



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 10:21 AM UTC

PDB ID : 8AJB / pdb_00008ajb
EMDB ID : EMD-15476
Title : Cryo-EM structure of crescentin filaments (stutter mutant, C2 symmetry and large box)
Authors : Liu, Y.; Lowe, J.
Deposited on : 2022-07-28
Resolution : 4.30 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:

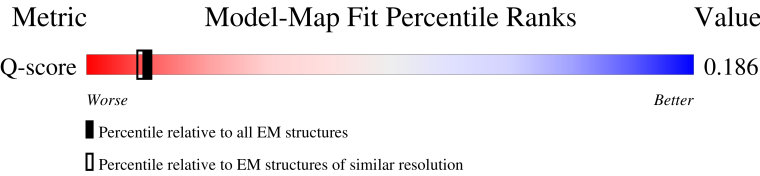
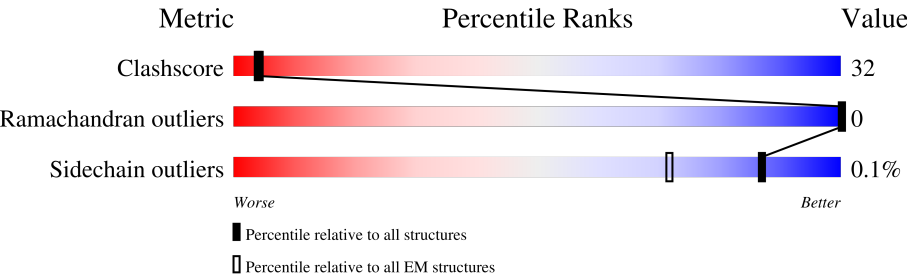
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.30 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.



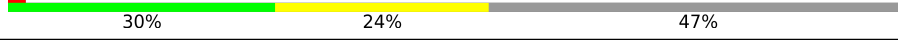
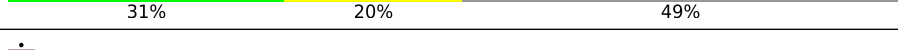
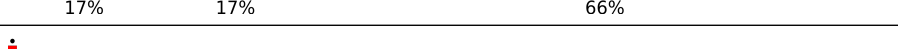
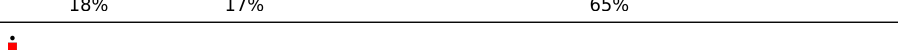
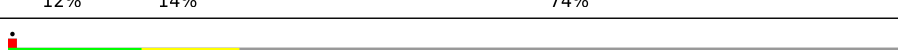
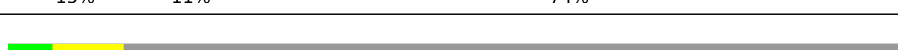
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	460	 29% 24% 47%
1	B	460	 32% 19% 48%
1	C	460	 31% 20% 49%
1	D	460	 31% 20% 49%

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Mol	Chain	Length	Quality of chain
1	G	460	 17% 16% 66%
1	H	460	 18% 17% 65%
1	I	460	 12% 15% 74%
1	J	460	 15% 11% 74%
1	M	460	 30% 24% 47%
1	N	460	 32% 19% 48%
1	O	460	 30% 20% 49%
1	P	460	 31% 20% 49%
1	S	460	 17% 17% 66%
1	T	460	 18% 17% 65%
1	U	460	 12% 14% 74%
1	V	460	 15% 11% 74%
2	E	907	 5% 8% 88%
2	F	907	 5% 7% 88%
2	K	907	 5% 8% 88%
2	L	907	 5% 7% 88%
2	Q	907	 5% 8% 88%
2	R	907	 5% 8% 88%
2	W	907	 5% 8% 88%
2	X	907	 5% 7% 88%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 30088 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	245	Total	C	N	O	S	0	0
			1876	1127	366	382	1		
1	B	238	Total	C	N	O	S	0	0
			1828	1099	358	370	1		
1	C	234	Total	C	N	O	S	0	0
			1793	1065	364	361	3		
1	D	234	Total	C	N	O	S	0	0
			1793	1065	364	361	3		
1	G	155	Total	C	N	O	S	0	0
			1203	727	234	241	1		
1	H	163	Total	C	N	O	S	0	0
			1264	764	244	255	1		
1	I	120	Total	C	N	O	S	0	0
			934	555	192	185	2		
1	J	120	Total	C	N	O	S	0	0
			934	555	192	185	2		
1	M	245	Total	C	N	O	S	0	0
			1876	1127	366	382	1		
1	N	238	Total	C	N	O	S	0	0
			1828	1099	358	370	1		
1	O	234	Total	C	N	O	S	0	0
			1793	1065	364	361	3		
1	P	234	Total	C	N	O	S	0	0
			1793	1065	364	361	3		
1	S	155	Total	C	N	O	S	0	0
			1203	727	234	241	1		
1	T	163	Total	C	N	O	S	0	0
			1264	764	244	255	1		
1	U	120	Total	C	N	O	S	0	0
			934	555	192	185	2		
1	V	120	Total	C	N	O	S	0	0
			934	555	192	185	2		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	insertion	UNP A0A8F8EC09
A	407	ALA	-	insertion	UNP A0A8F8EC09
A	408	THR	-	insertion	UNP A0A8F8EC09
B	406	SER	-	insertion	UNP A0A8F8EC09
B	407	ALA	-	insertion	UNP A0A8F8EC09
B	408	THR	-	insertion	UNP A0A8F8EC09
C	406	SER	-	insertion	UNP A0A8F8EC09
C	407	ALA	-	insertion	UNP A0A8F8EC09
C	408	THR	-	insertion	UNP A0A8F8EC09
D	406	SER	-	insertion	UNP A0A8F8EC09
D	407	ALA	-	insertion	UNP A0A8F8EC09
D	408	THR	-	insertion	UNP A0A8F8EC09
G	406	SER	-	insertion	UNP A0A8F8EC09
G	407	ALA	-	insertion	UNP A0A8F8EC09
G	408	THR	-	insertion	UNP A0A8F8EC09
H	406	SER	-	insertion	UNP A0A8F8EC09
H	407	ALA	-	insertion	UNP A0A8F8EC09
H	408	THR	-	insertion	UNP A0A8F8EC09
I	406	SER	-	insertion	UNP A0A8F8EC09
I	407	ALA	-	insertion	UNP A0A8F8EC09
I	408	THR	-	insertion	UNP A0A8F8EC09
J	406	SER	-	insertion	UNP A0A8F8EC09
J	407	ALA	-	insertion	UNP A0A8F8EC09
J	408	THR	-	insertion	UNP A0A8F8EC09
M	406	SER	-	insertion	UNP A0A8F8EC09
M	407	ALA	-	insertion	UNP A0A8F8EC09
M	408	THR	-	insertion	UNP A0A8F8EC09
N	406	SER	-	insertion	UNP A0A8F8EC09
N	407	ALA	-	insertion	UNP A0A8F8EC09
N	408	THR	-	insertion	UNP A0A8F8EC09
O	406	SER	-	insertion	UNP A0A8F8EC09
O	407	ALA	-	insertion	UNP A0A8F8EC09
O	408	THR	-	insertion	UNP A0A8F8EC09
P	406	SER	-	insertion	UNP A0A8F8EC09
P	407	ALA	-	insertion	UNP A0A8F8EC09
P	408	THR	-	insertion	UNP A0A8F8EC09
S	406	SER	-	insertion	UNP A0A8F8EC09
S	407	ALA	-	insertion	UNP A0A8F8EC09
S	408	THR	-	insertion	UNP A0A8F8EC09
T	406	SER	-	insertion	UNP A0A8F8EC09
T	407	ALA	-	insertion	UNP A0A8F8EC09
T	408	THR	-	insertion	UNP A0A8F8EC09
U	406	SER	-	insertion	UNP A0A8F8EC09

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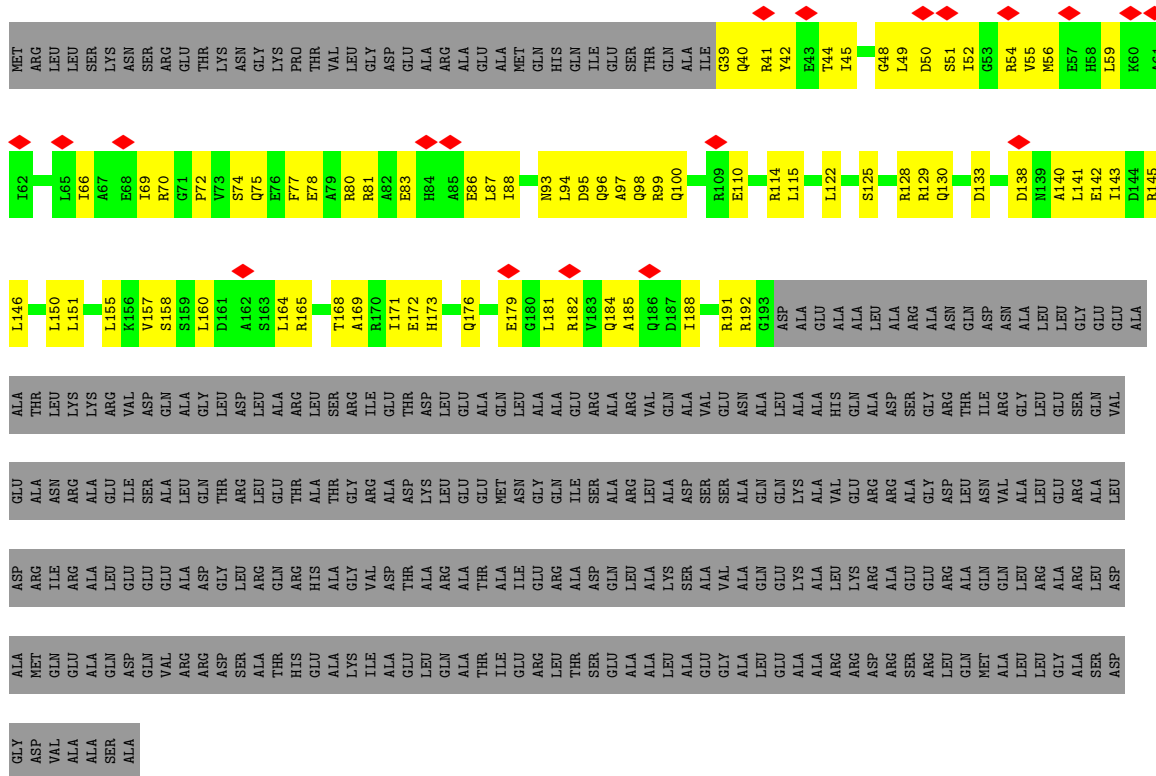
Chain	Residue	Modelled	Actual	Comment	Reference
U	407	ALA	-	insertion	UNP A0A8F8EC09
U	408	THR	-	insertion	UNP A0A8F8EC09
V	406	SER	-	insertion	UNP A0A8F8EC09
V	407	ALA	-	insertion	UNP A0A8F8EC09
V	408	THR	-	insertion	UNP A0A8F8EC09

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

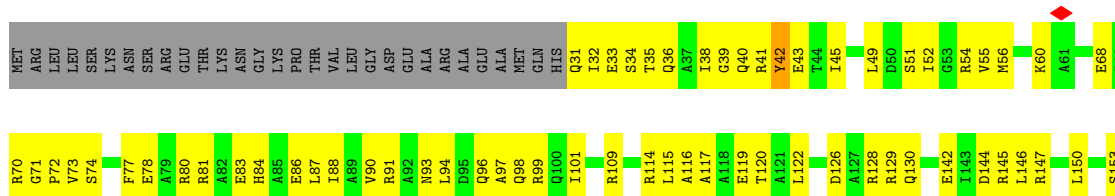
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	F	111	Total	C	N	O	S	0	0
			861	535	154	167	5		
2	K	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	L	105	Total	C	N	O	S	0	0
			820	508	148	159	5		
2	Q	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	R	111	Total	C	N	O	S	0	0
			861	535	154	167	5		
2	W	112	Total	C	N	O	S	0	0
			869	539	155	170	5		
2	X	105	Total	C	N	O	S	0	0
			820	508	148	159	5		



