2:K:29[B]:GLN:HE22	0.77	0.88
1:E:21:LYS:NZ	2:K:33:THR:HB	1.89	0.88
1:G:170:LEU:CD1	1:G:424:LEU:CD2	2.29	0.88
1:A:470:GLU:HG3	1:A:471:THR:N	1.85	0.88
1:C:465:ILE:HD12	2:Q:24:ARG:CG	2.01	0.88
1:G:52:GLU:CD	2:I:29[B]:GLN:OE1	2.12	0.88
1:G:465:ILE:CG1	2:U:24:ARG:HB3	2.04	0.88
1:B:391:VAL:HG11	1:B:437:LEU:HD13	0.89	0.87
1:F:465:ILE:CG1	2:I:24:ARG:HB3	2.03	0.87
1:A:410:PRO:HA	1:H:15:ALA:CB	2.03	0.87
1:C:19:ASP:OD1	2:M:29[A]:GLN:HA	1.03	0.87
1:D:391:VAL:HG11	1:D:437:LEU:HD13	0.89	0.87
1:E:470:GLU:HG3	1:E:471:THR:N	1.85	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:391:VAL:HG11	1:F:437:LEU:HD13	0.89	0.87
1:B:465:ILE:HD12	2:M:24:ARG:CA	2.03	0.87
1:H:21:LYS:HG3	2:W:33:THR:CG2	2.04	0.87
1:E:21:LYS:HG3	2:K:33:THR:CG2	2.05	0.87
1:E:391:VAL:HG11	1:E:437:LEU:HD13	0.89	0.87
1:F:18:LYS:HB3	2:U:32:GLU:CA	1.98	0.87
1:F:49:PRO:CD	2:U:29[A]:GLN:NE2	2.37	0.87
1:G:19:ASP:OD1	2:I:29[B]:GLN:HA	0.89	0.87
1:G:391:VAL:HG11	1:G:437:LEU:HD13	0.89	0.87
1:H:391:VAL:HG11	1:H:437:LEU:HD13	0.89	0.87
1:C:45:GLN:OE1	2:N:3:LEU:HD12	1.74	0.87
1:D:409:HIS:NE2	1:D:454:GLU:O	2.07	0.87
1:C:18:LYS:HA	2:M:31:GLY:C	1.94	0.87
1:D:473:ASP:OD2	2:L:24:ARG:NE	2.08	0.87
1:B:409:HIS:NE2	1:B:454:GLU:O	2.07	0.87
1:H:18:LYS:CB	2:W:32:GLU:CA	2.40	0.87
1:A:52:GLU:OE2	2:S:29[B]:GLN:OE1	1.92	0.87
1:C:391:VAL:HG11	1:C:437:LEU:HD13	0.89	0.87
1:F:409:HIS:NE2	1:F:454:GLU:O	2.07	0.87
1:H:18:LYS:HA	2:W:32:GLU:N	1.89	0.87
1:E:409:HIS:NE2	1:E:454:GLU:O	2.07	0.86
1:F:21:LYS:HG2	2:U:33:THR:CG2	2.04	0.86
1:G:409:HIS:NE2	1:G:454:GLU:O	2.07	0.86
1:F:170:LEU:CG	1:F:424:LEU:CD1	2.50	0.86
1:A:167:ARG:NE	1:A:428:VAL:HG21	1.91	0.86
1:C:167:ARG:NE	1:C:428:VAL:HG21	1.91	0.86
1:H:409:HIS:NE2	1:H:454:GLU:O	2.07	0.86
1:A:19:ASP:HB2	2:S:33:THR:N	1.90	0.86
1:A:391:VAL:HG11	1:A:437:LEU:HD13	0.89	0.86
1:D:46:PRO:HG2	2:O:80:GLU:HG3	0.87	0.86
1:E:19:ASP:OD1	2:K:29[B]:GLN:HA	1.03	0.86
1:H:392:GLU:CB	1:H:438:TYR:CD1	2.49	0.86
1:C:409:HIS:NE2	1:C:454:GLU:O	2.07	0.86
1:E:167:ARG:NE	1:E:428:VAL:HG21	1.91	0.86
1:F:167:ARG:NE	1:F:428:VAL:HG21	1.91	0.86
1:B:46:PRO:CA	2:Q:76:HIS:CG	2.56	0.86
1:F:52:GLU:CG	2:U:29[B]:GLN:OE1	2.23	0.86
1:F:45:GLN:OE1	2:V:3:LEU:HD11	1.76	0.86
1:A:46:PRO:CA	2:S:76:HIS:NE2	2.36	0.86
1:A:409:HIS:NE2	1:A:454:GLU:O	2.07	0.86
1:B:196:GLY:N	1:B:421:ARG:HH11	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196:GLY:N	1:H:421:ARG:HH11	1.74	0.86
1:B:167:ARG:NE	1:B:428:VAL:HG21	1.91	0.85
1:E:21:LYS:HZ2	2:K:33:THR:HB	1.39	0.85
1:H:167:ARG:NE	1:H:428:VAL:HG21	1.91	0.85
1:D:46:PRO:CA	2:O:76:HIS:CG	2.54	0.85
1:E:196:GLY:N	1:E:421:ARG:HH11	1.74	0.85
1:C:196:GLY:N	1:C:421:ARG:HH11	1.74	0.85
1:D:196:GLY:N	1:D:421:ARG:HH11	1.74	0.85
1:F:196:GLY:N	1:F:421:ARG:HH11	1.74	0.85
1:G:196:GLY:N	1:G:421:ARG:HH11	1.74	0.85
1:H:19:ASP:OD1	2:W:29[A]:GLN:HA	0.98	0.85
1:E:18:LYS:HB3	2:K:32:GLU:CA	2.06	0.85
1:F:19:ASP:HB2	2:U:33:THR:N	1.90	0.85
1:A:196:GLY:N	1:A:421:ARG:HH11	1.74	0.85
1:H:18:LYS:HA	2:W:31:GLY:C	1.97	0.85
1:D:167:ARG:NE	1:D:428:VAL:HG21	1.91	0.85
1:G:167:ARG:NE	1:G:428:VAL:HG21	1.91	0.85
1:H:52:GLU:CG	2:W:29[B]:GLN:NE2	1.94	0.85
1:C:384:VAL:CG2	1:C:459:LEU:HD23	2.07	0.84
1:F:465:ILE:HD12	2:I:24:ARG:CG	2.03	0.84
1:A:384:VAL:CG2	1:A:459:LEU:HD23	2.07	0.84
1:D:384:VAL:CG2	1:D:459:LEU:HD23	2.07	0.84
1:E:384:VAL:CG2	1:E:459:LEU:HD23	2.07	0.84
1:F:384:VAL:CG2	1:F:459:LEU:HD23	2.07	0.84
1:A:385:TRP:NE1	1:A:463:LYS:HA	1.93	0.84
1:C:45:GLN:CD	2:N:3:LEU:HD12	1.97	0.84
1:F:15:ALA:HB3	1:G:410:PRO:HA	1.58	0.84
1:G:384:VAL:CG2	1:G:459:LEU:HD23	2.07	0.84
1:B:384:VAL:CG2	1:B:459:LEU:HD23	2.07	0.84
1:D:465:ILE:HG13	2:K:24:ARG:CB	2.07	0.84
1:A:46:PRO:HD3	2:S:80:GLU:OE1	1.29	0.84
1:C:21:LYS:HZ1	2:M:33:THR:CG2	1.80	0.84
1:D:465:ILE:HD11	2:K:24:ARG:HB3	1.57	0.84
1:F:45:GLN:C	2:V:1:MET:CE	2.46	0.84
1:H:384:VAL:CG2	1:H:459:LEU:HD23	2.07	0.84
1:C:385:TRP:NE1	1:C:463:LYS:HA	1.93	0.84
1:E:385:TRP:NE1	1:E:463:LYS:HA	1.93	0.84
1:E:465:ILE:CG1	2:O:24:ARG:HB3	2.08	0.84
1:A:409:HIS:CG	1:A:416:GLY:CA	2.58	0.83
1:E:46:PRO:HB3	2:K:76:HIS:HD2	1.06	0.83
1:F:385:TRP:NE1	1:F:463:LYS:HA	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:HIS:CG	1:E:416:GLY:CA	2.58	0.83
1:E:21:LYS:HZ1	2:K:33:THR:HG21	1.25	0.83
1:F:409:HIS:CG	1:F:416:GLY:CA	2.58	0.83
1:D:47:GLY:N	2:O:76:HIS:CG	2.45	0.83
1:D:385:TRP:NE1	1:D:463:LYS:HA	1.92	0.83
1:E:52:GLU:CG	2:K:29[B]:GLN:NE2	2.05	0.83
1:B:21:LYS:HZ3	2:Q:33:THR:CB	1.87	0.83
1:D:47:GLY:H	2:O:76:HIS:CG	1.97	0.83
1:D:385:TRP:NE1	1:D:459:LEU:O	2.12	0.83
1:H:392:GLU:CB	1:H:438:TYR:HB2	2.05	0.83
1:E:385:TRP:NE1	1:E:459:LEU:O	2.12	0.83
1:G:385:TRP:NE1	1:G:463:LYS:HA	1.93	0.83
1:F:385:TRP:NE1	1:F:459:LEU:O	2.12	0.82
1:G:385:TRP:NE1	1:G:459:LEU:O	2.12	0.82
1:H:385:TRP:NE1	1:H:463:LYS:HA	1.93	0.82
1:C:21:LYS:CE	2:M:33:THR:HG21	2.09	0.82
1:D:21:LYS:HZ3	2:O:33:THR:HB	1.43	0.82
1:F:267:HIS:HD2	1:F:277:ASN:HD22	1.26	0.82
1:H:18:LYS:HB3	2:W:32:GLU:HA	0.83	0.82
1:B:385:TRP:NE1	1:B:463:LYS:HA	1.92	0.82
1:A:46:PRO:CB	2:S:76:HIS:O	2.27	0.82
1:E:21:LYS:NZ	2:K:33:THR:OG1	2.12	0.82
1:B:45:GLN:C	2:R:1:MET:HE2	1.92	0.82
1:B:267:HIS:HD2	1:B:277:ASN:HD22	1.26	0.82
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.26	0.82
1:G:47:GLY:N	2:I:76:HIS:CG	2.46	0.82
1:H:21:LYS:CG	2:W:33:THR:CG2	2.58	0.82
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.26	0.82
1:B:392:GLU:CB	1:B:438:TYR:HB2	2.05	0.82
1:C:385:TRP:NE1	1:C:459:LEU:O	2.12	0.82
1:A:385:TRP:NE1	1:A:459:LEU:O	2.12	0.82
1:D:170:LEU:HD11	1:D:424:LEU:HB2	0.82	0.82
1:E:22:LEU:HD11	2:K:33:THR:C	1.99	0.82
1:F:170:LEU:HD11	1:F:424:LEU:HB2	0.82	0.82
1:G:170:LEU:HD11	1:G:424:LEU:HB2	0.82	0.82
1:B:52:GLU:HB3	2:Q:29[B]:GLN:NE2	1.84	0.81
1:H:473:ASP:OD2	2:T:24:ARG:NE	2.13	0.81
1:E:170:LEU:HD11	1:E:424:LEU:HB2	0.82	0.81
1:C:409:HIS:CG	1:C:416:GLY:CA	2.58	0.81
1:G:19:ASP:OD1	2:I:29[A]:GLN:CA	1.85	0.81
2:Q:71:MET:HE3	2:R:100:LYS:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:71:MET:HE3	2:X:100:LYS:HB2	1.63	0.81
1:A:170:LEU:HD11	1:A:424:LEU:HB2	0.82	0.81
1:A:385:TRP:CD1	1:A:463:LYS:CA	2.62	0.81
1:B:46:PRO:CA	2:Q:76:HIS:CE1	2.60	0.81
1:C:52:GLU:HG2	2:M:29[B]:GLN:CD	1.99	0.81
1:C:170:LEU:HD11	1:C:424:LEU:HB2	0.82	0.81
1:F:52:GLU:HG2	2:U:29[B]:GLN:OE1	1.79	0.81
1:A:392:GLU:CB	1:A:438:TYR:HB2	2.05	0.81
1:B:131:ARG:NE	2:Q:80:GLU:OE1	2.14	0.81
1:B:46:PRO:CA	2:Q:76:HIS:NE2	2.41	0.81
1:D:385:TRP:CD1	1:D:463:LYS:CA	2.62	0.81
1:E:22:LEU:CD2	2:K:33:THR:CB	2.56	0.81
1:G:267:HIS:HD2	1:G:277:ASN:HD22	1.26	0.81
1:B:52:GLU:OE2	2:Q:32:GLU:OE2	1.99	0.81
1:E:167:ARG:HB3	1:E:431:ARG:NH2	1.96	0.81
1:F:167:ARG:HB3	1:F:431:ARG:NH2	1.96	0.81
1:C:267:HIS:HD2	1:C:277:ASN:HD22	1.26	0.81
1:C:385:TRP:CD1	1:C:463:LYS:CA	2.62	0.81
1:A:391:VAL:HG11	1:A:437:LEU:HD12	1.25	0.81
1:G:385:TRP:CD1	1:G:463:LYS:CA	2.62	0.80
1:A:46:PRO:HD2	2:S:80:GLU:OE1	1.81	0.80
1:B:15:ALA:HB3	1:C:410:PRO:HA	1.62	0.80
1:D:170:LEU:HD12	1:D:424:LEU:HD22	0.81	0.80
1:E:18:LYS:HA	2:K:31:GLY:C	2.02	0.80
1:B:21:LYS:HG3	2:Q:33:THR:HG22	0.84	0.80
1:C:392:GLU:CB	1:C:438:TYR:HB2	2.05	0.80
1:G:170:LEU:HD12	1:G:424:LEU:HD22	0.81	0.80
1:H:46:PRO:HB2	2:W:76:HIS:O	1.82	0.80
1:D:21:LYS:CD	2:O:33:THR:HG21	2.11	0.80
1:D:267:HIS:HD2	1:D:277:ASN:HD22	1.26	0.80
1:D:391:VAL:HG11	1:D:437:LEU:CB	2.11	0.80
1:F:391:VAL:HG11	1:F:437:LEU:CB	2.11	0.80
1:G:391:VAL:HG11	1:G:437:LEU:CB	2.11	0.80
1:A:267:HIS:HD2	1:A:277:ASN:HD22	1.26	0.80
1:B:170:LEU:HD12	1:B:424:LEU:HD22	0.81	0.80
1:E:46:PRO:CB	2:K:76:HIS:CG	2.62	0.80
1:E:391:VAL:HG11	1:E:437:LEU:CB	2.11	0.80
1:F:15:ALA:HB2	1:G:410:PRO:HA	1.63	0.80
1:F:18:LYS:HA	2:U:31:GLY:C	2.01	0.80
1:H:170:LEU:HD12	1:H:424:LEU:HD22	0.81	0.80
1:F:52:GLU:HB2	2:U:29[B]:GLN:NE2	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LEU:HD12	1:C:424:LEU:HD22	0.81	0.80
1:G:21:LYS:HZ3	2:I:33:THR:CB	1.95	0.80
1:G:167:ARG:HB3	1:G:431:ARG:NH2	1.96	0.80
1:B:385:TRP:NE1	1:B:459:LEU:O	2.12	0.80
1:A:167:ARG:HB3	1:A:431:ARG:NH2	1.96	0.80
1:A:170:LEU:HD12	1:A:424:LEU:HD22	0.81	0.80
1:A:391:VAL:HG11	1:A:437:LEU:CB	2.11	0.80
1:C:391:VAL:HG11	1:C:437:LEU:HD12	1.25	0.80
1:D:18:LYS:HA	2:O:31:GLY:C	2.02	0.80
1:D:167:ARG:HB3	1:D:431:ARG:NH2	1.96	0.80
1:H:385:TRP:NE1	1:H:459:LEU:O	2.12	0.80
1:A:46:PRO:CA	2:S:76:HIS:CE1	2.61	0.79
1:B:170:LEU:HD11	1:B:424:LEU:HB2	0.82	0.79
1:D:15:ALA:HB3	1:E:410:PRO:HA	1.63	0.79
1:H:391:VAL:HG11	1:H:437:LEU:CB	2.11	0.79
1:B:391:VAL:HG11	1:B:437:LEU:CB	2.11	0.79
1:G:19:ASP:CB	2:I:33:THR:HG23	2.12	0.79
1:A:46:PRO:HB3	2:S:76:HIS:HD2	1.45	0.79
1:B:410:PRO:HA	1:C:15:ALA:HB2	1.64	0.79
1:C:167:ARG:HB3	1:C:431:ARG:NH2	1.96	0.79
1:C:391:VAL:HG11	1:C:437:LEU:CB	2.11	0.79
1:H:170:LEU:HD11	1:H:424:LEU:HB2	0.82	0.79
1:A:392:GLU:CB	1:A:438:TYR:CD1	2.49	0.79
1:F:170:LEU:HD12	1:F:424:LEU:HD22	0.81	0.79
1:G:409:HIS:CG	1:G:416:GLY:CA	2.58	0.79
1:A:21:LYS:HG3	2:S:33:THR:HG22	0.81	0.79
1:D:45:GLN:HB3	2:P:3:LEU:HD11	1.63	0.79
1:E:47:GLY:N	2:K:76:HIS:CG	2.51	0.79
1:A:15:ALA:HB2	1:H:410:PRO:HA	1.65	0.79
1:D:392:GLU:CB	1:D:438:TYR:HB2	2.05	0.79
1:E:170:LEU:HD12	1:E:424:LEU:HD22	0.81	0.79
1:C:392:GLU:CB	1:C:438:TYR:CD1	2.49	0.79
1:D:49:PRO:CD	2:O:29[A]:GLN:NE2	2.46	0.79
1:D:409:HIS:CG	1:D:416:GLY:CA	2.58	0.79
1:G:392:GLU:CB	1:G:438:TYR:HB2	2.05	0.79
1:G:469:PHE:HB2	1:G:470:GLU:O	1.83	0.79
1:A:45:GLN:HB3	2:T:3:LEU:HD11	1.63	0.79
1:A:49:PRO:HD2	2:S:29[A]:GLN:HE21	1.45	0.79
1:D:469:PHE:HB2	1:D:470:GLU:O	1.83	0.79
1:F:410:PRO:HA	1:G:15:ALA:HB3	1.63	0.79
1:F:469:PHE:HB2	1:F:470:GLU:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLY:N	2:S:76:HIS:ND1	2.31	0.79
1:B:167:ARG:HB3	1:B:431:ARG:NH2	1.96	0.79
1:B:409:HIS:CG	1:B:416:GLY:CA	2.58	0.79
1:D:410:PRO:HA	1:E:15:ALA:HB3	1.64	0.79
1:E:469:PHE:HB2	1:E:470:GLU:O	1.83	0.79
1:G:21:LYS:CG	2:I:33:THR:HG21	2.03	0.79
1:H:52:GLU:HG2	2:W:29[B]:GLN:HE22	0.69	0.78
1:A:131:ARG:NE	2:S:80:GLU:OE1	2.15	0.78
1:D:52:GLU:HB2	2:O:29[B]:GLN:NE2	1.97	0.78
1:F:410:PRO:HA	1:G:15:ALA:HB2	1.63	0.78
1:H:409:HIS:CG	1:H:416:GLY:CA	2.58	0.78
1:D:19:ASP:CB	2:O:33:THR:HG23	2.14	0.78
1:D:465:ILE:HG13	2:K:24:ARG:HB3	1.65	0.78
1:H:167:ARG:HB3	1:H:431:ARG:NH2	1.96	0.78
1:A:48:VAL:HG23	2:T:1:MET:HB2	1.64	0.78
1:B:49:PRO:HD2	2:Q:29[A]:GLN:HE21	1.47	0.78
1:C:19:ASP:HB2	2:M:33:THR:CG2	2.14	0.78
1:A:469:PHE:HB2	1:A:470:GLU:O	1.83	0.78
1:B:385:TRP:CD1	1:B:463:LYS:CA	2.62	0.78
1:C:21:LYS:HZ2	2:M:33:THR:CB	1.94	0.78
1:D:15:ALA:HB2	1:E:410:PRO:HA	1.64	0.78
1:E:45:GLN:OE1	2:L:3:LEU:HD11	1.84	0.78
1:D:45:GLN:OE1	2:P:3:LEU:HD11	1.82	0.77
1:D:410:PRO:HA	1:E:15:ALA:HB2	1.64	0.77
1:A:196:GLY:CA	1:A:421:ARG:NH1	2.28	0.77
1:C:469:PHE:HB2	1:C:470:GLU:O	1.83	0.77
1:H:469:PHE:HB2	1:H:470:GLU:O	1.83	0.77
1:B:52:GLU:OE2	2:Q:29[B]:GLN:OE1	2.00	0.77
1:F:19:ASP:CB	2:U:33:THR:HG23	2.15	0.77
1:H:52:GLU:CD	2:W:29[B]:GLN:OE1	2.22	0.77
1:F:47:GLY:N	2:U:76:HIS:CG	2.51	0.77
1:B:469:PHE:HB2	1:B:470:GLU:O	1.83	0.77
1:G:465:ILE:CG1	2:U:24:ARG:CB	2.62	0.77
1:B:18:LYS:HA	2:Q:31:GLY:C	2.05	0.77
1:H:385:TRP:CD1	1:H:463:LYS:CA	2.62	0.77
1:B:15:ALA:HB2	1:C:410:PRO:HA	1.67	0.77
1:H:45:GLN:HB3	2:X:3:LEU:HD11	1.66	0.77
1:C:196:GLY:CA	1:C:421:ARG:NH1	2.28	0.76
1:D:406:THR:HA	1:D:420:ASN:OD1	1.86	0.76
1:F:385:TRP:CD1	1:F:463:LYS:CA	2.62	0.76
1:B:465:ILE:HG13	2:M:24:ARG:HB2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:ILE:CG1	2:Q:24:ARG:HB3	2.15	0.76
1:F:406:THR:HA	1:F:420:ASN:OD1	1.85	0.76
1:G:406:THR:HA	1:G:420:ASN:OD1	1.86	0.76
1:C:465:ILE:HD13	2:Q:24:ARG:NH2	1.96	0.76
1:E:471:THR:CA	1:E:472:MET:N	2.49	0.76
1:H:167:ARG:CG	1:H:428:VAL:HG21	1.85	0.76
1:A:471:THR:CA	1:A:472:MET:N	2.49	0.76
1:D:52:GLU:CG	2:O:29[B]:GLN:OE1	2.33	0.76
1:F:471:THR:CA	1:F:472:MET:N	2.49	0.76
1:A:15:ALA:HB3	1:H:410:PRO:HA	1.66	0.76
1:A:410:PRO:HA	1:H:15:ALA:HB2	1.66	0.76
1:A:465:ILE:HG13	2:W:24:ARG:CB	2.15	0.76
1:C:21:LYS:HG3	2:M:33:THR:HG22	1.65	0.76
1:C:471:THR:CA	1:C:472:MET:N	2.49	0.76
1:E:406:THR:HA	1:E:420:ASN:OD1	1.86	0.76
1:F:392:GLU:CB	1:F:438:TYR:HB2	2.05	0.76
1:H:46:PRO:C	2:W:76:HIS:CG	2.49	0.76
1:A:18:LYS:HA	2:S:31:GLY:C	2.05	0.76
1:C:170:LEU:HD11	1:C:424:LEU:HD13	1.63	0.76
1:G:19:ASP:HB2	2:I:33:THR:N	2.01	0.76
1:H:406:THR:HA	1:H:420:ASN:OD1	1.85	0.76
1:B:167:ARG:CG	1:B:428:VAL:HG21	1.85	0.76
1:F:49:PRO:HD3	2:U:29[A]:GLN:NE2	2.00	0.76
1:H:21:LYS:CG	2:W:33:THR:HG21	2.14	0.76
1:B:46:PRO:CB	2:Q:76:HIS:O	2.33	0.76
1:D:19:ASP:HB2	2:O:33:THR:N	2.00	0.76
1:D:465:ILE:HD12	2:K:24:ARG:CG	2.15	0.76
1:B:170:LEU:HD11	1:B:424:LEU:HD13	1.62	0.76
1:A:170:LEU:HD11	1:A:424:LEU:HD13	1.63	0.76
1:C:167:ARG:CG	1:C:428:VAL:HG21	1.85	0.76
1:E:385:TRP:CD1	1:E:463:LYS:CA	2.62	0.76
1:E:392:GLU:CB	1:E:438:TYR:HB2	2.05	0.76
1:B:406:THR:HA	1:B:420:ASN:OD1	1.86	0.75
1:D:45:GLN:C	2:P:1:MET:CE	2.53	0.75
1:F:52:GLU:HB3	2:U:29[B]:GLN:HE22	1.46	0.75
1:B:410:PRO:HA	1:C:15:ALA:HB3	1.66	0.75
1:D:46:PRO:HG2	2:O:80:GLU:CG	1.58	0.75
1:H:170:LEU:HD11	1:H:424:LEU:HD13	1.63	0.75
1:H:410:PRO:HD3	1:H:461:LEU:HD22	1.68	0.75
1:A:167:ARG:CG	1:A:428:VAL:HG21	1.85	0.75
1:B:410:PRO:HD3	1:B:461:LEU:HD22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:GLY:H	2:U:76:HIS:CG	2.03	0.75
1:C:406:THR:HA	1:C:420:ASN:OD1	1.86	0.75
1:B:471:THR:CA	1:B:472:MET:N	2.49	0.75
1:B:473:ASP:OD2	2:N:24:ARG:HD3	1.85	0.75
1:G:471:THR:CA	1:G:472:MET:N	2.49	0.75
1:H:465:ILE:CG1	2:S:24:ARG:HB3	2.17	0.75
1:D:410:PRO:HD3	1:D:461:LEU:HD22	1.68	0.75
1:E:196:GLY:CA	1:E:421:ARG:NH1	2.28	0.75
1:A:406:THR:HA	1:A:420:ASN:OD1	1.86	0.75
1:A:410:PRO:HD3	1:A:461:LEU:HD22	1.68	0.75
1:A:52:GLU:OE2	2:S:32:GLU:OE2	2.03	0.75
1:A:410:PRO:HA	1:H:15:ALA:HB3	1.68	0.75
1:D:471:THR:CA	1:D:472:MET:N	2.49	0.75
1:E:21:LYS:CG	2:K:33:THR:HG21	2.13	0.75
1:F:52:GLU:OE2	2:U:29[B]:GLN:OE1	2.03	0.75
1:F:196:GLY:CA	1:F:421:ARG:NH1	2.28	0.75
1:G:45:GLN:OE1	2:J:3:LEU:HD11	1.87	0.75
2:U:71:MET:HE3	2:V:100:LYS:HB2	1.69	0.75
1:E:22:LEU:CD1	2:K:33:THR:C	2.53	0.75
1:E:409:HIS:CB	1:E:416:GLY:HA3	2.09	0.75
1:G:410:PRO:HD3	1:G:461:LEU:HD22	1.68	0.75
1:H:471:THR:CA	1:H:472:MET:N	2.49	0.75
2:K:71:MET:HE3	2:L:100:LYS:HB2	1.69	0.75
1:C:19:ASP:CB	2:M:33:THR:CG2	2.63	0.74
1:F:392:GLU:CB	1:F:438:TYR:CD1	2.49	0.74
1:E:19:ASP:HB2	2:K:33:THR:HG23	1.69	0.74
1:A:45:GLN:O	2:T:1:MET:HE1	1.86	0.74
1:A:46:PRO:HB3	2:S:76:HIS:O	1.85	0.74
1:A:391:VAL:HG13	1:A:437:LEU:CD1	2.15	0.74
1:E:52:GLU:CB	2:K:29[B]:GLN:NE2	2.42	0.74
1:F:21:LYS:HZ1	2:U:33:THR:CB	1.80	0.74
1:B:391:VAL:HG13	1:B:437:LEU:CD1	2.15	0.74
1:C:52:GLU:HG2	2:M:29[B]:GLN:HE22	0.60	0.74
1:C:410:PRO:HD3	1:C:461:LEU:HD22	1.68	0.74
1:A:45:GLN:C	2:T:1:MET:HE2	1.98	0.74
1:B:472:MET:CA	1:B:473:ASP:N	2.51	0.74
1:H:350:ARG:NH2	1:H:394:PHE:O	2.21	0.74
1:H:472:MET:CA	1:H:473:ASP:N	2.51	0.74
1:F:15:ALA:CB	1:G:410:PRO:CA	2.65	0.74
1:H:465:ILE:HG22	2:S:20:TYR:CZ	2.22	0.74
1:B:350:ARG:NH2	1:B:394:PHE:O	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:MET:CA	1:C:473:ASP:N	2.51	0.74
1:H:391:VAL:HG13	1:H:437:LEU:CD1	2.15	0.74
1:A:409:HIS:CB	1:A:416:GLY:HA3	2.09	0.74
1:C:391:VAL:HG13	1:C:437:LEU:CD1	2.15	0.74
1:A:472:MET:CA	1:A:473:ASP:N	2.51	0.74
1:H:20:TYR:CA	2:W:32:GLU:OE1	2.36	0.74
1:A:409:HIS:HB2	1:A:416:GLY:HA2	1.70	0.73
1:G:350:ARG:NH2	1:G:394:PHE:O	2.21	0.73
1:B:46:PRO:HB3	2:Q:76:HIS:HD2	1.49	0.73
1:C:409:HIS:HB2	1:C:416:GLY:HA2	1.70	0.73
1:E:392:GLU:CB	1:E:438:TYR:CD1	2.49	0.73
1:G:47:GLY:H	2:I:76:HIS:CG	2.03	0.73
1:D:350:ARG:NH2	1:D:394:PHE:O	2.21	0.73
1:G:21:LYS:CD	2:I:33:THR:HG21	2.18	0.73
1:H:52:GLU:CB	2:W:29[B]:GLN:NE2	2.40	0.73
1:A:383:HIS:H	1:A:386:HIS:HD2	1.37	0.73
1:F:410:PRO:HD3	1:F:461:LEU:HD22	1.68	0.73
1:F:472:MET:CA	1:F:473:ASP:N	2.51	0.73
1:C:409:HIS:CB	1:C:416:GLY:HA3	2.09	0.73
1:E:167:ARG:CD	1:E:428:VAL:HG21	2.19	0.73
1:E:410:PRO:HD3	1:E:461:LEU:HD22	1.68	0.73
1:F:167:ARG:CD	1:F:428:VAL:HG21	2.19	0.73
1:H:21:LYS:HZ1	2:W:33:THR:CG2	1.87	0.73
1:C:383:HIS:H	1:C:386:HIS:HD2	1.37	0.73
1:E:472:MET:CA	1:E:473:ASP:N	2.51	0.73
1:F:49:PRO:HD2	2:U:29[A]:GLN:NE2	2.03	0.73
1:G:383:HIS:H	1:G:386:HIS:HD2	1.37	0.73
1:H:167:ARG:CD	1:H:428:VAL:HG21	2.19	0.73
2:M:71:MET:HE3	2:N:100:LYS:HB2	1.71	0.73
1:B:48:VAL:HG23	2:R:1:MET:HB2	1.70	0.73
1:D:21:LYS:HG2	2:O:33:THR:CG2	2.16	0.73
1:G:472:MET:CA	1:G:473:ASP:N	2.51	0.73
1:B:167:ARG:CD	1:B:428:VAL:HG21	2.19	0.73
1:D:472:MET:CA	1:D:473:ASP:N	2.51	0.73
1:E:396:ASP:OD1	1:E:431:ARG:CD	2.37	0.73
1:F:396:ASP:OD1	1:F:431:ARG:CD	2.37	0.73
1:D:383:HIS:H	1:D:386:HIS:HD2	1.37	0.72
1:F:383:HIS:H	1:F:386:HIS:HD2	1.37	0.72
1:H:391:VAL:CG1	1:H:437:LEU:CB	2.67	0.72
1:A:396:ASP:OD1	1:A:431:ARG:CD	2.37	0.72
1:B:391:VAL:CG1	1:B:437:LEU:CB	2.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ASP:OD1	1:B:431:ARG:CD	2.37	0.72
1:D:396:ASP:OD1	1:D:431:ARG:CD	2.37	0.72
1:E:46:PRO:CB	2:K:76:HIS:NE2	2.40	0.72
1:G:396:ASP:OD1	1:G:431:ARG:CD	2.37	0.72
1:D:21:LYS:HZ2	2:O:33:THR:HG21	1.13	0.72
1:E:383:HIS:H	1:E:386:HIS:HD2	1.37	0.72
1:H:396:ASP:OD1	1:H:431:ARG:CD	2.37	0.72
1:C:21:LYS:HG3	2:M:33:THR:CG2	2.20	0.72
1:D:391:VAL:CG1	1:D:437:LEU:CB	2.67	0.72
1:E:391:VAL:CG1	1:E:437:LEU:CB	2.67	0.72
1:F:391:VAL:CG1	1:F:437:LEU:CB	2.67	0.72
1:B:21:LYS:NZ	2:Q:33:THR:HB	1.99	0.72
1:C:396:ASP:OD1	1:C:431:ARG:CD	2.37	0.72
1:G:391:VAL:CG1	1:G:437:LEU:CB	2.67	0.72
1:D:167:ARG:CD	1:D:428:VAL:HG21	2.19	0.72
2:I:71:MET:HE3	2:J:100:LYS:HB2	1.72	0.72
2:S:71:MET:HE3	2:T:100:LYS:HB2	1.72	0.72
1:A:47:GLY:H	2:S:76:HIS:CG	2.07	0.72
1:C:465:ILE:HG22	2:Q:20:TYR:CZ	2.24	0.72
1:F:49:PRO:HD3	2:U:29[A]:GLN:HE22	1.53	0.72
2:O:71:MET:HE3	2:P:100:LYS:HB2	1.72	0.72
1:C:46:PRO:HB2	2:M:76:HIS:O	1.87	0.72
1:F:45:GLN:HB3	2:V:3:LEU:HD11	1.70	0.72
1:A:15:ALA:CB	1:H:410:PRO:CA	2.68	0.72
1:C:47:GLY:C	2:N:1:MET:SD	2.69	0.72
1:D:52:GLU:OE2	2:O:29[B]:GLN:OE1	2.06	0.72
1:F:46:PRO:HD2	2:V:3:LEU:HD11	1.72	0.72
1:G:383:HIS:CG	1:G:462:TRP:HB3	2.25	0.72
1:H:383:HIS:H	1:H:386:HIS:HD2	1.37	0.72
1:A:167:ARG:CD	1:A:428:VAL:HG21	2.19	0.71
1:B:46:PRO:HB3	2:Q:76:HIS:O	1.89	0.71
1:B:383:HIS:H	1:B:386:HIS:HD2	1.37	0.71
1:C:18:LYS:HG2	2:M:31:GLY:O	1.89	0.71
1:C:167:ARG:CD	1:C:428:VAL:HG21	2.19	0.71
1:C:350:ARG:NH2	1:C:394:PHE:O	2.21	0.71
1:D:383:HIS:CG	1:D:462:TRP:HB3	2.25	0.71
1:E:167:ARG:CG	1:E:428:VAL:HG21	1.85	0.71
1:G:167:ARG:CD	1:G:428:VAL:HG21	2.19	0.71
1:A:350:ARG:NH2	1:A:394:PHE:O	2.21	0.71
1:A:391:VAL:CG1	1:A:437:LEU:CB	2.67	0.71
1:F:465:ILE:CG1	2:I:24:ARG:CB	2.65	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:409:HIS:CB	1:G:416:GLY:HA3	2.09	0.71
1:C:391:VAL:CG1	1:C:437:LEU:CB	2.67	0.71
1:D:392:GLU:CB	1:D:438:TYR:CD1	2.49	0.71
1:E:409:HIS:HB2	1:E:416:GLY:HA2	1.70	0.71
1:F:383:HIS:CG	1:F:462:TRP:HB3	2.25	0.71
1:H:18:LYS:HG2	2:W:31:GLY:O	1.90	0.71
1:A:465:ILE:HD12	2:W:24:ARG:HB3	0.74	0.71
1:D:46:PRO:HB2	2:O:76:HIS:O	1.91	0.71
1:E:383:HIS:CG	1:E:462:TRP:HB3	2.25	0.71
1:G:21:LYS:HG2	2:I:33:THR:CG2	2.20	0.71
1:B:47:GLY:N	2:Q:76:HIS:ND1	2.36	0.71
1:D:409:HIS:CB	1:D:416:GLY:HA3	2.09	0.71
1:B:196:GLY:CA	1:B:421:ARG:NH1	2.28	0.71
1:G:21:LYS:NZ	2:I:33:THR:HB	2.02	0.71
1:B:410:PRO:CA	1:C:15:ALA:CB	2.68	0.71
1:F:45:GLN:O	2:V:1:MET:CE	2.38	0.71
1:E:170:LEU:HD11	1:E:424:LEU:HD13	1.63	0.71
1:F:409:HIS:HB2	1:F:416:GLY:HA2	1.70	0.71
1:E:465:ILE:CG1	2:O:24:ARG:CB	2.66	0.70
1:B:15:ALA:CB	1:C:410:PRO:CA	2.69	0.70
1:E:21:LYS:HG2	2:K:33:THR:CG2	2.18	0.70
1:F:167:ARG:CG	1:F:428:VAL:HG21	1.85	0.70
1:C:383:HIS:CG	1:C:462:TRP:HB3	2.25	0.70
2:N:24:ARG:HH11	2:N:24:ARG:CG	2.05	0.70
2:T:24:ARG:HH11	2:T:24:ARG:CG	2.05	0.70
1:A:383:HIS:CG	1:A:462:TRP:HB3	2.25	0.70
1:H:383:HIS:CG	1:H:462:TRP:HB3	2.25	0.70
1:B:46:PRO:HD2	2:Q:80:GLU:OE1	1.90	0.70
1:E:52:GLU:CD	2:K:29[B]:GLN:OE1	2.29	0.70
1:F:15:ALA:HB3	1:G:410:PRO:CA	2.20	0.70
1:G:392:GLU:CB	1:G:438:TYR:CD1	2.49	0.70
1:B:383:HIS:CG	1:B:462:TRP:HB3	2.25	0.70
1:E:350:ARG:NH2	1:E:394:PHE:O	2.21	0.70
1:F:19:ASP:OD1	2:U:28:ALA:O	2.10	0.70
1:F:170:LEU:HD11	1:F:424:LEU:HD13	1.62	0.70
1:A:46:PRO:HB2	2:S:76:HIS:O	1.89	0.70
1:F:350:ARG:NH2	1:F:394:PHE:O	2.21	0.70
1:H:19:ASP:OD1	2:W:29[A]:GLN:CA	1.68	0.70
1:H:196:GLY:CA	1:H:421:ARG:NH1	2.28	0.70
1:D:410:PRO:CA	1:E:15:ALA:CB	2.69	0.70
1:F:410:PRO:CA	1:G:15:ALA:CB	2.69	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:GLN:HB3	2:J:3:LEU:HD11	1.72	0.70
1:C:167:ARG:HB3	1:C:428:VAL:HG13	1.74	0.70
1:A:45:GLN:HB3	2:T:3:LEU:CD1	2.22	0.69
1:C:52:GLU:CG	2:M:29[B]:GLN:NE2	2.02	0.69
1:A:167:ARG:HB3	1:A:428:VAL:HG13	1.74	0.69
1:B:167:ARG:HB3	1:B:428:VAL:HG13	1.74	0.69
1:D:21:LYS:HZ2	2:O:33:THR:CB	1.88	0.69
1:B:383:HIS:CD2	1:B:462:TRP:HB3	2.28	0.69
1:B:473:ASP:HB3	2:N:20:TYR:OH	1.93	0.69
2:J:24:ARG:HH11	2:J:24:ARG:CG	2.05	0.69
