



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:10 AM UTC

PDB ID : 8AIX / pdb_00008aix
EMDB ID : EMD-15473
Title : Cryo-EM structure of crescentin filaments (wildtype, C2 symmetry and large box)
Authors : Liu, Y.; Lowe, J.
Deposited on : 2022-07-27
Resolution : 5.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

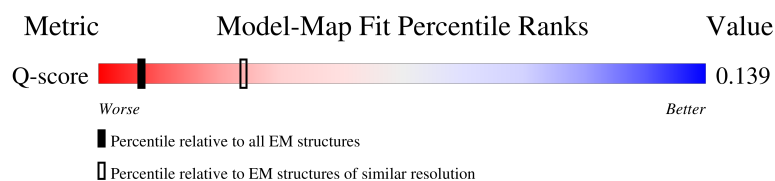
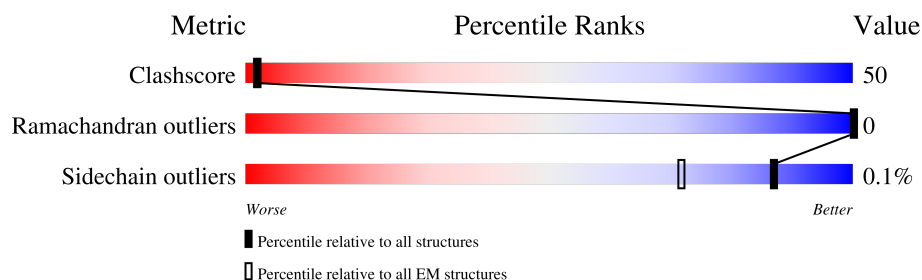
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.80 Å.

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



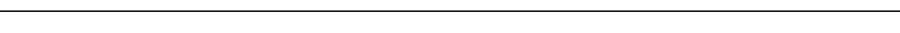
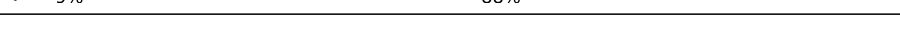
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	511 (5.30 - 6.30)

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

Mol	Chain	Length	Quality of chain
1	A	457	
1	B	457	
1	E	457	
1	F	457	

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Mol	Chain	Length	Quality of chain
1	G	457	 14% 26% 60%
1	H	457	 10% 30% 61%
1	K	457	 7% 9% 84%
1	L	457	 9% 9% 82%
1	M	457	 9% 24% 68%
1	N	457	 13% 21% 66%
1	Q	457	 14% 26% 60%
1	R	457	 10% 30% 61%
1	U	457	 6% 10% 84%
1	V	457	 9% 10% 82%
1	W	457	 9% 24% 68%
1	X	457	 14% 20% 66%
2	C	907	 7% 90%
2	D	907	 8% 88%
2	I	907	 9% 88%
2	J	907	 8% 88%
2	O	907	 7% 90%
2	P	907	 8% 88%
2	S	907	 9% 88%
2	T	907	 8% 88%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21924 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 Crescentin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	84	Total	C	N	O	S	0	0
			655	390	134	130	1		
1	B	85	Total	C	N	O	S	0	0
			664	395	136	132	1		
1	G	183	Total	C	N	O	S	0	0
			1400	844	269	286	1		
1	H	179	Total	C	N	O	S	0	0
			1373	829	264	279	1		
1	K	72	Total	C	N	O	S	0	0
			556	341	104	110	1		
1	L	84	Total	C	N	O	S	0	0
			643	393	124	125	1		
1	M	147	Total	C	N	O	S	0	0
			1142	677	234	228	3		
1	N	156	Total	C	N	O	S	0	0
			1207	714	247	243	3		
1	E	84	Total	C	N	O	S	0	0
			655	390	134	130	1		
1	F	85	Total	C	N	O	S	0	0
			664	395	136	132	1		
1	Q	183	Total	C	N	O	S	0	0
			1400	844	269	286	1		
1	R	179	Total	C	N	O	S	0	0
			1373	829	264	279	1		
1	U	72	Total	C	N	O	S	0	0
			556	341	104	110	1		
1	V	84	Total	C	N	O	S	0	0
			643	393	124	125	1		
1	W	147	Total	C	N	O	S	0	0
			1142	677	234	228	3		
1	X	156	Total	C	N	O	S	0	0
			1207	714	247	243	3		

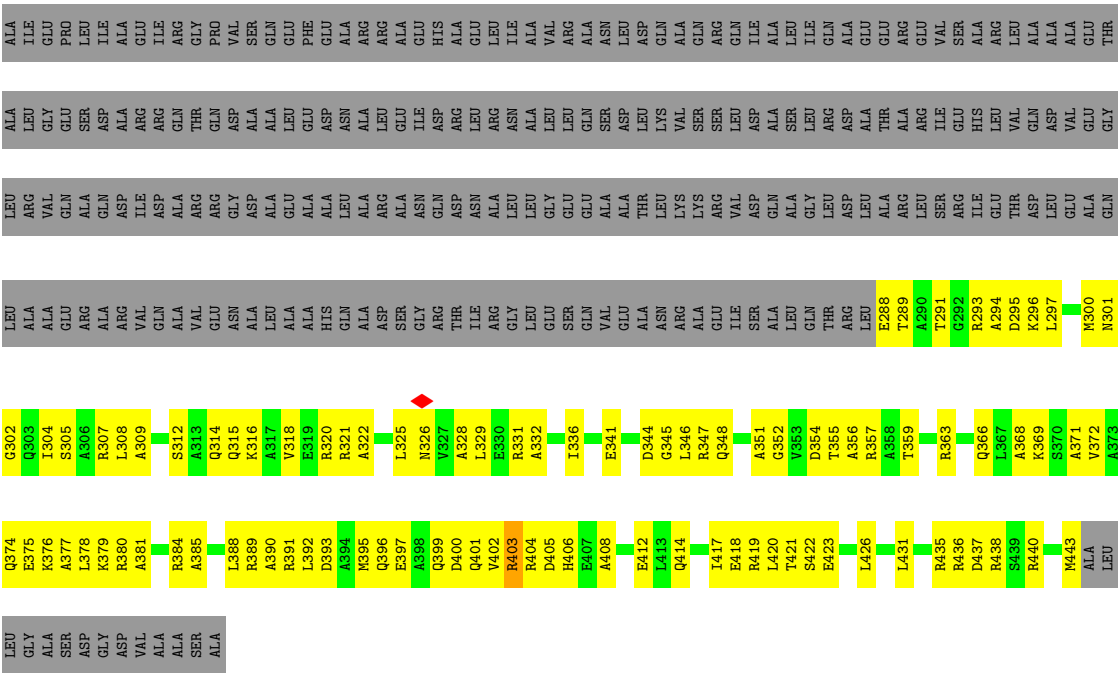
- Molecule 2 is a protein called Crescentin-specific megabody MB13.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	J	111	Total	C	N	O	S	0	0
			860	534	154	167	5		
2	C	94	Total	C	N	O	S	0	0
			724	449	129	142	4		
2	I	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	P	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	T	111	Total	C	N	O	S	0	0
			860	534	154	167	5		
2	O	94	Total	C	N	O	S	0	0
			724	449	129	142	4		
2	S	112	Total	C	N	O	S	0	0
			869	539	155	170	5		

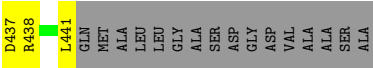
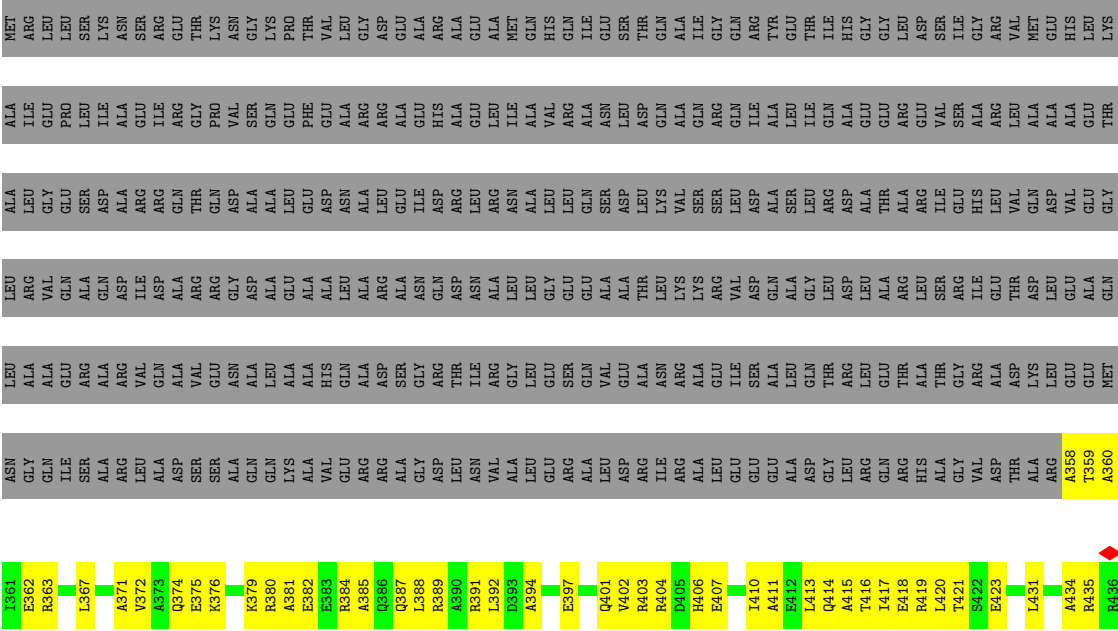
Chain H: 10% 30% 61%







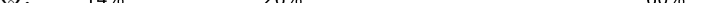
● Molecule 1: Crescentin

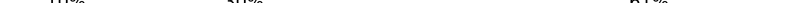


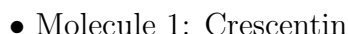
● Molecule 1: Crescentin



R436	R438	R440	R442	MET
D437	S439	L441	Q442	ALA
				LEU
				LEU
				GLY
				ALA
				SER
				ASP
				GLY
				ASP
				VAL
				ALA
				ALA
				SER
				ALA

Chain Q:  14% 26% 60%

Chain R:  10% 30% 61%



ARG	LEU	VAL	HIS	ALA	ASP	E63
SER	LYS	GLU	GLN	ALA	ASN	P64
ARG	ARG	ARG	ALA	ALA	ALA	P65
LEU	ALA	ARG	ASP	ALA	LEU	I66
GLN	GLU	ALA	SER	ALA	GLU	A67
MET	GLU	GLY	GLY	ASN	ILE	E68
ALA	ARG	ASP	ARG	GLN	ASP	I69
LEU	ALA	LEU	THR	ASP	ARG	R70
LEU	ALA	ASN	ILE	ASN	LEU	G71
GLY	GLN	VAL	ARG	ALA	ARG	P72
ALA	LEU	ALA	GLY	LEU	ASN	V73
SER	ARG	LEU	LEU	GLY	LEU	S74
ASP	ALA	GLU	SER	GLU	LEU	Q75
GLY	ARG	ARG	SER	GLU	GLN	E78
ASP	LEU	ALA	GLN	GLU	LEU	A79
VAL	ASP	LEU	VAL	ALA	SER	R80
ALA	ALA	ASP	GLU	ALA	ASP	E84
SER	MET	ARG	ALA	THR	LEU	H84
ALA	GLN	ILE	ASN	LEU	LYS	A85
SER	GLN	ARG	ARG	LEU	VAL	E86
ALA	ALA	ALA	ALA	LYS	SER	L87
VAL	GLN	LEU	GLU	ARG	SER	V90
ASP	ASP	GLU	ILE	VAL	LEU	R91
GLN	GLN	ARG	SER	ASP	ASP	A92
VAL	VAL	GLU	ALA	GLN	ALA	D95
ARG	ARG	ALA	LEU	ALA	SER	Q96
ARG	ARG	ALA	LEU	ALA	LEU	A97
LYS	LYS	GLN	LEU	ALA	THR	Q100
ILE	ILE	HIS	THR	ARG	ALA	I101
GLU	GLU	THR	ALA	LEU	ARG	E104
SER	SER	THR	ALA	LEU	ILE	Q105
THR	THR	GLY	GLY	ARG	GLU	A106
GLN	GLN	ARG	ILE	ILE	HIS	E107
ALA	ALA	ASP	ALA	THR	LEU	E108
ILE	ALA	THR	ASP	ASP	GLN	R109
GLY	ILE	ARG	LYS	LEU	VAL	V111
ARG	ARG	ALA	LEU	GLU	GLU	E114
THR	THR	THR	ALA	GLY	GLY	R114
SER	SER	ILE	ASN	LEU	LEU	A117
GLU	GLU	ARG	GLY	ALA	ARG	A118
ALA	ALA	GLN	GLN	VAL	VAL	E119
ALA	ALA	ILE	ILE	GLU	GLN	T120
LEU	LEU	ALA	ALA	ALA	GLN	R128
ALA	ALA	GLN	ARG	ALA	ASP	ARG
GLU	GLU	LEU	LEU	VAL	ILE	GLN
GLY	LYS	LYS	ASP	GLN	ASP	THR
LEU	ALA	ASP	ALA	VAL	ARG	GLN
LEU	VAL	VAL	SER	GLU	ARG	ASP
ALA	ALA	ALA	ALA	ASN	GLY	ALA
ARG	ALA	GLN	GLN	ALA	ASP	ALA
ASP	LYS	LYS	LYS	LEU	ALA	LEU
ARG	ALA	ALA	ALA	ALA	GLU	GLU
ASP	ASP	ALA	ALA	ALA	ALA	ALA

Chain W: 9% 24% 68%

A433	E362	N301	LEU	LEU	ARG	ALA
A434	G302	Q302	ALA	ALA	VAL	GLY
R435	A371	Q303	GLU	GLU	GLN	GLU
R436		I304	ARG	ALA	GLN	SER
D437	Q374	S305	ALA	GLN	ASP	ILE
R438	E375	A306	ALA	GLN	ASP	ALA
S439	K376	R307	ARG	ASP	ALA	ASN
R440	A377	L308	VAL	ILE	ARG	SER
L441	L378	A399	GLN	GLN	ARG	ARG
Q442	K379	D310	ALA	ALA	GLN	ARG
M443	R380	S311	VAL	VAL	THR	THR
ALA	A381	S312	GLU	GLU	GLN	PRO
LEU	E362	A313	ASN	ASN	ASP	VAL
LEU	E383	Q314	ALA	ALA	ASP	VAL
GLY	R384	Q315	LEU	LEU	ALA	SER
ALA	A385	A316	ALA	ALA	GLN	GLY
SER	Q386	K317	ALA	ALA	GLU	PHE
ASP	Q387	V318	HIS	ALA	ASP	GLU
GLY	L388	E319	GLN	GLN	ASN	ALA
ASP	R389	R320	ALA	ALA	LEU	ALA
VAL	A390	R321	ASP	ARG	LEU	ARG
ALA	R391	A322	SER	ALA	GLU	ASP
ALA	L392	G323	GLY	ASN	ILE	GLU
SER	D393	D324	ARG	GLN	ASP	ALA
ALA	A394	L325	THR	ASP	ARG	ALA
	M395	N326	ILE	ASN	LEU	ALA
	Q399	A328	GLY	LEU	ASN	ILE
D400	D400	L329	LEU	LEU	ALA	ALA
		E330	GLU	GLY	LEU	VAL
R403		R331	SER	GLU	LEU	ARG
A404	A332	A332	GLN	GLU	GLN	ALA
D405	L333	D334	VAL	ALA	SER	ALA
H406	D334	D334	GLU	ALA	ASP	ASN
E407	E407	R335	ALA	THR	LEU	SER
A408	A408	I336	ASN	LEU	LYS	GLN
K409	R337	R337	ARG	LYS	VAL	ALA
I410	A338	A338	ALA	LYS	SER	ALA
A411	L339	L339	GLU	ARG	SER	GLY
E412	E340	E340	ILE	VAL	LEU	GLN
L413	E341	E341	SER	ASP	ASP	GLN
Q414	E342	E342	ALA	GLN	ALA	ALA
A415	A343	A343	LEU	LEU	SER	LEU
T416	D344	D344	GLN	GLY	LEU	ILE
I417	G345	G345	THR	LEU	ARG	ILE
E418	L346	L346	ARG	ASP	ASP	ALA
R419	R347	R347	LEU	LEU	ALA	GLU
L420	Q348	Q348	GLU	ALA	THR	GLY
T421	R349	R349	THR	ARG	ALA	ARG
S422			ALA	LEU	ASP	LEU
E423	G352	G352	THR	SER	ILE	SER
A424	V353	V353	GLY	ARG	GLU	VAL
A425	D354	D354	ILE	ILE	ALA	GLE
L426	T355	T355	ALA	GLU	LEU	ALA
A427	A356	A356	ASP	THR	VAL	ARG
E428	R357	R357	LYS	ASP	GLN	VAL
G429	A358	A358	LEU	LEU	ALA	ALA
A430	T359	T359	GLU	GLU	VAL	ALA
L431	A360	A360	ALA	GLU	GLY	GLU
E432	I361	I361	GLN	GLN	THR	LYS

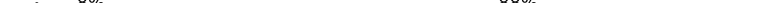
[illegible]

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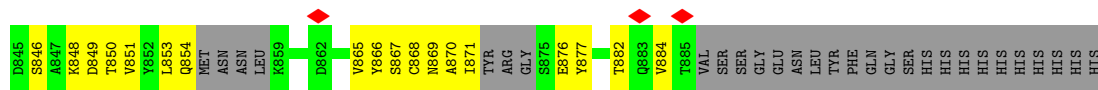
- Molecule 2: Crescentin-specific megabody MB13

Chain J:  8% 88%

[illegible]

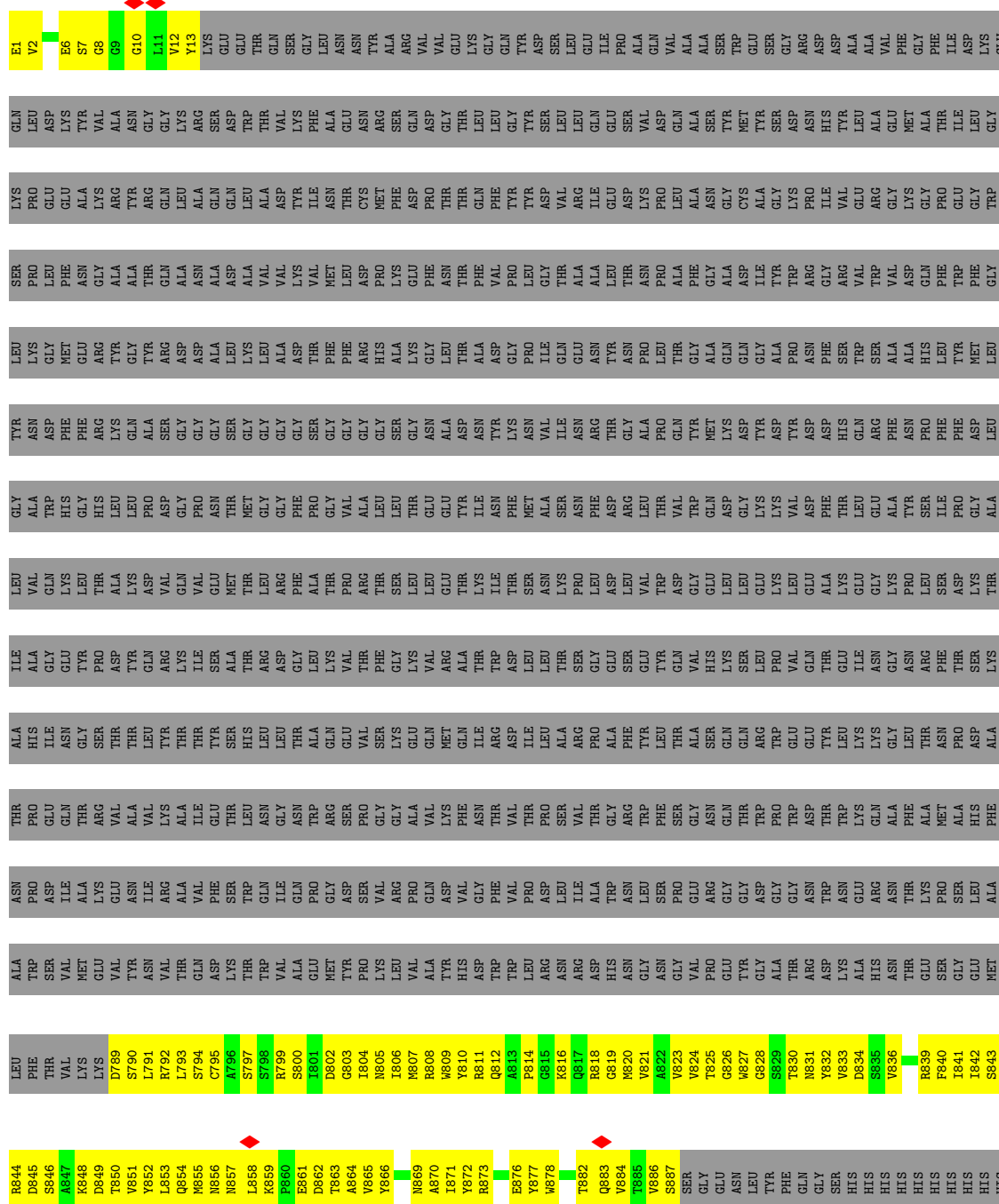
[illegible]

Chain C: 7% 90%



• Molecule 2: Crescentin-specific megabody MB13

Chain I: 9% 88%



• Molecule 2: Crescentin-specific megabody MB13

Chain P: 8% 88%



Chain T: 8%



[illegible]

Chain 0: 7% 90%



B844	D845	S846	A847	K848	D849	T850	V851	Y852	L853	Q854	M855	N856	N857	L858	K859	P860	E861	D862	T863	A864	V865	V866		N869	A870	I871	Y872	B873		E876	Y877	W878		T882	Q883	V884	T885	V886	S887	SER	GLY	GLU	ASN	LEU	TYR	PHE	GLN	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS					
LEU	PHE	THR	VAL	LYS	D789	S790	L791	R792	L793	S794	C795	A796	S797	S798	R799	S800	I801	D802	G803	I804	N805	I806	M807	R808	W809	Y810	R811	Q812	A813	P814	G815	K816	R818	G819	M820	V821	A822	V823	V824	T825	G826	W827	S829	T830	N831	Y832	V833	D834	S835	V836		R839	F840	I841	I842	S843								
ALA	TRP	ASP	ILE	MET	VAL	TYR	ASN	VAL	THR	GLN	ASP	LYS	THR	TRP	GLN	ALA	GLU	MET	TYR	PRO	LYS	LEU	VAL	R808	W809	Y810	R811	Q812	A813	P814	G815	K816	R818	G819	M820	V821	A822	V823	V824	T825	G826	W827	S829	T830	N831	Y832	V833	D834	S835	V836		R839	F840	I841	I842	S843								
ASN	PRO	ASP	ILE	MET	GLU	ASN	ILE	ARG	ALA	VAL	PHE	SER	THR	LEU	ASN	GLN	PRO	GLY	TYR	ASP	VAL	ARG	PRO	GLN	ASP	VAL	ASP	PHE	VAL	PRO	ASP	ILE	VAL	ASP	HIS	ASN	GLY	LEU	PRO	GLY	VAL	GLU	PRO	ARG	GLN	GLY	THR	ALA	ASP	LYS	ASN	GLU	ARG	THR	LYS	PRO	SER	GLY	LEU	ALA				
THR	PRO	GLU	GLN	THR	ARG	VAL	ALA	LYS	THR	ALA	ILE	GLU	THR	LEU	ASN	GLY	TRP	ARG	SER	PRO	VAL	PHE	GLY	LYS	GLN	VAL	PHE	ASN	THR	VAL	THR	PRO	ILE	VAL	THR	GLY	ASN	GLN	VAL	ALA	GLY	ASN	GLN	THR	TRP	ASP	THR	THR	TRP	GLU	ILE	LYS	ASN	GLY	THR	ALA	PHE	THR	ASN	PRO	THR	ASP	LEU	ALA
ILE	ALA	GLY	GLU	TYR	PRO	ASP	THR	SER	LYS	ARG	VAL	THR	ALA	THR	HIS	LEU	ASP	GLY	LEU	THR	PHE	GLY	LYS	GLN	VAL	MET	GLN	ILE	THR	ARG	ASP	ILE	VAL	THR	GLY	ASN	GLN	VAL	ALA	GLY	ASN	GLN	THR	TRP	VAL	PRO	THR	LEU	ILE	LYS	ASN	GLY	THR	ALA	ARG	PHE	THR	ASN	PRO	THR	ASP	LEU	ALA	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	550574	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.942	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	972.0, 972.0, 972.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.944, 1.944, 1.944	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	0.35	0/655	0.75	0/875
1	B	0.41	0/664	0.89	0/887
1	E	0.35	0/655	0.75	0/875
1	F	0.41	0/664	0.88	0/887
1	G	0.28	0/1407	0.65	0/1899
1	H	0.30	0/1380	0.64	0/1862
1	K	0.21	0/560	0.49	0/755
1	L	0.25	0/648	0.55	0/872
1	M	0.29	0/1143	0.63	0/1528
1	N	0.35	0/1208	0.78	1/1615 (0.1%)
1	Q	0.28	0/1407	0.65	0/1899
1	R	0.31	0/1380	0.64	0/1862
1	U	0.21	0/560	0.49	0/755
1	V	0.24	0/648	0.55	0/872
1	W	0.29	0/1143	0.63	0/1528
1	X	0.35	0/1208	0.78	1/1615 (0.1%)
2	C	0.46	0/734	0.75	1/988 (0.1%)
2	D	0.34	0/883	0.61	0/1192
2	I	0.43	0/883	0.73	0/1192
2	J	0.37	0/874	0.67	0/1180
2	O	0.46	0/734	0.75	1/988 (0.1%)
2	P	0.34	0/883	0.60	0/1192
2	S	0.43	0/883	0.73	0/1192
2	T	0.38	0/874	0.67	0/1180
All	All	0.34	0/22078	0.68	4/29690 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	403	ARG	CB-CG-CD	6.24	125.66	111.30
1	X	403	ARG	CB-CG-CD	6.21	125.59	111.30
2	O	798	SER	N-CA-C	-5.43	107.20	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	798	SER	N-CA-C	-5.43	107.20	113.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	655	0	667	72	0
1	B	664	0	674	70	0
1	E	655	0	667	71	0
1	F	664	0	674	71	0
1	G	1400	0	1389	138	0
1	H	1373	0	1364	179	0
1	K	556	0	557	44	0
1	L	643	0	646	49	0
1	M	1142	0	1151	145	0
1	N	1207	0	1214	119	0
1	Q	1400	0	1389	139	0
1	R	1373	0	1364	179	0
1	U	556	0	557	47	0
1	V	643	0	646	51	0
1	W	1142	0	1151	141	0
1	X	1207	0	1214	118	0
2	C	724	0	697	106	0
2	D	869	0	846	95	0
2	I	869	0	846	130	0
2	J	860	0	837	103	0
2	O	724	0	697	103	0
2	P	869	0	846	92	0
2	S	869	0	846	127	0
2	T	860	0	837	99	0
All	All	21924	0	21776	2187	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 50.

