



Full wwPDB EM Validation Report ⓘ

Apr 23, 2024 – 01:17 am BST

PDB ID : 6ZXK
EMDB ID : EMD-11523
Title : Fully-loaded anthrax lethal toxin in its heptameric pre-pore state and PA7LF(2+1B) arrangement
Authors : Quentin, D.; Antoni, C.; Gatsogiannis, C.; Raunser, S.
Deposited on : 2020-07-29
Resolution : 3.80 Å(reported)
Based on initial model : 6ZXJ

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:

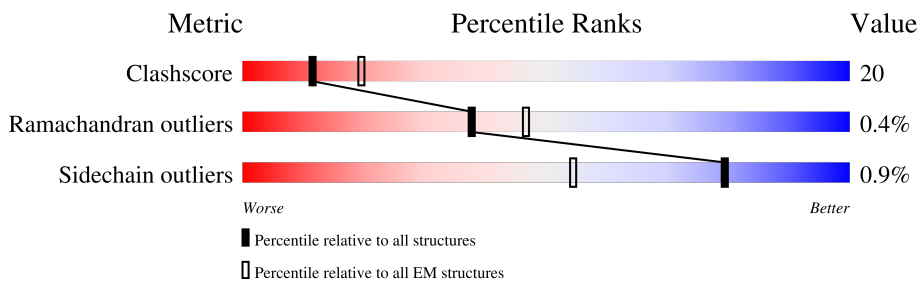
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	759	 42% 27% 30%
1	B	759	 47% 21% 30%
1	C	759	 44% 25% 30%
1	D	759	 44% 25% 30%
1	E	759	 45% 23% 30%
1	F	759	 45% 24% 30%
1	G	759	 46% 23% 30%
2	H	809	 10% 52% 33% 14%

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Mol	Chain	Length	Quality of chain
2	I	809	
2	J	809	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 42292 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 Protective antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	529	3984	2495	694	791	4	0	0
1	B	529	3977	2488	692	793	4	0	0
1	C	529	3977	2488	692	793	4	0	0
1	D	528	3970	2483	691	792	4	0	0
1	E	529	3977	2488	692	793	4	0	0
1	F	529	3977	2488	692	793	4	0	0
1	G	529	3977	2488	692	793	4	0	0