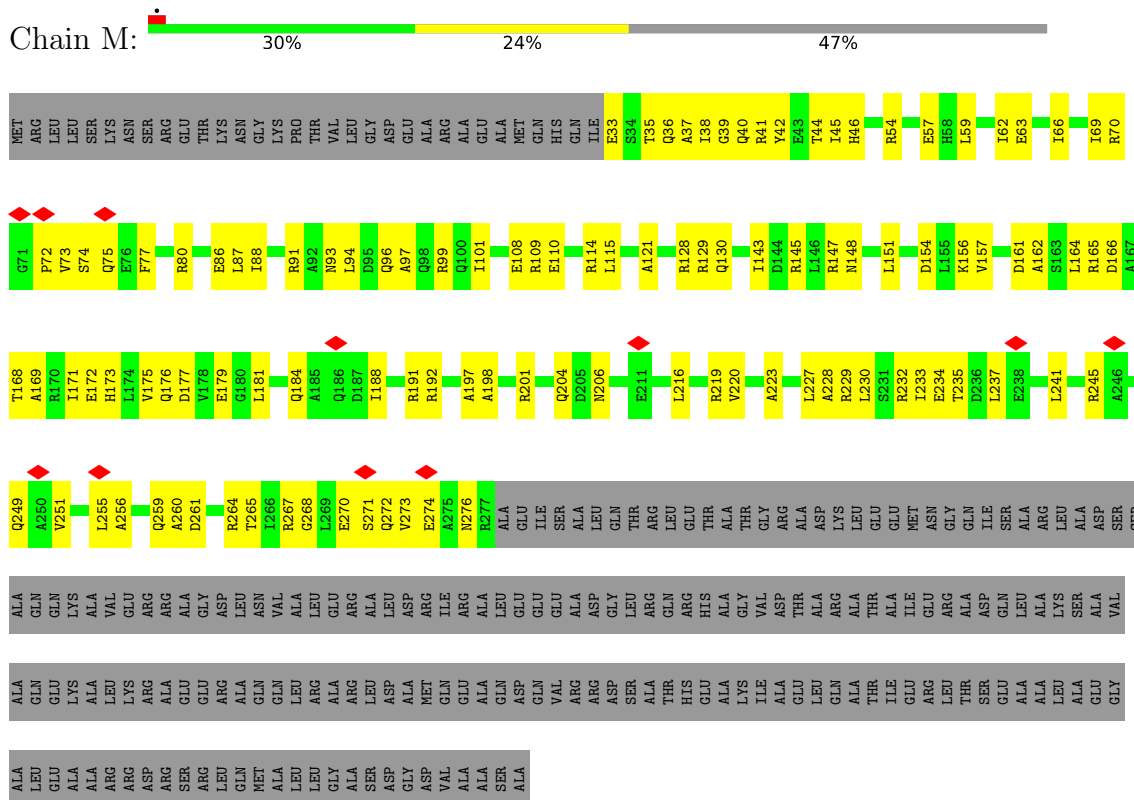
- Molecule 1: Crescentin



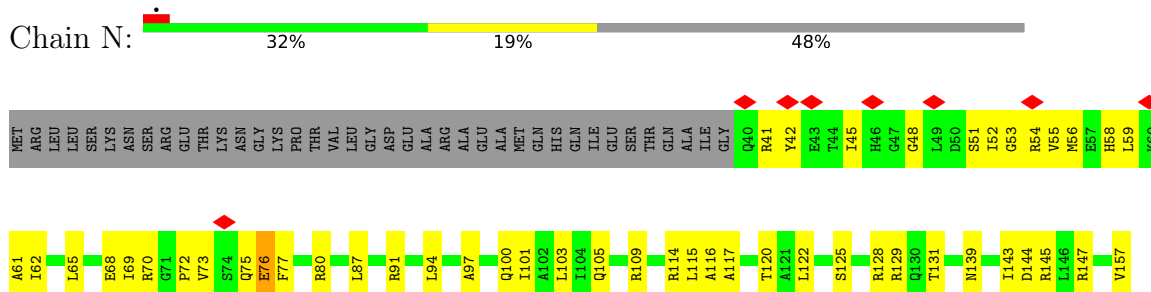
- Molecule 1: Crescentin



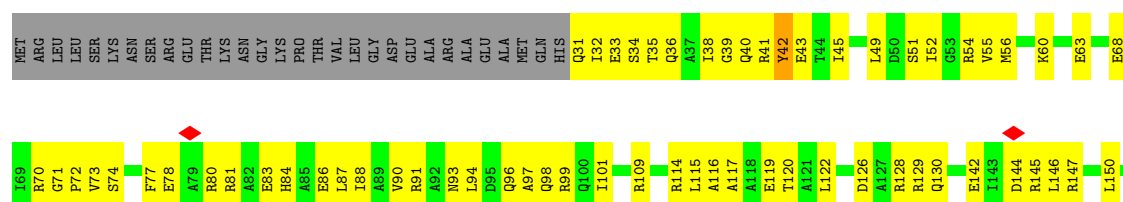
- Molecule 1: Crescentin



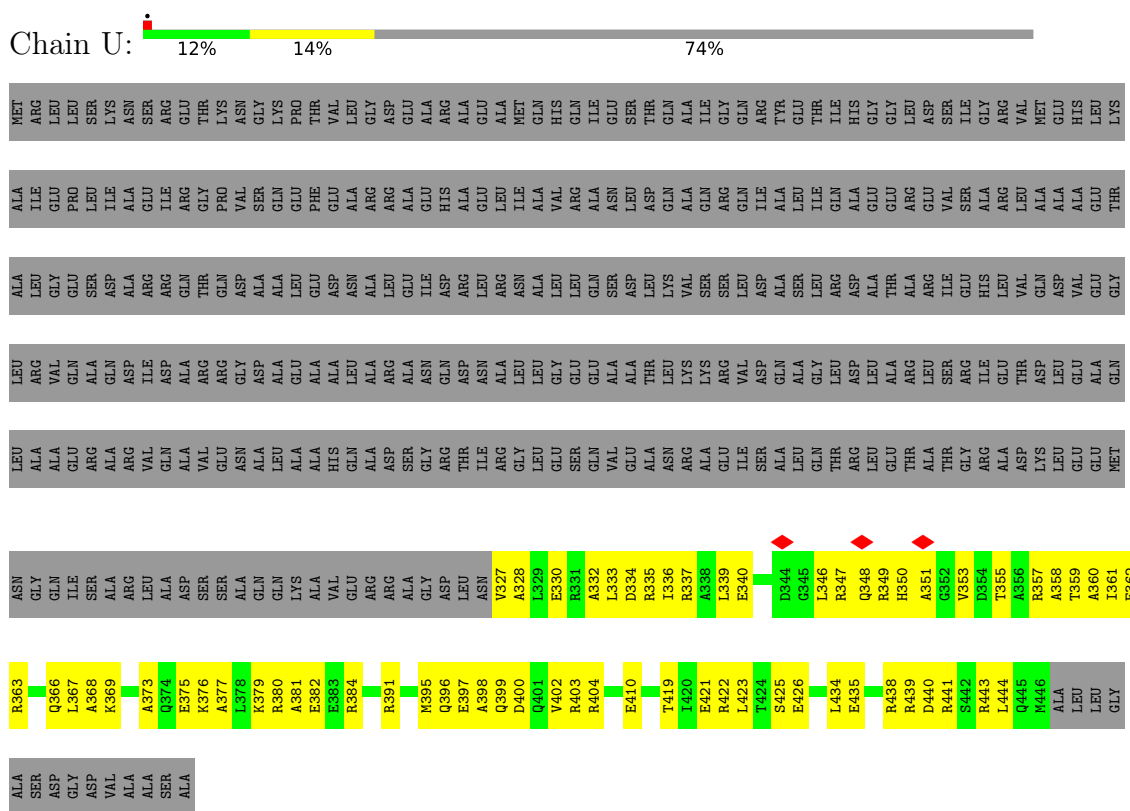
- Molecule 1: Crescentin



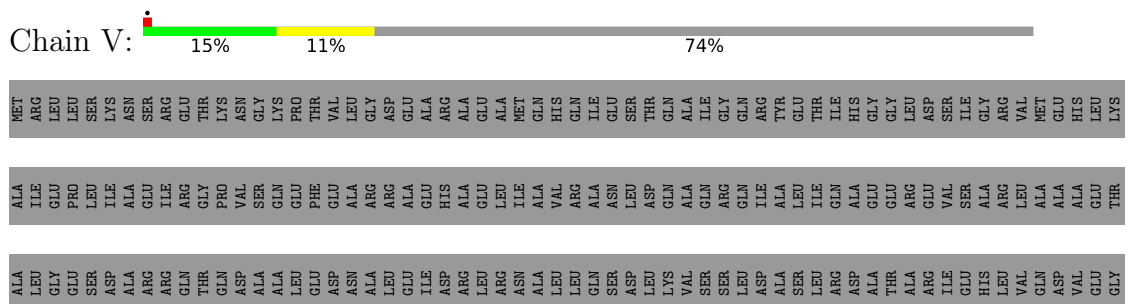


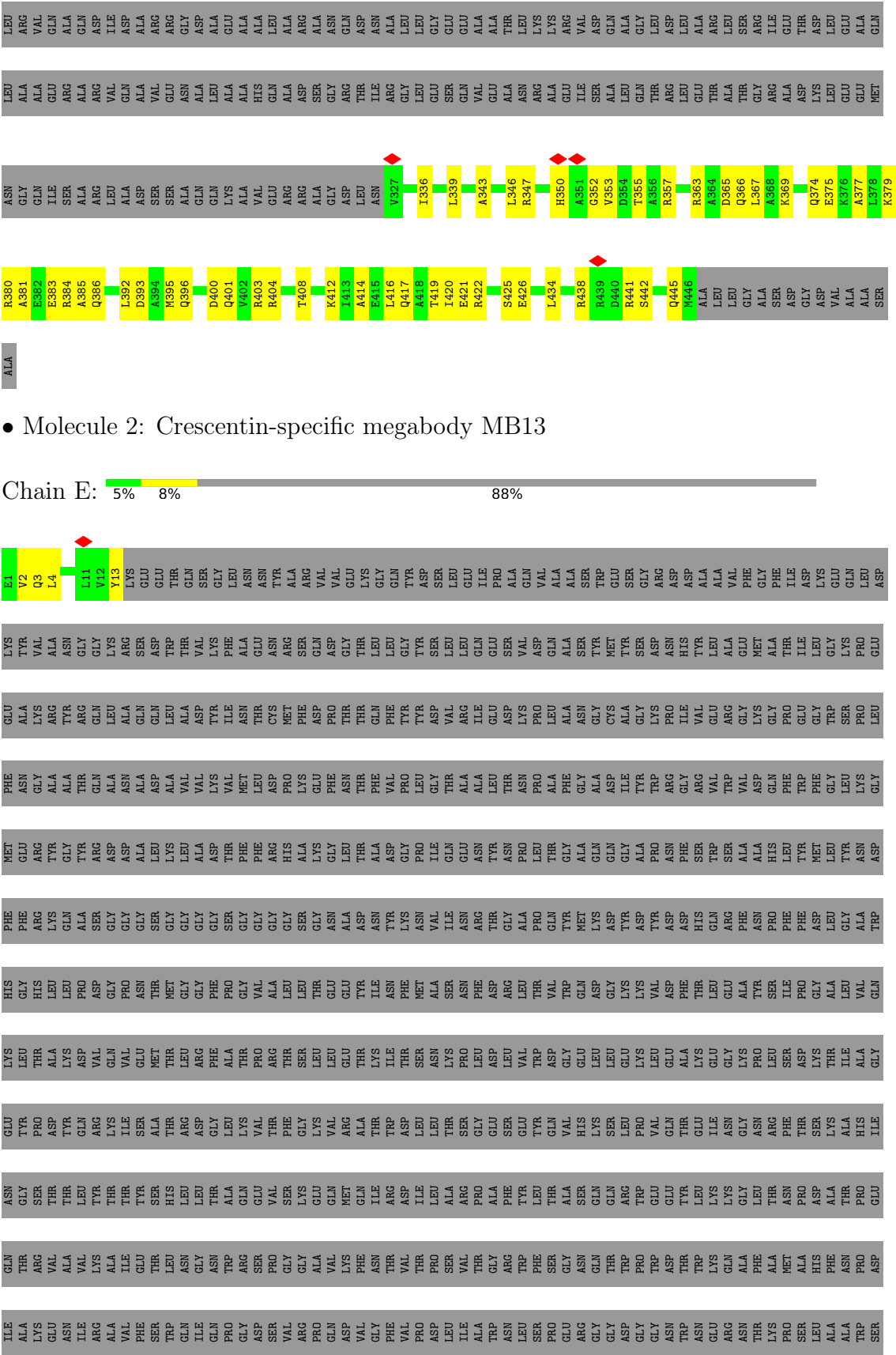


- Molecule 1: Crescentin



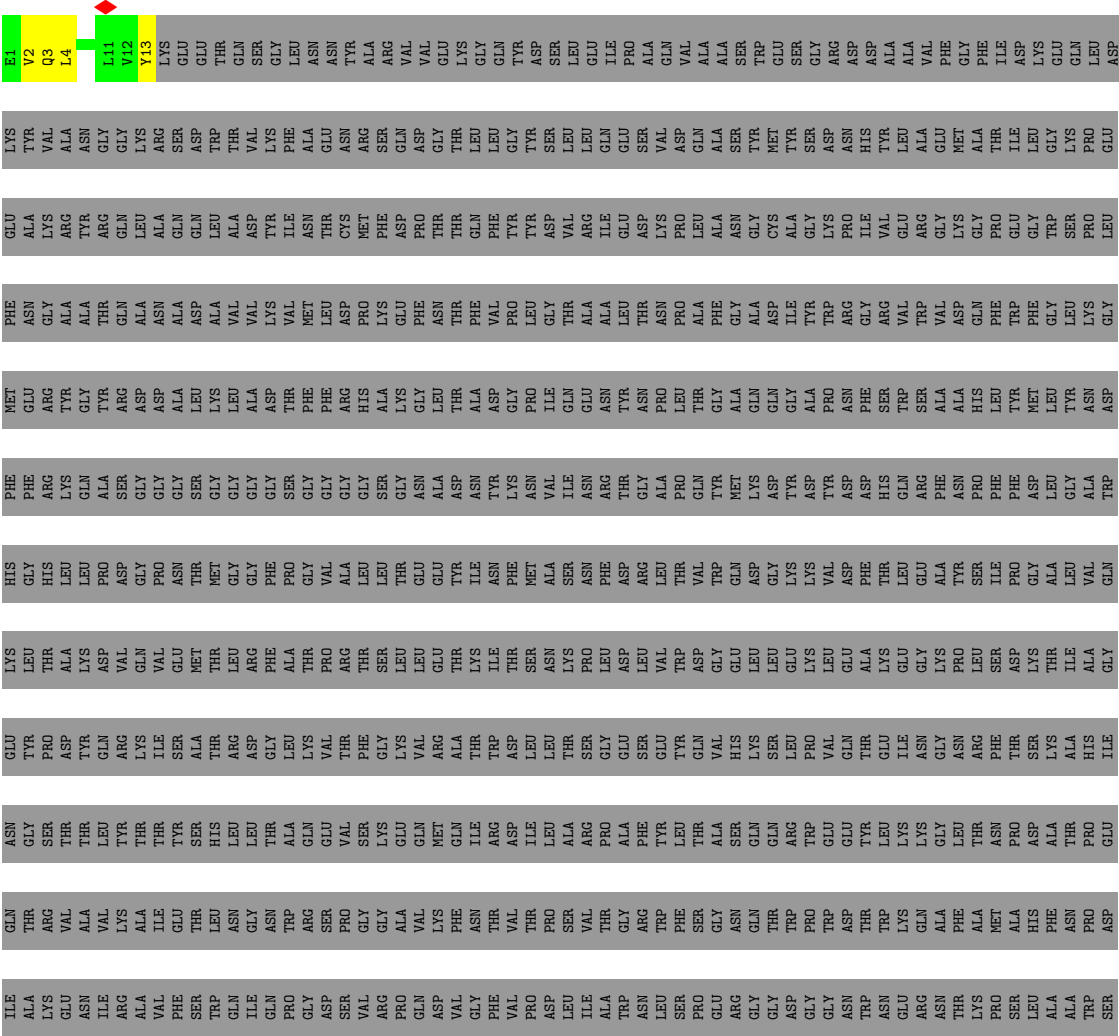
- Molecule 1: Crescentin



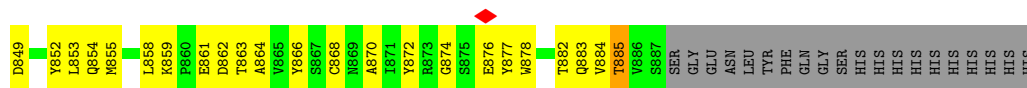


• Molecule 2: Crescentin-specific megabody MB13

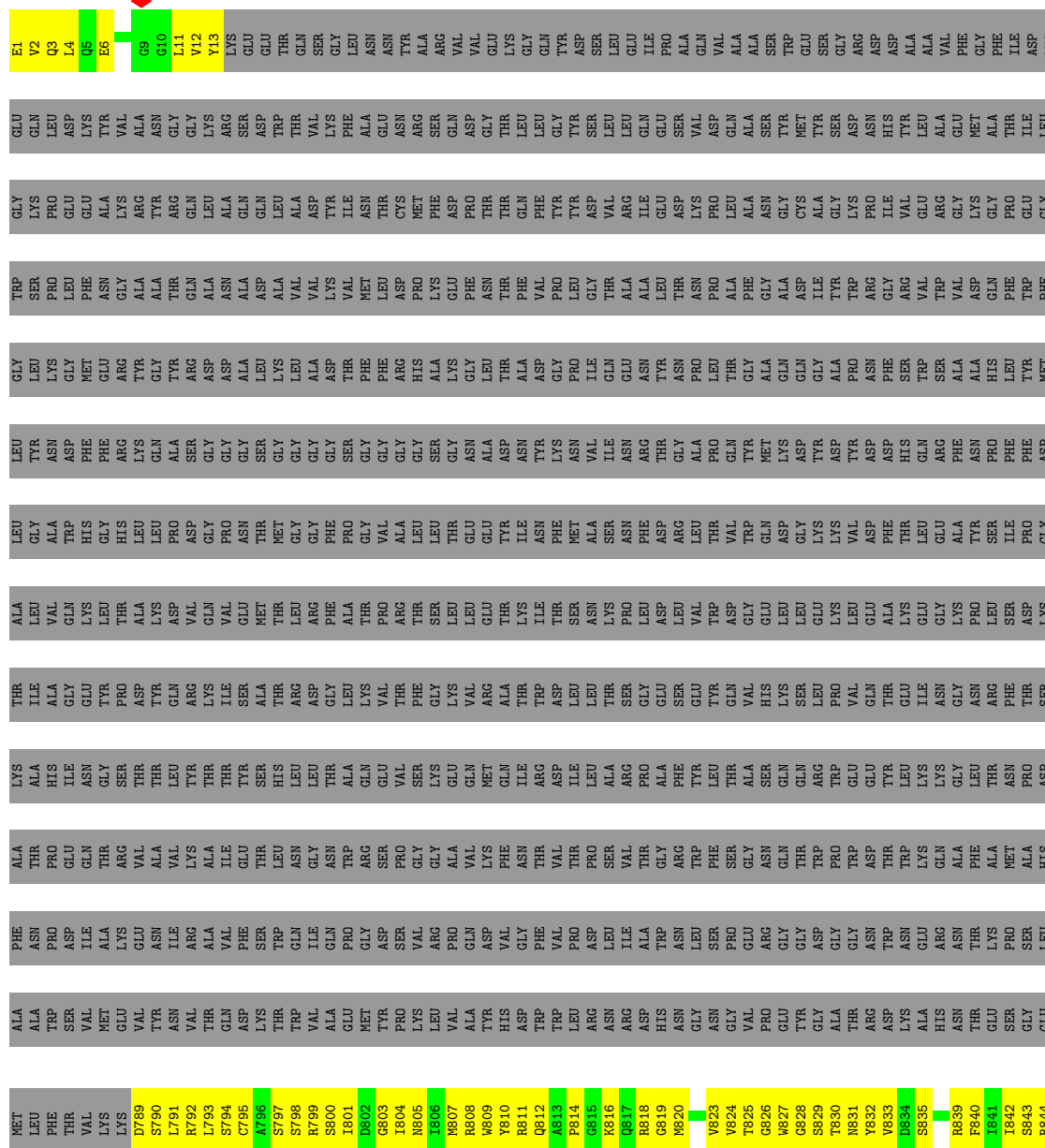
Chain E: 5% 8% 88%







• Molecule 2: Crescentin-specific megabody MB13



• Molecule 2: Crescentin-specific megabody MB13





A	D849		MET	LEU	ALA	ASN	PHE	ALA	THR	ALA	LYS	THR	ILE	THR
	T850		PHE	THR	TRP	ASP	ASN	PRO	PRO	HIS	ALA	GLY	GLY	THR
	W851		THR	VAL	VAL	ILE	ILE	GLN	GLN	ASN	GLY	THR	TVR	GLY
	Y852		VAL	MET	GLU	LYS	ALA	LYS	ARG	THR	SER	ARG	PRO	THR
	L853		LYS	GLU	VAL	GLN	VAL	GLU	VAL	VAL	SER	THR	ASP	ASP
	R854		D789	T790	T791	T792	T793	T794	T795	T796	T797	T798	T799	T800
	R855		R789	R790	R791	R792	R793	R794	R795	R796	R797	R798	R799	R800
	R856		L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802
	R857		R792	R793	R794	R795	R796	R797	R798	R799	R800	R801	R802	R803
	R858		L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804
B	R859		L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805
	R860		L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806
	E861		L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807
	T862		L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808
	L863		L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809
	R864		L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810
	R865		L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811
	R866		L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812
	R867		L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813
	R868		L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814
C	R869		L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815
	A870		L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816
	L871		L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817
	R872		L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818
	R873		L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819
	R874		L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820
	R875		L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821
	R876		L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822
	R877		L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823
	R878		L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824
D	T882		R808	R809	R810	R811	R812	R813	R814	R815	R816	R817	R818	R819
	R883		R809	R810	R811	R812	R813	R814	R815	R816	R817	R818	R819	R820
	R884		R810	R811	R812	R813	R814	R815	R816	R817	R818	R819	R820	R821
	T885		R811	R812	R813	R814	R815	R816	R817	R818	R819	R820	R821	R822
	R886		R812	R813	R814	R815	R816	R817	R818	R819	R820	R821	R822	R823
	R887		R813	R814	R815	R816	R817	R818	R819	R820	R821	R822	R823	R824
	R888		R814	R815	R816	R817	R818	R819	R820	R821	R822	R823	R824	R825
	R889		R815	R816	R817	R818	R819	R820	R821	R822	R823	R824	R825	R826
	R890		R816	R817	R818	R819	R820	R821	R822	R823	R824	R825	R826	R827
	R891		R817	R818	R819	R820	R821	R822	R823	R824	R825	R826	R827	R828
E	R892		R818	R819	R820	R821	R822	R823	R824	R825	R826	R827	R828	R829
	R893		R819	R820	R821	R822	R823	R824	R825	R826	R827	R828	R829	R830
	R894		R820	R821	R822	R823	R824	R825	R826	R827	R828	R829	R830	R831
	R895		R821	R822	R823	R824	R825	R826	R827	R828	R829	R830	R831	R832
	R896		R822	R823	R824	R825	R826	R827	R828	R829	R830	R831	R832	R833
	R897		R823	R824	R825	R826	R827	R828	R829	R830	R831	R832	R833	R834
	R898		R824	R825	R826	R827	R828	R829	R830	R831	R832	R833	R834	R835
	R899		R825	R826	R827	R828	R829	R830	R831	R832	R833	R834	R835	R836
	R900		R826	R827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837
	R901		R827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838

- Molecule 2: Crescentin-specific megabody MB13

Chain X: 7% 88%

[illegible]