All (2187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:802:ASP:OD1	2:O:844:ARG:HD3	1.52	1.09
2:C:802:ASP:OD1	2:C:844:ARG:HD3	1.52	1.08
2:J:832:TYR:HB2	2:J:836:VAL:HG21	1.42	1.01
1:A:404:ARG:NH2	1:X:320:ARG:HD2	1.76	1.01
2:I:805:ASN:HD21	2:I:872:TYR:HD1	1.01	1.01
2:O:866:TYR:H	2:O:884:VAL:HG21	1.28	0.99
2:T:832:TYR:HB2	2:T:836:VAL:HG21	1.42	0.98
2:S:805:ASN:HD21	2:S:872:TYR:HD1	1.01	0.96
1:N:296:LYS:NZ	1:N:300:MET:SD	2.39	0.96
2:C:866:TYR:H	2:C:884:VAL:HG21	1.28	0.96
2:C:808:ARG:CB	2:C:823:VAL:HA	1.96	0.95
1:X:296:LYS:NZ	1:X:300:MET:SD	2.39	0.95
2:O:808:ARG:CB	2:O:823:VAL:HA	1.96	0.94
1:A:367:LEU:HB3	1:B:367:LEU:HD22	1.50	0.93
2:C:804:ILE:HG21	2:C:807:MET:HB3	1.50	0.93
1:E:367:LEU:HB3	1:F:367:LEU:HD22	1.50	0.93
2:C:808:ARG:HB3	2:C:823:VAL:HA	1.50	0.93
1:G:80:ARG:HA	1:G:83:GLU:HB2	1.50	0.93
2:O:804:ILE:HG21	2:O:807:MET:HB3	1.50	0.93
1:Q:80:ARG:HA	1:Q:83:GLU:HB2	1.50	0.93
2:O:808:ARG:HB3	2:O:823:VAL:HA	1.50	0.91
2:S:805:ASN:OD1	2:S:806:ILE:N	2.04	0.90
1:R:88:ILE:HD12	1:R:91:ARG:HD2	1.53	0.90
1:H:128:ARG:NH1	1:H:131:THR:OG1	2.07	0.88
2:I:805:ASN:OD1	2:I:806:ILE:N	2.04	0.88
1:H:88:ILE:HD12	1:H:91:ARG:HD2	1.54	0.88
1:R:128:ARG:NH1	1:R:131:THR:OG1	2.07	0.87
2:O:805:ASN:HB3	2:O:871:ILE:O	1.75	0.87
1:M:437:ASP:OD1	1:M:440:ARG:NH1	2.08	0.87
1:W:437:ASP:OD1	1:W:440:ARG:NH1	2.08	0.87
1:Q:146:LEU:HG	1:R:146:LEU:HB3	1.54	0.87
2:J:863:THR:HG23	2:J:885:THR:HA	1.55	0.87
1:G:146:LEU:HG	1:H:146:LEU:HB3	1.54	0.86
2:T:863:THR:HG23	2:T:885:THR:HA	1.55	0.86
2:I:792:ARG:HE	2:I:852:TYR:HA	1.39	0.86
1:A:358:ALA:O	1:A:362:GLU:HB2	1.75	0.85
2:S:792:ARG:HE	2:S:852:TYR:HA	1.39	0.85
2:C:805:ASN:HB3	2:C:871:ILE:O	1.75	0.85
1:E:358:ALA:O	1:E:362:GLU:HB2	1.75	0.85
2:I:805:ASN:ND2	2:I:872:TYR:HD1	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:790:SER:HA	2:P:856:ASN:HD21	1.41	0.83
1:H:181:LEU:O	1:H:184:GLN:NE2	2.12	0.83
1:R:181:LEU:O	1:R:184:GLN:NE2	2.12	0.83
1:W:322:ALA:O	1:W:326:ASN:N	2.11	0.82
2:O:797:SER:HB3	2:O:849:ASP:HB3	1.61	0.82
2:S:805:ASN:ND2	2:S:872:TYR:HD1	1.77	0.82
2:D:790:SER:HA	2:D:856:ASN:HD21	1.41	0.82
1:M:322:ALA:O	1:M:326:ASN:N	2.11	0.82
1:G:148:ASN:O	1:G:152:GLN:N	2.12	0.82
2:I:805:ASN:O	2:I:806:ILE:HD13	1.79	0.82
1:X:352:GLY:O	1:X:355:THR:OG1	1.98	0.82
1:K:93:ASN:OD1	1:K:96:GLN:NE2	2.13	0.81
1:U:93:ASN:OD1	1:U:96:GLN:NE2	2.13	0.81
2:S:805:ASN:O	2:S:806:ILE:HD13	1.79	0.81
1:Q:148:ASN:O	1:Q:152:GLN:N	2.12	0.81
1:Q:173:HIS:HB3	1:W:331:ARG:HH21	1.45	0.81
2:J:11:LEU:HD13	2:J:885:THR:H	1.44	0.81
2:C:797:SER:HB3	2:C:849:ASP:HB3	1.61	0.81
2:T:792:ARG:HE	2:T:793:LEU:H	1.28	0.81
1:L:66:ILE:HA	1:L:69:ILE:HB	1.63	0.81
2:T:11:LEU:HD13	2:T:885:THR:H	1.44	0.81
1:G:170:ARG:HA	1:G:173:HIS:HB2	1.62	0.81
2:S:6:GLU:HB3	2:S:793:LEU:HB3	1.61	0.81
1:R:209:LEU:O	1:R:213:ALA:N	2.15	0.80
1:N:354:ASP:OD1	1:N:357:ARG:NH2	2.15	0.80
2:I:6:GLU:HB3	2:I:793:LEU:HB3	1.61	0.80
1:G:173:HIS:HB3	1:M:331:ARG:HH21	1.45	0.80
2:J:792:ARG:HE	2:J:793:LEU:H	1.27	0.80
1:R:73:VAL:HA	1:R:76:GLU:HB2	1.63	0.80
1:V:66:ILE:HA	1:V:69:ILE:HB	1.63	0.80
2:C:809:TRP:HA	2:C:868:CYS:HA	1.64	0.80
1:G:87:LEU:O	1:G:91:ARG:N	2.15	0.80
1:R:168:THR:O	1:R:172:GLU:N	2.15	0.80
1:W:403:ARG:HA	1:W:406:HIS:CD2	2.17	0.80
1:G:201:ARG:NH1	1:G:205:ASP:OD2	2.15	0.80
1:Q:87:LEU:O	1:Q:91:ARG:N	2.15	0.80
1:Q:170:ARG:HA	1:Q:173:HIS:HB2	1.62	0.80
1:N:288:GLU:HG2	1:N:289:THR:H	1.47	0.80
1:X:354:ASP:OD1	1:X:357:ARG:NH2	2.15	0.80
1:H:45:ILE:HG12	1:L:70:ARG:HH11	1.46	0.79
1:G:76:GLU:OE1	1:H:80:ARG:NH1	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:320:ARG:HD2	1:E:404:ARG:NH2	1.96	0.79
1:N:352:GLY:O	1:N:355:THR:OG1	1.98	0.79
1:H:168:THR:O	1:H:172:GLU:N	2.15	0.79
2:O:809:TRP:HA	2:O:868:CYS:HA	1.64	0.79
1:X:288:GLU:HG2	1:X:289:THR:H	1.47	0.79
1:H:209:LEU:O	1:H:213:ALA:N	2.15	0.79
1:G:150:LEU:O	1:G:154:ASP:N	2.16	0.79
1:Q:76:GLU:OE1	1:R:80:ARG:NH1	2.15	0.79
1:M:403:ARG:HA	1:M:406:HIS:CD2	2.17	0.79
1:E:435:ARG:NH2	2:P:817:GLN:OE1	2.16	0.79
1:L:59:LEU:O	1:L:62:ILE:N	2.15	0.79
1:H:73:VAL:HA	1:H:76:GLU:HB2	1.63	0.79
2:I:848:LYS:NZ	2:I:850:THR:OG1	2.14	0.79
1:Q:201:ARG:NH1	1:Q:205:ASP:OD2	2.15	0.79
1:Q:150:LEU:O	1:Q:154:ASP:N	2.16	0.78
1:H:96:GLN:O	1:H:99:ARG:NH1	2.17	0.78
1:A:435:ARG:NH2	2:D:817:GLN:OE1	2.16	0.78
1:V:59:LEU:O	1:V:62:ILE:N	2.15	0.78
1:R:96:GLN:O	1:R:99:ARG:NH1	2.16	0.78
1:W:412:GLU:CB	2:S:873:ARG:HH11	1.98	0.77
2:S:848:LYS:NZ	2:S:850:THR:OG1	2.14	0.77
1:H:46:HIS:HA	1:H:49:LEU:HB2	1.66	0.77
1:R:45:ILE:HG12	1:V:70:ARG:HH11	1.47	0.77
2:O:811:ARG:O	2:O:819:GLY:N	2.18	0.77
2:C:844:ARG:HA	2:C:851:VAL:HG12	1.67	0.77
1:M:428:GLU:O	1:M:432:GLU:N	2.16	0.77
2:C:811:ARG:O	2:C:819:GLY:N	2.18	0.77
2:T:824:VAL:HG11	2:T:842:ILE:HG12	1.67	0.77
1:N:391:ARG:HG2	1:N:395:MET:HE1	1.66	0.77
2:I:844:ARG:HA	2:I:851:VAL:HA	1.67	0.77
1:R:153:SER:HA	1:R:156:LYS:HE2	1.67	0.77
1:G:175:VAL:HG21	1:H:170:ARG:HH12	1.50	0.77
2:J:824:VAL:HG11	2:J:842:ILE:HG12	1.67	0.77
1:H:143:ILE:O	1:H:147:ARG:N	2.18	0.76
1:U:83:GLU:OE1	1:V:84:HIS:NE2	2.18	0.76
2:S:844:ARG:HA	2:S:851:VAL:HA	1.67	0.76
1:R:46:HIS:HA	1:R:49:LEU:HB2	1.66	0.76
1:X:391:ARG:HG2	1:X:395:MET:HE1	1.66	0.76
2:O:808:ARG:HB3	2:O:823:VAL:CA	2.15	0.76
1:R:101:ILE:O	1:R:105:GLN:NE2	2.18	0.76
2:O:844:ARG:HA	2:O:851:VAL:HG12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:412:GLU:CB	2:I:873:ARG:HH11	1.98	0.76
1:H:101:ILE:O	1:H:105:GLN:NE2	2.18	0.76
1:M:383:GLU:O	1:M:387:GLN:NE2	2.19	0.76
1:A:389:ARG:HH21	1:A:392:LEU:HD22	1.51	0.76
2:I:805:ASN:O	2:I:806:ILE:CD1	2.33	0.76
1:R:143:ILE:O	1:R:147:ARG:N	2.18	0.76
1:H:137:GLU:O	1:H:141:LEU:N	2.16	0.76
2:O:808:ARG:O	2:O:869:ASN:N	2.18	0.76
1:E:389:ARG:HH21	1:E:392:LEU:HD22	1.51	0.76
2:J:789:ASP:N	2:J:855:MET:O	2.19	0.75
1:G:207:ALA:O	1:G:211:GLU:N	2.20	0.75
2:T:789:ASP:N	2:T:855:MET:O	2.19	0.75
2:C:808:ARG:HB3	2:C:823:VAL:CA	2.15	0.75
1:E:372:VAL:HG12	1:E:376:LYS:HZ1	1.50	0.75
1:W:383:GLU:O	1:W:387:GLN:NE2	2.19	0.75
2:S:805:ASN:O	2:S:806:ILE:CD1	2.33	0.75
1:A:372:VAL:HG12	1:A:376:LYS:HZ1	1.51	0.75
1:H:153:SER:HA	1:H:156:LYS:HE2	1.67	0.75
1:Q:175:VAL:HG21	1:R:170:ARG:HH12	1.50	0.75
2:D:13:TYR:HA	2:D:887:SER:HB2	1.69	0.75
2:P:13:TYR:HA	2:P:887:SER:HB2	1.69	0.75
2:P:862:ASP:HB2	2:P:886:VAL:HB	1.68	0.75
1:R:54:ARG:HG2	1:R:58:HIS:CE1	2.22	0.75
2:I:797:SER:OG	2:I:799:ARG:O	2.05	0.74
2:C:808:ARG:O	2:C:869:ASN:N	2.18	0.74
1:Q:207:ALA:O	1:Q:211:GLU:N	2.20	0.74
1:E:389:ARG:HH22	1:F:388:LEU:HD13	1.52	0.74
1:R:137:GLU:O	1:R:141:LEU:N	2.16	0.74
1:H:54:ARG:HG2	1:H:58:HIS:CE1	2.22	0.73
1:R:122:LEU:O	1:R:126:ASP:N	2.21	0.73
1:H:60:LYS:HA	1:H:63:GLU:HG2	1.70	0.73
1:X:419:ARG:NH1	2:T:876:GLU:OE1	2.21	0.73
1:A:435:ARG:HH12	2:D:816:LYS:HB3	1.52	0.73
2:J:800:SER:HB2	2:J:873:ARG:HE	1.54	0.73
1:G:205:ASP:HA	1:G:208:LEU:HB3	1.71	0.73
1:M:337:ARG:HA	1:M:340:GLU:HB2	1.71	0.73
1:W:390:ALA:O	1:W:394:ALA:N	2.22	0.73
1:N:419:ARG:NH1	2:J:876:GLU:OE1	2.21	0.73
1:M:436:ARG:HH22	2:J:811:ARG:HH21	1.37	0.73
2:J:803:GLY:O	2:J:873:ARG:NH2	2.19	0.73
1:M:390:ALA:O	1:M:394:ALA:N	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:80:ARG:O	1:Q:84:HIS:ND1	2.22	0.72
2:S:797:SER:OG	2:S:799:ARG:O	2.05	0.72
1:A:389:ARG:HH22	1:B:388:LEU:HD13	1.52	0.72
1:K:83:GLU:OE1	1:L:84:HIS:NE2	2.18	0.72
2:J:835:SER:O	2:J:839:ARG:NE	2.17	0.72
2:C:808:ARG:HB3	2:C:823:VAL:HG23	1.71	0.72
1:E:435:ARG:HH12	2:P:816:LYS:HB3	1.52	0.72
1:R:70:ARG:O	1:R:74:SER:N	2.22	0.72
2:D:862:ASP:HB2	2:D:886:VAL:HB	1.68	0.72
2:P:7:SER:N	2:P:794:SER:O	2.22	0.72
1:Q:101:ILE:O	1:Q:105:GLN:N	2.22	0.72
1:X:288:GLU:O	1:X:291:THR:OG1	2.06	0.72
2:T:800:SER:HB2	2:T:873:ARG:HE	1.54	0.72
2:O:808:ARG:HB3	2:O:823:VAL:HG23	1.71	0.72
2:I:7:SER:O	2:I:794:SER:N	2.20	0.72
1:Q:99:ARG:O	1:Q:103:LEU:N	2.21	0.72
1:R:60:LYS:HA	1:R:63:GLU:HG2	1.70	0.72
1:H:70:ARG:O	1:H:74:SER:N	2.22	0.72
1:L:114:ARG:O	1:L:118:ALA:N	2.20	0.72
1:W:337:ARG:HA	1:W:340:GLU:HB2	1.71	0.72
1:G:101:ILE:O	1:G:105:GLN:N	2.22	0.71
1:R:123:GLY:O	1:R:127:ALA:N	2.22	0.71
1:G:80:ARG:O	1:G:84:HIS:ND1	2.22	0.71
1:H:123:GLY:O	1:H:127:ALA:N	2.22	0.71
1:Q:205:ASP:HA	1:Q:208:LEU:HB3	1.71	0.71
1:H:168:THR:HA	1:H:171:ILE:HG22	1.73	0.71
2:D:7:SER:N	2:D:794:SER:O	2.22	0.71
1:G:102:ALA:HA	1:G:105:GLN:HB3	1.73	0.71
2:J:792:ARG:NH2	2:J:853:LEU:O	2.24	0.71
2:J:812:GLN:HB2	2:J:818:ARG:HD3	1.72	0.71
1:W:436:ARG:HH22	2:T:811:ARG:HH21	1.37	0.71
1:V:114:ARG:O	1:V:118:ALA:N	2.20	0.71
2:T:812:GLN:HB2	2:T:818:ARG:HD3	1.72	0.71
1:M:411:ALA:O	1:M:414:GLN:NE2	2.24	0.71
1:K:87:LEU:HD22	1:L:87:LEU:HB3	1.73	0.71
2:C:835:SER:O	2:C:839:ARG:NH2	2.18	0.71
1:Q:102:ALA:HA	1:Q:105:GLN:HB3	1.73	0.71
1:Q:192:ARG:NE	1:Q:196:GLU:OE2	2.24	0.71
1:G:99:ARG:O	1:G:103:LEU:N	2.21	0.71
1:F:417:ILE:HD12	1:F:420:LEU:HD11	1.73	0.71
1:V:92:ALA:O	1:V:96:GLN:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:434:ALA:O	1:W:438:ARG:N	2.24	0.71
2:I:811:ARG:HB2	2:I:821:VAL:HG23	1.73	0.71
1:G:192:ARG:NE	1:G:196:GLU:OE2	2.24	0.70
2:I:865:VAL:HA	2:I:883:GLN:HA	1.73	0.70
1:G:148:ASN:HA	1:G:151:LEU:HB2	1.73	0.70
1:H:92:ALA:O	1:H:96:GLN:N	2.24	0.70
1:B:417:ILE:HD12	1:B:420:LEU:HD11	1.73	0.70
1:G:63:GLU:HG2	1:G:64:PRO:HD3	1.72	0.70
1:L:92:ALA:O	1:L:96:GLN:N	2.23	0.70
2:J:808:ARG:NH1	2:J:820:MET:SD	2.65	0.70
1:H:122:LEU:O	1:H:126:ASP:N	2.21	0.70
2:S:811:ARG:HB2	2:S:821:VAL:HG23	1.73	0.70
1:W:411:ALA:O	1:W:414:GLN:NE2	2.24	0.70
2:S:865:VAL:HA	2:S:883:GLN:HA	1.73	0.70
2:D:869:ASN:OD1	2:D:870:ALA:N	2.25	0.70
1:R:168:THR:HA	1:R:171:ILE:HG22	1.72	0.70
2:T:808:ARG:NH1	2:T:820:MET:SD	2.65	0.70
1:M:434:ALA:O	1:M:438:ARG:N	2.24	0.70
1:Q:148:ASN:HA	1:Q:151:LEU:HB2	1.73	0.70
2:O:835:SER:O	2:O:839:ARG:NH2	2.18	0.70
1:M:412:GLU:HB3	2:I:873:ARG:HH11	1.57	0.70
2:J:841:ILE:O	2:J:854:GLN:N	2.23	0.70
2:T:792:ARG:NH2	2:T:853:LEU:O	2.24	0.69
2:I:821:VAL:HG13	2:I:836:VAL:HG11	1.74	0.69
2:P:869:ASN:OD1	2:P:870:ALA:N	2.25	0.69
1:H:81:ARG:O	1:H:85:ALA:N	2.25	0.69
1:Q:63:GLU:HG2	1:Q:64:PRO:HD3	1.72	0.69
1:U:87:LEU:HD22	1:V:87:LEU:HB3	1.73	0.69
2:T:818:ARG:NH1	2:T:865:VAL:O	2.25	0.69
2:J:818:ARG:NH1	2:J:865:VAL:O	2.25	0.69
2:T:845:ASP:OD1	2:T:846:SER:N	2.25	0.69
2:O:812:GLN:HB3	2:O:818:ARG:HA	1.74	0.69
2:C:808:ARG:HB3	2:C:823:VAL:CB	2.23	0.69
1:E:431:LEU:HD23	1:E:435:ARG:HB2	1.75	0.69
2:S:821:VAL:HG13	2:S:836:VAL:HG11	1.74	0.69
1:A:431:LEU:HD23	1:A:435:ARG:HB2	1.75	0.69
2:T:805:ASN:OD1	2:T:873:ARG:NH2	2.26	0.69
1:K:102:ALA:O	1:K:106:ALA:N	2.23	0.69
2:J:845:ASP:OD1	2:J:846:SER:N	2.25	0.69
2:I:862:ASP:N	2:I:887:SER:O	2.26	0.69
1:W:344:ASP:O	1:W:348:GLN:N	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:808:ARG:CB	2:O:823:VAL:CA	2.71	0.69
2:O:808:ARG:HB3	2:O:823:VAL:CB	2.23	0.69
1:G:169:ALA:O	1:G:173:HIS:N	2.26	0.69
1:U:102:ALA:O	1:U:106:ALA:N	2.23	0.69
1:W:412:GLU:HB3	2:S:873:ARG:HH11	1.57	0.69
1:G:105:GLN:O	1:G:109:ARG:NH1	2.26	0.69
1:F:417:ILE:HG12	2:O:806:ILE:HG21	1.75	0.69
1:Q:151:LEU:HD13	1:X:355:THR:HG22	1.74	0.69
1:X:294:ALA:O	1:X:297:LEU:N	2.26	0.69
1:H:70:ARG:HH21	1:L:45:ILE:HD13	1.57	0.68
2:C:812:GLN:HB3	2:C:818:ARG:HA	1.74	0.68
2:P:866:TYR:N	2:P:882:THR:O	2.25	0.68
2:D:822:ALA:HA	2:D:832:TYR:HA	1.75	0.68
1:Q:150:LEU:HD13	1:R:150:LEU:HA	1.75	0.68
1:W:428:GLU:O	1:W:432:GLU:N	2.16	0.68
2:T:835:SER:O	2:T:839:ARG:NE	2.17	0.68
1:M:344:ASP:O	1:M:348:GLN:N	2.22	0.68
1:M:428:GLU:HA	1:M:431:LEU:HB2	1.74	0.68
1:R:70:ARG:HH21	1:V:45:ILE:HD13	1.57	0.68
2:S:7:SER:O	2:S:794:SER:N	2.20	0.68
1:G:79:ALA:O	1:G:83:GLU:N	2.26	0.68
1:G:150:LEU:HD13	1:H:150:LEU:HA	1.75	0.68
1:N:288:GLU:O	1:N:291:THR:OG1	2.06	0.68
1:N:294:ALA:O	1:N:297:LEU:N	2.26	0.68
1:F:432:GLU:OE1	1:F:435:ARG:NE	2.27	0.68
2:O:813:ALA:HB3	2:O:816:LYS:HD3	1.75	0.68
1:H:110:GLU:O	1:H:114:ARG:N	2.24	0.68
1:M:335:ARG:HA	1:M:338:ALA:HB3	1.75	0.68
1:Q:79:ALA:O	1:Q:83:GLU:N	2.26	0.68
1:Q:105:GLN:O	1:Q:109:ARG:NH1	2.26	0.68
1:R:81:ARG:O	1:R:85:ALA:N	2.26	0.68
1:W:428:GLU:HA	1:W:431:LEU:HB2	1.74	0.68
2:D:804:ILE:HA	2:D:872:TYR:HE1	1.59	0.68
2:J:863:THR:OG1	2:J:886:VAL:O	2.12	0.68
1:A:419:ARG:NH1	1:A:423:GLU:OE2	2.27	0.68
1:B:399:GLN:HE22	1:B:403:ARG:HD3	1.59	0.68
1:G:151:LEU:HD13	1:N:355:THR:HG22	1.74	0.68
1:E:419:ARG:NH1	1:E:423:GLU:OE2	2.27	0.68
1:Q:169:ALA:O	1:Q:173:HIS:N	2.26	0.68
1:W:335:ARG:HA	1:W:338:ALA:HB3	1.75	0.68
2:T:809:TRP:N	2:T:822:ALA:O	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:825:THR:HG22	2:O:827:TRP:H	1.59	0.68
2:T:863:THR:OG1	2:T:886:VAL:O	2.12	0.68
2:J:805:ASN:OD1	2:J:873:ARG:NH2	2.26	0.67
2:P:836:VAL:HG12	2:P:839:ARG:CZ	2.25	0.67
1:R:92:ALA:O	1:R:96:GLN:N	2.24	0.67
1:R:163:SER:HA	1:R:166:ASP:HB2	1.75	0.67
1:X:399:GLN:HB3	1:X:403:ARG:NH1	2.10	0.67
2:I:6:GLU:HG3	2:I:795:CYS:HA	1.76	0.67
2:S:862:ASP:N	2:S:887:SER:O	2.26	0.67
1:G:205:ASP:O	1:G:209:LEU:N	2.22	0.67
1:R:110:GLU:O	1:R:114:ARG:N	2.24	0.67
2:D:809:TRP:HZ3	2:D:853:LEU:HD22	1.59	0.67
2:C:813:ALA:HB3	2:C:816:LYS:HD3	1.75	0.67
1:R:148:ASN:O	1:R:152:GLN:N	2.24	0.67
1:V:45:ILE:HG13	1:V:46:HIS:H	1.59	0.67
2:D:836:VAL:HG12	2:D:839:ARG:CZ	2.25	0.67
1:F:417:ILE:HD11	2:O:806:ILE:HD13	1.77	0.67
2:T:803:GLY:O	2:T:873:ARG:NH2	2.19	0.67
1:B:432:GLU:OE1	1:B:435:ARG:NE	2.27	0.67
1:F:399:GLN:HE22	1:F:403:ARG:HD3	1.59	0.67
2:S:825:THR:O	2:S:844:ARG:NH2	2.28	0.67
1:H:42:TYR:HA	1:H:45:ILE:HD12	1.77	0.67
1:Q:44:THR:O	1:Q:48:GLY:N	2.22	0.67
2:C:825:THR:HG22	2:C:827:TRP:H	1.59	0.67
2:P:804:ILE:HA	2:P:872:TYR:HE1	1.59	0.67
2:D:808:ARG:NH1	2:D:876:GLU:OE2	2.28	0.67
1:A:420:LEU:HD13	1:B:420:LEU:HD13	1.77	0.67
1:B:382:GLU:OE2	1:B:389:ARG:NH2	2.28	0.67
1:H:117:ALA:O	1:H:121:ALA:N	2.28	0.67
1:N:399:GLN:HB3	1:N:403:ARG:NH1	2.10	0.66
1:F:382:GLU:OE2	1:F:389:ARG:NH2	2.28	0.66
2:P:808:ARG:NH1	2:P:876:GLU:OE2	2.28	0.66
2:P:809:TRP:HZ3	2:P:853:LEU:HD22	1.59	0.66
1:W:424:ALA:O	1:W:427:ALA:N	2.28	0.66
1:M:424:ALA:O	1:M:427:ALA:N	2.28	0.66
1:E:381:ALA:O	1:E:384:ARG:HG2	1.95	0.66
1:H:163:SER:HA	1:H:166:ASP:HB2	1.75	0.66
2:P:5:GLN:O	2:P:796:ALA:N	2.29	0.66
1:R:40:GLN:HE21	1:U:70:ARG:HA	1.60	0.66
2:J:809:TRP:N	2:J:822:ALA:O	2.24	0.66
2:S:6:GLU:HG3	2:S:795:CYS:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ALA:O	1:B:364:ALA:HB3	1.96	0.66
1:B:417:ILE:HG12	2:C:806:ILE:HG21	1.75	0.66
1:M:375:GLU:HA	1:M:378:LEU:HD23	1.78	0.66
2:I:825:THR:O	2:I:844:ARG:NH2	2.28	0.66
1:Q:181:LEU:HA	1:Q:184:GLN:CD	2.21	0.66
2:P:822:ALA:HA	2:P:832:TYR:HA	1.75	0.66
1:X:301:ASN:O	1:X:305:SER:OG	2.05	0.66
1:A:381:ALA:O	1:A:384:ARG:HG2	1.95	0.66
1:L:45:ILE:HG13	1:L:46:HIS:H	1.59	0.66
2:C:809:TRP:CE2	2:C:853:LEU:HB2	2.31	0.66
2:T:841:ILE:O	2:T:854:GLN:N	2.22	0.66
2:D:866:TYR:N	2:D:882:THR:O	2.26	0.66
1:M:384:ARG:NH1	1:M:384:ARG:O	2.29	0.66
1:L:45:ILE:HG13	1:L:46:HIS:N	2.11	0.66
1:R:42:TYR:HA	1:R:45:ILE:HD12	1.77	0.66
1:V:45:ILE:HG13	1:V:46:HIS:N	2.11	0.66
1:B:417:ILE:HD11	2:C:806:ILE:HD13	1.77	0.66
1:W:384:ARG:NH1	1:W:384:ARG:O	2.28	0.66
1:B:423:GLU:OE1	2:D:808:ARG:NH2	2.30	0.65
1:E:376:LYS:HB2	1:E:380:ARG:NH2	2.12	0.65
1:E:420:LEU:HD13	1:F:420:LEU:HD13	1.77	0.65
1:R:117:ALA:O	1:R:121:ALA:N	2.29	0.65
1:A:376:LYS:HB2	1:A:380:ARG:NH2	2.11	0.65
1:H:124:GLU:CD	1:N:380:ARG:HH21	2.04	0.65
1:F:360:ALA:O	1:F:364:ALA:HB3	1.96	0.65
2:P:801:ILE:HG23	2:P:849:ASP:HB2	1.78	0.65
2:D:5:GLN:O	2:D:796:ALA:N	2.29	0.65
1:H:40:GLN:HE21	1:K:70:ARG:HA	1.60	0.65
1:H:164:LEU:HD12	1:H:165:ARG:HE	1.61	0.65
2:J:857:ASN:O	2:J:859:LYS:NZ	2.28	0.65
2:P:13:TYR:O	2:P:887:SER:N	2.27	0.65
1:R:167:ALA:O	1:R:171:ILE:N	2.28	0.65
1:V:72:PRO:O	1:V:75:GLN:NE2	2.30	0.65
1:W:392:LEU:HD11	1:X:388:LEU:HD12	1.79	0.65
1:M:299:GLU:O	1:M:303:GLN:N	2.29	0.65
1:W:375:GLU:HA	1:W:378:LEU:HD23	1.78	0.65
1:L:72:PRO:O	1:L:75:GLN:NE2	2.30	0.65
1:H:62:ILE:HA	1:H:65:LEU:HD12	1.79	0.65
1:R:62:ILE:HA	1:R:65:LEU:HD12	1.79	0.65
2:O:809:TRP:CE2	2:O:853:LEU:HB2	2.31	0.65
2:D:801:ILE:HG23	2:D:849:ASP:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:392:LEU:HD11	1:N:388:LEU:HD12	1.79	0.65
1:N:393:ASP:O	1:N:396:GLN:HG3	1.97	0.65
1:Q:34:SER:O	1:Q:38:ILE:N	2.28	0.65
1:X:393:ASP:O	1:X:396:GLN:HG3	1.97	0.65
2:T:792:ARG:NE	2:T:793:LEU:H	1.95	0.65
1:H:59:LEU:HD13	1:H:62:ILE:HD13	1.78	0.64
1:K:86:GLU:O	1:K:90:VAL:N	2.30	0.64
1:R:164:LEU:HD12	1:R:165:ARG:HE	1.61	0.64
1:W:299:GLU:O	1:W:303:GLN:N	2.29	0.64
2:J:792:ARG:NE	2:J:793:LEU:H	1.95	0.64
1:F:423:GLU:OE1	2:P:808:ARG:NH2	2.29	0.64
1:Q:206:ASN:OD1	1:Q:207:ALA:N	2.31	0.64
1:Q:205:ASP:O	1:Q:209:LEU:N	2.22	0.64
1:R:124:GLU:CD	1:X:380:ARG:HH21	2.04	0.64
2:D:13:TYR:O	2:D:887:SER:N	2.27	0.64
1:G:181:LEU:HA	1:G:184:GLN:CD	2.21	0.64
2:T:857:ASN:O	2:T:859:LYS:NZ	2.28	0.64
2:I:805:ASN:HD21	2:I:872:TYR:HA	1.63	0.64
2:O:804:ILE:CG2	2:O:807:MET:HB3	2.26	0.64
2:D:859:LYS:N	2:D:862:ASP:OD2	2.26	0.64
1:G:191:ARG:NH2	1:H:196:GLU:OE1	2.30	0.64
1:N:301:ASN:O	1:N:305:SER:OG	2.05	0.64
1:Q:197:ALA:O	1:Q:201:ARG:N	2.29	0.64
1:X:297:LEU:O	1:X:301:ASN:ND2	2.31	0.64
1:B:386:GLN:HG3	1:B:389:ARG:HH12	1.63	0.64
1:Q:191:ARG:NH2	1:R:196:GLU:OE1	2.30	0.64
1:G:34:SER:O	1:G:38:ILE:N	2.28	0.64
1:G:206:ASN:OD1	1:G:207:ALA:N	2.31	0.64
1:K:71:GLY:O	1:K:75:GLN:N	2.22	0.64
2:J:886:VAL:O	2:J:887:SER:OG	2.16	0.64
1:U:86:GLU:O	1:U:90:VAL:N	2.30	0.64
1:R:59:LEU:HD13	1:R:62:ILE:HD13	1.78	0.63
1:R:148:ASN:OD1	1:R:149:ALA:N	2.32	0.63
1:R:175:VAL:O	1:R:178:VAL:N	2.32	0.63
1:R:72:PRO:HA	1:R:75:GLN:HG2	1.80	0.63
2:S:805:ASN:HD21	2:S:872:TYR:HA	1.63	0.63
1:G:118:ALA:O	1:G:122:LEU:N	2.32	0.63
1:M:328:ALA:O	1:M:331:ARG:HG2	1.99	0.63
2:C:9:GLY:HA3	2:C:793:LEU:HD23	1.81	0.63
1:Q:88:ILE:O	1:Q:92:ALA:N	2.30	0.63
1:Q:118:ALA:O	1:Q:122:LEU:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:834:ASP:HA	2:D:837:LYS:HE3	1.81	0.63
1:H:52:ILE:HG13	1:H:53:GLY:N	2.14	0.63
1:H:148:ASN:OD1	1:H:149:ALA:N	2.32	0.63
1:H:167:ALA:O	1:H:171:ILE:N	2.28	0.63
1:W:319:GLU:HA	1:W:322:ALA:HB3	1.79	0.63
1:W:319:GLU:O	1:W:323:GLY:N	2.22	0.63
1:G:34:SER:HB2	1:G:37:ALA:HB3	1.80	0.63
1:G:197:ALA:O	1:G:201:ARG:N	2.29	0.63
1:F:386:GLN:HG3	1:F:389:ARG:HH12	1.63	0.63
1:R:52:ILE:HG13	1:R:53:GLY:N	2.14	0.63
2:O:9:GLY:HA3	2:O:793:LEU:HD23	1.81	0.63
1:A:410:ILE:O	1:A:414:GLN:NE2	2.32	0.62
1:G:128:ARG:O	1:G:132:GLN:NE2	2.32	0.62
1:H:152:GLN:HA	1:H:155:LEU:HD13	1.81	0.62
1:M:346:LEU:HD13	1:M:349:ARG:HH22	1.64	0.62
1:N:375:GLU:O	1:N:379:LYS:HG2	1.99	0.62
2:I:812:GLN:HB3	2:I:818:ARG:HA	1.81	0.62
2:P:809:TRP:NE1	2:P:868:CYS:SG	2.72	0.62
2:S:839:ARG:HB3	2:S:839:ARG:CZ	2.29	0.62
1:N:297:LEU:O	1:N:301:ASN:ND2	2.31	0.62
2:T:825:THR:OG1	2:T:826:GLY:N	2.29	0.62
1:A:431:LEU:O	1:A:435:ARG:N	2.30	0.62
1:H:72:PRO:HA	1:H:75:GLN:HG2	1.80	0.62
1:M:319:GLU:HA	1:M:322:ALA:HB3	1.79	0.62
2:C:804:ILE:CG2	2:C:807:MET:HB3	2.26	0.62
1:X:304:ILE:HG13	1:X:307:ARG:HD3	1.82	0.62
1:X:375:GLU:O	1:X:379:LYS:HG2	1.99	0.62
2:D:11:LEU:HA	2:D:885:THR:HG21	1.81	0.62
2:C:808:ARG:CB	2:C:823:VAL:CA	2.71	0.62
2:P:6:GLU:HA	2:P:795:CYS:HA	1.81	0.62
2:P:845:ASP:OD1	2:P:846:SER:N	2.32	0.62
1:R:152:GLN:HA	1:R:155:LEU:HD13	1.81	0.62
2:T:834:ASP:HA	2:T:837:LYS:HZ2	1.64	0.62
2:T:840:PHE:CZ	2:T:855:MET:HE2	2.34	0.62
2:J:809:TRP:HA	2:J:868:CYS:HA	1.81	0.62
2:J:840:PHE:CZ	2:J:855:MET:HE2	2.34	0.62
1:E:410:ILE:O	1:E:414:GLN:NE2	2.32	0.62
2:P:834:ASP:HA	2:P:837:LYS:HE3	1.81	0.62
1:W:328:ALA:O	1:W:331:ARG:HG2	1.99	0.62
1:G:44:THR:O	1:G:48:GLY:N	2.22	0.62
2:J:825:THR:OG1	2:J:826:GLY:N	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:834:ASP:HA	2:J:837:LYS:NZ	2.14	0.62
1:W:346:LEU:HD13	1:W:349:ARG:HH22	1.64	0.62
1:B:403:ARG:NH1	1:B:407:GLU:OE1	2.33	0.62
2:I:804:ILE:HG13	2:I:804:ILE:O	2.00	0.62
1:F:403:ARG:NH1	1:F:407:GLU:OE1	2.33	0.62
2:P:789:ASP:O	2:P:856:ASN:ND2	2.33	0.62
1:Q:34:SER:HB2	1:Q:37:ALA:HB3	1.80	0.62
1:R:91:ARG:O	1:R:95:ASP:N	2.30	0.62
2:T:834:ASP:HA	2:T:837:LYS:NZ	2.14	0.62
2:D:6:GLU:HA	2:D:795:CYS:HA	1.81	0.62
2:D:809:TRP:NE1	2:D:868:CYS:SG	2.72	0.62
1:H:54:ARG:O	1:H:58:HIS:ND1	2.33	0.62
1:H:80:ARG:O	1:H:84:HIS:N	2.30	0.62
1:M:434:ALA:O	1:N:438:ARG:NH2	2.33	0.62
1:N:304:ILE:HG13	1:N:307:ARG:HD3	1.81	0.62
2:J:812:GLN:NE2	2:J:816:LYS:O	2.33	0.62
1:U:71:GLY:O	1:U:75:GLN:N	2.22	0.62
2:D:845:ASP:OD1	2:D:846:SER:N	2.32	0.62
1:G:143:ILE:O	1:G:147:ARG:N	2.33	0.62
2:T:809:TRP:HA	2:T:868:CYS:HA	1.81	0.62
2:O:804:ILE:CG2	2:O:870:ALA:HB1	2.30	0.62
1:A:372:VAL:HG12	1:A:376:LYS:NZ	2.15	0.61
1:R:144:ASP:HA	1:R:147:ARG:HD2	1.82	0.61
1:U:103:LEU:O	1:U:107:GLU:N	2.33	0.61
1:H:144:ASP:HA	1:H:147:ARG:HD2	1.82	0.61
1:Q:115:LEU:HG	1:R:114:ARG:HH12	1.66	0.61
1:W:378:LEU:HD22	1:X:378:LEU:HD21	1.81	0.61
2:P:11:LEU:HD13	2:P:885:THR:HG21	1.82	0.61
2:P:840:PHE:HB3	2:P:853:LEU:HD11	1.82	0.61
1:V:74:SER:O	1:V:78:GLU:N	2.28	0.61
1:W:388:LEU:HB2	1:X:389:ARG:HH22	1.65	0.61
2:S:812:GLN:HB3	2:S:818:ARG:HA	1.81	0.61
1:A:435:ARG:HH22	2:D:816:LYS:HA	1.65	0.61
1:H:175:VAL:O	1:H:178:VAL:N	2.32	0.61
2:I:839:ARG:HB3	2:I:839:ARG:CZ	2.29	0.61
1:E:431:LEU:O	1:E:435:ARG:N	2.30	0.61
1:A:385:ALA:O	1:A:389:ARG:NH1	2.34	0.61
1:M:388:LEU:HB2	1:N:389:ARG:HH22	1.65	0.61
2:C:804:ILE:CG2	2:C:870:ALA:HB1	2.30	0.61
2:P:11:LEU:HA	2:P:885:THR:HG21	1.81	0.61
1:Q:128:ARG:O	1:Q:132:GLN:NE2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:LEU:HG	1:H:114:ARG:HH12	1.66	0.61
1:H:91:ARG:O	1:H:95:ASP:N	2.30	0.61
2:I:12:VAL:O	2:I:886:VAL:HA	2.00	0.61
1:Q:126:ASP:OD1	1:Q:127:ALA:N	2.33	0.61
1:R:144:ASP:OD1	1:R:145:ARG:N	2.33	0.61
2:T:812:GLN:NE2	2:T:816:LYS:O	2.33	0.61
2:S:12:VAL:O	2:S:886:VAL:HA	2.00	0.61
2:D:11:LEU:HD13	2:D:885:THR:HG21	1.82	0.61
2:D:805:ASN:HD21	2:D:871:ILE:HG23	1.66	0.61
1:K:105:GLN:OE1	1:K:109:ARG:NH1	2.34	0.61
1:L:74:SER:O	1:L:78:GLU:N	2.27	0.61
1:Q:143:ILE:O	1:Q:147:ARG:N	2.33	0.61
1:V:91:ARG:O	1:V:95:ASP:N	2.25	0.61
2:O:810:TYR:HE2	2:O:869:ASN:HD22	1.47	0.61
2:D:789:ASP:O	2:D:856:ASN:ND2	2.33	0.61
1:E:406:HIS:ND1	1:F:406:HIS:CE1	2.69	0.61
1:W:311:SER:O	1:W:314:GLN:NE2	2.33	0.61
1:W:420:LEU:HA	1:W:423:GLU:CD	2.26	0.61
1:W:435:ARG:HH21	1:X:431:LEU:HD11	1.66	0.61
1:G:126:ASP:OD1	1:G:127:ALA:N	2.33	0.61
1:M:308:LEU:HG	1:N:308:LEU:HD11	1.83	0.61
2:J:842:ILE:HA	2:J:853:LEU:HD12	1.83	0.61
2:C:808:ARG:HB3	2:C:823:VAL:CG2	2.31	0.61
1:A:406:HIS:ND1	1:B:406:HIS:CE1	2.69	0.61
1:G:147:ARG:NH1	1:N:359:THR:HG22	2.16	0.61
1:H:144:ASP:OD1	1:H:145:ARG:N	2.33	0.61
1:M:435:ARG:HH21	1:N:431:LEU:HD11	1.66	0.61
1:R:54:ARG:O	1:R:58:HIS:ND1	2.33	0.61
1:U:105:GLN:OE1	1:U:109:ARG:NH1	2.34	0.61
1:W:434:ALA:O	1:X:438:ARG:NH2	2.33	0.61
2:S:804:ILE:HG13	2:S:804:ILE:O	2.00	0.61
1:H:62:ILE:HA	1:H:65:LEU:HB2	1.83	0.60
1:E:372:VAL:HG12	1:E:376:LYS:NZ	2.15	0.60
2:C:834:ASP:HA	2:C:837:LYS:HZ3	1.66	0.60
1:W:308:LEU:HG	1:X:308:LEU:HD11	1.83	0.60
1:H:109:ARG:O	1:H:112:SER:OG	2.19	0.60
1:M:420:LEU:HA	1:M:423:GLU:CD	2.26	0.60
2:C:810:TYR:HE2	2:C:869:ASN:HD22	1.47	0.60
1:E:435:ARG:HH22	2:P:816:LYS:HA	1.66	0.60
2:T:842:ILE:HA	2:T:853:LEU:HD12	1.83	0.60
2:S:812:GLN:CB	2:S:818:ARG:HA	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:792:ARG:HA	2:D:792:ARG:HE	1.66	0.60
1:K:103:LEU:O	1:K:107:GLU:N	2.33	0.60
1:M:311:SER:O	1:M:314:GLN:NE2	2.33	0.60
1:E:385:ALA:O	1:E:389:ARG:NH1	2.34	0.60
1:R:45:ILE:O	1:R:49:LEU:N	2.31	0.60
2:O:808:ARG:HB3	2:O:823:VAL:CG2	2.31	0.60
2:O:810:TYR:N	2:O:867:SER:O	2.35	0.60
1:M:384:ARG:O	1:M:388:LEU:N	2.35	0.60
2:J:840:PHE:CE1	2:J:855:MET:HG3	2.36	0.60
1:V:80:ARG:O	1:V:84:HIS:N	2.35	0.60
1:W:384:ARG:O	1:W:388:LEU:N	2.35	0.60
1:W:416:THR:HG22	2:S:806:ILE:HG12	1.84	0.60
1:G:194:ASP:OD1	1:G:195:ALA:N	2.35	0.60
2:T:840:PHE:CE1	2:T:855:MET:HG3	2.36	0.60
1:H:148:ASN:O	1:H:152:GLN:N	2.24	0.60
1:R:111:VAL:HA	1:R:114:ARG:HB3	1.84	0.60
2:D:840:PHE:HB3	2:D:853:LEU:HD11	1.82	0.60
1:L:91:ARG:O	1:L:95:ASP:N	2.25	0.60
1:M:319:GLU:O	1:M:323:GLY:N	2.22	0.60
1:M:378:LEU:HD22	1:N:378:LEU:HD21	1.81	0.60
2:C:826:GLY:HA2	2:C:844:ARG:HH22	1.67	0.60
2:P:805:ASN:HD21	2:P:871:ILE:HG23	1.65	0.60
1:Q:194:ASP:OD1	1:Q:195:ALA:N	2.35	0.60
1:Q:206:ASN:O	1:Q:210:GLY:N	2.33	0.60
1:W:359:THR:HA	1:W:362:GLU:HB2	1.84	0.60
1:X:288:GLU:HG2	1:X:289:THR:N	2.17	0.60
1:M:416:THR:HG22	2:I:806:ILE:HG12	1.84	0.60
2:J:800:SER:O	2:J:873:ARG:NH1	2.35	0.60
1:Q:147:ARG:NH1	1:X:359:THR:HG22	2.16	0.60
1:R:97:ALA:O	1:R:101:ILE:N	2.31	0.60
1:V:72:PRO:HA	1:V:75:GLN:HG3	1.83	0.60