There are 161 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP Q68GS1
A	-22	GLY	-	expression tag	UNP Q68GS1
A	-21	HIS	-	expression tag	UNP Q68GS1
A	-20	HIS	-	expression tag	UNP Q68GS1
A	-19	HIS	-	expression tag	UNP Q68GS1
A	-18	HIS	-	expression tag	UNP Q68GS1
A	-17	HIS	-	expression tag	UNP Q68GS1
A	-16	HIS	-	expression tag	UNP Q68GS1
A	-15	HIS	-	expression tag	UNP Q68GS1
A	-14	HIS	-	expression tag	UNP Q68GS1
A	-13	HIS	-	expression tag	UNP Q68GS1
A	-12	HIS	-	expression tag	UNP Q68GS1
A	-11	SER	-	expression tag	UNP Q68GS1
A	-10	SER	-	expression tag	UNP Q68GS1
A	-9	GLY	-	expression tag	UNP Q68GS1
A	-8	HIS	-	expression tag	UNP Q68GS1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ILE	-	expression tag	UNP Q68GS1
A	-6	ASP	-	expression tag	UNP Q68GS1
A	-5	ASP	-	expression tag	UNP Q68GS1
A	-4	ASP	-	expression tag	UNP Q68GS1
A	-3	ASP	-	expression tag	UNP Q68GS1
A	-2	LYS	-	expression tag	UNP Q68GS1
A	-1	HIS	-	expression tag	UNP Q68GS1
B	-23	MET	-	initiating methionine	UNP Q68GS1
B	-22	GLY	-	expression tag	UNP Q68GS1
B	-21	HIS	-	expression tag	UNP Q68GS1
B	-20	HIS	-	expression tag	UNP Q68GS1
B	-19	HIS	-	expression tag	UNP Q68GS1
B	-18	HIS	-	expression tag	UNP Q68GS1
B	-17	HIS	-	expression tag	UNP Q68GS1
B	-16	HIS	-	expression tag	UNP Q68GS1
B	-15	HIS	-	expression tag	UNP Q68GS1
B	-14	HIS	-	expression tag	UNP Q68GS1
B	-13	HIS	-	expression tag	UNP Q68GS1
B	-12	HIS	-	expression tag	UNP Q68GS1
B	-11	SER	-	expression tag	UNP Q68GS1
B	-10	SER	-	expression tag	UNP Q68GS1
B	-9	GLY	-	expression tag	UNP Q68GS1
B	-8	HIS	-	expression tag	UNP Q68GS1
B	-7	ILE	-	expression tag	UNP Q68GS1
B	-6	ASP	-	expression tag	UNP Q68GS1
B	-5	ASP	-	expression tag	UNP Q68GS1
B	-4	ASP	-	expression tag	UNP Q68GS1
B	-3	ASP	-	expression tag	UNP Q68GS1
B	-2	LYS	-	expression tag	UNP Q68GS1
B	-1	HIS	-	expression tag	UNP Q68GS1
C	-23	MET	-	initiating methionine	UNP Q68GS1
C	-22	GLY	-	expression tag	UNP Q68GS1
C	-21	HIS	-	expression tag	UNP Q68GS1
C	-20	HIS	-	expression tag	UNP Q68GS1
C	-19	HIS	-	expression tag	UNP Q68GS1
C	-18	HIS	-	expression tag	UNP Q68GS1
C	-17	HIS	-	expression tag	UNP Q68GS1
C	-16	HIS	-	expression tag	UNP Q68GS1
C	-15	HIS	-	expression tag	UNP Q68GS1
C	-14	HIS	-	expression tag	UNP Q68GS1
C	-13	HIS	-	expression tag	UNP Q68GS1
C	-12	HIS	-	expression tag	UNP Q68GS1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	SER	-	expression tag	UNP Q68GS1
C	-10	SER	-	expression tag	UNP Q68GS1
C	-9	GLY	-	expression tag	UNP Q68GS1
C	-8	HIS	-	expression tag	UNP Q68GS1
C	-7	ILE	-	expression tag	UNP Q68GS1
C	-6	ASP	-	expression tag	UNP Q68GS1
C	-5	ASP	-	expression tag	UNP Q68GS1
C	-4	ASP	-	expression tag	UNP Q68GS1
C	-3	ASP	-	expression tag	UNP Q68GS1
C	-2	LYS	-	expression tag	UNP Q68GS1
C	-1	HIS	-	expression tag	UNP Q68GS1
D	-23	MET	-	initiating methionine	UNP Q68GS1