2:L:24:ARG:HH11	2:L:24:ARG:CG	2.05	0.69
1:H:383:HIS:CD2	1:H:462:TRP:HB3	2.28	0.69
2:P:24:ARG:HH11	2:P:24:ARG:CG	2.05	0.69
2:V:24:ARG:HH11	2:V:24:ARG:CG	2.05	0.69
1:F:46:PRO:HB2	2:U:76:HIS:O	1.93	0.69
1:H:21:LYS:CG	2:W:33:THR:HG22	2.22	0.69
1:H:167:ARG:HB3	1:H:428:VAL:HG13	1.75	0.69
1:H:409:HIS:HB2	1:H:416:GLY:HA2	1.70	0.69
1:D:15:ALA:CB	1:E:410:PRO:CA	2.69	0.69
1:C:383:HIS:CD2	1:C:462:TRP:HB3	2.28	0.69
1:D:52:GLU:HG2	2:O:29[B]:GLN:OE1	1.89	0.69
1:E:167:ARG:HB3	1:E:428:VAL:HG13	1.75	0.69
1:G:167:ARG:HB3	1:G:428:VAL:HG13	1.74	0.69
1:H:18:LYS:CA	2:W:32:GLU:N	2.54	0.69
1:A:383:HIS:CD2	1:A:462:TRP:HB3	2.28	0.69
1:D:167:ARG:HB3	1:D:428:VAL:HG13	1.74	0.69
1:E:46:PRO:CA	2:K:76:HIS:ND1	2.34	0.69
1:F:167:ARG:HB3	1:F:428:VAL:HG13	1.74	0.69
1:G:49:PRO:CD	2:I:29[A]:GLN:NE2	2.56	0.69
1:G:196:GLY:CA	1:G:421:ARG:NH1	2.28	0.69
1:G:467:PHE:HA	1:G:468:GLU:CA	2.21	0.69
1:D:45:GLN:CD	2:P:3:LEU:CD1	2.46	0.69
1:A:22:LEU:HD13	2:S:35:PRO:HD3	1.75	0.69
1:B:45:GLN:HB3	2:R:3:LEU:HD11	1.73	0.69
1:D:467:PHE:HA	1:D:468:GLU:CA	2.21	0.69
1:B:409:HIS:HB2	1:B:416:GLY:HA2	1.70	0.68
1:G:18:LYS:HA	2:I:31:GLY:C	2.12	0.68
1:A:47:GLY:N	2:S:76:HIS:CG	2.62	0.68
1:A:409:HIS:CD2	1:A:419:ALA:CB	2.77	0.68
1:D:46:PRO:HD2	2:P:3:LEU:HD11	1.74	0.68
1:F:46:PRO:CB	2:U:76:HIS:O	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASP:OD1	1:A:431:ARG:HD2	1.94	0.68
1:C:409:HIS:CD2	1:C:419:ALA:CB	2.77	0.68
1:D:196:GLY:CA	1:D:421:ARG:NH1	2.28	0.68
1:D:383:HIS:CD2	1:D:462:TRP:HB3	2.28	0.68
1:E:46:PRO:C	2:K:76:HIS:ND1	2.46	0.68
1:G:465:ILE:HG13	2:U:24:ARG:CB	2.23	0.68
1:C:396:ASP:OD1	1:C:431:ARG:HD2	1.94	0.68
1:H:52:GLU:OE2	2:W:29[B]:GLN:OE1	2.11	0.68
1:G:383:HIS:CD2	1:G:462:TRP:HB3	2.28	0.68
1:H:396:ASP:OD1	1:H:431:ARG:HD2	1.94	0.68
2:X:24:ARG:HH11	2:X:24:ARG:CG	2.05	0.68
1:B:409:HIS:CB	1:B:416:GLY:HA3	2.09	0.68
1:C:45:GLN:HB3	2:N:3:LEU:HD11	1.76	0.68
2:K:85:LEU:HD23	2:K:88:MET:HE3	1.76	0.68
2:R:24:ARG:HH11	2:R:24:ARG:CG	2.05	0.68
2:Q:14:LEU:CD2	2:R:89[A]:VAL:HG21	2.17	0.68
1:A:410:PRO:CA	1:H:15:ALA:CB	2.72	0.68
1:D:391:VAL:HG13	1:D:437:LEU:CD1	2.15	0.68
1:E:467:PHE:HA	1:E:468:GLU:CA	2.21	0.68
2:S:85:LEU:HD23	2:S:88:MET:HE3	1.76	0.68
1:B:396:ASP:OD1	1:B:431:ARG:HD2	1.94	0.67
1:C:21:LYS:CG	2:M:33:THR:CG2	2.72	0.67
1:D:384:VAL:HG21	1:D:459:LEU:HD23	1.76	0.67
1:D:391:VAL:HG13	1:D:437:LEU:HD12	1.73	0.67
1:E:383:HIS:CD2	1:E:462:TRP:HB3	2.28	0.67
1:F:467:PHE:HA	1:F:468:GLU:CA	2.21	0.67
1:G:295:ARG:HD3	1:G:298:HIS:CD2	2.29	0.67
1:G:384:VAL:HG21	1:G:459:LEU:HD23	1.76	0.67
2:W:14:LEU:CD2	2:X:89[A]:VAL:HG21	2.17	0.67
1:D:45:GLN:O	2:P:1:MET:CE	2.42	0.67
1:D:46:PRO:CB	2:O:76:HIS:O	2.42	0.67
1:D:295:ARG:HD3	1:D:298:HIS:CD2	2.29	0.67
1:D:409:HIS:CD2	1:D:419:ALA:CB	2.77	0.67
1:F:391:VAL:HG13	1:F:437:LEU:HD12	1.73	0.67
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.41	0.67
1:A:384:VAL:HG21	1:A:459:LEU:HD23	1.76	0.67
1:B:409:HIS:CD2	1:B:419:ALA:CB	2.77	0.67
1:E:19:ASP:HB3	2:K:33:THR:HG23	1.76	0.67
1:E:295:ARG:HD3	1:E:298:HIS:CD2	2.29	0.67
1:E:409:HIS:CD2	1:E:419:ALA:CB	2.77	0.67
1:G:396:ASP:OD1	1:G:431:ARG:HD2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:409:HIS:CD2	1:G:419:ALA:CB	2.77	0.67
1:A:48:VAL:HG23	2:T:1:MET:CB	2.24	0.67
1:D:396:ASP:OD1	1:D:431:ARG:HD2	1.94	0.67
1:G:391:VAL:HG13	1:G:437:LEU:CD1	2.15	0.67
1:G:391:VAL:HG13	1:G:437:LEU:HD12	1.73	0.67
1:C:384:VAL:HG21	1:C:459:LEU:HD23	1.76	0.67
1:F:295:ARG:HD3	1:F:298:HIS:CD2	2.29	0.67
1:F:383:HIS:CD2	1:F:462:TRP:HB3	2.28	0.67
1:F:409:HIS:CD2	1:F:419:ALA:CB	2.77	0.67
1:H:467:PHE:HA	1:H:468:GLU:CA	2.21	0.67
2:U:85:LEU:HD23	2:U:88:MET:HE3	1.77	0.67
1:A:295:ARG:HD3	1:A:298:HIS:CD2	2.29	0.67
1:E:391:VAL:HG13	1:E:437:LEU:HD12	1.73	0.67
1:A:167:ARG:CD	1:A:428:VAL:CG2	2.71	0.67
1:C:239:TYR:HE2	1:C:401:GLN:HE22	1.41	0.67
1:E:396:ASP:OD1	1:E:431:ARG:HD2	1.94	0.67
1:F:396:ASP:OD1	1:F:431:ARG:HD2	1.94	0.67
1:G:52:GLU:HG2	2:I:29[B]:GLN:OE1	1.94	0.67
1:H:295:ARG:HD3	1:H:298:HIS:CD2	2.29	0.67
1:H:409:HIS:CD2	1:H:419:ALA:CB	2.77	0.67
1:C:295:ARG:HD3	1:C:298:HIS:CD2	2.29	0.67
1:D:52:GLU:CG	2:O:29[B]:GLN:CD	2.40	0.67
1:H:409:HIS:CB	1:H:416:GLY:HA3	2.09	0.67
1:B:295:ARG:HD3	1:B:298:HIS:CD2	2.29	0.67
1:C:167:ARG:CD	1:C:428:VAL:CG2	2.71	0.67
1:E:19:ASP:OD1	2:K:29[A]:GLN:CA	1.92	0.67
1:F:239:TYR:HE2	1:F:401:GLN:HE22	1.41	0.67
1:H:384:VAL:HG21	1:H:459:LEU:HD23	1.76	0.67
1:A:465:ILE:HD12	2:W:24:ARG:CA	2.22	0.67
1:C:473:ASP:OD2	2:R:24:ARG:NE	2.27	0.66
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.41	0.66
1:E:384:VAL:HG21	1:E:459:LEU:HD23	1.76	0.66
1:E:472:MET:O	1:E:474:LYS:HE2	1.95	0.66
1:F:384:VAL:HG21	1:F:459:LEU:HD23	1.76	0.66
1:G:52:GLU:CG	2:I:29[B]:GLN:OE1	2.43	0.66
1:E:18:LYS:HA	2:K:32:GLU:N	2.07	0.66
1:F:472:MET:O	1:F:474:LYS:HE2	1.95	0.66
1:G:409:HIS:HB2	1:G:416:GLY:HA2	1.70	0.66
1:H:239:TYR:HE2	1:H:401:GLN:HE22	1.41	0.66
1:B:15:ALA:HB3	1:C:410:PRO:CA	2.25	0.66
1:D:49:PRO:HD3	2:O:29[A]:GLN:NE2	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:472:MET:O	1:H:474:LYS:HE2	1.95	0.66
1:B:467:PHE:HA	1:B:468:GLU:CA	2.21	0.66
1:A:473:ASP:HB3	2:X:20:TYR:OH	1.96	0.66
1:B:384:VAL:HG21	1:B:459:LEU:HD23	1.76	0.66
1:B:472:MET:O	1:B:474:LYS:HE2	1.95	0.66
1:C:465:ILE:HG13	2:Q:24:ARG:CB	2.26	0.66
1:B:239:TYR:HE2	1:B:401:GLN:HE22	1.41	0.66
1:C:467:PHE:HA	1:C:468:GLU:CA	2.21	0.66
1:A:472:MET:O	1:A:474:LYS:HE2	1.95	0.66
1:D:15:ALA:HB3	1:E:410:PRO:CA	2.26	0.66
1:D:409:HIS:HB2	1:D:416:GLY:HA2	1.70	0.66
1:C:472:MET:O	1:C:474:LYS:HE2	1.95	0.66
1:A:15:ALA:HB3	1:H:410:PRO:CA	2.24	0.66
1:D:239:TYR:HE2	1:D:401:GLN:HE22	1.41	0.66
1:G:46:PRO:HB2	2:I:76:HIS:O	1.96	0.66
1:D:472:MET:O	1:D:474:LYS:HE2	1.95	0.65
1:F:410:PRO:CA	1:G:15:ALA:HB3	2.26	0.65
1:A:467:PHE:HA	1:A:468:GLU:CA	2.21	0.65
1:D:385:TRP:NE1	1:D:463:LYS:CA	2.59	0.65
1:G:472:MET:O	1:G:474:LYS:HE2	1.95	0.65
1:H:45:GLN:CD	2:X:3:LEU:CD1	2.61	0.65
1:G:170:LEU:HD11	1:G:424:LEU:HD13	1.63	0.65
1:H:19:ASP:HB2	2:W:33:THR:N	2.11	0.65
1:E:167:ARG:CD	1:E:428:VAL:CG2	2.71	0.65
1:E:391:VAL:HG13	1:E:437:LEU:CD1	2.15	0.65
1:G:239:TYR:HE2	1:G:401:GLN:HE22	1.41	0.65
1:G:385:TRP:NE1	1:G:463:LYS:CA	2.59	0.65
1:E:52:GLU:HG2	2:K:29[B]:GLN:OE1	1.96	0.65
1:F:167:ARG:CD	1:F:428:VAL:CG2	2.71	0.65
1:F:391:VAL:HG13	1:F:437:LEU:CD1	2.15	0.65
1:G:45:GLN:C	2:J:1:MET:CE	2.63	0.65
1:D:170:LEU:HD11	1:D:424:LEU:HD13	1.62	0.65
1:C:391:VAL:HG13	1:C:437:LEU:HD12	1.73	0.65
1:D:49:PRO:HD3	2:O:29[A]:GLN:HE22	1.62	0.65
1:B:19:ASP:CB	2:Q:33:THR:HG23	2.27	0.65
1:C:21:LYS:CG	2:M:33:THR:HG21	2.26	0.65
1:F:385:TRP:NE1	1:F:463:LYS:CA	2.59	0.65
1:H:385:TRP:NE1	1:H:463:LYS:CA	2.59	0.65
2:S:14:LEU:CD2	2:T:89[A]:VAL:HG21	2.17	0.65
1:F:473:ASP:CB	2:J:20:TYR:OH	2.44	0.65
1:H:465:ILE:HD12	2:S:24:ARG:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:HD3	2:T:2:ASN:ND2	2.13	0.64
1:E:385:TRP:NE1	1:E:463:LYS:CA	2.60	0.64
1:A:409:HIS:NE2	1:A:419:ALA:HB2	2.13	0.64
1:B:167:ARG:CD	1:B:428:VAL:CG2	2.71	0.64
1:B:385:TRP:NE1	1:B:463:LYS:CA	2.59	0.64
1:C:409:HIS:NE2	1:C:419:ALA:HB2	2.13	0.64
1:D:45:GLN:HB3	2:P:3:LEU:CD1	2.27	0.64
1:D:46:PRO:HG3	2:O:80:GLU:CG	0.28	0.64
1:D:49:PRO:HD2	2:O:29[A]:GLN:NE2	2.12	0.64
1:D:410:PRO:CA	1:E:15:ALA:HB3	2.26	0.64
2:W:85:LEU:HD23	2:W:88:MET:HE3	1.78	0.64
1:B:14:LYS:HE3	1:B:14:LYS:O	1.98	0.64
1:B:409:HIS:NE2	1:B:419:ALA:HB2	2.13	0.64
1:C:19:ASP:HB2	2:M:33:THR:N	2.12	0.64
1:G:14:LYS:HE3	1:G:14:LYS:O	1.98	0.64
1:H:409:HIS:NE2	1:H:419:ALA:HB2	2.13	0.64
2:M:14:LEU:CD2	2:N:89[A]:VAL:HG21	2.17	0.64
2:Q:85:LEU:HD23	2:Q:88:MET:HE3	1.78	0.64
1:B:410:PRO:CA	1:C:15:ALA:HB3	2.26	0.64
1:H:21:LYS:NZ	2:W:33:THR:OG1	2.29	0.64
1:H:14:LYS:O	1:H:14:LYS:HE3	1.98	0.64
1:D:14:LYS:O	1:D:14:LYS:HE3	1.98	0.64
1:H:465:ILE:CG1	2:S:24:ARG:CB	2.75	0.64
2:I:74:ARG:HG2	2:I:75:GLU:N	2.13	0.64
2:O:74:ARG:HG2	2:O:75:GLU:N	2.13	0.64
1:A:14:LYS:O	1:A:14:LYS:HE3	1.98	0.64
1:B:391:VAL:HG13	1:B:437:LEU:HD12	1.73	0.64
2:I:85:LEU:HD23	2:I:88:MET:HE3	1.79	0.64
2:M:74:ARG:HG2	2:M:75:GLU:N	2.13	0.64
1:E:409:HIS:NE2	1:E:419:ALA:HB2	2.13	0.64
1:H:167:ARG:CD	1:H:428:VAL:CG2	2.71	0.64
2:O:85:LEU:HD23	2:O:88:MET:HE3	1.79	0.64
2:S:74:ARG:HG2	2:S:75:GLU:N	2.13	0.64
1:C:14:LYS:O	1:C:14:LYS:HE3	1.98	0.64
1:E:46:PRO:C	2:K:76:HIS:CG	2.72	0.64
1:F:409:HIS:NE2	1:F:419:ALA:HB2	2.13	0.64
1:C:52:GLU:CD	2:M:29[B]:GLN:OE1	2.37	0.63
1:C:385:TRP:NE1	1:C:463:LYS:CA	2.59	0.63
1:D:45:GLN:O	2:P:1:MET:HE1	1.98	0.63
1:D:46:PRO:CG	2:O:80:GLU:CG	0.90	0.63
1:F:52:GLU:HB3	2:U:29[B]:GLN:NE2	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:HIS:NE2	1:D:419:ALA:HB2	2.13	0.63
1:E:14:LYS:O	1:E:14:LYS:HE3	1.98	0.63
1:E:45:GLN:C	2:L:1:MET:CE	2.67	0.63
1:F:14:LYS:O	1:F:14:LYS:HE3	1.98	0.63
1:H:170:LEU:CD1	1:H:424:LEU:CD2	2.29	0.63
2:M:85:LEU:HD23	2:M:88:MET:HE3	1.80	0.63
2:U:14:LEU:CD2	2:V:89[A]:VAL:HG21	2.17	0.63
1:A:385:TRP:NE1	1:A:463:LYS:CA	2.59	0.63
1:A:409:HIS:CD2	1:A:419:ALA:HB2	2.34	0.63
1:F:392:GLU:HB3	1:F:438:TYR:HD1	1.64	0.63
1:H:465:ILE:HG13	2:S:24:ARG:CB	2.28	0.63
1:C:409:HIS:CD2	1:C:419:ALA:HB2	2.34	0.63
1:E:392:GLU:HB3	1:E:438:TYR:HD1	1.64	0.63
1:H:391:VAL:HG13	1:H:437:LEU:HD12	1.73	0.63
1:D:278:THR:O	1:D:282:LYS:HG2	1.99	0.63
1:E:465:ILE:HG13	2:O:24:ARG:CB	2.28	0.63
1:E:469:PHE:HD2	1:E:470:GLU:C	2.02	0.63
1:G:167:ARG:CG	1:G:428:VAL:HG21	1.85	0.63
1:G:278:THR:O	1:G:282:LYS:HG2	1.99	0.63
1:G:409:HIS:NE2	1:G:419:ALA:HB2	2.13	0.63
2:K:74:ARG:HG2	2:K:75:GLU:N	2.13	0.63
2:O:14:LEU:CD2	2:P:89[A]:VAL:HG21	2.17	0.63
1:B:45:GLN:O	2:R:1:MET:HE1	1.89	0.63
1:C:469:PHE:HD2	1:C:470:GLU:C	2.02	0.63
1:D:409:HIS:CD2	1:D:458:ALA:HB2	2.34	0.63
1:F:469:PHE:HD2	1:F:470:GLU:C	2.02	0.63
1:G:409:HIS:CD2	1:G:458:ALA:HB2	2.34	0.63
1:H:21:LYS:HZ2	2:W:33:THR:HG21	0.93	0.63
2:U:74:ARG:HG2	2:U:75:GLU:N	2.13	0.63
1:A:392:GLU:HB3	1:A:438:TYR:HD1	1.64	0.63
1:A:469:PHE:HD2	1:A:470:GLU:C	2.02	0.63
1:B:46:PRO:HB2	2:Q:76:HIS:O	1.98	0.63
1:B:47:GLY:H	2:Q:76:HIS:CG	2.16	0.63
2:K:14:LEU:CD2	2:L:89[A]:VAL:HG21	2.17	0.63
1:C:392:GLU:HB3	1:C:438:TYR:HD1	1.64	0.63
1:B:167:ARG:HG3	1:B:428:VAL:HG22	0.64	0.62
1:B:409:HIS:HB2	1:B:416:GLY:CA	2.27	0.62
1:B:409:HIS:CD2	1:B:419:ALA:HB2	2.34	0.62
1:E:409:HIS:CD2	1:E:419:ALA:HB2	2.34	0.62
1:F:465:ILE:HG13	2:I:24:ARG:CB	2.29	0.62
1:H:409:HIS:CD2	1:H:458:ALA:HB2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ILE:HG13	2:W:24:ARG:HB2	1.81	0.62
1:B:48:VAL:HG23	2:R:1:MET:CB	2.29	0.62
1:B:278:THR:O	1:B:282:LYS:HG2	1.99	0.62
1:B:469:PHE:HD2	1:B:470:GLU:C	2.02	0.62
1:G:469:PHE:HD2	1:G:470:GLU:C	2.02	0.62
1:H:278:THR:O	1:H:282:LYS:HG2	1.99	0.62
1:H:469:PHE:HD2	1:H:470:GLU:C	2.02	0.62
2:I:14:LEU:CD2	2:J:89[A]:VAL:HG21	2.17	0.62
1:A:167:ARG:HG3	1:A:428:VAL:HG22	0.64	0.62
1:B:409:HIS:CD2	1:B:458:ALA:HB2	2.34	0.62
1:H:409:HIS:CD2	1:H:419:ALA:HB2	2.34	0.62
2:W:74:ARG:HG2	2:W:75:GLU:N	2.13	0.62
1:D:469:PHE:HD2	1:D:470:GLU:C	2.02	0.62
1:F:409:HIS:CD2	1:F:458:ALA:HB2	2.34	0.62
1:F:409:HIS:CD2	1:F:419:ALA:HB2	2.34	0.62
1:H:409:HIS:HB2	1:H:416:GLY:CA	2.27	0.62
1:C:167:ARG:HG3	1:C:428:VAL:HG22	0.64	0.62
1:D:167:ARG:HG3	1:D:428:VAL:HG22	0.64	0.62
1:D:167:ARG:HB2	1:D:428:VAL:HG22	1.77	0.62
1:G:19:ASP:HB2	2:I:33:THR:HG23	1.81	0.62
1:G:170:LEU:HD13	1:G:424:LEU:HB2	1.72	0.62
1:H:167:ARG:HG3	1:H:428:VAL:HG22	0.64	0.62
1:A:48:VAL:HG23	2:T:1:MET:HG3	1.81	0.62
1:E:19:ASP:CB	2:K:33:THR:CG2	2.75	0.62
1:E:47:GLY:N	2:K:76:HIS:CE1	2.64	0.62
1:E:409:HIS:CD2	1:E:458:ALA:HB2	2.34	0.62
1:H:46:PRO:CB	2:W:76:HIS:O	2.48	0.62
2:Q:74:ARG:HG2	2:Q:75:GLU:N	2.13	0.62
1:A:18:LYS:HB3	2:S:32:GLU:CA	2.04	0.62
1:A:48:VAL:HG23	2:T:1:MET:CG	2.30	0.62
1:C:409:HIS:CD2	1:C:458:ALA:HB2	2.34	0.62
1:G:409:HIS:HB2	1:G:416:GLY:CA	2.27	0.62
1:B:22:LEU:HD13	2:Q:35:PRO:HD3	1.81	0.62
1:D:167:ARG:CD	1:D:428:VAL:CG2	2.71	0.62
1:F:45:GLN:O	2:V:1:MET:HE1	1.99	0.62
1:G:167:ARG:HG3	1:G:428:VAL:HG22	0.64	0.62
1:G:167:ARG:CD	1:G:428:VAL:CG2	2.71	0.62
1:A:48:VAL:CG2	2:T:1:MET:HG3	2.30	0.62
1:F:52:GLU:OE2	2:U:32:GLU:OE2	2.18	0.62
1:F:167:ARG:HG3	1:F:428:VAL:HG22	0.64	0.62
1:G:167:ARG:HB2	1:G:428:VAL:HG22	1.77	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:GLU:CB	1:B:438:TYR:CD1	2.49	0.62
1:D:19:ASP:HB2	2:O:33:THR:HG23	1.81	0.62
1:E:167:ARG:HG3	1:E:428:VAL:HG22	0.64	0.62
1:A:409:HIS:CD2	1:A:458:ALA:HB2	2.34	0.61
1:B:128:LYS:HD3	2:R:2:ASN:ND2	2.15	0.61
1:B:392:GLU:HB3	1:B:438:TYR:HD1	1.64	0.61
1:C:278:THR:O	1:C:282:LYS:HG2	1.99	0.61
1:D:170:LEU:HD13	1:D:424:LEU:HB2	1.72	0.61
1:A:278:THR:O	1:A:282:LYS:HG2	1.99	0.61
1:A:410:PRO:CA	1:H:15:ALA:HB3	2.29	0.61
1:B:48:VAL:HG23	2:R:1:MET:HG3	1.82	0.61
1:D:19:ASP:OD1	2:O:28:ALA:O	2.18	0.61
1:D:409:HIS:HB2	1:D:416:GLY:CA	2.28	0.61
1:E:19:ASP:OD2	2:K:33:THR:HG23	2.00	0.61
1:E:278:THR:O	1:E:282:LYS:HG2	1.99	0.61
1:D:167:ARG:CG	1:D:428:VAL:HG21	1.85	0.61
1:D:409:HIS:CD2	1:D:419:ALA:HB2	2.34	0.61
1:F:473:ASP:HB3	2:J:20:TYR:OH	2.01	0.61
1:G:49:PRO:HD3	2:I:29[A]:GLN:NE2	2.15	0.61
1:H:45:GLN:OE1	2:X:3:LEU:HD11	1.97	0.61
1:A:19:ASP:CB	2:S:33:THR:HG23	2.30	0.61
1:B:19:ASP:OD1	2:Q:28:ALA:C	2.38	0.61
1:F:45:GLN:C	2:V:1:MET:HE2	2.20	0.61
1:F:278:THR:O	1:F:282:LYS:HG2	1.99	0.61
1:C:465:ILE:CG1	2:Q:24:ARG:CB	2.75	0.61
1:B:465:ILE:HD12	2:M:24:ARG:HB3	0.66	0.61
1:G:409:HIS:CD2	1:G:419:ALA:HB2	2.34	0.61
1:H:19:ASP:HB2	2:W:33:THR:CG2	2.30	0.61
1:B:45:GLN:HB3	2:R:3:LEU:CD1	2.30	0.61
1:D:46:PRO:HG2	2:O:80:GLU:CB	2.02	0.61
1:E:19:ASP:HB2	2:K:32:GLU:C	2.18	0.61
1:D:18:LYS:HA	2:O:32:GLU:N	2.15	0.60
1:F:45:GLN:O	2:V:1:MET:HE2	2.00	0.60
1:G:45:GLN:CD	2:J:3:LEU:CD1	2.57	0.60
1:C:52:GLU:OE2	2:M:29[B]:GLN:OE1	2.19	0.60
2:O:63:LYS:HG2	2:O:66:LEU:HD22	1.83	0.60
1:G:47:GLY:N	2:I:76:HIS:CE1	2.68	0.60
1:G:52:GLU:OE2	2:I:29[B]:GLN:OE1	2.18	0.60
2:I:63:LYS:HG2	2:I:66:LEU:HD22	1.83	0.60
1:G:52:GLU:HB2	2:I:29[B]:GLN:NE2	2.12	0.60
2:Q:63:LYS:HG2	2:Q:66:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HD21	1:E:146:LYS:HD2	1.84	0.60
2:W:63:LYS:HG2	2:W:66:LEU:HD22	1.83	0.60
1:A:22:LEU:CD1	2:S:35:PRO:HD3	2.32	0.60
1:C:392:GLU:HB2	1:C:438:TYR:CD1	2.37	0.60
2:S:63:LYS:HG2	2:S:66:LEU:HD22	1.83	0.60
1:B:47:GLY:N	2:Q:76:HIS:CG	2.70	0.59
1:D:392:GLU:HB3	1:D:438:TYR:HD1	1.64	0.59
2:M:63:LYS:HG2	2:M:66:LEU:HD22	1.83	0.59
1:A:392:GLU:HB2	1:A:438:TYR:CD1	2.37	0.59
1:B:22:LEU:CD1	2:Q:35:PRO:HD3	2.33	0.59
1:G:392:GLU:HB3	1:G:438:TYR:HD1	1.64	0.59
1:G:465:ILE:HG22	2:U:20:TYR:CZ	2.36	0.59
2:U:63:LYS:HG2	2:U:66:LEU:HD22	1.83	0.59
1:A:53:ALA:HB1	1:A:130:ILE:HD11	1.85	0.59
1:D:53:ALA:HB1	1:D:130:ILE:HD11	1.85	0.59
2:K:63:LYS:HG2	2:K:66:LEU:HD22	1.83	0.59
1:A:473:ASP:OD2	2:X:24:ARG:CZ	2.47	0.59
1:G:53:ALA:HB1	1:G:130:ILE:HD11	1.85	0.59
1:A:396:ASP:OD1	1:A:431:ARG:HD3	2.03	0.59
1:A:409:HIS:C	1:A:410:PRO:N	2.56	0.59
1:C:53:ALA:HB1	1:C:130:ILE:HD11	1.85	0.59
1:C:396:ASP:OD1	1:C:431:ARG:HD3	2.03	0.59
1:C:409:HIS:C	1:C:410:PRO:N	2.56	0.59
1:B:48:VAL:HG23	2:R:1:MET:CG	2.33	0.59
1:G:409:HIS:C	1:G:410:PRO:N	2.56	0.59
1:D:409:HIS:C	1:D:410:PRO:N	2.56	0.59
1:D:473:ASP:CB	2:L:20:TYR:OH	2.51	0.59
1:F:392:GLU:HB2	1:F:438:TYR:CD1	2.37	0.59
1:G:46:PRO:CB	2:I:76:HIS:O	2.51	0.58
1:B:53:ALA:HB1	1:B:130:ILE:HD11	1.85	0.58
1:D:48:VAL:HG23	2:P:1:MET:HB2	1.84	0.58
1:E:396:ASP:OD1	1:E:431:ARG:HD3	2.03	0.58
1:H:53:ALA:HB1	1:H:130:ILE:HD11	1.85	0.58
2:L:23:LEU:O	2:L:27:LEU:HB2	2.04	0.58
2:V:23:LEU:O	2:V:27:LEU:HB2	2.04	0.58
1:B:19:ASP:HB2	2:Q:33:THR:H	1.67	0.58
1:B:473:ASP:OD2	2:N:24:ARG:CZ	2.48	0.58
1:E:53:ALA:HB1	1:E:130:ILE:HD11	1.85	0.58
1:F:53:ALA:HB1	1:F:130:ILE:HD11	1.85	0.58
1:G:465:ILE:HD12	2:U:24:ARG:HG2	1.83	0.58
1:E:392:GLU:HB2	1:E:438:TYR:CD1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:396:ASP:OD1	1:F:431:ARG:HD3	2.03	0.58
1:E:409:HIS:C	1:E:410:PRO:N	2.56	0.58
1:F:146:LYS:HD2	1:H:105:LEU:HD21	1.85	0.58
2:J:23:LEU:O	2:J:27:LEU:HB2	2.04	0.58
1:A:15:ALA:HB2	1:H:410:PRO:CA	2.33	0.58
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.87	0.58
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.87	0.58
1:B:409:HIS:C	1:B:410:PRO:N	2.56	0.58
2:P:23:LEU:O	2:P:27:LEU:HB2	2.04	0.58
2:R:23:LEU:O	2:R:27:LEU:HB2	2.04	0.58
1:D:52:GLU:HB3	2:O:29[B]:GLN:NE2	2.15	0.58
1:H:20:TYR:H	2:W:32:GLU:CD	2.02	0.58
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.87	0.58
1:H:409:HIS:C	1:H:410:PRO:N	2.56	0.58
2:N:23:LEU:O	2:N:27:LEU:HB2	2.04	0.58
2:X:23:LEU:O	2:X:27:LEU:HB2	2.04	0.58
1:C:202:ASP:OD1	1:C:238:HIS:HE1	1.87	0.58
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.87	0.58
1:F:45:GLN:HB3	2:V:3:LEU:CD1	2.34	0.58
1:F:409:HIS:C	1:F:410:PRO:N	2.56	0.58
2:T:23:LEU:O	2:T:27:LEU:HB2	2.04	0.58
1:B:469:PHE:C	2:M:50:GLN:HA	2.24	0.58
1:F:202:ASP:OD1	1:F:238:HIS:HE1	1.87	0.58
1:F:409:HIS:CB	1:F:416:GLY:HA3	2.09	0.58
1:G:46:PRO:CB	2:I:76:HIS:CG	2.82	0.58
1:A:388:PRO:HG3	1:A:442:GLY:N	2.19	0.58
1:F:45:GLN:CD	2:V:3:LEU:CD1	2.45	0.58
1:G:18:LYS:HA	2:I:32:GLU:N	2.19	0.58
1:C:388:PRO:HG3	1:C:442:GLY:N	2.19	0.57
1:H:392:GLU:HB3	1:H:438:TYR:HD1	1.64	0.57
1:B:392:GLU:HB2	1:B:438:TYR:CD1	2.37	0.57
1:C:19:ASP:CG	2:M:33:THR:HG23	2.25	0.57
1:D:202:ASP:OD1	1:D:238:HIS:HE1	1.87	0.57
1:H:396:ASP:OD1	1:H:431:ARG:HD3	2.03	0.57
2:K:90:VAL:O	2:K:94:GLN:HG3	2.04	0.57
2:U:90:VAL:O	2:U:94:GLN:HG3	2.04	0.57
1:B:48:VAL:CG2	2:R:1:MET:HG3	2.35	0.57
1:B:410:PRO:CA	1:C:15:ALA:HB2	2.33	0.57
1:D:18:LYS:HG2	2:O:31:GLY:O	2.04	0.57
1:E:21:LYS:HZ1	2:K:33:THR:CB	1.83	0.57
1:E:21:LYS:CD	2:K:33:THR:HG21	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:202:ASP:OD1	1:G:238:HIS:HE1	1.87	0.57
2:I:90:VAL:O	2:I:94:GLN:HG3	2.04	0.57
1:B:167:ARG:HB2	1:B:428:VAL:HG22	1.77	0.57
1:E:52:GLU:CG	2:K:29[B]:GLN:OE1	2.52	0.57
1:F:167:ARG:HB2	1:F:428:VAL:HG22	1.78	0.57
2:O:90:VAL:O	2:O:94:GLN:HG3	2.04	0.57
1:H:392:GLU:HB2	1:H:438:TYR:CD1	2.37	0.57
2:P:69:ARG:O	2:P:73:VAL:HG23	2.05	0.57
2:Q:90:VAL:O	2:Q:94:GLN:HG3	2.04	0.57
1:B:396:ASP:OD1	1:B:431:ARG:HD3	2.03	0.57
1:D:442:GLY:O	1:D:446:ARG:HD3	2.05	0.57
1:G:388:PRO:HG3	1:G:442:GLY:N	2.19	0.57
1:G:442:GLY:O	1:G:446:ARG:HD3	2.05	0.57
1:H:48:VAL:HG23	2:X:1:MET:HE2	1.85	0.57
2:J:69:ARG:O	2:J:73:VAL:HG23	2.05	0.57
2:W:90:VAL:O	2:W:94:GLN:HG3	2.04	0.57
1:D:388:PRO:HG3	1:D:442:GLY:N	2.19	0.57
1:E:465:ILE:HG22	2:O:20:TYR:CZ	2.40	0.57
1:G:392:GLU:HB2	1:G:438:TYR:CD1	2.37	0.57
2:R:75:GLU:O	2:R:79:GLU:HG3	2.05	0.57
2:X:75:GLU:O	2:X:79:GLU:HG3	2.05	0.57
1:C:465:ILE:HD12	2:Q:24:ARG:HG2	1.83	0.57
1:E:388:PRO:HG3	1:E:442:GLY:N	2.19	0.57
1:F:388:PRO:HG3	1:F:442:GLY:N	2.19	0.57
1:G:46:PRO:HD2	2:J:3:LEU:HD11	1.86	0.57
2:L:69:ARG:O	2:L:73:VAL:HG23	2.05	0.57
2:R:69:ARG:O	2:R:73:VAL:HG23	2.05	0.57
2:X:69:ARG:O	2:X:73:VAL:HG23	2.05	0.57
1:D:392:GLU:HB2	1:D:438:TYR:CD1	2.37	0.57
1:H:167:ARG:HB2	1:H:428:VAL:HG22	1.78	0.57
1:H:388:PRO:HG3	1:H:442:GLY:N	2.19	0.57
1:H:442:GLY:O	1:H:446:ARG:HD3	2.05	0.57
2:L:75:GLU:O	2:L:79:GLU:HG3	2.05	0.57
2:V:69:ARG:O	2:V:73:VAL:HG23	2.05	0.57
1:B:442:GLY:O	1:B:446:ARG:HD3	2.05	0.57
1:D:396:ASP:OD1	1:D:431:ARG:HD3	2.03	0.57
2:M:90:VAL:O	2:M:94:GLN:HG3	2.04	0.57
2:S:90:VAL:O	2:S:94:GLN:HG3	2.04	0.57
2:V:75:GLU:O	2:V:79:GLU:HG3	2.05	0.57
1:B:388:PRO:HG3	1:B:442:GLY:N	2.19	0.56
1:F:19:ASP:HB2	2:U:32:GLU:C	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:LEU:CD2	2:K:33:THR:HB	2.34	0.56
1:E:409:HIS:HB2	1:E:416:GLY:CA	2.27	0.56
1:F:442:GLY:O	1:F:446:ARG:HD3	2.05	0.56
1:G:46:PRO:C	2:I:76:HIS:CG	2.77	0.56
2:M:14:LEU:HD23	2:N:89[A]:VAL:CG2	2.20	0.56
2:P:75:GLU:O	2:P:79:GLU:HG3	2.05	0.56
1:A:45:GLN:CB	2:T:3:LEU:HD11	2.33	0.56
1:D:409:HIS:HE2	1:D:454:GLU:C	2.06	0.56
1:E:167:ARG:HB2	1:E:428:VAL:HG22	1.78	0.56
1:E:442:GLY:O	1:E:446:ARG:HD3	2.05	0.56
1:G:396:ASP:OD1	1:G:431:ARG:HD3	2.03	0.56
1:G:409:HIS:HE2	1:G:454:GLU:C	2.06	0.56
2:J:75:GLU:O	2:J:79:GLU:HG3	2.05	0.56
2:N:75:GLU:O	2:N:79:GLU:HG3	2.05	0.56
2:T:69:ARG:O	2:T:73:VAL:HG23	2.05	0.56
1:A:46:PRO:HB2	2:S:76:HIS:C	2.25	0.56
1:F:409:HIS:HB2	1:F:416:GLY:CA	2.27	0.56
1:G:21:LYS:HZ3	2:I:33:THR:HB	1.64	0.56
1:H:469:PHE:O	1:H:470:GLU:N	2.39	0.56
2:T:75:GLU:O	2:T:79:GLU:HG3	2.05	0.56
1:A:409:HIS:HB2	1:A:416:GLY:CA	2.27	0.56
1:C:409:HIS:HE2	1:C:454:GLU:C	2.06	0.56
1:G:384:VAL:HG23	1:G:459:LEU:HD23	1.87	0.56
2:N:69:ARG:O	2:N:73:VAL:HG23	2.05	0.56
1:A:442:GLY:O	1:A:446:ARG:HD3	2.05	0.56
1:B:469:PHE:O	1:B:470:GLU:N	2.39	0.56
1:C:45:GLN:OE1	2:N:3:LEU:HD11	2.02	0.56
1:D:384:VAL:HG23	1:D:459:LEU:HD23	1.87	0.56
1:C:20:TYR:CA	2:M:32:GLU:OE1	2.53	0.56
1:C:442:GLY:O	1:C:446:ARG:HD3	2.05	0.56
1:D:46:PRO:CG	2:O:80:GLU:HG3	0.20	0.56
1:A:19:ASP:HB2	2:S:33:THR:H	1.68	0.56
1:F:48:VAL:HG23	2:V:1:MET:HB2	1.86	0.56
1:C:21:LYS:HZ2	2:M:33:THR:HB	1.70	0.56