1:W:319:GLU:OE1	1:X:315:GLN:NE2	2.34	0.60
2:O:826:GLY:HA2	2:O:844:ARG:HH22	1.67	0.60
1:G:88:ILE:O	1:G:92:ALA:N	2.30	0.60
1:H:111:VAL:HA	1:H:114:ARG:HB3	1.84	0.60
1:W:301:ASN:HD21	1:X:301:ASN:HD21	1.50	0.60
1:W:435:ARG:HE	1:X:431:LEU:HD11	1.66	0.60
1:L:66:ILE:HG22	1:L:70:ARG:HG3	1.84	0.59
2:P:858:LEU:HB3	2:P:886:VAL:HG23	1.83	0.59
1:N:345:GLY:HA2	1:N:348:GLN:OE1	2.01	0.59
1:N:356:ALA:O	1:N:359:THR:OG1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:859:LYS:N	2:I:862:ASP:OD2	2.35	0.59
2:O:796:ALA:HA	2:O:850:THR:HA	1.84	0.59
1:H:70:ARG:HA	1:H:73:VAL:HB	1.84	0.59
1:H:97:ALA:O	1:H:101:ILE:N	2.31	0.59
2:C:806:ILE:O	2:C:806:ILE:HG13	2.02	0.59
1:Q:170:ARG:HE	1:R:171:ILE:HG12	1.68	0.59
2:S:842:ILE:HD11	2:S:853:LEU:HD12	1.84	0.59
2:C:802:ASP:HB2	2:C:846:SER:HA	1.84	0.59
2:I:842:ILE:HD11	2:I:853:LEU:HD12	1.84	0.59
1:R:142:GLU:HG3	1:R:146:LEU:HD12	1.85	0.59
2:O:806:ILE:HG13	2:O:806:ILE:O	2.02	0.59
2:S:2:VAL:HG22	2:S:877:TYR:CZ	2.38	0.59
1:G:117:ALA:O	1:G:121:ALA:N	2.30	0.59
2:I:824:VAL:HG11	2:I:842:ILE:HG21	1.84	0.59
2:P:813:ALA:HB3	2:P:816:LYS:HD2	1.85	0.59
2:S:805:ASN:ND2	2:S:872:TYR:CD1	2.62	0.59
1:M:359:THR:HA	1:M:362:GLU:HB2	1.84	0.59
1:M:435:ARG:HE	1:N:431:LEU:HD11	1.66	0.59
2:C:810:TYR:N	2:C:867:SER:O	2.35	0.59
1:Q:129:ARG:O	1:Q:133:ASP:N	2.35	0.59
1:R:62:ILE:HA	1:R:65:LEU:HB2	1.83	0.59
1:A:415:ALA:O	1:A:418:GLU:HG3	2.03	0.59
1:G:129:ARG:O	1:G:133:ASP:N	2.35	0.59
1:N:399:GLN:HA	1:N:402:VAL:HG22	1.84	0.59
2:C:796:ALA:HA	2:C:850:THR:HA	1.84	0.59
2:P:792:ARG:HA	2:P:792:ARG:HE	1.67	0.59
2:P:853:LEU:HG	2:P:854:GLN:H	1.67	0.59
1:W:298:GLU:O	1:W:302:GLY:N	2.30	0.59
1:X:345:GLY:HA2	1:X:348:GLN:OE1	2.01	0.59
2:S:13:TYR:O	2:S:887:SER:N	2.36	0.59
1:B:367:LEU:O	1:B:370:SER:OG	2.20	0.59
2:I:812:GLN:CB	2:I:818:ARG:HA	2.32	0.59
1:R:109:ARG:O	1:R:112:SER:OG	2.19	0.59
1:W:377:ALA:O	1:W:380:ARG:NH1	2.36	0.59
2:T:886:VAL:O	2:T:887:SER:OG	2.16	0.59
2:D:12:VAL:N	2:D:885:THR:OG1	2.35	0.59
2:D:858:LEU:HB3	2:D:886:VAL:HG23	1.83	0.59
1:M:319:GLU:OE1	1:N:315:GLN:NE2	2.34	0.59
2:C:804:ILE:HG22	2:C:805:ASN:N	2.17	0.59
2:D:813:ALA:HB3	2:D:816:LYS:HD2	1.85	0.59
1:K:84:HIS:HA	1:K:87:LEU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:804:ILE:HA	2:P:872:TYR:CE1	2.38	0.59
1:H:142:GLU:HG3	1:H:146:LEU:HD12	1.85	0.58
1:L:72:PRO:HA	1:L:75:GLN:HG3	1.83	0.58
1:L:80:ARG:O	1:L:84:HIS:N	2.35	0.58
1:N:423:GLU:OE1	2:J:808:ARG:NH2	2.35	0.58
1:E:406:HIS:HD1	1:F:406:HIS:HE1	1.50	0.58
1:E:415:ALA:O	1:E:418:GLU:HG3	2.03	0.58
2:T:800:SER:O	2:T:873:ARG:NH1	2.35	0.58
2:O:802:ASP:HB2	2:O:846:SER:HA	1.84	0.58
2:S:859:LYS:N	2:S:862:ASP:OD2	2.35	0.58
1:H:66:ILE:O	1:H:69:ILE:N	2.29	0.58
1:M:301:ASN:HD21	1:N:301:ASN:HD21	1.50	0.58
2:I:2:VAL:HG22	2:I:877:TYR:CZ	2.38	0.58
2:I:805:ASN:ND2	2:I:872:TYR:CD1	2.62	0.58
2:I:805:ASN:O	2:I:806:ILE:CG1	2.51	0.58
2:I:845:ASP:N	2:I:850:THR:O	2.36	0.58
1:V:66:ILE:HG22	1:V:70:ARG:HG3	1.84	0.58
2:S:824:VAL:HG11	2:S:842:ILE:HG21	1.84	0.58
1:G:147:ARG:HH22	1:N:359:THR:HA	1.68	0.58
1:Q:147:ARG:HH22	1:X:359:THR:HA	1.68	0.58
1:X:399:GLN:HA	1:X:402:VAL:HG22	1.84	0.58
2:O:804:ILE:HG22	2:O:805:ASN:N	2.17	0.58
2:I:10:GLY:H	2:I:791:LEU:HD21	1.68	0.58
1:X:423:GLU:OE1	2:T:808:ARG:NH2	2.35	0.58
1:G:112:SER:O	1:G:116:ALA:N	2.35	0.58
1:G:170:ARG:HE	1:H:171:ILE:HG12	1.68	0.58
1:M:377:ALA:O	1:M:380:ARG:NH1	2.36	0.58
1:R:70:ARG:HA	1:R:73:VAL:HB	1.84	0.58
1:W:345:GLY:HA2	1:W:348:GLN:HB3	1.85	0.58
1:G:59:LEU:O	1:G:62:ILE:HG22	2.04	0.58
2:P:12:VAL:N	2:P:885:THR:OG1	2.35	0.58
2:O:834:ASP:HA	2:O:837:LYS:HZ3	1.69	0.58
1:B:386:GLN:HA	1:B:389:ARG:NH1	2.19	0.58
2:C:832:TYR:OH	2:C:842:ILE:N	2.30	0.58
2:C:834:ASP:OD1	2:C:835:SER:N	2.37	0.58
2:I:845:ASP:O	2:I:850:THR:N	2.36	0.58
1:X:351:ALA:O	1:X:355:THR:HG23	2.04	0.58
2:D:853:LEU:HG	2:D:854:GLN:H	1.67	0.58
1:G:96:GLN:O	1:G:99:ARG:NH1	2.37	0.58
1:F:382:GLU:O	1:F:386:GLN:NE2	2.37	0.58
1:Q:59:LEU:O	1:Q:62:ILE:N	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:371:ALA:O	1:X:374:GLN:N	2.37	0.58
2:S:805:ASN:O	2:S:806:ILE:CG1	2.51	0.58
2:I:799:ARG:HD2	2:I:800:SER:N	2.19	0.58
1:F:386:GLN:HA	1:F:389:ARG:NH1	2.19	0.58
1:R:152:GLN:HG2	1:R:156:LYS:NZ	2.19	0.58
1:X:355:THR:O	1:X:359:THR:HG23	2.04	0.58
2:O:834:ASP:OD1	2:O:835:SER:N	2.37	0.58
1:B:382:GLU:O	1:B:386:GLN:NE2	2.37	0.57
1:G:206:ASN:O	1:G:210:GLY:N	2.33	0.57
1:H:152:GLN:HG2	1:H:156:LYS:NZ	2.19	0.57
2:P:869:ASN:ND2	2:P:876:GLU:OE2	2.31	0.57
1:W:305:SER:HA	1:W:308:LEU:HB2	1.86	0.57
1:X:309:ALA:O	1:X:312:SER:OG	2.20	0.57
2:D:821:VAL:O	2:D:833:VAL:N	2.38	0.57
2:P:839:ARG:O	2:P:840:PHE:HD1	1.87	0.57
1:U:84:HIS:HA	1:U:87:LEU:HB2	1.85	0.57
2:S:845:ASP:N	2:S:850:THR:O	2.36	0.57
1:M:305:SER:HA	1:M:308:LEU:HB2	1.86	0.57
1:M:338:ALA:O	1:M:341:GLU:HG3	2.04	0.57
1:N:351:ALA:O	1:N:355:THR:HG23	2.04	0.57
1:N:355:THR:O	1:N:359:THR:HG23	2.04	0.57
1:N:400:ASP:OD1	1:N:404:ARG:NH1	2.36	0.57
1:R:105:GLN:HA	1:R:108:GLU:HG3	1.85	0.57
1:Q:80:ARG:NH1	1:R:79:ALA:O	2.38	0.57
1:W:334:ASP:O	1:W:337:ARG:NH1	2.37	0.57
2:S:10:GLY:H	2:S:791:LEU:HD21	1.68	0.57
2:D:804:ILE:HA	2:D:872:TYR:CE1	2.38	0.57
2:J:2:VAL:HA	2:J:799:ARG:HD2	1.87	0.57
2:J:3:GLN:HB3	2:J:798:SER:HB3	1.87	0.57
1:W:414:GLN:HB2	2:T:827:TRP:CZ2	2.40	0.57
1:X:422:SER:HA	2:S:831:ASN:ND2	2.20	0.57
2:T:2:VAL:HA	2:T:799:ARG:HD2	1.87	0.57
2:T:804:ILE:HG13	2:T:826:GLY:HA2	1.87	0.57
2:S:799:ARG:HD2	2:S:800:SER:N	2.19	0.57
2:D:869:ASN:ND2	2:D:876:GLU:OE2	2.31	0.57
1:M:345:GLY:HA2	1:M:348:GLN:HB3	1.85	0.57
1:R:120:THR:HG22	1:X:384:ARG:NH2	2.19	0.57
1:X:435:ARG:HH21	2:S:816:LYS:HA	1.70	0.57
2:S:839:ARG:NH1	2:S:856:ASN:O	2.38	0.57
1:A:406:HIS:HD1	1:B:406:HIS:HE1	1.50	0.57
1:Q:96:GLN:O	1:Q:99:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:117:ALA:O	1:Q:121:ALA:N	2.30	0.57
1:W:338:ALA:O	1:W:341:GLU:HG3	2.04	0.57
2:T:792:ARG:HH22	2:T:854:GLN:HA	1.70	0.57
2:O:804:ILE:HG23	2:O:870:ALA:HB1	1.87	0.57
1:G:80:ARG:NH1	1:H:79:ALA:O	2.38	0.57
1:M:298:GLU:HA	1:M:301:ASN:HB2	1.87	0.57
2:C:804:ILE:HG23	2:C:870:ALA:HB1	1.87	0.57
2:O:808:ARG:N	2:O:869:ASN:O	2.34	0.57
2:S:836:VAL:HB	2:S:840:PHE:CD1	2.39	0.57
1:Q:71:GLY:O	1:Q:75:GLN:HB2	2.05	0.57
1:R:66:ILE:O	1:R:69:ILE:N	2.29	0.57
2:S:792:ARG:NH2	2:S:851:VAL:O	2.27	0.57
1:M:334:ASP:O	1:M:337:ARG:NH1	2.38	0.57
2:I:792:ARG:HG2	2:I:853:LEU:H	1.69	0.57
1:R:80:ARG:O	1:R:84:HIS:N	2.30	0.57
1:W:298:GLU:HA	1:W:301:ASN:HB2	1.87	0.57
1:W:312:SER:O	1:W:316:LYS:N	2.35	0.57
2:O:832:TYR:OH	2:O:842:ILE:N	2.30	0.57
2:S:792:ARG:HG2	2:S:853:LEU:H	1.69	0.57
1:M:414:GLN:HB2	2:J:827:TRP:CZ2	2.40	0.56
2:C:6:GLU:HG2	2:C:794:SER:C	2.30	0.56
2:I:836:VAL:HB	2:I:840:PHE:CD1	2.39	0.56
1:R:210:GLY:O	1:R:213:ALA:N	2.38	0.56
1:W:379:LYS:O	1:W:383:GLU:N	2.32	0.56
2:O:882:THR:OG1	2:O:884:VAL:HG22	2.05	0.56
1:H:45:ILE:O	1:H:49:LEU:N	2.31	0.56
1:N:371:ALA:O	1:N:374:GLN:N	2.37	0.56
1:F:365:ASP:O	1:F:369:LYS:HD2	2.06	0.56
1:F:419:ARG:HH11	1:F:419:ARG:HG3	1.70	0.56
1:X:356:ALA:O	1:X:359:THR:OG1	2.19	0.56
2:S:792:ARG:HH22	2:S:850:THR:HG22	1.70	0.56
1:A:388:LEU:HD22	1:A:389:ARG:HH22	1.71	0.56
1:B:419:ARG:HH11	1:B:419:ARG:HG3	1.70	0.56
1:H:105:GLN:HA	1:H:108:GLU:HG3	1.85	0.56
1:M:312:SER:O	1:M:316:LYS:N	2.35	0.56
1:N:288:GLU:HG2	1:N:289:THR:N	2.16	0.56
2:J:792:ARG:HH22	2:J:854:GLN:HA	1.69	0.56
2:C:882:THR:OG1	2:C:884:VAL:HG22	2.05	0.56
2:I:839:ARG:NH1	2:I:856:ASN:O	2.38	0.56
2:P:792:ARG:NH2	2:P:854:GLN:OE1	2.38	0.56
1:X:400:ASP:OD1	1:X:404:ARG:NH1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:3:GLN:HB3	2:T:798:SER:HB3	1.87	0.56
2:D:792:ARG:NH2	2:D:854:GLN:OE1	2.38	0.56
1:G:163:SER:O	1:G:167:ALA:N	2.28	0.56
1:R:62:ILE:HG13	1:R:65:LEU:HD12	1.88	0.56
2:D:839:ARG:O	2:D:840:PHE:HD1	1.87	0.56
1:H:120:THR:HG22	1:N:384:ARG:NH2	2.19	0.56
1:M:318:VAL:HB	1:N:315:GLN:HE21	1.70	0.56
2:I:805:ASN:O	2:I:806:ILE:HG12	2.05	0.56
2:P:821:VAL:O	2:P:833:VAL:N	2.38	0.56
2:P:859:LYS:N	2:P:862:ASP:OD2	2.26	0.56
1:G:71:GLY:O	1:G:75:GLN:HB2	2.05	0.56
1:H:75:GLN:O	1:H:79:ALA:HB3	2.05	0.56
1:Q:59:LEU:O	1:Q:62:ILE:HG22	2.04	0.56
1:W:352:GLY:O	1:W:355:THR:OG1	2.17	0.56
2:T:797:SER:H	2:T:849:ASP:HB3	1.71	0.56
2:S:805:ASN:O	2:S:806:ILE:HG12	2.05	0.56
2:S:859:LYS:O	2:S:861:GLU:N	2.38	0.56
1:B:383:GLU:HA	1:B:386:GLN:NE2	2.21	0.56
1:H:210:GLY:O	1:H:213:ALA:N	2.38	0.56
1:M:352:GLY:O	1:M:355:THR:OG1	2.17	0.56
2:I:792:ARG:HH22	2:I:850:THR:HG22	1.70	0.56
1:E:388:LEU:HD22	1:E:389:ARG:HH22	1.71	0.56
1:F:383:GLU:HA	1:F:386:GLN:NE2	2.20	0.56
1:Q:80:ARG:HH11	1:R:83:GLU:HG3	1.70	0.56
1:R:75:GLN:O	1:R:79:ALA:HB3	2.05	0.56
1:W:346:LEU:HB3	1:X:346:LEU:HD13	1.88	0.56
2:O:832:TYR:HE1	2:O:842:ILE:HG22	1.71	0.56
1:B:363:ARG:O	1:B:366:GLN:HG3	2.06	0.56
1:M:354:ASP:OD1	1:M:357:ARG:NE	2.35	0.56
2:C:808:ARG:N	2:C:869:ASN:O	2.34	0.56
2:I:13:TYR:O	2:I:887:SER:N	2.36	0.56
2:I:808:ARG:O	2:I:869:ASN:N	2.30	0.56
1:F:363:ARG:O	1:F:366:GLN:HG3	2.06	0.56
1:G:153:SER:O	1:G:156:LYS:HB2	2.06	0.56
1:M:303:GLN:OE1	1:M:307:ARG:NH2	2.39	0.56
1:M:334:ASP:O	1:M:337:ARG:HD3	2.05	0.56
1:N:422:SER:HA	2:I:831:ASN:ND2	2.20	0.56
2:I:802:ASP:O	2:I:804:ILE:HG23	2.06	0.56
1:E:360:ALA:HA	1:F:360:ALA:HB2	1.88	0.56
1:A:360:ALA:HA	1:B:360:ALA:HB2	1.88	0.56
1:G:152:GLN:O	1:G:155:LEU:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:406:HIS:HB2	1:N:406:HIS:CE1	2.41	0.56
2:C:832:TYR:HE1	2:C:842:ILE:HG22	1.71	0.56
1:W:303:GLN:HE22	1:W:307:ARG:HG3	1.71	0.56
1:W:334:ASP:O	1:W:337:ARG:HD3	2.05	0.56
2:O:6:GLU:HG2	2:O:794:SER:C	2.30	0.56
1:B:365:ASP:O	1:B:369:LYS:HD2	2.06	0.55
1:M:301:ASN:HA	1:M:304:ILE:HG22	1.88	0.55
2:J:804:ILE:HG13	2:J:826:GLY:HA2	1.87	0.55
2:I:859:LYS:O	2:I:861:GLU:N	2.38	0.55
2:S:802:ASP:O	2:S:804:ILE:HG23	2.06	0.55
1:G:101:ILE:HG21	1:H:100:GLN:HE22	1.71	0.55
1:G:155:LEU:HD11	1:N:348:GLN:HG3	1.89	0.55
1:H:62:ILE:HG13	1:H:65:LEU:HD12	1.88	0.55
1:F:367:LEU:O	1:F:370:SER:OG	2.20	0.55
1:X:312:SER:O	1:X:316:LYS:HG2	2.06	0.55
1:N:435:ARG:HH21	2:I:816:LYS:HA	1.70	0.55
1:Q:112:SER:O	1:Q:116:ALA:N	2.35	0.55
1:W:301:ASN:HA	1:W:304:ILE:HG22	1.89	0.55
1:W:406:HIS:HB2	1:X:406:HIS:CE1	2.41	0.55
2:T:822:ALA:HB1	2:T:832:TYR:HD1	1.72	0.55
1:G:59:LEU:O	1:G:62:ILE:N	2.27	0.55
1:M:303:GLN:HE22	1:M:307:ARG:HG3	1.71	0.55
1:N:312:SER:O	1:N:316:LYS:HG2	2.06	0.55
2:J:844:ARG:HB2	2:J:851:VAL:HG23	1.87	0.55
2:P:802:ASP:OD1	2:P:844:ARG:NH2	2.39	0.55
1:Q:153:SER:O	1:Q:156:LYS:HB2	2.06	0.55
2:T:869:ASN:ND2	2:T:879:GLY:H	2.05	0.55
2:J:869:ASN:ND2	2:J:879:GLY:H	2.05	0.55
1:Q:152:GLN:O	1:Q:155:LEU:HB2	2.06	0.55
1:R:71:GLY:O	1:R:74:SER:OG	2.17	0.55
1:G:80:ARG:HH11	1:H:83:GLU:HG3	1.71	0.55
1:H:40:GLN:NE2	1:K:74:SER:OG	2.40	0.55
1:M:379:LYS:O	1:M:383:GLU:N	2.32	0.55
1:R:52:ILE:HG13	1:R:53:GLY:H	1.71	0.55
1:W:318:VAL:HB	1:X:315:GLN:HE21	1.71	0.55
1:G:66:ILE:O	1:G:69:ILE:HG22	2.07	0.55
1:M:376:LYS:O	1:M:379:LYS:HG2	2.07	0.55
2:J:834:ASP:OD1	2:J:835:SER:N	2.40	0.55
1:F:358:ALA:O	1:F:361:ILE:N	2.40	0.55
2:T:836:VAL:HA	2:T:839:ARG:HG3	1.89	0.55
2:S:809:TRP:CE2	2:S:853:LEU:HD13	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:848:LYS:HG3	2:S:850:THR:OG1	2.07	0.55
1:B:424:ALA:O	1:B:428:GLU:HB3	2.06	0.55
2:D:802:ASP:OD1	2:D:844:ARG:NH2	2.39	0.55
2:D:841:ILE:O	2:D:853:LEU:HD12	2.07	0.55
1:H:58:HIS:O	1:H:62:ILE:HD12	2.07	0.55
1:H:90:VAL:O	1:H:94:LEU:N	2.25	0.55
2:J:797:SER:H	2:J:849:ASP:HB3	1.71	0.55
1:F:424:ALA:O	1:F:428:GLU:HB3	2.06	0.55
1:Q:101:ILE:HG21	1:R:100:GLN:HE22	1.71	0.55
1:R:90:VAL:O	1:R:94:LEU:N	2.25	0.55
1:V:59:LEU:HG	1:V:63:GLU:OE1	2.07	0.55
1:W:303:GLN:OE1	1:W:307:ARG:NH2	2.39	0.55
1:H:62:ILE:O	1:H:66:ILE:N	2.38	0.55
2:I:848:LYS:HG3	2:I:850:THR:OG1	2.07	0.55
2:T:834:ASP:OD1	2:T:835:SER:N	2.40	0.55
1:H:97:ALA:O	1:H:101:ILE:HG13	2.07	0.55
1:K:56:MET:SD	1:K:60:LYS:HG3	2.47	0.55
2:I:792:ARG:NH2	2:I:851:VAL:O	2.27	0.55
2:T:836:VAL:O	2:T:839:ARG:N	2.30	0.55
2:O:832:TYR:CE1	2:O:842:ILE:HG22	2.42	0.55
2:S:839:ARG:NH1	2:S:858:LEU:HA	2.22	0.55
1:G:128:ARG:O	1:G:131:THR:OG1	2.22	0.54
1:G:143:ILE:O	1:G:147:ARG:HG3	2.08	0.54
1:H:52:ILE:HG13	1:H:53:GLY:H	1.71	0.54
2:P:797:SER:OG	2:P:849:ASP:HB3	2.07	0.54
2:P:841:ILE:O	2:P:853:LEU:HD12	2.07	0.54
1:Q:66:ILE:O	1:Q:69:ILE:HG22	2.07	0.54
1:R:59:LEU:HA	1:R:62:ILE:HD13	1.89	0.54
1:B:358:ALA:O	1:B:361:ILE:N	2.40	0.54
2:C:832:TYR:CE1	2:C:842:ILE:HG22	2.42	0.54
1:A:374:GLN:CD	1:B:374:GLN:HG3	2.33	0.54
1:G:111:VAL:O	1:G:115:LEU:N	2.33	0.54
1:H:69:ILE:O	1:H:70:ARG:NH1	2.41	0.54
2:J:822:ALA:HB1	2:J:832:TYR:HD1	1.71	0.54
2:J:836:VAL:HA	2:J:839:ARG:HG3	1.89	0.54
1:E:401:GLN:NE2	1:E:402:VAL:HG23	2.22	0.54
1:R:69:ILE:O	1:R:70:ARG:NH1	2.41	0.54
1:W:416:THR:HG22	2:S:806:ILE:CG1	2.37	0.54
1:X:385:ALA:O	1:X:389:ARG:HG2	2.07	0.54
2:T:809:TRP:CD1	2:T:853:LEU:HD22	2.43	0.54
1:L:110:GLU:O	1:L:114:ARG:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:416:THR:HG22	2:I:806:ILE:CG1	2.37	0.54
1:N:402:VAL:HA	1:N:405:ASP:OD2	2.07	0.54
2:I:836:VAL:HB	2:I:840:PHE:HB2	1.90	0.54
2:T:844:ARG:HB2	2:T:851:VAL:HG23	1.88	0.54
1:A:401:GLN:NE2	1:A:402:VAL:HG23	2.22	0.54
1:M:346:LEU:HB3	1:N:346:LEU:HD13	1.88	0.54
1:N:309:ALA:O	1:N:312:SER:OG	2.20	0.54
1:N:401:GLN:NE2	1:N:405:ASP:OD1	2.41	0.54
2:J:809:TRP:CD1	2:J:853:LEU:HD22	2.42	0.54
2:J:836:VAL:O	2:J:839:ARG:N	2.30	0.54
1:E:407:GLU:HA	1:E:410:ILE:HG12	1.89	0.54
2:S:845:ASP:O	2:S:850:THR:N	2.36	0.54
1:G:37:ALA:O	1:G:41:ARG:NH1	2.40	0.54
1:N:385:ALA:O	1:N:389:ARG:HG2	2.07	0.54
2:I:802:ASP:N	2:I:849:ASP:OD2	2.41	0.54
1:R:40:GLN:NE2	1:U:74:SER:OG	2.40	0.54
1:R:62:ILE:O	1:R:66:ILE:HG12	2.08	0.54
1:H:62:ILE:O	1:H:66:ILE:HG12	2.08	0.54
1:L:59:LEU:HG	1:L:63:GLU:OE1	2.07	0.54
2:C:808:ARG:HB2	2:C:822:ALA:C	2.33	0.54
2:I:825:THR:HG22	2:I:827:TRP:HD1	1.73	0.54
1:Q:155:LEU:HD11	1:X:348:GLN:HG3	1.89	0.54
2:D:797:SER:OG	2:D:849:ASP:HB3	2.07	0.54
1:G:174:LEU:HD21	1:H:171:ILE:HD11	1.90	0.54
1:M:388:LEU:HD12	1:M:389:ARG:N	2.23	0.54
2:J:811:ARG:HB3	2:J:866:TYR:CD1	2.43	0.54
2:I:809:TRP:CE2	2:I:853:LEU:HD13	2.42	0.54
2:I:809:TRP:CZ2	2:I:853:LEU:HB2	2.43	0.54
2:I:839:ARG:NH1	2:I:858:LEU:HA	2.22	0.54
1:E:384:ARG:O	1:E:387:GLN:HG3	2.07	0.54
1:Q:164:LEU:HD12	1:Q:165:ARG:HG3	1.90	0.54
1:R:58:HIS:O	1:R:62:ILE:HD12	2.07	0.54
1:R:97:ALA:O	1:R:101:ILE:HG13	2.07	0.54
1:W:376:LYS:O	1:W:379:LYS:HG2	2.07	0.54
2:O:808:ARG:HB2	2:O:823:VAL:HA	1.87	0.54
1:A:384:ARG:O	1:A:387:GLN:HG3	2.07	0.54
1:G:83:GLU:HA	1:G:86:GLU:HG3	1.90	0.54
1:M:330:GLU:O	1:M:334:ASP:N	2.29	0.54
2:I:792:ARG:NH2	2:I:850:THR:HG22	2.23	0.54
2:I:828:GLY:H	2:I:844:ARG:HH22	1.56	0.54
1:U:56:MET:SD	1:U:60:LYS:HG3	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:288:GLU:HG2	1:X:289:THR:HG23	1.90	0.54
1:X:402:VAL:HA	1:X:405:ASP:OD2	2.07	0.54
2:O:808:ARG:HB2	2:O:822:ALA:C	2.33	0.54
2:S:792:ARG:NH2	2:S:850:THR:HG22	2.23	0.54
2:S:792:ARG:NE	2:S:852:TYR:HA	2.17	0.54
1:M:302:GLY:O	1:M:305:SER:OG	2.21	0.54
2:C:811:ARG:HG3	2:C:866:TYR:CZ	2.43	0.54
1:F:420:LEU:HD12	1:F:421:THR:N	2.23	0.54
1:Q:93:ASN:HA	1:Q:96:GLN:OE1	2.08	0.54
1:R:72:PRO:O	1:R:76:GLU:N	2.41	0.54
1:A:407:GLU:HA	1:A:410:ILE:HG12	1.89	0.53
1:N:288:GLU:HG2	1:N:289:THR:HG23	1.90	0.53
2:S:836:VAL:HB	2:S:840:PHE:HB2	1.90	0.53
1:H:72:PRO:O	1:H:76:GLU:N	2.42	0.53
1:N:414:GLN:NE2	2:I:827:TRP:CD2	2.77	0.53
2:I:805:ASN:ND2	2:I:872:TYR:HA	2.23	0.53
1:Q:143:ILE:O	1:Q:147:ARG:HG3	2.08	0.53
1:X:321:ARG:O	1:X:325:LEU:HD13	2.09	0.53
2:O:811:ARG:HG3	2:O:866:TYR:CZ	2.43	0.53
1:B:420:LEU:HD12	1:B:421:THR:N	2.23	0.53
1:G:97:ALA:HA	1:G:100:GLN:HG3	1.89	0.53
1:G:117:ALA:O	1:G:120:THR:OG1	2.18	0.53
1:K:76:GLU:O	1:K:80:ARG:N	2.30	0.53
1:E:374:GLN:CD	1:F:374:GLN:HG3	2.33	0.53
1:Q:37:ALA:O	1:Q:41:ARG:NH1	2.40	0.53
1:A:404:ARG:CZ	1:X:320:ARG:HD2	2.37	0.53
2:C:882:THR:O	2:C:884:VAL:HG23	2.08	0.53
1:U:76:GLU:O	1:U:80:ARG:N	2.30	0.53
1:X:401:GLN:NE2	1:X:405:ASP:OD1	2.41	0.53
2:S:809:TRP:CZ2	2:S:853:LEU:HB2	2.43	0.53
1:N:321:ARG:O	1:N:325:LEU:HD13	2.09	0.53
1:X:414:GLN:NE2	2:S:827:TRP:CD2	2.77	0.53
1:A:375:GLU:HB3	1:A:379:LYS:HZ3	1.72	0.53
1:G:192:ARG:HD2	1:H:192:ARG:HE	1.74	0.53
2:T:811:ARG:HB3	2:T:866:TYR:CD1	2.43	0.53
1:M:384:ARG:HH12	1:M:388:LEU:N	2.07	0.53
2:I:805:ASN:C	2:I:806:ILE:HG12	2.34	0.53
1:Q:41:ARG:NH1	1:U:78:GLU:OE2	2.42	0.53
1:Q:97:ALA:HA	1:Q:100:GLN:HG3	1.89	0.53
1:Q:168:THR:O	1:Q:172:GLU:N	2.30	0.53
1:W:432:GLU:OE1	1:W:436:ARG:NE	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:802:ASP:N	2:S:849:ASP:OD2	2.41	0.53
2:S:866:TYR:N	2:S:882:THR:O	2.34	0.53
2:D:812:GLN:HB2	2:D:818:ARG:HG2	1.91	0.53
2:D:840:PHE:CD2	2:D:853:LEU:HD21	2.44	0.53
1:M:312:SER:O	1:M:316:LYS:HG2	2.09	0.53
1:Q:174:LEU:HD21	1:R:171:ILE:HD11	1.90	0.53
1:V:110:GLU:O	1:V:114:ARG:HG2	2.07	0.53
2:S:825:THR:HG22	2:S:827:TRP:HD1	1.73	0.53
1:G:164:LEU:HD12	1:G:165:ARG:HG3	1.90	0.53
1:G:179:GLU:HA	1:G:182:ARG:HD2	1.91	0.53
1:H:59:LEU:HA	1:H:62:ILE:HD13	1.89	0.53
1:W:388:LEU:HD12	1:W:389:ARG:N	2.23	0.53
2:O:882:THR:O	2:O:884:VAL:HG23	2.08	0.53
1:H:44:THR:HG22	1:K:69:ILE:HG13	1.91	0.53
1:H:49:LEU:O	1:H:52:ILE:HG12	2.09	0.53
2:C:804:ILE:CG2	2:C:805:ASN:N	2.72	0.53
2:P:795:CYS:O	2:P:850:THR:HA	2.09	0.53
1:R:152:GLN:O	1:R:155:LEU:HB2	2.09	0.53
1:A:358:ALA:O	1:A:362:GLU:CB	2.55	0.52
1:G:93:ASN:HA	1:G:96:GLN:OE1	2.08	0.52
1:H:38:ILE:HG22	1:H:40:GLN:HB3	1.91	0.52
1:N:397:GLU:HA	1:N:400:ASP:OD2	2.09	0.52
1:N:436:ARG:NH1	1:N:437:ASP:OD1	2.42	0.52
2:I:807:MET:HG3	2:I:869:ASN:O	2.09	0.52
2:I:869:ASN:OD1	2:I:870:ALA:N	2.41	0.52
2:P:840:PHE:CD2	2:P:853:LEU:HD21	2.44	0.52
1:X:397:GLU:HA	1:X:400:ASP:OD2	2.09	0.52
2:T:848:LYS:HD2	2:T:848:LYS:O	2.10	0.52
1:H:128:ARG:HH11	1:H:131:THR:HG1	1.58	0.52
1:M:302:GLY:O	1:M:306:ALA:N	2.37	0.52
1:Q:179:GLU:HA	1:Q:182:ARG:HD2	1.91	0.52
1:R:142:GLU:O	1:R:146:LEU:N	2.38	0.52
1:W:416:THR:CG2	2:S:806:ILE:CG1	2.88	0.52
2:S:807:MET:HG3	2:S:869:ASN:O	2.09	0.52
1:H:152:GLN:O	1:H:155:LEU:HB2	2.09	0.52
2:J:848:LYS:HD2	2:J:848:LYS:O	2.10	0.52
1:F:361:ILE:O	1:F:365:ASP:HB2	2.10	0.52
2:P:812:GLN:HB2	2:P:818:ARG:HG2	1.91	0.52
1:Q:163:SER:O	1:Q:167:ALA:N	2.28	0.52
1:Q:214:ALA:O	1:Q:216:LEU:N	2.40	0.52
1:R:139:ASN:O	1:R:142:GLU:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:436:ARG:NH1	1:X:437:ASP:OD1	2.42	0.52
2:D:795:CYS:O	2:D:850:THR:HA	2.09	0.52
1:M:406:HIS:HB2	1:N:406:HIS:NE2	2.25	0.52
2:J:801:ILE:HD12	2:J:849:ASP:HB2	1.92	0.52
1:E:434:ALA:O	1:F:438:ARG:NH2	2.43	0.52
1:Q:83:GLU:HA	1:Q:86:GLU:HG3	1.90	0.52
1:R:38:ILE:HG22	1:R:40:GLN:HB3	1.91	0.52
2:S:869:ASN:OD1	2:S:870:ALA:N	2.41	0.52
1:A:434:ALA:O	1:B:438:ARG:NH2	2.43	0.52
1:B:361:ILE:O	1:B:365:ASP:HB2	2.10	0.52
1:G:143:ILE:HD11	1:H:143:ILE:HG12	1.92	0.52
1:K:104:ILE:HA	1:K:107:GLU:HB2	1.91	0.52
1:M:416:THR:CG2	2:I:806:ILE:CG1	2.88	0.52
2:C:827:TRP:O	2:C:829:SER:N	2.42	0.52
1:Q:164:LEU:HD12	1:Q:165:ARG:N	2.25	0.52
1:Q:174:LEU:O	1:Q:178:VAL:HG23	2.09	0.52
1:U:104:ILE:HA	1:U:107:GLU:HB2	1.91	0.52
2:I:809:TRP:CD2	2:I:853:LEU:HD13	2.45	0.52
1:Q:192:ARG:HD2	1:R:192:ARG:HE	1.74	0.52
2:O:827:TRP:O	2:O:829:SER:N	2.42	0.52
2:S:805:ASN:ND2	2:S:872:TYR:HA	2.23	0.52
2:S:828:GLY:H	2:S:844:ARG:HH22	1.56	0.52
1:B:432:GLU:O	1:B:435:ARG:HG3	2.10	0.52
1:G:90:VAL:HA	1:G:93:ASN:HB2	1.92	0.52
1:G:96:GLN:O	1:G:99:ARG:HD3	2.10	0.52
1:E:375:GLU:HB3	1:E:379:LYS:HZ3	1.75	0.52
1:E:416:THR:HG21	2:O:805:ASN:ND2	2.25	0.52
1:W:312:SER:O	1:W:316:LYS:HG2	2.09	0.52
1:X:399:GLN:HB3	1:X:403:ARG:HH12	1.75	0.52
1:B:365:ASP:HB3	1:B:369:LYS:NZ	2.25	0.52
1:G:180:GLY:O	1:G:184:GLN:HG3	2.10	0.52
1:M:307:ARG:O	1:M:311:SER:N	2.32	0.52
1:M:425:ALA:HB1	2:J:832:TYR:O	2.10	0.52
2:J:836:VAL:O	2:J:839:ARG:HG3	2.10	0.52
2:I:846:SER:C	2:I:849:ASP:H	2.18	0.52
1:W:371:ALA:O	1:W:374:GLN:N	2.43	0.52
2:S:809:TRP:CD2	2:S:853:LEU:HD13	2.45	0.52
1:M:339:LEU:HA	1:M:342:GLU:HG3	1.91	0.52
1:F:432:GLU:O	1:F:435:ARG:HG3	2.10	0.52
1:Q:90:VAL:HA	1:Q:93:ASN:HB2	1.92	0.52
1:Q:111:VAL:O	1:Q:115:LEU:N	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:49:LEU:O	1:R:52:ILE:HG12	2.09	0.52
1:G:91:ARG:O	1:G:94:LEU:HG	2.10	0.51
1:G:214:ALA:O	1:G:216:LEU:N	2.40	0.51
2:I:845:ASP:HB3	2:I:850:THR:HB	1.92	0.51
1:F:365:ASP:HB3	1:F:369:LYS:NZ	2.25	0.51
1:R:55:VAL:HA	1:R:58:HIS:ND1	2.25	0.51
1:V:105:GLN:C	1:V:109:ARG:HH21	2.18	0.51
1:W:412:GLU:CB	2:S:873:ARG:NH1	2.70	0.51
1:W:417:ILE:HD11	1:X:417:ILE:HG12	1.92	0.51
2:T:801:ILE:HD12	2:T:849:ASP:HB2	1.91	0.51
2:S:805:ASN:C	2:S:806:ILE:HG12	2.34	0.51
1:K:111:VAL:O	1:K:115:LEU:N	2.41	0.51
1:M:371:ALA:O	1:M:374:GLN:N	2.43	0.51
1:U:111:VAL:O	1:U:115:LEU:N	2.41	0.51
1:V:100:GLN:NE2	1:V:104:ILE:HD13	2.24	0.51
1:A:416:THR:HG21	2:C:805:ASN:ND2	2.25	0.51
1:Q:96:GLN:O	1:Q:99:ARG:HD3	2.10	0.51
1:W:381:ALA:O	1:W:385:ALA:N	2.42	0.51
1:W:384:ARG:HH12	1:W:388:LEU:N	2.07	0.51
1:B:372:VAL:C	1:B:376:LYS:HZ2	2.18	0.51
1:L:105:GLN:C	1:L:109:ARG:HH21	2.18	0.51
1:Q:91:ARG:O	1:Q:94:LEU:HG	2.10	0.51
1:R:189:ASP:O	1:R:192:ARG:HB2	2.11	0.51
1:W:339:LEU:HA	1:W:342:GLU:HG3	1.91	0.51
2:S:808:ARG:O	2:S:869:ASN:N	2.30	0.51
1:B:370:SER:O	1:B:374:GLN:OE1	2.28	0.51
1:G:176:GLN:HA	1:G:179:GLU:OE2	2.10	0.51
1:M:432:GLU:OE1	1:M:436:ARG:NE	2.42	0.51
1:Q:180:GLY:O	1:Q:184:GLN:HG3	2.10	0.51
1:R:44:THR:HG22	1:U:69:ILE:HG13	1.91	0.51
2:T:836:VAL:O	2:T:839:ARG:HG3	2.10	0.51
2:S:869:ASN:ND2	2:S:876:GLU:OE2	2.30	0.51
1:N:372:VAL:C	1:N:376:LYS:HZ3	2.18	0.51
1:Q:176:GLN:HA	1:Q:179:GLU:OE2	2.10	0.51
1:W:403:ARG:HA	1:W:406:HIS:HD2	1.74	0.51
2:S:839:ARG:NE	2:S:857:ASN:O	2.44	0.51
1:H:98:GLN:HA	1:H:101:ILE:HD12	1.92	0.51
2:O:804:ILE:CG2	2:O:805:ASN:N	2.72	0.51
1:A:379:LYS:O	1:A:380:ARG:C	2.53	0.51
1:A:420:LEU:HD12	1:A:421:THR:N	2.26	0.51
1:G:41:ARG:NH1	1:K:78:GLU:OE2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:189:ASP:O	1:H:192:ARG:HB2	2.11	0.51
1:N:294:ALA:O	1:N:295:ASP:C	2.54	0.51
1:F:381:ALA:HA	1:F:384:ARG:NH1	2.26	0.51
1:R:62:ILE:O	1:R:66:ILE:N	2.38	0.51
1:R:98:GLN:HA	1:R:101:ILE:HD12	1.92	0.51
1:R:161:ASP:O	1:R:164:LEU:HG	2.11	0.51
1:R:200:ALA:O	1:R:204:GLN:N	2.41	0.51
1:V:75:GLN:HA	1:V:78:GLU:HB3	1.93	0.51
1:X:372:VAL:C	1:X:376:LYS:HZ3	2.19	0.51
1:B:381:ALA:HA	1:B:384:ARG:NH1	2.26	0.51
2:D:825:THR:OG1	2:D:828:GLY:N	2.44	0.51
1:L:100:GLN:NE2	1:L:104:ILE:HD13	2.24	0.51
2:I:814:PRO:HG3	2:I:883:GLN:NE2	2.26	0.51
1:R:204:GLN:HE21	1:X:297:LEU:HD21	1.76	0.51
1:R:212:GLU:OE2	1:X:293:ARG:NH1	2.44	0.51
1:W:425:ALA:HB1	2:T:832:TYR:O	2.10	0.51
1:W:435:ARG:HA	1:W:438:ARG:HB3	1.92	0.51
2:O:796:ALA:HB1	2:O:848:LYS:HZ2	1.76	0.51
2:S:814:PRO:HG3	2:S:883:GLN:NE2	2.26	0.51
2:S:846:SER:C	2:S:849:ASP:H	2.18	0.51
1:G:128:ARG:HG2	1:G:132:GLN:HE22	1.76	0.51
1:G:174:LEU:O	1:G:178:VAL:HG23	2.09	0.51
1:H:55:VAL:HA	1:H:58:HIS:ND1	2.25	0.51
1:N:399:GLN:HB3	1:N:403:ARG:HH12	1.75	0.51
2:J:812:GLN:O	2:J:864:ALA:HB1	2.11	0.51
1:F:370:SER:O	1:F:374:GLN:OE1	2.28	0.51
2:O:812:GLN:O	2:O:865:VAL:N	2.34	0.51
1:H:54:ARG:HG2	1:H:58:HIS:HE1	1.73	0.50
1:H:142:GLU:O	1:H:146:LEU:N	2.38	0.50
1:K:76:GLU:HA	1:K:79:ALA:HB3	1.94	0.50
1:N:426:LEU:HD12	2:I:834:ASP:OD2	2.11	0.50
2:J:809:TRP:HB2	2:J:822:ALA:HB3	1.94	0.50
2:I:839:ARG:NE	2:I:857:ASN:O	2.44	0.50
1:Q:35:THR:HA	1:Q:38:ILE:HB	1.93	0.50
1:Q:143:ILE:HD11	1:R:143:ILE:HG12	1.92	0.50
1:R:54:ARG:HG2	1:R:58:HIS:HE1	1.73	0.50
1:U:76:GLU:HA	1:U:79:ALA:HB3	1.93	0.50
1:W:299:GLU:HG2	1:W:300:MET:N	2.27	0.50
1:W:302:GLY:O	1:W:306:ALA:N	2.37	0.50
1:W:406:HIS:HB2	1:X:406:HIS:NE2	2.25	0.50
1:X:426:LEU:HD12	2:S:834:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLN:HA	1:A:417:ILE:HG12	1.92	0.50
1:B:416:THR:HG22	2:D:805:ASN:HD22	1.75	0.50
1:G:35:THR:HA	1:G:38:ILE:HB	1.93	0.50
1:G:164:LEU:HD12	1:G:165:ARG:N	2.25	0.50
1:M:435:ARG:HA	1:M:438:ARG:HB3	1.92	0.50
2:I:809:TRP:CH2	2:I:853:LEU:HD22	2.46	0.50
1:E:414:GLN:HA	1:E:417:ILE:HG12	1.92	0.50
1:F:372:VAL:C	1:F:376:LYS:HZ2	2.19	0.50
1:F:384:ARG:O	1:F:387:GLN:HG3	2.11	0.50
1:B:384:ARG:O	1:B:387:GLN:HG3	2.11	0.50
2:D:834:ASP:O	2:D:837:LYS:HG2	2.12	0.50
1:H:204:GLN:HE21	1:N:297:LEU:HD21	1.76	0.50
1:L:97:ALA:HA	1:L:100:GLN:HB3	1.93	0.50
1:N:328:ALA:O	1:N:331:ARG:HG3	2.12	0.50
1:E:402:VAL:O	1:E:406:HIS:HD2	1.94	0.50
2:O:811:ARG:N	2:O:819:GLY:O	2.31	0.50
1:A:402:VAL:O	1:A:406:HIS:HD2	1.94	0.50
1:H:91:ARG:HA	1:H:94:LEU:HB2	1.93	0.50