D	-22	GLY	-	expression tag	UNP Q68GS1
D	-21	HIS	-	expression tag	UNP Q68GS1
D	-20	HIS	-	expression tag	UNP Q68GS1
D	-19	HIS	-	expression tag	UNP Q68GS1
D	-18	HIS	-	expression tag	UNP Q68GS1
D	-17	HIS	-	expression tag	UNP Q68GS1
D	-16	HIS	-	expression tag	UNP Q68GS1
D	-15	HIS	-	expression tag	UNP Q68GS1
D	-14	HIS	-	expression tag	UNP Q68GS1
D	-13	HIS	-	expression tag	UNP Q68GS1
D	-12	HIS	-	expression tag	UNP Q68GS1
D	-11	SER	-	expression tag	UNP Q68GS1
D	-10	SER	-	expression tag	UNP Q68GS1
D	-9	GLY	-	expression tag	UNP Q68GS1
D	-8	HIS	-	expression tag	UNP Q68GS1
D	-7	ILE	-	expression tag	UNP Q68GS1
D	-6	ASP	-	expression tag	UNP Q68GS1
D	-5	ASP	-	expression tag	UNP Q68GS1
D	-4	ASP	-	expression tag	UNP Q68GS1
D	-3	ASP	-	expression tag	UNP Q68GS1
D	-2	LYS	-	expression tag	UNP Q68GS1
D	-1	HIS	-	expression tag	UNP Q68GS1
E	-23	MET	-	initiating methionine	UNP Q68GS1
E	-22	GLY	-	expression tag	UNP Q68GS1
E	-21	HIS	-	expression tag	UNP Q68GS1
E	-20	HIS	-	expression tag	UNP Q68GS1
E	-19	HIS	-	expression tag	UNP Q68GS1
E	-18	HIS	-	expression tag	UNP Q68GS1
E	-17	HIS	-	expression tag	UNP Q68GS1
E	-16	HIS	-	expression tag	UNP Q68GS1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	HIS	-	expression tag	UNP Q68GS1
E	-14	HIS	-	expression tag	UNP Q68GS1
E	-13	HIS	-	expression tag	UNP Q68GS1
E	-12	HIS	-	expression tag	UNP Q68GS1
E	-11	SER	-	expression tag	UNP Q68GS1
E	-10	SER	-	expression tag	UNP Q68GS1
E	-9	GLY	-	expression tag	UNP Q68GS1
E	-8	HIS	-	expression tag	UNP Q68GS1
E	-7	ILE	-	expression tag	UNP Q68GS1
E	-6	ASP	-	expression tag	UNP Q68GS1
E	-5	ASP	-	expression tag	UNP Q68GS1
E	-4	ASP	-	expression tag	UNP Q68GS1
E	-3	ASP	-	expression tag	UNP Q68GS1
E	-2	LYS	-	expression tag	UNP Q68GS1
E	-1	HIS	-	expression tag	UNP Q68GS1
F	-23	MET	-	initiating methionine	UNP Q68GS1
F	-22	GLY	-	expression tag	UNP Q68GS1
F	-21	HIS	-	expression tag	UNP Q68GS1
F	-20	HIS	-	expression tag	UNP Q68GS1
F	-19	HIS	-	expression tag	UNP Q68GS1
F	-18	HIS	-	expression tag	UNP Q68GS1
F	-17	HIS	-	expression tag	UNP Q68GS1
F	-16	HIS	-	expression tag	UNP Q68GS1
F	-15	HIS	-	expression tag	UNP Q68GS1
F	-14	HIS	-	expression tag	UNP Q68GS1
F	-13	HIS	-	expression tag	UNP Q68GS1
F	-12	HIS	-	expression tag	UNP Q68GS1
F	-11	SER	-	expression tag	UNP Q68GS1
F	-10	SER	-	expression tag	UNP Q68GS1
F	-9	GLY	-	expression tag	UNP Q68GS1
F	-8	HIS	-	expression tag	UNP Q68GS1
F	-7	ILE	-	expression tag	UNP Q68GS1
F	-6	ASP	-	expression tag	UNP Q68GS1
F	-5	ASP	-	expression tag	UNP Q68GS1
F	-4	ASP	-	expression tag	UNP Q68GS1
F	-3	ASP	-	expression tag	UNP Q68GS1
F	-2	LYS	-	expression tag	UNP Q68GS1
F	-1	HIS	-	expression tag	UNP Q68GS1
G	-23	MET	-	initiating methionine	UNP Q68GS1
G	-22	GLY	-	expression tag	UNP Q68GS1
G	-21	HIS	-	expression tag	UNP Q68GS1
G	-20	HIS	-	expression tag	UNP Q68GS1