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	585252	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.736	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	954.0, 954.0, 954.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.59, 1.59, 1.59	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	0.31	0/1884	0.61	0/2540
1	B	0.31	0/1836	0.63	1/2475 (0.0%)
1	C	0.29	0/1795	0.61	0/2407
1	D	0.30	0/1795	0.59	0/2407
1	G	0.29	0/1210	0.67	0/1630
1	H	0.30	0/1271	0.68	2/1713 (0.1%)
1	I	0.34	0/935	0.60	0/1251
1	J	0.29	0/935	0.62	0/1251
1	M	0.31	0/1884	0.61	0/2540
1	N	0.31	0/1836	0.63	1/2475 (0.0%)
1	O	0.29	0/1795	0.61	0/2407
1	P	0.30	0/1795	0.59	0/2407
1	S	0.29	0/1210	0.66	0/1630
1	T	0.30	0/1271	0.68	2/1713 (0.1%)
1	U	0.34	0/935	0.60	0/1251
1	V	0.29	0/935	0.62	0/1251
2	E	0.44	0/883	0.69	0/1192
2	F	0.39	0/875	0.73	1/1181 (0.1%)
2	K	0.37	0/883	0.55	0/1192
2	L	0.35	0/833	0.65	0/1124
2	Q	0.43	0/883	0.69	0/1192
2	R	0.39	0/875	0.73	1/1181 (0.1%)
2	W	0.37	0/883	0.55	0/1192
2	X	0.35	0/833	0.65	0/1124
All	All	0.33	0/30270	0.63	8/40726 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	42	TYR	CA-C-N	-5.71	112.63	120.28
1	H	42	TYR	C-N-CA	-5.71	112.63	120.28
1	T	42	TYR	CA-C-N	-5.70	112.64	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	42	TYR	C-N-CA	-5.70	112.64	120.28
2	R	885	THR	N-CA-C	5.67	115.90	108.07
2	F	885	THR	N-CA-C	5.66	115.88	108.07
1	B	76	GLU	CA-CB-CG	-5.29	103.53	114.10
1	N	76	GLU	CA-CB-CG	-5.28	103.54	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1876	0	1869	140	0
1	B	1828	0	1824	131	0
1	C	1793	0	1815	111	0
1	D	1793	0	1813	104	0
1	G	1203	0	1200	104	0
1	H	1264	0	1261	107	0
1	I	934	0	946	84	0
1	J	934	0	946	71	0
1	M	1876	0	1869	142	0
1	N	1828	0	1824	128	0
1	O	1793	0	1815	109	0
1	P	1793	0	1813	107	0
1	S	1203	0	1200	104	0
1	T	1264	0	1261	105	0
1	U	934	0	946	81	0
1	V	934	0	946	73	0
2	E	869	0	846	83	0
2	F	861	0	842	74	0
2	K	869	0	846	121	0
2	L	820	0	802	79	0
2	Q	869	0	846	83	0
2	R	861	0	842	79	0
2	W	869	0	846	122	0
2	X	820	0	802	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	30088	0	30020	1926	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (1926) 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:K:804:ILE:HB	2:K:872:TYR:CZ	1.30	1.66
2:K:804:ILE:HD13	2:K:872:TYR:CD2	1.28	1.64
2:W:804:ILE:HD13	2:W:872:TYR:CD2	1.28	1.63
2:W:804:ILE:HB	2:W:872:TYR:CZ	1.29	1.62
2:W:804:ILE:CB	2:W:872:TYR:CE1	1.85	1.60
2:K:804:ILE:CB	2:K:872:TYR:CE1	1.85	1.57
2:K:804:ILE:HB	2:K:872:TYR:CE1	1.00	1.51
2:W:804:ILE:HB	2:W:872:TYR:CE1	1.00	1.50
2:K:870:ALA:HB1	2:K:872:TYR:CE2	1.59	1.37
2:W:870:ALA:HB1	2:W:872:TYR:CE2	1.59	1.35
2:W:804:ILE:HD13	2:W:872:TYR:CE2	1.62	1.34
2:K:804:ILE:HD13	2:K:872:TYR:CE2	1.62	1.33
2:K:804:ILE:HD13	2:K:872:TYR:CG	1.64	1.32
2:W:804:ILE:HD13	2:W:872:TYR:CG	1.65	1.32
2:K:804:ILE:HG12	2:K:807:MET:SD	1.74	1.27
2:K:803:GLY:O	2:K:872:TYR:CD1	1.88	1.26
2:W:804:ILE:HG12	2:W:807:MET:SD	1.74	1.26
2:W:803:GLY:O	2:W:872:TYR:CD1	1.88	1.24
2:K:804:ILE:CD1	2:K:872:TYR:CD2	2.22	1.21
2:W:804:ILE:CD1	2:W:872:TYR:CD2	2.22	1.20
2:K:804:ILE:CB	2:K:872:TYR:CZ	2.08	1.16
2:W:804:ILE:CB	2:W:872:TYR:CZ	2.08	1.15
2:K:804:ILE:CD1	2:K:872:TYR:CG	2.35	1.08
2:W:804:ILE:CD1	2:W:872:TYR:CG	2.35	1.08
1:V:419:THR:HG21	2:W:805:ASN:ND2	1.71	1.06
1:J:419:THR:HG21	2:K:805:ASN:ND2	1.71	1.04
2:W:804:ILE:CA	2:W:872:TYR:CE1	2.40	1.04
2:K:804:ILE:CG1	2:K:872:TYR:CZ	2.42	1.03
2:W:804:ILE:CG1	2:W:872:TYR:CZ	2.42	1.03
2:K:804:ILE:CA	2:K:872:TYR:CE1	2.40	1.02
2:K:804:ILE:CD1	2:K:872:TYR:CE2	2.41	1.02
2:W:804:ILE:CD1	2:W:872:TYR:CE2	2.41	1.02
2:W:870:ALA:CB	2:W:872:TYR:HE2	1.74	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:803:GLY:O	2:W:872:TYR:HD1	1.33	1.00
1:N:120:THR:HG22	1:P:384:ARG:HH22	1.24	0.99
2:W:804:ILE:HG21	2:W:807:MET:SD	2.02	0.99
1:B:120:THR:HG22	1:D:384:ARG:HH22	1.24	0.99
2:K:804:ILE:HG21	2:K:807:MET:SD	2.01	0.99
2:K:870:ALA:CB	2:K:872:TYR:HE2	1.74	0.99
2:W:804:ILE:CG1	2:W:807:MET:SD	2.52	0.98
2:W:803:GLY:O	2:W:872:TYR:CE1	2.18	0.97
2:K:804:ILE:CG1	2:K:807:MET:SD	2.52	0.97
2:K:804:ILE:HB	2:K:872:TYR:HE1	1.16	0.96
2:Q:804:ILE:HG22	2:Q:826:GLY:HA2	1.48	0.96
2:K:803:GLY:O	2:K:872:TYR:CE1	2.18	0.95
2:K:870:ALA:CB	2:K:872:TYR:CE2	2.48	0.95
1:M:129:ARG:HE	1:N:128:ARG:HH12	1.06	0.94
1:P:422:ARG:HE	2:Q:871:ILE:HD12	1.32	0.94
2:E:804:ILE:HG22	2:E:826:GLY:HA2	1.48	0.94
2:W:870:ALA:CB	2:W:872:TYR:CE2	2.48	0.94
2:L:792:ARG:HH12	2:L:852:TYR:HB3	1.33	0.93
2:X:792:ARG:HH12	2:X:852:TYR:HB3	1.32	0.93
1:D:422:ARG:HE	2:E:871:ILE:HD12	1.32	0.93
1:A:129:ARG:HE	1:B:128:ARG:HH12	1.07	0.92
2:W:804:ILE:HB	2:W:872:TYR:HE1	1.16	0.92
1:M:73:VAL:HG12	1:M:77:PHE:HE2	1.38	0.88
1:A:73:VAL:HG22	1:H:41:ARG:HH12	1.38	0.88
1:P:422:ARG:HH12	1:P:426:GLU:HB2	1.39	0.88
2:W:870:ALA:HB1	2:W:872:TYR:HE2	1.07	0.88
2:K:803:GLY:O	2:K:872:TYR:HD1	1.33	0.88
1:I:346:LEU:HA	1:I:349:ARG:HG2	1.56	0.88
1:D:422:ARG:HH12	1:D:426:GLU:HB2	1.38	0.87
1:U:346:LEU:HA	1:U:349:ARG:HG2	1.56	0.86
2:E:802:ASP:HA	2:E:804:ILE:HG13	1.56	0.86
1:M:73:VAL:HG22	1:T:41:ARG:HH12	1.38	0.85
1:P:438:ARG:HH12	1:P:442:SER:HB3	1.42	0.84
1:U:395:MET:HE1	1:V:395:MET:HB3	1.58	0.84
2:W:804:ILE:CG2	2:W:807:MET:SD	2.66	0.84
1:N:62:ILE:HG21	1:T:56:MET:HG3	1.59	0.84
2:Q:802:ASP:HA	2:Q:804:ILE:HG13	1.56	0.84
1:A:73:VAL:HG12	1:A:77:PHE:HE2	1.38	0.84
1:I:395:MET:HE1	1:J:395:MET:HB3	1.58	0.83
2:K:804:ILE:HD11	2:K:871:ILE:N	1.93	0.83
2:W:12:VAL:O	2:W:887:SER:N	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:12:VAL:O	2:K:887:SER:N	2.09	0.83
2:K:804:ILE:CG2	2:K:807:MET:SD	2.66	0.83
2:W:804:ILE:HD11	2:W:871:ILE:N	1.93	0.83
1:B:62:ILE:HG21	1:H:56:MET:HG3	1.59	0.83
2:L:865:VAL:HA	2:L:883:GLN:HA	1.61	0.83
2:W:804:ILE:CD1	2:W:872:TYR:CD1	2.62	0.82
1:D:438:ARG:HH12	1:D:442:SER:HB3	1.42	0.82
2:K:870:ALA:HB1	2:K:872:TYR:HE2	1.07	0.82
2:K:804:ILE:CD1	2:K:872:TYR:CD1	2.62	0.82
2:F:795:CYS:HB3	2:F:809:TRP:CH2	2.14	0.82
1:P:428:ALA:HA	2:R:820:MET:HE1	1.62	0.82
2:R:795:CYS:HB3	2:R:809:TRP:CH2	2.14	0.82
2:W:804:ILE:HD13	2:W:872:TYR:CD1	2.15	0.82
2:K:804:ILE:HD13	2:K:872:TYR:CZ	2.14	0.81
1:D:428:ALA:HA	2:F:820:MET:HE1	1.62	0.81
1:J:426:GLU:OE1	2:K:808:ARG:NH1	2.13	0.81
1:B:59:LEU:HD13	1:H:60:LYS:HG2	1.63	0.81
1:M:166:ASP:OD1	1:O:335:ARG:NH2	2.13	0.81
1:V:426:GLU:OE1	2:W:808:ARG:NH1	2.13	0.81
2:W:804:ILE:HD13	2:W:872:TYR:CZ	2.14	0.81
2:K:804:ILE:HD13	2:K:872:TYR:CD1	2.15	0.81
1:U:434:LEU:HD21	1:V:438:ARG:HH12	1.45	0.81
2:W:803:GLY:C	2:W:872:TYR:CE1	2.59	0.81
1:A:166:ASP:OD1	1:C:335:ARG:NH2	2.13	0.81
2:X:836:VAL:HB	2:X:840:PHE:HD2	1.45	0.81
2:K:803:GLY:C	2:K:872:TYR:CE1	2.59	0.81
1:U:358:ALA:HA	1:U:361:ILE:HD12	1.62	0.80
2:L:836:VAL:HB	2:L:840:PHE:HD2	1.45	0.80
1:A:129:ARG:NE	1:B:128:ARG:HH12	1.79	0.80
1:M:129:ARG:NE	1:N:128:ARG:HH12	1.79	0.80
2:F:843:SER:HB3	2:F:852:TYR:HB2	1.63	0.80
1:C:264:ARG:HG3	1:U:348:GLN:HE21	1.46	0.80
2:X:865:VAL:HA	2:X:883:GLN:HA	1.61	0.80
1:I:358:ALA:HA	1:I:361:ILE:HD12	1.62	0.80
2:R:843:SER:HB3	2:R:852:TYR:HB2	1.63	0.80
1:I:434:LEU:HD21	1:J:438:ARG:HH12	1.45	0.80
1:N:52:ILE:HG22	1:N:56:MET:HE1	1.64	0.79
1:N:255:LEU:O	1:N:259:GLN:NE2	2.16	0.79
1:D:282:ALA:O	1:D:285:THR:OG1	2.00	0.79
1:N:59:LEU:HD13	1:T:60:LYS:HG2	1.63	0.79
1:I:348:GLN:HE21	1:O:264:ARG:HG3	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:826:GLY:O	2:K:844:ARG:NH1	2.15	0.79
2:L:824:VAL:HG13	2:L:842:ILE:HD12	1.64	0.79
1:J:419:THR:CG2	2:K:805:ASN:ND2	2.45	0.79
2:X:824:VAL:HG13	2:X:842:ILE:HD12	1.64	0.79
1:B:52:ILE:HG22	1:B:56:MET:HE1	1.64	0.78
1:P:282:ALA:O	1:P:285:THR:OG1	2.00	0.78
2:K:803:GLY:C	2:K:872:TYR:HE1	1.92	0.78
2:W:826:GLY:O	2:W:844:ARG:NH1	2.15	0.78
2:Q:825:THR:HG23	2:Q:827:TRP:H	1.48	0.78
2:E:825:THR:HG23	2:E:827:TRP:H	1.48	0.78
1:B:255:LEU:O	1:B:259:GLN:NE2	2.16	0.77
1:U:435:GLU:HA	1:U:438:ARG:HE	1.49	0.77
1:I:435:GLU:HA	1:I:438:ARG:HE	1.49	0.77
1:V:419:THR:CG2	2:W:805:ASN:ND2	2.45	0.77
1:A:156:LYS:NZ	1:B:157:VAL:HG11	2.00	0.77
1:U:434:LEU:HB3	1:V:434:LEU:HD13	1.66	0.77
2:Q:13:TYR:HA	2:Q:887:SER:HA	1.67	0.77
2:W:803:GLY:C	2:W:872:TYR:HE1	1.92	0.77
1:I:434:LEU:HB3	1:J:434:LEU:HD13	1.66	0.76
1:N:204:GLN:HE21	1:O:301:ASN:HD21	1.33	0.76
1:H:38:ILE:HG23	1:H:42:TYR:HE1	1.51	0.76
2:L:854:GLN:OE1	2:L:856:ASN:ND2	2.19	0.76
1:M:156:LYS:NZ	1:N:157:VAL:HG11	2.00	0.76
1:C:283:LEU:HD13	1:C:286:ARG:HH12	1.51	0.75
1:A:59:LEU:HD21	1:G:59:LEU:HD13	1.68	0.75
2:K:804:ILE:CD1	2:K:872:TYR:CZ	2.68	0.75
2:E:13:TYR:HA	2:E:887:SER:HA	1.67	0.75
1:M:59:LEU:HD21	1:S:59:LEU:HD13	1.68	0.75
1:N:128:ARG:HA	1:N:131:THR:HG22	1.68	0.75
1:B:144:ASP:HA	1:B:147:ARG:HD2	1.69	0.75
2:K:804:ILE:CG1	2:K:872:TYR:CE1	2.69	0.75
2:R:863:THR:HA	2:R:884:VAL:HB	1.67	0.75
2:X:854:GLN:OE1	2:X:856:ASN:ND2	2.19	0.75
2:F:863:THR:HA	2:F:884:VAL:HB	1.67	0.75
1:B:204:GLN:HE21	1:C:301:ASN:HD21	1.33	0.74
2:K:804:ILE:HB	2:K:872:TYR:OH	1.87	0.74
1:H:94:LEU:O	1:H:98:GLN:NE2	2.21	0.74
2:K:839:ARG:HH12	2:K:858:LEU:HA	1.52	0.74
1:O:283:LEU:HD13	1:O:286:ARG:HH12	1.50	0.74
1:T:38:ILE:HG23	1:T:42:TYR:HE1	1.51	0.74
1:M:129:ARG:HE	1:N:128:ARG:NH1	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:129:ARG:NH1	1:M:130:GLN:OE1	2.21	0.74
1:A:74:SER:HA	1:A:77:PHE:HD2	1.53	0.74
1:B:128:ARG:HA	1:B:131:THR:HG22	1.68	0.74
2:E:839:ARG:NH1	2:E:857:ASN:O	2.18	0.74
1:M:74:SER:HA	1:M:77:PHE:HD2	1.53	0.73
1:I:423:LEU:HD21	2:L:806:ILE:HG21	1.71	0.73
1:N:219:ARG:HH11	1:P:288:GLU:HG2	1.53	0.73
1:A:33:GLU:HA	1:A:36:GLN:HE21	1.54	0.73
1:B:219:ARG:HH11	1:D:288:GLU:HG2	1.53	0.73
1:A:129:ARG:NH1	1:A:130:GLN:OE1	2.21	0.73
1:T:94:LEU:O	1:T:98:GLN:NE2	2.21	0.73
2:W:839:ARG:HH12	2:W:858:LEU:HA	1.52	0.73
1:A:72:PRO:HG2	1:H:41:ARG:HH21	1.54	0.73
1:B:41:ARG:HH12	1:H:81:ARG:HG3	1.54	0.73
2:W:804:ILE:HB	2:W:872:TYR:OH	1.87	0.73
1:M:33:GLU:HA	1:M:36:GLN:HE21	1.54	0.73
1:B:184:GLN:HE22	1:B:188:ILE:HD11	1.54	0.72
1:M:72:PRO:HG2	1:T:41:ARG:HH21	1.54	0.72
1:M:162:ALA:HA	1:M:165:ARG:HD3	1.72	0.72
1:N:144:ASP:HA	1:N:147:ARG:HD2	1.69	0.72
1:O:378:LEU:HB2	1:P:378:LEU:HD21	1.71	0.72
2:F:872:TYR:HB3	2:F:877:TYR:HE2	1.54	0.72
1:H:109:ARG:NH2	1:I:397:GLU:OE1	2.22	0.72
2:R:872:TYR:HB3	2:R:877:TYR:HE2	1.54	0.72
1:C:378:LEU:HB2	1:D:378:LEU:HD21	1.71	0.72
1:N:41:ARG:HH12	1:T:81:ARG:HG3	1.54	0.72
1:T:109:ARG:NH2	1:U:397:GLU:OE1	2.22	0.72
1:A:129:ARG:HE	1:B:128:ARG:NH1	1.85	0.72
1:H:161:ASP:HB3	1:H:165:ARG:HH12	1.54	0.72
2:L:791:LEU:HB3	2:L:855:MET:HB2	1.72	0.72
1:N:184:GLN:HE22	1:N:188:ILE:HD11	1.54	0.71
1:U:423:LEU:HD21	2:X:806:ILE:HG21	1.71	0.71
1:O:401:GLN:HA	1:O:404:ARG:HE	1.56	0.71
1:J:419:THR:HG21	2:K:805:ASN:CG	2.16	0.71
2:K:866:TYR:N	2:K:882:THR:O	2.24	0.71
2:W:804:ILE:CG1	2:W:872:TYR:CE2	2.73	0.71
2:W:804:ILE:CG1	2:W:872:TYR:CE1	2.69	0.71
2:W:870:ALA:HB1	2:W:872:TYR:CD2	2.25	0.71
1:C:401:GLN:HA	1:C:404:ARG:HE	1.56	0.71
2:K:804:ILE:CG1	2:K:872:TYR:CE2	2.73	0.71
2:K:870:ALA:HB1	2:K:872:TYR:CD2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:839:ARG:NH1	2:Q:857:ASN:O	2.17	0.71
2:X:791:LEU:HB3	2:X:855:MET:HB2	1.72	0.71
1:P:249:GLN:O	1:P:253:ASN:ND2	2.17	0.70
1:T:161:ASP:HB3	1:T:165:ARG:HH12	1.54	0.70
2:W:804:ILE:CD1	2:W:872:TYR:CZ	2.68	0.70
2:K:804:ILE:HG21	2:K:872:TYR:OH	1.92	0.70
2:E:836:VAL:HG11	2:E:840:PHE:CD2	2.26	0.70
2:K:839:ARG:NH2	2:K:857:ASN:O	2.23	0.70
2:Q:836:VAL:HG11	2:Q:840:PHE:CD2	2.26	0.70
1:A:162:ALA:HA	1:A:165:ARG:HD3	1.72	0.70
1:D:249:GLN:O	1:D:253:ASN:ND2	2.17	0.70
2:W:839:ARG:NH2	2:W:857:ASN:O	2.23	0.70
1:V:419:THR:HG21	2:W:805:ASN:CG	2.16	0.70
2:L:6:GLU:CD	2:L:881:GLY:H	2.00	0.70
2:X:6:GLU:CD	2:X:881:GLY:H	2.00	0.70
1:A:73:VAL:HG22	1:H:41:ARG:NH1	2.07	0.70
1:D:424:THR:HG23	2:F:831:ASN:HD21	1.57	0.69
1:C:392:LEU:HD22	1:D:392:LEU:HD13	1.74	0.69
2:W:804:ILE:CB	2:W:872:TYR:OH	2.39	0.69
2:W:804:ILE:CG2	2:W:872:TYR:OH	2.40	0.69
2:W:804:ILE:HA	2:W:872:TYR:CD1	2.28	0.69
1:G:168:THR:O	1:G:171:ILE:HG22	1.92	0.69
2:K:804:ILE:HA	2:K:872:TYR:CD1	2.28	0.69
2:W:804:ILE:HG21	2:W:872:TYR:OH	1.92	0.69
2:K:804:ILE:CG2	2:K:872:TYR:OH	2.40	0.69
1:O:401:GLN:HA	1:O:404:ARG:NE	2.08	0.69
2:X:792:ARG:NH1	2:X:852:TYR:HB3	2.07	0.69
2:F:6:GLU:HA	2:F:795:CYS:HA	1.73	0.69
2:K:804:ILE:CB	2:K:872:TYR:OH	2.39	0.69
2:Q:863:THR:HG23	2:Q:885:THR:HA	1.74	0.69
2:R:6:GLU:HA	2:R:795:CYS:HA	1.73	0.69
2:W:866:TYR:N	2:W:882:THR:O	2.24	0.69
1:C:214:ALA:HA	1:C:217:LYS:HE2	1.75	0.69
1:O:214:ALA:HA	1:O:217:LYS:HE2	1.75	0.69
2:X:792:ARG:HA	2:X:854:GLN:HA	1.75	0.69
2:K:839:ARG:NH2	2:K:857:ASN:OD1	2.26	0.69
2:L:792:ARG:HA	2:L:854:GLN:HA	1.75	0.69
2:L:836:VAL:HA	2:L:839:ARG:HD3	1.75	0.69
2:X:830:THR:HG23	2:X:842:ILE:HD11	1.75	0.69
1:C:264:ARG:HG3	1:U:348:GLN:NE2	2.08	0.68
1:O:392:LEU:HD22	1:P:392:LEU:HD13	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:424:THR:HG23	2:R:831:ASN:HD21	1.57	0.68
1:S:168:THR:O	1:S:171:ILE:HG22	1.92	0.68
1:T:109:ARG:NH2	1:U:400:ASP:OD2	2.26	0.68
2:W:839:ARG:NH2	2:W:857:ASN:OD1	2.26	0.68
1:G:96:GLN:HA	1:G:99:ARG:HH12	1.59	0.68
1:C:401:GLN:HA	1:C:404:ARG:NE	2.08	0.68
2:K:804:ILE:CB	2:K:872:TYR:HE1	1.82	0.68
2:W:804:ILE:HD11	2:W:871:ILE:C	2.19	0.68
1:H:126:ASP:O	1:H:130:GLN:NE2	2.27	0.68
2:L:830:THR:HG23	2:L:842:ILE:HD11	1.75	0.68
2:X:836:VAL:HA	2:X:839:ARG:HD3	1.75	0.68
1:B:120:THR:HG22	1:D:384:ARG:NH2	2.04	0.67
2:E:863:THR:HG23	2:E:885:THR:HA	1.74	0.67
2:L:832:TYR:HE1	2:L:842:ILE:HG12	1.59	0.67
1:I:440:ASP:OD2	1:I:441:ARG:NH1	2.25	0.67
2:R:791:LEU:HD22	2:R:858:LEU:HD12	1.76	0.67
1:T:126:ASP:O	1:T:130:GLN:NE2	2.27	0.67
2:E:859:LYS:NZ	2:E:861:GLU:OE2	2.27	0.67
2:K:804:ILE:CD1	2:K:872:TYR:CE1	2.78	0.67
2:R:6:GLU:HG3	2:R:795:CYS:HB2	1.76	0.67
1:G:40:GLN:HE21	1:G:41:ARG:HG2	1.59	0.67
1:J:422:ARG:NH2	1:J:425:SER:OG	2.28	0.67
2:K:804:ILE:HD11	2:K:871:ILE:C	2.19	0.67
2:Q:808:ARG:HB3	2:Q:823:VAL:HG22	1.76	0.67
2:E:804:ILE:HD13	2:E:844:ARG:HD2	1.77	0.67
2:F:6:GLU:HG3	2:F:795:CYS:HB2	1.77	0.67
2:F:791:LEU:HD22	2:F:858:LEU:HD12	1.76	0.67
1:H:33:GLU:OE1	1:H:33:GLU:N	2.27	0.67
1:H:109:ARG:NH2	1:I:400:ASP:OD2	2.26	0.67
1:S:40:GLN:HE21	1:S:41:ARG:HG2	1.59	0.67
1:S:96:GLN:HA	1:S:99:ARG:HH12	1.58	0.67
1:V:422:ARG:NH2	1:V:425:SER:OG	2.28	0.67
2:X:832:TYR:HE1	2:X:842:ILE:HG12	1.59	0.67
1:H:161:ASP:HB3	1:H:165:ARG:NH1	2.10	0.67
1:M:73:VAL:HG22	1:T:41:ARG:NH1	2.07	0.67
1:M:156:LYS:HZ2	1:N:157:VAL:HG11	1.57	0.67
2:Q:853:LEU:HB3	2:Q:855:MET:HE3	1.77	0.67
2:E:808:ARG:HB3	2:E:823:VAL:HG22	1.76	0.67
1:T:38:ILE:HG23	1:T:42:TYR:CE1	2.30	0.67
2:W:804:ILE:HD12	2:W:872:TYR:CG	2.30	0.67
1:A:73:VAL:HG12	1:A:77:PHE:CE2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:ARG:HH12	1:G:133:ASP:HB2	1.59	0.66
1:H:38:ILE:HG23	1:H:42:TYR:CE1	2.30	0.66
2:L:832:TYR:HB2	2:L:837:LYS:HE2	1.76	0.66
1:I:350:HIS:HE1	1:J:350:HIS:HA	1.61	0.66
2:Q:811:ARG:HH22	2:Q:836:VAL:HG21	1.60	0.66
2:L:792:ARG:NH1	2:L:852:TYR:HB3	2.07	0.66
1:S:129:ARG:HH12	1:S:133:ASP:HB2	1.59	0.66
1:T:161:ASP:HB3	1:T:165:ARG:NH1	2.10	0.66
1:A:38:ILE:HB	1:H:80:ARG:HH12	1.59	0.66
2:E:811:ARG:HH22	2:E:836:VAL:HG21	1.60	0.66
2:X:832:TYR:HB2	2:X:837:LYS:HE2	1.76	0.66
1:I:350:HIS:CE1	1:J:350:HIS:HA	2.31	0.66
1:M:38:ILE:HG13	1:T:80:ARG:HH22	1.61	0.66
1:J:414:ALA:O	1:J:417:GLN:HG3	1.95	0.66
2:Q:793:LEU:HB2	2:Q:809:TRP:HZ3	1.61	0.66
2:Q:804:ILE:HD13	2:Q:844:ARG:HD2	1.77	0.66
2:E:853:LEU:HB3	2:E:855:MET:HE3	1.77	0.65
1:M:38:ILE:HB	1:T:80:ARG:HH12	1.59	0.65
1:N:120:THR:HG22	1:P:384:ARG:NH2	2.04	0.65
1:T:33:GLU:OE1	1:T:33:GLU:N	2.28	0.65
1:A:38:ILE:HG13	1:H:80:ARG:HH22	1.61	0.65
1:V:416:LEU:HD23	2:W:805:ASN:OD1	1.96	0.65
1:J:400:ASP:HB3	1:J:404:ARG:HH21	1.62	0.65
2:W:804:ILE:CD1	2:W:872:TYR:CE1	2.78	0.65
2:W:804:ILE:CA	2:W:872:TYR:CD1	2.80	0.65
1:B:55:VAL:O	1:B:59:LEU:HG	1.97	0.65
2:K:863:THR:OG1	2:K:883:GLN:OE1	2.15	0.65
1:M:73:VAL:HG12	1:M:77:PHE:CE2	2.27	0.65
1:O:443:ARG:HH21	1:O:444:LEU:HD21	1.62	0.65
2:Q:859:LYS:NZ	2:Q:861:GLU:OE2	2.28	0.65
1:V:375:GLU:OE2	1:V:379:LYS:NZ	2.28	0.65
1:U:350:HIS:CE1	1:V:350:HIS:HA	2.31	0.65
2:K:804:ILE:CA	2:K:872:TYR:CD1	2.80	0.65
1:V:414:ALA:O	1:V:417:GLN:HG3	1.95	0.65
1:I:357:ARG:HD3	1:J:357:ARG:HB2	1.79	0.65
1:M:69:ILE:HD11	1:T:45:ILE:HG23	1.79	0.65
1:U:357:ARG:HD3	1:V:357:ARG:HB2	1.79	0.65
1:C:443:ARG:HH21	1:C:444:LEU:HD21	1.62	0.65
1:J:416:LEU:HD23	2:K:805:ASN:OD1	1.96	0.65
1:V:400:ASP:HB3	1:V:404:ARG:HH21	1.62	0.65
2:K:804:ILE:HD12	2:K:872:TYR:CG	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:31:GLN:HG3	1:T:32:ILE:H	1.61	0.64
2:E:793:LEU:HB2	2:E:809:TRP:HZ3	1.61	0.64
1:I:375:GLU:HB3	1:I:379:LYS:HZ1	1.63	0.64
1:P:337:ARG:O	1:P:340:GLU:HG3	1.97	0.64
2:Q:834:ASP:HA	2:Q:837:LYS:HB2	1.78	0.64
2:W:804:ILE:CB	2:W:872:TYR:HE1	1.82	0.64
1:D:337:ARG:O	1:D:340:GLU:HG3	1.97	0.64
1:H:31:GLN:HG3	1:H:32:ILE:H	1.61	0.64
2:K:804:ILE:CD1	2:K:871:ILE:C	2.70	0.64
1:N:55:VAL:O	1:N:59:LEU:HG	1.97	0.64
1:U:440:ASP:OD2	1:U:441:ARG:NH1	2.25	0.64
1:A:184:GLN:HE22	1:A:188:ILE:HD11	1.62	0.64
1:U:350:HIS:HE1	1:V:350:HIS:HA	1.61	0.64
2:W:804:ILE:CD1	2:W:871:ILE:C	2.70	0.64
1:A:69:ILE:HD11	1:H:45:ILE:HG23	1.79	0.64
2:R:1:GLU:OE2	2:R:3:GLN:NE2	2.30	0.64
1:T:36:GLN:O	1:T:40:GLN:NE2	2.30	0.64
1:H:36:GLN:O	1:H:40:GLN:NE2	2.30	0.64
1:M:184:GLN:HE22	1:M:188:ILE:HD11	1.62	0.64
1:C:261:ASP:O	1:C:265:THR:HG23	1.98	0.63
1:N:42:TYR:HA	1:N:45:ILE:HD12	1.80	0.63
2:E:834:ASP:HA	2:E:837:LYS:HB2	1.78	0.63
1:P:401:GLN:HA	1:P:404:ARG:HE	1.63	0.63
1:B:42:TYR:HA	1:B:45:ILE:HD12	1.80	0.63
1:T:144:ASP:OD1	1:T:147:ARG:NH2	2.32	0.63
2:F:813:ALA:HB3	2:F:816:LYS:HD2	1.81	0.63
2:F:884:VAL:HG12	2:F:885:THR:H	1.63	0.63
2:W:804:ILE:N	2:W:872:TYR:HE1	1.96	0.63
2:X:791:LEU:O	2:X:855:MET:N	2.31	0.63
1:A:42:TYR:CZ	1:G:77:PHE:HB3	2.33	0.63
2:L:791:LEU:O	2:L:855:MET:N	2.31	0.63
1:O:442:SER:HA	1:O:446:MET:HG2	1.81	0.63
2:R:813:ALA:HB3	2:R:816:LYS:HD2	1.81	0.63
2:R:884:VAL:HG12	2:R:885:THR:H	1.62	0.63
1:A:87:LEU:HB2	1:B:87:LEU:HD21	1.81	0.63
1:A:216:LEU:HD23	1:A:219:ARG:HD2	1.81	0.63
1:M:42:TYR:CZ	1:S:77:PHE:HB3	2.33	0.63
1:D:401:GLN:HA	1:D:404:ARG:HE	1.63	0.62
1:M:87:LEU:HB2	1:N:87:LEU:HD21	1.81	0.62
2:R:839:ARG:NH1	2:R:862:ASP:OD2	2.32	0.62
1:V:381:ALA:HA	1:V:384:ARG:NE	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:375:GLU:OE2	1:J:379:LYS:NZ	2.28	0.62
1:O:261:ASP:O	1:O:265:THR:HG23	1.98	0.62
1:T:94:LEU:HG	1:T:98:GLN:HE22	1.64	0.62
2:W:863:THR:OG1	2:W:883:GLN:OE1	2.15	0.62
1:A:272:GLN:NE2	1:A:276:ASN:HD21	1.97	0.62
2:F:797:SER:OG	2:F:849:ASP:OD1	2.17	0.62
2:K:804:ILE:N	2:K:872:TYR:HE1	1.97	0.62
1:C:442:SER:HA	1:C:446:MET:HG2	1.81	0.62
1:H:144:ASP:OD1	1:H:147:ARG:NH2	2.32	0.62
1:N:241:LEU:HD12	1:N:245:ARG:HH22	1.63	0.62
1:A:38:ILE:HG13	1:H:80:ARG:NH2	2.15	0.62
1:B:241:LEU:HD12	1:B:245:ARG:HH22	1.63	0.62
1:M:38:ILE:HG13	1:T:80:ARG:NH2	2.14	0.62
1:T:179:GLU:OE2	1:T:182:ARG:NH1	2.32	0.62
1:B:59:LEU:HD22	1:H:60:LYS:HG3	1.81	0.62
2:E:811:ARG:HG3	2:E:866:TYR:HE1	1.65	0.62
2:F:1:GLU:OE2	2:F:3:GLN:NE2	2.30	0.62
1:O:423:LEU:HD13	2:R:806:ILE:HD13	1.82	0.62
1:P:435:GLU:OE1	2:R:817:GLN:NE2	2.26	0.62
1:B:231:SER:O	1:B:234:GLU:HG3	2.00	0.62
1:M:272:GLN:NE2	1:M:276:ASN:HD21	1.97	0.62
2:F:810:TYR:CE1	2:F:820:MET:HB2	2.35	0.61
2:Q:811:ARG:HG3	2:Q:866:TYR:HE1	1.65	0.61
2:R:1:GLU:N	2:R:877:TYR:OH	2.33	0.61
1:G:188:ILE:HG23	1:H:188:ILE:HD13	1.82	0.61
1:J:381:ALA:HA	1:J:384:ARG:NE	2.14	0.61
2:K:832:TYR:OH	2:K:842:ILE:N	2.32	0.61
1:G:155:LEU:O	1:G:158:SER:OG	2.13	0.61
2:R:810:TYR:CE1	2:R:820:MET:HB2	2.35	0.61
1:V:417:GLN:HB2	2:X:827:TRP:NE1	2.16	0.61
1:A:156:LYS:HZ2	1:B:157:VAL:HG11	1.65	0.61
1:H:94:LEU:HG	1:H:98:GLN:HE22	1.64	0.61
1:I:382:GLU:OE2	1:J:384:ARG:NH1	2.33	0.61
1:I:421:GLU:OE1	2:K:829:SER:OG	2.15	0.61
2:L:836:VAL:HB	2:L:840:PHE:CD2	2.32	0.61
1:M:216:LEU:HD23	1:M:219:ARG:HD2	1.81	0.61
1:N:59:LEU:HD22	1:T:60:LYS:HG3	1.81	0.61
2:R:797:SER:OG	2:R:849:ASP:OD1	2.17	0.61
1:H:179:GLU:OE2	1:H:182:ARG:NH1	2.32	0.61
1:S:188:ILE:HG23	1:T:188:ILE:HD13	1.82	0.61
1:C:230:LEU:HD22	1:D:230:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ALA:HA	1:D:277:ARG:HD2	1.82	0.61
1:O:230:LEU:HD22	1:P:230:LEU:HD23	1.81	0.61
1:S:66:ILE:O	1:S:70:ARG:HG2	2.01	0.61
1:U:375:GLU:HA	1:V:374:GLN:HE22	1.66	0.61
1:U:382:GLU:OE2	1:V:384:ARG:NH1	2.33	0.61
1:A:72:PRO:HG2	1:H:41:ARG:NH2	2.16	0.61
1:A:143:ILE:O	1:A:147:ARG:HG3	2.01	0.61
1:I:348:GLN:NE2	1:O:264:ARG:HG3	2.13	0.61
1:O:420:ILE:O	1:O:424:THR:HG23	2.00	0.61
2:Q:860:PRO:HA	2:Q:886:VAL:HG23	1.82	0.61
1:D:420:ILE:HD11	2:F:806:ILE:HD11	1.83	0.61
1:M:143:ILE:O	1:M:147:ARG:HG3	2.01	0.61
1:M:264:ARG:HE	1:M:267:ARG:NH1	1.99	0.61
1:T:71:GLY:O	1:T:74:SER:OG	2.11	0.61
1:V:343:ALA:O	1:V:347:ARG:HG2	2.01	0.61
1:C:266:ILE:HG22	1:C:267:ARG:HH22	1.66	0.61
1:J:417:GLN:HB2	2:L:827:TRP:NE1	2.15	0.61
1:N:231:SER:O	1:N:234:GLU:HG3	2.00	0.61
1:C:420:ILE:O	1:C:424:THR:HG23	2.01	0.60
2:E:789:ASP:O	2:E:858:LEU:N	2.27	0.60
2:L:827:TRP:H	2:L:827:TRP:HE3	1.49	0.60
1:M:228:ALA:HA	1:P:277:ARG:HD2	1.82	0.60
1:G:66:ILE:O	1:G:70:ARG:HG2	2.01	0.60
1:I:375:GLU:HA	1:J:374:GLN:HE22	1.66	0.60
2:L:825:THR:HB	2:L:827:TRP:CE3	2.36	0.60
1:N:48:GLY:HA2	1:S:70:ARG:HH22	1.67	0.60
2:W:789:ASP:O	2:W:857:ASN:N	2.34	0.60
2:X:825:THR:HB	2:X:827:TRP:CE3	2.36	0.60
1:C:263:GLY:O	1:C:267:ARG:HG2	2.02	0.60
1:N:192:ARG:HA	1:N:192:ARG:NH1	2.17	0.60
1:N:216:LEU:O	1:N:220:VAL:HG23	2.02	0.60
1:O:266:ILE:HG22	1:O:267:ARG:HH22	1.66	0.60
1:A:264:ARG:HE	1:A:267:ARG:NH1	1.99	0.60
1:B:216:LEU:O	1:B:220:VAL:HG23	2.02	0.60
2:Q:855:MET:HB3	2:Q:858:LEU:HD21	1.84	0.60
2:F:1:GLU:N	2:F:877:TYR:OH	2.33	0.60
1:B:48:GLY:HA2	1:G:70:ARG:HH22	1.67	0.60
2:E:839:ARG:HH12	2:E:859:LYS:N	2.00	0.60
1:M:147:ARG:HE	1:P:359:THR:HG22	1.66	0.60
2:E:813:ALA:HB3	2:E:816:LYS:HB3	1.84	0.60
2:E:855:MET:HB3	2:E:858:LEU:HD21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:249:GLN:O	1:O:253:ASN:ND2	2.35	0.60
2:Q:813:ALA:HB3	2:Q:816:LYS:HB3	1.84	0.60
2:W:832:TYR:OH	2:W:842:ILE:N	2.32	0.60
1:C:423:LEU:HD13	2:F:806:ILE:HD13	1.82	0.60
1:D:435:GLU:OE1	2:F:817:GLN:NE2	2.26	0.60
1:J:343:ALA:O	1:J:347:ARG:HG2	2.01	0.60
2:K:804:ILE:HG12	2:K:872:TYR:CZ	2.36	0.60
1:M:251:VAL:HG13	1:M:255:LEU:HD23	1.84	0.60
1:O:263:GLY:O	1:O:267:ARG:HG2	2.02	0.60