1:M:399:GLN:HB2	1:N:399:GLN:HG2	1.92	0.50
1:M:417:ILE:HD11	1:N:417:ILE:HG12	1.92	0.50
1:E:403:ARG:HA	1:E:406:HIS:CD2	2.47	0.50
1:E:420:LEU:HD12	1:E:421:THR:N	2.26	0.50
2:S:809:TRP:CH2	2:S:853:LEU:HD22	2.46	0.50
2:S:828:GLY:H	2:S:844:ARG:NH2	2.09	0.50
2:S:845:ASP:HB3	2:S:850:THR:HB	1.92	0.50
1:A:403:ARG:HA	1:A:406:HIS:CD2	2.47	0.50
1:A:416:THR:HG21	2:C:805:ASN:CG	2.37	0.50
1:A:417:ILE:O	1:A:421:THR:HG23	2.12	0.50
1:H:212:GLU:OE2	1:N:293:ARG:NH1	2.44	0.50
1:L:75:GLN:HA	1:L:78:GLU:HB3	1.93	0.50
1:A:388:LEU:HD22	1:B:388:LEU:HD13	1.93	0.50
2:J:3:GLN:H	2:J:799:ARG:HE	1.60	0.50
1:E:379:LYS:O	1:E:380:ARG:C	2.53	0.50
1:X:414:GLN:NE2	2:S:827:TRP:CE2	2.80	0.50
2:T:809:TRP:HB2	2:T:822:ALA:HB3	1.93	0.50
1:B:380:ARG:HA	1:B:383:GLU:OE1	2.12	0.50
1:G:150:LEU:HD12	1:G:153:SER:OG	2.12	0.50
1:G:174:LEU:HA	1:G:177:ASP:OD2	2.12	0.50
1:H:139:ASN:O	1:H:142:GLU:HG2	2.10	0.50
1:L:100:GLN:HE21	1:L:104:ILE:HD13	1.76	0.50
1:N:414:GLN:NE2	2:I:827:TRP:CE2	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:810:TYR:HA	2:I:820:MET:HA	1.94	0.50
1:Q:128:ARG:HG2	1:Q:132:GLN:HE22	1.76	0.50
1:V:100:GLN:HE21	1:V:104:ILE:HD13	1.76	0.50
1:W:399:GLN:HB2	1:X:399:GLN:HG2	1.92	0.50
2:S:810:TYR:HA	2:S:820:MET:HA	1.94	0.50
1:H:203:ASN:O	1:H:206:ASN:HB3	2.12	0.50
1:K:110:GLU:O	1:K:114:ARG:N	2.36	0.50
2:C:808:ARG:HB2	2:C:823:VAL:HA	1.87	0.50
1:E:406:HIS:ND1	1:F:406:HIS:HE1	2.09	0.50
1:F:416:THR:HG22	2:P:805:ASN:HD22	1.75	0.50
2:P:812:GLN:HG3	2:P:817:GLN:O	2.12	0.50
2:P:825:THR:OG1	2:P:828:GLY:N	2.44	0.50
1:Q:60:LYS:HA	1:Q:63:GLU:OE2	2.12	0.50
2:D:796:ALA:HA	2:D:850:THR:OG1	2.11	0.50
1:H:71:GLY:O	1:H:74:SER:OG	2.17	0.50
1:H:86:GLU:HG3	1:H:87:LEU:HD12	1.94	0.50
1:M:432:GLU:OE2	1:M:435:ARG:NH1	2.45	0.50
1:E:359:THR:HG23	1:E:360:ALA:N	2.27	0.50
1:F:419:ARG:HH22	2:P:876:GLU:HB2	1.77	0.50
1:R:179:GLU:O	1:R:183:VAL:N	2.43	0.50
2:T:841:ILE:HB	2:T:854:GLN:HB3	1.94	0.50
2:J:841:ILE:HB	2:J:854:GLN:HB3	1.94	0.49
2:C:796:ALA:HB1	2:C:848:LYS:NZ	2.27	0.49
1:V:96:GLN:O	1:V:100:GLN:N	2.45	0.49
1:V:97:ALA:HA	1:V:100:GLN:HB3	1.93	0.49
1:X:328:ALA:O	1:X:331:ARG:HG3	2.12	0.49
2:O:796:ALA:HB1	2:O:848:LYS:NZ	2.27	0.49
2:O:825:THR:HG22	2:O:827:TRP:HE3	1.77	0.49
1:H:161:ASP:O	1:H:164:LEU:HG	2.11	0.49
2:I:828:GLY:H	2:I:844:ARG:NH2	2.09	0.49
1:W:354:ASP:OD1	1:W:357:ARG:NE	2.35	0.49
1:X:294:ALA:O	1:X:295:ASP:C	2.54	0.49
1:N:344:ASP:HA	1:N:347:ARG:NH1	2.28	0.49
2:I:882:THR:HG23	2:I:884:VAL:HG23	1.94	0.49
1:E:388:LEU:HD22	1:F:388:LEU:HD13	1.93	0.49
1:E:416:THR:HG21	2:O:805:ASN:CG	2.37	0.49
1:F:380:ARG:HA	1:F:383:GLU:OE1	2.12	0.49
1:F:414:GLN:NE2	1:F:418:GLU:OE2	2.44	0.49
2:P:834:ASP:O	2:P:837:LYS:HG2	2.12	0.49
1:W:307:ARG:O	1:W:311:SER:N	2.32	0.49
1:W:357:ARG:HD2	1:W:358:ALA:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:363:ARG:O	1:X:366:GLN:HG3	2.13	0.49
2:T:811:ARG:HB3	2:T:866:TYR:CE1	2.47	0.49
1:M:357:ARG:HD2	1:M:358:ALA:N	2.28	0.49
1:M:380:ARG:O	1:M:384:ARG:N	2.33	0.49
1:M:389:ARG:O	1:M:392:LEU:HB2	2.12	0.49
1:M:400:ASP:O	1:M:404:ARG:HG2	2.12	0.49
2:J:811:ARG:HH12	2:J:839:ARG:HH12	1.61	0.49
1:Q:174:LEU:HA	1:Q:177:ASP:OD2	2.12	0.49
1:U:94:LEU:O	1:U:98:GLN:N	2.42	0.49
1:X:344:ASP:HA	1:X:347:ARG:NH1	2.28	0.49
1:G:99:ARG:HA	1:G:102:ALA:HB3	1.95	0.49
2:C:795:CYS:O	2:C:850:THR:HA	2.12	0.49
2:C:807:MET:HE1	2:C:851:VAL:HG21	1.94	0.49
2:P:796:ALA:HA	2:P:850:THR:OG1	2.11	0.49
1:Q:99:ARG:HA	1:Q:102:ALA:HB3	1.95	0.49
1:Q:150:LEU:HD12	1:Q:153:SER:OG	2.12	0.49
1:R:91:ARG:HA	1:R:94:LEU:HB2	1.93	0.49
1:W:400:ASP:O	1:W:404:ARG:HG2	2.12	0.49
2:T:3:GLN:H	2:T:799:ARG:HE	1.60	0.49
1:A:359:THR:HG23	1:A:360:ALA:N	2.27	0.49
1:G:60:LYS:HA	1:G:63:GLU:OE2	2.12	0.49
1:F:367:LEU:C	1:F:370:SER:HG	2.17	0.49
1:Q:128:ARG:O	1:Q:131:THR:OG1	2.22	0.49
1:Q:173:HIS:HB3	1:W:331:ARG:NH2	2.22	0.49
1:R:207:ALA:O	1:R:211:GLU:N	2.38	0.49
1:W:432:GLU:OE2	1:W:435:ARG:NH1	2.45	0.49
2:O:802:ASP:H	2:O:849:ASP:HB2	1.78	0.49
1:B:414:GLN:NE2	1:B:418:GLU:OE2	2.44	0.49
1:B:419:ARG:HH22	2:D:876:GLU:HB2	1.77	0.49
2:D:812:GLN:HG3	2:D:817:GLN:O	2.12	0.49
1:G:168:THR:O	1:G:172:GLU:N	2.30	0.49
1:H:207:ALA:O	1:H:211:GLU:N	2.38	0.49
1:M:298:GLU:O	1:M:302:GLY:N	2.30	0.49
1:M:381:ALA:O	1:M:385:ALA:N	2.42	0.49
2:C:825:THR:HG22	2:C:827:TRP:HE3	1.77	0.49
2:I:841:ILE:HG22	2:I:854:GLN:NE2	2.28	0.49
2:P:858:LEU:C	2:P:859:LYS:HD3	2.38	0.49
1:R:203:ASN:O	1:R:206:ASN:HB3	2.12	0.49
2:T:811:ARG:HH12	2:T:839:ARG:HH12	1.60	0.49
2:T:812:GLN:O	2:T:864:ALA:HB1	2.11	0.49
2:O:795:CYS:O	2:O:850:THR:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:299:GLU:HG2	1:M:300:MET:N	2.27	0.49
2:C:2:VAL:HG21	2:C:877:TYR:CD2	2.48	0.49
1:Q:123:GLY:HA2	1:Q:126:ASP:OD2	2.13	0.49
1:R:86:GLU:HG3	1:R:87:LEU:HD12	1.94	0.49
2:O:807:MET:HE1	2:O:851:VAL:HG21	1.94	0.49
2:D:802:ASP:N	2:D:849:ASP:OD2	2.46	0.49
1:N:363:ARG:O	1:N:366:GLN:HG3	2.13	0.49
1:E:388:LEU:HD22	1:E:389:ARG:NH2	2.28	0.49
1:R:175:VAL:O	1:R:178:VAL:HG12	2.13	0.49
1:B:383:GLU:HA	1:B:386:GLN:HE21	1.78	0.49
2:D:792:ARG:HA	2:D:792:ARG:NE	2.28	0.49
2:J:812:GLN:HB2	2:J:818:ARG:CD	2.42	0.49
2:I:811:ARG:CZ	2:I:864:ALA:HA	2.43	0.49
1:E:417:ILE:O	1:E:421:THR:HG23	2.12	0.49
1:M:310:ASP:O	1:M:314:GLN:HG3	2.13	0.48
1:N:372:VAL:HG12	1:N:376:LYS:NZ	2.28	0.48
1:Q:171:ILE:HG23	1:R:170:ARG:NH1	2.28	0.48
1:W:310:ASP:O	1:W:314:GLN:HG3	2.13	0.48
2:S:807:MET:HA	2:S:870:ALA:HA	1.95	0.48
2:D:809:TRP:CD1	2:D:868:CYS:SG	3.06	0.48
1:H:73:VAL:C	1:H:76:GLU:H	2.21	0.48
1:H:175:VAL:O	1:H:178:VAL:HG12	2.13	0.48
1:K:75:GLN:O	1:K:79:ALA:N	2.43	0.48
1:M:422:SER:HA	2:J:831:ASN:HD22	1.77	0.48
1:N:289:THR:O	1:N:293:ARG:HG2	2.13	0.48
2:C:802:ASP:H	2:C:849:ASP:HB2	1.78	0.48
2:I:792:ARG:NE	2:I:852:TYR:HA	2.18	0.48
2:P:802:ASP:N	2:P:849:ASP:OD2	2.46	0.48
1:W:389:ARG:O	1:W:392:LEU:HB2	2.12	0.48
1:H:185:ALA:HA	1:H:188:ILE:HD12	1.95	0.48
2:J:811:ARG:HB3	2:J:866:TYR:CE1	2.47	0.48
1:F:410:ILE:O	1:F:413:LEU:HG	2.13	0.48
2:P:792:ARG:HA	2:P:792:ARG:NE	2.28	0.48
1:V:45:ILE:O	1:V:49:LEU:HG	2.14	0.48
1:X:300:MET:O	1:X:304:ILE:HG22	2.13	0.48
2:C:796:ALA:HB1	2:C:848:LYS:HZ2	1.79	0.48
1:Q:72:PRO:O	1:Q:76:GLU:HG3	2.14	0.48
1:R:185:ALA:HA	1:R:188:ILE:HD12	1.95	0.48
1:V:60:LYS:O	1:V:64:PRO:HG3	2.14	0.48
1:W:395:MET:HE2	1:W:395:MET:HA	1.96	0.48
2:T:789:ASP:N	2:T:789:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:836:VAL:HA	2:T:839:ARG:NE	2.28	0.48
1:B:407:GLU:HA	1:B:410:ILE:HD12	1.95	0.48
1:G:72:PRO:O	1:G:76:GLU:HG3	2.14	0.48
1:H:200:ALA:O	1:H:204:GLN:N	2.41	0.48
1:M:417:ILE:HD13	1:M:420:LEU:HD12	1.96	0.48
2:C:848:LYS:HD3	2:C:848:LYS:O	2.14	0.48
1:F:417:ILE:HG12	2:O:806:ILE:CG2	2.43	0.48
2:P:809:TRP:CD1	2:P:868:CYS:SG	3.06	0.48
2:P:809:TRP:HD1	2:P:868:CYS:HA	1.78	0.48
1:W:405:ASP:O	1:W:408:ALA:N	2.46	0.48
2:D:836:VAL:O	2:D:839:ARG:N	2.38	0.48
1:M:405:ASP:O	1:M:408:ALA:N	2.46	0.48
2:J:869:ASN:HD22	2:J:879:GLY:H	1.62	0.48
1:W:417:ILE:HD13	1:W:420:LEU:HD12	1.96	0.48
2:T:811:ARG:HD3	2:T:866:TYR:CE1	2.49	0.48
2:O:804:ILE:HG21	2:O:870:ALA:HB1	1.95	0.48
2:O:812:GLN:N	2:O:865:VAL:O	2.30	0.48
2:J:811:ARG:HH12	2:J:839:ARG:HH22	1.62	0.48
2:J:811:ARG:HD3	2:J:866:TYR:CE1	2.49	0.48
1:F:407:GLU:HA	1:F:410:ILE:HD12	1.95	0.48
2:S:841:ILE:HG22	2:S:854:GLN:NE2	2.28	0.48
2:S:882:THR:HG23	2:S:884:VAL:HG23	1.95	0.48
1:A:388:LEU:HD22	1:A:389:ARG:NH2	2.28	0.48
2:D:858:LEU:C	2:D:859:LYS:HD3	2.38	0.48
1:G:96:GLN:HA	1:G:99:ARG:CZ	2.43	0.48
1:G:149:ALA:O	1:G:152:GLN:HG3	2.14	0.48
1:G:171:ILE:HG23	1:H:170:ARG:NH1	2.28	0.48
1:G:186:GLN:O	1:G:189:ASP:HB2	2.14	0.48
1:L:66:ILE:HG22	1:L:70:ARG:HE	1.79	0.48
1:N:300:MET:O	1:N:304:ILE:HG22	2.13	0.48
1:Q:73:VAL:O	1:Q:76:GLU:HB2	2.13	0.48
1:Q:96:GLN:HA	1:Q:99:ARG:CZ	2.44	0.48
1:Q:117:ALA:O	1:Q:120:THR:OG1	2.18	0.48
1:Q:124:GLU:O	1:Q:128:ARG:HB2	2.14	0.48
1:W:422:SER:HA	2:T:831:ASN:HD22	1.77	0.48
1:W:431:LEU:HB3	1:X:431:LEU:HG	1.96	0.48
1:L:65:LEU:O	1:L:68:GLU:HG3	2.14	0.48
1:M:431:LEU:HB3	1:N:431:LEU:HG	1.95	0.48
1:Q:100:GLN:O	1:Q:104:ILE:HG12	2.14	0.48
1:R:73:VAL:C	1:R:76:GLU:H	2.21	0.48
2:O:848:LYS:O	2:O:848:LYS:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:841:ILE:O	2:D:853:LEU:HA	2.14	0.48
2:J:809:TRP:CE3	2:J:868:CYS:HB3	2.49	0.48
2:C:825:THR:C	2:C:827:TRP:N	2.70	0.48
2:I:843:SER:O	2:I:852:TYR:N	2.29	0.48
1:Q:59:LEU:HD12	1:Q:62:ILE:CG2	2.44	0.48
1:V:66:ILE:HG22	1:V:70:ARG:HE	1.79	0.48
1:X:289:THR:O	1:X:293:ARG:HG2	2.13	0.48
2:T:812:GLN:HB2	2:T:818:ARG:CD	2.42	0.48
2:O:825:THR:C	2:O:827:TRP:N	2.70	0.48
1:G:55:VAL:HB	1:K:56:MET:HE1	1.96	0.47
1:G:124:GLU:O	1:G:128:ARG:HB2	2.14	0.47
1:L:60:LYS:O	1:L:64:PRO:HG3	2.14	0.47
1:M:412:GLU:CB	2:I:873:ARG:NH1	2.70	0.47
1:M:412:GLU:HB2	2:I:873:ARG:HH11	1.77	0.47
1:E:435:ARG:NH1	2:P:816:LYS:HB3	2.26	0.47
1:F:406:HIS:HA	1:F:409:LYS:HG2	1.95	0.47
1:W:330:GLU:HA	1:W:333:LEU:HB3	1.96	0.47
1:G:73:VAL:O	1:G:76:GLU:HB2	2.13	0.47
1:H:128:ARG:HH12	1:H:132:GLN:N	2.12	0.47
1:H:152:GLN:HG2	1:H:156:LYS:HZ3	1.79	0.47
1:N:417:ILE:O	1:N:420:LEU:HG	2.14	0.47
2:I:807:MET:HA	2:I:870:ALA:HA	1.95	0.47
2:P:841:ILE:O	2:P:853:LEU:HA	2.14	0.47
1:U:77:PHE:HB3	1:U:81:ARG:NH2	2.29	0.47
1:U:84:HIS:O	1:U:88:ILE:HG12	2.14	0.47
2:T:811:ARG:HH12	2:T:839:ARG:HH22	1.62	0.47
1:G:100:GLN:O	1:G:104:ILE:HG12	2.14	0.47
1:L:87:LEU:HA	1:L:90:VAL:HB	1.97	0.47
1:M:395:MET:HE2	1:M:395:MET:HA	1.95	0.47
2:J:797:SER:OG	2:J:799:ARG:O	2.26	0.47
2:J:834:ASP:HA	2:J:837:LYS:HZ3	1.76	0.47
2:J:836:VAL:HA	2:J:839:ARG:NE	2.28	0.47
1:R:70:ARG:NH1	1:R:73:VAL:HG21	2.29	0.47
1:V:71:GLY:O	1:V:74:SER:OG	2.21	0.47
1:W:330:GLU:O	1:W:334:ASP:N	2.29	0.47
2:O:869:ASN:HD21	2:O:876:GLU:HG3	1.80	0.47
2:S:811:ARG:CZ	2:S:864:ALA:HA	2.43	0.47
1:B:410:ILE:O	1:B:413:LEU:HG	2.13	0.47
2:D:809:TRP:HD1	2:D:868:CYS:HA	1.78	0.47
1:K:84:HIS:O	1:K:88:ILE:HG12	2.14	0.47
1:M:386:GLN:HA	1:M:389:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:426:LEU:HD12	2:I:834:ASP:CG	2.40	0.47
2:C:804:ILE:HG21	2:C:870:ALA:HB1	1.95	0.47
2:I:825:THR:HG22	2:I:827:TRP:CD1	2.49	0.47
1:E:410:ILE:HG13	1:E:411:ALA:N	2.30	0.47
1:Q:96:GLN:HA	1:Q:99:ARG:NE	2.29	0.47
1:R:128:ARG:HH11	1:R:131:THR:HG1	1.61	0.47
1:W:358:ALA:O	1:W:362:GLU:N	2.38	0.47
1:X:390:ALA:O	1:X:393:ASP:HB2	2.14	0.47
1:X:414:GLN:HE22	2:S:827:TRP:CD1	2.32	0.47
2:T:797:SER:OG	2:T:801:ILE:HD13	2.15	0.47
2:O:2:VAL:HG21	2:O:877:TYR:CD2	2.48	0.47
1:A:359:THR:HG23	1:A:360:ALA:H	1.79	0.47
1:B:406:HIS:HA	1:B:409:LYS:HG2	1.95	0.47
2:D:833:VAL:O	2:D:836:VAL:HG22	2.15	0.47
1:M:330:GLU:HA	1:M:333:LEU:HB3	1.96	0.47
1:M:403:ARG:NH1	1:M:404:ARG:HB3	2.30	0.47
2:J:792:ARG:HE	2:J:793:LEU:N	2.04	0.47
1:E:359:THR:HG23	1:E:360:ALA:H	1.79	0.47
1:Q:186:GLN:O	1:Q:189:ASP:HB2	2.14	0.47
1:V:46:HIS:ND1	1:V:49:LEU:HD12	2.29	0.47
1:V:65:LEU:O	1:V:68:GLU:HG3	2.14	0.47
1:V:101:ILE:HG13	1:V:105:GLN:HG2	1.95	0.47
1:X:341:GLU:O	1:X:344:ASP:HB2	2.15	0.47
1:X:372:VAL:HG12	1:X:376:LYS:NZ	2.28	0.47
1:X:423:GLU:CD	2:T:808:ARG:HH22	2.23	0.47
2:S:859:LYS:O	2:S:862:ASP:N	2.43	0.47
1:A:406:HIS:HB2	1:B:406:HIS:CE1	2.50	0.47
1:G:96:GLN:HA	1:G:99:ARG:NE	2.29	0.47
1:G:123:GLY:HA2	1:G:126:ASP:OD2	2.13	0.47
1:G:175:VAL:HG22	1:H:174:LEU:HG	1.97	0.47
1:L:101:ILE:HG13	1:L:105:GLN:HG2	1.95	0.47
1:F:372:VAL:HA	1:F:375:GLU:CD	2.40	0.47
2:P:833:VAL:O	2:P:836:VAL:HG22	2.15	0.47
2:P:840:PHE:CG	2:P:853:LEU:HD21	2.50	0.47
1:R:120:THR:HG22	1:X:384:ARG:HH21	1.80	0.47
1:R:128:ARG:HH12	1:R:132:GLN:N	2.12	0.47
1:U:56:MET:O	1:U:60:LYS:N	2.33	0.47
1:V:87:LEU:HA	1:V:90:VAL:HB	1.97	0.47
1:V:104:ILE:H	1:V:104:ILE:HD12	1.80	0.47
1:X:417:ILE:O	1:X:420:LEU:HG	2.15	0.47
1:B:372:VAL:HA	1:B:375:GLU:CD	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:840:PHE:CG	2:D:853:LEU:HD21	2.50	0.47
1:G:59:LEU:HD12	1:G:62:ILE:CG2	2.44	0.47
1:H:55:VAL:O	1:H:58:HIS:HB2	2.15	0.47
1:M:420:LEU:HD13	1:N:420:LEU:HD11	1.97	0.47
1:N:368:ALA:O	1:N:372:VAL:HG23	2.15	0.47
1:N:390:ALA:O	1:N:393:ASP:HB2	2.14	0.47
2:J:6:GLU:HG2	2:J:881:GLY:H	1.80	0.47
2:J:797:SER:OG	2:J:801:ILE:HD13	2.15	0.47
2:C:869:ASN:HD21	2:C:876:GLU:HG3	1.80	0.47
1:E:379:LYS:O	1:E:382:GLU:HG2	2.15	0.47
2:P:836:VAL:O	2:P:839:ARG:N	2.39	0.47
1:Q:55:VAL:HB	1:U:56:MET:HE1	1.96	0.47
1:Q:74:SER:O	1:Q:77:PHE:HB2	2.15	0.47
1:Q:149:ALA:O	1:Q:152:GLN:HG3	2.14	0.47
1:W:301:ASN:ND2	1:X:301:ASN:HD21	2.13	0.47
1:W:420:LEU:HD13	1:X:420:LEU:HD11	1.97	0.47
2:T:6:GLU:HG2	2:T:881:GLY:H	1.80	0.47
2:T:809:TRP:CE3	2:T:868:CYS:HB3	2.49	0.47
2:O:806:ILE:HG13	2:O:871:ILE:HD12	1.97	0.47
2:D:802:ASP:C	2:D:804:ILE:H	2.23	0.47
1:H:40:GLN:O	1:H:44:THR:HG23	2.14	0.47
2:C:808:ARG:HB2	2:C:822:ALA:O	2.15	0.47
1:E:406:HIS:HB2	1:F:406:HIS:CE1	2.50	0.47
1:F:383:GLU:HA	1:F:386:GLN:HE21	1.78	0.47
1:X:368:ALA:O	1:X:372:VAL:HG23	2.15	0.47
1:H:173:HIS:ND1	1:H:174:LEU:HD22	2.30	0.47
1:N:422:SER:HA	2:I:831:ASN:HD22	1.79	0.47
1:E:402:VAL:O	1:E:406:HIS:CD2	2.68	0.47
1:F:432:GLU:HA	1:F:435:ARG:HG3	1.97	0.47
1:R:173:HIS:ND1	1:R:174:LEU:HD22	2.30	0.47
1:U:75:GLN:O	1:U:79:ALA:N	2.43	0.47
1:W:386:GLN:HA	1:W:389:ARG:NH1	2.29	0.47
2:O:793:LEU:HB3	2:O:809:TRP:CH2	2.49	0.47
2:O:817:GLN:OE1	2:O:817:GLN:N	2.48	0.47
1:H:38:ILE:CG2	1:H:40:GLN:HB3	2.45	0.47
1:H:70:ARG:NH1	1:H:73:VAL:HG21	2.29	0.47
1:K:77:PHE:HB3	1:K:81:ARG:NH2	2.29	0.47
1:L:46:HIS:ND1	1:L:49:LEU:HD12	2.29	0.47
2:J:789:ASP:N	2:J:789:ASP:OD1	2.46	0.47
1:Q:175:VAL:HG22	1:R:174:LEU:HG	1.97	0.47
1:X:371:ALA:O	1:X:372:VAL:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:843:SER:O	2:S:852:TYR:N	2.29	0.47
1:A:379:LYS:O	1:A:382:GLU:HG2	2.15	0.46
1:A:388:LEU:HG	1:A:391:ARG:NH2	2.30	0.46
1:N:372:VAL:HA	1:N:375:GLU:OE2	2.15	0.46
1:N:414:GLN:HE22	2:I:827:TRP:CD1	2.32	0.46
1:N:423:GLU:CD	2:J:808:ARG:HH22	2.23	0.46
2:C:793:LEU:HB3	2:C:809:TRP:CH2	2.49	0.46
2:C:826:GLY:CA	2:C:844:ARG:HH22	2.28	0.46
2:I:7:SER:OG	2:I:8:GLY:N	2.48	0.46
1:R:55:VAL:O	1:R:58:HIS:HB2	2.15	0.46
1:U:108:GLU:HA	1:U:111:VAL:HB	1.97	0.46
1:W:403:ARG:NH1	1:W:404:ARG:HB3	2.30	0.46
2:O:836:VAL:HB	2:O:840:PHE:HB2	1.97	0.46
2:S:1:GLU:HA	2:S:877:TYR:HE1	1.80	0.46
2:S:811:ARG:O	2:S:819:GLY:N	2.48	0.46
1:A:402:VAL:O	1:A:406:HIS:CD2	2.68	0.46
2:D:864:ALA:O	2:D:884:VAL:N	2.48	0.46
1:L:104:ILE:HD12	1:L:104:ILE:H	1.80	0.46
2:J:834:ASP:HA	2:J:837:LYS:HZ2	1.80	0.46
2:C:806:ILE:HG13	2:C:871:ILE:HD12	1.97	0.46
2:C:808:ARG:HB2	2:C:823:VAL:CA	2.44	0.46
2:C:836:VAL:HB	2:C:840:PHE:HB2	1.97	0.46
1:X:426:LEU:HD12	2:S:834:ASP:CG	2.40	0.46
1:K:81:ARG:HG3	1:K:84:HIS:CD2	2.50	0.46
1:M:297:LEU:HB3	1:M:298:GLU:H	1.58	0.46
1:E:388:LEU:HG	1:E:391:ARG:NH2	2.30	0.46
2:P:802:ASP:C	2:P:804:ILE:H	2.23	0.46
1:R:38:ILE:CG2	1:R:40:GLN:HB3	2.45	0.46
1:R:40:GLN:O	1:R:44:THR:HG23	2.14	0.46
1:U:81:ARG:HG3	1:U:84:HIS:CD2	2.50	0.46
2:S:825:THR:HG22	2:S:827:TRP:CD1	2.49	0.46
1:A:419:ARG:HH21	2:C:871:ILE:HG23	1.80	0.46
1:G:53:GLY:HA2	1:G:56:MET:CE	2.46	0.46
1:L:66:ILE:O	1:L:70:ARG:N	2.34	0.46
1:M:384:ARG:HH12	1:M:387:GLN:C	2.24	0.46
1:M:392:LEU:HD11	1:N:388:LEU:CD1	2.45	0.46
2:J:833:VAL:O	2:J:836:VAL:HG13	2.16	0.46
2:J:855:MET:HG2	2:J:858:LEU:HD11	1.97	0.46
2:J:858:LEU:HD23	2:J:858:LEU:HA	1.75	0.46
2:I:811:ARG:O	2:I:819:GLY:N	2.48	0.46
1:E:406:HIS:CE1	1:E:407:GLU:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:805:ASN:ND2	2:P:871:ILE:HG23	2.30	0.46
1:Q:53:GLY:HA2	1:Q:56:MET:CE	2.46	0.46
1:R:70:ARG:HA	1:R:70:ARG:HD3	1.71	0.46
1:U:77:PHE:HB3	1:U:81:ARG:HH21	1.80	0.46
1:W:385:ALA:HA	1:W:388:LEU:CD2	2.46	0.46
2:I:866:TYR:N	2:I:882:THR:O	2.34	0.46
1:E:419:ARG:HH21	2:O:871:ILE:HG23	1.80	0.46
1:X:332:ALA:O	1:X:336:ILE:HG12	2.16	0.46
1:A:434:ALA:HB1	1:B:438:ARG:HH22	1.80	0.46
1:G:147:ARG:HH22	1:N:359:THR:CA	2.29	0.46
1:K:77:PHE:HB3	1:K:81:ARG:HH21	1.80	0.46
1:L:45:ILE:O	1:L:49:LEU:HG	2.14	0.46
1:N:332:ALA:O	1:N:336:ILE:HG12	2.16	0.46
1:R:70:ARG:HA	1:R:70:ARG:HH11	1.81	0.46
1:R:118:ALA:HA	1:R:121:ALA:HB3	1.98	0.46
1:R:124:GLU:OE1	1:X:380:ARG:NH2	2.47	0.46
1:W:384:ARG:HH12	1:W:387:GLN:C	2.24	0.46
2:T:855:MET:HG2	2:T:858:LEU:HD11	1.97	0.46
1:A:406:HIS:CE1	1:A:407:GLU:HG3	2.51	0.46
1:A:435:ARG:NH1	2:D:816:LYS:HB3	2.26	0.46
1:B:432:GLU:HA	1:B:435:ARG:HG3	1.97	0.46
1:H:51:SER:HB3	1:K:59:LEU:HD21	1.98	0.46
1:H:70:ARG:NH2	1:L:45:ILE:HG21	2.31	0.46
1:H:148:ASN:O	1:H:151:LEU:N	2.47	0.46
1:H:161:ASP:HA	1:H:164:LEU:HG	1.98	0.46
1:M:421:THR:HG23	2:J:831:ASN:HD21	1.81	0.46
1:N:341:GLU:O	1:N:344:ASP:HB2	2.15	0.46
2:C:799:ARG:HG2	2:C:800:SER:H	1.81	0.46
2:I:2:VAL:HG21	2:I:872:TYR:HD2	1.81	0.46
1:F:371:ALA:HA	1:F:374:GLN:NE2	2.31	0.46
2:P:864:ALA:O	2:P:884:VAL:N	2.48	0.46
1:R:70:ARG:NH2	1:V:45:ILE:HG21	2.31	0.46
1:R:160:LEU:HD23	1:R:164:LEU:HD23	1.97	0.46
1:G:181:LEU:CD1	1:H:181:LEU:HD22	2.46	0.46
1:H:52:ILE:HG22	1:L:63:GLU:HG3	1.98	0.46
1:H:160:LEU:HD23	1:H:164:LEU:HD23	1.97	0.46
1:K:108:GLU:HA	1:K:111:VAL:HB	1.97	0.46
2:P:856:ASN:HA	2:P:858:LEU:HG	1.98	0.46
1:Q:147:ARG:HH22	1:X:359:THR:CA	2.29	0.46
1:W:380:ARG:O	1:W:384:ARG:N	2.33	0.46
1:X:422:SER:HA	2:S:831:ASN:HD22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:789:ASP:O	2:T:856:ASN:ND2	2.48	0.46
1:A:376:LYS:HB2	1:A:380:ARG:HH21	1.80	0.46
1:A:410:ILE:HG13	1:A:411:ALA:N	2.30	0.46
1:B:433:ALA:HA	1:B:436:ARG:HD2	1.98	0.46
1:H:186:GLN:HG2	1:M:320:ARG:HH22	1.81	0.46
1:K:74:SER:HA	1:K:77:PHE:CD2	2.51	0.46
1:N:414:GLN:NE2	2:I:827:TRP:CG	2.84	0.46
1:N:426:LEU:HA	2:I:834:ASP:OD1	2.15	0.46
2:C:834:ASP:CA	2:C:837:LYS:HZ3	2.28	0.46
1:F:385:ALA:O	1:F:388:LEU:HG	2.16	0.46
1:R:186:GLN:HG2	1:W:320:ARG:HH22	1.81	0.46
1:U:110:GLU:O	1:U:114:ARG:N	2.36	0.46
1:W:302:GLY:O	1:W:305:SER:OG	2.21	0.46
1:W:416:THR:CG2	2:S:806:ILE:HG12	2.46	0.46
1:X:414:GLN:HE22	2:S:827:TRP:NE1	2.14	0.46
2:T:869:ASN:HD22	2:T:879:GLY:H	1.62	0.46
2:O:799:ARG:HG2	2:O:800:SER:H	1.81	0.46
2:O:802:ASP:HB2	2:O:846:SER:CA	2.46	0.46
2:O:808:ARG:HB2	2:O:822:ALA:O	2.15	0.46
1:B:423:GLU:OE2	2:D:808:ARG:NH1	2.49	0.46
2:D:795:CYS:C	2:D:850:THR:HG23	2.41	0.46
2:D:805:ASN:ND2	2:D:871:ILE:HG23	2.31	0.46
2:D:843:SER:OG	2:D:844:ARG:N	2.49	0.46
1:H:202:ALA:O	1:H:206:ASN:N	2.49	0.46
1:N:371:ALA:O	1:N:372:VAL:C	2.58	0.46
1:E:434:ALA:HB1	1:F:438:ARG:HH22	1.80	0.46
1:R:70:ARG:NH2	1:V:45:ILE:HD13	2.29	0.46
1:R:202:ALA:O	1:R:206:ASN:N	2.49	0.46
1:U:105:GLN:HA	1:U:108:GLU:HG2	1.97	0.46
2:O:802:ASP:CB	2:O:846:SER:HB2	2.46	0.46
2:O:826:GLY:CA	2:O:844:ARG:HH22	2.28	0.46
2:D:865:VAL:HA	2:D:883:GLN:HA	1.98	0.45
1:G:74:SER:O	1:G:77:PHE:HB2	2.15	0.45
1:G:109:ARG:HG2	1:G:109:ARG:HH11	1.80	0.45
1:H:70:ARG:HA	1:H:70:ARG:HD3	1.71	0.45
1:K:119:GLU:O	1:K:122:LEU:HB2	2.16	0.45
2:P:793:LEU:HD11	2:P:866:TYR:HD2	1.81	0.45
1:Q:108:GLU:HA	1:Q:111:VAL:HG23	1.99	0.45
1:R:161:ASP:HA	1:R:164:LEU:HG	1.98	0.45
1:W:410:ILE:O	1:W:414:GLN:HG3	2.16	0.45
2:O:793:LEU:HB3	2:O:809:TRP:CZ3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:811:ARG:HG2	2:O:865:VAL:O	2.16	0.45
2:D:793:LEU:HD11	2:D:866:TYR:HD2	1.81	0.45
2:D:856:ASN:HA	2:D:858:LEU:HG	1.98	0.45
1:G:213:ALA:O	1:G:216:LEU:HB2	2.16	0.45
1:K:108:GLU:O	1:K:112:SER:N	2.35	0.45
1:M:301:ASN:ND2	1:N:301:ASN:HD21	2.13	0.45
1:M:442:GLN:OE1	1:M:443:MET:HB2	2.16	0.45
1:N:414:GLN:HE22	2:I:827:TRP:NE1	2.14	0.45
1:Q:181:LEU:CD1	1:R:181:LEU:HD22	2.46	0.45
1:U:119:GLU:O	1:U:122:LEU:HB2	2.16	0.45
1:V:47:GLY:O	1:V:51:SER:HB3	2.15	0.45
1:H:120:THR:HG22	1:N:384:ARG:HH21	1.80	0.45
1:L:47:GLY:O	1:L:51:SER:HB3	2.16	0.45
2:C:793:LEU:HB3	2:C:809:TRP:CZ3	2.51	0.45
2:C:817:GLN:N	2:C:817:GLN:OE1	2.48	0.45
2:I:799:ARG:NH1	2:I:800:SER:HB3	2.32	0.45
2:P:801:ILE:C	2:P:803:GLY:H	2.24	0.45
1:R:38:ILE:HD12	1:R:41:ARG:NH2	2.31	0.45
1:X:372:VAL:HA	1:X:375:GLU:OE2	2.16	0.45
2:T:833:VAL:O	2:T:836:VAL:HG13	2.16	0.45
2:S:7:SER:OG	2:S:8:GLY:N	2.48	0.45
1:H:156:LYS:O	1:H:160:LEU:N	2.44	0.45
1:K:56:MET:O	1:K:60:LYS:N	2.33	0.45
1:K:105:GLN:HA	1:K:108:GLU:HG2	1.97	0.45
1:L:96:GLN:O	1:L:100:GLN:N	2.45	0.45
1:N:379:LYS:HA	1:N:379:LYS:HD3	1.88	0.45
2:C:811:ARG:HA	2:C:866:TYR:HA	1.99	0.45
2:I:832:TYR:HE2	2:I:842:ILE:HG12	1.81	0.45
1:E:372:VAL:HA	1:E:375:GLU:OE1	2.17	0.45
2:P:795:CYS:C	2:P:850:THR:HG23	2.41	0.45
1:R:51:SER:HB3	1:U:59:LEU:HD21	1.98	0.45
1:W:421:THR:HG23	2:T:831:ASN:HD21	1.81	0.45
1:W:442:GLN:OE1	1:W:443:MET:HB2	2.16	0.45
2:O:811:ARG:HA	2:O:866:TYR:HA	1.99	0.45
2:O:835:SER:C	2:O:839:ARG:HH22	2.17	0.45
1:H:38:ILE:HD12	1:H:41:ARG:NH2	2.31	0.45
1:L:72:PRO:HA	1:L:75:GLN:CG	2.46	0.45
1:F:433:ALA:HA	1:F:436:ARG:HD2	1.98	0.45
1:W:412:GLU:HB2	2:S:873:ARG:HH11	1.77	0.45
1:X:414:GLN:NE2	2:S:827:TRP:CG	2.84	0.45
1:X:426:LEU:HA	2:S:834:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:2:VAL:HG21	2:S:872:TYR:HD2	1.81	0.45
2:D:801:ILE:C	2:D:803:GLY:H	2.24	0.45
1:H:118:ALA:HA	1:H:121:ALA:HB3	1.98	0.45
1:M:358:ALA:O	1:M:362:GLU:N	2.38	0.45
2:C:802:ASP:HB2	2:C:846:SER:CA	2.46	0.45
1:R:60:LYS:O	1:R:63:GLU:HB2	2.17	0.45
1:R:105:GLN:HA	1:R:108:GLU:CG	2.47	0.45
1:W:337:ARG:O	1:W:341:GLU:N	2.39	0.45
2:O:825:THR:CG2	2:O:827:TRP:H	2.28	0.45
2:S:832:TYR:HE2	2:S:842:ILE:HG12	1.81	0.45
1:B:371:ALA:HA	1:B:374:GLN:NE2	2.31	0.45
1:B:385:ALA:O	1:B:388:LEU:HG	2.16	0.45
1:B:417:ILE:CG1	2:C:806:ILE:HG21	2.45	0.45
2:D:802:ASP:HA	2:D:844:ARG:HH21	1.82	0.45
1:H:58:HIS:CE1	1:K:55:VAL:HA	2.52	0.45
1:M:385:ALA:HA	1:M:388:LEU:CD2	2.46	0.45
1:E:376:LYS:HB2	1:E:380:ARG:HH21	1.80	0.45
1:F:423:GLU:OE2	2:P:808:ARG:NH1	2.49	0.45
1:Q:109:ARG:HG2	1:Q:109:ARG:HH11	1.80	0.45
1:R:41:ARG:HA	1:R:44:THR:HG23	1.99	0.45
1:V:117:ALA:O	1:V:120:THR:OG1	2.24	0.45
2:T:840:PHE:HA	2:T:854:GLN:O	2.17	0.45
1:A:385:ALA:O	1:A:389:ARG:HG2	2.17	0.45
1:G:58:HIS:CE1	1:L:52:ILE:HB	2.52	0.45
2:P:862:ASP:HB2	2:P:886:VAL:CB	2.43	0.45
1:Q:150:LEU:HD22	1:R:149:ALA:HB1	1.99	0.45
1:R:53:GLY:O	1:R:57:GLU:N	2.37	0.45
1:U:74:SER:HA	1:U:77:PHE:CD2	2.51	0.45
1:W:357:ARG:O	1:W:361:ILE:HG12	2.17	0.45
2:T:812:GLN:HE21	2:T:816:LYS:C	2.25	0.45
2:S:800:SER:HB2	2:S:803:GLY:HA3	1.99	0.45
1:A:394:ALA:HA	1:A:397:GLU:OE2	2.17	0.45
1:G:173:HIS:HB3	1:M:331:ARG:NH2	2.22	0.45
2:C:802:ASP:CB	2:C:846:SER:HB2	2.46	0.45
2:C:811:ARG:HG2	2:C:865:VAL:O	2.16	0.45
2:I:811:ARG:NH2	2:I:864:ALA:HA	2.31	0.45
1:Q:127:ALA:HA	1:Q:130:GLN:OE1	2.17	0.45
1:R:52:ILE:HG22	1:V:63:GLU:HG3	1.98	0.45
1:R:148:ASN:O	1:R:151:LEU:N	2.47	0.45
1:R:152:GLN:HG2	1:R:156:LYS:HZ3	1.82	0.45
2:O:805:ASN:CB	2:O:871:ILE:O	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:GLU:HA	1:G:111:VAL:HG23	1.99	0.45
1:H:76:GLU:C	1:H:80:ARG:HE	2.25	0.45
1:H:103:LEU:HD12	1:H:104:ILE:HD13	1.99	0.45
1:K:86:GLU:O	1:K:90:VAL:HG22	2.17	0.45
1:M:297:LEU:HB3	1:M:298:GLU:OE1	2.17	0.45
1:M:410:ILE:O	1:M:414:GLN:HG3	2.16	0.45
2:J:789:ASP:O	2:J:856:ASN:ND2	2.48	0.45
2:J:812:GLN:HE21	2:J:816:LYS:C	2.25	0.45
1:E:394:ALA:HA	1:E:397:GLU:OE2	2.17	0.45
1:Q:167:ALA:HA	1:Q:170:ARG:HG2	1.99	0.45
1:R:53:GLY:HA2	1:R:56:MET:HG3	1.98	0.45
1:W:349:ARG:CZ	1:W:349:ARG:HB3	2.46	0.45
1:W:400:ASP:O	1:W:403:ARG:HD3	2.17	0.45
2:O:832:TYR:O	2:O:837:LYS:NZ	2.45	0.45
1:M:349:ARG:HB3	1:M:349:ARG:CZ	2.46	0.44
2:J:840:PHE:HA	2:J:854:GLN:O	2.17	0.44
1:E:385:ALA:O	1:E:389:ARG:HG2	2.17	0.44
1:Q:213:ALA:O	1:Q:216:LEU:HB2	2.16	0.44
1:V:86:GLU:O	1:V:90:VAL:HG23	2.17	0.44
1:W:325:LEU:HD12	1:X:322:ALA:HB1	1.99	0.44
1:W:424:ALA:HA	1:W:427:ALA:HB3	1.98	0.44
2:O:841:ILE:HG22	2:O:854:GLN:HB3	1.99	0.44
2:S:799:ARG:NH1	2:S:800:SER:HB3	2.32	0.44
2:S:811:ARG:NH2	2:S:864:ALA:HA	2.31	0.44
2:D:7:SER:OG	2:D:794:SER:HB2	2.18	0.44
1:H:156:LYS:HA	1:H:159:SER:OG	2.18	0.44
1:M:435:ARG:HH21	1:N:431:LEU:CD1	2.29	0.44
2:J:789:ASP:N	2:J:856:ASN:HA	2.32	0.44
2:I:805:ASN:OD1	2:I:871:ILE:O	2.35	0.44
2:P:843:SER:OG	2:P:844:ARG:N	2.49	0.44
1:Q:58:HIS:CE1	1:V:52:ILE:HB	2.52	0.44
1:R:45:ILE:HG12	1:V:70:ARG:NH1	2.25	0.44
1:W:297:LEU:HB3	1:W:298:GLU:OE1	2.17	0.44
1:B:419:ARG:HH12	2:D:875:SER:C	2.26	0.44
1:H:72:PRO:HB2	1:H:76:GLU:OE2	2.17	0.44
1:H:153:SER:O	1:H:157:VAL:HG23	2.17	0.44
1:H:201:ARG:O	1:H:204:GLN:HB3	2.17	0.44
1:K:94:LEU:O	1:K:98:GLN:HG2	2.17	0.44
1:L:86:GLU:O	1:L:90:VAL:HG23	2.17	0.44
2:I:800:SER:HB2	2:I:803:GLY:HA3	1.99	0.44
1:E:371:ALA:O	1:E:375:GLU:OE1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:63:GLU:HG2	1:Q:64:PRO:CD	2.43	0.44
1:Q:177:ASP:CG	1:W:331:ARG:HH12	2.24	0.44
1:R:48:GLY:O	1:R:52:ILE:HG23	2.17	0.44