1:E:18:LYS:HA	2:K:31:GLY:O	2.04	0.56
1:H:170:LEU:HD13	1:H:424:LEU:HB2	1.72	0.56
1:H:392:GLU:HB2	1:H:438:TYR:CA	2.37	0.56
1:B:392:GLU:HB2	1:B:438:TYR:CA	2.37	0.55
1:C:52:GLU:CB	2:M:29[B]:GLN:NE2	2.55	0.55
1:D:469:PHE:O	1:D:470:GLU:N	2.39	0.55
1:F:15:ALA:HB2	1:G:410:PRO:CA	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:ASP:HB2	2:U:33:THR:HG23	1.87	0.55
1:A:46:PRO:HD2	2:T:3:LEU:CD1	2.34	0.55
1:A:409:HIS:HE2	1:A:454:GLU:C	2.06	0.55
1:C:469:PHE:O	1:C:470:GLU:N	2.39	0.55
1:E:49:PRO:CD	2:K:29[A]:GLN:NE2	2.69	0.55
1:F:19:ASP:HB3	2:U:33:THR:HG23	1.85	0.55
1:G:469:PHE:O	1:G:470:GLU:N	2.39	0.55
1:H:409:HIS:HE2	1:H:454:GLU:C	2.06	0.55
1:B:146:LYS:HD2	1:E:105:LEU:HD21	1.88	0.55
1:D:473:ASP:HB3	2:L:20:TYR:OH	2.06	0.55
2:N:90:VAL:O	2:N:94:GLN:HG3	2.07	0.55
1:C:384:VAL:HG23	1:C:459:LEU:HD23	1.87	0.55
1:D:105:LEU:HD21	1:G:146:LYS:HD2	1.89	0.55
1:D:392:GLU:HB2	1:D:438:TYR:CA	2.36	0.55
1:F:49:PRO:HD2	2:U:29[A]:GLN:HE21	1.72	0.55
1:G:392:GLU:HB2	1:G:438:TYR:CA	2.37	0.55
1:H:170:LEU:CD2	1:H:424:LEU:HD13	2.34	0.55
2:J:90:VAL:O	2:J:94:GLN:HG3	2.07	0.55
2:L:30:LEU:HD12	2:L:69:ARG:NH2	2.21	0.55
2:P:90:VAL:O	2:P:94:GLN:HG3	2.07	0.55
2:T:90:VAL:O	2:T:94:GLN:HG3	2.07	0.55
1:B:46:PRO:HD2	2:R:3:LEU:CD1	2.29	0.55
1:F:469:PHE:O	1:F:470:GLU:N	2.39	0.55
2:V:30:LEU:HD12	2:V:69:ARG:NH2	2.21	0.55
1:E:19:ASP:CG	2:K:33:THR:HG23	2.26	0.55
1:E:46:PRO:HB2	2:K:76:HIS:O	2.05	0.55
1:E:384:VAL:HG23	1:E:459:LEU:HD23	1.87	0.55
1:E:469:PHE:O	1:E:470:GLU:N	2.39	0.55
1:F:384:VAL:HG23	1:F:459:LEU:HD23	1.87	0.55
2:Q:14:LEU:HD23	2:R:89[A]:VAL:CG2	2.20	0.55
1:B:170:LEU:CD2	1:B:424:LEU:HD13	2.34	0.55
1:C:19:ASP:OD2	2:M:33:THR:HG23	2.06	0.55
1:F:473:ASP:HB2	2:J:20:TYR:OH	2.07	0.55
1:G:46:PRO:CA	2:I:76:HIS:ND1	2.54	0.55
1:B:409:HIS:HE2	1:B:454:GLU:C	2.06	0.55
1:G:47:GLY:H	2:I:76:HIS:CE1	2.11	0.55
2:L:90:VAL:O	2:L:94:GLN:HG3	2.07	0.55
2:X:30:LEU:HD12	2:X:69:ARG:NH2	2.21	0.55
1:A:19:ASP:HB2	2:S:32:GLU:C	2.18	0.55
1:A:384:VAL:HG23	1:A:459:LEU:HD23	1.88	0.55
1:B:170:LEU:HD13	1:B:424:LEU:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:392:GLU:HB2	1:F:438:TYR:CA	2.36	0.55
1:H:19:ASP:HB3	2:W:33:THR:HG23	1.83	0.55
1:H:21:LYS:HG2	2:W:33:THR:CG2	2.37	0.55
2:R:30:LEU:HD12	2:R:69:ARG:NH2	2.21	0.55
2:V:90:VAL:O	2:V:94:GLN:HG3	2.07	0.55
1:A:128:LYS:HD3	2:T:2:ASN:HD21	1.72	0.55
1:E:392:GLU:HB2	1:E:438:TYR:CA	2.37	0.55
1:F:105:LEU:HD21	1:H:146:LYS:HD2	1.89	0.55
2:X:90:VAL:O	2:X:94:GLN:HG3	2.07	0.55
2:P:30:LEU:HD12	2:P:69:ARG:NH2	2.21	0.54
2:R:90:VAL:O	2:R:94:GLN:HG3	2.07	0.54
2:W:14:LEU:HD23	2:X:89[A]:VAL:CG2	2.20	0.54
1:A:410:PRO:CA	1:H:15:ALA:HB2	2.37	0.54
1:H:19:ASP:N	2:W:32:GLU:N	2.19	0.54
2:J:30:LEU:HD12	2:J:69:ARG:NH2	2.21	0.54
1:A:406:THR:OG1	1:A:420:ASN:OD1	2.24	0.54
1:C:465:ILE:HG13	2:Q:24:ARG:HB3	1.86	0.54
1:E:52:GLU:OE2	2:K:29[B]:GLN:OE1	2.25	0.54
1:A:469:PHE:O	1:A:470:GLU:N	2.39	0.54
1:F:18:LYS:HA	2:U:32:GLU:N	2.21	0.54
1:G:49:PRO:HD2	2:I:29[A]:GLN:NE2	2.23	0.54
1:A:167:ARG:HB2	1:A:428:VAL:HG22	1.78	0.54
1:A:473:ASP:CB	2:X:20:TYR:OH	2.54	0.54
1:B:384:VAL:HG23	1:B:459:LEU:HD23	1.87	0.54
1:B:391:VAL:CG1	1:B:437:LEU:HB2	2.38	0.54
1:C:406:THR:OG1	1:C:420:ASN:OD1	2.24	0.54
1:E:170:LEU:HD13	1:E:424:LEU:HB2	1.72	0.54
1:E:409:HIS:HE2	1:E:454:GLU:C	2.06	0.54
1:F:22:LEU:HD11	2:U:34:ASN:N	2.22	0.54
1:H:391:VAL:CG1	1:H:437:LEU:HB2	2.38	0.54
1:B:15:ALA:HB2	1:C:410:PRO:CA	2.37	0.54
1:F:409:HIS:HE2	1:F:454:GLU:C	2.06	0.54
1:G:49:PRO:HD3	2:I:29[A]:GLN:HE22	1.72	0.54
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.91	0.54
1:E:170:LEU:CG	1:E:424:LEU:CD1	2.50	0.54
1:E:391:VAL:CG1	1:E:437:LEU:HB2	2.38	0.54
1:F:391:VAL:CG1	1:F:437:LEU:HB2	2.38	0.54
1:G:19:ASP:HB2	2:I:32:GLU:C	2.27	0.54
2:T:30:LEU:HD12	2:T:69:ARG:NH2	2.21	0.54
1:C:167:ARG:HB2	1:C:428:VAL:HG22	1.78	0.54
1:E:170:LEU:CG	1:E:424:LEU:HD22	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:LEU:HD13	1:F:424:LEU:HB2	1.72	0.54
2:N:30:LEU:HD12	2:N:69:ARG:NH2	2.21	0.54
1:A:48:VAL:HG22	2:T:1:MET:N	2.23	0.54
1:B:19:ASP:HB3	2:Q:33:THR:HG23	1.89	0.54
1:A:392:GLU:HB2	1:A:438:TYR:CA	2.36	0.54
1:D:410:PRO:CA	1:E:15:ALA:HB2	2.36	0.54
1:F:170:LEU:CG	1:F:424:LEU:HD22	2.36	0.54
1:F:200:THR:OG1	1:F:238:HIS:HD2	1.91	0.54
1:B:49:PRO:HG2	2:Q:29[B]:GLN:HE21	1.72	0.53
1:C:392:GLU:HB2	1:C:438:TYR:CA	2.37	0.53
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.91	0.53
1:H:19:ASP:CB	2:W:33:THR:CG2	2.78	0.53
1:H:200:THR:OG1	1:H:238:HIS:HD2	1.91	0.53
1:C:464:GLU:O	2:Q:24:ARG:NH2	2.41	0.53
1:C:466:LYS:C	2:Q:20:TYR:OH	2.47	0.53
1:F:46:PRO:CA	2:U:76:HIS:ND1	2.59	0.53
1:D:170:LEU:HD12	1:D:424:LEU:CB	2.09	0.53
1:H:464:GLU:O	2:S:24:ARG:NH2	2.41	0.53
1:G:52:GLU:CG	2:I:29[B]:GLN:CD	2.52	0.53
1:A:170:LEU:CG	1:A:424:LEU:HD22	2.35	0.53
1:G:170:LEU:HD12	1:G:424:LEU:CB	2.09	0.53
1:H:21:LYS:HZ2	2:W:33:THR:HB	1.69	0.53
1:F:18:LYS:HG2	2:U:31:GLY:O	2.08	0.53
1:G:200:THR:OG1	1:G:238:HIS:HD2	1.91	0.53
1:B:48:VAL:HG22	2:R:1:MET:N	2.24	0.53
1:D:18:LYS:CA	2:O:32:GLU:N	2.71	0.53
1:D:22:LEU:HD11	2:O:34:ASN:N	2.23	0.53
1:B:18:LYS:HA	2:Q:31:GLY:O	2.09	0.53
1:C:170:LEU:HD13	1:C:424:LEU:HB2	1.72	0.53
1:C:391:VAL:CG1	1:C:437:LEU:HB2	2.38	0.53
1:D:200:THR:OG1	1:D:238:HIS:HD2	1.91	0.53
1:F:410:PRO:CA	1:G:15:ALA:HB2	2.35	0.53
1:A:200:THR:OG1	1:A:238:HIS:HD2	1.91	0.53
1:A:391:VAL:CG1	1:A:437:LEU:HB2	2.38	0.53
1:D:46:PRO:C	2:O:76:HIS:CG	2.82	0.53
1:E:170:LEU:CD2	1:E:424:LEU:HD13	2.34	0.53
1:A:49:PRO:HG2	2:S:29[B]:GLN:HE21	1.73	0.53
1:A:170:LEU:HD13	1:A:424:LEU:HB2	1.72	0.53
1:C:409:HIS:HB2	1:C:416:GLY:CA	2.27	0.53
1:G:21:LYS:HZ1	2:I:33:THR:CG2	2.07	0.53
1:C:170:LEU:CG	1:C:424:LEU:HD22	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:THR:OG1	1:C:238:HIS:HD2	1.91	0.52
1:D:52:GLU:OE2	2:O:32:GLU:OE2	2.26	0.52
1:C:45:GLN:CD	2:N:3:LEU:CD1	2.70	0.52
1:F:46:PRO:HB3	2:U:76:HIS:O	2.09	0.52
1:H:384:VAL:HG23	1:H:459:LEU:HD23	1.88	0.52
1:A:15:ALA:CB	1:H:410:PRO:N	2.72	0.52
1:E:465:ILE:HD12	2:O:24:ARG:HG2	1.88	0.52
1:H:465:ILE:HG22	2:S:20:TYR:CE2	2.44	0.52
1:A:146:LYS:HD2	1:C:105:LEU:HD21	1.92	0.52
1:E:19:ASP:HB2	2:K:33:THR:CG2	2.38	0.52
1:F:170:LEU:CD2	1:F:424:LEU:HD13	2.34	0.52
1:G:45:GLN:O	2:J:1:MET:CE	2.56	0.52
1:H:52:GLU:CG	2:W:29[B]:GLN:CD	2.64	0.52
1:D:15:ALA:HB2	1:E:410:PRO:CA	2.35	0.52
1:D:19:ASP:HB3	2:O:33:THR:HG23	1.90	0.52
1:E:406:THR:CA	1:E:420:ASN:OD1	2.57	0.52
1:B:48:VAL:N	2:R:1:MET:HG3	2.24	0.52
1:D:47:GLY:N	2:O:76:HIS:CE1	2.77	0.52
1:F:15:ALA:CB	1:G:410:PRO:N	2.72	0.52
1:G:391:VAL:CG1	1:G:437:LEU:HB2	2.38	0.52
1:G:170:LEU:CG	1:G:424:LEU:HD22	2.36	0.52
1:F:22:LEU:HD13	2:U:35:PRO:HD3	1.91	0.52
1:F:406:THR:CA	1:F:420:ASN:OD1	2.57	0.52
1:C:21:LYS:NZ	2:M:33:THR:OG1	2.42	0.52
1:C:48:VAL:HG23	2:N:1:MET:HE2	1.92	0.52
1:D:391:VAL:CG1	1:D:437:LEU:HB2	2.38	0.52
1:E:473:ASP:CB	2:P:20:TYR:OH	2.58	0.52
1:H:383:HIS:H	1:H:386:HIS:CD2	2.23	0.52
1:D:170:LEU:CG	1:D:424:LEU:HD22	2.35	0.52
1:H:22:LEU:HD11	2:W:34:ASN:N	2.18	0.52
2:R:30:LEU:CD1	2:R:69:ARG:NH2	2.73	0.52
2:X:30:LEU:CD1	2:X:69:ARG:NH2	2.73	0.52
1:B:406:THR:CA	1:B:420:ASN:OD1	2.57	0.51
1:C:19:ASP:HB3	2:M:33:THR:HG23	1.79	0.51
1:G:19:ASP:OD1	2:I:28:ALA:O	2.28	0.51
1:G:406:THR:OG1	1:G:420:ASN:OD1	2.24	0.51
2:N:30:LEU:CD1	2:N:69:ARG:NH2	2.73	0.51
2:P:30:LEU:CD1	2:P:69:ARG:NH2	2.73	0.51
2:T:30:LEU:CD1	2:T:69:ARG:NH2	2.73	0.51
1:A:22:LEU:HD11	2:S:34:ASN:N	2.24	0.51
1:D:45:GLN:O	2:P:1:MET:HE2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:THR:OG1	1:D:420:ASN:OD1	2.24	0.51
1:G:45:GLN:O	2:J:1:MET:HE1	2.11	0.51
2:J:30:LEU:CD1	2:J:69:ARG:NH2	2.73	0.51
2:V:30:LEU:CD1	2:V:69:ARG:NH2	2.73	0.51
1:B:46:PRO:HB2	2:Q:76:HIS:C	2.30	0.51
1:B:383:HIS:H	1:B:386:HIS:CD2	2.23	0.51
1:C:465:ILE:CD1	2:Q:24:ARG:NH2	2.41	0.51
1:D:45:GLN:C	2:P:1:MET:HE2	2.30	0.51
2:L:30:LEU:CD1	2:L:69:ARG:NH2	2.73	0.51
2:T:24:ARG:CG	2:T:24:ARG:NH1	2.71	0.51
1:D:406:THR:CA	1:D:420:ASN:OD1	2.57	0.51
1:G:473:ASP:CB	2:V:20:TYR:OH	2.58	0.51
1:E:18:LYS:CA	2:K:32:GLU:N	2.70	0.51
1:A:406:THR:CA	1:A:420:ASN:OD1	2.57	0.51
1:D:146:LYS:HD2	1:G:105:LEU:HD21	1.93	0.51
1:H:406:THR:CA	1:H:420:ASN:OD1	2.56	0.51
1:C:21:LYS:HZ1	2:M:33:THR:CB	2.14	0.51
1:C:46:PRO:CB	2:M:76:HIS:O	2.56	0.51
1:C:229:GLN:HE21	1:C:236:LYS:H	1.59	0.51
1:E:46:PRO:C	2:K:76:HIS:CE1	2.76	0.51
1:G:406:THR:CA	1:G:420:ASN:OD1	2.57	0.51
1:H:465:ILE:HG13	2:S:24:ARG:HB3	1.91	0.51
1:B:48:VAL:HG22	2:R:1:MET:H1	1.76	0.51
1:C:170:LEU:CD2	1:C:424:LEU:HD13	2.34	0.51
1:D:383:HIS:H	1:D:386:HIS:CD2	2.23	0.51
1:E:45:GLN:CD	2:L:3:LEU:CD1	2.66	0.51
1:G:312:ARG:HB2	1:G:345:PHE:HB3	1.93	0.51
1:G:464:GLU:O	2:U:24:ARG:NH2	2.44	0.51
1:A:19:ASP:HB3	2:S:33:THR:HG23	1.91	0.51
1:A:48:VAL:N	2:T:1:MET:HG3	2.25	0.51
1:D:239:TYR:HB3	1:D:266:MET:HB3	1.93	0.51
1:E:45:GLN:HB3	2:L:3:LEU:HD11	1.93	0.51
1:F:21:LYS:HG2	2:U:33:THR:HG21	1.76	0.51
1:F:131:ARG:NE	2:U:80:GLU:OE1	2.33	0.51
1:G:239:TYR:HB3	1:G:266:MET:HB3	1.93	0.51
1:G:383:HIS:H	1:G:386:HIS:CD2	2.23	0.51
1:A:229:GLN:HE21	1:A:236:LYS:H	1.58	0.51
1:A:466:LYS:N	2:W:20:TYR:OH	2.40	0.51
1:B:410:PRO:N	1:C:15:ALA:CB	2.74	0.51
1:C:406:THR:CA	1:C:420:ASN:OD1	2.57	0.51
1:D:465:ILE:HG13	2:K:24:ARG:HB2	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:406:THR:OG1	1:H:420:ASN:OD1	2.24	0.51
1:C:21:LYS:CG	2:M:33:THR:HG22	2.34	0.50
1:D:312:ARG:HB2	1:D:345:PHE:HB3	1.93	0.50
1:D:465:ILE:HD12	2:K:24:ARG:CA	2.37	0.50
1:H:229:GLN:HE21	1:H:236:LYS:H	1.58	0.50
1:A:170:LEU:CD2	1:A:424:LEU:HD13	2.34	0.50
1:D:93:GLU:CD	1:D:305:ARG:HH22	2.15	0.50
1:E:49:PRO:HD3	2:K:29[A]:GLN:NE2	2.26	0.50
1:F:46:PRO:C	2:U:76:HIS:CG	2.84	0.50
1:G:46:PRO:C	2:I:76:HIS:ND1	2.62	0.50
1:H:93:GLU:CD	1:H:305:ARG:HH22	2.15	0.50
1:B:229:GLN:HE21	1:B:236:LYS:H	1.58	0.50
1:E:229:GLN:HE21	1:E:236:LYS:H	1.58	0.50
1:F:18:LYS:CA	2:U:32:GLU:N	2.73	0.50
1:F:312:ARG:HB2	1:F:345:PHE:HB3	1.93	0.50
1:G:93:GLU:CD	1:G:305:ARG:HH22	2.15	0.50
1:H:466:LYS:C	2:S:20:TYR:OH	2.45	0.50
1:B:93:GLU:CD	1:B:305:ARG:HH22	2.15	0.50
1:E:312:ARG:HB2	1:E:345:PHE:HB3	1.93	0.50
1:G:229:GLN:HE21	1:G:236:LYS:H	1.59	0.50
1:B:473:ASP:CB	2:N:20:TYR:OH	2.57	0.50
1:D:46:PRO:HB3	2:O:76:HIS:O	2.12	0.50
1:E:46:PRO:CB	2:K:76:HIS:O	2.60	0.50
2:M:85:LEU:HD23	2:M:88:MET:CE	2.42	0.50
1:B:170:LEU:CG	1:B:424:LEU:HD22	2.36	0.50
1:C:312:ARG:HB2	1:C:345:PHE:HB3	1.93	0.50
1:C:465:ILE:HG22	2:Q:20:TYR:OH	2.12	0.50
1:D:128:LYS:HD3	2:P:2:ASN:ND2	2.27	0.50
1:F:46:PRO:CB	2:U:76:HIS:CG	2.87	0.50
1:G:45:GLN:HB3	2:J:3:LEU:CD1	2.40	0.50
2:K:85:LEU:HD23	2:K:88:MET:CE	2.42	0.50
2:M:74:ARG:NH1	2:N:97:ASN:OD1	2.44	0.50
2:N:24:ARG:CG	2:N:24:ARG:NH1	2.71	0.50
2:U:85:LEU:HD23	2:U:88:MET:CE	2.42	0.50
1:A:239:TYR:HB3	1:A:266:MET:HB3	1.93	0.50
1:B:22:LEU:HD11	2:Q:34:ASN:N	2.26	0.50
1:B:239:TYR:HB3	1:B:266:MET:HB3	1.93	0.50
1:F:229:GLN:HE21	1:F:236:LYS:H	1.58	0.50
1:G:465:ILE:HG22	2:U:20:TYR:CE2	2.47	0.50
1:H:239:TYR:HB3	1:H:266:MET:HB3	1.93	0.50
2:K:71:MET:CE	2:L:100:LYS:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:74:ARG:NH1	2:X:97:ASN:OD1	2.44	0.50
1:A:105:LEU:HD21	1:C:146:LYS:HD2	1.94	0.50
1:A:312:ARG:HB2	1:A:345:PHE:HB3	1.93	0.50
1:A:391:VAL:HG13	1:A:437:LEU:HD12	1.73	0.50
1:G:19:ASP:HB3	2:I:33:THR:HG23	1.92	0.50
1:H:170:LEU:CG	1:H:424:LEU:HD22	2.36	0.50
2:S:74:ARG:NH1	2:T:97:ASN:OD1	2.44	0.50
1:B:312:ARG:HB2	1:B:345:PHE:HB3	1.93	0.50
1:D:47:GLY:H	2:O:76:HIS:CE1	2.17	0.50
1:D:229:GLN:HE21	1:D:236:LYS:H	1.59	0.50
2:M:71:MET:CE	2:N:100:LYS:HB2	2.41	0.50
2:Q:74:ARG:NH1	2:R:97:ASN:OD1	2.44	0.50
2:U:71:MET:CE	2:V:100:LYS:HB2	2.41	0.50
1:D:21:LYS:HG2	2:O:33:THR:HG21	1.86	0.49
1:G:170:LEU:CD2	1:G:424:LEU:HD13	2.34	0.49
1:H:312:ARG:HB2	1:H:345:PHE:HB3	1.93	0.49
2:S:71:MET:CE	2:T:100:LYS:HB2	2.41	0.49
1:B:406:THR:HG1	1:B:420:ASN:CG	2.14	0.49
1:C:45:GLN:O	2:M:76:HIS:CE1	2.66	0.49
1:C:239:TYR:HB3	1:C:266:MET:HB3	1.93	0.49
1:F:128:LYS:HD3	2:V:2:ASN:ND2	2.27	0.49
2:Q:85:LEU:HD23	2:Q:88:MET:CE	2.42	0.49
1:F:93:GLU:CD	1:F:305:ARG:HH22	2.15	0.49
2:W:85:LEU:HD23	2:W:88:MET:CE	2.42	0.49
1:C:134:ARG:HA	1:C:308:GLY:O	2.13	0.49
1:E:22:LEU:HD11	2:K:34:ASN:N	2.27	0.49
2:K:74:ARG:NH1	2:L:97:ASN:OD1	2.44	0.49
2:Q:100:LYS:HG2	2:R:56:ILE:HG22	1.94	0.49
2:U:71:MET:HA	2:U:74:ARG:HD2	1.94	0.49
2:W:100:LYS:HG2	2:X:56:ILE:HG22	1.94	0.49
1:A:134:ARG:HA	1:A:308:GLY:O	2.13	0.49
1:D:170:LEU:CD2	1:D:424:LEU:HD13	2.34	0.49
1:E:93:GLU:CD	1:E:305:ARG:HH22	2.15	0.49
1:F:239:TYR:HB3	1:F:266:MET:HB3	1.93	0.49
2:I:85:LEU:HD23	2:I:88:MET:CE	2.42	0.49
2:K:35:PRO:HB2	2:K:36:PRO:HD3	1.95	0.49
2:K:71:MET:HA	2:K:74:ARG:HD2	1.94	0.49
2:M:100:LYS:HG2	2:N:56:ILE:HG22	1.94	0.49
2:S:71:MET:HA	2:S:74:ARG:HD2	1.94	0.49
2:S:100:LYS:HG2	2:T:56:ILE:HG22	1.94	0.49
2:U:35:PRO:HB2	2:U:36:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:74:ARG:NH1	2:V:97:ASN:OD1	2.44	0.49
1:E:239:TYR:HB3	1:E:266:MET:HB3	1.93	0.49
1:F:134:ARG:HA	1:F:308:GLY:O	2.13	0.49
2:I:100:LYS:HG2	2:J:56:ILE:HG22	1.94	0.49
2:M:71:MET:HA	2:M:74:ARG:HD2	1.94	0.49
2:O:100:LYS:HG2	2:P:56:ILE:HG22	1.94	0.49
1:C:170:LEU:HD12	1:C:424:LEU:CB	2.09	0.49
1:E:134:ARG:HA	1:E:308:GLY:O	2.13	0.49
2:O:71:MET:HA	2:O:74:ARG:HD2	1.94	0.49
2:O:85:LEU:HD23	2:O:88:MET:CE	2.42	0.49
1:A:18:LYS:HG2	2:S:31:GLY:O	2.13	0.49
1:C:19:ASP:OD1	2:M:29[A]:GLN:CA	1.73	0.49
1:C:391:VAL:HG12	1:C:437:LEU:HB2	1.95	0.49
1:D:134:ARG:HA	1:D:308:GLY:O	2.13	0.49
1:F:170:LEU:HD12	1:F:424:LEU:CB	2.09	0.49
2:I:71:MET:HA	2:I:74:ARG:HD2	1.94	0.49
2:O:71:MET:CE	2:P:100:LYS:HB2	2.41	0.49
2:O:74:ARG:NH1	2:P:97:ASN:OD1	2.44	0.49
2:Q:71:MET:HA	2:Q:74:ARG:HD2	1.94	0.49
1:A:391:VAL:HG12	1:A:437:LEU:HB2	1.95	0.49
1:B:128:LYS:HD3	2:R:2:ASN:HD21	1.77	0.49
1:E:391:VAL:HG12	1:E:437:LEU:HB2	1.95	0.49
1:F:391:VAL:HG12	1:F:437:LEU:HB2	1.95	0.49
1:G:134:ARG:HA	1:G:308:GLY:O	2.13	0.49
1:G:391:VAL:HG12	1:G:437:LEU:HB2	1.95	0.49
2:I:71:MET:CE	2:J:100:LYS:HB2	2.41	0.49
2:I:74:ARG:NH1	2:J:97:ASN:OD1	2.44	0.49
2:N:2:ASN:C	2:N:2:ASN:HD22	2.16	0.49
2:T:2:ASN:HD22	2:T:2:ASN:C	2.16	0.49
2:U:100:LYS:HG2	2:V:56:ILE:HG22	1.94	0.49
2:W:71:MET:HA	2:W:74:ARG:HD2	1.94	0.49
1:A:48:VAL:CG2	2:T:1:MET:HB2	2.39	0.49
1:C:19:ASP:HB3	2:M:33:THR:CG2	2.40	0.49
1:D:391:VAL:HG12	1:D:437:LEU:HB2	1.95	0.49
1:F:18:LYS:HA	2:U:31:GLY:O	2.12	0.49
1:F:21:LYS:HZ2	2:U:33:THR:HG21	1.21	0.49
2:K:100:LYS:HG2	2:L:56:ILE:HG22	1.94	0.49
1:A:383:HIS:H	1:A:386:HIS:CD2	2.23	0.48
1:B:353:HIS:HD2	1:B:367:ASP:OD1	1.96	0.48
1:C:383:HIS:H	1:C:386:HIS:CD2	2.24	0.48
1:E:170:LEU:HD12	1:E:424:LEU:CB	2.09	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:285:ARG:HG3	1:H:285:ARG:O	2.13	0.48
2:L:2:ASN:HD22	2:L:2:ASN:C	2.16	0.48
2:P:2:ASN:C	2:P:2:ASN:HD22	2.16	0.48
2:V:2:ASN:C	2:V:2:ASN:HD22	2.16	0.48
1:A:353:HIS:HD2	1:A:367:ASP:OD1	1.96	0.48
2:J:2:ASN:C	2:J:2:ASN:HD22	2.16	0.48
1:B:285:ARG:O	1:B:285:ARG:HG3	2.13	0.48
1:C:19:ASP:OD2	2:M:29[B]:GLN:HB3	2.13	0.48
1:E:353:HIS:HD2	1:E:367:ASP:OD1	1.97	0.48
1:F:396:ASP:CG	1:F:431:ARG:HD2	2.34	0.48
1:H:391:VAL:HG12	1:H:437:LEU:HB2	1.95	0.48
2:I:35:PRO:HB2	2:I:36:PRO:HD3	1.95	0.48
1:B:391:VAL:HG12	1:B:437:LEU:HB2	1.95	0.48
1:C:353:HIS:HD2	1:C:367:ASP:OD1	1.97	0.48
1:E:396:ASP:CG	1:E:431:ARG:HD2	2.34	0.48
1:F:353:HIS:HD2	1:F:367:ASP:OD1	1.97	0.48
1:H:353:HIS:HD2	1:H:367:ASP:OD1	1.97	0.48
2:O:35:PRO:HB2	2:O:36:PRO:HD3	1.95	0.48
1:B:396:ASP:CG	1:B:431:ARG:HD2	2.34	0.48
1:B:467:PHE:HB3	2:M:17:TYR:HE1	1.78	0.48
1:D:353:HIS:HD2	1:D:367:ASP:OD1	1.97	0.48
1:F:46:PRO:HB2	2:U:76:HIS:C	2.34	0.48
1:G:52:GLU:OE2	2:I:32:GLU:OE2	2.31	0.48
1:G:353:HIS:HD2	1:G:367:ASP:OD1	1.96	0.48
2:W:71:MET:CE	2:X:100:LYS:HB2	2.41	0.48
1:A:93:GLU:CD	1:A:305:ARG:HH22	2.15	0.48
1:F:383:HIS:H	1:F:386:HIS:CD2	2.23	0.48
1:C:396:ASP:CG	1:C:431:ARG:HD2	2.34	0.48
1:E:385:TRP:CE2	1:E:463:LYS:HG3	2.49	0.48
1:F:21:LYS:HZ1	2:U:33:THR:HG21	1.22	0.48
1:H:396:ASP:CG	1:H:431:ARG:HD2	2.33	0.48
2:Q:71:MET:CE	2:R:100:LYS:HB2	2.41	0.48
1:A:396:ASP:CG	1:A:431:ARG:HD2	2.34	0.48
1:C:93:GLU:CD	1:C:305:ARG:HH22	2.15	0.48
1:D:385:TRP:CE2	1:D:463:LYS:HG3	2.49	0.48
1:E:383:HIS:H	1:E:386:HIS:CD2	2.24	0.48
1:H:134:ARG:HA	1:H:308:GLY:O	2.13	0.48
2:W:35:PRO:HB2	2:W:36:PRO:HD3	1.95	0.48
1:B:134:ARG:HA	1:B:308:GLY:O	2.13	0.48
1:F:385:TRP:CE2	1:F:463:LYS:HG3	2.49	0.48
1:G:385:TRP:CE2	1:G:463:LYS:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:35:PRO:HB2	2:Q:36:PRO:HD3	1.95	0.48
2:S:35:PRO:HB2	2:S:36:PRO:HD3	1.95	0.48
1:A:170:LEU:HD12	1:A:424:LEU:CB	2.09	0.48
1:B:472:MET:CG	1:B:473:ASP:N	2.70	0.48
2:M:35:PRO:HB2	2:M:36:PRO:HD3	1.95	0.48
1:A:385:TRP:CE2	1:A:463:LYS:HG3	2.49	0.47
1:A:396:ASP:OD2	1:A:431:ARG:HD2	2.14	0.47
1:C:385:TRP:CE2	1:C:463:LYS:HG3	2.49	0.47
1:C:396:ASP:OD2	1:C:431:ARG:HD2	2.14	0.47
1:D:131:ARG:NE	2:O:80:GLU:OE1	2.39	0.47
1:E:21:LYS:HG2	2:K:33:THR:HG21	1.89	0.47
1:F:285:ARG:O	1:F:285:ARG:HG3	2.13	0.47
1:G:52:GLU:HB3	2:I:29[B]:GLN:HE22	1.63	0.47
2:P:24:ARG:CG	2:P:24:ARG:NH1	2.71	0.47
1:E:46:PRO:HD2	2:L:3:LEU:HD11	1.96	0.47
2:I:71:MET:HE2	2:J:97:ASN:HA	1.96	0.47
2:O:14:LEU:HD23	2:P:89[A]:VAL:CG2	2.20	0.47
2:O:71:MET:HE2	2:P:97:ASN:HA	1.96	0.47
1:B:471:THR:HA	1:B:472:MET:N	2.28	0.47
1:C:471:THR:HA	1:C:472:MET:N	2.28	0.47
1:D:471:THR:HA	1:D:472:MET:N	2.28	0.47
1:H:45:GLN:O	2:W:76:HIS:CE1	2.67	0.47
1:E:473:ASP:HB2	2:P:20:TYR:OH	2.15	0.47
1:H:472:MET:CG	1:H:473:ASP:N	2.70	0.47
2:J:24:ARG:CG	2:J:24:ARG:NH1	2.71	0.47
2:S:71:MET:HE2	2:T:97:ASN:HA	1.96	0.47
1:E:285:ARG:O	1:E:285:ARG:HG3	2.13	0.47
1:E:465:ILE:HG22	2:O:20:TYR:CE2	2.49	0.47
1:F:391:VAL:CB	1:F:437:LEU:HD13	2.40	0.47
1:H:396:ASP:OD2	1:H:431:ARG:HD2	2.14	0.47
1:H:471:THR:HA	1:H:472:MET:N	2.28	0.47
1:B:167:ARG:HG2	1:B:168:PRO:O	2.15	0.47
1:B:396:ASP:OD2	1:B:431:ARG:HD2	2.14	0.47
1:C:21:LYS:NZ	2:M:33:THR:HB	2.25	0.47
1:E:167:ARG:HG2	1:E:168:PRO:O	2.15	0.47
1:E:406:THR:HG1	1:E:420:ASN:CG	2.16	0.47
1:F:167:ARG:HG2	1:F:168:PRO:O	2.15	0.47
1:F:406:THR:HG1	1:F:420:ASN:CG	2.17	0.47
1:G:396:ASP:CG	1:G:431:ARG:HD2	2.34	0.47
1:A:285:ARG:HG3	1:A:285:ARG:O	2.13	0.47
1:B:171:GLY:HA2	1:B:199:PHE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:PRO:CA	2:O:76:HIS:ND1	2.65	0.47
1:D:167:ARG:HG2	1:D:168:PRO:O	2.15	0.47
1:D:396:ASP:CG	1:D:431:ARG:HD2	2.34	0.47
1:F:466:LYS:HA	1:F:467:PHE:O	2.15	0.47
1:G:167:ARG:HG2	1:G:168:PRO:O	2.15	0.47
1:G:471:THR:HA	1:G:472:MET:N	2.28	0.47
1:H:45:GLN:C	2:X:1:MET:CE	2.83	0.47
1:H:167:ARG:HG2	1:H:168:PRO:O	2.15	0.47
1:H:171:GLY:HA2	1:H:199:PHE:O	2.15	0.47
1:H:385:TRP:CE2	1:H:463:LYS:HG3	2.49	0.47
2:I:14:LEU:HD23	2:J:89[A]:VAL:CG2	2.20	0.47
1:C:285:ARG:HG3	1:C:285:ARG:O	2.13	0.47
1:C:472:MET:CG	1:C:473:ASP:N	2.70	0.47
1:D:49:PRO:HD2	2:O:29[A]:GLN:HE21	1.79	0.47
1:D:171:GLY:HA2	1:D:199:PHE:O	2.15	0.47
1:F:396:ASP:OD2	1:F:431:ARG:HD2	2.14	0.47
1:H:465:ILE:HG22	2:S:20:TYR:OH	2.14	0.47
2:S:85:LEU:HD23	2:S:88:MET:CE	2.42	0.47
1:B:385:TRP:CE2	1:B:463:LYS:HG3	2.49	0.47
1:D:396:ASP:OD2	1:D:431:ARG:HD2	2.15	0.47
1:E:396:ASP:OD2	1:E:431:ARG:HD2	2.15	0.47
1:E:466:LYS:HA	1:E:467:PHE:O	2.15	0.47
2:L:24:ARG:CG	2:L:24:ARG:NH1	2.71	0.47
1:A:435:ARG:HH22	1:A:447:GLU:CD	2.16	0.47
1:B:15:ALA:CB	1:C:410:PRO:N	2.77	0.47
1:C:171:GLY:HA2	1:C:199:PHE:O	2.15	0.47
1:C:464:GLU:O	1:C:465:ILE:N	2.48	0.47
1:E:391:VAL:CB	1:E:437:LEU:HD13	2.40	0.47
1:E:406:THR:OG1	1:E:420:ASN:OD1	2.24	0.47
1:G:171:GLY:HA2	1:G:199:PHE:O	2.15	0.47
1:G:466:LYS:HA	1:G:467:PHE:O	2.15	0.47
2:R:2:ASN:C	2:R:2:ASN:HD22	2.16	0.47
2:X:2:ASN:C	2:X:2:ASN:HD22	2.16	0.47
1:A:167:ARG:HG2	1:A:168:PRO:O	2.15	0.46
1:A:472:MET:CG	1:A:473:ASP:N	2.70	0.46
1:C:435:ARG:HH22	1:C:447:GLU:CD	2.16	0.46
1:E:464:GLU:O	2:O:24:ARG:NH2	2.48	0.46
1:H:464:GLU:O	1:H:465:ILE:N	2.48	0.46
2:L:74:ARG:HG2	2:L:75:GLU:N	2.30	0.46
2:V:74:ARG:HG2	2:V:75:GLU:N	2.30	0.46
1:D:15:ALA:CB	1:E:410:PRO:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:PRO:N	2:K:76:HIS:CE1	2.79	0.46
1:F:406:THR:OG1	1:F:420:ASN:OD1	2.24	0.46
1:F:410:PRO:N	1:G:15:ALA:CB	2.78	0.46
1:G:396:ASP:OD2	1:G:431:ARG:HD2	2.14	0.46
1:G:464:GLU:O	1:G:465:ILE:N	2.48	0.46
1:H:170:LEU:HD12	1:H:424:LEU:CB	2.09	0.46
2:V:24:ARG:CG	2:V:24:ARG:NH1	2.71	0.46
1:A:171:GLY:HA2	1:A:199:PHE:O	2.15	0.46
1:D:466:LYS:HA	1:D:467:PHE:O	2.15	0.46
1:F:471:THR:HA	1:F:472:MET:N	2.28	0.46
1:H:21:LYS:CD	2:W:33:THR:HG21	2.45	0.46
1:A:466:LYS:HA	1:A:467:PHE:O	2.15	0.46
1:B:47:GLY:CA	2:Q:73:VAL:HG13	2.45	0.46
1:C:167:ARG:HG2	1:C:168:PRO:O	2.15	0.46
1:D:285:ARG:HG3	1:D:285:ARG:O	2.13	0.46
1:F:464:GLU:O	1:F:465:ILE:N	2.48	0.46
1:G:285:ARG:HG3	1:G:285:ARG:O	2.13	0.46
1:G:473:ASP:HB2	2:V:20:TYR:OH	2.15	0.46
2:M:71:MET:HE2	2:N:97:ASN:HA	1.97	0.46
1:B:45:GLN:CB	2:R:3:LEU:HD11	2.42	0.46