2:R:882:THR:HG22	2:R:883:GLN:H	1.67	0.60
1:C:249:GLN:O	1:C:253:ASN:ND2	2.35	0.59
1:M:72:PRO:HG2	1:T:41:ARG:NH2	2.16	0.59
1:M:115:LEU:HD21	1:N:114:ARG:HH12	1.67	0.59
1:P:420:ILE:HD11	2:R:806:ILE:HD11	1.83	0.59
2:R:826:GLY:HA2	2:R:844:ARG:CZ	2.32	0.59
1:O:318:VAL:HG13	1:O:321:ARG:HH21	1.68	0.59
1:S:179:GLU:HA	1:S:182:ARG:HD2	1.83	0.59
2:F:826:GLY:HA2	2:F:844:ARG:CZ	2.32	0.59
1:I:346:LEU:HD22	1:I:349:ARG:HD3	1.85	0.59
2:Q:839:ARG:HH12	2:Q:859:LYS:N	2.00	0.59
1:I:346:LEU:CA	1:I:349:ARG:HG2	2.30	0.59
2:L:807:MET:SD	2:L:824:VAL:HG23	2.43	0.59
1:B:192:ARG:NH1	1:B:192:ARG:HA	2.17	0.59
2:F:839:ARG:NH1	2:F:862:ASP:OD2	2.32	0.59
1:H:71:GLY:O	1:H:74:SER:OG	2.11	0.59
1:M:35:THR:O	1:M:38:ILE:HG22	2.02	0.59
2:W:804:ILE:HG12	2:W:872:TYR:CZ	2.36	0.59
1:A:251:VAL:HG13	1:A:255:LEU:HD23	1.84	0.59
1:C:245:ARG:O	1:C:249:GLN:NE2	2.36	0.59
2:F:882:THR:HG22	2:F:883:GLN:H	1.67	0.59
1:G:179:GLU:HA	1:G:182:ARG:HD2	1.83	0.59
2:W:804:ILE:HD13	2:W:872:TYR:CE1	2.36	0.59
2:W:804:ILE:N	2:W:872:TYR:CE1	2.70	0.59
1:A:114:ARG:NH1	1:A:114:ARG:HB2	2.18	0.59
1:N:219:ARG:NH1	1:P:288:GLU:HG2	2.18	0.59
1:S:155:LEU:O	1:S:158:SER:OG	2.13	0.59
1:A:86:GLU:HG3	1:H:31:GLN:OE1	2.03	0.59
1:A:147:ARG:HE	1:D:359:THR:HG22	1.66	0.59
1:B:69:ILE:O	1:B:72:PRO:HD2	2.03	0.59
2:F:807:MET:HA	2:F:870:ALA:HA	1.84	0.59
1:G:49:LEU:O	1:G:52:ILE:HG22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:245:ARG:O	1:O:249:GLN:NE2	2.36	0.59
1:B:208:LEU:HD22	1:D:296:LYS:HZ1	1.67	0.59
2:E:860:PRO:HA	2:E:886:VAL:HG23	1.82	0.59
2:K:804:ILE:HD13	2:K:872:TYR:CE1	2.36	0.59
1:A:77:PHE:HE1	1:H:42:TYR:HH	1.51	0.59
1:A:115:LEU:HD21	1:B:114:ARG:HH12	1.67	0.59
1:J:380:ARG:HA	1:J:383:GLU:OE1	2.03	0.59
2:R:807:MET:HA	2:R:870:ALA:HA	1.84	0.59
2:X:836:VAL:HB	2:X:840:PHE:CD2	2.32	0.59
1:S:49:LEU:O	1:S:52:ILE:HG22	2.03	0.58
2:W:840:PHE:CE2	2:W:855:MET:HG3	2.38	0.58
1:U:350:HIS:HE1	1:V:350:HIS:CA	2.17	0.58
1:V:380:ARG:HA	1:V:383:GLU:OE1	2.03	0.58
2:X:827:TRP:HE3	2:X:827:TRP:H	1.49	0.58
2:X:840:PHE:CE1	2:X:855:MET:HA	2.38	0.58
1:A:35:THR:O	1:A:38:ILE:HG22	2.02	0.58
1:M:114:ARG:NH1	1:M:114:ARG:HB2	2.18	0.58
1:P:440:ASP:HA	1:P:443:ARG:HG2	1.86	0.58
2:X:807:MET:SD	2:X:824:VAL:HG23	2.43	0.58
2:K:804:ILE:N	2:K:872:TYR:CE1	2.70	0.58
2:W:797:SER:OG	2:W:849:ASP:OD2	2.21	0.58
2:K:811:ARG:N	2:K:819:GLY:O	2.35	0.58
1:A:173:HIS:O	1:C:331:ARG:NH2	2.37	0.58
2:K:840:PHE:CE2	2:K:855:MET:HG3	2.38	0.58
1:M:86:GLU:HG3	1:T:31:GLN:OE1	2.03	0.58
1:M:173:HIS:O	1:O:331:ARG:NH2	2.37	0.58
2:Q:789:ASP:O	2:Q:858:LEU:N	2.27	0.58
1:S:96:GLN:HA	1:S:99:ARG:NH1	2.19	0.58
1:G:96:GLN:HA	1:G:99:ARG:NH1	2.19	0.58
2:K:797:SER:OG	2:K:849:ASP:OD2	2.21	0.58
1:D:269:LEU:O	1:D:273:VAL:HG13	2.03	0.58
2:R:802:ASP:C	2:R:804:ILE:H	2.12	0.58
2:W:810:TYR:HA	2:W:820:MET:HA	1.85	0.58
2:F:825:THR:HG23	2:F:827:TRP:H	1.69	0.58
1:I:327:VAL:O	1:I:330:GLU:N	2.37	0.58
2:L:812:GLN:HB2	2:L:865:VAL:HG13	1.85	0.58
2:R:792:ARG:HA	2:R:854:GLN:NE2	2.18	0.58
2:R:830:THR:HA	2:R:842:ILE:HD11	1.86	0.58
1:U:346:LEU:HD22	1:U:349:ARG:HD3	1.85	0.58
1:D:440:ASP:HA	1:D:443:ARG:HG2	1.85	0.58
2:F:792:ARG:HA	2:F:854:GLN:NE2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:802:ASP:C	2:F:804:ILE:H	2.12	0.58
1:M:110:GLU:CD	1:M:114:ARG:HH12	2.12	0.58
1:N:69:ILE:O	1:N:72:PRO:HD2	2.03	0.58
1:N:77:PHE:HA	1:N:80:ARG:HE	1.69	0.58
1:A:260:ALA:O	1:A:264:ARG:HG2	2.04	0.57
2:K:810:TYR:HA	2:K:820:MET:HA	1.85	0.57
2:K:3:GLN:HB2	2:K:798:SER:HB3	1.86	0.57
2:K:789:ASP:O	2:K:857:ASN:N	2.34	0.57
1:B:267:ARG:HA	1:B:270:GLU:HG3	1.87	0.57
2:L:840:PHE:CE1	2:L:855:MET:HA	2.38	0.57
1:N:254:ALA:O	1:N:258:HIS:ND1	2.24	0.57
1:P:269:LEU:O	1:P:273:VAL:HG13	2.03	0.57
1:I:350:HIS:HE1	1:J:350:HIS:CA	2.17	0.57
1:U:327:VAL:O	1:U:330:GLU:N	2.37	0.57
1:U:375:GLU:HB3	1:U:379:LYS:HZ1	1.70	0.57
2:W:811:ARG:N	2:W:819:GLY:O	2.35	0.57
1:A:41:ARG:O	1:A:45:ILE:HG12	2.05	0.57
1:J:438:ARG:O	1:J:442:SER:OG	2.20	0.57
2:K:793:LEU:HB2	2:K:855:MET:HE1	1.87	0.57
1:S:87:LEU:HD21	1:T:91:ARG:HH21	1.69	0.57
1:U:346:LEU:CA	1:U:349:ARG:HG2	2.30	0.57
2:X:812:GLN:HB2	2:X:865:VAL:HG13	1.84	0.57
1:U:434:LEU:HD21	1:V:438:ARG:NH1	2.18	0.57
1:A:110:GLU:CD	1:A:114:ARG:HH12	2.12	0.57
1:M:260:ALA:O	1:M:264:ARG:HG2	2.04	0.57
1:N:267:ARG:HA	1:N:270:GLU:HG3	1.87	0.57
1:A:264:ARG:HE	1:A:267:ARG:HH11	1.53	0.57
1:C:318:VAL:HG13	1:C:321:ARG:HH21	1.68	0.57
1:M:41:ARG:O	1:M:45:ILE:HG12	2.05	0.57
1:O:431:GLU:HG2	2:Q:820:MET:HG3	1.87	0.57
2:W:4:LEU:HD23	2:W:797:SER:HA	1.87	0.57
2:W:824:VAL:HG11	2:W:844:ARG:HG3	1.87	0.57
2:W:825:THR:HG1	2:W:827:TRP:CD1	2.23	0.57
1:G:87:LEU:HD21	1:H:91:ARG:HH21	1.69	0.57
1:N:72:PRO:HA	1:N:75:GLN:HE21	1.70	0.57
1:O:441:ARG:NH2	1:P:437:ALA:O	2.38	0.57
1:A:272:GLN:O	1:A:276:ASN:ND2	2.38	0.57
1:B:219:ARG:NH1	1:D:288:GLU:HG2	2.18	0.57
2:R:825:THR:HG23	2:R:827:TRP:H	1.69	0.57
2:W:825:THR:HG23	2:W:827:TRP:H	1.70	0.57
1:A:206:ASN:ND2	1:B:205:ASP:OD2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:ARG:NH2	1:D:437:ALA:O	2.38	0.56
2:E:805:ASN:H	2:E:807:MET:HE2	1.70	0.56
1:N:58:HIS:O	1:N:61:ALA:N	2.36	0.56
2:F:791:LEU:HD13	2:F:858:LEU:HG	1.87	0.56
1:M:77:PHE:HE1	1:T:42:TYR:HH	1.54	0.56
1:M:264:ARG:HE	1:M:267:ARG:HH11	1.53	0.56
1:B:72:PRO:HA	1:B:75:GLN:HE21	1.70	0.56
1:B:77:PHE:HA	1:B:80:ARG:HE	1.69	0.56
1:B:232:ARG:O	1:B:235:THR:OG1	2.22	0.56
2:K:4:LEU:HD23	2:K:797:SER:HA	1.87	0.56
1:M:62:ILE:HG21	1:T:56:MET:HE3	1.88	0.56
1:M:206:ASN:ND2	1:N:205:ASP:OD2	2.37	0.56
2:Q:805:ASN:H	2:Q:807:MET:HE2	1.70	0.56
2:W:793:LEU:HB2	2:W:855:MET:HE1	1.87	0.56
2:W:832:TYR:CZ	2:W:842:ILE:HG22	2.41	0.56
2:X:869:ASN:OD1	2:X:870:ALA:N	2.38	0.56
1:C:417:GLN:OE1	2:E:827:TRP:NE1	2.39	0.56
1:D:264:ARG:HA	1:D:267:ARG:NH2	2.20	0.56
1:J:419:THR:HG21	2:K:805:ASN:HD22	1.64	0.56
2:L:869:ASN:OD1	2:L:870:ALA:N	2.38	0.56
1:M:97:ALA:O	1:M:101:ILE:HG12	2.05	0.56
1:M:245:ARG:O	1:M:249:GLN:NE2	2.39	0.56
1:N:116:ALA:O	1:N:120:THR:HG23	2.05	0.56
1:B:69:ILE:HG12	1:G:45:ILE:HG22	1.86	0.56
1:I:339:LEU:HD13	1:J:339:LEU:HD22	1.87	0.56
1:J:377:ALA:HA	1:J:380:ARG:HD2	1.87	0.56
2:K:824:VAL:HG11	2:K:844:ARG:HG3	1.87	0.56
1:N:208:LEU:HD22	1:P:296:LYS:HZ1	1.71	0.56
1:N:219:ARG:NH2	1:P:284:GLN:OE1	2.38	0.56
1:A:38:ILE:HG23	1:G:81:ARG:HG2	1.87	0.56
1:A:62:ILE:HG21	1:H:56:MET:HE3	1.88	0.56
2:F:804:ILE:HD12	2:F:844:ARG:HH21	1.71	0.56
1:N:69:ILE:HG12	1:S:45:ILE:HG22	1.86	0.56
1:P:264:ARG:HA	1:P:267:ARG:NH2	2.20	0.56
1:U:339:LEU:HD13	1:V:339:LEU:HD22	1.87	0.56
1:U:421:GLU:OE1	2:W:829:SER:OG	2.15	0.56
2:E:796:ALA:HA	2:E:850:THR:HG22	1.88	0.56
1:H:70:ARG:NH2	1:H:71:GLY:HA2	2.21	0.56
2:L:839:ARG:HH12	2:L:859:LYS:H	1.54	0.56
1:M:66:ILE:HA	1:M:69:ILE:HG22	1.88	0.56
1:V:377:ALA:HA	1:V:380:ARG:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:3:GLN:HB2	2:W:798:SER:HB3	1.86	0.56
2:X:812:GLN:HE22	2:X:818:ARG:HA	1.71	0.56
2:R:791:LEU:HD13	2:R:858:LEU:HG	1.88	0.56
1:A:156:LYS:HZ3	1:B:157:VAL:HG11	1.69	0.56
1:D:285:THR:O	1:D:288:GLU:HG3	2.06	0.56
2:K:832:TYR:CZ	2:K:842:ILE:HG22	2.41	0.56
1:P:285:THR:O	1:P:288:GLU:HG3	2.06	0.56
2:W:804:ILE:HD12	2:W:872:TYR:CD1	2.41	0.56
1:B:116:ALA:O	1:B:120:THR:HG23	2.05	0.55
1:C:431:GLU:HG2	2:E:820:MET:HG3	1.87	0.55
2:F:830:THR:HA	2:F:842:ILE:HD11	1.86	0.55
1:I:346:LEU:HA	1:I:349:ARG:CG	2.34	0.55
2:K:794:SER:HB2	2:K:850:THR:HB	1.88	0.55
1:N:277:ARG:HD3	1:O:227:LEU:HD11	1.87	0.55
1:O:417:GLN:OE1	2:Q:827:TRP:NE1	2.39	0.55
2:X:3:GLN:H	2:X:798:SER:HB2	1.71	0.55
1:A:97:ALA:O	1:A:101:ILE:HG12	2.06	0.55
1:A:255:LEU:HD11	1:B:255:LEU:HD12	1.88	0.55
1:B:277:ARG:HD3	1:C:227:LEU:HD11	1.87	0.55
2:K:825:THR:HG23	2:K:827:TRP:H	1.70	0.55
2:L:812:GLN:HE22	2:L:818:ARG:HA	1.71	0.55
2:R:804:ILE:HD12	2:R:844:ARG:HH21	1.71	0.55
1:B:105:GLN:O	1:B:109:ARG:HG2	2.06	0.55
1:D:268:GLY:O	1:D:271:SER:OG	2.20	0.55
1:H:49:LEU:HA	1:H:52:ILE:HG22	1.89	0.55
1:M:38:ILE:HG23	1:S:81:ARG:HG2	1.87	0.55
1:M:191:ARG:HG2	1:N:192:ARG:HE	1.72	0.55
2:Q:796:ALA:HA	2:Q:850:THR:HG22	1.88	0.55
1:B:219:ARG:NH2	1:D:284:GLN:OE1	2.38	0.55
1:B:254:ALA:O	1:B:258:HIS:ND1	2.24	0.55
1:C:318:VAL:HG13	1:C:321:ARG:NH2	2.22	0.55
1:A:147:ARG:NH1	1:D:362:GLU:OE2	2.40	0.55
1:G:100:GLN:NE2	1:H:101:ILE:HG12	2.22	0.55
1:H:96:GLN:HA	1:H:99:ARG:HG2	1.88	0.55
1:M:54:ARG:HH21	1:M:57:GLU:CD	2.15	0.55
1:T:49:LEU:HA	1:T:52:ILE:HG22	1.89	0.55
1:U:347:ARG:HH12	1:V:346:LEU:HD21	1.70	0.55
2:W:794:SER:HB2	2:W:850:THR:HB	1.88	0.55
1:A:66:ILE:HA	1:A:69:ILE:HG22	1.88	0.55
1:A:245:ARG:O	1:A:249:GLN:NE2	2.39	0.55
1:G:78:GLU:OE1	1:G:81:ARG:NE	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:347:ARG:HH12	1:J:346:LEU:HD21	1.70	0.55
1:N:117:ALA:O	1:N:120:THR:OG1	2.19	0.55
1:C:434:LEU:HG	1:D:434:LEU:HD23	1.88	0.55
1:T:142:GLU:OE2	1:T:145:ARG:NH2	2.39	0.55
1:I:434:LEU:HD21	1:J:438:ARG:NH1	2.18	0.55
2:K:825:THR:HG1	2:K:827:TRP:CD1	2.25	0.55
1:O:276:ASN:OD1	1:P:280:ILE:HD11	2.06	0.55
2:R:836:VAL:HB	2:R:840:PHE:HB2	1.89	0.55
1:S:129:ARG:HD2	1:T:128:ARG:CZ	2.37	0.55
1:U:357:ARG:HG2	1:V:357:ARG:HH11	1.72	0.55
1:A:191:ARG:HG2	1:B:192:ARG:HE	1.72	0.55
1:C:276:ASN:OD1	1:D:280:ILE:HD11	2.06	0.55
1:H:142:GLU:OE2	1:H:145:ARG:NH2	2.40	0.55
1:T:96:GLN:HA	1:T:99:ARG:HG2	1.89	0.55
1:T:109:ARG:CZ	1:U:396:GLN:HE22	2.20	0.55
2:X:801:ILE:HA	2:X:804:ILE:HG22	1.89	0.55
1:B:184:GLN:NE2	1:B:188:ILE:HD11	2.22	0.55
1:I:357:ARG:HG2	1:J:357:ARG:HH11	1.72	0.55
1:M:272:GLN:O	1:M:276:ASN:ND2	2.38	0.55
1:S:100:GLN:NE2	1:T:101:ILE:HG12	2.22	0.55
1:V:343:ALA:O	1:V:347:ARG:NH1	2.40	0.55
2:X:839:ARG:HH12	2:X:859:LYS:H	1.54	0.55
2:F:859:LYS:HZ3	2:F:861:GLU:HB3	1.72	0.54
2:K:804:ILE:CB	2:K:872:TYR:CD1	2.78	0.54
2:L:3:GLN:H	2:L:798:SER:HB2	1.71	0.54
2:L:845:ASP:OD2	2:L:848:LYS:NZ	2.36	0.54
1:M:147:ARG:NH1	1:P:362:GLU:OE2	2.40	0.54
1:S:78:GLU:OE1	1:S:81:ARG:NE	2.40	0.54
1:T:70:ARG:NH2	1:T:71:GLY:HA2	2.21	0.54
2:F:836:VAL:HA	2:F:839:ARG:HB2	1.90	0.54
1:O:242:ALA:HA	1:O:245:ARG:NE	2.22	0.54
1:O:318:VAL:HG13	1:O:321:ARG:NH2	2.22	0.54
1:O:434:LEU:HG	1:P:434:LEU:HD23	1.88	0.54
1:T:68:GLU:O	1:T:72:PRO:HD3	2.07	0.54
2:W:2:VAL:HB	2:W:877:TYR:HD2	1.73	0.54
1:B:45:ILE:HG12	1:H:70:ARG:NH1	2.23	0.54
1:C:288:GLU:HA	1:C:291:THR:HG22	1.89	0.54
1:J:343:ALA:O	1:J:347:ARG:NH1	2.40	0.54
1:M:33:GLU:O	1:M:37:ALA:HB3	2.08	0.54
1:M:255:LEU:HD11	1:N:255:LEU:HD12	1.88	0.54
1:A:35:THR:O	1:A:39:GLY:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:422:ARG:NH2	2:L:876:GLU:HG3	2.23	0.54
2:K:1:GLU:HA	2:K:799:ARG:HH21	1.73	0.54
2:L:866:TYR:N	2:L:882:THR:O	2.34	0.54
1:M:115:LEU:HD11	1:N:114:ARG:CZ	2.37	0.54
1:P:417:GLN:NE2	2:R:827:TRP:HB2	2.22	0.54
1:A:115:LEU:HD11	1:B:114:ARG:CZ	2.37	0.54
1:N:184:GLN:NE2	1:N:188:ILE:HD11	2.22	0.54
2:R:859:LYS:HZ3	2:R:861:GLU:HB3	1.72	0.54
1:A:33:GLU:O	1:A:37:ALA:HB3	2.08	0.54
1:A:54:ARG:HH21	1:A:57:GLU:CD	2.15	0.54
1:D:262:SER:O	1:D:266:ILE:HG12	2.08	0.54
1:N:105:GLN:O	1:N:109:ARG:HG2	2.06	0.54
1:C:242:ALA:HA	1:C:245:ARG:NE	2.22	0.54
1:C:250:ALA:HA	1:C:253:ASN:HD22	1.73	0.54
1:G:95:ASP:O	1:G:98:GLN:HG3	2.08	0.54
1:H:109:ARG:CZ	1:I:396:GLN:HE22	2.20	0.54
1:I:434:LEU:CB	1:J:434:LEU:HD13	2.37	0.54
2:K:2:VAL:HB	2:K:877:TYR:HD2	1.73	0.54
2:L:801:ILE:HA	2:L:804:ILE:HG22	1.89	0.54
2:L:828:GLY:HA2	2:L:844:ARG:HH12	1.72	0.54
1:M:77:PHE:O	1:S:39:GLY:N	2.41	0.54
1:M:223:ALA:O	1:M:227:LEU:HD23	2.08	0.54
1:U:422:ARG:HG2	1:U:426:GLU:OE1	2.08	0.54
1:V:417:GLN:HB2	2:X:827:TRP:CE2	2.43	0.54
1:A:77:PHE:O	1:G:39:GLY:N	2.41	0.54
1:A:223:ALA:O	1:A:227:LEU:HD23	2.08	0.54
1:O:421:GLU:HB3	2:Q:827:TRP:HZ2	1.73	0.54
1:B:58:HIS:O	1:B:61:ALA:N	2.36	0.54
1:D:417:GLN:NE2	2:F:827:TRP:HB2	2.23	0.54
1:G:129:ARG:HD2	1:H:128:ARG:CZ	2.37	0.54
2:R:812:GLN:HG3	2:R:818:ARG:HA	1.90	0.54
1:T:153:SER:O	1:T:157:VAL:HG23	2.09	0.54
2:F:836:VAL:HB	2:F:840:PHE:HB2	1.89	0.53
2:L:839:ARG:NH1	2:L:858:LEU:HA	2.22	0.53
1:S:95:ASP:O	1:S:98:GLN:HG3	2.08	0.53
2:X:828:GLY:HA2	2:X:844:ARG:HH12	1.72	0.53
1:A:232:ARG:O	1:A:235:THR:OG1	2.23	0.53
1:H:68:GLU:O	1:H:72:PRO:HD3	2.07	0.53
1:M:232:ARG:O	1:M:235:THR:OG1	2.23	0.53
1:A:169:ALA:O	1:A:173:HIS:ND1	2.32	0.53
1:M:72:PRO:HA	1:M:75:GLN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:422:ARG:NH2	2:X:876:GLU:HG3	2.23	0.53
1:O:250:ALA:HA	1:O:253:ASN:HD22	1.73	0.53
2:X:866:TYR:N	2:X:882:THR:O	2.34	0.53
2:E:804:ILE:HG21	2:E:844:ARG:CZ	2.38	0.53
2:E:869:ASN:OD1	2:E:870:ALA:N	2.41	0.53
1:G:140:ALA:O	1:G:143:ILE:HG22	2.09	0.53
1:J:417:GLN:HB2	2:L:827:TRP:CE2	2.43	0.53
1:O:308:LEU:CD1	1:P:304:ILE:HG12	2.39	0.53
1:P:262:SER:O	1:P:266:ILE:HG12	2.08	0.53
2:Q:790:SER:HB2	2:Q:857:ASN:H	1.73	0.53
2:Q:869:ASN:OD1	2:Q:870:ALA:N	2.41	0.53
1:V:408:THR:C	1:V:412:LYS:HZ2	2.17	0.53
2:X:8:GLY:HA3	2:X:793:LEU:HG	1.91	0.53
1:C:416:LEU:HA	1:C:419:THR:HG22	1.91	0.53
2:E:790:SER:HB2	2:E:857:ASN:H	1.73	0.53
2:F:818:ARG:HG3	2:F:818:ARG:HH21	1.74	0.53
1:H:172:GLU:O	1:H:175:VAL:HG12	2.09	0.53
1:N:255:LEU:HG	1:N:259:GLN:HE22	1.74	0.53
1:O:288:GLU:HA	1:O:291:THR:HG22	1.89	0.53
2:R:836:VAL:HA	2:R:839:ARG:HB2	1.90	0.53
2:X:839:ARG:NH1	2:X:858:LEU:HA	2.22	0.53
1:I:359:THR:O	1:I:362:GLU:HG2	2.09	0.53
1:J:347:ARG:HG2	1:J:347:ARG:HH11	1.73	0.53
1:N:45:ILE:HG12	1:T:70:ARG:NH1	2.23	0.53
2:W:1:GLU:HA	2:W:799:ARG:HH21	1.73	0.53
1:B:255:LEU:HG	1:B:259:GLN:HE22	1.74	0.53
1:C:282:ALA:O	1:C:286:ARG:HG2	2.09	0.53
1:C:308:LEU:CD1	1:D:304:ILE:HG12	2.39	0.53
1:D:270:GLU:O	1:D:273:VAL:HG22	2.09	0.53
2:L:834:ASP:OD1	2:L:835:SER:N	2.42	0.53
1:O:418:ALA:O	1:O:421:GLU:HG3	2.08	0.53
1:U:434:LEU:CB	1:V:434:LEU:HD13	2.37	0.53
1:V:347:ARG:HG2	1:V:347:ARG:HH11	1.73	0.53
1:G:129:ARG:N	1:H:129:ARG:HH22	2.07	0.53
1:H:40:GLN:HA	1:H:43:GLU:OE1	2.09	0.53
1:I:384:ARG:HH12	1:J:385:ALA:HB1	1.73	0.53
2:Q:804:ILE:HG21	2:Q:844:ARG:CZ	2.38	0.53
1:S:115:LEU:HD21	1:T:114:ARG:CZ	2.39	0.53
1:A:148:ASN:O	1:A:151:LEU:HB2	2.09	0.53
2:E:3:GLN:C	2:E:4:LEU:HD12	2.34	0.53
1:G:66:ILE:HA	1:G:69:ILE:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:804:ILE:HD12	2:K:871:ILE:O	2.08	0.53
2:K:804:ILE:HD12	2:K:872:TYR:CD1	2.41	0.53
2:K:869:ASN:OD1	2:K:870:ALA:N	2.42	0.53
1:O:268:GLY:O	1:O:271:SER:OG	2.26	0.53
2:Q:3:GLN:C	2:Q:4:LEU:HD12	2.34	0.53
2:W:824:VAL:HG12	2:W:825:THR:O	2.09	0.53
1:A:72:PRO:HA	1:A:75:GLN:HB2	1.90	0.52
1:S:129:ARG:N	1:T:129:ARG:HH22	2.07	0.52
1:U:359:THR:O	1:U:362:GLU:HG2	2.09	0.52
2:W:869:ASN:OD1	2:W:870:ALA:N	2.42	0.52
1:B:100:GLN:HA	1:B:103:LEU:HG	1.91	0.52
1:G:115:LEU:HD21	1:H:114:ARG:CZ	2.39	0.52
1:S:140:ALA:O	1:S:143:ILE:HG22	2.09	0.52
1:U:444:LEU:HB3	1:V:445:GLN:CD	2.34	0.52
1:C:418:ALA:O	1:C:421:GLU:HG3	2.08	0.52
1:G:150:LEU:HD13	1:H:150:LEU:HD13	1.91	0.52
1:J:408:THR:C	1:J:412:LYS:HZ2	2.17	0.52
1:M:35:THR:O	1:M:39:GLY:N	2.39	0.52
1:S:66:ILE:HA	1:S:69:ILE:HG12	1.91	0.52
1:T:172:GLU:O	1:T:175:VAL:HG12	2.09	0.52
1:I:422:ARG:HG2	1:I:426:GLU:OE1	2.08	0.52
1:O:282:ALA:O	1:O:286:ARG:HG2	2.09	0.52
1:U:384:ARG:HH12	1:V:385:ALA:HB1	1.73	0.52
2:W:11:LEU:HD12	2:W:886:VAL:HA	1.91	0.52
2:W:804:ILE:HD12	2:W:871:ILE:O	2.08	0.52
2:W:833:VAL:HG12	2:W:835:SER:H	1.75	0.52
2:X:860:PRO:HB3	2:X:887:SER:H	1.75	0.52
1:H:153:SER:O	1:H:157:VAL:HG23	2.09	0.52
2:K:824:VAL:HG12	2:K:825:THR:O	2.09	0.52
1:S:87:LEU:HD11	1:T:91:ARG:NH2	2.25	0.52
2:X:834:ASP:OD1	2:X:835:SER:N	2.42	0.52
1:C:308:LEU:HB3	1:D:307:ARG:HH12	1.75	0.52
1:C:421:GLU:HB3	2:E:827:TRP:HZ2	1.73	0.52
1:I:434:LEU:HD13	1:J:434:LEU:CB	2.40	0.52
2:K:863:THR:OG1	2:K:885:THR:OG1	2.27	0.52
1:M:115:LEU:HD21	1:N:114:ARG:NH1	2.24	0.52
1:O:266:ILE:HG22	1:O:267:ARG:NH2	2.24	0.52
1:U:434:LEU:HD13	1:V:434:LEU:CB	2.40	0.52
1:C:266:ILE:HG22	1:C:267:ARG:NH2	2.24	0.52
2:F:792:ARG:HA	2:F:854:GLN:HE22	1.75	0.52
2:F:812:GLN:HG3	2:F:818:ARG:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:377:ALA:O	1:I:380:ARG:HG3	2.10	0.52
1:M:148:ASN:O	1:M:151:LEU:HB2	2.09	0.52
1:O:308:LEU:HB3	1:P:307:ARG:HH12	1.75	0.52
1:O:416:LEU:HA	1:O:419:THR:HG22	1.91	0.52
1:B:97:ALA:O	1:B:101:ILE:HG12	2.10	0.52
1:M:63:GLU:N	1:S:56:MET:SD	2.83	0.52
2:Q:793:LEU:HB2	2:Q:809:TRP:CZ3	2.43	0.52
2:R:866:TYR:HB2	2:R:882:THR:H	1.75	0.52
1:S:150:LEU:HD13	1:T:150:LEU:HD13	1.91	0.52
1:A:63:GLU:N	1:G:56:MET:SD	2.83	0.52
1:P:270:GLU:O	1:P:273:VAL:HG22	2.08	0.52
2:R:818:ARG:HH21	2:R:818:ARG:HG3	1.74	0.52
1:S:138:ASP:O	1:S:141:LEU:HG	2.10	0.52
1:U:377:ALA:O	1:U:380:ARG:HG3	2.10	0.52
1:A:201:ARG:O	1:A:204:GLN:HG3	2.10	0.52
2:E:802:ASP:C	2:E:804:ILE:H	2.18	0.52
2:K:823:VAL:HG22	2:K:831:ASN:O	2.10	0.52
1:T:40:GLN:HA	1:T:43:GLU:OE1	2.09	0.52
2:K:791:LEU:HD23	2:K:792:ARG:N	2.26	0.51
2:K:833:VAL:HG12	2:K:835:SER:H	1.75	0.51
2:L:8:GLY:HA3	2:L:793:LEU:HG	1.91	0.51
2:L:791:LEU:CB	2:L:855:MET:HB2	2.40	0.51
1:N:97:ALA:O	1:N:101:ILE:HG12	2.10	0.51
1:U:375:GLU:HB3	1:U:379:LYS:NZ	2.25	0.51
1:V:438:ARG:O	1:V:442:SER:OG	2.20	0.51
1:G:87:LEU:HD11	1:H:91:ARG:NH2	2.25	0.51
2:K:11:LEU:HD12	2:K:886:VAL:HA	1.91	0.51
2:Q:802:ASP:C	2:Q:804:ILE:H	2.18	0.51
2:R:832:TYR:OH	2:R:842:ILE:HG12	2.10	0.51
1:A:80:ARG:CZ	1:B:80:ARG:HG2	2.41	0.51
1:B:117:ALA:O	1:B:120:THR:OG1	2.19	0.51
2:F:833:VAL:C	2:F:837:LYS:HZ3	2.17	0.51
2:K:809:TRP:CG	2:K:853:LEU:HD22	2.46	0.51
1:N:238:GLU:HA	1:N:241:LEU:HG	1.93	0.51
1:O:283:LEU:HD22	1:O:286:ARG:HH22	1.76	0.51
1:U:360:ALA:HA	1:U:363:ARG:HG2	1.93	0.51
2:W:866:TYR:O	2:W:882:THR:N	2.44	0.51
2:K:814:PRO:O	2:K:816:LYS:N	2.43	0.51
2:L:860:PRO:HB3	2:L:887:SER:H	1.75	0.51
2:W:809:TRP:CG	2:W:853:LEU:HD22	2.46	0.51
1:B:75:GLN:CD	1:B:76:GLU:HG3	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:806:ILE:CD1	2:L:825:THR:HG22	2.41	0.51
1:M:273:VAL:HG13	1:N:276:ASN:OD1	2.11	0.51
1:P:244:GLU:O	1:P:248:VAL:HG23	2.11	0.51
2:R:833:VAL:C	2:R:837:LYS:HZ3	2.18	0.51
2:W:791:LEU:HD23	2:W:792:ARG:N	2.26	0.51
1:A:77:PHE:CD1	1:G:42:TYR:CG	2.99	0.51
1:A:273:VAL:HG13	1:B:276:ASN:OD1	2.11	0.51
2:F:866:TYR:HB2	2:F:882:THR:H	1.75	0.51
1:G:138:ASP:O	1:G:141:LEU:HG	2.10	0.51
1:I:444:LEU:HB3	1:J:445:GLN:CD	2.34	0.51
1:M:115:LEU:HA	1:N:115:LEU:HD13	1.93	0.51
1:N:125:SER:O	1:N:129:ARG:HG3	2.11	0.51
1:U:373:ALA:HA	1:U:376:LYS:HD3	1.93	0.51
1:A:115:LEU:HD21	1:B:114:ARG:NH1	2.24	0.51
1:C:283:LEU:HD22	1:C:286:ARG:HH22	1.76	0.51
2:E:839:ARG:HH12	2:E:859:LYS:H	1.59	0.51
1:G:173:HIS:HA	1:G:176:GLN:OE1	2.11	0.51
1:I:334:ASP:O	1:I:337:ARG:HG3	2.11	0.51
1:M:77:PHE:CD1	1:S:42:TYR:CG	2.99	0.51
1:M:96:GLN:HA	1:M:99:ARG:CD	2.41	0.51
1:A:96:GLN:HA	1:A:99:ARG:CD	2.41	0.51
2:F:825:THR:HG22	2:F:829:SER:OG	2.11	0.51
2:F:832:TYR:OH	2:F:842:ILE:HG12	2.10	0.51
2:F:843:SER:N	2:F:852:TYR:O	2.32	0.51
1:M:62:ILE:HB	1:S:56:MET:SD	2.51	0.51
2:Q:836:VAL:HG13	2:Q:839:ARG:HB3	1.92	0.51
1:S:173:HIS:HA	1:S:176:GLN:OE1	2.11	0.51
2:W:823:VAL:HG22	2:W:831:ASN:O	2.10	0.51
2:X:806:ILE:CD1	2:X:825:THR:HG22	2.41	0.51
1:D:422:ARG:NE	2:E:871:ILE:HD12	2.14	0.51
1:G:48:GLY:O	1:G:51:SER:OG	2.17	0.51
2:K:866:TYR:O	2:K:882:THR:N	2.44	0.51
2:W:859:LYS:HE2	2:W:861:GLU:OE2	2.11	0.51
1:D:297:LEU:HA	1:D:300:MET:SD	2.51	0.51
1:N:100:GLN:HA	1:N:103:LEU:HG	1.92	0.51
1:U:346:LEU:HA	1:U:349:ARG:CG	2.34	0.51
1:B:125:SER:O	1:B:129:ARG:HG3	2.11	0.50
1:I:441:ARG:HB3	1:J:441:ARG:HD2	1.93	0.50
1:M:201:ARG:O	1:M:204:GLN:HG3	2.10	0.50
1:N:145:ARG:HG2	1:N:145:ARG:HH11	1.76	0.50
1:P:357:ARG:O	1:P:361:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:863:THR:OG1	2:W:885:THR:OG1	2.27	0.50
2:X:793:LEU:N	2:X:853:LEU:O	2.28	0.50
1:A:62:ILE:HB	1:G:56:MET:SD	2.51	0.50
1:A:115:LEU:HA	1:B:115:LEU:HD13	1.93	0.50
1:D:282:ALA:HB1	1:D:286:ARG:HH21	1.76	0.50
1:D:345:GLY:HA2	1:D:348:GLN:NE2	2.27	0.50
2:E:805:ASN:O	2:E:807:MET:HE2	2.12	0.50
2:L:832:TYR:CE1	2:L:842:ILE:HG12	2.44	0.50
1:B:145:ARG:HG2	1:B:145:ARG:HH11	1.76	0.50
2:E:836:VAL:HG13	2:E:839:ARG:HB3	1.92	0.50
1:M:80:ARG:CZ	1:N:80:ARG:HG2	2.41	0.50
1:M:173:HIS:HB3	1:O:331:ARG:CZ	2.42	0.50
1:N:68:GLU:O	1:N:72:PRO:HD3	2.11	0.50
1:A:164:LEU:HD12	1:B:164:LEU:HB2	1.93	0.50
1:B:68:GLU:O	1:B:72:PRO:HD3	2.11	0.50
1:C:425:SER:HA	2:E:831:ASN:HD22	1.76	0.50
1:N:232:ARG:O	1:N:235:THR:OG1	2.22	0.50
1:O:353:VAL:O	1:O:353:VAL:HG12	2.12	0.50
1:S:181:LEU:HA	1:S:184:GLN:HG3	1.93	0.50
1:T:35:THR:HA	1:T:38:ILE:HD12	1.94	0.50
1:V:419:THR:HG21	2:W:805:ASN:HD22	1.64	0.50
2:W:803:GLY:C	2:W:872:TYR:CD1	2.81	0.50
1:D:244:GLU:O	1:D:248:VAL:HG23	2.11	0.50
1:M:93:ASN:O	1:M:96:GLN:HG3	2.12	0.50
1:P:282:ALA:HB1	1:P:286:ARG:HH21	1.76	0.50
1:U:334:ASP:O	1:U:337:ARG:HG3	2.11	0.50
1:V:393:ASP:HA	1:V:396:GLN:HG3	1.93	0.50
1:A:70:ARG:NH1	1:G:50:ASP:OD1	2.45	0.50
1:C:276:ASN:O	1:C:280:ILE:HG12	2.12	0.50
1:M:70:ARG:NH1	1:S:50:ASP:OD1	2.45	0.50
1:N:75:GLN:CD	1:N:76:GLU:HG3	2.35	0.50
2:R:12:VAL:HG11	2:R:790:SER:HB2	1.93	0.50
1:A:173:HIS:HB3	1:C:331:ARG:CZ	2.41	0.50
1:B:238:GLU:HA	1:B:241:LEU:HG	1.93	0.50
1:D:357:ARG:O	1:D:361:ILE:HG12	2.11	0.50
1:G:122:LEU:HB2	1:H:122:LEU:HD21	1.93	0.50
1:H:31:GLN:CG	1:H:32:ILE:H	2.25	0.50
1:I:441:ARG:HB3	1:J:441:ARG:CD	2.42	0.50
1:O:403:ARG:HH12	1:P:402:VAL:HG11	1.77	0.50
1:P:297:LEU:HA	1:P:300:MET:SD	2.51	0.50
2:Q:805:ASN:O	2:Q:807:MET:HE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:441:ARG:HB3	1:V:441:ARG:HD2	1.93	0.50
1:A:256:ALA:O	1:A:259:GLN:NE2	2.45	0.50
2:E:812:GLN:O	2:E:865:VAL:HG12	2.12	0.50
1:G:168:THR:O	1:G:169:ALA:C	2.55	0.50
1:H:35:THR:HA	1:H:38:ILE:HD12	1.94	0.50
1:H:97:ALA:O	1:H:101:ILE:HG13	2.12	0.50
1:O:276:ASN:O	1:O:280:ILE:HG12	2.12	0.50
2:X:845:ASP:OD2	2:X:848:LYS:NZ	2.36	0.50
1:D:263:GLY:C	1:D:267:ARG:HH12	2.20	0.50
2:F:834:ASP:HA	2:F:837:LYS:NZ	2.27	0.50
1:H:84:HIS:O	1:H:88:ILE:HG13	2.12	0.50
1:J:393:ASP:HA	1:J:396:GLN:HG3	1.93	0.50
2:K:859:LYS:HE2	2:K:861:GLU:OE2	2.11	0.50
1:P:241:LEU:HD13	1:P:245:ARG:NH2	2.27	0.50
1:P:263:GLY:C	1:P:267:ARG:HH12	2.20	0.50
2:R:825:THR:HG22	2:R:829:SER:OG	2.11	0.50
1:T:97:ALA:O	1:T:101:ILE:HG13	2.12	0.50
2:X:791:LEU:CB	2:X:855:MET:HB2	2.40	0.50
1:I:360:ALA:HA	1:I:363:ARG:HG2	1.93	0.49
1:I:373:ALA:O	1:I:376:LYS:HG2	2.11	0.49
1:U:373:ALA:O	1:U:376:LYS:HG2	2.11	0.49
1:C:213:ALA:O	1:C:216:LEU:HB2	2.12	0.49
1:C:353:VAL:O	1:C:353:VAL:HG12	2.12	0.49
1:M:268:GLY:O	1:M:271:SER:OG	2.25	0.49
1:O:213:ALA:O	1:O:216:LEU:HB2	2.12	0.49
1:C:416:LEU:HD21	2:F:827:TRP:CH2	2.47	0.49