1:R:58:HIS:CE1	1:U:55:VAL:HA	2.52	0.44
1:R:103:LEU:HD12	1:R:104:ILE:HD13	1.99	0.44
1:X:366:GLN:HA	1:X:369:LYS:NZ	2.33	0.44
1:X:388:LEU:HD13	1:X:388:LEU:HA	1.77	0.44
1:B:417:ILE:HG12	2:C:806:ILE:CG2	2.44	0.44
2:D:793:LEU:HD11	2:D:866:TYR:CD2	2.53	0.44
1:G:127:ALA:HA	1:G:130:GLN:OE1	2.17	0.44
1:G:150:LEU:HD22	1:H:149:ALA:HB1	1.99	0.44
1:H:48:GLY:O	1:H:52:ILE:HG23	2.17	0.44
1:H:53:GLY:HA2	1:H:56:MET:HG3	1.98	0.44
1:H:70:ARG:HA	1:H:70:ARG:HH11	1.81	0.44
1:M:424:ALA:HA	1:M:427:ALA:HB3	1.98	0.44
2:I:1:GLU:HA	2:I:877:TYR:HE1	1.80	0.44
2:I:808:ARG:HB3	2:I:823:VAL:HG23	2.00	0.44
2:I:811:ARG:HG2	2:I:865:VAL:H	1.82	0.44
2:P:865:VAL:HA	2:P:883:GLN:HA	1.98	0.44
1:R:153:SER:O	1:R:157:VAL:HG23	2.17	0.44
1:R:201:ARG:O	1:R:204:GLN:HB3	2.17	0.44
1:U:86:GLU:O	1:U:90:VAL:HG22	2.17	0.44
1:G:102:ALA:HA	1:G:105:GLN:CB	2.46	0.44
1:G:127:ALA:O	1:G:131:THR:HG23	2.18	0.44
1:H:90:VAL:HG12	1:H:94:LEU:HD23	2.00	0.44
1:H:105:GLN:HA	1:H:108:GLU:CG	2.47	0.44
1:H:171:ILE:HD12	1:H:171:ILE:HA	1.91	0.44
1:M:416:THR:CG2	2:I:806:ILE:HG12	2.46	0.44
1:N:314:GLN:O	1:N:318:VAL:HG23	2.18	0.44
2:J:839:ARG:HD2	2:J:840:PHE:CD1	2.53	0.44
2:C:799:ARG:HG2	2:C:800:SER:N	2.32	0.44
2:C:841:ILE:HG22	2:C:854:GLN:HB3	1.99	0.44
1:E:363:ARG:HG2	1:E:367:LEU:CD1	2.48	0.44
1:R:156:LYS:HA	1:R:159:SER:OG	2.18	0.44
1:R:185:ALA:O	1:R:189:ASP:N	2.45	0.44
1:W:339:LEU:O	1:W:343:ALA:N	2.50	0.44
2:O:812:GLN:CB	2:O:818:ARG:HA	2.46	0.44
2:D:820:MET:O	2:D:833:VAL:HG21	2.17	0.44
1:M:357:ARG:O	1:M:361:ILE:HG12	2.17	0.44
1:N:366:GLN:HA	1:N:369:LYS:NZ	2.33	0.44
2:I:812:GLN:H	2:I:865:VAL:HB	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:792:ARG:HE	2:T:793:LEU:N	2.04	0.44
2:S:812:GLN:H	2:S:865:VAL:HB	1.82	0.44
1:B:365:ASP:HB3	1:B:369:LYS:HZ3	1.82	0.44
2:D:833:VAL:O	2:D:835:SER:N	2.51	0.44
1:G:177:ASP:CG	1:M:331:ARG:HH12	2.24	0.44
1:H:60:LYS:O	1:H:63:GLU:HB2	2.17	0.44
2:C:812:GLN:CB	2:C:818:ARG:HA	2.46	0.44
1:E:413:LEU:O	1:E:416:THR:OG1	2.35	0.44
1:W:392:LEU:HD11	1:X:388:LEU:CD1	2.45	0.44
1:X:314:GLN:O	1:X:318:VAL:HG23	2.18	0.44
2:T:789:ASP:N	2:T:856:ASN:HA	2.32	0.44
2:O:834:ASP:HA	2:O:837:LYS:HD3	2.00	0.44
2:S:811:ARG:HG2	2:S:865:VAL:H	1.82	0.44
1:A:371:ALA:O	1:A:375:GLU:OE1	2.35	0.44
1:A:372:VAL:HA	1:A:375:GLU:OE1	2.17	0.44
1:H:59:LEU:HA	1:H:62:ILE:CD1	2.48	0.44
1:H:179:GLU:O	1:H:183:VAL:N	2.42	0.44
1:M:400:ASP:O	1:M:403:ARG:HD3	2.17	0.44
1:F:376:LYS:O	1:F:380:ARG:HG2	2.18	0.44
2:P:809:TRP:HA	2:P:868:CYS:HA	2.00	0.44
1:Q:181:LEU:HD12	1:R:181:LEU:HD22	2.00	0.44
2:T:834:ASP:C	2:T:836:VAL:H	2.25	0.44
2:O:799:ARG:HG2	2:O:800:SER:N	2.32	0.44
2:S:808:ARG:HB3	2:S:823:VAL:HG23	2.00	0.44
2:D:792:ARG:HD3	2:D:793:LEU:H	1.83	0.44
1:G:63:GLU:HG2	1:G:64:PRO:CD	2.43	0.44
1:G:181:LEU:HD12	1:H:181:LEU:HD22	2.00	0.44
1:H:70:ARG:NH2	1:L:45:ILE:HD13	2.29	0.44
1:M:418:GLU:HA	1:M:421:THR:HG22	2.00	0.44
1:N:372:VAL:HG12	1:N:376:LYS:HZ2	1.83	0.44
1:N:388:LEU:HD13	1:N:388:LEU:HA	1.77	0.44
1:F:435:ARG:HD2	1:F:436:ARG:N	2.33	0.44
2:P:806:ILE:H	2:P:806:ILE:HD12	1.82	0.44
1:R:90:VAL:HG12	1:R:94:LEU:HD23	2.00	0.44
2:T:839:ARG:HD2	2:T:840:PHE:CD1	2.53	0.44
2:D:809:TRP:CD1	2:D:868:CYS:HA	2.52	0.43
2:C:811:ARG:N	2:C:819:GLY:O	2.31	0.43
2:I:811:ARG:HD3	2:I:812:GLN:N	2.33	0.43
2:I:814:PRO:HG3	2:I:883:GLN:HE22	1.82	0.43
1:E:410:ILE:C	1:E:414:GLN:HE22	2.25	0.43
1:F:417:ILE:CG1	2:O:806:ILE:HG21	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:792:ARG:HD3	2:P:793:LEU:H	1.83	0.43
2:P:836:VAL:HG11	2:P:840:PHE:CD2	2.53	0.43
1:R:40:GLN:NE2	1:U:74:SER:HG	2.15	0.43
1:R:76:GLU:C	1:R:80:ARG:HE	2.25	0.43
1:V:72:PRO:HA	1:V:75:GLN:CG	2.46	0.43
1:X:379:LYS:HA	1:X:379:LYS:HD3	1.88	0.43
1:A:406:HIS:ND1	1:B:406:HIS:HE1	2.09	0.43
2:D:845:ASP:OD1	2:D:847:ALA:N	2.49	0.43
2:D:866:TYR:O	2:D:881:GLY:HA2	2.18	0.43
1:H:122:LEU:O	1:H:125:SER:OG	2.32	0.43
1:H:189:ASP:OD1	1:H:192:ARG:NH1	2.51	0.43
1:N:302:GLY:O	1:N:305:SER:OG	2.36	0.43
2:J:835:SER:CB	2:J:839:ARG:HH11	2.31	0.43
2:P:809:TRP:CD1	2:P:868:CYS:HA	2.52	0.43
1:Q:84:HIS:O	1:Q:88:ILE:HG13	2.18	0.43
1:W:380:ARG:HD3	1:W:380:ARG:H	1.83	0.43
1:W:418:GLU:HA	1:W:421:THR:HG22	2.00	0.43
2:O:808:ARG:HB2	2:O:823:VAL:CA	2.44	0.43
2:S:805:ASN:OD1	2:S:871:ILE:O	2.35	0.43
2:S:811:ARG:HD3	2:S:812:GLN:N	2.33	0.43
2:S:826:GLY:C	2:S:844:ARG:HH22	2.26	0.43
1:A:410:ILE:C	1:A:414:GLN:HE22	2.25	0.43
1:B:435:ARG:HD2	1:B:436:ARG:N	2.33	0.43
2:D:835:SER:O	2:D:839:ARG:NH1	2.51	0.43
2:D:836:VAL:HG11	2:D:840:PHE:CD2	2.53	0.43
1:G:84:HIS:O	1:G:88:ILE:HG13	2.18	0.43
1:M:312:SER:O	1:M:315:GLN:HB3	2.18	0.43
1:M:325:LEU:HD12	1:N:322:ALA:HB1	1.99	0.43
1:M:339:LEU:O	1:M:343:ALA:N	2.50	0.43
1:M:388:LEU:HD13	1:N:388:LEU:HG	2.00	0.43
2:J:790:SER:O	2:J:790:SER:OG	2.32	0.43
2:I:869:ASN:ND2	2:I:876:GLU:OE2	2.30	0.43
1:F:419:ARG:HH12	2:P:875:SER:C	2.26	0.43
1:U:94:LEU:O	1:U:98:GLN:HG2	2.17	0.43
2:T:797:SER:OG	2:T:799:ARG:O	2.26	0.43
2:T:801:ILE:CD1	2:T:849:ASP:HB2	2.49	0.43
2:T:835:SER:CB	2:T:839:ARG:HH11	2.31	0.43
2:S:814:PRO:HG3	2:S:883:GLN:HE22	1.82	0.43
1:A:392:LEU:HD11	1:B:391:ARG:NH1	2.34	0.43
1:B:372:VAL:HA	1:B:375:GLU:OE2	2.18	0.43
2:D:809:TRP:HA	2:D:868:CYS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:339:LEU:HD12	1:N:336:ILE:HD12	2.00	0.43
1:R:153:SER:O	1:R:157:VAL:N	2.42	0.43
1:W:312:SER:O	1:W:315:GLN:HB3	2.18	0.43
1:X:302:GLY:O	1:X:305:SER:OG	2.36	0.43
2:T:811:ARG:O	2:T:818:ARG:HD3	2.18	0.43
1:A:363:ARG:HG2	1:A:367:LEU:CD1	2.48	0.43
1:A:420:LEU:HA	1:A:423:GLU:HB3	2.00	0.43
2:D:806:ILE:H	2:D:806:ILE:HD12	1.82	0.43
1:G:100:GLN:O	1:G:104:ILE:N	2.47	0.43
1:G:167:ALA:HA	1:G:170:ARG:HG2	1.99	0.43
2:C:834:ASP:HA	2:C:837:LYS:HD3	2.00	0.43
2:I:808:ARG:NH1	2:I:810:TYR:OH	2.52	0.43
2:I:826:GLY:C	2:I:844:ARG:HH22	2.26	0.43
1:E:392:LEU:HD11	1:F:391:ARG:NH1	2.34	0.43
2:P:793:LEU:HD11	2:P:866:TYR:CD2	2.53	0.43
1:Q:127:ALA:O	1:Q:131:THR:HG23	2.18	0.43
1:R:45:ILE:HG22	1:R:49:LEU:HG	2.01	0.43
1:V:63:GLU:N	1:V:64:PRO:HD2	2.33	0.43
1:W:339:LEU:HD12	1:X:336:ILE:HD12	2.00	0.43
2:T:802:ASP:O	2:T:804:ILE:N	2.51	0.43
2:O:865:VAL:HA	2:O:884:VAL:HG11	2.01	0.43
1:A:389:ARG:NH1	1:B:388:LEU:HD22	2.34	0.43
1:B:376:LYS:O	1:B:380:ARG:HG2	2.18	0.43
1:G:177:ASP:OD2	1:M:331:ARG:NH2	2.51	0.43
1:H:96:GLN:O	1:H:99:ARG:HD3	2.19	0.43
2:J:801:ILE:CD1	2:J:849:ASP:HB2	2.49	0.43
2:J:810:TYR:N	2:J:867:SER:O	2.52	0.43
2:P:802:ASP:HA	2:P:844:ARG:HH21	1.82	0.43
2:P:833:VAL:O	2:P:835:SER:N	2.51	0.43
1:Q:100:GLN:O	1:Q:104:ILE:N	2.47	0.43
1:R:59:LEU:HA	1:R:62:ILE:CD1	2.48	0.43
1:R:155:LEU:O	1:R:159:SER:N	2.33	0.43
1:W:416:THR:HG21	2:S:806:ILE:HD11	2.01	0.43
2:D:862:ASP:HB2	2:D:886:VAL:CB	2.42	0.43
1:G:45:ILE:HD12	1:G:45:ILE:HA	1.89	0.43
1:H:41:ARG:HA	1:H:44:THR:HG23	1.99	0.43
1:H:45:ILE:HG22	1:H:49:LEU:HG	2.01	0.43
1:N:377:ALA:HA	1:N:380:ARG:CZ	2.49	0.43
2:J:802:ASP:O	2:J:804:ILE:N	2.52	0.43
1:F:372:VAL:HA	1:F:375:GLU:OE2	2.18	0.43
2:P:3:GLN:C	2:P:4:LEU:HD22	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:175:VAL:O	1:Q:178:VAL:N	2.51	0.43
1:Q:177:ASP:OD2	1:W:331:ARG:NH2	2.51	0.43
1:R:72:PRO:HB2	1:R:76:GLU:OE2	2.17	0.43
1:U:87:LEU:HA	1:U:90:VAL:HG22	2.01	0.43
1:W:329:LEU:HD21	1:X:325:LEU:O	2.19	0.43
2:O:795:CYS:HB3	2:O:851:VAL:HG22	2.01	0.43
2:D:859:LYS:O	2:D:886:VAL:HG11	2.19	0.43
1:G:175:VAL:O	1:G:178:VAL:N	2.51	0.43
1:L:106:ALA:O	1:L:109:ARG:HG2	2.19	0.43
1:M:403:ARG:HA	1:M:406:HIS:HD2	1.74	0.43
2:C:797:SER:CB	2:C:849:ASP:HB3	2.41	0.43
2:P:802:ASP:OD1	2:P:802:ASP:O	2.37	0.43
2:P:820:MET:O	2:P:833:VAL:HG21	2.18	0.43
2:P:832:TYR:CZ	2:P:842:ILE:HG22	2.54	0.43
1:R:96:GLN:O	1:R:99:ARG:HD3	2.19	0.43
1:R:154:ASP:HA	1:R:157:VAL:HB	2.01	0.43
1:W:388:LEU:HD13	1:X:388:LEU:HG	2.00	0.43
1:W:410:ILE:HG13	1:X:406:HIS:HE1	1.84	0.43
2:S:808:ARG:NH1	2:S:810:TYR:OH	2.52	0.43
1:B:406:HIS:HA	1:B:409:LYS:NZ	2.34	0.43
1:M:409:LYS:O	1:M:413:LEU:HD23	2.19	0.43
1:M:435:ARG:O	1:M:438:ARG:HB3	2.19	0.43
2:J:836:VAL:HA	2:J:839:ARG:CG	2.49	0.43
2:P:7:SER:OG	2:P:794:SER:HB2	2.18	0.43
1:Q:74:SER:HA	1:Q:77:PHE:HD2	1.84	0.43
1:Q:102:ALA:HA	1:Q:105:GLN:CB	2.46	0.43
1:R:189:ASP:OD1	1:R:192:ARG:NH1	2.51	0.43
1:V:106:ALA:O	1:V:109:ARG:HG2	2.19	0.43
1:X:408:ALA:O	1:X:412:GLU:OE1	2.37	0.43
1:X:414:GLN:CD	2:S:827:TRP:CG	2.97	0.43
1:A:413:LEU:O	1:A:416:THR:OG1	2.35	0.43
2:D:802:ASP:OD1	2:D:802:ASP:O	2.37	0.43
1:G:83:GLU:HA	1:G:86:GLU:CG	2.49	0.43
1:K:87:LEU:HA	1:K:90:VAL:HG22	2.01	0.43
1:M:380:ARG:H	1:M:380:ARG:HD3	1.83	0.43
2:J:811:ARG:O	2:J:818:ARG:HD3	2.18	0.43
2:P:859:LYS:O	2:P:886:VAL:HG11	2.19	0.43
1:R:41:ARG:O	1:R:45:ILE:HG13	2.19	0.43
1:V:65:LEU:O	1:V:69:ILE:N	2.52	0.43
1:W:409:LYS:O	1:W:413:LEU:HD23	2.19	0.43
2:T:796:ALA:HB1	2:T:848:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ARG:C	1:A:437:ASP:H	2.27	0.42
1:H:41:ARG:O	1:H:45:ILE:HG13	2.19	0.42
1:L:65:LEU:O	1:L:69:ILE:N	2.52	0.42
1:M:416:THR:HG21	2:I:806:ILE:HD11	2.01	0.42
2:J:809:TRP:CG	2:J:853:LEU:HD22	2.54	0.42
2:C:832:TYR:O	2:C:837:LYS:NZ	2.45	0.42
2:I:790:SER:HA	2:I:854:GLN:HA	2.01	0.42
2:P:835:SER:O	2:P:839:ARG:NH1	2.51	0.42
1:W:435:ARG:HH21	1:X:431:LEU:CD1	2.29	0.42
1:X:372:VAL:HG12	1:X:376:LYS:HZ2	1.84	0.42
2:T:796:ALA:HB1	2:T:848:LYS:HD2	2.01	0.42
1:G:147:ARG:HH12	1:N:359:THR:HA	1.84	0.42
2:C:809:TRP:CD2	2:C:853:LEU:HB2	2.54	0.42
2:C:823:VAL:HG12	2:C:831:ASN:HD21	1.84	0.42
1:E:358:ALA:O	1:E:362:GLU:CB	2.55	0.42
2:P:866:TYR:O	2:P:881:GLY:HA2	2.18	0.42
1:Q:147:ARG:HH12	1:X:359:THR:HA	1.84	0.42
1:Q:192:ARG:HB2	1:R:192:ARG:HE	1.85	0.42
1:W:354:ASP:O	1:W:357:ARG:HG3	2.20	0.42
1:A:388:LEU:HG	1:A:391:ARG:HH21	1.84	0.42
1:G:74:SER:HA	1:G:77:PHE:HD2	1.84	0.42
1:H:154:ASP:HA	1:H:157:VAL:HB	2.01	0.42
1:K:55:VAL:O	1:K:59:LEU:HD12	2.19	0.42
1:L:63:GLU:N	1:L:64:PRO:HD2	2.33	0.42
1:M:386:GLN:HA	1:M:389:ARG:HH12	1.84	0.42
2:J:834:ASP:C	2:J:836:VAL:H	2.25	0.42
2:C:795:CYS:HB3	2:C:851:VAL:HG22	2.01	0.42
1:R:96:GLN:HA	1:R:99:ARG:NE	2.34	0.42
1:R:129:ARG:O	1:R:132:GLN:HB2	2.19	0.42
1:X:377:ALA:HA	1:X:380:ARG:CZ	2.49	0.42
2:O:809:TRP:CD2	2:O:853:LEU:HB2	2.54	0.42
1:M:410:ILE:HG13	1:N:406:HIS:HE1	1.84	0.42
1:N:440:ARG:HA	1:N:443:MET:HG3	2.01	0.42
2:I:807:MET:HG2	2:I:808:ARG:N	2.35	0.42
1:E:420:LEU:HA	1:E:423:GLU:HB3	2.00	0.42
1:Q:192:ARG:HD2	1:R:192:ARG:HH21	1.85	0.42
1:X:440:ARG:HA	1:X:443:MET:HG3	2.01	0.42
2:O:795:CYS:HB2	2:O:809:TRP:CZ2	2.54	0.42
2:S:832:TYR:CE2	2:S:841:ILE:HA	2.54	0.42
1:B:371:ALA:O	1:B:374:GLN:N	2.52	0.42
2:D:832:TYR:CZ	2:D:842:ILE:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:PRO:O	1:H:75:GLN:HG2	2.20	0.42
1:H:124:GLU:OE1	1:N:380:ARG:NH2	2.47	0.42
2:J:796:ALA:HB1	2:J:848:LYS:O	2.19	0.42
2:J:796:ALA:HB2	2:J:850:THR:OG1	2.19	0.42
2:C:812:GLN:O	2:C:865:VAL:N	2.34	0.42
2:C:812:GLN:HG3	2:C:865:VAL:HB	2.01	0.42
1:Q:59:LEU:HD12	1:Q:62:ILE:HG22	2.02	0.42
2:T:865:VAL:HA	2:T:882:THR:O	2.20	0.42
2:O:797:SER:CB	2:O:849:ASP:HB3	2.41	0.42
2:S:824:VAL:HA	2:S:830:THR:HA	2.02	0.42
1:G:192:ARG:HB2	1:H:192:ARG:HE	1.85	0.42
1:H:153:SER:O	1:H:157:VAL:N	2.42	0.42
1:N:414:GLN:CD	2:I:827:TRP:CG	2.97	0.42
2:J:812:GLN:OE1	2:J:818:ARG:HB2	2.20	0.42
2:C:795:CYS:HB2	2:C:809:TRP:CZ2	2.54	0.42
2:I:809:TRP:CZ3	2:I:853:LEU:HD22	2.54	0.42
1:R:72:PRO:O	1:R:75:GLN:HG2	2.20	0.42
1:R:153:SER:O	1:R:156:LYS:N	2.53	0.42
1:R:161:ASP:OD1	1:R:164:LEU:HD21	2.20	0.42
1:U:108:GLU:O	1:U:112:SER:N	2.35	0.42
2:T:809:TRP:CG	2:T:853:LEU:HD22	2.54	0.42
2:T:810:TYR:N	2:T:867:SER:O	2.52	0.42
2:O:812:GLN:HG3	2:O:865:VAL:HB	2.01	0.42
2:S:790:SER:HA	2:S:854:GLN:HA	2.01	0.42
2:S:854:GLN:OE1	2:S:854:GLN:N	2.53	0.42
2:D:3:GLN:C	2:D:4:LEU:HD22	2.44	0.42
1:G:171:ILE:HD11	1:H:167:ALA:HA	2.02	0.42
1:H:129:ARG:O	1:H:132:GLN:HB2	2.20	0.42
1:N:408:ALA:O	1:N:412:GLU:OE1	2.37	0.42
2:C:805:ASN:CB	2:C:871:ILE:O	2.58	0.42
2:C:835:SER:C	2:C:839:ARG:HH22	2.18	0.42
1:X:378:LEU:HA	1:X:378:LEU:HD13	1.87	0.42
2:T:836:VAL:HA	2:T:839:ARG:CG	2.49	0.42
1:A:417:ILE:HD13	1:A:420:LEU:HD21	2.02	0.42
1:A:435:ARG:HH22	2:D:816:LYS:CA	2.32	0.42
1:M:329:LEU:HD21	1:N:325:LEU:O	2.19	0.42
1:M:354:ASP:O	1:M:357:ARG:HG3	2.19	0.42
2:J:865:VAL:HA	2:J:882:THR:O	2.20	0.42
2:I:832:TYR:CE2	2:I:841:ILE:HA	2.54	0.42
1:E:414:GLN:HA	1:E:417:ILE:CG1	2.50	0.42
1:F:371:ALA:O	1:F:374:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:83:GLU:HA	1:Q:86:GLU:CG	2.49	0.42
1:Q:171:ILE:HD11	1:R:167:ALA:HA	2.02	0.42
1:W:435:ARG:O	1:W:438:ARG:HB3	2.19	0.42
1:X:393:ASP:O	1:X:397:GLU:OE1	2.38	0.42
2:T:811:ARG:HA	2:T:865:VAL:O	2.20	0.42
2:S:789:ASP:HB2	2:S:855:MET:C	2.45	0.42
1:A:414:GLN:HA	1:A:417:ILE:CG1	2.50	0.42
1:G:148:ASN:N	1:G:148:ASN:OD1	2.51	0.42
1:G:192:ARG:HD2	1:H:192:ARG:HH21	1.85	0.42
1:H:205:ASP:O	1:H:208:LEU:HB3	2.20	0.42
2:J:796:ALA:HB1	2:J:848:LYS:HD2	2.01	0.42
2:J:810:TYR:CE1	2:J:869:ASN:HB2	2.55	0.42
2:C:825:THR:CG2	2:C:827:TRP:H	2.28	0.42
2:P:865:VAL:HG13	2:P:882:THR:C	2.45	0.42
1:R:92:ALA:HA	1:R:95:ASP:HB3	2.02	0.42
1:V:66:ILE:C	1:V:69:ILE:H	2.28	0.42
1:M:381:ALA:HA	1:M:384:ARG:HB2	2.02	0.42
2:C:865:VAL:HA	2:C:884:VAL:HG11	2.01	0.42
1:U:98:GLN:O	1:U:101:ILE:HG22	2.20	0.42
1:U:111:VAL:HG21	1:V:108:GLU:HG3	2.02	0.42
1:W:386:GLN:HA	1:W:389:ARG:HH12	1.84	0.42
1:W:430:ALA:HA	1:W:433:ALA:HB3	2.02	0.42
2:T:796:ALA:HB2	2:T:850:THR:OG1	2.19	0.42
2:S:7:SER:H	2:S:794:SER:N	2.18	0.42
1:G:206:ASN:HA	1:G:209:LEU:HB2	2.02	0.41
1:H:47:GLY:C	1:K:66:ILE:HD11	2.45	0.41
1:H:155:LEU:O	1:H:159:SER:N	2.33	0.41
1:H:161:ASP:OD1	1:H:164:LEU:HD21	2.20	0.41
1:K:98:GLN:O	1:K:101:ILE:HG22	2.20	0.41
2:I:7:SER:H	2:I:794:SER:N	2.18	0.41
2:I:824:VAL:HA	2:I:830:THR:HA	2.02	0.41
1:E:388:LEU:HG	1:E:391:ARG:HH21	1.84	0.41
1:W:435:ARG:NH2	1:X:431:LEU:HD11	2.34	0.41
2:S:809:TRP:CZ3	2:S:853:LEU:HD22	2.54	0.41
1:B:440:ARG:O	1:B:442:GLN:N	2.53	0.41
1:H:154:ASP:O	1:H:158:SER:N	2.50	0.41
1:M:301:ASN:HD21	1:N:297:LEU:HD22	1.85	0.41
2:C:812:GLN:N	2:C:865:VAL:O	2.30	0.41
1:E:389:ARG:NH1	1:F:388:LEU:HD22	2.34	0.41
1:F:406:HIS:HA	1:F:409:LYS:NZ	2.34	0.41
1:F:406:HIS:O	1:F:410:ILE:HG13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:104:ILE:O	1:R:108:GLU:HG3	2.21	0.41
1:W:298:GLU:H	1:W:298:GLU:CD	2.28	0.41
2:S:836:VAL:HB	2:S:840:PHE:CG	2.55	0.41
1:H:92:ALA:HA	1:H:95:ASP:HB3	2.02	0.41
1:K:93:ASN:O	1:K:96:GLN:NE2	2.47	0.41
1:L:111:VAL:O	1:L:114:ARG:HB2	2.20	0.41
2:C:832:TYR:OH	2:C:841:ILE:HD12	2.21	0.41
2:I:805:ASN:C	2:I:806:ILE:CG1	2.93	0.41
1:E:417:ILE:HD13	1:E:420:LEU:HD21	2.02	0.41
2:P:809:TRP:CZ3	2:P:853:LEU:HD22	2.47	0.41
1:U:55:VAL:O	1:U:59:LEU:HD12	2.20	0.41
2:S:807:MET:HG2	2:S:808:ARG:N	2.35	0.41
1:A:416:THR:CG2	2:C:805:ASN:ND2	2.83	0.41
1:B:379:LYS:O	1:B:383:GLU:OE1	2.38	0.41
2:D:857:ASN:O	2:D:859:LYS:NZ	2.54	0.41
1:G:88:ILE:HA	1:G:91:ARG:HB2	2.03	0.41
1:F:440:ARG:O	1:F:442:GLN:N	2.53	0.41
1:W:385:ALA:HA	1:W:388:LEU:HD23	2.03	0.41
2:T:858:LEU:HD23	2:T:858:LEU:HA	1.76	0.41
2:O:821:VAL:HG13	2:O:836:VAL:HG11	2.01	0.41
1:B:406:HIS:O	1:B:410:ILE:HG13	2.20	0.41
1:H:153:SER:O	1:H:156:LYS:N	2.53	0.41
1:L:66:ILE:C	1:L:69:ILE:H	2.28	0.41
1:M:385:ALA:O	1:M:389:ARG:NH1	2.54	0.41
2:J:807:MET:C	2:J:808:ARG:HG3	2.46	0.41
2:C:802:ASP:OD1	2:C:844:ARG:CD	2.45	0.41
2:I:821:VAL:O	2:I:833:VAL:HG12	2.20	0.41
2:I:854:GLN:OE1	2:I:854:GLN:N	2.53	0.41
1:W:300:MET:HA	1:W:303:GLN:CB	2.50	0.41
1:W:385:ALA:O	1:W:389:ARG:NH1	2.54	0.41
2:T:807:MET:HB2	2:T:870:ALA:CB	2.51	0.41
2:T:812:GLN:OE1	2:T:818:ARG:HB2	2.20	0.41
2:O:807:MET:HE2	2:O:807:MET:HB2	1.86	0.41
2:O:832:TYR:OH	2:O:841:ILE:HD12	2.21	0.41
1:H:45:ILE:HG12	1:L:70:ARG:NH1	2.25	0.41
1:H:168:THR:O	1:H:171:ILE:HG22	2.21	0.41
1:M:299:GLU:OE1	1:M:299:GLU:N	2.47	0.41
1:N:393:ASP:O	1:N:397:GLU:OE1	2.38	0.41
2:J:811:ARG:HA	2:J:865:VAL:O	2.20	0.41
2:C:802:ASP:HB2	2:C:846:SER:CB	2.51	0.41
2:I:789:ASP:HB2	2:I:855:MET:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:802:ASP:O	2:I:804:ILE:N	2.54	0.41
2:I:836:VAL:HB	2:I:840:PHE:CG	2.55	0.41
1:E:416:THR:CG2	2:O:805:ASN:ND2	2.83	0.41
1:E:441:LEU:HD12	1:E:441:LEU:HA	1.87	0.41
1:U:109:ARG:O	1:U:113:ALA:N	2.36	0.41
1:V:66:ILE:HB	1:V:70:ARG:HH21	1.85	0.41
1:X:381:ALA:O	1:X:384:ARG:HB2	2.21	0.41
1:X:400:ASP:CG	1:X:404:ARG:HH12	2.27	0.41
2:T:810:TYR:CE1	2:T:869:ASN:HB2	2.55	0.41
2:S:833:VAL:HG12	2:S:836:VAL:HG22	2.02	0.41
2:D:808:ARG:HH11	2:D:869:ASN:ND2	2.19	0.41
1:H:96:GLN:HA	1:H:99:ARG:NE	2.34	0.41
1:K:94:LEU:O	1:K:98:GLN:N	2.42	0.41
2:C:797:SER:HB2	2:C:799:ARG:O	2.21	0.41
2:C:821:VAL:HG13	2:C:836:VAL:HG11	2.01	0.41
1:Q:88:ILE:HA	1:Q:91:ARG:HB2	2.03	0.41
1:W:301:ASN:HD21	1:X:297:LEU:HD22	1.85	0.41
2:O:823:VAL:HG12	2:O:831:ASN:HD21	1.84	0.41
1:B:360:ALA:O	1:B:361:ILE:C	2.62	0.41
2:D:865:VAL:HG13	2:D:882:THR:C	2.45	0.41
1:G:59:LEU:HD12	1:G:62:ILE:HG22	2.02	0.41
1:G:201:ARG:O	1:G:204:GLN:NE2	2.54	0.41
1:G:205:ASP:OD1	1:G:208:LEU:HD13	2.21	0.41
1:M:300:MET:O	1:M:304:ILE:N	2.26	0.41
1:M:435:ARG:NE	1:N:431:LEU:HD11	2.35	0.41
2:J:865:VAL:HG13	2:J:882:THR:N	2.35	0.41
1:E:435:ARG:C	1:E:437:ASP:H	2.28	0.41
1:R:38:ILE:HG23	1:U:77:PHE:HZ	1.85	0.41
1:R:205:ASP:O	1:R:208:LEU:HB3	2.20	0.41
2:O:797:SER:HB2	2:O:799:ARG:O	2.21	0.41
1:H:38:ILE:HG23	1:K:77:PHE:HZ	1.85	0.41
1:K:111:VAL:HG21	1:L:108:GLU:HG3	2.02	0.41
1:M:303:GLN:NE2	1:M:307:ARG:HG3	2.35	0.41
1:M:385:ALA:HA	1:M:388:LEU:HD23	2.03	0.41
1:M:417:ILE:HA	1:M:420:LEU:HD12	2.03	0.41
1:M:430:ALA:HA	1:M:433:ALA:HB3	2.02	0.41
1:M:432:GLU:HA	1:M:435:ARG:CZ	2.51	0.41
1:M:435:ARG:NH2	1:N:431:LEU:HD11	2.34	0.41
1:N:378:LEU:HD13	1:N:378:LEU:HA	1.87	0.41
1:N:418:GLU:O	1:N:421:THR:HG22	2.21	0.41
2:J:811:ARG:C	2:J:818:ARG:HD3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:818:ARG:HH22	2:I:878:TRP:HZ3	1.69	0.41
2:I:861:GLU:O	2:I:863:THR:N	2.54	0.41
1:E:420:LEU:HD12	1:E:420:LEU:C	2.46	0.41
1:F:365:ASP:HB3	1:F:369:LYS:HZ3	1.85	0.41
2:P:845:ASP:OD1	2:P:847:ALA:N	2.49	0.41
1:Q:69:ILE:O	1:Q:73:VAL:HB	2.21	0.41
1:Q:148:ASN:OD1	1:Q:148:ASN:N	2.51	0.41
1:R:47:GLY:C	1:U:66:ILE:HD11	2.45	0.41
1:R:168:THR:O	1:R:171:ILE:HG22	2.21	0.41
1:R:179:GLU:O	1:R:183:VAL:HG23	2.21	0.41
1:V:111:VAL:O	1:V:114:ARG:HB2	2.20	0.41
1:W:377:ALA:O	1:X:378:LEU:HD11	2.21	0.41
1:W:385:ALA:O	1:W:388:LEU:HG	2.21	0.41
2:T:12:VAL:HG23	2:T:886:VAL:HA	2.03	0.41
2:T:795:CYS:O	2:T:851:VAL:HG12	2.21	0.41
2:S:818:ARG:HH22	2:S:878:TRP:HZ3	1.69	0.41
2:S:821:VAL:O	2:S:833:VAL:HG12	2.20	0.41
2:S:861:GLU:O	2:S:863:THR:N	2.54	0.41
1:H:53:GLY:O	1:H:57:GLU:N	2.37	0.41
1:K:84:HIS:NE2	1:L:84:HIS:HB2	2.36	0.41
1:M:300:MET:HA	1:M:303:GLN:CB	2.50	0.41
1:N:421:THR:OG1	2:I:823:VAL:HG13	2.21	0.41
2:J:796:ALA:HA	2:J:849:ASP:O	2.21	0.41
2:C:804:ILE:CG2	2:C:805:ASN:H	2.34	0.41
2:C:807:MET:HE2	2:C:807:MET:HB2	1.86	0.41
1:Q:192:ARG:CG	1:R:192:ARG:HE	2.34	0.41
1:U:84:HIS:NE2	1:V:84:HIS:HB2	2.36	0.41
2:T:811:ARG:C	2:T:818:ARG:HD3	2.46	0.41
2:O:3:GLN:HB2	2:O:798:SER:HB3	2.03	0.41
2:S:812:GLN:HB3	2:S:818:ARG:HG2	2.03	0.41
1:A:435:ARG:NH2	1:A:438:ARG:HH22	2.19	0.40
1:H:104:ILE:HG22	1:H:108:GLU:HG2	2.03	0.40
1:H:139:ASN:O	1:H:143:ILE:HG13	2.21	0.40
1:H:185:ALA:O	1:H:189:ASP:N	2.45	0.40
2:C:807:MET:HB2	2:C:869:ASN:O	2.21	0.40
2:I:804:ILE:HD12	2:I:826:GLY:HA3	2.03	0.40
2:I:833:VAL:HG12	2:I:836:VAL:HG22	2.02	0.40
2:I:859:LYS:C	2:I:861:GLU:N	2.79	0.40
1:F:360:ALA:O	1:F:361:ILE:C	2.62	0.40
2:P:857:ASN:O	2:P:859:LYS:NZ	2.54	0.40
1:Q:135:ALA:HA	1:Q:138:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:205:ASP:CA	1:Q:208:LEU:HB3	2.48	0.40
1:R:54:ARG:CZ	1:U:58:HIS:HB2	2.51	0.40
1:R:73:VAL:O	1:R:76:GLU:N	2.53	0.40
1:W:354:ASP:O	1:W:357:ARG:NE	2.54	0.40
1:B:415:ALA:HA	1:B:418:GLU:OE1	2.21	0.40
1:G:192:ARG:CG	1:H:192:ARG:HE	2.34	0.40
1:H:104:ILE:O	1:H:108:GLU:HG3	2.21	0.40
1:L:66:ILE:HB	1:L:70:ARG:HH21	1.85	0.40
1:N:326:ASN:O	1:N:329:LEU:HB3	2.21	0.40
1:N:371:ALA:O	1:N:375:GLU:OE1	2.39	0.40
1:N:389:ARG:HH21	1:N:392:LEU:CD1	2.35	0.40
2:J:795:CYS:O	2:J:851:VAL:HG12	2.21	0.40
2:J:802:ASP:HB2	2:J:846:SER:OG	2.21	0.40
2:J:807:MET:HB2	2:J:870:ALA:CB	2.51	0.40
2:I:863:THR:N	2:I:886:VAL:O	2.55	0.40
1:R:176:GLN:HA	1:R:179:GLU:OE2	2.21	0.40
1:V:66:ILE:O	1:V:70:ARG:N	2.35	0.40
1:W:371:ALA:O	1:W:374:GLN:HB2	2.21	0.40
1:X:379:LYS:O	1:X:383:GLU:OE1	2.39	0.40
1:G:56:MET:O	1:G:60:LYS:N	2.40	0.40
1:G:69:ILE:O	1:G:73:VAL:HB	2.21	0.40
1:M:377:ALA:HA	1:M:380:ARG:NE	2.36	0.40
1:N:381:ALA:O	1:N:384:ARG:HB2	2.21	0.40
1:Q:201:ARG:O	1:Q:204:GLN:NE2	2.54	0.40
1:Q:206:ASN:HA	1:Q:209:LEU:HB2	2.02	0.40
1:R:104:ILE:HG22	1:R:108:GLU:HG2	2.03	0.40
1:R:128:ARG:O	1:R:131:THR:OG1	2.34	0.40
1:R:155:LEU:O	1:R:158:SER:OG	2.28	0.40
2:T:856:ASN:O	2:T:857:ASN:C	2.65	0.40
1:A:417:ILE:O	1:A:420:LEU:HG	2.22	0.40
2:D:826:GLY:HA2	2:D:844:ARG:HH12	1.87	0.40
1:H:128:ARG:NH2	1:H:132:GLN:OE1	2.54	0.40
1:H:151:LEU:HD12	1:H:151:LEU:HA	1.77	0.40
1:M:298:GLU:H	1:M:298:GLU:CD	2.28	0.40
1:F:379:LYS:O	1:F:383:GLU:OE1	2.38	0.40
1:F:415:ALA:HA	1:F:418:GLU:OE1	2.21	0.40
1:Q:100:GLN:O	1:Q:103:LEU:HB3	2.21	0.40
1:U:95:ASP:O	1:U:99:ARG:HG2	2.21	0.40
1:W:381:ALA:HA	1:W:384:ARG:HB2	2.01	0.40
2:S:792:ARG:HH22	2:S:850:THR:CG2	2.34	0.40
1:B:403:ARG:HG2	1:B:403:ARG:HH11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:814:PRO:O	2:D:816:LYS:HG3	2.21	0.40
1:G:97:ALA:HA	1:G:100:GLN:HE21	1.86	0.40
1:H:179:GLU:O	1:H:183:VAL:HG23	2.21	0.40
1:M:354:ASP:O	1:M:357:ARG:NE	2.54	0.40
2:C:825:THR:HG22	2:C:826:GLY:N	2.37	0.40
2:I:812:GLN:HB3	2:I:818:ARG:HG2	2.03	0.40
1:E:435:ARG:NH2	1:E:438:ARG:HH22	2.19	0.40
1:F:403:ARG:HG2	1:F:403:ARG:HH11	1.85	0.40
1:Q:56:MET:O	1:Q:60:LYS:N	2.40	0.40
1:Q:97:ALA:HA	1:Q:100:GLN:HE21	1.86	0.40
1:R:139:ASN:O	1:R:143:ILE:HG13	2.21	0.40
1:X:418:GLU:O	1:X:421:THR:HG22	2.21	0.40
2:O:807:MET:HB2	2:O:869:ASN:O	2.22	0.40
2:O:836:VAL:O	2:O:837:LYS:C	2.64	0.40
2:S:802:ASP:O	2:S:804:ILE:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	82/457 (18%)	76 (93%)	6 (7%)	0	100	100
1	B	83/457 (18%)	72 (87%)	11 (13%)	0	100	100
1	E	82/457 (18%)	76 (93%)	6 (7%)	0	100	100
1	F	83/457 (18%)	72 (87%)	11 (13%)	0	100	100
1	G	181/457 (40%)	166 (92%)	15 (8%)	0	100	100
1	H	177/457 (39%)	166 (94%)	11 (6%)	0	100	100
1	K	70/457 (15%)	67 (96%)	3 (4%)	0	100	100
1	L	82/457 (18%)	77 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	145/457 (32%)	139 (96%)	6 (4%)	0	100	100
1	N	154/457 (34%)	151 (98%)	3 (2%)	0	100	100
1	Q	181/457 (40%)	166 (92%)	15 (8%)	0	100	100
1	R	177/457 (39%)	166 (94%)	11 (6%)	0	100	100
1	U	70/457 (15%)	67 (96%)	3 (4%)	0	100	100
1	V	82/457 (18%)	77 (94%)	5 (6%)	0	100	100
1	W	145/457 (32%)	139 (96%)	6 (4%)	0	100	100
1	X	154/457 (34%)	151 (98%)	3 (2%)	0	100	100
2	C	86/907 (10%)	70 (81%)	16 (19%)	0	100	100
2	D	108/907 (12%)	88 (82%)	20 (18%)	0	100	100
2	I	108/907 (12%)	81 (75%)	27 (25%)	0	100	100
2	J	107/907 (12%)	80 (75%)	27 (25%)	0	100	100
2	O	86/907 (10%)	70 (81%)	16 (19%)	0	100	100
2	P	108/907 (12%)	88 (82%)	20 (18%)	0	100	100
2	S	108/907 (12%)	81 (75%)	27 (25%)	0	100	100
2	T	107/907 (12%)	80 (75%)	27 (25%)	0	100	100
All	All	2766/14568 (19%)	2466 (89%)	300 (11%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	62/345 (18%)	62 (100%)	0	100	100
1	B	63/345 (18%)	63 (100%)	0	100	100
1	E	62/345 (18%)	62 (100%)	0	100	100
1	F	63/345 (18%)	63 (100%)	0	100	100
1	G	140/345 (41%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	137/345 (40%)	137 (100%)	0	100	100
1	K	55/345 (16%)	55 (100%)	0	100	100
1	L	63/345 (18%)	63 (100%)	0	100	100
1	M	110/345 (32%)	110 (100%)	0	100	100
1	N	116/345 (34%)	116 (100%)	0	100	100
1	Q	140/345 (41%)	140 (100%)	0	100	100
1	R	137/345 (40%)	137 (100%)	0	100	100
1	U	55/345 (16%)	55 (100%)	0	100	100
1	V	63/345 (18%)	63 (100%)	0	100	100
1	W	110/345 (32%)	110 (100%)	0	100	100
1	X	116/345 (34%)	116 (100%)	0	100	100
2	C	78/749 (10%)	77 (99%)	1 (1%)	61	73
2	D	94/749 (13%)	94 (100%)	0	100	100
2	I	94/749 (13%)	94 (100%)	0	100	100
2	J	93/749 (12%)	93 (100%)	0	100	100
2	O	78/749 (10%)	77 (99%)	1 (1%)	61	73
2	P	94/749 (13%)	94 (100%)	0	100	100
2	S	94/749 (13%)	94 (100%)	0	100	100
2	T	93/749 (12%)	93 (100%)	0	100	100
All	All	2210/11512 (19%)	2208 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	808	ARG
2	O	808	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	399	GLN
1	B	406	HIS
2	D	856	ASN
1	G	132	GLN