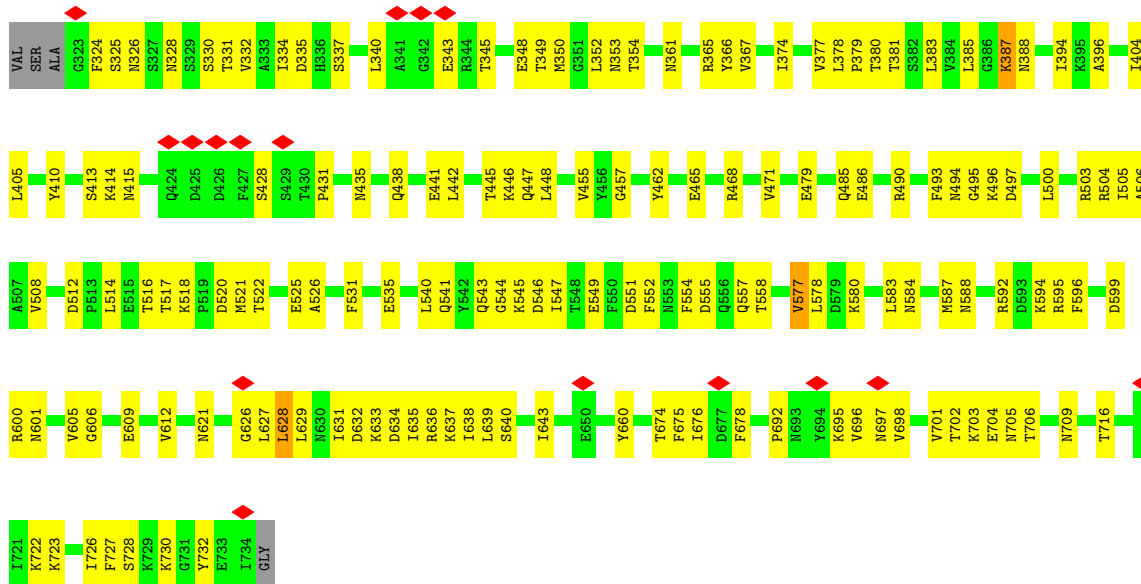
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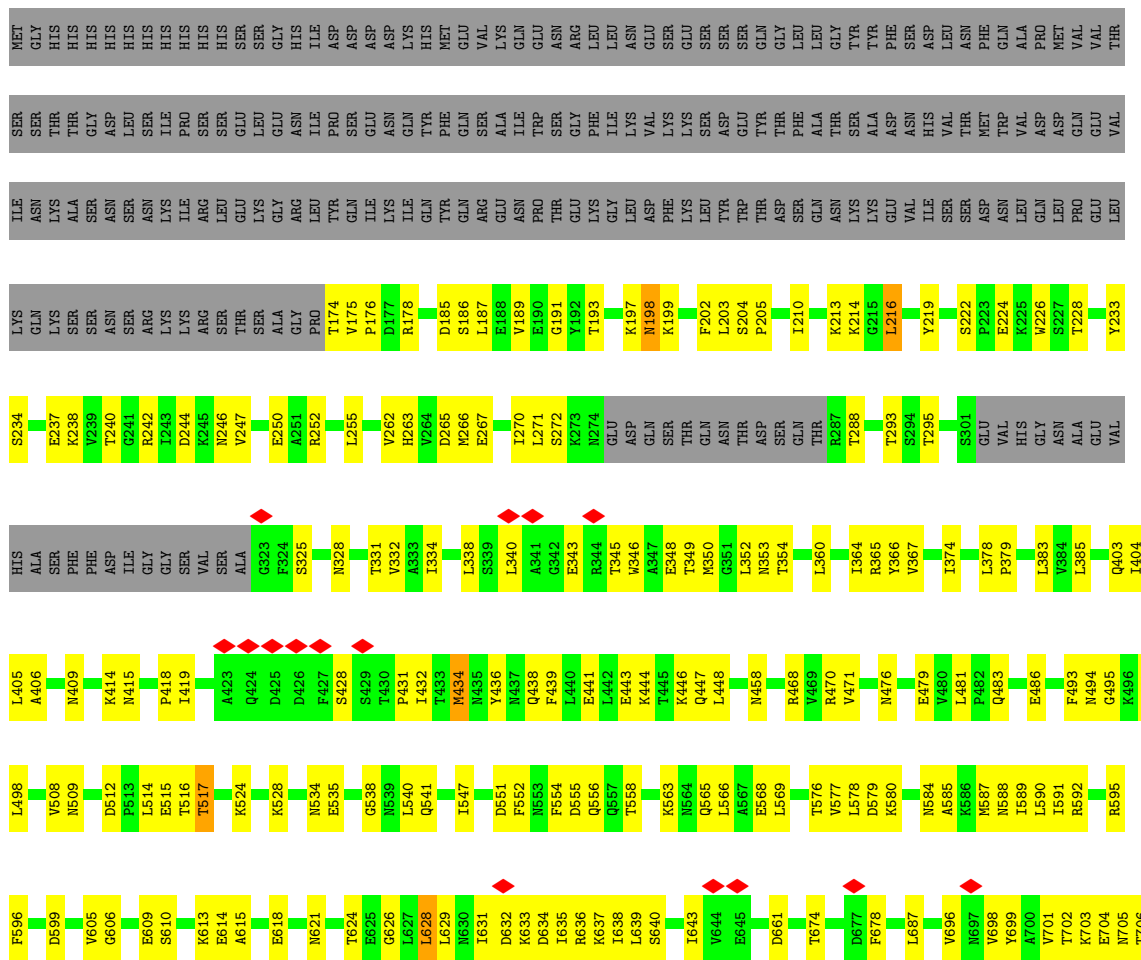
Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	HIS	-	expression tag	UNP Q68GS1
G	-18	HIS	-	expression tag	UNP Q68GS1
G	-17	HIS	-	expression tag	UNP Q68GS1
G	-16	HIS	-	expression tag	UNP Q68GS1
G	-15	HIS	-	expression tag	UNP Q68GS1
G	-14	HIS	-	expression tag	UNP Q68GS1
G	-13	HIS	-	expression tag	UNP Q68GS1
G	-12	HIS	-	expression tag	UNP Q68GS1
G	-11	SER	-	expression tag	UNP Q68GS1
G	-10	SER	-	expression tag	UNP Q68GS1
G	-9	GLY	-	expression tag	UNP Q68GS1
G	-8	HIS	-	expression tag	UNP Q68GS1
G	-7	ILE	-	expression tag	UNP Q68GS1
G	-6	ASP	-	expression tag	UNP Q68GS1
G	-5	ASP	-	expression tag	UNP Q68GS1
G	-4	ASP	-	expression tag	UNP Q68GS1
G	-3	ASP	-	expression tag	UNP Q68GS1
G	-2	LYS	-	expression tag	UNP Q68GS1
G	-1	HIS	-	expression tag	UNP Q68GS1