1:D:401:GLN:HA	1:D:401:GLN:OE1	2.13	0.49
2:E:793:LEU:HB2	2:E:809:TRP:CZ3	2.43	0.49
1:G:74:SER:O	1:G:78:GLU:HG2	2.13	0.49
2:Q:812:GLN:O	2:Q:865:VAL:HG12	2.12	0.49
2:W:832:TYR:OH	2:W:842:ILE:HG22	2.13	0.49
2:Q:824:VAL:HG23	2:Q:842:ILE:HG12	1.95	0.49
2:K:809:TRP:CE3	2:K:868:CYS:HB3	2.47	0.49
2:K:863:THR:OG1	2:K:884:VAL:O	2.30	0.49
2:L:805:ASN:CG	2:L:806:ILE:H	2.21	0.49
1:M:35:THR:HA	1:M:38:ILE:HG22	1.94	0.49
1:M:232:ARG:HG3	1:P:274:GLU:OE1	2.12	0.49
1:P:297:LEU:O	1:P:301:ASN:ND2	2.45	0.49
1:S:74:SER:O	1:S:78:GLU:HG2	2.13	0.49
1:U:441:ARG:HB3	1:V:441:ARG:CD	2.42	0.49
2:X:805:ASN:CG	2:X:806:ILE:H	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:THR:HA	1:A:38:ILE:HG22	1.94	0.49
1:A:232:ARG:HG3	1:D:274:GLU:OE1	2.12	0.49
1:A:268:GLY:O	1:A:271:SER:OG	2.25	0.49
1:I:373:ALA:HA	1:I:376:LYS:HD3	1.93	0.49
1:I:375:GLU:HB3	1:I:379:LYS:NZ	2.25	0.49
1:M:164:LEU:HD12	1:N:164:LEU:HB2	1.93	0.49
1:M:192:ARG:HE	1:N:191:ARG:HH22	1.61	0.49
1:N:59:LEU:HB3	1:T:60:LYS:HE2	1.94	0.49
1:O:425:SER:HA	2:Q:831:ASN:HD22	1.76	0.49
2:R:884:VAL:HG12	2:R:885:THR:N	2.27	0.49
1:S:51:SER:O	1:S:55:VAL:HG23	2.13	0.49
2:W:855:MET:HB3	2:W:858:LEU:HD11	1.93	0.49
1:A:220:VAL:HG11	1:B:216:LEU:HD11	1.95	0.49
1:C:423:LEU:HD23	1:D:423:LEU:HD23	1.94	0.49
1:D:241:LEU:HD13	1:D:245:ARG:NH2	2.27	0.49
1:J:417:GLN:HB2	2:L:827:TRP:HE1	1.77	0.49
2:L:833:VAL:HG12	2:L:836:VAL:HG22	1.94	0.49
2:R:834:ASP:HA	2:R:837:LYS:NZ	2.27	0.49
1:S:182:ARG:HG3	1:T:181:LEU:HD11	1.95	0.49
1:T:84:HIS:O	1:T:88:ILE:HG13	2.12	0.49
1:U:375:GLU:OE2	1:U:379:LYS:NZ	2.46	0.49
2:W:804:ILE:CB	2:W:872:TYR:CD1	2.78	0.49
2:W:809:TRP:CE3	2:W:868:CYS:HB3	2.47	0.49
1:B:59:LEU:HB3	1:H:60:LYS:HE2	1.94	0.49
2:K:855:MET:HB3	2:K:858:LEU:HD11	1.93	0.49
1:N:269:LEU:O	1:N:273:VAL:HG23	2.13	0.49
1:P:345:GLY:HA2	1:P:348:GLN:NE2	2.27	0.49
1:S:165:ARG:O	1:S:168:THR:OG1	2.29	0.49
1:S:168:THR:O	1:S:169:ALA:C	2.55	0.49
2:W:863:THR:OG1	2:W:884:VAL:O	2.30	0.49
1:A:93:ASN:O	1:A:96:GLN:HG3	2.12	0.49
1:I:351:ALA:O	1:I:355:THR:HG23	2.13	0.49
2:R:792:ARG:HA	2:R:854:GLN:HE22	1.75	0.49
1:S:122:LEU:HB2	1:T:122:LEU:HD21	1.93	0.49
1:V:417:GLN:HB2	2:X:827:TRP:HE1	1.77	0.49
2:W:791:LEU:HD23	2:W:792:ARG:H	1.78	0.49
2:E:811:ARG:NE	2:E:866:TYR:OH	2.46	0.49
2:F:12:VAL:HG11	2:F:790:SER:HB2	1.93	0.49
1:G:51:SER:O	1:G:55:VAL:HG23	2.13	0.49
1:G:181:LEU:HA	1:G:184:GLN:HG3	1.93	0.49
2:K:832:TYR:OH	2:K:842:ILE:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:284:GLN:O	1:O:288:GLU:HG2	2.13	0.49
1:O:423:LEU:HD23	1:P:423:LEU:HD23	1.94	0.49
2:R:843:SER:N	2:R:852:TYR:O	2.32	0.49
1:S:48:GLY:O	1:S:51:SER:OG	2.17	0.49
1:S:77:PHE:O	1:S:80:ARG:HB2	2.13	0.49
1:I:332:ALA:O	1:I:336:ILE:HG13	2.14	0.48
1:J:363:ARG:HE	1:J:367:LEU:HD11	1.78	0.48
1:M:96:GLN:HA	1:M:99:ARG:NE	2.28	0.48
1:T:83:GLU:O	1:T:86:GLU:HG3	2.12	0.48
1:U:391:ARG:NH2	1:V:392:LEU:HD21	2.28	0.48
1:A:73:VAL:CG1	1:A:77:PHE:HE2	2.19	0.48
1:A:96:GLN:O	1:A:99:ARG:NH1	2.46	0.48
1:B:269:LEU:O	1:B:273:VAL:HG23	2.13	0.48
1:C:403:ARG:HH12	1:D:402:VAL:HG11	1.77	0.48
1:C:422:ARG:HD2	2:F:874:GLY:O	2.13	0.48
2:E:832:TYR:OH	2:E:842:ILE:N	2.34	0.48
2:F:882:THR:HG22	2:F:883:GLN:N	2.28	0.48
1:G:182:ARG:HG3	1:H:181:LEU:HD11	1.95	0.48
1:I:391:ARG:NH2	1:J:392:LEU:HD21	2.29	0.48
1:M:154:ASP:HA	1:M:157:VAL:HG12	1.94	0.48
1:M:169:ALA:O	1:M:173:HIS:ND1	2.32	0.48
1:M:220:VAL:HG11	1:N:216:LEU:HD11	1.95	0.48
1:N:53:GLY:HA2	1:N:56:MET:HE2	1.96	0.48
1:N:76:GLU:HB3	1:S:42:TYR:OH	2.13	0.48
1:O:416:LEU:HD21	2:R:827:TRP:CH2	2.47	0.48
1:O:422:ARG:HD2	2:R:874:GLY:O	2.13	0.48
1:P:401:GLN:HA	1:P:401:GLN:OE1	2.13	0.48
2:Q:825:THR:OG1	2:Q:827:TRP:NE1	2.47	0.48
1:G:77:PHE:CD1	1:G:80:ARG:HD2	2.49	0.48
2:R:824:VAL:HB	2:R:842:ILE:HD12	1.95	0.48
1:S:80:ARG:HD3	1:T:81:ARG:NE	2.29	0.48
1:U:351:ALA:O	1:U:355:THR:HG23	2.13	0.48
2:W:820:MET:O	2:W:833:VAL:HG21	2.13	0.48
1:C:363:ARG:NH1	1:D:364:ALA:HB1	2.29	0.48
1:D:405:ASP:O	1:D:408:THR:OG1	2.24	0.48
2:E:825:THR:OG1	2:E:827:TRP:NE1	2.46	0.48
1:G:80:ARG:HD3	1:H:81:ARG:NE	2.28	0.48
1:I:375:GLU:OE2	1:I:379:LYS:NZ	2.46	0.48
1:P:268:GLY:O	1:P:271:SER:OG	2.20	0.48
1:S:97:ALA:O	1:S:100:GLN:HG3	2.14	0.48
1:S:181:LEU:CB	1:T:181:LEU:HD13	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ARG:NE	1:B:191:ARG:HH12	2.12	0.48
1:B:245:ARG:HB2	1:B:245:ARG:NH1	2.29	0.48
1:C:308:LEU:HA	1:C:308:LEU:HD23	1.54	0.48
1:C:423:LEU:HD23	1:D:423:LEU:HB3	1.96	0.48
2:F:824:VAL:HB	2:F:842:ILE:HD12	1.95	0.48
2:K:791:LEU:HD23	2:K:792:ARG:H	1.78	0.48
2:L:797:SER:OG	2:L:849:ASP:OD1	2.25	0.48
1:O:235:THR:O	1:O:238:GLU:HG3	2.14	0.48
1:O:363:ARG:NH1	1:P:364:ALA:HB1	2.29	0.48
2:Q:811:ARG:NE	2:Q:866:TYR:OH	2.46	0.48
1:B:76:GLU:HB3	1:G:42:TYR:OH	2.13	0.48
1:D:422:ARG:NH1	1:D:426:GLU:HB2	2.20	0.48
1:G:72:PRO:O	1:G:75:GLN:HG3	2.14	0.48
1:G:97:ALA:O	1:G:100:GLN:HG3	2.14	0.48
2:K:820:MET:O	2:K:833:VAL:HG21	2.13	0.48
1:S:72:PRO:O	1:S:75:GLN:HG3	2.14	0.48
2:X:832:TYR:OH	2:X:841:ILE:HD12	2.13	0.48
1:C:284:GLN:O	1:C:288:GLU:HG2	2.13	0.48
1:I:335:ARG:HH22	1:J:336:ILE:HD13	1.79	0.48
1:P:422:ARG:NE	2:Q:871:ILE:HD12	2.14	0.48
1:S:51:SER:O	1:S:54:ARG:HG2	2.13	0.48
1:B:87:LEU:HD12	1:B:91:ARG:NH1	2.29	0.48
1:G:86:GLU:HG2	2:L:873:ARG:HD2	1.96	0.48
2:L:832:TYR:OH	2:L:841:ILE:HD12	2.13	0.48
1:O:423:LEU:HD23	1:P:423:LEU:HB3	1.96	0.48
2:X:801:ILE:HB	2:X:849:ASP:HA	1.95	0.48
2:X:818:ARG:HH21	2:X:818:ARG:HG3	1.79	0.48
2:X:833:VAL:HG12	2:X:836:VAL:HG22	1.94	0.48
1:A:154:ASP:HA	1:A:157:VAL:HG12	1.94	0.48
1:D:271:SER:HA	1:D:274:GLU:OE1	2.14	0.48
1:G:51:SER:O	1:G:54:ARG:HG2	2.13	0.48
1:G:77:PHE:O	1:G:80:ARG:HB2	2.13	0.48
1:G:181:LEU:CB	1:H:181:LEU:HD13	2.44	0.48
1:H:83:GLU:O	1:H:86:GLU:HG3	2.12	0.48
1:P:271:SER:HA	1:P:274:GLU:OE1	2.14	0.48
1:S:77:PHE:CD1	1:S:80:ARG:HD2	2.49	0.48
1:S:125:SER:O	1:T:129:ARG:NH2	2.47	0.48
1:T:73:VAL:HG13	1:T:77:PHE:CD2	2.49	0.48
1:U:332:ALA:O	1:U:336:ILE:HG13	2.13	0.48
1:U:335:ARG:HH22	1:V:336:ILE:HD13	1.79	0.48
2:X:6:GLU:HG3	2:X:795:CYS:SG	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:832:TYR:CE1	2:X:842:ILE:HG12	2.44	0.48
1:A:270:GLU:O	1:A:273:VAL:HB	2.14	0.48
1:B:53:GLY:HA2	1:B:56:MET:HE2	1.95	0.48
1:C:403:ARG:HA	1:C:403:ARG:CZ	2.44	0.48
2:E:824:VAL:HG23	2:E:842:ILE:HG12	1.95	0.48
1:H:70:ARG:HH12	1:H:74:SER:HB3	1.79	0.48
1:H:88:ILE:HG12	1:H:91:ARG:NH2	2.29	0.48
2:L:806:ILE:HD13	2:L:825:THR:HG22	1.96	0.48
1:M:41:ARG:O	1:M:44:THR:OG1	2.25	0.48
2:Q:792:ARG:CZ	2:Q:854:GLN:HE22	2.27	0.48
2:R:882:THR:HG22	2:R:883:GLN:N	2.28	0.48
1:S:86:GLU:HG2	2:X:873:ARG:HD2	1.96	0.48
1:S:169:ALA:HA	1:S:172:GLU:OE2	2.14	0.48
2:X:827:TRP:CE3	2:X:827:TRP:N	2.82	0.48
1:C:259:GLN:HE22	1:D:258:HIS:CG	2.32	0.47
1:G:125:SER:O	1:H:129:ARG:NH2	2.47	0.47
1:I:419:THR:HG21	2:L:805:ASN:HB3	1.95	0.47
1:N:219:ARG:HH12	1:P:284:GLN:CD	2.22	0.47
1:O:281:SER:O	1:O:285:THR:HG23	2.14	0.47
1:U:419:THR:HG21	2:X:805:ASN:HB3	1.95	0.47
2:W:843:SER:O	2:W:852:TYR:N	2.32	0.47
1:A:70:ARG:O	1:A:73:VAL:HB	2.14	0.47
1:C:270:GLU:O	1:C:274:GLU:OE1	2.32	0.47
2:F:884:VAL:HG12	2:F:885:THR:N	2.27	0.47
2:L:6:GLU:HG3	2:L:795:CYS:SG	2.54	0.47
2:L:801:ILE:HB	2:L:849:ASP:HA	1.95	0.47
1:O:403:ARG:CZ	1:O:403:ARG:HA	2.44	0.47
2:Q:805:ASN:H	2:Q:807:MET:CE	2.27	0.47
2:W:814:PRO:O	2:W:816:LYS:N	2.43	0.47
2:X:872:TYR:OH	2:X:873:ARG:NH1	2.47	0.47
1:G:40:GLN:HG2	1:G:41:ARG:HD3	1.96	0.47
1:I:357:ARG:NE	1:J:357:ARG:HD2	2.29	0.47
1:M:192:ARG:NE	1:N:191:ARG:HH12	2.12	0.47
1:T:70:ARG:HH12	1:T:74:SER:HB3	1.79	0.47
1:C:230:LEU:HB3	1:D:230:LEU:HD23	1.95	0.47
1:J:417:GLN:HB2	2:L:827:TRP:CZ2	2.49	0.47
1:M:96:GLN:O	1:M:99:ARG:NH1	2.46	0.47
1:O:230:LEU:HB3	1:P:230:LEU:HD23	1.95	0.47
1:A:69:ILE:C	1:A:73:VAL:HG21	2.39	0.47
1:A:96:GLN:HA	1:A:99:ARG:NE	2.28	0.47
1:A:115:LEU:HD12	1:B:115:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:ALA:HB1	1:D:286:ARG:NH2	2.29	0.47
1:I:357:ARG:NH1	1:J:353:VAL:HG12	2.29	0.47
2:L:818:ARG:HH21	2:L:818:ARG:HG3	1.79	0.47
1:M:270:GLU:O	1:M:273:VAL:HB	2.14	0.47
1:O:259:GLN:HE22	1:P:258:HIS:CG	2.32	0.47
2:Q:839:ARG:HH12	2:Q:859:LYS:H	1.59	0.47
2:X:840:PHE:HE1	2:X:855:MET:HA	1.80	0.47
1:A:94:LEU:HD21	1:B:94:LEU:HB2	1.96	0.47
1:H:73:VAL:HG13	1:H:77:PHE:CD2	2.49	0.47
1:M:256:ALA:O	1:M:259:GLN:NE2	2.45	0.47
1:O:308:LEU:HD23	1:O:308:LEU:HA	1.54	0.47
1:P:296:LYS:CD	1:P:300:MET:HE1	2.45	0.47
2:Q:832:TYR:OH	2:Q:842:ILE:N	2.34	0.47
1:U:434:LEU:HD22	1:V:434:LEU:HB3	1.97	0.47
1:A:192:ARG:HE	1:B:191:ARG:HH22	1.61	0.47
1:B:69:ILE:HG13	1:G:49:LEU:HG	1.96	0.47
1:B:219:ARG:HH12	1:D:284:GLN:CD	2.22	0.47
1:C:235:THR:O	1:C:238:GLU:HG3	2.14	0.47
1:C:336:ILE:HD13	1:D:339:LEU:HD12	1.97	0.47
2:E:869:ASN:ND2	2:E:876:GLU:OE2	2.44	0.47
2:L:6:GLU:OE2	2:L:881:GLY:N	2.39	0.47
2:L:825:THR:HB	2:L:827:TRP:HE3	1.80	0.47
1:M:156:LYS:HZ3	1:N:157:VAL:HG11	1.78	0.47
1:V:363:ARG:HE	1:V:367:LEU:HD11	1.78	0.47
1:C:230:LEU:HA	1:C:233:ILE:HG22	1.97	0.47
1:C:425:SER:HA	2:E:831:ASN:ND2	2.30	0.47
1:D:232:ARG:O	1:D:235:THR:OG1	2.27	0.47
2:F:864:ALA:O	2:F:883:GLN:HA	2.15	0.47
1:G:169:ALA:HA	1:G:172:GLU:OE2	2.14	0.47
2:K:812:GLN:OE1	2:K:818:ARG:HB2	2.14	0.47
1:M:69:ILE:C	1:M:73:VAL:HG21	2.39	0.47
1:M:109:ARG:NE	1:M:109:ARG:HA	2.30	0.47
1:N:87:LEU:HD12	1:N:91:ARG:NH1	2.29	0.47
1:N:266:ILE:O	1:N:269:LEU:HG	2.15	0.47
1:P:232:ARG:O	1:P:235:THR:OG1	2.27	0.47
1:U:357:ARG:NH1	1:V:353:VAL:HG12	2.29	0.47
1:V:417:GLN:HB2	2:X:827:TRP:CZ2	2.49	0.47
2:W:793:LEU:HD23	2:W:853:LEU:HD23	1.97	0.47
1:C:268:GLY:O	1:C:271:SER:OG	2.26	0.47
1:D:297:LEU:O	1:D:301:ASN:ND2	2.45	0.47
1:I:336:ILE:O	1:I:340:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:793:LEU:HD23	2:K:853:LEU:HD23	1.97	0.47
1:O:425:SER:HA	2:Q:831:ASN:ND2	2.30	0.47
2:R:812:GLN:CG	2:R:818:ARG:HA	2.45	0.47
1:T:109:ARG:NH2	1:U:396:GLN:OE1	2.48	0.47
1:A:35:THR:HG23	1:G:88:ILE:HD11	1.96	0.47
1:B:266:ILE:O	1:B:269:LEU:HG	2.15	0.47
1:D:296:LYS:CD	1:D:300:MET:HE1	2.45	0.47
1:D:329:LEU:HD12	1:D:329:LEU:HA	1.76	0.47
2:E:2:VAL:HG11	2:E:872:TYR:CD2	2.50	0.47
2:E:792:ARG:CZ	2:E:854:GLN:HE22	2.27	0.47
2:E:825:THR:HG21	2:E:827:TRP:CE2	2.50	0.47
1:G:110:GLU:OE1	1:G:114:ARG:HG3	2.15	0.47
2:K:804:ILE:HG12	2:K:872:TYR:CE2	2.50	0.47
1:M:35:THR:HG23	1:S:88:ILE:HD11	1.96	0.47
1:M:94:LEU:HD21	1:N:94:LEU:HB2	1.96	0.47
1:M:241:LEU:O	1:M:245:ARG:HG2	2.15	0.47
1:N:245:ARG:NH1	1:N:245:ARG:HB2	2.29	0.47
1:O:270:GLU:O	1:O:274:GLU:OE1	2.32	0.47
1:O:435:GLU:OE2	1:O:438:ARG:NH2	2.48	0.47
1:V:346:LEU:HB3	1:V:347:ARG:HH22	1.80	0.47
1:B:70:ARG:NH1	1:H:49:LEU:HB3	2.30	0.46
1:C:281:SER:O	1:C:285:THR:HG23	2.14	0.46
1:C:308:LEU:HD21	1:D:308:LEU:CB	2.45	0.46
2:F:833:VAL:HG12	2:F:836:VAL:HG22	1.97	0.46
1:H:81:ARG:NE	1:H:81:ARG:HA	2.30	0.46
1:N:70:ARG:NH1	1:T:49:LEU:HB3	2.30	0.46
1:N:261:ASP:HA	1:N:264:ARG:HG2	1.97	0.46
1:P:282:ALA:HB1	1:P:286:ARG:NH2	2.29	0.46
1:P:405:ASP:O	1:P:408:THR:OG1	2.24	0.46
1:S:115:LEU:HA	1:T:115:LEU:HD13	1.98	0.46
1:T:81:ARG:NE	1:T:81:ARG:HA	2.30	0.46
1:T:88:ILE:HG12	1:T:91:ARG:NH2	2.29	0.46
1:A:241:LEU:O	1:A:245:ARG:HG2	2.15	0.46
1:C:339:LEU:HA	1:C:342:GLU:HG3	1.97	0.46
2:E:800:SER:O	2:E:803:GLY:N	2.49	0.46
1:G:115:LEU:HA	1:H:115:LEU:HD13	1.98	0.46
1:O:384:ARG:HG2	1:O:384:ARG:HH11	1.80	0.46
1:S:168:THR:O	1:S:172:GLU:OE1	2.34	0.46
1:T:31:GLN:CG	1:T:32:ILE:H	2.25	0.46
2:X:806:ILE:HD13	2:X:825:THR:HG22	1.96	0.46
1:B:188:ILE:O	1:B:192:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:ARG:NH2	1:I:396:GLN:OE1	2.48	0.46
1:J:401:GLN:O	1:J:404:ARG:HG2	2.15	0.46
1:O:230:LEU:HA	1:O:233:ILE:HG22	1.97	0.46
2:W:812:GLN:OE1	2:W:818:ARG:HB2	2.14	0.46
1:C:435:GLU:OE2	1:C:438:ARG:NH2	2.48	0.46
1:M:70:ARG:O	1:M:73:VAL:HB	2.14	0.46
1:O:283:LEU:HD13	1:O:286:ARG:NH1	2.26	0.46
2:Q:2:VAL:HG11	2:Q:872:TYR:CD2	2.50	0.46
2:Q:810:TYR:CZ	2:Q:820:MET:HB3	2.51	0.46
2:Q:825:THR:HG21	2:Q:827:TRP:CE2	2.50	0.46
2:W:824:VAL:HG22	2:W:830:THR:HG22	1.97	0.46
1:B:261:ASP:HA	1:B:264:ARG:HG2	1.97	0.46
1:C:337:ARG:O	1:C:341:GLU:HG3	2.15	0.46
1:C:384:ARG:HG2	1:C:384:ARG:HH11	1.80	0.46
1:I:422:ARG:O	1:I:425:SER:N	2.48	0.46
2:L:805:ASN:OD1	2:L:806:ILE:N	2.49	0.46
2:L:872:TYR:OH	2:L:873:ARG:NH1	2.47	0.46
1:N:76:GLU:O	1:N:80:ARG:HG3	2.16	0.46
2:Q:836:VAL:O	2:Q:836:VAL:HG12	2.16	0.46
2:R:864:ALA:O	2:R:883:GLN:HA	2.15	0.46
1:U:336:ILE:O	1:U:340:GLU:HG2	2.15	0.46
1:A:191:ARG:HG2	1:B:192:ARG:HH21	1.81	0.46
2:F:812:GLN:CG	2:F:818:ARG:HA	2.45	0.46
1:O:308:LEU:HD21	1:P:308:LEU:CB	2.45	0.46
1:A:66:ILE:HD13	1:G:52:ILE:HG23	1.97	0.46
1:A:128:ARG:NH2	1:B:129:ARG:HB3	2.31	0.46
1:D:417:GLN:HA	1:D:420:ILE:HG22	1.98	0.46
1:D:438:ARG:NH2	1:D:439:ARG:HA	2.31	0.46
1:M:191:ARG:HG2	1:N:192:ARG:HH21	1.81	0.46
1:N:69:ILE:HG13	1:S:49:LEU:HG	1.96	0.46
1:O:422:ARG:NH2	2:R:876:GLU:OE2	2.48	0.46
1:O:428:ALA:HA	2:Q:820:MET:SD	2.56	0.46
1:P:438:ARG:NH2	1:P:439:ARG:HA	2.31	0.46
2:Q:866:TYR:O	2:Q:882:THR:N	2.34	0.46
2:Q:869:ASN:ND2	2:Q:876:GLU:OE2	2.44	0.46
2:R:11:LEU:HB3	2:R:885:THR:HB	1.98	0.46
1:U:357:ARG:NE	1:V:357:ARG:HD2	2.30	0.46
1:B:76:GLU:O	1:B:80:ARG:HG3	2.16	0.46
1:B:208:LEU:HD22	1:D:296:LYS:NZ	2.30	0.46
2:F:884:VAL:CG1	2:F:885:THR:H	2.29	0.46
2:K:804:ILE:HG23	2:K:804:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:115:LEU:HD12	1:N:115:LEU:HB2	1.97	0.46
1:N:208:LEU:HD22	1:P:296:LYS:NZ	2.30	0.46
1:S:40:GLN:HG2	1:S:41:ARG:HD3	1.97	0.46
1:U:422:ARG:O	1:U:425:SER:N	2.48	0.46
1:C:422:ARG:NH2	2:F:876:GLU:OE2	2.48	0.46
2:E:805:ASN:H	2:E:807:MET:CE	2.27	0.46
2:F:802:ASP:C	2:F:804:ILE:N	2.74	0.46
1:I:434:LEU:HD22	1:J:434:LEU:HB3	1.97	0.46
1:J:346:LEU:HB3	1:J:347:ARG:HH22	1.80	0.46
1:M:69:ILE:HG13	1:M:69:ILE:O	2.16	0.46
1:N:65:LEU:HD12	1:S:52:ILE:HD13	1.98	0.46
1:N:188:ILE:O	1:N:192:ARG:HG2	2.15	0.46
1:O:339:LEU:HA	1:O:342:GLU:HG3	1.97	0.46
2:Q:789:ASP:OD1	2:Q:790:SER:N	2.47	0.46
2:Q:812:GLN:HB3	2:Q:865:VAL:CG1	2.46	0.46
1:T:117:ALA:O	1:T:120:THR:OG1	2.31	0.46
2:W:790:SER:HA	2:W:855:MET:O	2.16	0.46
2:W:804:ILE:HG12	2:W:872:TYR:CE2	2.51	0.46
2:X:805:ASN:OD1	2:X:806:ILE:N	2.49	0.46
1:A:109:ARG:NE	1:A:109:ARG:HA	2.30	0.46
2:K:13:TYR:O	2:K:887:SER:OG	2.27	0.46
2:K:790:SER:HA	2:K:855:MET:O	2.16	0.46
2:L:812:GLN:NE2	2:L:818:ARG:HA	2.31	0.46
1:O:336:ILE:HD13	1:P:339:LEU:HD12	1.97	0.46
1:O:337:ARG:O	1:O:341:GLU:HG3	2.15	0.46
2:Q:805:ASN:C	2:Q:807:MET:HE2	2.41	0.46
2:R:833:VAL:HG12	2:R:836:VAL:HG22	1.97	0.46
1:S:110:GLU:OE1	1:S:114:ARG:HG3	2.15	0.46
1:V:352:GLY:O	1:V:355:THR:OG1	2.30	0.46
1:V:416:LEU:O	1:V:419:THR:OG1	2.28	0.46
1:C:315:GLN:OE1	1:C:316:LYS:HD2	2.15	0.45
1:C:428:ALA:HA	2:E:820:MET:SD	2.56	0.45
1:G:142:GLU:HG3	1:G:145:ARG:NH2	2.31	0.45
1:J:416:LEU:O	1:J:419:THR:OG1	2.28	0.45
1:M:66:ILE:HD13	1:S:52:ILE:HG23	1.97	0.45
1:M:114:ARG:HD2	1:N:115:LEU:HD21	1.98	0.45
1:O:315:GLN:OE1	1:O:316:LYS:HD2	2.15	0.45
2:Q:3:GLN:HB2	2:Q:798:SER:HB3	1.98	0.45
2:R:791:LEU:HD21	2:R:855:MET:HE2	1.98	0.45
1:S:129:ARG:NH2	1:S:130:GLN:OE1	2.26	0.45
1:S:191:ARG:HB3	1:S:192:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:401:GLN:O	1:V:404:ARG:HG2	2.15	0.45
1:A:114:ARG:HD2	1:B:115:LEU:HD21	1.98	0.45
1:A:177:ASP:O	1:A:181:LEU:HD23	2.17	0.45
1:G:168:THR:O	1:G:172:GLU:OE1	2.34	0.45
1:I:443:ARG:NH2	1:I:444:LEU:HD21	2.32	0.45
1:N:230:LEU:HA	1:N:233:ILE:HG22	1.98	0.45
1:U:443:ARG:NH2	1:U:444:LEU:HD21	2.32	0.45
2:W:804:ILE:CD1	2:W:871:ILE:O	2.65	0.45
1:A:69:ILE:O	1:A:69:ILE:HG13	2.16	0.45
2:E:812:GLN:HB3	2:E:865:VAL:CG1	2.46	0.45
2:E:840:PHE:HD1	2:E:856:ASN:H	1.64	0.45
2:K:824:VAL:HG22	2:K:830:THR:HG22	1.97	0.45
1:N:62:ILE:HG12	1:T:56:MET:SD	2.57	0.45
2:Q:809:TRP:O	2:Q:821:VAL:N	2.44	0.45
1:S:142:GLU:HG3	1:S:145:ARG:NH2	2.31	0.45
1:S:164:LEU:O	1:S:168:THR:HG23	2.16	0.45
1:A:38:ILE:HG12	1:A:42:TYR:CE2	2.52	0.45
2:E:802:ASP:HA	2:E:804:ILE:CG1	2.39	0.45
2:E:836:VAL:O	2:E:836:VAL:HG12	2.16	0.45
2:F:793:LEU:HD23	2:F:840:PHE:HE1	1.81	0.45
1:G:87:LEU:HD23	1:H:87:LEU:HB3	1.98	0.45
1:G:157:VAL:HG11	1:H:156:LYS:HE2	1.99	0.45
1:G:164:LEU:O	1:G:168:THR:HG23	2.16	0.45
1:M:77:PHE:HE1	1:T:42:TYR:OH	1.99	0.45
1:O:357:ARG:HH11	1:O:357:ARG:HG3	1.81	0.45
1:O:417:GLN:OE1	2:Q:827:TRP:CD1	2.70	0.45
2:Q:791:LEU:HG	2:Q:792:ARG:H	1.81	0.45
2:Q:800:SER:O	2:Q:803:GLY:N	2.49	0.45
2:R:884:VAL:CG1	2:R:885:THR:H	2.29	0.45
2:W:865:VAL:HG22	2:W:883:GLN:HB2	1.98	0.45
1:C:267:ARG:HH21	1:C:270:GLU:HG2	1.81	0.45
1:C:347:ARG:NH1	1:D:346:LEU:HD21	2.32	0.45
1:C:396:GLN:NE2	1:C:400:ASP:OD2	2.50	0.45
1:C:417:GLN:OE1	2:E:827:TRP:CD1	2.70	0.45
2:E:805:ASN:C	2:E:807:MET:HE2	2.41	0.45
2:F:11:LEU:HB3	2:F:885:THR:HB	1.98	0.45
1:M:128:ARG:NH2	1:N:129:ARG:HB3	2.31	0.45
2:E:795:CYS:HB2	2:E:809:TRP:HZ2	1.82	0.45
1:G:52:ILE:HD12	1:G:52:ILE:HA	1.73	0.45
1:J:352:GLY:O	1:J:355:THR:OG1	2.30	0.45
1:O:396:GLN:NE2	1:O:400:ASP:OD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:77:PHE:HA	1:S:80:ARG:HD2	1.99	0.45
2:W:804:ILE:O	2:W:804:ILE:HG23	2.15	0.45
2:W:807:MET:HE3	2:W:807:MET:HB3	1.78	0.45
2:E:808:ARG:O	2:E:809:TRP:HD1	2.00	0.45
1:G:191:ARG:HB3	1:G:192:ARG:NH2	2.31	0.45
1:H:54:ARG:CZ	1:H:55:VAL:HG22	2.46	0.45
1:T:54:ARG:CZ	1:T:55:VAL:HG22	2.46	0.45
1:A:41:ARG:O	1:A:44:THR:OG1	2.25	0.45
1:B:168:THR:HA	1:B:171:ILE:HG22	1.99	0.45
2:Q:808:ARG:O	2:Q:809:TRP:HD1	2.00	0.45
2:R:4:LEU:HD12	2:R:878:TRP:C	2.42	0.45
1:A:171:ILE:O	1:A:175:VAL:HG23	2.17	0.45
1:C:308:LEU:HD22	1:D:307:ARG:NH1	2.32	0.45
1:C:357:ARG:HH11	1:C:357:ARG:HG3	1.81	0.45
2:E:810:TYR:CZ	2:E:820:MET:HB3	2.51	0.45
2:K:6:GLU:HG3	2:K:795:CYS:HB3	1.99	0.45
2:L:793:LEU:N	2:L:853:LEU:O	2.28	0.45
2:L:840:PHE:HE1	2:L:855:MET:HA	1.80	0.45
1:M:177:ASP:O	1:M:181:LEU:HD23	2.16	0.45
2:R:840:PHE:CD1	2:R:853:LEU:HD21	2.52	0.45
1:S:99:ARG:NH1	1:S:99:ARG:HB3	2.32	0.45
1:V:383:GLU:O	1:V:386:GLN:HG3	2.17	0.45
1:A:108:GLU:HG2	1:A:109:ARG:NH2	2.32	0.45
1:B:73:VAL:HG13	1:B:77:PHE:HE2	1.82	0.45
2:E:809:TRP:O	2:E:821:VAL:N	2.44	0.45
1:G:77:PHE:HA	1:G:80:ARG:HD2	1.99	0.45
1:G:185:ALA:HA	1:G:188:ILE:HG22	1.99	0.45
1:M:42:TYR:HE1	1:T:77:PHE:CZ	2.35	0.45
1:M:176:GLN:O	1:M:179:GLU:HG3	2.17	0.45
1:O:347:ARG:NH1	1:P:346:LEU:HD21	2.32	0.45
1:S:181:LEU:HB2	1:T:181:LEU:HD13	1.99	0.45
2:X:801:ILE:HB	2:X:849:ASP:OD1	2.17	0.45
1:B:65:LEU:HD12	1:G:52:ILE:HD13	1.98	0.44
1:C:357:ARG:HG3	1:C:357:ARG:NH1	2.31	0.44
2:F:791:LEU:HD21	2:F:855:MET:HE2	1.98	0.44
1:H:117:ALA:O	1:H:120:THR:OG1	2.31	0.44
2:L:801:ILE:HB	2:L:849:ASP:OD1	2.17	0.44
1:M:45:ILE:HG13	1:T:77:PHE:HZ	1.82	0.44
1:N:62:ILE:HG13	1:S:52:ILE:CG1	2.47	0.44
2:Q:809:TRP:CZ3	2:Q:853:LEU:HB2	2.52	0.44
1:T:175:VAL:HA	1:T:178:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:801:ILE:HA	2:W:849:ASP:OD2	2.17	0.44
2:X:806:ILE:HD11	2:X:823:VAL:CG1	2.47	0.44
2:X:812:GLN:NE2	2:X:818:ARG:HA	2.31	0.44
1:A:176:GLN:O	1:A:179:GLU:HG3	2.17	0.44
2:E:791:LEU:HG	2:E:792:ARG:H	1.81	0.44
1:G:99:ARG:NH1	1:G:99:ARG:HB3	2.32	0.44
1:J:383:GLU:O	1:J:386:GLN:HG3	2.17	0.44
2:K:825:THR:HG23	2:K:828:GLY:H	1.82	0.44
1:O:267:ARG:HH21	1:O:270:GLU:HG2	1.81	0.44
1:P:424:THR:OG1	2:R:823:VAL:HG11	2.16	0.44
2:Q:840:PHE:HD1	2:Q:856:ASN:H	1.64	0.44
2:R:793:LEU:HD23	2:R:840:PHE:HE1	1.81	0.44
1:T:38:ILE:O	1:T:42:TYR:HD1	2.00	0.44
2:W:855:MET:HB3	2:W:858:LEU:HD21	1.99	0.44
1:A:77:PHE:HE1	1:H:42:TYR:OH	1.99	0.44
1:A:229:ARG:HH22	1:A:230:LEU:CD2	2.31	0.44
1:B:252:GLU:O	1:B:255:LEU:HB3	2.17	0.44
2:E:846:SER:HA	2:E:849:ASP:HA	2.00	0.44
2:F:4:LEU:HD12	2:F:878:TRP:C	2.42	0.44
2:F:841:ILE:O	2:F:853:LEU:HA	2.17	0.44
1:G:181:LEU:HB2	1:H:181:LEU:HD13	1.99	0.44
1:H:168:THR:HA	1:H:171:ILE:HG22	1.99	0.44
1:J:401:GLN:HA	1:J:404:ARG:NE	2.32	0.44
2:K:804:ILE:CD1	2:K:871:ILE:O	2.65	0.44
2:K:804:ILE:HD12	2:K:871:ILE:C	2.42	0.44
1:M:46:HIS:CE1	1:S:78:GLU:OE2	2.70	0.44
1:M:191:ARG:NH1	1:N:192:ARG:HE	2.16	0.44
1:M:229:ARG:HH22	1:M:230:LEU:CD2	2.31	0.44
1:N:266:ILE:HA	1:N:269:LEU:HG	2.00	0.44
1:P:219:ARG:O	1:P:222:GLN:HG2	2.17	0.44
1:P:417:GLN:O	1:P:420:ILE:HG22	2.17	0.44
1:P:422:ARG:NH1	1:P:426:GLU:HB2	2.20	0.44
1:S:185:ALA:HA	1:S:188:ILE:HG22	1.99	0.44
1:T:115:LEU:O	1:T:119:GLU:OE1	2.36	0.44
1:A:46:HIS:CE1	1:G:78:GLU:OE2	2.70	0.44
1:B:62:ILE:HG13	1:G:52:ILE:HD11	2.00	0.44
1:B:62:ILE:HG12	1:H:56:MET:SD	2.57	0.44
1:B:242:ALA:HA	1:B:245:ARG:NH2	2.32	0.44
1:C:224:GLY:O	1:C:227:LEU:HG	2.17	0.44
1:C:417:GLN:OE1	1:C:417:GLN:HA	2.18	0.44
2:E:3:GLN:HB2	2:E:798:SER:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:800:SER:O	2:K:803:GLY:N	2.50	0.44
2:L:827:TRP:CE3	2:L:827:TRP:N	2.82	0.44
1:M:171:ILE:O	1:M:175:VAL:HG23	2.17	0.44
1:O:423:LEU:HB3	1:P:423:LEU:HD23	2.00	0.44
1:T:168:THR:HA	1:T:171:ILE:HG22	1.99	0.44
1:A:121:ALA:HB3	1:B:122:LEU:HD11	1.98	0.44
1:B:41:ARG:NH1	1:H:81:ARG:HG3	2.28	0.44
1:B:62:ILE:HG13	1:G:52:ILE:CG1	2.47	0.44
1:B:230:LEU:HA	1:B:233:ILE:HG22	1.98	0.44
1:D:219:ARG:O	1:D:222:GLN:HG2	2.17	0.44
2:F:840:PHE:CD1	2:F:853:LEU:HD21	2.52	0.44
1:G:94:LEU:HA	1:H:94:LEU:HD13	1.99	0.44
1:H:38:ILE:O	1:H:42:TYR:HD1	2.00	0.44
2:L:806:ILE:HD11	2:L:823:VAL:CG1	2.47	0.44
1:M:161:ASP:O	1:M:165:ARG:HG3	2.18	0.44
1:P:263:GLY:C	1:P:267:ARG:NH1	2.76	0.44
2:W:6:GLU:HG3	2:W:795:CYS:HB3	1.99	0.44
2:X:797:SER:OG	2:X:849:ASP:OD1	2.25	0.44
2:X:839:ARG:O	2:X:856:ASN:HB2	2.18	0.44
1:A:191:ARG:NH1	1:B:192:ARG:HE	2.15	0.44
1:B:51:SER:HA	1:B:54:ARG:HH11	1.82	0.44
1:C:423:LEU:HB3	1:D:423:LEU:HD23	2.00	0.44
1:D:314:GLN:O	1:D:318:VAL:HG22	2.17	0.44
1:D:424:THR:OG1	2:F:823:VAL:HG11	2.16	0.44
2:F:810:TYR:CZ	2:F:820:MET:HB2	2.52	0.44
1:I:398:ALA:O	1:I:402:VAL:HG23	2.18	0.44
1:P:417:GLN:HA	1:P:420:ILE:HG22	1.98	0.44
2:R:810:TYR:CZ	2:R:820:MET:HB2	2.52	0.44
2:R:817:GLN:HG3	2:R:818:ARG:O	2.18	0.44
1:S:176:GLN:O	1:S:179:GLU:HG3	2.18	0.44
1:V:365:ASP:HB3	1:V:369:LYS:HZ1	1.83	0.44
1:V:366:GLN:HA	1:V:369:LYS:HE2	2.00	0.44
1:V:401:GLN:HA	1:V:404:ARG:NE	2.32	0.44
1:D:263:GLY:C	1:D:267:ARG:NH1	2.75	0.44
2:F:817:GLN:HG3	2:F:818:ARG:O	2.18	0.44
1:H:157:VAL:O	1:H:160:LEU:HG	2.18	0.44
2:K:865:VAL:HG22	2:K:883:GLN:HB2	1.98	0.44
1:M:40:GLN:O	1:M:44:THR:HG23	2.18	0.44
1:M:108:GLU:HG2	1:M:109:ARG:NH2	2.32	0.44
1:M:230:LEU:HA	1:M:233:ILE:HG22	2.00	0.44
1:N:41:ARG:NH2	1:T:78:GLU:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:62:ILE:HG13	1:S:52:ILE:HD11	2.00	0.44
1:N:73:VAL:HG13	1:N:77:PHE:HE2	1.82	0.44