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Mol	Chain	Res	Type
1	H	40	GLN
1	H	100	GLN
1	H	139	ASN
1	L	100	GLN
1	L	105	GLN
1	M	387	GLN
1	N	301	ASN
1	N	315	GLN
1	N	387	GLN
1	N	414	GLN
2	C	3	GLN
2	C	5	GLN
2	I	883	GLN
1	F	399	GLN
1	F	406	HIS
2	P	856	ASN
1	Q	46	HIS
1	Q	132	GLN
1	R	40	GLN
1	R	100	GLN
1	R	139	ASN
1	R	206	ASN
1	V	100	GLN
1	V	105	GLN
1	W	387	GLN
1	X	301	ASN
1	X	315	GLN
1	X	414	GLN
2	O	3	GLN
2	O	5	GLN
2	S	883	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

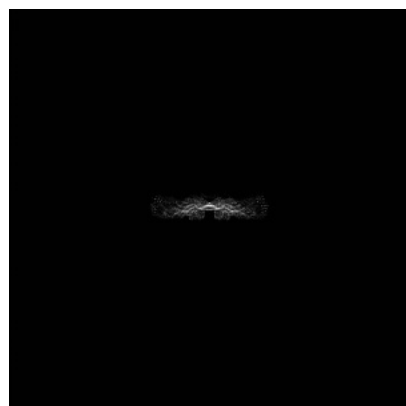
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15473. These allow visual inspection of the internal detail of the map and identification of artifacts.