1:B:465:ILE:CD1	2:M:24:ARG:CG	2.66	0.46
1:H:46:PRO:HB2	2:W:76:HIS:C	2.34	0.46
2:R:74:ARG:HG2	2:R:75:GLU:N	2.30	0.46
1:A:48:VAL:H	2:T:1:MET:CE	2.27	0.46
1:C:466:LYS:HA	1:C:467:PHE:O	2.15	0.46
1:D:435:ARG:HH22	1:D:447:GLU:CD	2.16	0.46
1:E:464:GLU:O	1:E:465:ILE:N	2.48	0.46
2:P:74:ARG:HG2	2:P:75:GLU:N	2.30	0.46
1:A:18:LYS:HA	2:S:31:GLY:O	2.16	0.46
1:B:435:ARG:HH22	1:B:447:GLU:CD	2.16	0.46
1:F:22:LEU:CD1	2:U:35:PRO:HD3	2.44	0.46
2:J:74:ARG:HG2	2:J:75:GLU:N	2.30	0.46
2:X:74:ARG:HG2	2:X:75:GLU:N	2.30	0.46
1:A:207:ASN:O	1:A:217:ARG:NH1	2.49	0.46
1:C:207:ASN:O	1:C:217:ARG:NH1	2.49	0.46
1:A:45:GLN:HB3	2:T:3:LEU:CG	2.46	0.46
1:A:391:VAL:HB	1:A:437:LEU:HB3	1.98	0.46
1:A:471:THR:HA	1:A:472:MET:N	2.28	0.46
1:B:21:LYS:HZ1	2:Q:33:THR:CG2	2.06	0.46
1:C:391:VAL:HB	1:C:437:LEU:HB3	1.98	0.46
1:D:391:VAL:CG2	1:D:437:LEU:HD13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:PRO:N	1:E:15:ALA:CB	2.79	0.46
1:E:45:GLN:C	2:L:1:MET:HE2	2.37	0.46
1:E:471:THR:HA	1:E:472:MET:N	2.28	0.46
1:F:391:VAL:CG2	1:F:437:LEU:HD13	2.46	0.46
1:G:391:VAL:CG2	1:G:437:LEU:HD13	2.46	0.46
1:G:409:HIS:CE1	1:G:454:GLU:HB2	2.51	0.46
1:G:435:ARG:HH22	1:G:447:GLU:CD	2.16	0.46
1:H:409:HIS:CE1	1:H:454:GLU:HB2	2.51	0.46
2:S:14:LEU:HD23	2:T:89[A]:VAL:CG2	2.20	0.46
1:B:409:HIS:CE1	1:B:454:GLU:HB2	2.51	0.46
1:D:409:HIS:CE1	1:D:454:GLU:HB2	2.51	0.46
1:E:19:ASP:HB3	2:K:33:THR:CG2	2.41	0.46
1:E:391:VAL:CG2	1:E:437:LEU:HD13	2.46	0.46
1:B:391:VAL:CG1	1:B:437:LEU:HB3	2.46	0.45
1:F:171:GLY:HA2	1:F:199:PHE:O	2.15	0.45
1:H:19:ASP:N	2:W:32:GLU:H	2.10	0.45
1:A:467:PHE:HB3	2:W:17:TYR:HE1	1.81	0.45
1:D:46:PRO:HB2	2:O:76:HIS:C	2.37	0.45
1:E:171:GLY:HA2	1:E:199:PHE:O	2.15	0.45
1:H:391:VAL:CG1	1:H:437:LEU:HB3	2.46	0.45
1:H:435:ARG:HH22	1:H:447:GLU:CD	2.16	0.45
2:T:74:ARG:HG2	2:T:75:GLU:N	2.30	0.45
1:A:273:GLY:HA3	1:H:273:GLY:HA3	1.98	0.45
1:H:52:GLU:HB2	2:W:29[B]:GLN:NE2	2.27	0.45
1:H:466:LYS:HA	1:H:467:PHE:O	2.15	0.45
2:N:74:ARG:HG2	2:N:75:GLU:N	2.30	0.45
1:E:409:HIS:CE1	1:E:454:GLU:HB2	2.52	0.45
1:G:18:LYS:CA	2:I:32:GLU:N	2.79	0.45
1:A:409:HIS:CE1	1:A:454:GLU:HB2	2.51	0.45
1:B:49:PRO:CG	2:Q:29[B]:GLN:HE21	2.29	0.45
1:B:391:VAL:HB	1:B:437:LEU:HB3	1.98	0.45
1:C:465:ILE:HG22	2:Q:20:TYR:CE2	2.51	0.45
1:C:467:PHE:CZ	2:Q:20:TYR:CD2	2.55	0.45
1:F:409:HIS:CE1	1:F:454:GLU:HB2	2.52	0.45
1:G:18:LYS:HG2	2:I:31:GLY:O	2.16	0.45
1:H:391:VAL:CG2	1:H:437:LEU:HD13	2.46	0.45
1:B:466:LYS:HA	1:B:467:PHE:O	2.15	0.45
1:B:469:PHE:CD2	1:B:470:GLU:C	2.89	0.45
1:C:21:LYS:HG2	2:M:33:THR:CG2	2.45	0.45
1:A:18:LYS:CA	2:S:32:GLU:N	2.80	0.45
1:A:464:GLU:O	1:A:465:ILE:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:LEU:HD12	1:B:424:LEU:CB	2.09	0.45
1:E:391:VAL:HB	1:E:437:LEU:HB3	1.98	0.45
1:F:391:VAL:HB	1:F:437:LEU:HB3	1.98	0.45
1:B:435:ARG:NH2	1:B:447:GLU:OE2	2.29	0.45
1:H:435:ARG:NH2	1:H:447:GLU:OE2	2.29	0.45
1:A:410:PRO:N	1:H:15:ALA:CB	2.80	0.45
1:B:391:VAL:CG2	1:B:437:LEU:HD13	2.46	0.45
1:C:409:HIS:CE1	1:C:454:GLU:HB2	2.52	0.45
1:E:22:LEU:HD21	2:K:33:THR:HB	1.92	0.45
1:H:391:VAL:HB	1:H:437:LEU:HB3	1.98	0.45
1:A:391:VAL:CG2	1:A:437:LEU:HD13	2.46	0.45
1:B:20:TYR:CG	2:Q:32:GLU:OE1	2.70	0.45
1:H:234:GLU:OE1	1:H:421:ARG:NH2	2.50	0.45
1:B:207:ASN:O	1:B:217:ARG:NH1	2.49	0.44
1:B:234:GLU:OE1	1:B:421:ARG:NH2	2.50	0.44
1:D:19:ASP:HB2	2:O:32:GLU:C	2.30	0.44
1:D:391:VAL:HB	1:D:437:LEU:HB3	1.98	0.44
1:G:391:VAL:HB	1:G:437:LEU:HB3	1.98	0.44
1:H:207:ASN:O	1:H:217:ARG:NH1	2.49	0.44
1:E:234:GLU:OE1	1:E:421:ARG:NH2	2.50	0.44
1:G:473:ASP:HB3	2:V:20:TYR:OH	2.18	0.44
1:A:47:GLY:CA	2:S:73:VAL:HG13	2.48	0.44
1:F:207:ASN:O	1:F:217:ARG:NH1	2.49	0.44
1:F:234:GLU:OE1	1:F:421:ARG:NH2	2.50	0.44
1:G:234:GLU:OE1	1:G:421:ARG:NH2	2.50	0.44
1:C:152:PRO:O	1:C:285:ARG:HD3	2.18	0.44
1:C:391:VAL:CG2	1:C:437:LEU:HD13	2.46	0.44
1:D:234:GLU:OE1	1:D:421:ARG:NH2	2.50	0.44
1:F:469:PHE:CD2	1:F:470:GLU:C	2.89	0.44
1:G:52:GLU:HB3	2:I:29[B]:GLN:NE2	2.27	0.44
1:B:14:LYS:HZ1	1:B:18:LYS:HG3	1.82	0.44
1:B:295:ARG:H	1:B:295:ARG:HG3	1.64	0.44
1:B:391:VAL:CB	1:B:437:LEU:HD13	2.40	0.44
1:D:18:LYS:HA	2:O:31:GLY:O	2.17	0.44
1:D:391:VAL:CG1	1:D:437:LEU:HB3	2.46	0.44
1:E:18:LYS:HG2	2:K:31:GLY:O	2.18	0.44
1:E:49:PRO:HD2	2:K:29[A]:GLN:NE2	2.32	0.44
1:E:469:PHE:CD2	1:E:470:GLU:C	2.89	0.44
1:H:295:ARG:H	1:H:295:ARG:HG3	1.64	0.44
1:A:152:PRO:O	1:A:285:ARG:HD3	2.18	0.44
1:E:207:ASN:O	1:E:217:ARG:NH1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:71:MET:HE2	2:L:97:ASN:HA	1.99	0.44
1:A:391:VAL:CG1	1:A:437:LEU:HB3	2.46	0.44
1:C:391:VAL:CG1	1:C:437:LEU:HB3	2.46	0.44
1:E:384:VAL:O	1:E:445:LEU:HD11	2.18	0.44
1:E:391:VAL:CG1	1:E:437:LEU:HB3	2.46	0.44
1:F:152:PRO:O	1:F:285:ARG:HD3	2.18	0.44
1:F:384:VAL:O	1:F:445:LEU:HD11	2.18	0.44
2:J:71:MET:HA	2:J:74:ARG:HD2	2.00	0.44
2:P:71:MET:HA	2:P:74:ARG:HD2	2.00	0.44
2:U:71:MET:HE2	2:V:97:ASN:HA	1.99	0.44
1:C:217:ARG:HE	1:C:217:ARG:HB3	1.45	0.44
1:D:384:VAL:O	1:D:445:LEU:HD11	2.18	0.44
1:G:384:VAL:O	1:G:445:LEU:HD11	2.18	0.44
2:M:4:LYS:O	2:M:8[B]:LYS:HB2	2.18	0.44
2:S:4:LYS:O	2:S:8[B]:LYS:HB2	2.18	0.44
1:C:234:GLU:OE1	1:C:421:ARG:NH2	2.50	0.44
1:E:152:PRO:O	1:E:285:ARG:HD3	2.18	0.44
1:E:392:GLU:HB2	1:E:438:TYR:HA	2.00	0.44
1:E:473:ASP:HB3	2:P:20:TYR:OH	2.18	0.44
1:G:48:VAL:HG23	2:J:1:MET:HB2	1.99	0.44
1:G:152:PRO:O	1:G:285:ARG:HD3	2.18	0.44
1:H:391:VAL:CB	1:H:437:LEU:HD13	2.40	0.44
1:A:234:GLU:OE1	1:A:421:ARG:NH2	2.50	0.43
1:C:384:VAL:O	1:C:445:LEU:HD11	2.18	0.43
1:D:152:PRO:O	1:D:285:ARG:HD3	2.18	0.43
1:F:391:VAL:CG1	1:F:437:LEU:HB3	2.46	0.43
2:V:71:MET:HA	2:V:74:ARG:HD2	2.00	0.43
1:B:406:THR:OG1	1:B:420:ASN:OD1	2.24	0.43
1:C:46:PRO:HB2	2:M:76:HIS:C	2.39	0.43
1:E:46:PRO:N	2:K:76:HIS:NE2	2.57	0.43
1:F:19:ASP:HB2	2:U:33:THR:H	1.75	0.43
1:F:392:GLU:HB2	1:F:438:TYR:HA	2.00	0.43
1:G:391:VAL:CG1	1:G:437:LEU:HB3	2.46	0.43
1:H:384:VAL:O	1:H:445:LEU:HD11	2.18	0.43
1:H:392:GLU:HB2	1:H:438:TYR:HA	2.00	0.43
2:L:71:MET:HA	2:L:74:ARG:HD2	2.00	0.43
1:A:18:LYS:CA	2:S:31:GLY:C	2.82	0.43
1:B:46:PRO:CD	2:R:3:LEU:HD11	2.32	0.43
1:B:273:GLY:HA3	1:C:273:GLY:HA3	2.00	0.43
1:B:392:GLU:HB2	1:B:438:TYR:HA	2.00	0.43
1:C:469:PHE:CD2	1:C:470:GLU:C	2.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4:LYS:O	2:I:8[B]:LYS:HB2	2.18	0.43
1:A:20:TYR:CG	2:S:32:GLU:OE1	2.69	0.43
1:A:217:ARG:HE	1:A:217:ARG:HB3	1.45	0.43
1:B:46:PRO:HG2	2:R:3:LEU:CD2	2.48	0.43
1:D:207:ASN:O	1:D:217:ARG:NH1	2.49	0.43
1:G:45:GLN:C	2:J:1:MET:HE2	2.38	0.43
1:G:207:ASN:O	1:G:217:ARG:NH1	2.48	0.43
2:O:4:LYS:O	2:O:8[B]:LYS:HB2	2.18	0.43
2:Q:4:LYS:O	2:Q:8[B]:LYS:HB2	2.18	0.43
2:U:4:LYS:O	2:U:8[B]:LYS:HB2	2.18	0.43
2:W:4:LYS:O	2:W:8[B]:LYS:HB2	2.18	0.43
1:A:384:VAL:O	1:A:445:LEU:HD11	2.18	0.43
1:B:384:VAL:O	1:B:445:LEU:HD11	2.18	0.43
1:C:18:LYS:HA	2:M:31:GLY:O	2.18	0.43
1:E:21:LYS:HG2	2:K:33:THR:HG22	1.89	0.43
1:H:21:LYS:NZ	2:W:33:THR:HB	2.24	0.43
1:A:167:ARG:HE	1:A:428:VAL:HG21	1.79	0.43
1:A:392:GLU:HB2	1:A:438:TYR:HA	2.00	0.43
1:A:469:PHE:CD2	1:A:470:GLU:C	2.89	0.43
1:C:392:GLU:HB2	1:C:438:TYR:HA	2.00	0.43
1:D:217:ARG:HE	1:D:217:ARG:HB3	1.45	0.43
1:D:472:MET:CG	1:D:473:ASP:N	2.70	0.43
2:K:4:LYS:O	2:K:8[B]:LYS:HB2	2.18	0.43
1:A:353:HIS:HE1	1:A:355:GLU:OE2	2.02	0.43
1:B:152:PRO:O	1:B:285:ARG:HD3	2.18	0.43
1:E:353:HIS:HE1	1:E:355:GLU:OE2	2.02	0.43
1:F:48:VAL:HG23	2:V:1:MET:HG3	2.01	0.43
1:F:353:HIS:HE1	1:F:355:GLU:OE2	2.02	0.43
1:G:229:GLN:NE2	1:G:236:LYS:H	2.17	0.43
1:H:353:HIS:HE1	1:H:355:GLU:OE2	2.02	0.43
2:I:71:MET:CE	2:J:97:ASN:HA	2.49	0.43
1:B:353:HIS:HE1	1:B:355:GLU:OE2	2.02	0.43
1:C:353:HIS:HE1	1:C:355:GLU:OE2	2.02	0.43
1:C:392:GLU:HG2	1:C:438:TYR:CE1	2.26	0.43
1:D:229:GLN:NE2	1:D:236:LYS:H	2.17	0.43
1:D:353:HIS:HE1	1:D:355:GLU:OE2	2.02	0.43
1:E:131:ARG:NE	2:K:80:GLU:OE1	2.45	0.43
2:O:71:MET:CE	2:P:97:ASN:HA	2.49	0.43
2:O:93:ILE:HD13	2:P:74:ARG:HG3	2.01	0.43
1:C:167:ARG:HE	1:C:428:VAL:HG21	1.79	0.43
1:E:167:ARG:HE	1:E:428:VAL:HG21	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:353:HIS:HE1	1:G:355:GLU:OE2	2.02	0.43
1:H:152:PRO:O	1:H:285:ARG:HD3	2.18	0.43
2:I:93:ILE:HD13	2:J:74:ARG:HG3	2.01	0.43
2:K:93:ILE:HD13	2:L:74:ARG:HG3	2.01	0.43
2:U:93:ILE:HD13	2:V:74:ARG:HG3	2.01	0.43
1:C:51:ASP:HA	1:C:87:ILE:CD1	2.49	0.43
1:F:273:GLY:HA3	1:G:273:GLY:HA3	1.99	0.43
1:G:472:MET:CG	1:G:473:ASP:N	2.70	0.43
1:H:14:LYS:HZ1	1:H:18:LYS:HG3	1.83	0.43
1:A:392:GLU:HG2	1:A:438:TYR:CE1	2.26	0.42
1:D:273:GLY:HA3	1:E:273:GLY:HA3	2.00	0.42
1:D:392:GLU:HB2	1:D:438:TYR:HA	2.00	0.42
1:D:406:THR:CB	1:D:420:ASN:OD1	2.67	0.42
1:G:406:THR:CB	1:G:420:ASN:OD1	2.67	0.42
2:J:94:GLN:O	2:J:98:MET:HB2	2.19	0.42
2:K:71:MET:CE	2:L:97:ASN:HA	2.49	0.42
2:N:71:MET:HA	2:N:74:ARG:HD2	2.00	0.42
2:P:94:GLN:O	2:P:98:MET:HB2	2.19	0.42
2:T:71:MET:HA	2:T:74:ARG:HD2	2.00	0.42
1:A:48:VAL:HG22	2:T:1:MET:H1	1.84	0.42
1:A:51:ASP:HA	1:A:87:ILE:CD1	2.50	0.42
1:D:51:ASP:HA	1:D:87:ILE:CD1	2.50	0.42
1:F:462:TRP:CD1	1:G:66:TRP:CZ3	3.07	0.42
1:G:51:ASP:HA	1:G:87:ILE:CD1	2.50	0.42
2:Q:71:MET:CE	2:R:97:ASN:HA	2.49	0.42
2:U:71:MET:CE	2:V:97:ASN:HA	2.49	0.42
2:W:71:MET:CE	2:X:97:ASN:HA	2.49	0.42
1:B:133:LEU:O	1:B:307:HIS:HA	2.19	0.42
1:C:152:PRO:HB2	1:C:153:HIS:CD2	2.55	0.42
1:E:385:TRP:CZ2	1:E:463:LYS:HG3	2.55	0.42
1:F:385:TRP:CZ2	1:F:463:LYS:HG3	2.55	0.42
1:F:435:ARG:HH22	1:F:447:GLU:CD	2.16	0.42
1:H:133:LEU:O	1:H:307:HIS:HA	2.19	0.42
1:H:229:GLN:NE2	1:H:236:LYS:H	2.17	0.42
2:J:11:ALA:O	2:J:15:GLN:HG3	2.20	0.42
2:L:94:GLN:O	2:L:98:MET:HB2	2.19	0.42
2:N:94:GLN:O	2:N:98:MET:HB2	2.19	0.42
2:T:94:GLN:O	2:T:98:MET:HB2	2.19	0.42
1:A:152:PRO:HB2	1:A:153:HIS:CD2	2.55	0.42
1:B:47:GLY:HA2	2:Q:73:VAL:HG13	2.00	0.42
1:B:383:HIS:NE2	1:B:462:TRP:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:THR:CB	1:B:420:ASN:OD1	2.67	0.42
1:C:133:LEU:O	1:C:307:HIS:HA	2.19	0.42
1:D:46:PRO:HG2	2:O:80:GLU:HB2	1.91	0.42
1:E:229:GLN:NE2	1:E:236:LYS:H	2.16	0.42
1:F:167:ARG:HE	1:F:428:VAL:HG21	1.79	0.42
1:F:229:GLN:NE2	1:F:236:LYS:H	2.17	0.42
1:G:133:LEU:O	1:G:307:HIS:HA	2.19	0.42
2:P:11:ALA:O	2:P:15:GLN:HG3	2.20	0.42
2:V:94:GLN:O	2:V:98:MET:HB2	2.19	0.42
2:X:94:GLN:O	2:X:98:MET:HB2	2.19	0.42
1:A:133:LEU:O	1:A:307:HIS:HA	2.19	0.42
1:C:385:TRP:CZ2	1:C:463:LYS:HG3	2.55	0.42
1:D:133:LEU:O	1:D:307:HIS:HA	2.19	0.42
1:G:217:ARG:HE	1:G:217:ARG:HB3	1.45	0.42
1:G:466:LYS:N	2:U:20:TYR:OH	2.52	0.42
1:H:45:GLN:HB3	2:X:3:LEU:CD1	2.43	0.42
2:M:85:LEU:HA	2:M:88:MET:HE2	2.02	0.42
2:R:94:GLN:O	2:R:98:MET:HB2	2.19	0.42
2:V:11:ALA:O	2:V:15:GLN:HG3	2.20	0.42
2:X:71:MET:HA	2:X:74:ARG:HD2	2.00	0.42
1:A:385:TRP:CZ2	1:A:463:LYS:HG3	2.55	0.42
1:B:18:LYS:HG2	2:Q:31:GLY:O	2.20	0.42
1:B:217:ARG:HE	1:B:217:ARG:HB3	1.45	0.42
1:B:229:GLN:NE2	1:B:236:LYS:H	2.16	0.42
1:F:31:PRO:HB3	1:F:37:LEU:HD21	2.02	0.42
1:G:392:GLU:HB2	1:G:438:TYR:HA	2.00	0.42
1:G:409:HIS:CD2	1:G:419:ALA:HB3	2.54	0.42
2:L:11:ALA:O	2:L:15:GLN:HG3	2.20	0.42
2:R:71:MET:HA	2:R:74:ARG:HD2	2.00	0.42
1:B:46:PRO:CB	2:Q:76:HIS:C	2.88	0.42
1:C:20:TYR:H	2:M:32:GLU:CD	2.17	0.42
1:E:31:PRO:HB3	1:E:37:LEU:HD21	2.02	0.42
1:F:409:HIS:CD2	1:F:419:ALA:HB3	2.54	0.42
1:G:383:HIS:NE2	1:G:462:TRP:O	2.50	0.42
1:H:406:THR:CB	1:H:420:ASN:OD1	2.67	0.42
1:A:406:THR:CB	1:A:420:ASN:OD1	2.67	0.42
1:B:51:ASP:HA	1:B:87:ILE:CD1	2.49	0.42
1:D:14:LYS:H	1:D:14:LYS:HG3	1.77	0.42
1:D:152:PRO:HB2	1:D:153:HIS:CD2	2.55	0.42
1:E:406:THR:CB	1:E:420:ASN:OD1	2.67	0.42
1:F:66:TRP:CZ3	1:G:462:TRP:CD1	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:LYS:H	1:G:14:LYS:HG3	1.77	0.42
1:H:51:ASP:HA	1:H:87:ILE:CD1	2.50	0.42
1:H:152:PRO:HB2	1:H:153:HIS:CD2	2.55	0.42
2:M:71:MET:CE	2:N:97:ASN:HA	2.49	0.42
2:S:71:MET:CE	2:T:97:ASN:HA	2.49	0.42
2:W:93:ILE:HD13	2:X:74:ARG:HG3	2.01	0.42
1:A:18:LYS:HA	2:S:32:GLU:N	2.35	0.42
1:A:229:GLN:NE2	1:A:236:LYS:H	2.17	0.42
1:B:152:PRO:HB2	1:B:153:HIS:CD2	2.55	0.42
1:D:382:ILE:HA	1:D:386:HIS:CD2	2.55	0.42
1:D:409:HIS:CD2	1:D:419:ALA:HB3	2.54	0.42
1:E:409:HIS:CD2	1:E:419:ALA:HB3	2.54	0.42
1:E:465:ILE:HG23	2:O:24:ARG:HG2	1.41	0.42
1:F:48:VAL:CG2	2:V:1:MET:HG3	2.50	0.42
1:F:51:ASP:HA	1:F:87:ILE:CD1	2.49	0.42
1:F:406:THR:CB	1:F:420:ASN:OD1	2.67	0.42
1:G:152:PRO:HB2	1:G:153:HIS:CD2	2.55	0.42
1:G:382:ILE:HA	1:G:386:HIS:CD2	2.55	0.42
1:H:382:ILE:HA	1:H:386:HIS:CD2	2.55	0.42
2:Q:93:ILE:HD13	2:R:74:ARG:HG3	2.01	0.42
1:B:18:LYS:CA	2:Q:32:GLU:N	2.82	0.42
1:B:45:GLN:HB3	2:R:3:LEU:CG	2.49	0.42
1:B:382:ILE:HA	1:B:386:HIS:CD2	2.55	0.42
1:B:447:GLU:O	1:B:450:LYS:HB2	2.20	0.42
1:C:229:GLN:NE2	1:C:236:LYS:H	2.17	0.42
1:C:406:THR:CB	1:C:420:ASN:OD1	2.67	0.42
1:C:465:ILE:HG23	2:Q:24:ARG:HG2	1.49	0.42
1:D:31:PRO:HB3	1:D:37:LEU:HD21	2.02	0.42
1:D:48:VAL:HG23	2:P:1:MET:HE2	2.00	0.42
1:D:391:VAL:CB	1:D:437:LEU:HD13	2.40	0.42
1:E:46:PRO:HB2	2:K:76:HIS:C	2.40	0.42
1:E:51:ASP:HA	1:E:87:ILE:CD1	2.50	0.42
1:E:382:ILE:HA	1:E:386:HIS:CD2	2.55	0.42
1:E:435:ARG:HH22	1:E:447:GLU:CD	2.16	0.42
1:F:152:PRO:HB2	1:F:153:HIS:CD2	2.55	0.42
1:F:382:ILE:HA	1:F:386:HIS:CD2	2.55	0.42
1:G:22:LEU:HD11	2:I:34:ASN:N	2.34	0.42
1:G:31:PRO:HB3	1:G:37:LEU:HD21	2.02	0.42
1:G:46:PRO:C	2:I:76:HIS:CE1	2.90	0.42
2:M:93:ILE:HD13	2:N:74:ARG:HG3	2.01	0.42
1:B:385:TRP:CZ2	1:B:463:LYS:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:GLN:HG3	1:D:157:VAL:N	2.35	0.41
1:D:383:HIS:NE2	1:D:462:TRP:O	2.50	0.41
1:D:462:TRP:CD1	1:E:66:TRP:CH2	3.08	0.41
1:E:152:PRO:HB2	1:E:153:HIS:CD2	2.55	0.41
1:F:462:TRP:CD1	1:G:66:TRP:CH2	3.07	0.41
1:H:385:TRP:CZ2	1:H:463:LYS:HG3	2.55	0.41
2:I:85:LEU:HA	2:I:88:MET:HE2	2.02	0.41
2:M:23:LEU:O	2:M:27:LEU:HB2	2.20	0.41
2:O:85:LEU:HA	2:O:88:MET:HE2	2.02	0.41
2:S:93:ILE:HD13	2:T:74:ARG:HG3	2.01	0.41
1:A:18:LYS:CB	2:S:31:GLY:O	2.68	0.41
1:B:156:GLN:HG3	1:B:157:VAL:N	2.35	0.41
1:D:385:TRP:CZ2	1:D:463:LYS:HG3	2.55	0.41
1:D:473:ASP:HB2	2:L:20:TYR:OH	2.19	0.41
1:G:385:TRP:CZ2	1:G:463:LYS:HG3	2.55	0.41
1:H:217:ARG:HE	1:H:217:ARG:HB3	1.45	0.41
1:H:447:GLU:O	1:H:450:LYS:HB2	2.20	0.41
2:S:23:LEU:O	2:S:27:LEU:HB2	2.20	0.41
2:W:23:LEU:O	2:W:27:LEU:HB2	2.20	0.41
1:A:46:PRO:CB	2:S:76:HIS:CG	2.97	0.41
1:A:156:GLN:HG3	1:A:157:VAL:N	2.35	0.41
1:A:319:ARG:HG2	1:A:368:TRP:CZ3	2.56	0.41
1:A:382:ILE:HA	1:A:386:HIS:CD2	2.55	0.41
1:C:295:ARG:H	1:C:295:ARG:HG3	1.64	0.41
1:C:319:ARG:HG2	1:C:368:TRP:CZ3	2.56	0.41
1:E:319:ARG:HG2	1:E:368:TRP:CZ3	2.56	0.41
1:F:48:VAL:HG23	2:V:1:MET:CB	2.50	0.41
1:G:156:GLN:HG3	1:G:157:VAL:N	2.35	0.41
2:Q:23:LEU:O	2:Q:27:LEU:HB2	2.20	0.41
2:R:11:ALA:O	2:R:15:GLN:HG3	2.20	0.41
1:B:117:LEU:O	1:B:121:VAL:HG22	2.21	0.41
1:D:462:TRP:CD1	1:E:66:TRP:CZ3	3.09	0.41
1:F:133:LEU:O	1:F:307:HIS:HA	2.19	0.41
1:F:319:ARG:HG2	1:F:368:TRP:CZ3	2.56	0.41
1:G:391:VAL:CB	1:G:437:LEU:HD13	2.40	0.41
1:H:52:GLU:CG	2:W:29[B]:GLN:OE1	2.67	0.41
1:H:156:GLN:HG3	1:H:157:VAL:N	2.35	0.41
2:X:11:ALA:O	2:X:15:GLN:HG3	2.20	0.41
1:A:31:PRO:HB3	1:A:37:LEU:HD21	2.02	0.41
1:A:447:GLU:O	1:A:450:LYS:HB2	2.20	0.41
1:B:21:LYS:CE	2:Q:33:THR:CG2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:THR:HA	1:B:31:PRO:HD3	1.94	0.41
1:B:48:VAL:CG2	2:R:1:MET:N	2.84	0.41
1:B:319:ARG:HG2	1:B:368:TRP:CZ3	2.56	0.41
1:C:31:PRO:HB3	1:C:37:LEU:HD21	2.02	0.41
1:C:382:ILE:HA	1:C:386:HIS:CD2	2.55	0.41
1:G:46:PRO:HB2	2:I:76:HIS:C	2.40	0.41
1:H:14:LYS:H	1:H:14:LYS:HG3	1.77	0.41
1:H:319:ARG:HG2	1:H:368:TRP:CZ3	2.55	0.41
1:C:156:GLN:HG3	1:C:157:VAL:N	2.35	0.41
1:C:447:GLU:O	1:C:450:LYS:HB2	2.21	0.41
1:E:22:LEU:HD23	2:K:33:THR:HB	2.03	0.41
1:E:133:LEU:O	1:E:307:HIS:HA	2.20	0.41
2:Q:85:LEU:HA	2:Q:88:MET:HE2	2.03	0.41
2:W:85:LEU:HA	2:W:88:MET:HE2	2.03	0.41
1:B:31:PRO:HB3	1:B:37:LEU:HD21	2.02	0.41
1:D:22:LEU:HD13	2:O:35:PRO:HD3	2.02	0.41
1:F:156:GLN:HG3	1:F:157:VAL:N	2.35	0.41
1:H:31:PRO:HB3	1:H:37:LEU:HD21	2.02	0.41
1:H:47:GLY:N	2:W:76:HIS:CB	2.81	0.41
1:H:117:LEU:O	1:H:121:VAL:HG22	2.21	0.41
2:K:23:LEU:O	2:K:27:LEU:HB2	2.20	0.41
1:B:396:ASP:OD1	1:B:431:ARG:NH1	2.47	0.41
1:D:66:TRP:CZ3	1:E:462:TRP:CD1	3.09	0.41
1:E:156:GLN:HG3	1:E:157:VAL:N	2.35	0.41
1:G:117:LEU:O	1:G:121:VAL:HG22	2.21	0.41
1:G:447:GLU:O	1:G:450:LYS:HB2	2.20	0.41
1:G:469:PHE:CD2	1:G:470:GLU:C	2.89	0.41
1:H:465:ILE:HG23	2:S:24:ARG:HG2	1.52	0.41
2:N:11:ALA:O	2:N:15:GLN:HG3	2.20	0.41
2:U:23:LEU:O	2:U:27:LEU:HB2	2.20	0.41
1:A:295:ARG:H	1:A:295:ARG:HG3	1.64	0.41
1:C:14:LYS:H	1:C:14:LYS:HG3	1.77	0.41
1:C:117:LEU:O	1:C:121:VAL:HG22	2.21	0.41
1:D:117:LEU:O	1:D:121:VAL:HG22	2.21	0.41
1:D:319:ARG:HG2	1:D:368:TRP:CZ3	2.55	0.41
1:D:447:GLU:O	1:D:450:LYS:HB2	2.20	0.41
1:E:52:GLU:CG	2:K:29[B]:GLN:CD	2.62	0.41
1:E:383:HIS:NE2	1:E:462:TRP:O	2.50	0.41
1:E:472:MET:CG	1:E:473:ASP:N	2.70	0.41
1:F:383:HIS:NE2	1:F:462:TRP:O	2.50	0.41
1:F:447:GLU:O	1:F:450:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:LYS:HB2	1:G:18:LYS:HE2	1.89	0.41
1:G:319:ARG:HG2	1:G:368:TRP:CZ3	2.56	0.41
1:G:465:ILE:HG23	2:U:24:ARG:HG2	1.39	0.41
1:H:49:PRO:CD	2:W:29[A]:GLN:NE2	2.83	0.41
1:H:467:PHE:CZ	2:S:20:TYR:CD2	2.52	0.41
2:I:23:LEU:O	2:I:27:LEU:HB2	2.20	0.41
2:L:24:ARG:HG3	2:L:24:ARG:NH1	2.14	0.41
2:O:23:LEU:O	2:O:27:LEU:HB2	2.20	0.41
2:T:11:ALA:O	2:T:15:GLN:HG3	2.20	0.41
2:U:14:LEU:HD23	2:V:89[A]:VAL:CG2	2.20	0.41
1:A:117:LEU:O	1:A:121:VAL:HG22	2.21	0.41
1:A:465:ILE:HG22	2:W:20:TYR:CE2	2.56	0.41
1:A:472:MET:C	1:A:474:LYS:HG3	2.42	0.41
1:B:42:PHE:HE1	1:B:99:ALA:HB2	1.87	0.41
1:C:18:LYS:HB3	2:M:32:GLU:C	2.35	0.41
1:E:472:MET:C	1:E:474:LYS:HG3	2.42	0.41
1:F:472:MET:CG	1:F:473:ASP:N	2.70	0.41
1:H:19:ASP:OD2	2:W:33:THR:HG23	2.21	0.41
1:H:42:PHE:HE1	1:H:99:ALA:HB2	1.87	0.41
2:V:24:ARG:HG3	2:V:24:ARG:NH1	2.14	0.41
1:A:48:VAL:CG2	2:T:1:MET:CB	2.96	0.40
1:C:22:LEU:HD11	2:M:34:ASN:N	2.16	0.40
1:E:447:GLU:O	1:E:450:LYS:HB2	2.20	0.40
1:F:117:LEU:O	1:F:121:VAL:HG22	2.21	0.40
1:F:472:MET:C	1:F:474:LYS:HG3	2.42	0.40
1:A:14:LYS:H	1:A:14:LYS:HG3	1.77	0.40
1:A:47:GLY:HA2	2:S:73:VAL:HG13	2.04	0.40
1:B:464:GLU:O	1:B:465:ILE:N	2.48	0.40
1:C:391:VAL:HG11	1:C:437:LEU:HB3	2.01	0.40
1:C:472:MET:C	1:C:474:LYS:HG3	2.42	0.40
1:E:117:LEU:O	1:E:121:VAL:HG22	2.21	0.40
1:G:409:HIS:CD2	1:G:416:GLY:HA2	2.43	0.40
1:H:30:THR:HA	1:H:31:PRO:HD3	1.94	0.40
1:H:396:ASP:OD1	1:H:431:ARG:NH1	2.47	0.40
2:X:76:HIS:O	2:X:80:GLU:HG3	2.22	0.40
1:E:49:PRO:HD3	2:K:29[A]:GLN:HE22	1.86	0.40
1:E:384:VAL:O	1:E:445:LEU:CD1	2.70	0.40
1:G:42:PHE:HE1	1:G:99:ALA:HB2	1.87	0.40
1:H:409:HIS:CD2	1:H:419:ALA:HB3	2.54	0.40
2:R:76:HIS:O	2:R:80:GLU:HG3	2.22	0.40
1:B:14:LYS:H	1:B:14:LYS:HG3	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:GLU:OE1	1:B:312:ARG:NH2	2.55	0.40
1:B:384:VAL:O	1:B:445:LEU:CD1	2.70	0.40
1:B:409:HIS:CD2	1:B:419:ALA:HB3	2.54	0.40
1:D:42:PHE:HE1	1:D:99:ALA:HB2	1.87	0.40
1:D:295:ARG:H	1:D:295:ARG:HG3	1.63	0.40
1:E:466:LYS:N	2:O:20:TYR:OH	2.55	0.40
1:F:42:PHE:HE1	1:F:99:ALA:HB2	1.87	0.40
1:H:136:GLU:OE1	1:H:312:ARG:NH2	2.55	0.40
2:K:14:LEU:HD23	2:L:89[A]:VAL:CG2	2.20	0.40
2:M:14:LEU:HD13	2:N:14:LEU:HD21	2.04	0.40
1:A:46:PRO:CD	2:T:3:LEU:HD11	2.38	0.40
1:A:46:PRO:CB	2:S:76:HIS:C	2.85	0.40
1:F:384:VAL:O	1:F:445:LEU:CD1	2.69	0.40
1:H:24:TYR:CE1	1:H:81:LYS:HB2	2.57	0.40
1:H:384:VAL:O	1:H:445:LEU:CD1	2.70	0.40
1:H:473:ASP:HB2	2:T:20:TYR:OH	2.21	0.40
2:S:14:LEU:HD13	2:T:14:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	47	81
1	B	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	47	81
1	C	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	47	81
1	D	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	47	81
1	E	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	47	81
1	F	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	47	81
1	G	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	454/472 (96%)	443 (98%)	10 (2%)	1 (0%)	47 81
2	I	106/155 (68%)	104 (98%)	2 (2%)	0	100 100
2	J	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	17 57
2	K	106/155 (68%)	104 (98%)	2 (2%)	0	100 100
2	L	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	17 57
2	M	106/155 (68%)	104 (98%)	2 (2%)	0	100 100
2	N	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	17 57
2	O	106/155 (68%)	104 (98%)	2 (2%)	0	100 100
2	P	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	17 57
2	Q	106/155 (68%)	104 (98%)	2 (2%)	0	100 100
2	R	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	17 57
2	S	106/155 (68%)	104 (98%)	2 (2%)	0	100 100
2	T	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	17 57
2	U	106/155 (68%)	104 (98%)	2 (2%)	0	100 100
2	V	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	17 57
2	W	106/155 (68%)	104 (98%)	2 (2%)	0	100 100
2	X	107/155 (69%)	102 (95%)	4 (4%)	1 (1%)	17 57
All	All	5336/6256 (85%)	5192 (97%)	128 (2%)	16 (0%)	44 77