1:O:224:GLY:O	1:O:227:LEU:HG	2.17	0.44
1:O:286:ARG:HA	1:O:289:THR:OG1	2.18	0.44
1:O:308:LEU:HD22	1:P:307:ARG:NH1	2.32	0.44
1:P:314:GLN:O	1:P:318:VAL:HG22	2.17	0.44
2:Q:841:ILE:HB	2:Q:854:GLN:HB3	2.00	0.44
1:S:80:ARG:HD3	1:T:81:ARG:CZ	2.48	0.44
1:S:87:LEU:HD23	1:T:87:LEU:HB3	1.98	0.44
1:V:434:LEU:HA	1:V:434:LEU:HD23	1.67	0.44
1:I:353:VAL:O	1:I:357:ARG:HG3	2.18	0.44
1:M:164:LEU:HB2	1:N:164:LEU:HD12	2.00	0.44
1:N:139:ASN:O	1:N:143:ILE:HG13	2.18	0.44
2:Q:804:ILE:HD13	2:Q:844:ARG:HH11	1.83	0.44
1:T:157:VAL:O	1:T:160:LEU:HG	2.17	0.44
1:A:42:TYR:HE1	1:H:77:PHE:CZ	2.35	0.44
1:A:114:ARG:HB2	1:A:114:ARG:HH11	1.83	0.44
1:A:147:ARG:HH22	1:D:358:ALA:HB3	1.83	0.44
1:I:434:LEU:HD23	1:I:434:LEU:HA	1.64	0.44
1:P:422:ARG:NH2	2:Q:808:ARG:HH12	2.16	0.44
2:Q:795:CYS:HB2	2:Q:809:TRP:HZ2	1.82	0.44
2:R:841:ILE:O	2:R:853:LEU:HA	2.17	0.44
1:A:45:ILE:HG13	1:H:77:PHE:HZ	1.82	0.43
1:A:161:ASP:O	1:A:165:ARG:HG3	2.18	0.43
1:A:198:ALA:HA	1:A:201:ARG:NE	2.33	0.43
1:G:80:ARG:HD3	1:H:81:ARG:CZ	2.48	0.43
1:G:80:ARG:NE	1:H:81:ARG:HD2	2.33	0.43
1:H:115:LEU:O	1:H:119:GLU:OE1	2.36	0.43
1:M:38:ILE:HG12	1:M:42:TYR:CE2	2.52	0.43
1:M:198:ALA:HA	1:M:201:ARG:NE	2.33	0.43
1:N:252:GLU:O	1:N:255:LEU:HB3	2.17	0.43
1:O:357:ARG:HG3	1:O:357:ARG:NH1	2.31	0.43
2:R:802:ASP:C	2:R:804:ILE:N	2.74	0.43
1:S:94:LEU:HA	1:T:94:LEU:HD13	1.99	0.43
1:B:139:ASN:O	1:B:143:ILE:HG13	2.18	0.43
1:C:312:SER:O	1:C:316:LYS:HG2	2.18	0.43
1:D:286:ARG:O	1:D:289:THR:OG1	2.33	0.43
2:E:804:ILE:HD13	2:E:844:ARG:HH11	1.83	0.43
2:F:843:SER:O	2:F:852:TYR:N	2.37	0.43
2:K:801:ILE:HA	2:K:849:ASP:OD2	2.18	0.43
2:L:839:ARG:O	2:L:856:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:121:ALA:HB3	1:N:122:LEU:HD11	1.99	0.43
1:M:147:ARG:HH22	1:P:358:ALA:HB3	1.83	0.43
1:M:151:LEU:HD23	1:P:355:THR:HG21	2.00	0.43
1:N:242:ALA:HA	1:N:245:ARG:NH2	2.32	0.43
2:Q:802:ASP:HA	2:Q:804:ILE:CG1	2.39	0.43
2:X:825:THR:HB	2:X:827:TRP:HE3	1.80	0.43
1:C:401:GLN:O	1:C:404:ARG:HG2	2.18	0.43
1:J:366:GLN:HA	1:J:369:LYS:HE2	2.00	0.43
1:N:168:THR:HA	1:N:171:ILE:HG22	1.99	0.43
1:O:401:GLN:O	1:O:404:ARG:HG2	2.18	0.43
1:O:421:GLU:HB3	2:Q:827:TRP:CZ2	2.53	0.43
1:S:80:ARG:NE	1:T:81:ARG:HD2	2.33	0.43
1:S:100:GLN:HE21	1:T:101:ILE:HG12	1.83	0.43
1:S:145:ARG:HG3	1:S:146:LEU:N	2.33	0.43
1:C:423:LEU:HD22	2:F:806:ILE:HD11	2.01	0.43
2:E:809:TRP:CZ3	2:E:853:LEU:HB2	2.52	0.43
1:G:188:ILE:HD12	1:G:192:ARG:HH11	1.83	0.43
1:M:59:LEU:HD21	1:S:59:LEU:CD1	2.43	0.43
1:N:51:SER:HA	1:N:54:ARG:HH11	1.82	0.43
1:N:58:HIS:O	1:N:62:ILE:HD12	2.18	0.43
1:N:62:ILE:HG13	1:S:52:ILE:HG12	2.01	0.43
2:Q:804:ILE:HD11	2:Q:849:ASP:OD1	2.18	0.43
1:U:353:VAL:O	1:U:357:ARG:HG3	2.18	0.43
1:U:398:ALA:O	1:U:402:VAL:HG23	2.18	0.43
1:A:197:ALA:HB1	1:A:201:ARG:HH12	1.83	0.43
1:B:76:GLU:OE1	1:G:42:TYR:CZ	2.71	0.43
1:B:122:LEU:HA	1:B:122:LEU:HD23	1.79	0.43
1:C:267:ARG:NE	1:C:267:ARG:HA	2.33	0.43
1:M:114:ARG:HG2	1:N:115:LEU:HD11	2.00	0.43
1:N:68:GLU:C	1:S:45:ILE:HG21	2.44	0.43
1:N:76:GLU:OE1	1:S:42:TYR:CZ	2.71	0.43
1:O:417:GLN:OE1	1:O:417:GLN:HA	2.18	0.43
1:A:40:GLN:O	1:A:44:THR:HG23	2.18	0.43
1:B:41:ARG:NH2	1:H:78:GLU:OE1	2.51	0.43
1:B:58:HIS:O	1:B:62:ILE:HD12	2.18	0.43
1:D:422:ARG:NH2	2:E:808:ARG:HH12	2.16	0.43
1:G:176:GLN:O	1:G:179:GLU:HG3	2.18	0.43
1:H:116:ALA:HA	1:H:119:GLU:OE1	2.18	0.43
1:N:267:ARG:HA	1:N:270:GLU:CG	2.49	0.43
2:Q:846:SER:HA	2:Q:849:ASP:HA	2.00	0.43
2:R:804:ILE:HD13	2:R:844:ARG:HE	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:189:ASP:O	1:T:192:ARG:HB3	2.19	0.43
2:W:804:ILE:HD12	2:W:871:ILE:C	2.42	0.43
2:W:839:ARG:HH22	2:W:857:ASN:C	2.23	0.43
1:B:58:HIS:O	1:B:59:LEU:C	2.62	0.43
1:B:266:ILE:HA	1:B:269:LEU:HG	2.00	0.43
1:C:255:LEU:O	1:C:259:GLN:HG2	2.18	0.43
1:D:417:GLN:O	1:D:420:ILE:HG22	2.17	0.43
2:F:812:GLN:C	2:F:864:ALA:HB1	2.44	0.43
2:R:834:ASP:HA	2:R:837:LYS:HZ3	1.84	0.43
2:W:13:TYR:HA	2:W:887:SER:HA	2.01	0.43
1:A:66:ILE:O	1:A:69:ILE:HG22	2.18	0.43
1:A:114:ARG:HG2	1:B:115:LEU:HD11	2.00	0.43
1:A:191:ARG:HG2	1:B:192:ARG:NE	2.33	0.43
1:B:80:ARG:HD3	1:H:38:ILE:HG21	2.00	0.43
1:B:219:ARG:NH1	1:D:284:GLN:OE1	2.52	0.43
1:C:255:LEU:HD13	1:D:255:LEU:HD22	2.01	0.43
1:C:336:ILE:HD11	1:D:335:ARG:HB3	2.01	0.43
1:D:288:GLU:HA	1:D:291:THR:HG22	2.01	0.43
1:G:169:ALA:O	1:G:173:HIS:ND1	2.52	0.43
1:H:175:VAL:HA	1:H:178:VAL:HG12	1.99	0.43
1:M:66:ILE:O	1:M:69:ILE:HG22	2.18	0.43
1:O:255:LEU:O	1:O:259:GLN:HG2	2.18	0.43
1:O:307:ARG:CZ	1:P:308:LEU:HD11	2.49	0.43
1:B:204:GLN:HE21	1:C:301:ASN:ND2	2.09	0.43
2:E:841:ILE:HB	2:E:854:GLN:HB3	2.00	0.43
1:G:100:GLN:HE21	1:H:101:ILE:HG12	1.83	0.43
1:G:145:ARG:HG3	1:G:146:LEU:N	2.33	0.43
2:K:844:ARG:HA	2:K:851:VAL:HA	2.01	0.43
2:K:855:MET:HB3	2:K:858:LEU:HD21	1.99	0.43
1:M:191:ARG:HG2	1:N:192:ARG:NE	2.33	0.43
1:N:219:ARG:NH1	1:P:284:GLN:OE1	2.52	0.43
1:O:266:ILE:O	1:O:270:GLU:HG3	2.19	0.43
2:R:10:GLY:H	2:R:883:GLN:HE22	1.65	0.43
1:S:157:VAL:HG11	1:T:156:LYS:HE2	1.99	0.43
1:T:116:ALA:HA	1:T:119:GLU:OE1	2.18	0.43
1:U:375:GLU:HA	1:V:374:GLN:NE2	2.32	0.43
2:X:808:ARG:C	2:X:809:TRP:HD1	2.27	0.43
1:B:62:ILE:HG13	1:G:52:ILE:HG12	2.01	0.43
1:B:68:GLU:C	1:G:45:ILE:HG21	2.43	0.43
1:B:192:ARG:HH12	1:B:195:ALA:HB3	1.84	0.43
1:B:208:LEU:HD13	1:D:296:LYS:HZ1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:GLU:HB3	2:E:827:TRP:CZ2	2.53	0.43
1:C:423:LEU:HD12	1:C:423:LEU:HA	1.83	0.43
2:E:866:TYR:O	2:E:882:THR:N	2.34	0.43
2:F:10:GLY:H	2:F:883:GLN:HE22	1.65	0.43
1:O:336:ILE:HD11	1:P:335:ARG:HB3	2.01	0.43
2:Q:852:TYR:O	2:Q:853:LEU:HD22	2.19	0.43
2:R:839:ARG:NH1	2:R:857:ASN:O	2.52	0.43
1:T:129:ARG:HD3	1:T:129:ARG:HA	1.75	0.43
1:A:148:ASN:HA	1:A:151:LEU:HD12	2.01	0.42
1:D:423:LEU:HD12	1:D:423:LEU:HA	1.90	0.42
2:E:804:ILE:HD11	2:E:849:ASP:OD1	2.18	0.42
1:I:368:ALA:HB2	1:J:363:ARG:HH21	1.84	0.42
1:J:417:GLN:O	1:J:421:GLU:OE1	2.37	0.42
1:N:192:ARG:HH12	1:N:195:ALA:HB3	1.84	0.42
1:O:267:ARG:NE	1:O:267:ARG:HA	2.33	0.42
1:O:312:SER:O	1:O:316:LYS:HG2	2.18	0.42
2:Q:808:ARG:H	2:Q:808:ARG:HG2	1.65	0.42
2:R:812:GLN:C	2:R:864:ALA:HB1	2.44	0.42
1:U:368:ALA:HB2	1:V:363:ARG:HH21	1.84	0.42
1:V:417:GLN:O	1:V:421:GLU:OE1	2.37	0.42
2:X:822:ALA:HB1	2:X:842:ILE:HD13	2.01	0.42
2:L:4:LEU:HD21	2:L:870:ALA:HB2	2.02	0.42
2:L:839:ARG:HH12	2:L:858:LEU:HA	1.84	0.42
1:M:77:PHE:CE1	1:S:42:TYR:CD1	3.07	0.42
1:M:154:ASP:O	1:M:157:VAL:HG12	2.19	0.42
1:P:270:GLU:HA	1:P:273:VAL:HG22	2.01	0.42
1:P:296:LYS:HE3	1:P:297:LEU:HD12	2.01	0.42
1:P:328:ALA:O	1:P:331:ARG:HG3	2.19	0.42
2:Q:802:ASP:C	2:Q:804:ILE:N	2.77	0.42
1:U:422:ARG:NE	2:X:871:ILE:HD12	2.34	0.42
2:W:825:THR:HG23	2:W:828:GLY:H	1.83	0.42
2:X:2:VAL:HB	2:X:877:TYR:CE1	2.54	0.42
1:B:48:GLY:HA2	1:G:70:ARG:NH2	2.32	0.42
1:B:58:HIS:HE2	1:G:59:LEU:HG	1.84	0.42
1:C:286:ARG:HA	1:C:289:THR:OG1	2.18	0.42
1:C:307:ARG:CZ	1:D:308:LEU:HD11	2.49	0.42
2:F:812:GLN:HE21	2:F:819:GLY:H	1.67	0.42
1:I:333:LEU:HA	1:I:336:ILE:HD12	2.01	0.42
1:I:357:ARG:HG2	1:J:357:ARG:NH1	2.35	0.42
1:I:366:GLN:HA	1:I:369:LYS:NZ	2.35	0.42
2:R:863:THR:HG23	2:R:884:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:169:ALA:O	1:S:173:HIS:ND1	2.52	0.42
2:W:804:ILE:CB	2:W:807:MET:SD	3.07	0.42
1:A:77:PHE:CE1	1:G:42:TYR:CD1	3.07	0.42
2:E:873:ARG:NE	1:P:396:GLN:HG3	2.35	0.42
2:F:804:ILE:HD13	2:F:844:ARG:HE	1.83	0.42
1:G:83:GLU:OE1	1:H:84:HIS:NE2	2.53	0.42
2:L:2:VAL:HB	2:L:877:TYR:CE1	2.55	0.42
1:M:230:LEU:O	1:M:234:GLU:HG3	2.19	0.42
1:O:423:LEU:HD22	2:R:806:ILE:HD11	2.01	0.42
1:U:346:LEU:O	1:U:349:ARG:HG2	2.19	0.42
1:A:164:LEU:HB2	1:B:164:LEU:HD12	2.01	0.42
1:A:230:LEU:HA	1:A:233:ILE:HG22	2.00	0.42
1:D:270:GLU:HA	1:D:273:VAL:HG22	2.01	0.42
1:D:328:ALA:O	1:D:331:ARG:HG3	2.20	0.42
2:E:807:MET:SD	2:E:870:ALA:HA	2.60	0.42
1:H:189:ASP:O	1:H:192:ARG:HB3	2.19	0.42
2:Q:792:ARG:NE	2:Q:854:GLN:OE1	2.53	0.42
1:U:366:GLN:HA	1:U:369:LYS:NZ	2.35	0.42
1:A:151:LEU:HD23	1:D:355:THR:HG21	2.00	0.42
1:A:230:LEU:O	1:A:234:GLU:HG3	2.19	0.42
1:C:248:VAL:HG22	1:D:248:VAL:HG22	2.01	0.42
1:C:283:LEU:HD13	1:C:286:ARG:NH1	2.26	0.42
1:D:422:ARG:NH2	1:D:423:LEU:HD12	2.34	0.42
2:E:4:LEU:HD23	2:E:868:CYS:HB3	2.02	0.42
1:G:128:ARG:HE	1:H:129:ARG:NE	2.18	0.42
1:G:165:ARG:O	1:G:168:THR:OG1	2.29	0.42
1:H:51:SER:O	1:H:55:VAL:HG23	2.20	0.42
1:I:335:ARG:NH2	1:J:336:ILE:HD13	2.34	0.42
1:I:439:ARG:HA	1:I:439:ARG:CZ	2.49	0.42
2:K:13:TYR:HA	2:K:887:SER:HA	2.01	0.42
2:K:843:SER:O	2:K:852:TYR:N	2.32	0.42
1:M:197:ALA:HB1	1:M:201:ARG:HH12	1.83	0.42
1:N:80:ARG:HD3	1:T:38:ILE:HG21	2.00	0.42
1:O:255:LEU:HD13	1:P:255:LEU:HD22	2.01	0.42
1:P:288:GLU:HA	1:P:291:THR:HG22	2.01	0.42
1:S:128:ARG:HE	1:T:129:ARG:NE	2.18	0.42
1:U:439:ARG:CZ	1:U:439:ARG:HA	2.49	0.42
1:A:233:ILE:O	1:A:237:LEU:HD23	2.20	0.42
1:C:266:ILE:O	1:C:270:GLU:HG3	2.19	0.42
1:D:417:GLN:HG3	2:F:827:TRP:CD2	2.55	0.42
2:E:789:ASP:OD1	2:E:790:SER:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:346:LEU:O	1:I:349:ARG:HG2	2.19	0.42
1:I:367:LEU:HD22	1:J:367:LEU:HD13	2.01	0.42
1:O:237:LEU:HB3	1:P:237:LEU:HD13	2.01	0.42
1:O:248:VAL:HG22	1:P:248:VAL:HG22	2.01	0.42
1:O:297:LEU:HD21	1:P:298:GLU:N	2.35	0.42
1:P:417:GLN:HG3	2:R:827:TRP:CD2	2.55	0.42
2:R:812:GLN:HE21	2:R:819:GLY:H	1.67	0.42
1:S:146:LEU:HB3	1:T:146:LEU:CD2	2.50	0.42
1:T:116:ALA:HA	1:T:119:GLU:CD	2.45	0.42
1:A:168:THR:O	1:A:172:GLU:OE1	2.37	0.42
1:C:237:LEU:HB3	1:D:237:LEU:HD13	2.01	0.42
1:C:435:GLU:OE2	1:D:434:LEU:HD21	2.20	0.42
2:F:863:THR:HG23	2:F:884:VAL:O	2.20	0.42
1:G:40:GLN:O	1:G:44:THR:HG23	2.20	0.42
1:H:172:GLU:HA	1:H:175:VAL:HG12	2.02	0.42
2:L:808:ARG:C	2:L:809:TRP:HD1	2.27	0.42
1:M:145:ARG:HD2	1:M:145:ARG:C	2.45	0.42
1:M:148:ASN:HA	1:M:151:LEU:HD12	2.01	0.42
1:P:422:ARG:NH2	1:P:423:LEU:HD12	2.34	0.42
2:Q:4:LEU:HD23	2:Q:868:CYS:HB3	2.02	0.42
1:S:188:ILE:HD12	1:S:192:ARG:HH11	1.83	0.42
2:X:806:ILE:HG23	2:X:871:ILE:HB	2.01	0.42
1:A:154:ASP:O	1:A:157:VAL:HG12	2.19	0.42
1:D:345:GLY:HA2	1:D:348:GLN:CD	2.45	0.42
1:M:143:ILE:HD13	1:M:143:ILE:HA	1.93	0.42
1:N:48:GLY:HA2	1:S:70:ARG:NH2	2.32	0.42
1:O:329:LEU:HG	1:O:333:LEU:HD23	2.02	0.42
2:R:812:GLN:HE21	2:R:818:ARG:HA	1.84	0.42
1:U:402:VAL:HG21	1:V:403:ARG:HH12	1.84	0.42
1:V:347:ARG:HG2	1:V:347:ARG:NH1	2.34	0.42
2:X:6:GLU:OE2	2:X:881:GLY:N	2.39	0.42
1:C:416:LEU:O	1:C:419:THR:HG22	2.20	0.42
1:D:263:GLY:O	1:D:267:ARG:NH1	2.53	0.42
1:D:277:ARG:HA	1:D:280:ILE:HD12	2.01	0.42
1:G:129:ARG:NH2	1:G:130:GLN:OE1	2.26	0.42
1:I:422:ARG:NE	2:L:871:ILE:HD12	2.34	0.42
1:N:165:ARG:O	1:N:168:THR:HG22	2.20	0.42
1:U:335:ARG:NH2	1:V:336:ILE:HD13	2.34	0.42
2:X:4:LEU:HD21	2:X:870:ALA:HB2	2.02	0.42
2:X:816:LYS:HB3	2:X:816:LYS:HE2	1.85	0.42
2:X:839:ARG:HH12	2:X:858:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:840:PHE:HE1	2:X:855:MET:SD	2.43	0.42
1:B:267:ARG:HA	1:B:270:GLU:CG	2.49	0.41
1:C:255:LEU:HA	1:D:255:LEU:HD11	2.02	0.41
1:C:361:ILE:HD13	1:C:361:ILE:HA	1.91	0.41
2:E:792:ARG:NE	2:E:854:GLN:OE1	2.53	0.41
1:I:367:LEU:CD2	1:J:367:LEU:HB3	2.51	0.41
2:K:825:THR:OG1	2:K:826:GLY:N	2.53	0.41
2:L:812:GLN:OE1	2:L:818:ARG:HG3	2.20	0.41
2:L:822:ALA:HB1	2:L:842:ILE:HD13	2.01	0.41
2:L:840:PHE:HB3	2:L:853:LEU:HD11	2.02	0.41
1:M:73:VAL:CG1	1:M:77:PHE:HE2	2.19	0.41
1:M:168:THR:O	1:M:172:GLU:OE1	2.37	0.41
1:N:69:ILE:N	1:S:45:ILE:HG21	2.35	0.41
1:O:314:GLN:HB3	1:P:315:GLN:HE22	1.85	0.41
1:P:277:ARG:HA	1:P:280:ILE:HD12	2.01	0.41
2:R:843:SER:O	2:R:852:TYR:N	2.37	0.41
1:S:80:ARG:HD3	1:T:81:ARG:HD2	2.02	0.41
2:W:800:SER:O	2:W:803:GLY:N	2.50	0.41
2:W:844:ARG:HA	2:W:851:VAL:HA	2.01	0.41
2:X:801:ILE:C	2:X:803:GLY:H	2.28	0.41
1:A:241:LEU:HD12	1:A:241:LEU:HA	1.86	0.41
1:B:58:HIS:ND1	1:B:62:ILE:HD11	2.35	0.41
1:B:165:ARG:O	1:B:168:THR:HG22	2.20	0.41
1:C:418:ALA:HA	1:C:421:GLU:HG3	2.01	0.41
2:E:852:TYR:O	2:E:853:LEU:HD22	2.19	0.41
1:G:80:ARG:HD3	1:H:81:ARG:HD2	2.02	0.41
1:G:146:LEU:HB3	1:H:146:LEU:CD2	2.50	0.41
1:H:144:ASP:HA	1:H:147:ARG:HE	1.85	0.41
1:I:389:ARG:HG2	1:J:388:LEU:HD11	2.02	0.41
1:I:402:VAL:CG2	1:J:403:ARG:HH12	2.34	0.41
2:L:812:GLN:HB2	2:L:865:VAL:CG1	2.50	0.41
1:O:418:ALA:HA	1:O:421:GLU:HG3	2.01	0.41
2:X:840:PHE:HB3	2:X:853:LEU:HD11	2.02	0.41
1:B:58:HIS:NE2	1:G:55:VAL:HG12	2.35	0.41
1:G:172:GLU:O	1:G:176:GLN:OE1	2.38	0.41
1:J:404:ARG:O	1:J:408:THR:HG23	2.20	0.41
1:M:70:ARG:HE	1:M:70:ARG:HB2	1.68	0.41
1:N:58:HIS:CD2	1:S:59:LEU:HD11	2.55	0.41
1:O:435:GLU:OE2	1:P:434:LEU:HD21	2.20	0.41
1:P:329:LEU:HA	1:P:329:LEU:HD12	1.76	0.41
1:P:345:GLY:HA2	1:P:348:GLN:CD	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:807:MET:SD	2:Q:870:ALA:HA	2.60	0.41
2:Q:810:TYR:HA	2:Q:819:GLY:O	2.21	0.41
1:S:151:LEU:HD13	1:V:355:THR:HG22	2.03	0.41
1:T:39:GLY:O	1:T:43:GLU:OE1	2.38	0.41
1:U:333:LEU:HA	1:U:336:ILE:HD12	2.02	0.41
1:A:45:ILE:HD12	1:H:73:VAL:HG22	2.02	0.41
1:C:297:LEU:HD21	1:D:298:GLU:N	2.35	0.41
2:E:810:TYR:HA	2:E:819:GLY:O	2.21	0.41
2:F:793:LEU:O	2:F:794:SER:OG	2.32	0.41
1:G:151:LEU:HD13	1:J:355:THR:HG22	2.03	0.41
2:L:801:ILE:C	2:L:803:GLY:H	2.28	0.41
2:L:840:PHE:HE1	2:L:855:MET:SD	2.43	0.41
1:M:241:LEU:HD21	1:N:240:GLN:CD	2.46	0.41
1:N:263:GLY:O	1:N:267:ARG:HG2	2.21	0.41
1:O:308:LEU:HB3	1:P:307:ARG:NH1	2.36	0.41
1:O:414:ALA:O	1:O:417:GLN:HB3	2.20	0.41
2:Q:840:PHE:CE1	2:Q:855:MET:HA	2.56	0.41
1:U:367:LEU:HD22	1:V:367:LEU:HD13	2.01	0.41
1:A:241:LEU:HD21	1:B:240:GLN:CD	2.46	0.41
1:B:58:HIS:CD2	1:G:59:LEU:HD11	2.56	0.41
1:B:263:GLY:O	1:B:267:ARG:HG2	2.21	0.41
1:D:296:LYS:HE3	1:D:297:LEU:HD12	2.01	0.41
1:I:339:LEU:HB3	1:J:339:LEU:HD21	2.03	0.41
1:I:410:GLU:OE2	1:I:410:GLU:HA	2.20	0.41
2:L:806:ILE:HG23	2:L:871:ILE:HB	2.01	0.41
1:O:255:LEU:HB2	1:P:255:LEU:HD21	2.03	0.41
2:Q:3:GLN:O	2:Q:4:LEU:HD12	2.20	0.41
1:T:144:ASP:HA	1:T:147:ARG:HE	1.85	0.41
1:U:367:LEU:CD2	1:V:367:LEU:HB3	2.50	0.41
1:U:410:GLU:HA	1:U:410:GLU:OE2	2.20	0.41
2:X:812:GLN:OE1	2:X:818:ARG:HG3	2.20	0.41
1:A:145:ARG:C	1:A:145:ARG:HD2	2.45	0.41
1:A:228:ALA:O	1:A:231:SER:OG	2.33	0.41
1:A:255:LEU:HA	1:A:255:LEU:HD13	1.88	0.41
1:C:248:VAL:O	1:C:252:GLU:HG2	2.21	0.41
1:C:329:LEU:HG	1:C:333:LEU:HD23	2.01	0.41
1:C:403:ARG:HA	1:C:403:ARG:NE	2.36	0.41
1:D:396:GLN:HG3	2:Q:873:ARG:NE	2.35	0.41
1:D:409:HIS:O	1:D:413:ILE:HG12	2.21	0.41
2:E:836:VAL:O	2:E:837:LYS:C	2.64	0.41
1:G:94:LEU:HD22	1:H:90:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:346:LEU:C	1:I:349:ARG:HG2	2.46	0.41
1:I:380:ARG:HD2	1:I:381:ALA:N	2.36	0.41
1:M:233:ILE:O	1:M:237:LEU:HD23	2.19	0.41
1:O:248:VAL:O	1:O:252:GLU:HG2	2.21	0.41
1:P:409:HIS:O	1:P:413:ILE:HG12	2.21	0.41
1:S:108:GLU:HA	1:S:111:VAL:HG12	2.03	0.41
1:U:357:ARG:HG2	1:V:357:ARG:NH1	2.35	0.41
2:W:12:VAL:O	2:W:886:VAL:HB	2.21	0.41
1:C:255:LEU:HB2	1:D:255:LEU:HD21	2.03	0.41
1:C:414:ALA:O	1:C:417:GLN:HB3	2.20	0.41
2:F:812:GLN:HE21	2:F:818:ARG:HA	1.85	0.41
1:G:129:ARG:NH1	1:G:133:ASP:HB2	2.32	0.41
1:H:42:TYR:HA	1:H:45:ILE:HB	2.03	0.41
1:N:144:ASP:O	1:N:147:ARG:HB2	2.20	0.41
1:P:264:ARG:HA	1:P:267:ARG:HH22	1.86	0.41
2:Q:811:ARG:HH12	2:Q:836:VAL:HG23	1.85	0.41
1:V:420:ILE:HD13	1:V:420:ILE:HA	1.92	0.41
1:B:69:ILE:N	1:G:45:ILE:HG21	2.35	0.41
2:E:811:ARG:HH12	2:E:836:VAL:HG23	1.85	0.41
2:E:822:ALA:HB3	2:E:853:LEU:HD11	2.02	0.41
1:I:402:VAL:HG21	1:J:403:ARG:HH12	1.84	0.41
2:L:863:THR:OG1	2:L:886:VAL:HA	2.21	0.41
1:M:45:ILE:HD12	1:T:73:VAL:HG22	2.02	0.41
1:P:263:GLY:O	1:P:267:ARG:NH1	2.53	0.41
1:P:344:ASP:O	1:P:348:GLN:OE1	2.39	0.41
1:S:94:LEU:HD22	1:T:90:VAL:HG13	2.02	0.41
1:U:327:VAL:O	1:U:328:ALA:C	2.64	0.41
1:U:339:LEU:HB3	1:V:339:LEU:HD21	2.02	0.41
1:U:402:VAL:CG2	1:V:403:ARG:HH12	2.33	0.41
2:X:6:GLU:OE2	2:X:880:GLN:N	2.54	0.41
1:A:88:ILE:O	1:A:91:ARG:HB2	2.21	0.41
1:B:241:LEU:CD1	1:B:245:ARG:HH12	2.34	0.41
1:C:435:GLU:CD	1:C:438:ARG:HH21	2.29	0.41
1:D:223:ALA:O	1:D:227:LEU:HG	2.21	0.41
1:D:333:LEU:O	1:D:337:ARG:HG2	2.21	0.41
2:E:840:PHE:CE1	2:E:855:MET:HA	2.56	0.41
1:H:39:GLY:O	1:H:43:GLU:OE1	2.38	0.41
1:I:400:ASP:O	1:I:404:ARG:HG3	2.21	0.41
1:J:347:ARG:HG2	1:J:347:ARG:NH1	2.34	0.41
2:K:12:VAL:O	2:K:886:VAL:HB	2.21	0.41
2:L:6:GLU:OE2	2:L:880:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:807:MET:SD	2:L:807:MET:N	2.94	0.41
2:L:816:LYS:HB3	2:L:816:LYS:HE2	1.86	0.41
1:M:74:SER:HA	1:M:77:PHE:CD2	2.44	0.41
1:N:58:HIS:HE2	1:S:59:LEU:HG	1.84	0.41
1:N:58:HIS:ND1	1:N:62:ILE:HD11	2.35	0.41
1:O:279:GLU:O	1:O:283:LEU:HD23	2.21	0.41
1:O:416:LEU:O	1:O:419:THR:HG22	2.20	0.41
2:R:805:ASN:O	2:R:806:ILE:C	2.63	0.41
1:S:83:GLU:OE1	1:T:84:HIS:NE2	2.53	0.41
1:T:51:SER:O	1:T:55:VAL:HG23	2.20	0.41
1:U:400:ASP:O	1:U:404:ARG:HG3	2.21	0.41
2:W:825:THR:OG1	2:W:826:GLY:N	2.53	0.41
1:A:261:ASP:O	1:A:265:THR:HG23	2.21	0.41
1:A:270:GLU:O	1:A:274:GLU:OE1	2.39	0.41
1:B:144:ASP:O	1:B:147:ARG:HB2	2.20	0.41
1:C:308:LEU:HB3	1:D:307:ARG:NH1	2.36	0.41
2:E:3:GLN:O	2:E:4:LEU:HD12	2.21	0.41
2:F:840:PHE:CD1	2:F:855:MET:HA	2.56	0.41
1:I:380:ARG:O	1:I:383:GLU:HG3	2.21	0.41
1:J:420:ILE:HD13	1:J:420:ILE:HA	1.92	0.41
1:M:88:ILE:O	1:M:91:ARG:HB2	2.21	0.41
1:M:169:ALA:HA	1:M:172:GLU:CD	2.46	0.41
1:N:77:PHE:CZ	1:T:42:TYR:CG	3.09	0.41
1:P:438:ARG:NH1	1:P:442:SER:HB3	2.23	0.41
1:U:380:ARG:HD2	1:U:381:ALA:N	2.36	0.41
1:B:59:LEU:HG	1:B:59:LEU:H	1.75	0.40
2:F:4:LEU:HD22	2:F:868:CYS:O	2.21	0.40
1:G:93:ASN:ND2	1:H:94:LEU:HD21	2.36	0.40
1:G:142:GLU:HA	1:G:145:ARG:NH1	2.36	0.40
1:G:160:LEU:HD13	1:G:160:LEU:HA	1.96	0.40
1:I:327:VAL:O	1:I:328:ALA:C	2.64	0.40
1:I:400:ASP:OD1	1:I:403:ARG:NH1	2.54	0.40
1:N:52:ILE:HG23	1:T:63:GLU:HG3	2.03	0.40
1:N:109:ARG:HH12	1:O:396:GLN:HG3	1.86	0.40
2:Q:822:ALA:HB3	2:Q:853:LEU:HD11	2.02	0.40
1:S:40:GLN:O	1:S:44:THR:HG23	2.20	0.40
1:T:80:ARG:HA	1:T:83:GLU:HB3	2.03	0.40
1:U:399:GLN:HB3	1:U:403:ARG:CZ	2.50	0.40
1:V:404:ARG:O	1:V:408:THR:HG23	2.20	0.40
1:B:77:PHE:CZ	1:H:42:TYR:CG	3.09	0.40
1:H:34:SER:O	1:H:38:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:ARG:HA	1:H:83:GLU:HB3	2.03	0.40
1:H:116:ALA:HA	1:H:119:GLU:CD	2.45	0.40
1:H:129:ARG:HA	1:H:129:ARG:HD3	1.75	0.40
2:K:804:ILE:CB	2:K:807:MET:SD	3.07	0.40
2:L:818:ARG:HG3	2:L:818:ARG:NH2	2.36	0.40
1:M:261:ASP:O	1:M:265:THR:HG23	2.21	0.40
1:M:270:GLU:O	1:M:274:GLU:OE1	2.39	0.40
1:N:58:HIS:NE2	1:S:55:VAL:HG12	2.35	0.40
1:N:75:GLN:OE1	1:N:76:GLU:HG3	2.22	0.40
1:N:77:PHE:N	1:N:80:ARG:NH2	2.70	0.40
1:N:87:LEU:O	1:N:91:ARG:HD2	2.22	0.40
1:N:267:ARG:HA	1:N:267:ARG:HD2	1.90	0.40
1:S:40:GLN:H	1:S:40:GLN:CD	2.29	0.40
1:T:172:GLU:HA	1:T:175:VAL:HG12	2.02	0.40
1:U:434:LEU:HD23	1:U:434:LEU:HA	1.64	0.40
2:X:818:ARG:HG3	2:X:818:ARG:NH2	2.36	0.40
1:A:83:GLU:OE1	1:H:34:SER:HB3	2.22	0.40
1:B:75:GLN:OE1	1:B:76:GLU:HG3	2.22	0.40
2:E:853:LEU:HD13	2:E:853:LEU:HA	1.84	0.40
1:I:357:ARG:CD	1:J:357:ARG:HB2	2.50	0.40
1:I:399:GLN:HB3	1:I:403:ARG:CZ	2.51	0.40
2:K:807:MET:HE3	2:K:807:MET:HB3	1.78	0.40
1:N:58:HIS:O	1:N:59:LEU:C	2.62	0.40
1:S:136:LEU:HA	1:S:136:LEU:HD23	1.78	0.40
1:S:146:LEU:HB3	1:T:146:LEU:HD22	2.03	0.40
1:U:367:LEU:HD22	1:V:367:LEU:HB3	2.02	0.40
1:B:109:ARG:HH12	1:C:396:GLN:HG3	1.86	0.40
1:I:374:GLN:OE1	1:J:375:GLU:N	2.54	0.40
1:M:114:ARG:HB2	1:M:114:ARG:HH11	1.83	0.40
1:O:255:LEU:HA	1:P:255:LEU:HD11	2.02	0.40
1:O:403:ARG:HA	1:O:403:ARG:NE	2.36	0.40
1:P:223:ALA:O	1:P:227:LEU:HG	2.21	0.40
1:P:271:SER:HA	1:P:274:GLU:CD	2.46	0.40
1:P:296:LYS:HD3	1:P:300:MET:HE1	2.03	0.40
1:P:333:LEU:O	1:P:337:ARG:HG2	2.21	0.40
2:R:793:LEU:O	2:R:794:SER:OG	2.32	0.40
2:R:832:TYR:OH	2:R:841:ILE:HA	2.22	0.40
2:R:833:VAL:C	2:R:835:SER:H	2.30	0.40
1:U:434:LEU:HD13	1:V:434:LEU:HB2	2.03	0.40
2:X:807:MET:SD	2:X:807:MET:N	2.94	0.40
2:X:863:THR:OG1	2:X:886:VAL:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:PHE:N	1:B:80:ARG:NH2	2.70	0.40
1:G:140:ALA:HA	1:G:143:ILE:HG22	2.04	0.40
1:M:77:PHE:HB3	1:S:39:GLY:N	2.37	0.40
2:R:795:CYS:SG	2:R:796:ALA:N	2.95	0.40
2:R:840:PHE:CD1	2:R:855:MET:HA	2.57	0.40
1:S:142:GLU:HA	1:S:145:ARG:NH1	2.36	0.40
1:T:34:SER:O	1:T:38:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	243/460 (53%)	239 (98%)	4 (2%)	0	100	100
1	B	236/460 (51%)	231 (98%)	5 (2%)	0	100	100
1	C	232/460 (50%)	230 (99%)	2 (1%)	0	100	100
1	D	232/460 (50%)	229 (99%)	3 (1%)	0	100	100
1	G	153/460 (33%)	152 (99%)	1 (1%)	0	100	100
1	H	161/460 (35%)	159 (99%)	2 (1%)	0	100	100
1	I	118/460 (26%)	117 (99%)	1 (1%)	0	100	100
1	J	118/460 (26%)	116 (98%)	2 (2%)	0	100	100
1	M	243/460 (53%)	239 (98%)	4 (2%)	0	100	100
1	N	236/460 (51%)	231 (98%)	5 (2%)	0	100	100
1	O	232/460 (50%)	230 (99%)	2 (1%)	0	100	100
1	P	232/460 (50%)	229 (99%)	3 (1%)	0	100	100
1	S	153/460 (33%)	152 (99%)	1 (1%)	0	100	100
1	T	161/460 (35%)	159 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	118/460 (26%)	117 (99%)	1 (1%)	0	100	100
1	V	118/460 (26%)	116 (98%)	2 (2%)	0	100	100
2	E	108/907 (12%)	90 (83%)	18 (17%)	0	100	100
2	F	107/907 (12%)	81 (76%)	26 (24%)	0	100	100
2	K	108/907 (12%)	92 (85%)	16 (15%)	0	100	100
2	L	101/907 (11%)	89 (88%)	12 (12%)	0	100	100
2	Q	108/907 (12%)	90 (83%)	18 (17%)	0	100	100
2	R	107/907 (12%)	81 (76%)	26 (24%)	0	100	100
2	W	108/907 (12%)	92 (85%)	16 (15%)	0	100	100
2	X	101/907 (11%)	90 (89%)	11 (11%)	0	100	100
All	All	3834/14616 (26%)	3651 (95%)	183 (5%)	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	187/347 (54%)	187 (100%)	0	100	100
1	B	182/347 (52%)	182 (100%)	0	100	100
1	C	174/347 (50%)	174 (100%)	0	100	100
1	D	174/347 (50%)	174 (100%)	0	100	100
1	G	122/347 (35%)	122 (100%)	0	100	100
1	H	129/347 (37%)	128 (99%)	1 (1%)	73	77
1	I	89/347 (26%)	89 (100%)	0	100	100
1	J	89/347 (26%)	89 (100%)	0	100	100
1	M	187/347 (54%)	187 (100%)	0	100	100
1	N	182/347 (52%)	182 (100%)	0	100	100
1	O	174/347 (50%)	174 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	174/347 (50%)	174 (100%)	0	100	100
1	S	122/347 (35%)	122 (100%)	0	100	100
1	T	129/347 (37%)	128 (99%)	1 (1%)	73	77
1	U	89/347 (26%)	89 (100%)	0	100	100
1	V	89/347 (26%)	89 (100%)	0	100	100
2	E	94/749 (13%)	94 (100%)	0	100	100
2	F	93/749 (12%)	93 (100%)	0	100	100
2	K	94/749 (13%)	94 (100%)	0	100	100
2	L	89/749 (12%)	89 (100%)	0	100	100
2	Q	94/749 (13%)	94 (100%)	0	100	100
2	R	93/749 (12%)	93 (100%)	0	100	100
2	W	94/749 (13%)	94 (100%)	0	100	100
2	X	89/749 (12%)	89 (100%)	0	100	100
All	All	3032/11544 (26%)	3030 (100%)	2 (0%)	87	88