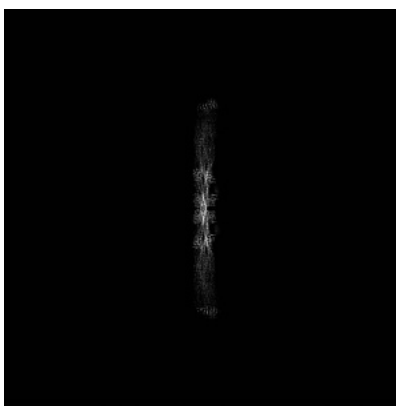
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

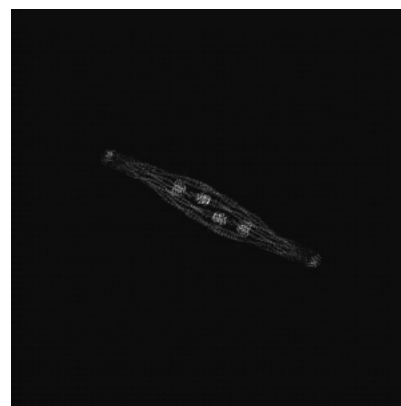
6.1.1 Primary map



X

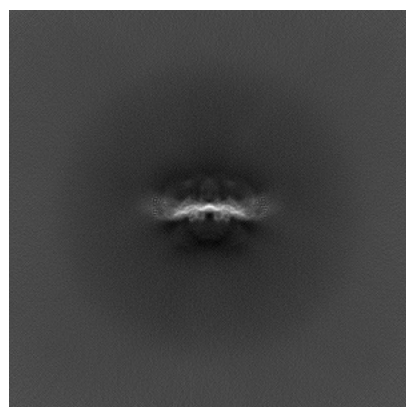


Y

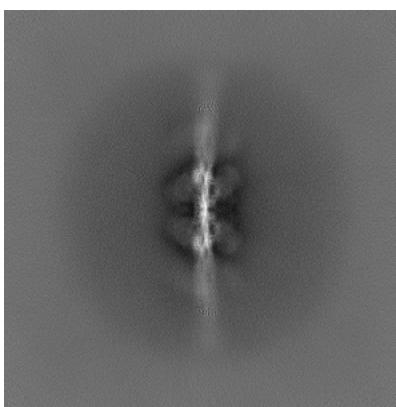


Z

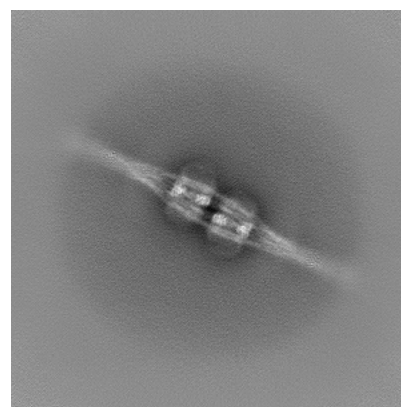
6.1.2 Raw map



X



Y

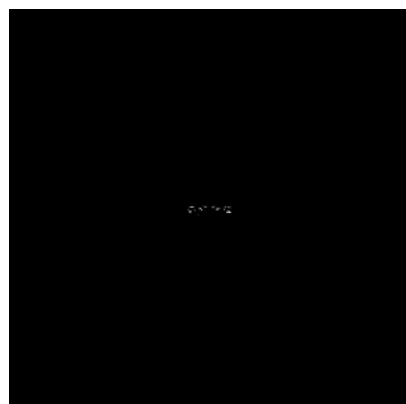


Z

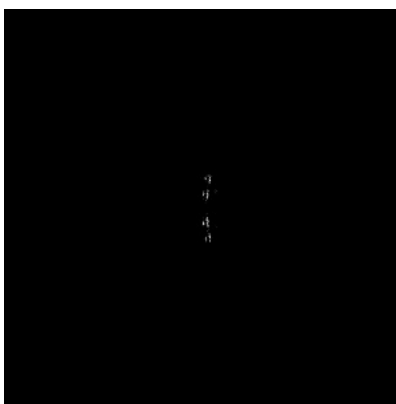
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 250