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	LYS
1	B	463	LYS
1	C	463	LYS
1	D	463	LYS
1	E	463	LYS
1	F	463	LYS
1	G	463	LYS
1	H	463	LYS
2	J	50	GLN
2	L	50	GLN
2	N	50	GLN
2	P	50	GLN
2	R	50	GLN
2	T	50	GLN

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Mol	Chain	Res	Type
2	V	50	GLN
2	X	50	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	377/383 (98%)	355 (94%)	22 (6%)	20 45
1	B	377/383 (98%)	355 (94%)	22 (6%)	20 45
1	C	377/383 (98%)	355 (94%)	22 (6%)	20 45
1	D	377/383 (98%)	355 (94%)	22 (6%)	20 45
1	E	377/383 (98%)	355 (94%)	22 (6%)	20 45
1	F	377/383 (98%)	355 (94%)	22 (6%)	20 45
1	G	377/383 (98%)	355 (94%)	22 (6%)	20 45
1	H	377/383 (98%)	355 (94%)	22 (6%)	20 45
2	I	85/137 (62%)	76 (89%)	9 (11%)	6 24
2	J	91/137 (66%)	82 (90%)	9 (10%)	8 26
2	K	85/137 (62%)	76 (89%)	9 (11%)	6 24
2	L	91/137 (66%)	82 (90%)	9 (10%)	8 26
2	M	85/137 (62%)	76 (89%)	9 (11%)	6 24
2	N	91/137 (66%)	82 (90%)	9 (10%)	8 26
2	O	85/137 (62%)	76 (89%)	9 (11%)	6 24
2	P	91/137 (66%)	82 (90%)	9 (10%)	8 26
2	Q	85/137 (62%)	76 (89%)	9 (11%)	6 24
2	R	91/137 (66%)	82 (90%)	9 (10%)	8 26
2	S	85/137 (62%)	76 (89%)	9 (11%)	6 24
2	T	91/137 (66%)	82 (90%)	9 (10%)	8 26
2	U	85/137 (62%)	76 (89%)	9 (11%)	6 24
2	V	91/137 (66%)	82 (90%)	9 (10%)	8 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	W	85/137 (62%)	76 (89%)	9 (11%)	6 24
2	X	91/137 (66%)	82 (90%)	9 (10%)	8 26
All	All	4424/5256 (84%)	4104 (93%)	320 (7%)	18 39