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

Mol	Chain	Res	Type
1	H	93	ASN
1	T	93	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	184	GLN
1	A	249	GLN
1	A	272	GLN
1	A	276	ASN
1	B	75	GLN
1	B	148	ASN
1	B	184	GLN
1	B	222	GLN
1	B	253	ASN
1	B	259	GLN
1	C	240	GLN

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Mol	Chain	Res	Type
1	C	253	ASN
1	C	259	GLN
1	C	301	ASN
1	D	272	GLN
1	D	374	GLN
1	D	409	HIS
2	F	5	GLN
2	F	812	GLN
1	G	40	GLN
1	G	100	GLN
1	G	139	ASN
1	H	31	GLN
1	H	40	GLN
1	H	93	ASN
1	H	130	GLN
1	H	132	GLN
1	I	348	GLN
1	I	350	HIS
1	I	409	HIS
1	I	445	GLN
1	J	374	GLN
2	K	880	GLN
1	M	36	GLN
1	M	184	GLN
1	M	272	GLN
1	M	276	ASN
1	N	75	GLN
1	N	148	ASN
1	N	184	GLN
1	N	253	ASN
1	N	259	GLN
1	O	240	GLN
1	O	249	GLN
1	O	253	ASN
1	O	259	GLN
1	O	301	ASN
1	P	272	GLN
1	P	374	GLN
1	P	409	HIS
2	R	5	GLN
2	R	812	GLN
1	S	40	GLN

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Mol	Chain	Res	Type
1	S	139	ASN
1	T	31	GLN
1	T	40	GLN
1	T	93	ASN
1	T	130	GLN
1	T	132	GLN
1	U	348	GLN
1	U	409	HIS
1	U	445	GLN
1	V	374	GLN
2	W	831	ASN
2	W	880	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

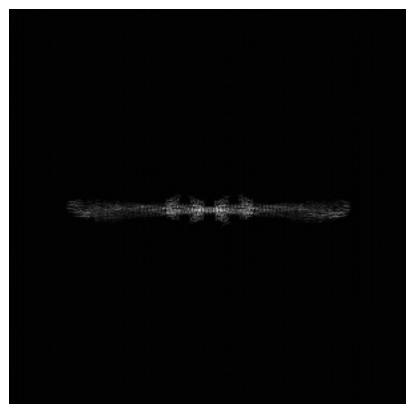
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15476. These allow visual inspection of the internal detail of the map and identification of artifacts.

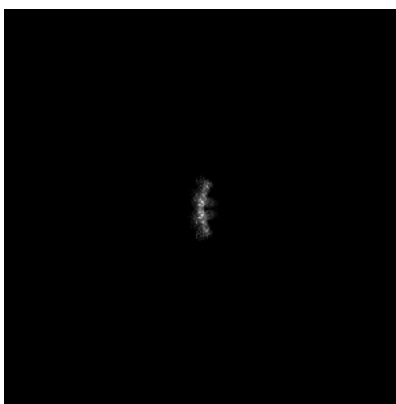
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

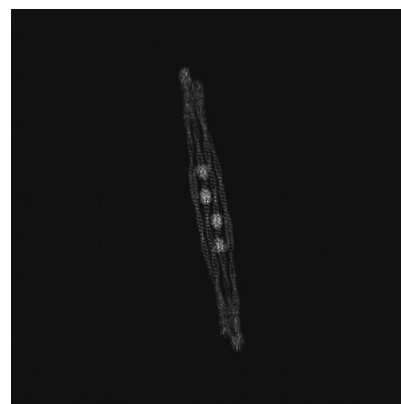
6.1.1 Primary map



X

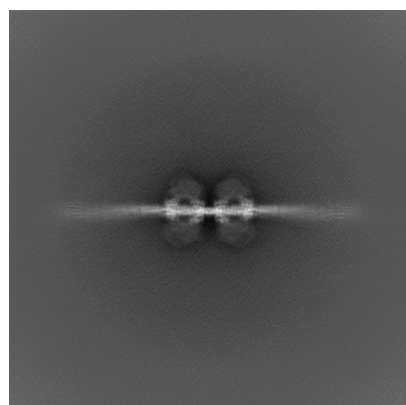


Y

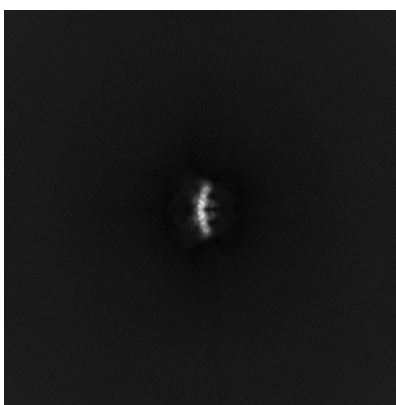


Z

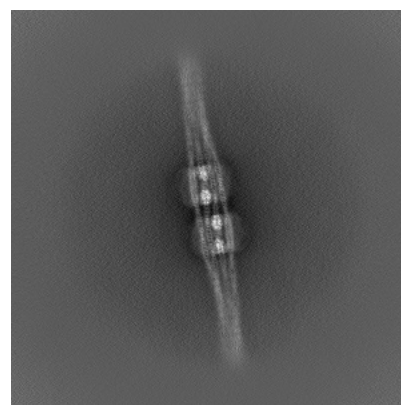
6.1.2 Raw map



X



Y

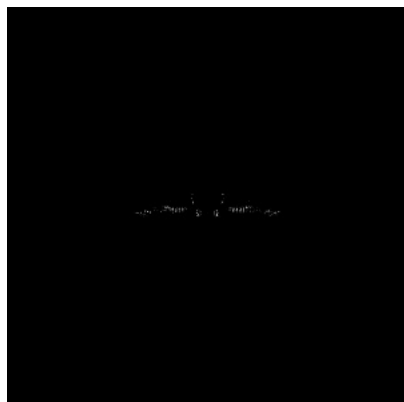


Z

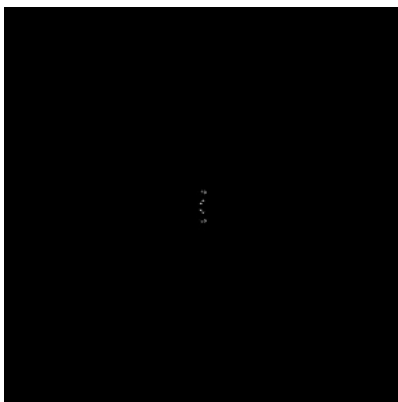
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 300

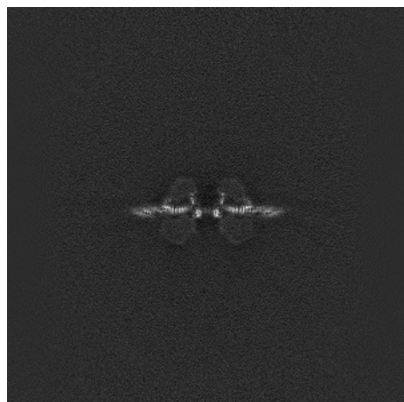


Y Index: 300

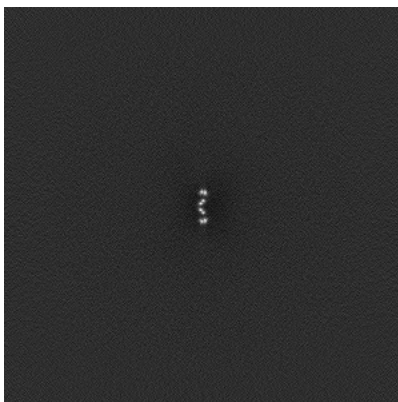


Z Index: 300

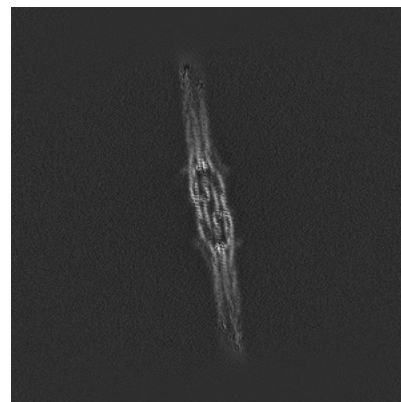
6.2.2 Raw map



X Index: 300



Y Index: 300



Z Index: 300

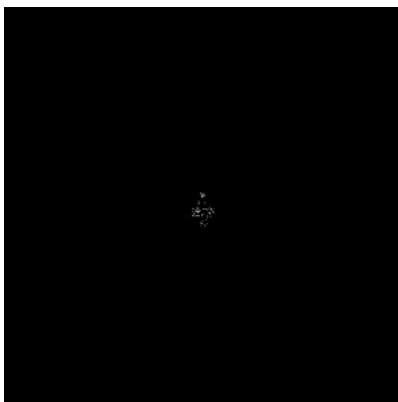
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 310

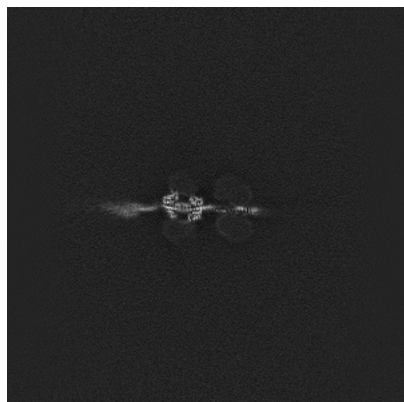


Y Index: 318

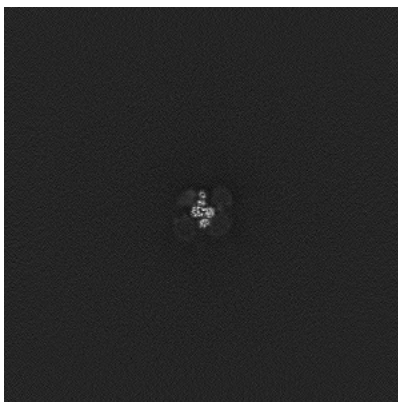


Z Index: 299

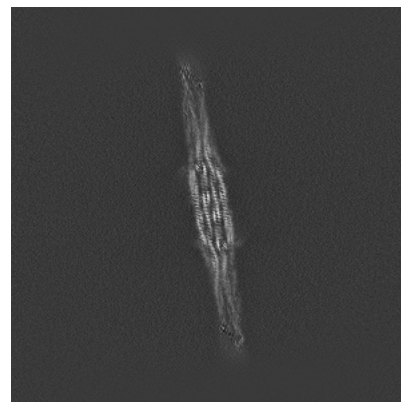
6.3.2 Raw map



X Index: 310



Y Index: 317

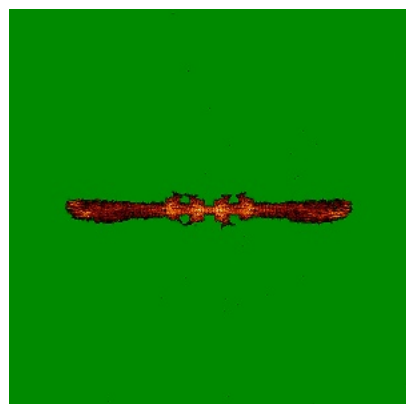


Z Index: 298

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

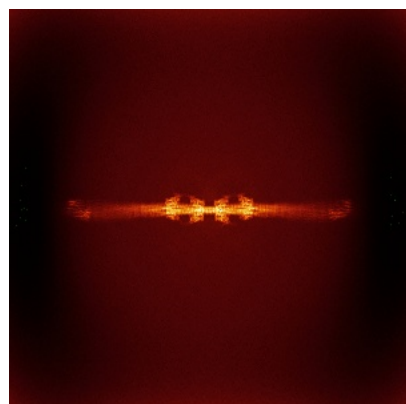


Y

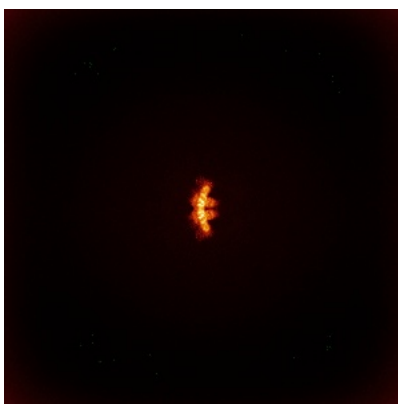


Z

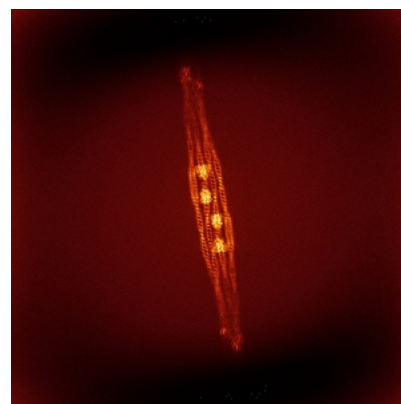
6.4.2 Raw map



X



Y

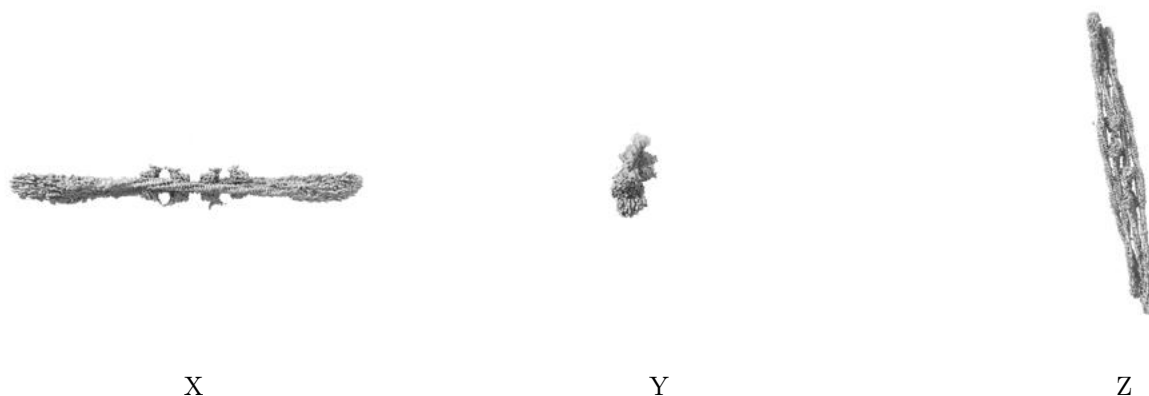


Z

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.