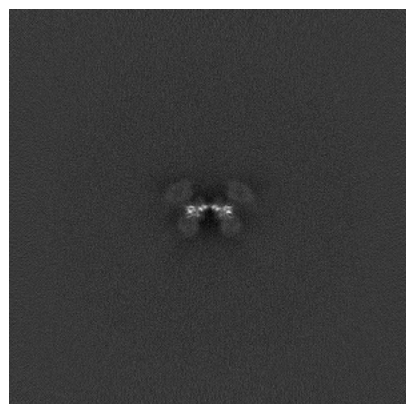


Y Index: 250

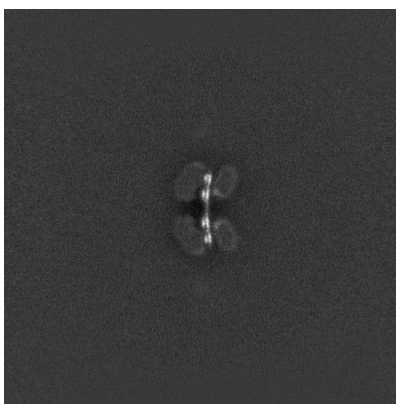


Z Index: 250

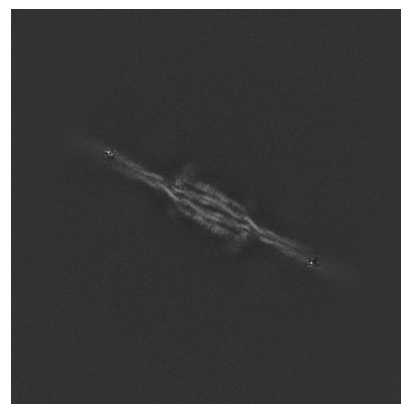
6.2.2 Raw map



X Index: 250



Y Index: 250

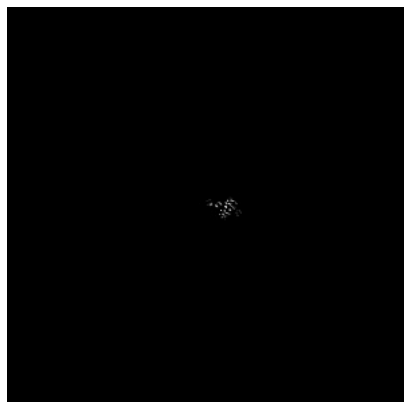


Z Index: 250

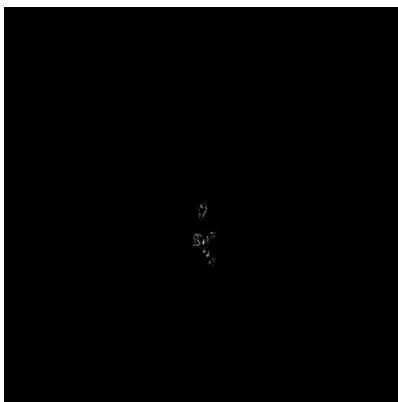
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 208

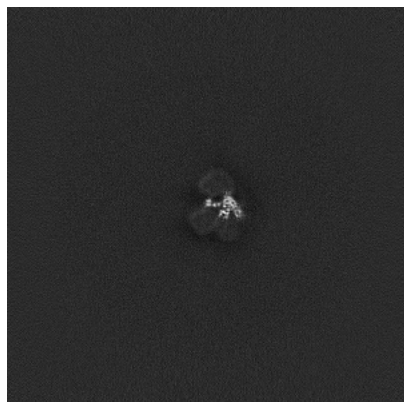


Y Index: 274

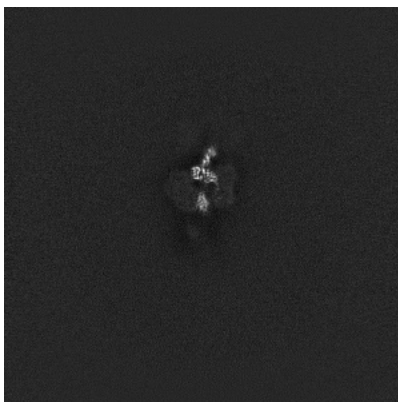


Z Index: 254

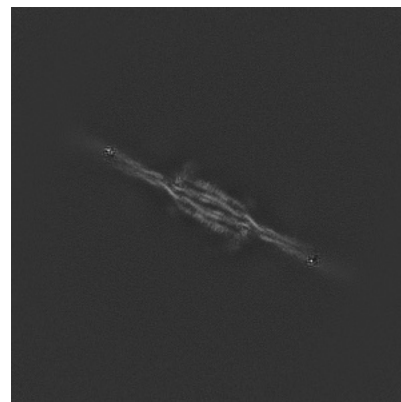
6.3.2 Raw map



X Index: 211



Y Index: 226



Z Index: 250

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

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X

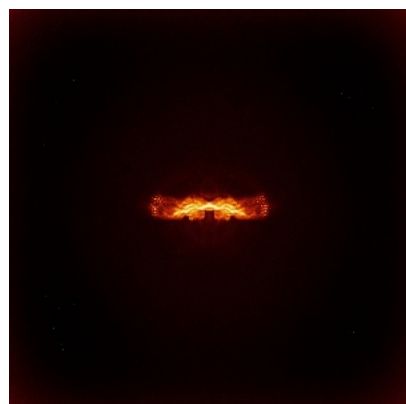


Y

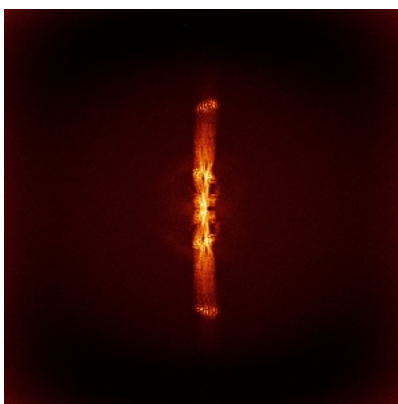


Z

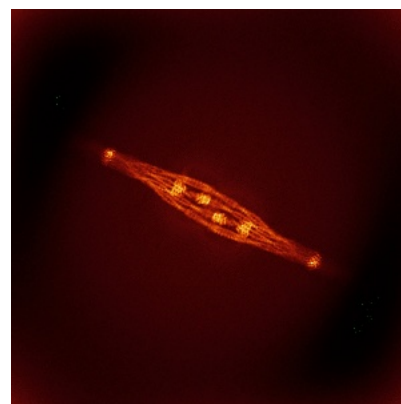
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

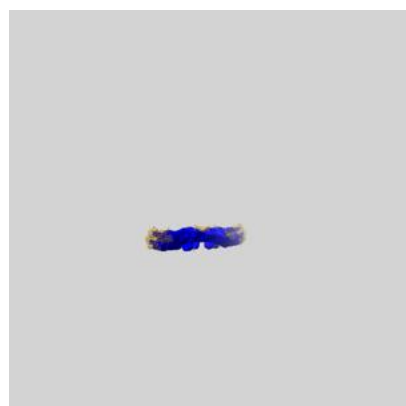
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

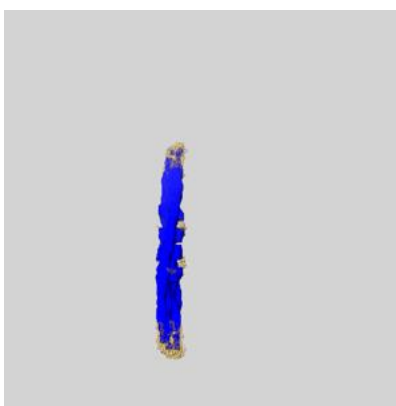
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

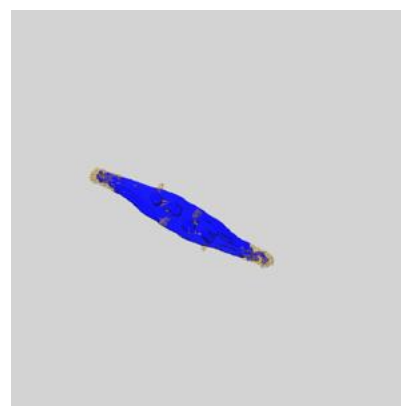
6.6.1 emd_15473_msk_1.map [i](#)



X



Y

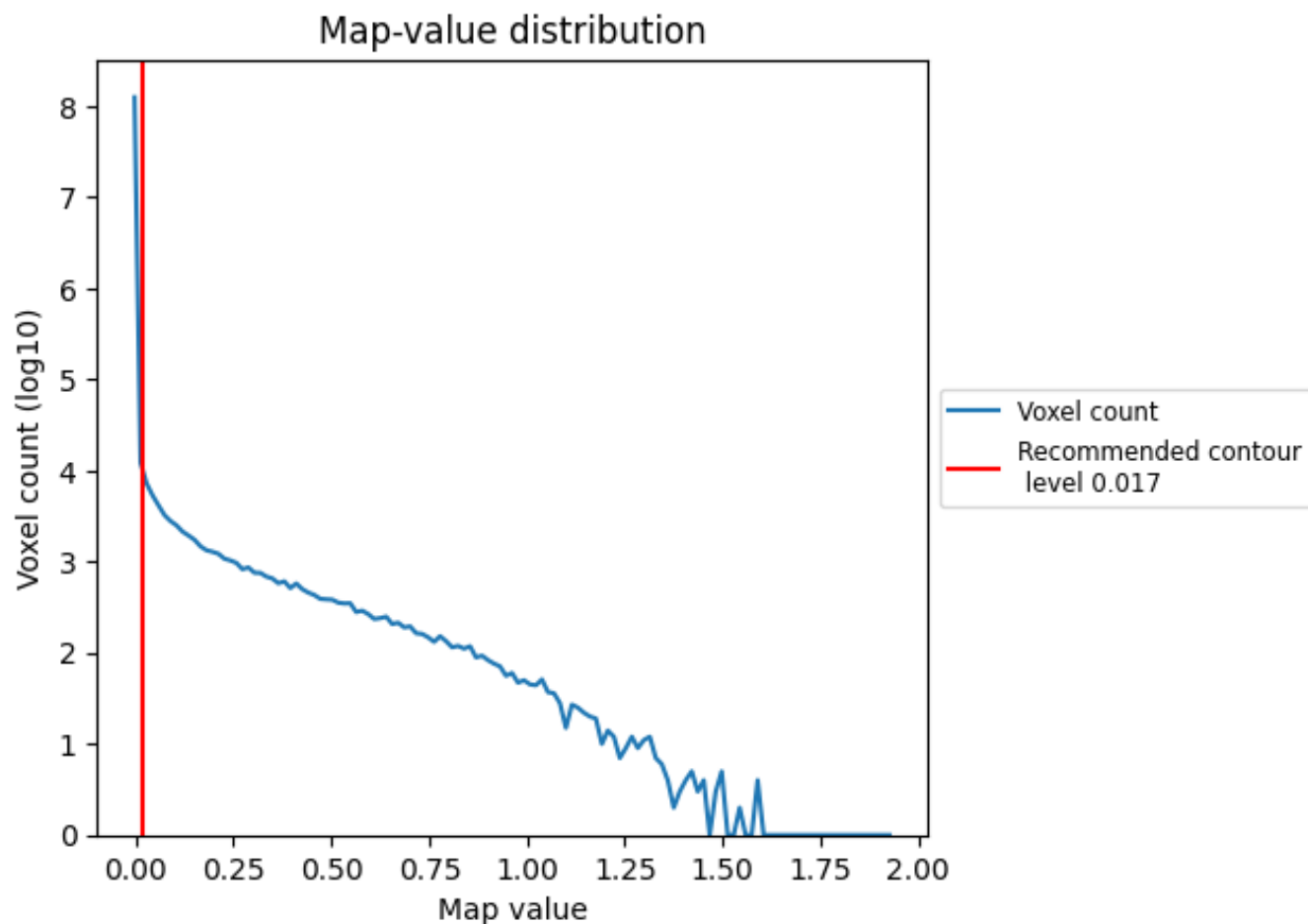


Z

7 Map analysis [i](#)

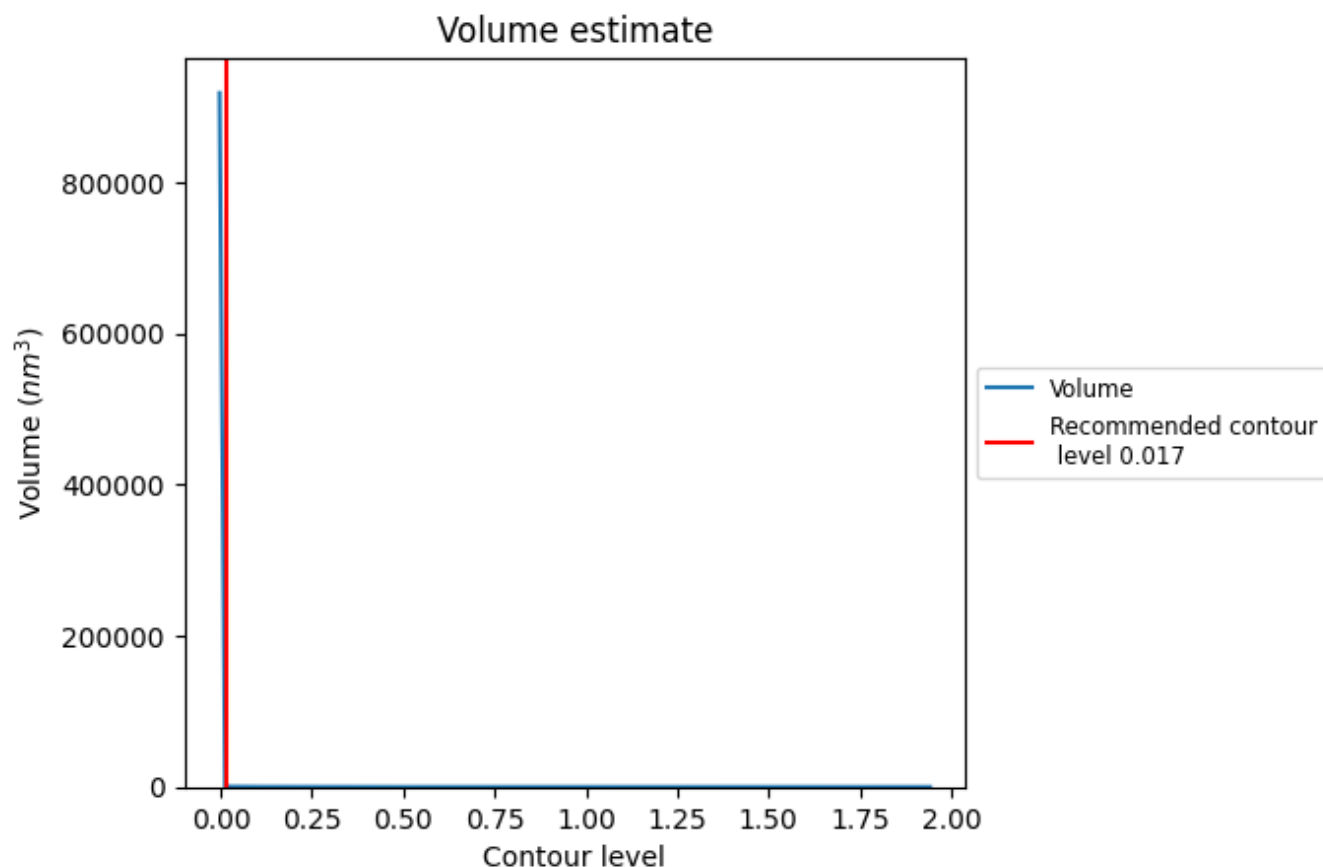
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

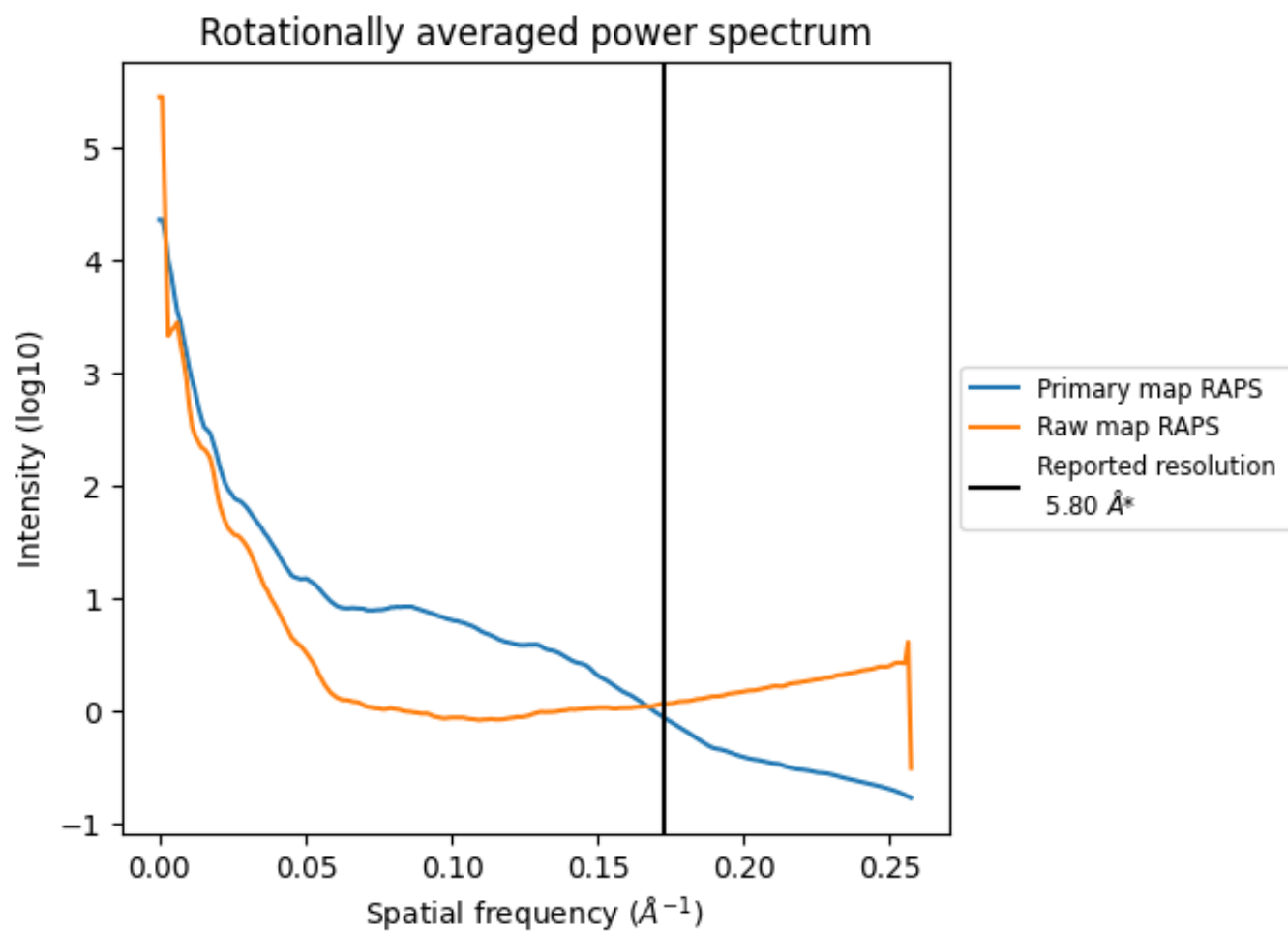
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 465 nm³; this corresponds to an approximate mass of 420 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

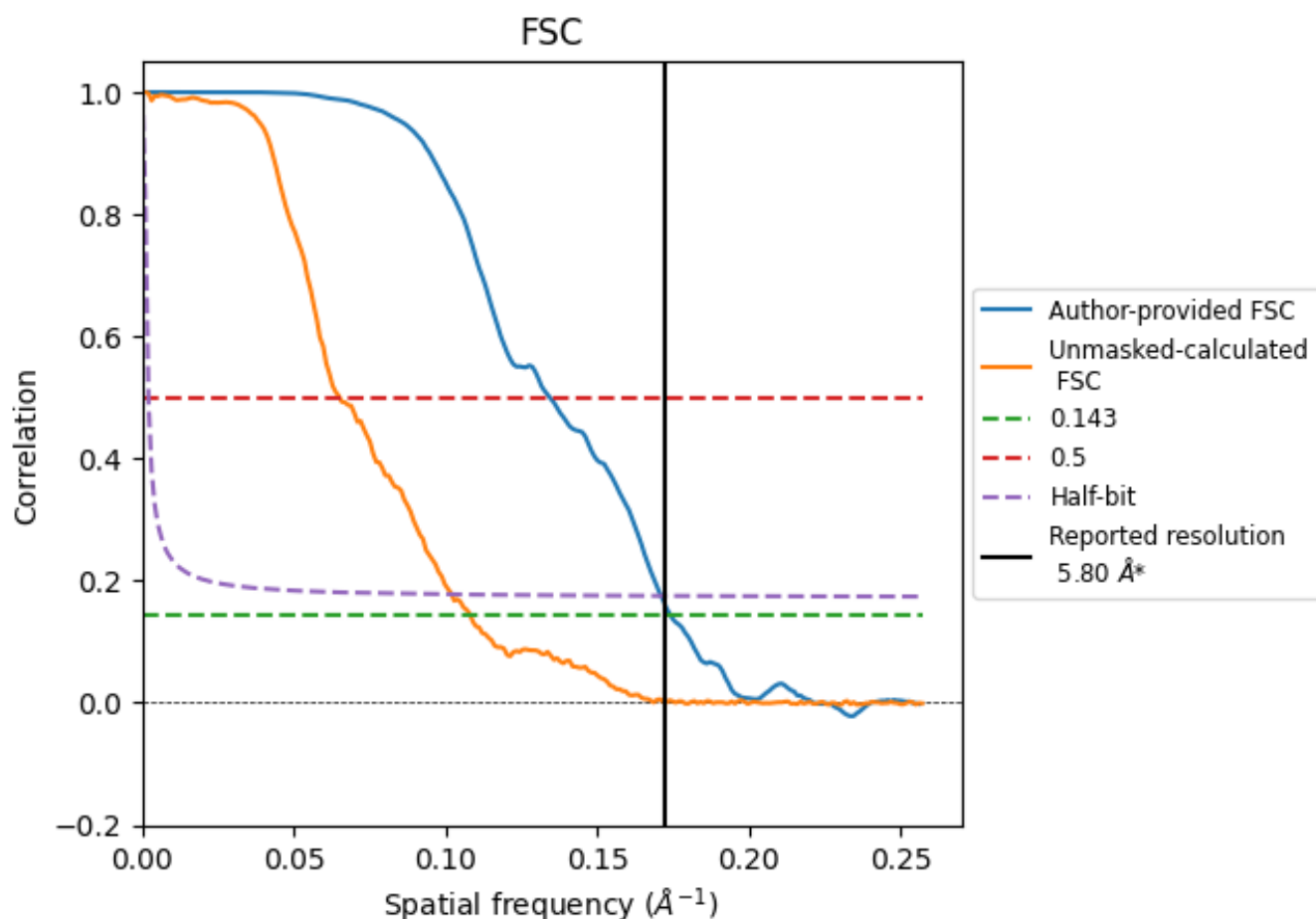


*Reported resolution corresponds to spatial frequency of 0.172 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.172 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.80	-	-
Author-provided FSC curve	5.74	7.44	5.84
Unmasked-calculated*	9.24	15.36	9.80

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.24 differs from the reported value 5.8 by more than 10 %

9 Map-model fit [i](#)

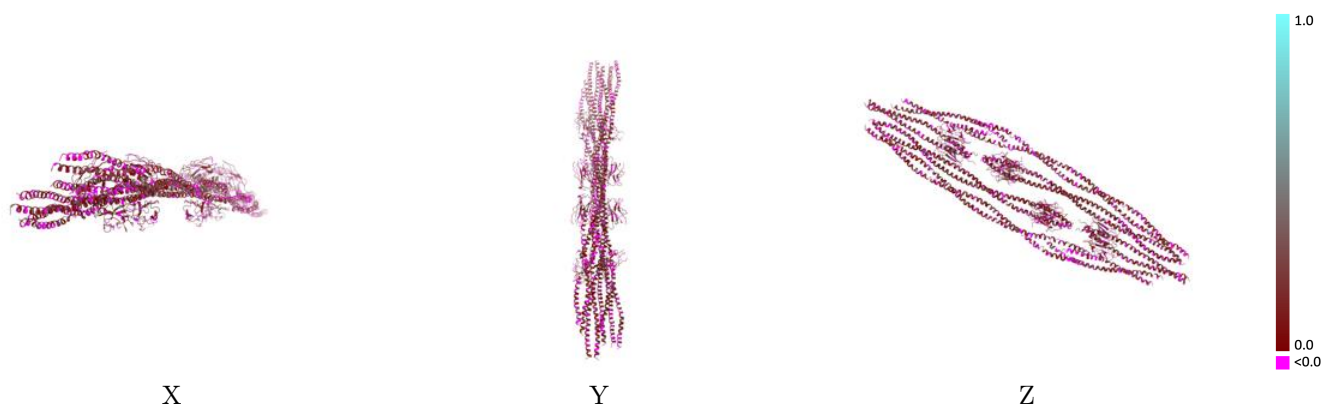
This section contains information regarding the fit between EMDB map EMD-15473 and PDB model 8AIX. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



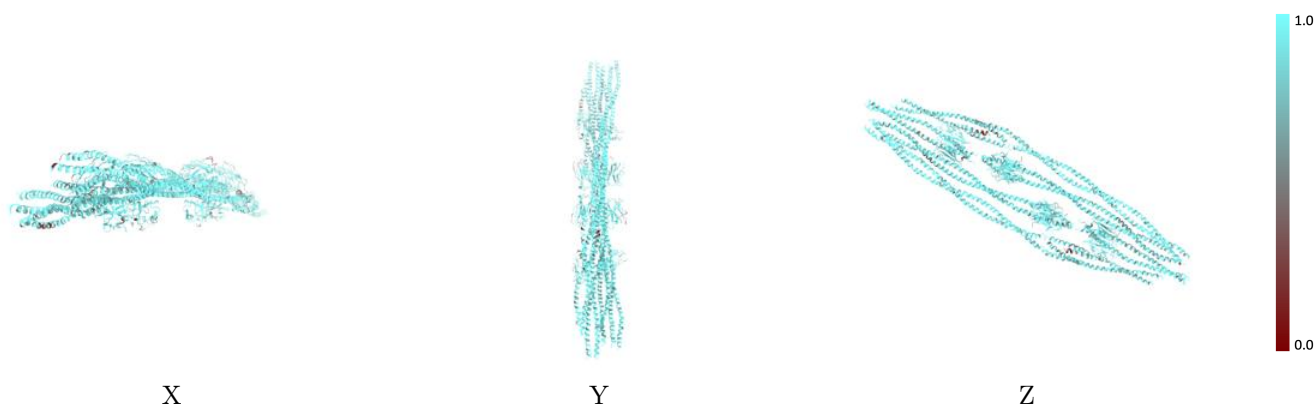
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



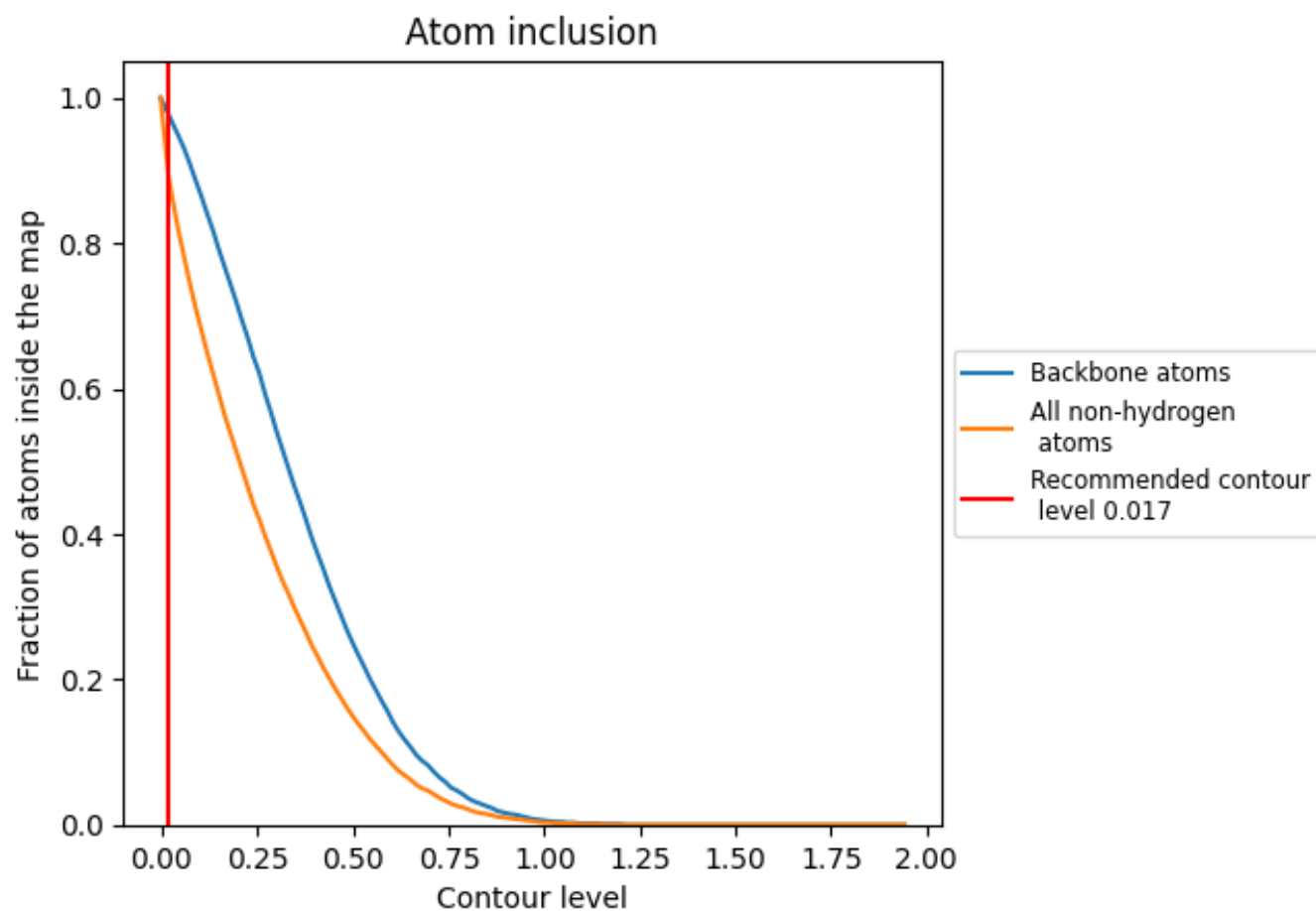
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8950	 0.1390
A	 0.8860	 0.1330
B	 0.9190	 0.1380
C	 0.8810	 0.1620
D	 0.8810	 0.1690
E	 0.8730	 0.1210
F	 0.9280	 0.1550
G	 0.9100	 0.1400
H	 0.9140	 0.1320
I	 0.8840	 0.1320
J	 0.8960	 0.1600
K	 0.7510	 0.0560
L	 0.8670	 0.1160
M	 0.9340	 0.1560
N	 0.9200	 0.1390
O	 0.8620	 0.1580
P	 0.9060	 0.1630
Q	 0.9050	 0.1390
R	 0.9170	 0.1240
S	 0.9090	 0.1630
T	 0.8670	 0.1560
U	 0.7730	 0.0570
V	 0.8930	 0.1130
W	 0.9200	 0.1670
X	 0.9070	 0.1250