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	36	LEU
1	A	41	ARG
1	A	78	ASP
1	A	127	PHE
1	A	134	ARG
1	A	156	GLN
1	A	167	ARG
1	A	203	ASP
1	A	213	ARG
1	A	215	ARG
1	A	217	ARG
1	A	219	LEU
1	A	239	TYR
1	A	241	ASN
1	A	295	ARG
1	A	303	ARG
1	A	319	ARG
1	A	339	LYS
1	A	341	SER
1	A	392	GLU
1	A	450	LYS
1	B	14	LYS
1	B	36	LEU
1	B	41	ARG
1	B	78	ASP
1	B	127	PHE
1	B	134	ARG
1	B	156	GLN
1	B	167	ARG
1	B	203	ASP
1	B	213	ARG
1	B	215	ARG
1	B	217	ARG

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Mol	Chain	Res	Type
1	B	219	LEU
1	B	239	TYR
1	B	241	ASN
1	B	295	ARG
1	B	303	ARG
1	B	319	ARG
1	B	339	LYS
1	B	341	SER
1	B	392	GLU
1	B	450	LYS
1	C	14	LYS
1	C	36	LEU
1	C	41	ARG
1	C	78	ASP
1	C	127	PHE
1	C	134	ARG
1	C	156	GLN
1	C	167	ARG
1	C	203	ASP
1	C	213	ARG
1	C	215	ARG
1	C	217	ARG
1	C	219	LEU
1	C	239	TYR
1	C	241	ASN
1	C	295	ARG
1	C	303	ARG
1	C	319	ARG
1	C	339	LYS
1	C	341	SER
1	C	392	GLU
1	C	450	LYS
1	D	14	LYS
1	D	36	LEU
1	D	41	ARG
1	D	78	ASP
1	D	127	PHE
1	D	134	ARG
1	D	156	GLN
1	D	167	ARG
1	D	203	ASP
1	D	213	ARG