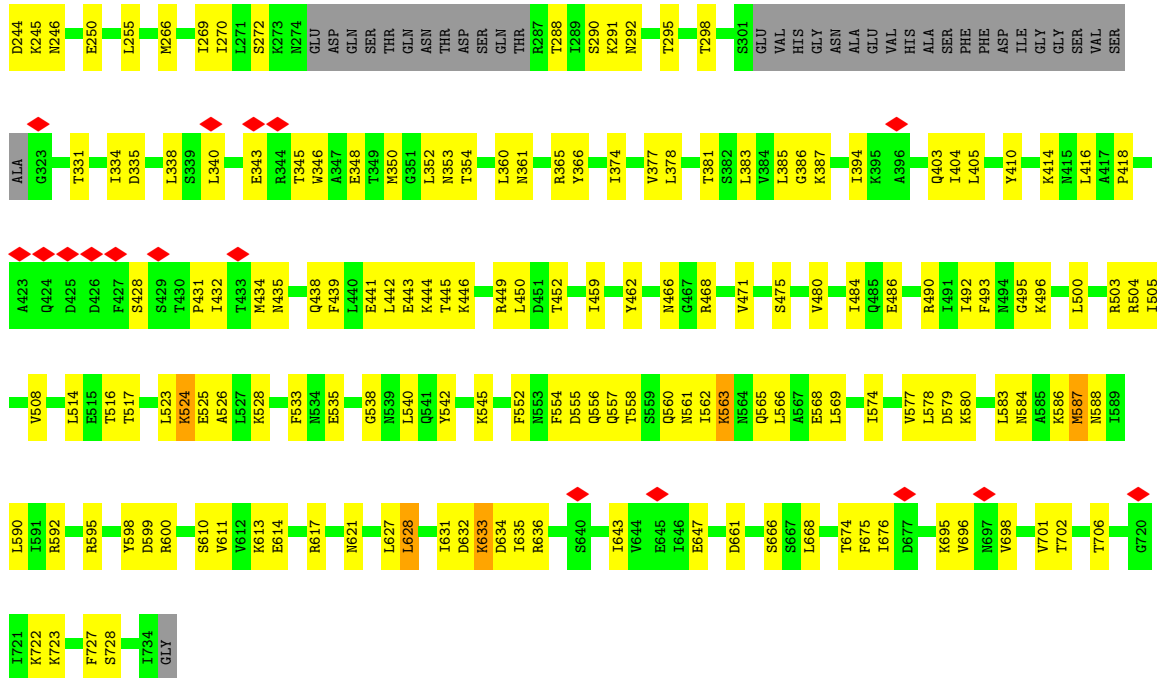
- Molecule 2 is a protein called Lethal factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	699	Total	C	N	O	S	0	0
			5401	3417	913	1065	6		
2	I	710	Total	C	N	O	S	0	0
			4734	2978	841	911	4		
2	J	661	Total	C	N	O	S	0	0
			4318	2717	758	841	2		