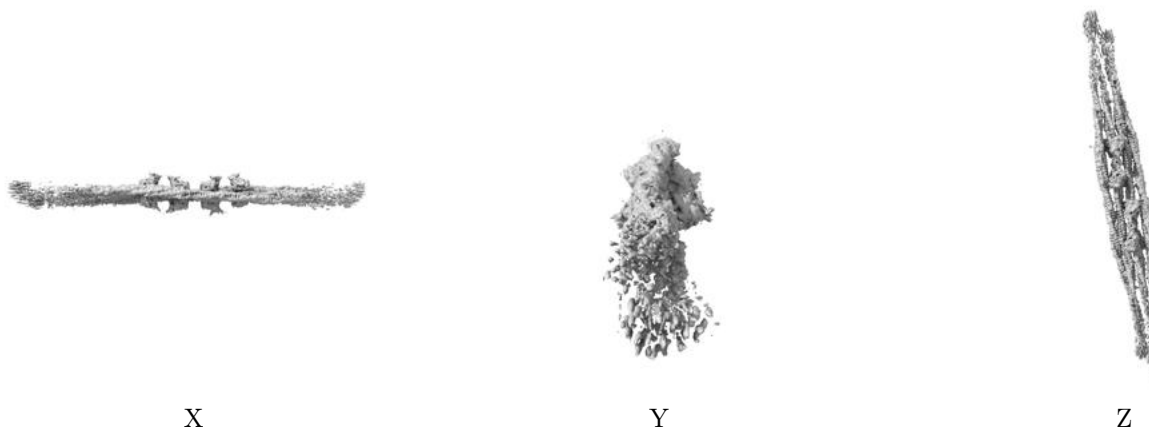
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. 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.

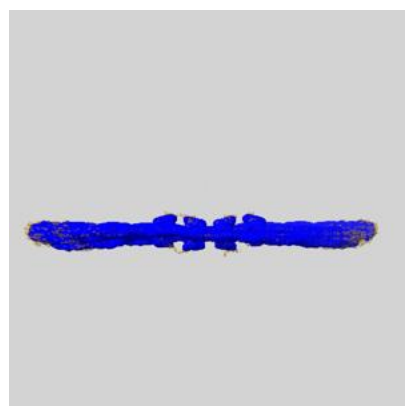
6.6 Mask visualisation [i](#)

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

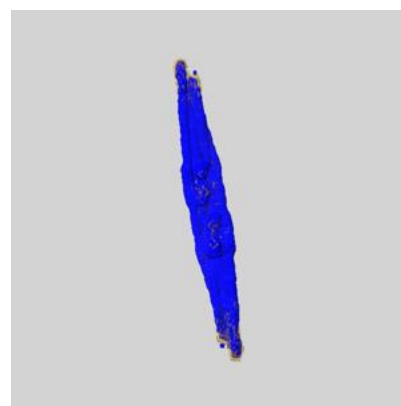
6.6.1 emd_15476_msk_1.map [i](#)



X



Y

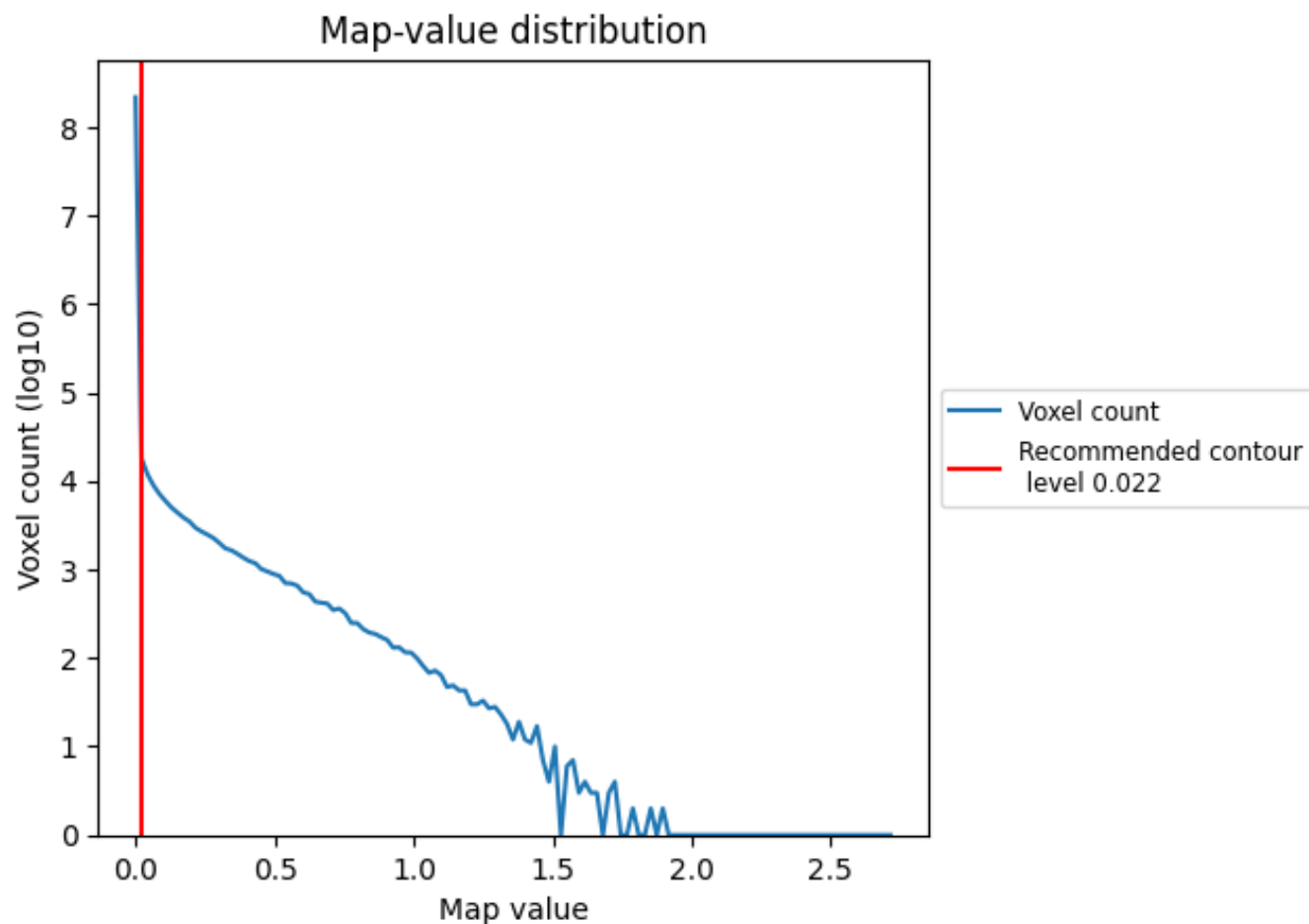


Z

7 Map analysis [i](#)

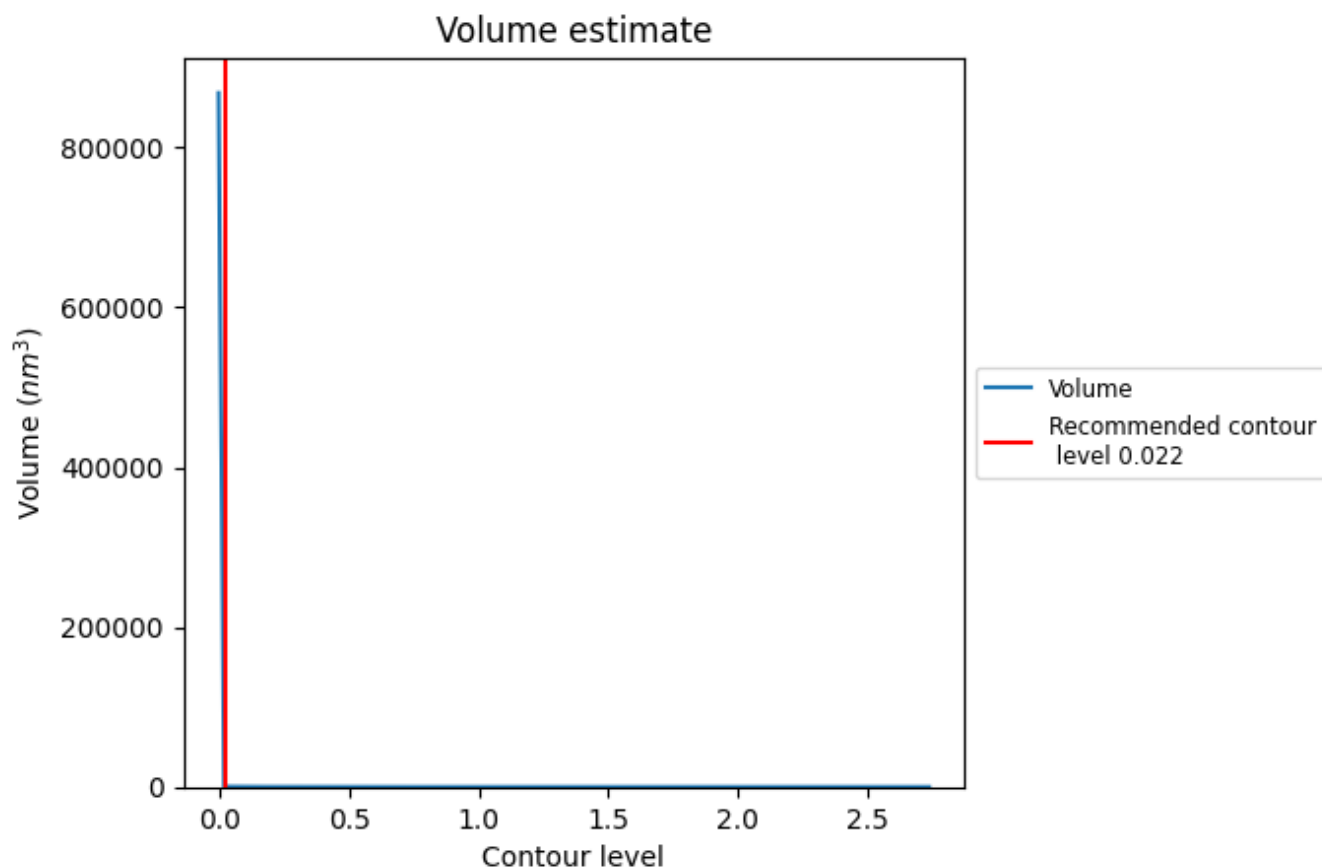
This section contains the results of statistical analysis of the map.

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.

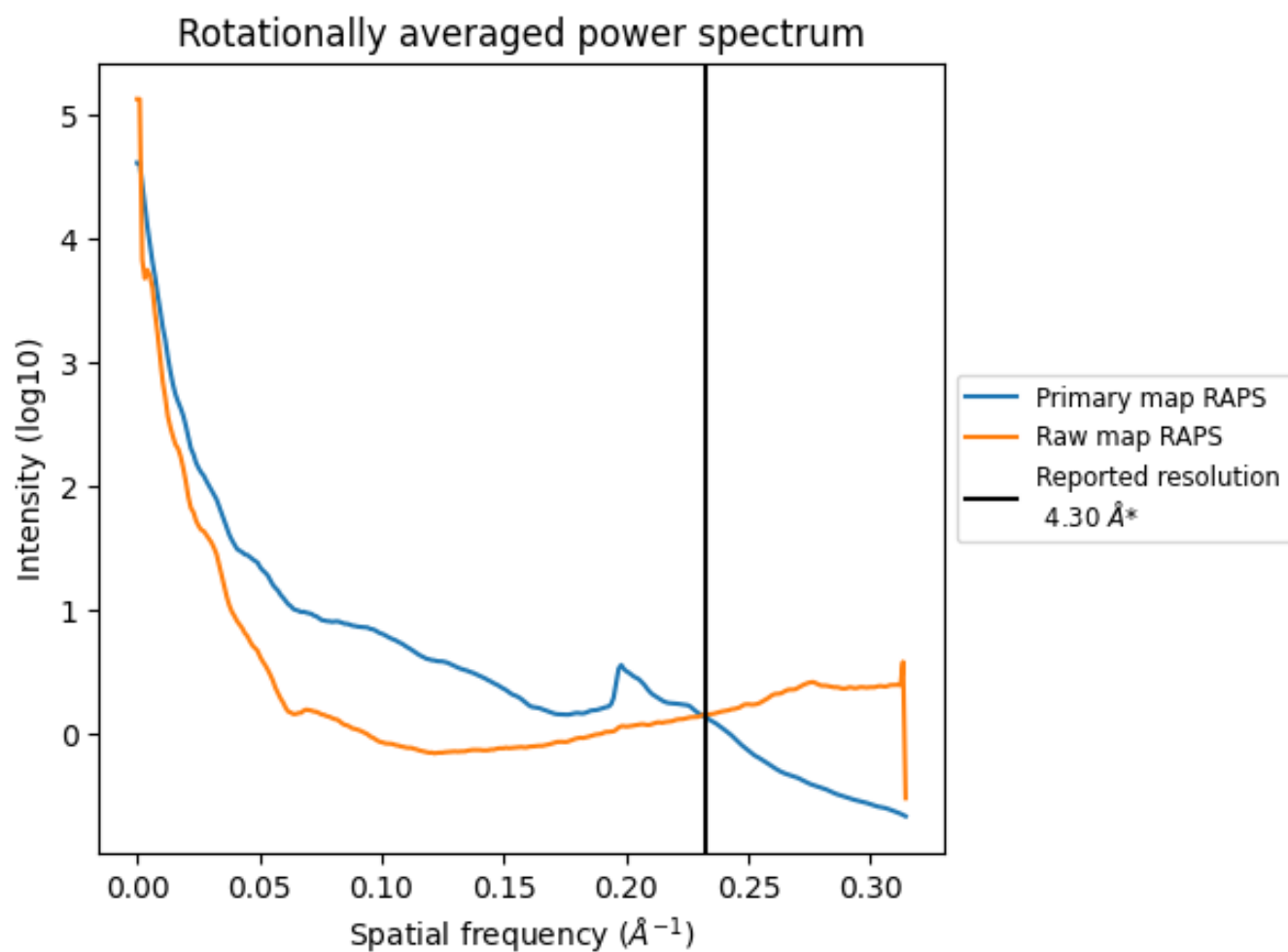
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 401 nm^3 ; this corresponds to an approximate mass of 362 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 ⓘ

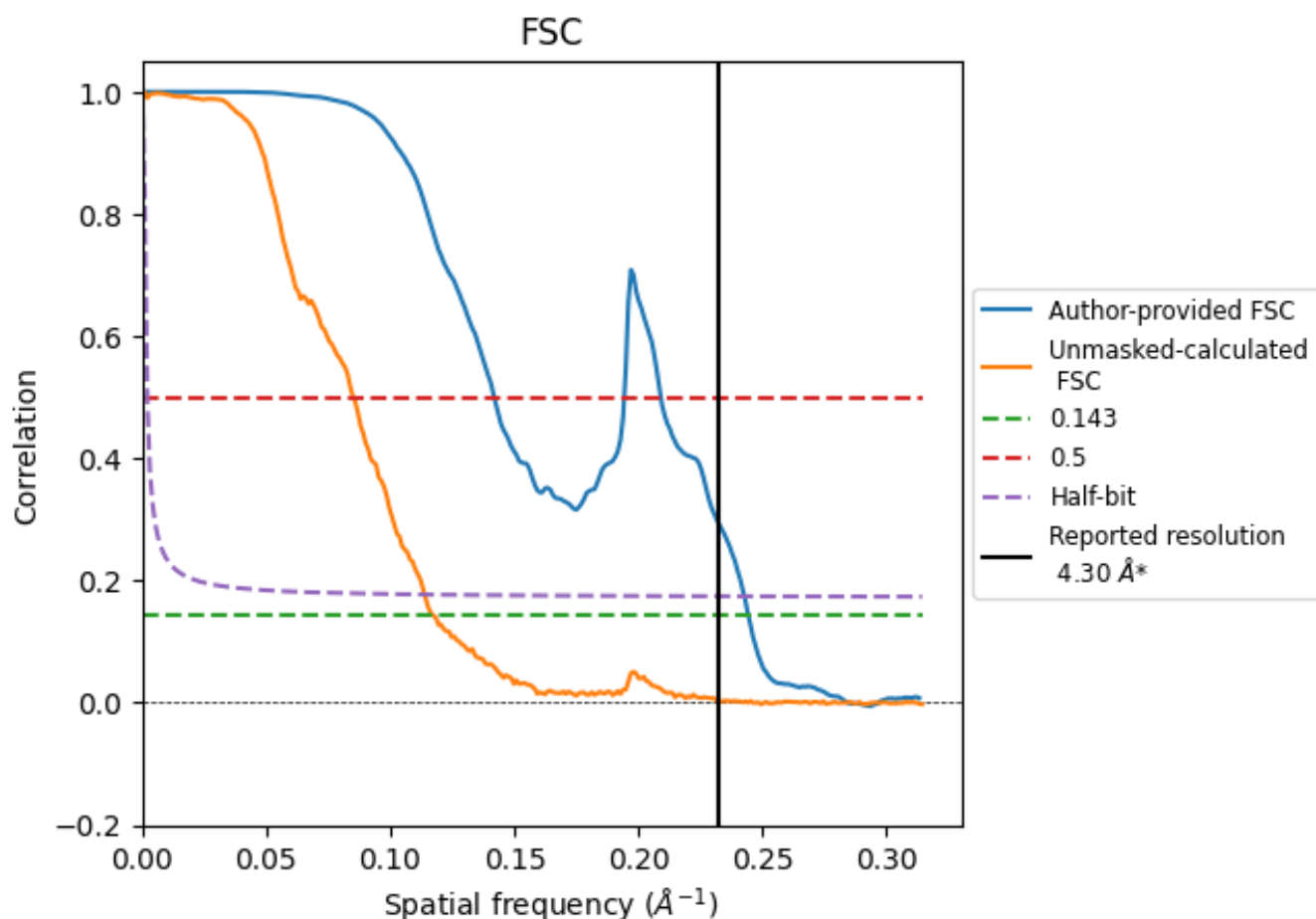


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

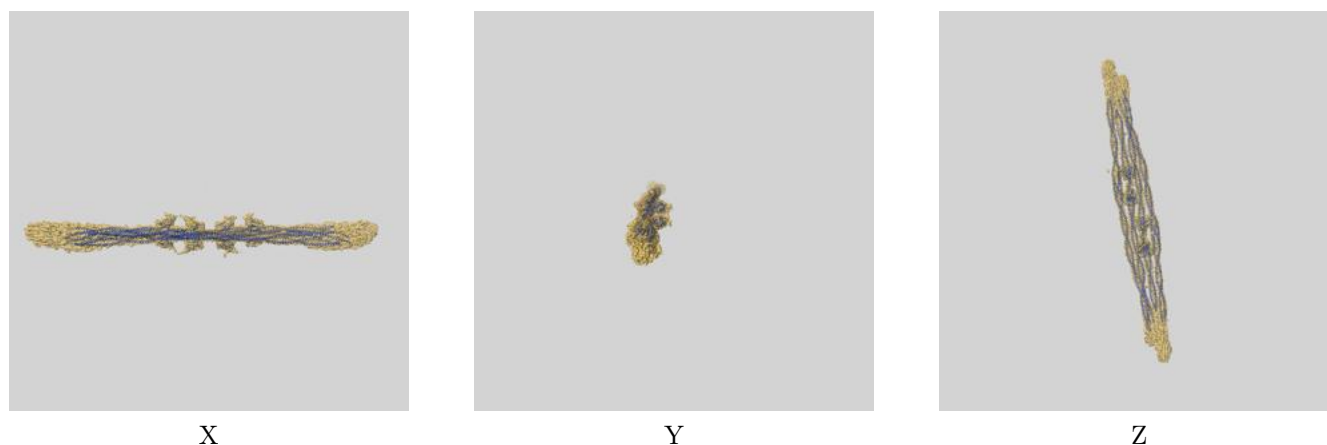
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.09	7.05	4.12
Unmasked-calculated*	8.53	11.75	8.78

*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 8.53 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15476 and PDB model 8AJB. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



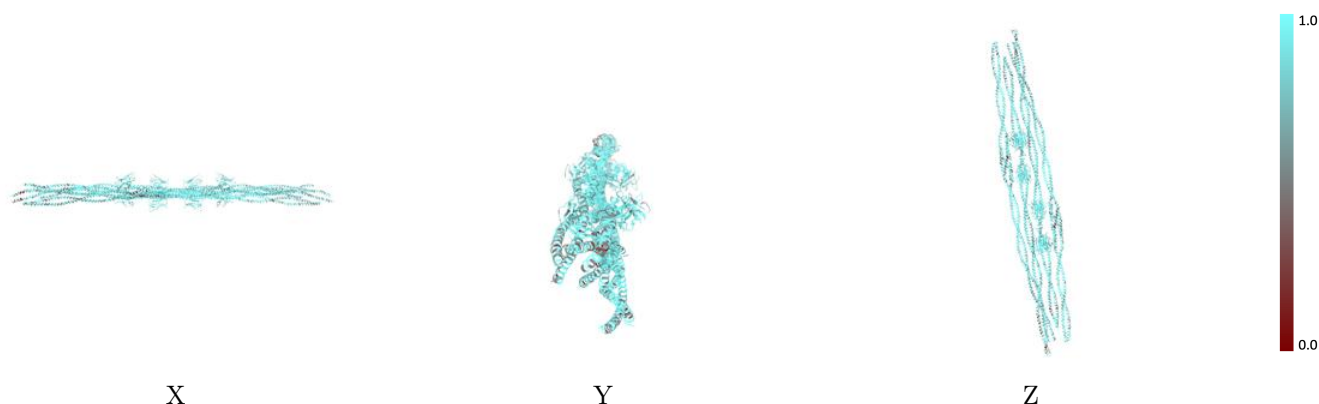
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



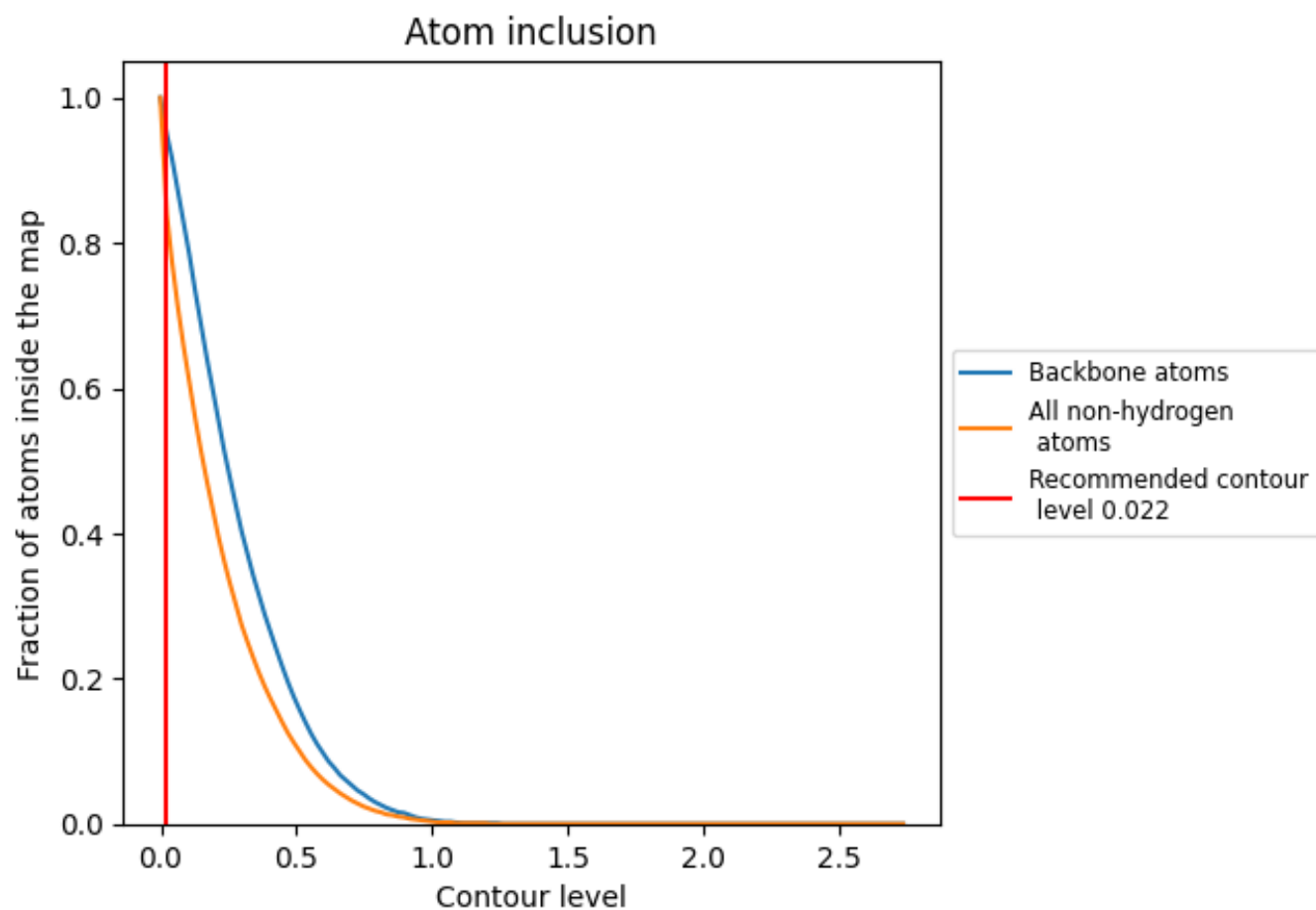
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 84% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8400	 0.1860
A	 0.8330	 0.1630
B	 0.8260	 0.1630
C	 0.8050	 0.1570
D	 0.8420	 0.1700
E	 0.9230	 0.3140
F	 0.9030	 0.2830
G	 0.7630	 0.0640
H	 0.8310	 0.0980
I	 0.8450	 0.1850
J	 0.8430	 0.1680
K	 0.9000	 0.2960
L	 0.8880	 0.3160
M	 0.8200	 0.1590
N	 0.8150	 0.1620
O	 0.8080	 0.1660
P	 0.8600	 0.1950
Q	 0.9050	 0.2970
R	 0.8990	 0.2710
S	 0.7620	 0.0650
T	 0.8280	 0.1230
U	 0.8440	 0.1940
V	 0.8330	 0.1830
W	 0.8920	 0.2850
X	 0.8960	 0.3280