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Mol	Chain	Res	Type
1	D	215	ARG
1	D	217	ARG
1	D	219	LEU
1	D	239	TYR
1	D	241	ASN
1	D	295	ARG
1	D	303	ARG
1	D	319	ARG
1	D	339	LYS
1	D	341	SER
1	D	392	GLU
1	D	450	LYS
1	E	14	LYS
1	E	36	LEU
1	E	41	ARG
1	E	78	ASP
1	E	127	PHE
1	E	134	ARG
1	E	156	GLN
1	E	167	ARG
1	E	203	ASP
1	E	213	ARG
1	E	215	ARG
1	E	217	ARG
1	E	219	LEU
1	E	239	TYR
1	E	241	ASN
1	E	295	ARG
1	E	303	ARG
1	E	319	ARG
1	E	339	LYS
1	E	341	SER
1	E	392	GLU
1	E	450	LYS
1	F	14	LYS
1	F	36	LEU
1	F	41	ARG
1	F	78	ASP
1	F	127	PHE
1	F	134	ARG
1	F	156	GLN
1	F	167	ARG

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Mol	Chain	Res	Type
1	F	203	ASP
1	F	213	ARG
1	F	215	ARG
1	F	217	ARG
1	F	219	LEU
1	F	239	TYR
1	F	241	ASN
1	F	295	ARG
1	F	303	ARG
1	F	319	ARG
1	F	339	LYS
1	F	341	SER
1	F	392	GLU
1	F	450	LYS
1	G	14	LYS
1	G	36	LEU
1	G	41	ARG
1	G	78	ASP
1	G	127	PHE
1	G	134	ARG
1	G	156	GLN
1	G	167	ARG
1	G	203	ASP
1	G	213	ARG
1	G	215	ARG
1	G	217	ARG
1	G	219	LEU
1	G	239	TYR
1	G	241	ASN
1	G	295	ARG
1	G	303	ARG
1	G	319	ARG
1	G	339	LYS
1	G	341	SER
1	G	392	GLU
1	G	450	LYS
1	H	14	LYS
1	H	36	LEU
1	H	41	ARG
1	H	78	ASP
1	H	127	PHE
1	H	134	ARG

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Mol	Chain	Res	Type
1	H	156	GLN
1	H	167	ARG
1	H	203	ASP
1	H	213	ARG
1	H	215	ARG
1	H	217	ARG
1	H	219	LEU
1	H	239	TYR
1	H	241	ASN
1	H	295	ARG
1	H	303	ARG
1	H	319	ARG
1	H	339	LYS
1	H	341	SER
1	H	392	GLU
1	H	450	LYS
2	I	26	VAL
2	I	27	LEU
2	I	49	VAL
2	I	60	PHE
2	I	65	ASP
2	I	66	LEU
2	I	74	ARG
2	I	98	MET
2	I	100	LYS
2	J	2	ASN
2	J	8	LYS
2	J	24	ARG
2	J	27	LEU
2	J	60	PHE
2	J	69	ARG
2	J	74	ARG
2	J	76	HIS
2	J	98	MET
2	K	26	VAL
2	K	27	LEU
2	K	49	VAL
2	K	60	PHE
2	K	65	ASP
2	K	66	LEU
2	K	74	ARG
2	K	98	MET

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Mol	Chain	Res	Type
2	K	100	LYS
2	L	2	ASN
2	L	8	LYS
2	L	24	ARG
2	L	27	LEU
2	L	60	PHE
2	L	69	ARG
2	L	74	ARG
2	L	76	HIS
2	L	98	MET
2	M	26	VAL
2	M	27	LEU
2	M	49	VAL
2	M	60	PHE
2	M	65	ASP
2	M	66	LEU
2	M	74	ARG
2	M	98	MET
2	M	100	LYS
2	N	2	ASN
2	N	8	LYS
2	N	24	ARG
2	N	27	LEU
2	N	60	PHE
2	N	69	ARG
2	N	74	ARG
2	N	76	HIS
2	N	98	MET
2	O	26	VAL
2	O	27	LEU
2	O	49	VAL
2	O	60	PHE
2	O	65	ASP
2	O	66	LEU
2	O	74	ARG
2	O	98	MET
2	O	100	LYS
2	P	2	ASN
2	P	8	LYS
2	P	24	ARG
2	P	27	LEU
2	P	60	PHE

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Mol	Chain	Res	Type
2	P	69	ARG
2	P	74	ARG
2	P	76	HIS
2	P	98	MET
2	Q	26	VAL
2	Q	27	LEU
2	Q	49	VAL
2	Q	60	PHE
2	Q	65	ASP
2	Q	66	LEU
2	Q	74	ARG
2	Q	98	MET
2	Q	100	LYS
2	R	2	ASN
2	R	8	LYS
2	R	24	ARG
2	R	27	LEU
2	R	60	PHE
2	R	69	ARG
2	R	74	ARG
2	R	76	HIS
2	R	98	MET
2	S	26	VAL
2	S	27	LEU
2	S	49	VAL
2	S	60	PHE
2	S	65	ASP
2	S	66	LEU
2	S	74	ARG
2	S	98	MET
2	S	100	LYS
2	T	2	ASN
2	T	8	LYS
2	T	24	ARG
2	T	27	LEU
2	T	60	PHE
2	T	69	ARG
2	T	74	ARG
2	T	76	HIS
2	T	98	MET
2	U	26	VAL
2	U	27	LEU

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Mol	Chain	Res	Type
2	U	49	VAL
2	U	60	PHE
2	U	65	ASP
2	U	66	LEU
2	U	74	ARG
2	U	98	MET
2	U	100	LYS
2	V	2	ASN
2	V	8	LYS
2	V	24	ARG
2	V	27	LEU
2	V	60	PHE
2	V	69	ARG
2	V	74	ARG
2	V	76	HIS
2	V	98	MET
2	W	26	VAL
2	W	27	LEU
2	W	49	VAL
2	W	60	PHE
2	W	65	ASP
2	W	66	LEU
2	W	74	ARG
2	W	98	MET
2	W	100	LYS
2	X	2	ASN
2	X	8	LYS
2	X	24	ARG
2	X	27	LEU
2	X	60	PHE
2	X	69	ARG
2	X	74	ARG
2	X	76	HIS
2	X	98	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	156	GLN
1	A	212	GLN
1	A	229	GLN

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Mol	Chain	Res	Type
1	A	238	HIS
1	A	241	ASN
1	A	267	HIS
1	A	277	ASN
1	A	304	GLN
1	A	353	HIS
1	A	383	HIS
1	A	386	HIS
1	A	401	GLN
1	B	153	HIS
1	B	156	GLN
1	B	212	GLN
1	B	229	GLN
1	B	238	HIS
1	B	241	ASN
1	B	267	HIS
1	B	277	ASN
1	B	304	GLN
1	B	353	HIS
1	B	383	HIS
1	B	386	HIS
1	B	401	GLN
1	C	153	HIS
1	C	156	GLN
1	C	212	GLN
1	C	229	GLN
1	C	238	HIS
1	C	241	ASN
1	C	267	HIS
1	C	277	ASN
1	C	304	GLN
1	C	353	HIS
1	C	383	HIS
1	C	386	HIS
1	C	401	GLN
1	D	153	HIS
1	D	156	GLN
1	D	212	GLN
1	D	229	GLN
1	D	238	HIS
1	D	241	ASN
1	D	267	HIS

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Mol	Chain	Res	Type
1	D	277	ASN
1	D	304	GLN
1	D	353	HIS
1	D	383	HIS
1	D	386	HIS
1	D	401	GLN
1	E	153	HIS
1	E	156	GLN
1	E	212	GLN
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN
1	E	267	HIS
1	E	277	ASN
1	E	304	GLN
1	E	353	HIS
1	E	383	HIS
1	E	386	HIS
1	E	401	GLN
1	F	153	HIS
1	F	156	GLN
1	F	212	GLN
1	F	229	GLN
1	F	238	HIS
1	F	241	ASN
1	F	267	HIS
1	F	277	ASN
1	F	304	GLN
1	F	353	HIS
1	F	383	HIS
1	F	386	HIS
1	F	401	GLN
1	G	153	HIS
1	G	156	GLN
1	G	212	GLN
1	G	229	GLN
1	G	238	HIS
1	G	241	ASN
1	G	267	HIS
1	G	277	ASN
1	G	304	GLN
1	G	353	HIS

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Mol	Chain	Res	Type
1	G	383	HIS
1	G	386	HIS
1	G	401	GLN
1	H	153	HIS
1	H	156	GLN
1	H	212	GLN
1	H	229	GLN
1	H	238	HIS
1	H	241	ASN
1	H	267	HIS
1	H	277	ASN
1	H	304	GLN
1	H	353	HIS
1	H	383	HIS
1	H	386	HIS
1	H	401	GLN
2	J	2	ASN
2	J	42	HIS
2	L	2	ASN
2	L	42	HIS
2	N	2	ASN
2	N	42	HIS
2	O	76	HIS
2	P	2	ASN
2	P	42	HIS
2	R	2	ASN
2	R	42	HIS
2	T	2	ASN
2	T	42	HIS
2	V	2	ASN
2	V	42	HIS
2	X	2	ASN
2	X	42	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	10
1	B	10
1	G	10
1	C	10
1	D	10
1	E	10
1	F	10
1	H	10

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	470:GLU	C	471:THR	N	3.94
1	B	470:GLU	C	471:THR	N	3.94
1	G	470:GLU	C	471:THR	N	3.94
1	C	470:GLU	C	471:THR	N	3.93
1	D	470:GLU	C	471:THR	N	3.93
1	E	470:GLU	C	471:THR	N	3.93
1	F	470:GLU	C	471:THR	N	3.93
1	H	470:GLU	C	471:THR	N	3.93
1	A	468:GLU	C	469:PHE	N	3.30
1	B	468:GLU	C	469:PHE	N	3.30
1	C	468:GLU	C	469:PHE	N	3.30
1	D	468:GLU	C	469:PHE	N	3.30
1	E	468:GLU	C	469:PHE	N	3.30

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	468:GLU	C	469:PHE	N	3.30
1	G	468:GLU	C	469:PHE	N	3.30
1	H	468:GLU	C	469:PHE	N	3.30
1	A	464:GLU	C	465:ILE	N	3.10
1	B	464:GLU	C	465:ILE	N	3.10
1	C	464:GLU	C	465:ILE	N	3.10
1	D	464:GLU	C	465:ILE	N	3.10
1	E	464:GLU	C	465:ILE	N	3.10
1	F	464:GLU	C	465:ILE	N	3.10
1	G	464:GLU	C	465:ILE	N	3.10
1	H	464:GLU	C	465:ILE	N	3.10
1	A	467:PHE	C	468:GLU	N	3.08
1	B	467:PHE	C	468:GLU	N	3.08
1	C	467:PHE	C	468:GLU	N	3.08
1	D	467:PHE	C	468:GLU	N	3.08
1	E	467:PHE	C	468:GLU	N	3.08
1	F	467:PHE	C	468:GLU	N	3.08
1	G	467:PHE	C	468:GLU	N	3.08
1	H	467:PHE	C	468:GLU	N	3.08
1	A	472:MET	C	473:ASP	N	2.89
1	B	472:MET	C	473:ASP	N	2.89
1	C	472:MET	C	473:ASP	N	2.89
1	D	472:MET	C	473:ASP	N	2.89
1	E	472:MET	C	473:ASP	N	2.89
1	F	472:MET	C	473:ASP	N	2.89
1	G	472:MET	C	473:ASP	N	2.89
1	H	472:MET	C	473:ASP	N	2.89
1	A	469:PHE	C	470:GLU	N	2.66
1	B	469:PHE	C	470:GLU	N	2.66
1	C	469:PHE	C	470:GLU	N	2.66
1	D	469:PHE	C	470:GLU	N	2.66
1	E	469:PHE	C	470:GLU	N	2.66
1	F	469:PHE	C	470:GLU	N	2.66
1	G	469:PHE	C	470:GLU	N	2.66
1	H	469:PHE	C	470:GLU	N	2.66
1	A	409:HIS	C	410:PRO	N	2.56
1	B	409:HIS	C	410:PRO	N	2.56
1	C	409:HIS	C	410:PRO	N	2.56
1	D	409:HIS	C	410:PRO	N	2.56
1	E	409:HIS	C	410:PRO	N	2.56
1	F	409:HIS	C	410:PRO	N	2.56
1	G	409:HIS	C	410:PRO	N	2.56

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	409:HIS	C	410:PRO	N	2.56
1	A	471:THR	C	472:MET	N	1.81
1	B	471:THR	C	472:MET	N	1.81
1	C	471:THR	C	472:MET	N	1.81
1	D	471:THR	C	472:MET	N	1.81
1	E	471:THR	C	472:MET	N	1.81
1	F	471:THR	C	472:MET	N	1.81
1	G	471:THR	C	472:MET	N	1.81
1	H	471:THR	C	472:MET	N	1.81
1	A	465:ILE	C	466:LYS	N	1.09
1	B	465:ILE	C	466:LYS	N	1.09
1	C	465:ILE	C	466:LYS	N	1.09
1	D	465:ILE	C	466:LYS	N	1.09
1	E	465:ILE	C	466:LYS	N	1.09
1	F	465:ILE	C	466:LYS	N	1.09
1	G	465:ILE	C	466:LYS	N	1.09
1	H	465:ILE	C	466:LYS	N	1.09
1	A	466:LYS	C	467:PHE	N	1.05
1	B	466:LYS	C	467:PHE	N	1.05
1	C	466:LYS	C	467:PHE	N	1.05
1	D	466:LYS	C	467:PHE	N	1.05
1	E	466:LYS	C	467:PHE	N	1.05
1	F	466:LYS	C	467:PHE	N	1.05
1	G	466:LYS	C	467:PHE	N	1.05
1	H	466:LYS	C	467:PHE	N	1.05

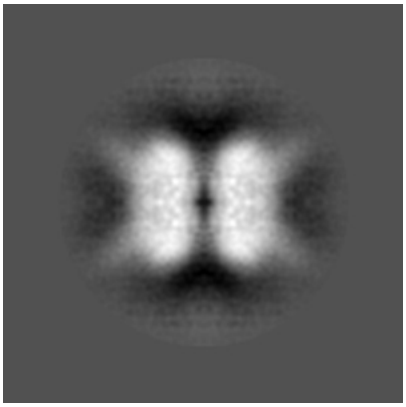
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1655. These allow visual inspection of the internal detail of the map and identification of artifacts.

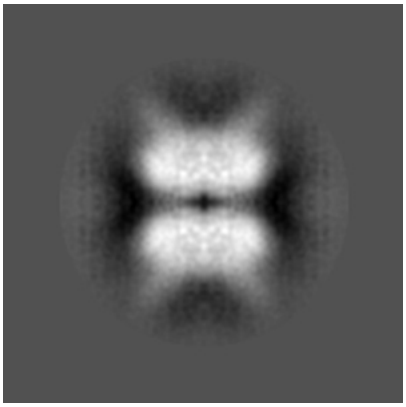
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

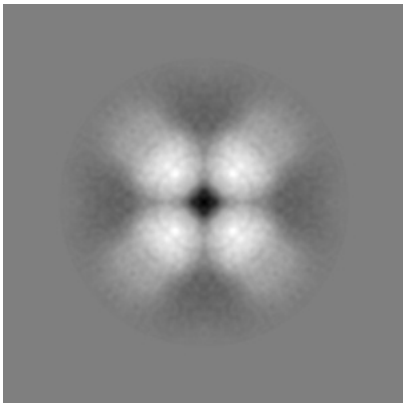
6.1.1 Primary map



X



Y

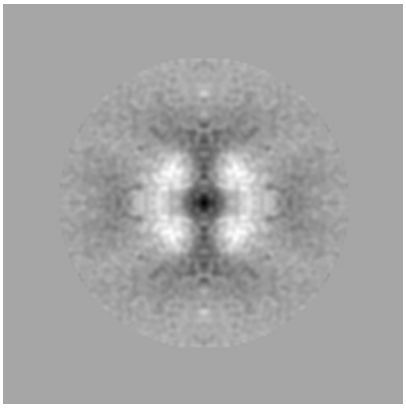


Z

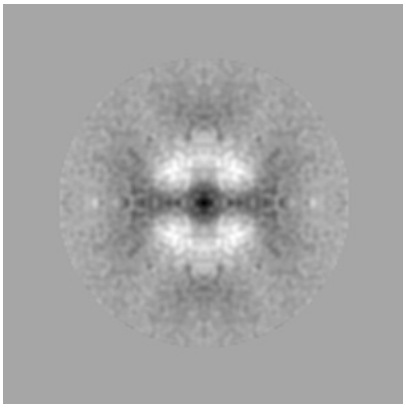
The images above show the map projected in three orthogonal directions.