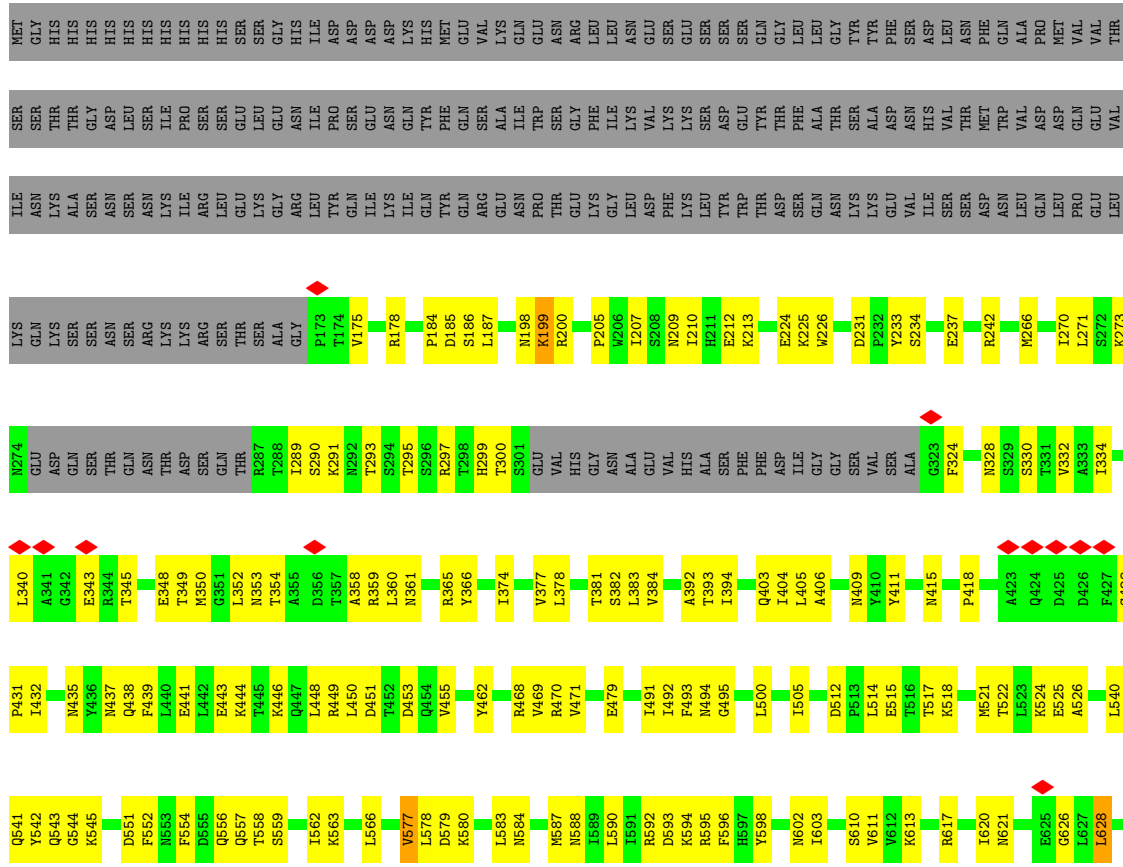


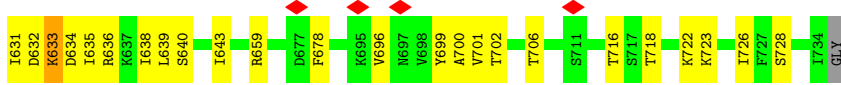
● Molecule 1: Protective antigen



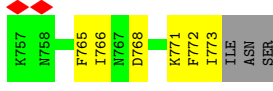
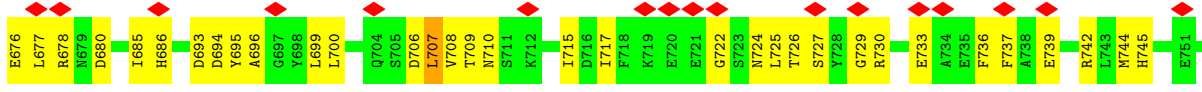
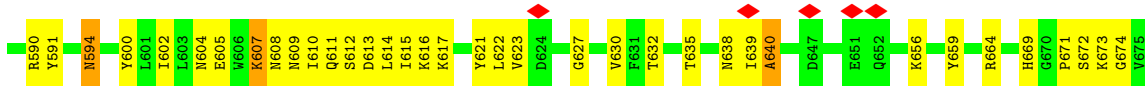
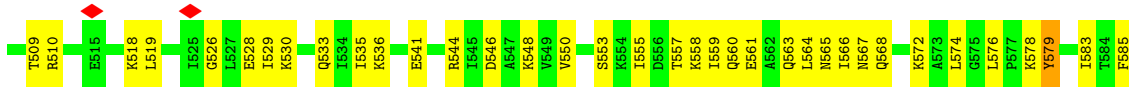
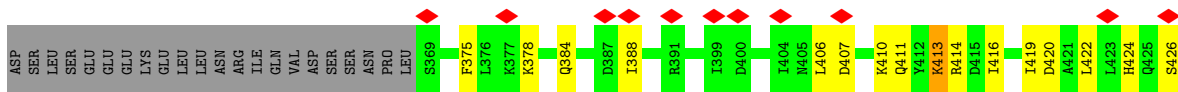
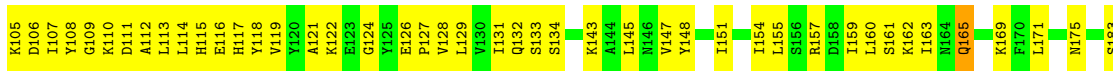
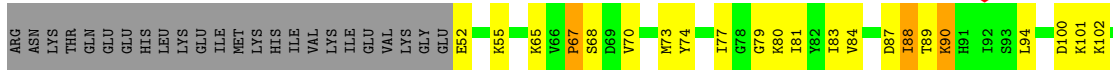
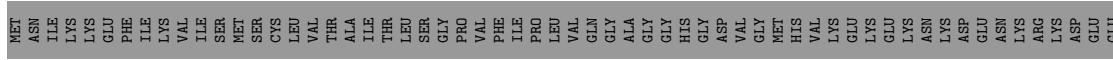