6.2 Central slices

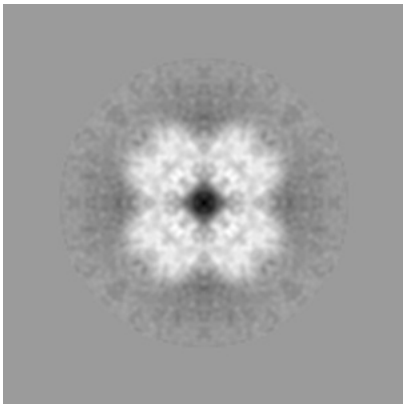
6.2.1 Primary map



X Index: 88



Y Index: 88

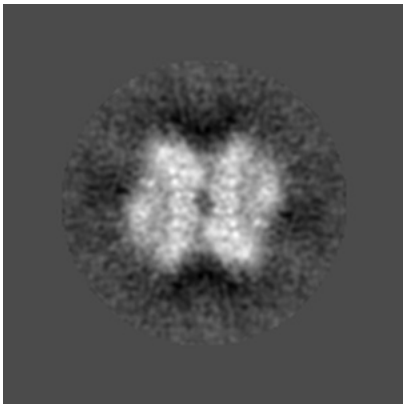


Z Index: 88

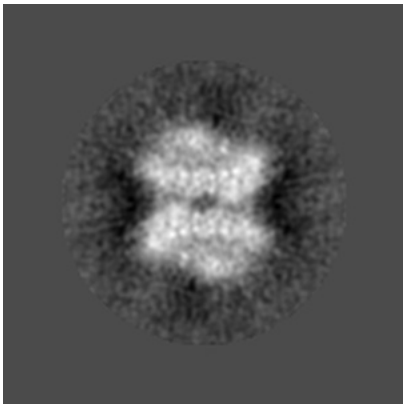
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

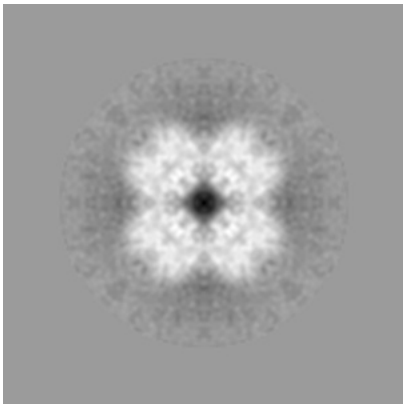
6.3.1 Primary map



X Index: 76



Y Index: 76

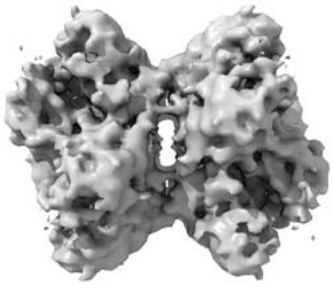


Z Index: 88

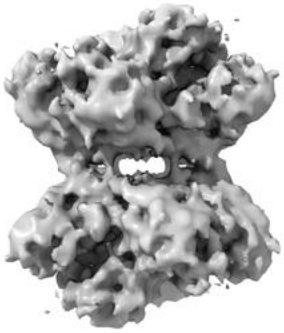
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

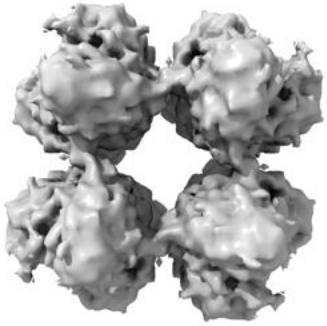
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

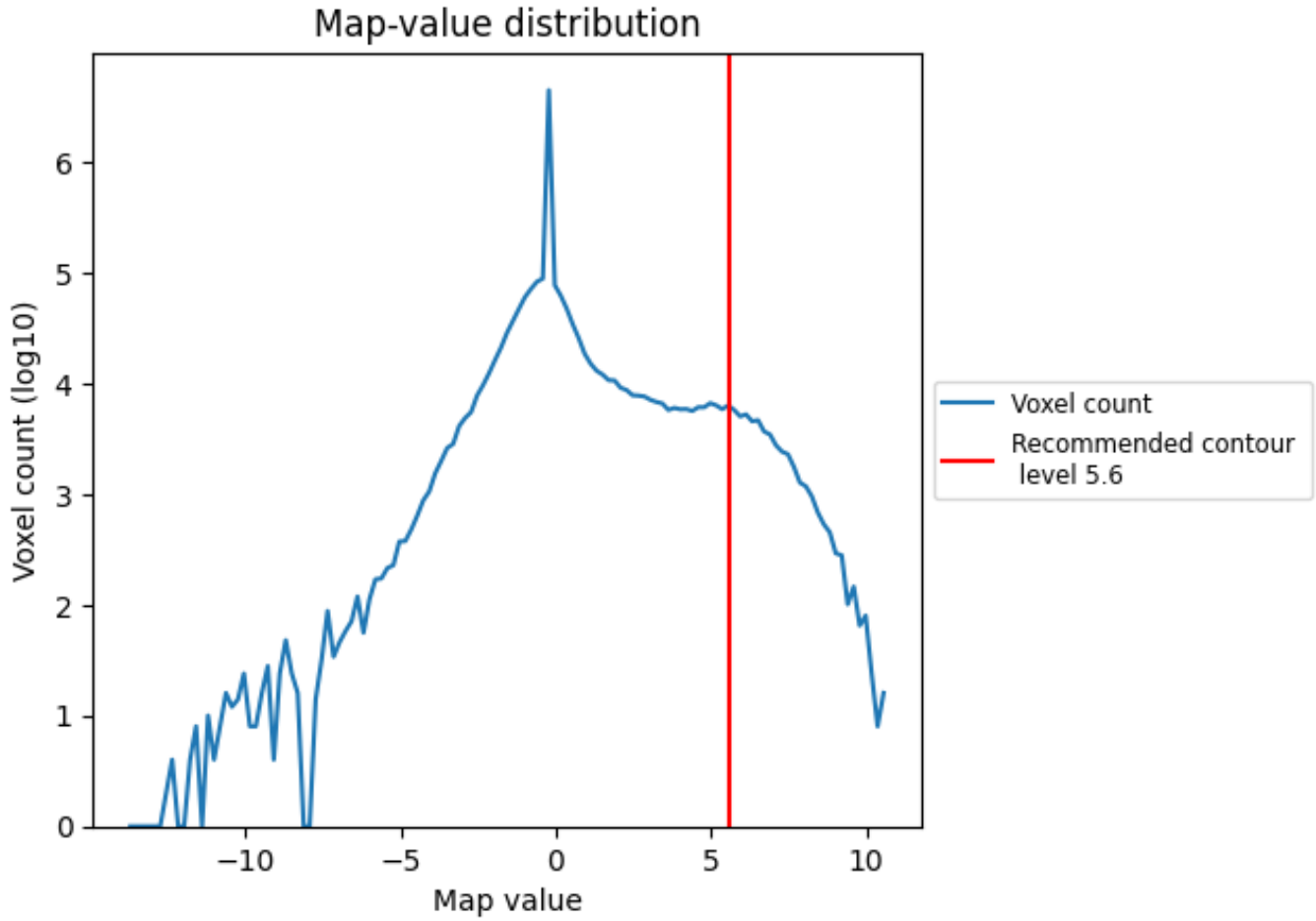
6.5 Mask visualisation (i)

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

7 Map analysis

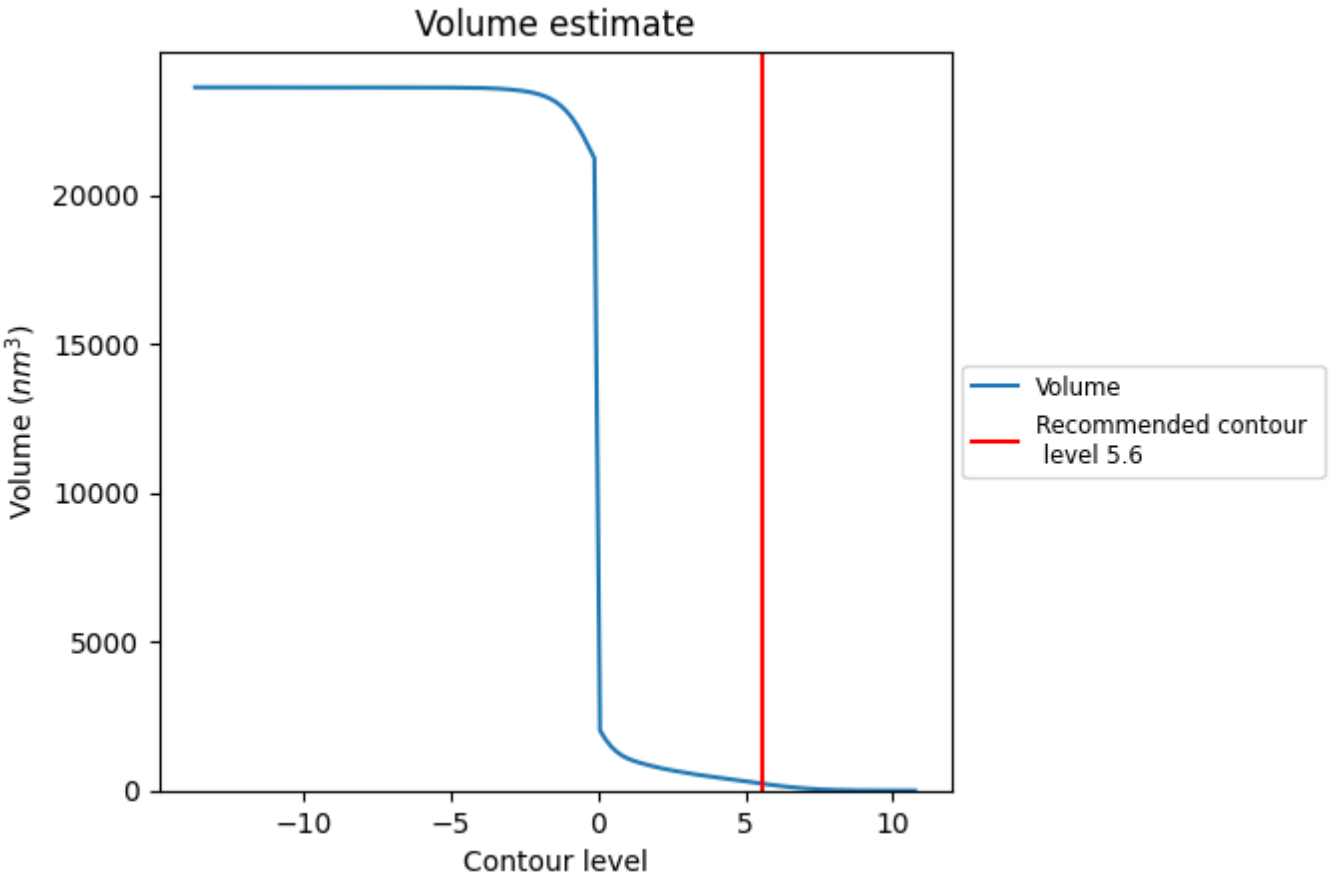
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

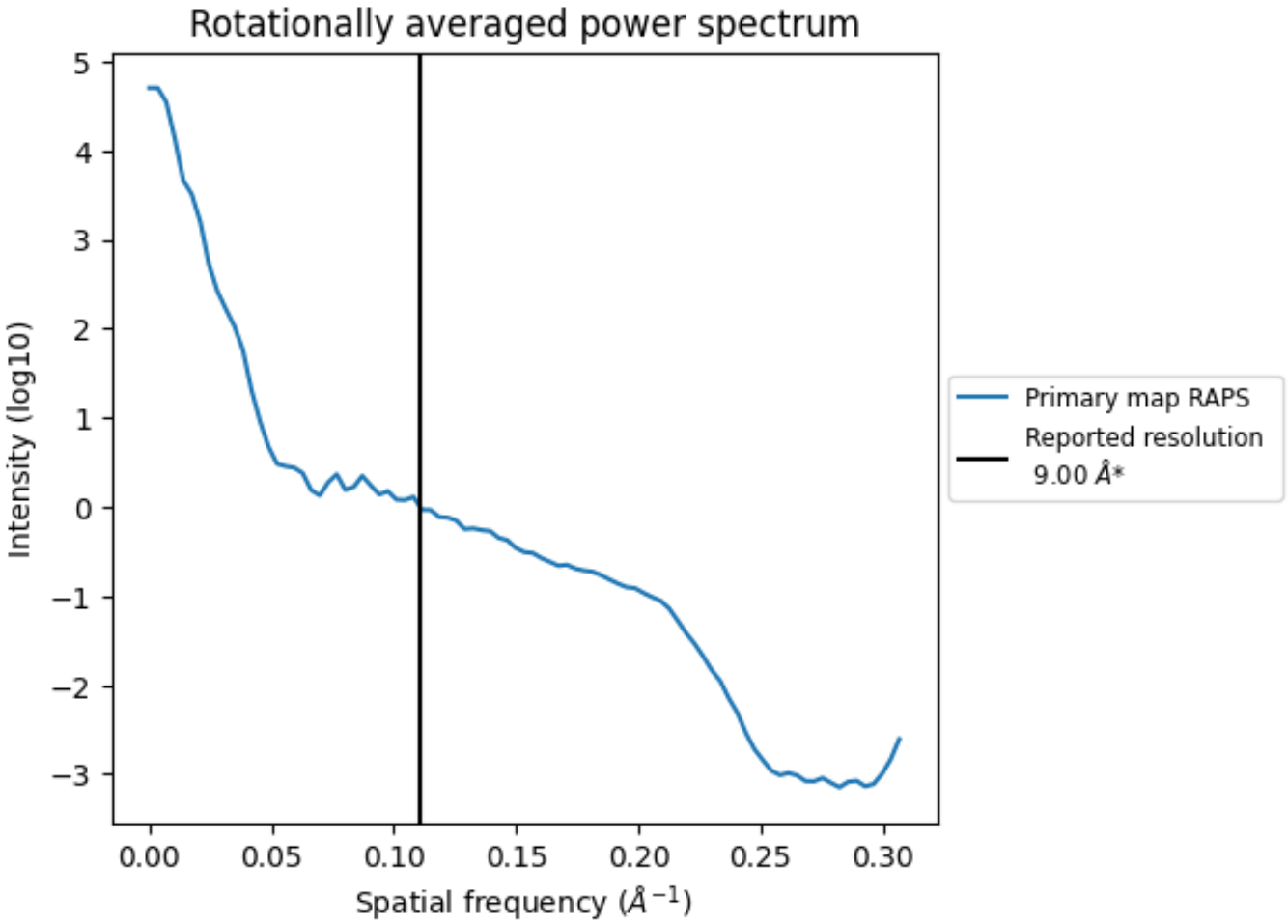
7.2 Volume estimate



The volume at the recommended contour level is 228 nm^3; this corresponds to an approximate mass of 206 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)



*Reported resolution corresponds to spatial frequency of 0.111 Å^{-1}

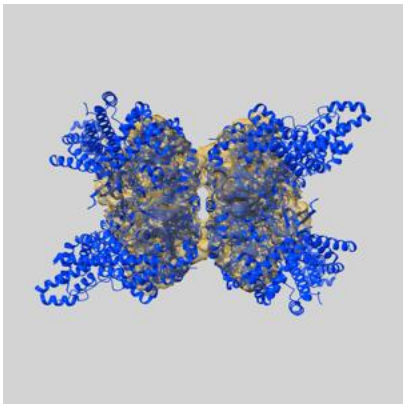
8 Fourier-Shell correlation

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

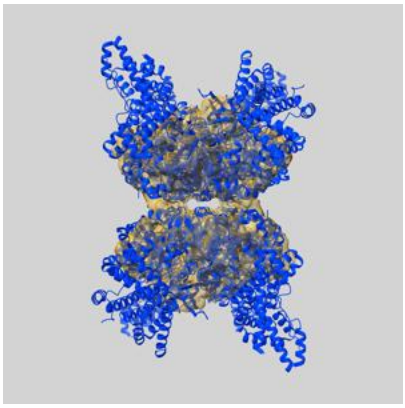
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1655 and PDB model 2WVW. Per-residue inclusion information can be found in section 3 on page 6.

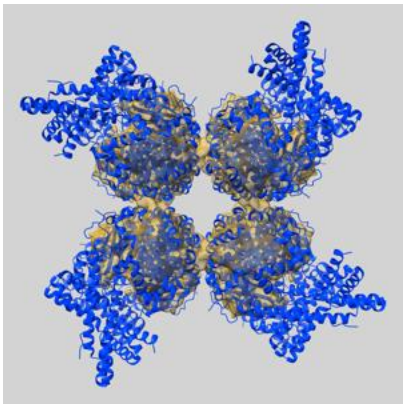
9.1 Map-model overlay



X



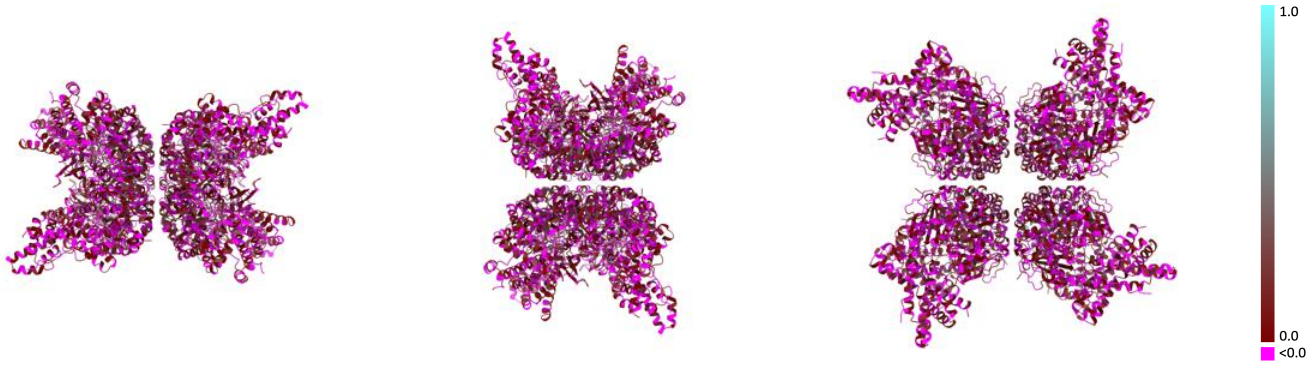
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.6 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.

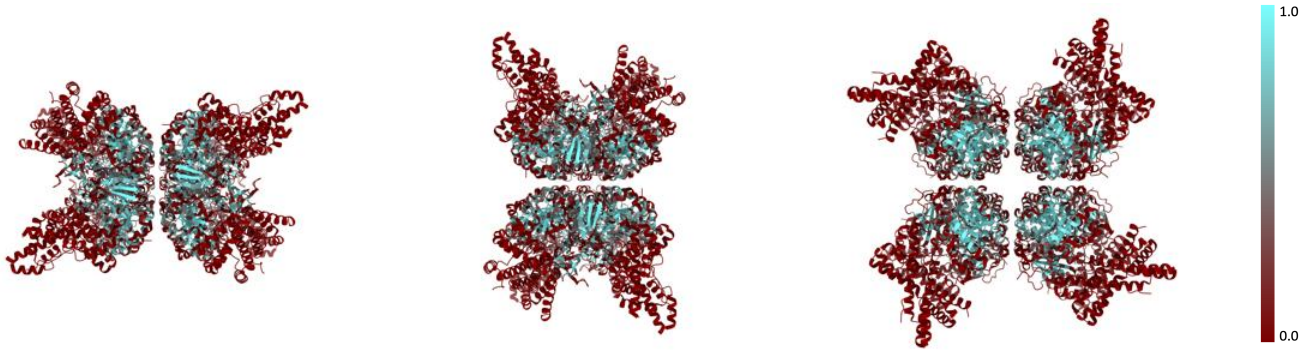
9.2 Q-score mapped to coordinate model



X Y Z

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.

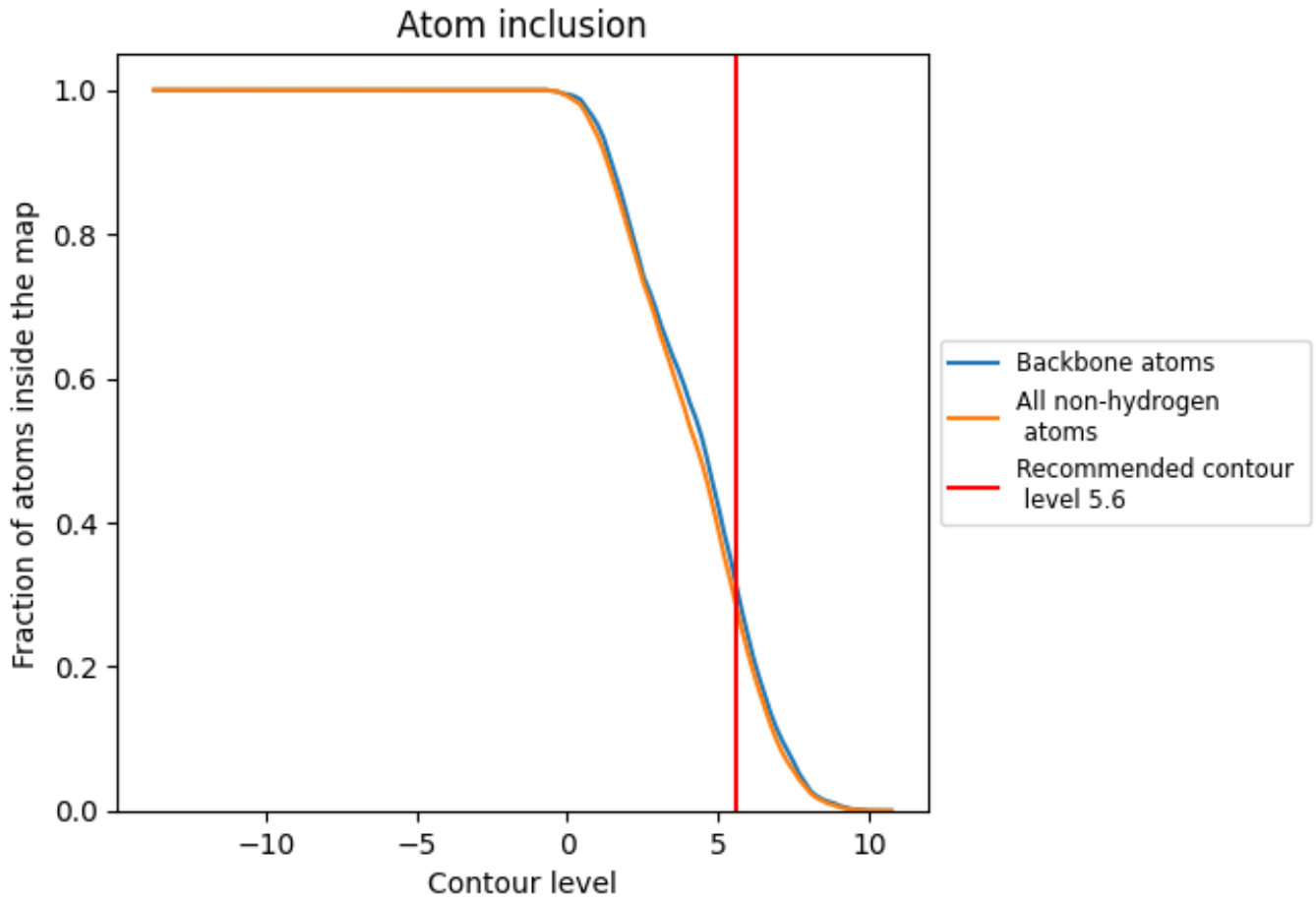
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (5.6).

9.4 Atom inclusion (i)



At the recommended contour level, 31% of all backbone atoms, 28% 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 (5.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2848	0.0300
A	0.4122	0.0390
B	0.4133	0.0370
C	0.4139	0.0320
D	0.4119	0.0340
E	0.4108	0.0320
F	0.4102	0.0360
G	0.4128	0.0300
H	0.4139	0.0300
I	0.0000	0.0010
J	0.0061	0.0380
K	0.0000	0.0010
L	0.0061	0.0360
M	0.0000	0.0060
N	0.0061	0.0380
O	0.0000	0.0030
P	0.0061	0.0400
Q	0.0000	0.0060
R	0.0061	0.0430
S	0.0000	0.0060
T	0.0061	0.0380
U	0.0000	0.0020
V	0.0061	0.0390
W	0.0000	0.0060
X	0.0061	0.0400