• Molecule 1: Protective antigen



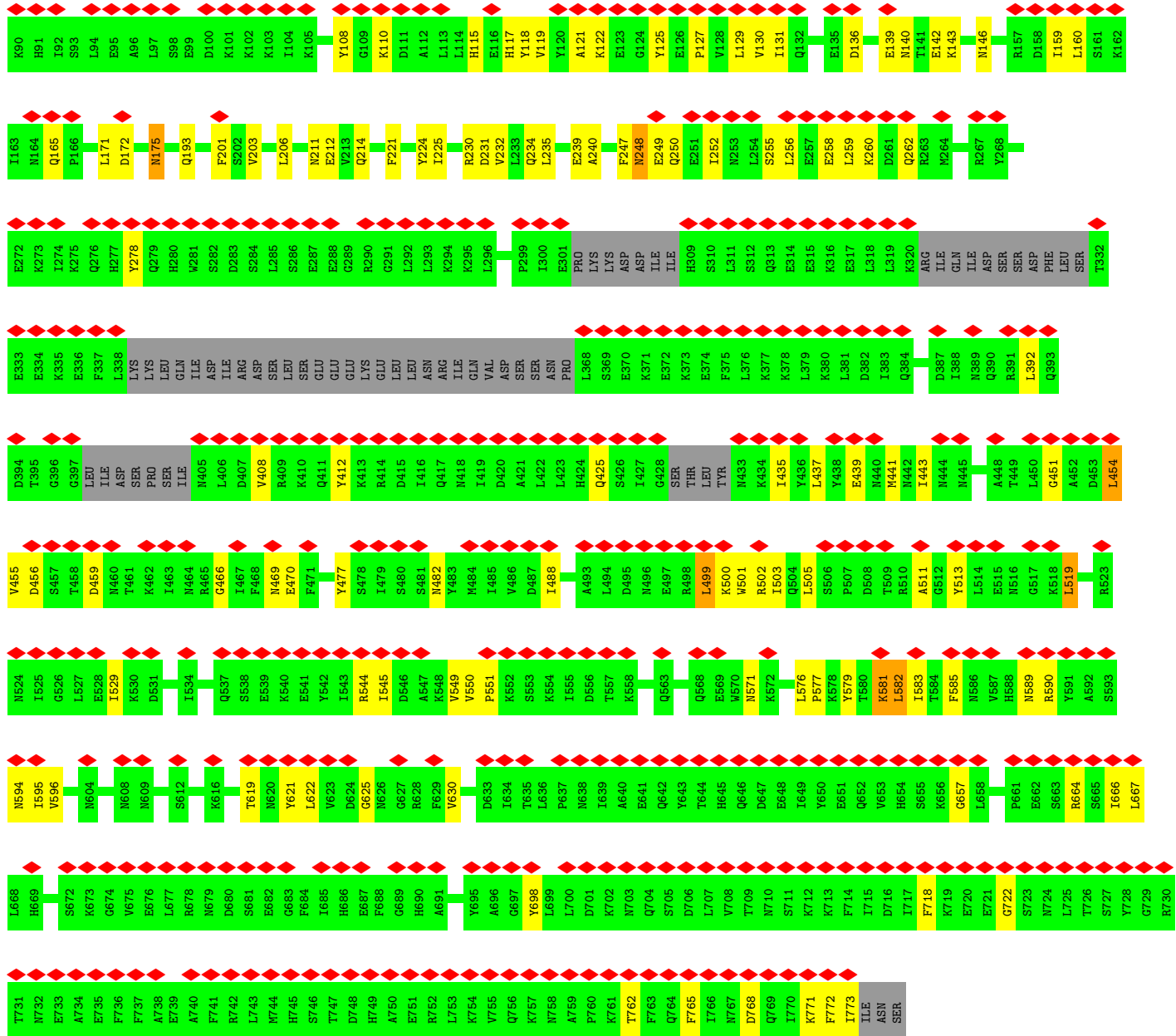


• Molecule 2: Lethal factor



• Molecule 2: Lethal factor





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	99000	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 ($e^-/\text{\AA}^2$)	74.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.696	Depositor
Minimum map value	-1.033	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	359.52002, 359.52002, 359.52002	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality i

5.1 Standard geometry i

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	0.62	1/4054 (0.0%)	0.68	3/5524 (0.1%)
1	B	0.65	1/4045 (0.0%)	0.70	5/5511 (0.1%)
1	C	0.63	0/4045	0.68	2/5511 (0.0%)
1	D	0.64	0/4037	0.72	4/5500 (0.1%)
1	E	0.60	0/4045	0.69	2/5511 (0.0%)
1	F	0.60	0/4045	0.68	3/5511 (0.1%)
1	G	0.61	0/4045	0.66	1/5511 (0.0%)
2	H	0.44	0/5499	0.67	3/7464 (0.0%)
2	I	0.40	0/4799	0.57	2/6559 (0.0%)
2	J	0.36	0/4380	0.59	7/6015 (0.1%)
All	All	0.56	2/42994 (0.0%)	0.66	32/58617 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	517	THR	C-N	-5.67	1.21	1.34
1	B	517	THR	C-N	-5.23	1.22	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	88	ILE	C-N-CA	14.34	157.54	121.70
2	J	499	LEU	CB-CG-CD2	-8.26	96.96	111.00
1	A	434	MET	CA-CB-CG	6.90	125.04	113.30
1	D	517	THR	C-N-CA	-6.83	104.64	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	628	LEU	CA-CB-CG	6.58	130.45	115.30
2	J	519	LEU	CA-CB-CG	6.53	130.32	115.30
1	F	587	MET	CB-CG-SD	-6.36	93.31	112.40
1	B	517	THR	C-N-CA	-6.33	105.89	121.70
1	D	216	LEU	CA-CB-CG	-6.13	101.20	115.30
1	A	517	THR	C-N-CA	-6.12	106.41	121.70
1	C	517	THR	C-N-CA	-6.04	106.60	121.70
1	E	517	THR	C-N-CA	-6.01	106.67	121.70
1	B	587	MET	CG-SD-CE	-6.00	90.59	100.20
1	B	216	LEU	CA-CB-CG	-5.96	101.58	115.30
2	J	67	PRO	CA-N-CD	-5.89	103.25	111.50
2	H	707	LEU	CA-CB-CG	5.80	128.65	115.30
1	A	527	LEU	CB-CG-CD1	-5.66	101.38	111.00
2	H	89	THR	O-C-N	5.61	131.68	122.70
2	J	67	PRO	N-CD-CG	-5.60	94.79	103.20
1	B	725	LEU	CA-CB-CG	5.58	128.14	115.30
1	D	628	LEU	CA-CB-CG	5.58	128.13	115.30
1	C	628	LEU	CA-CB-CG	5.52	128.00	115.30
1	F	517	THR	C-N-CA	-5.46	108.04	121.70
1	F	628	LEU	CA-CB-CG	5.45	127.84	115.30
2	J	454	LEU	CA-CB-CG	5.45	127.83	115.30
1	G	628	LEU	CA-CB-CG	5.39	127.70	115.30
1	E	628	LEU	CA-CB-CG	5.28	127.44	115.30
2	J	499	LEU	CA-CB-CG	5.25	127.37	115.30
1	D	434	MET	CA-CB-CG	5.24	122.20	113.30
2	I	235	LEU	CA-CB-CG	-5.23	103.27	115.30
2	J	172	ASP	CB-CG-OD2	5.20	122.98	118.30
2	I	172	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	165	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3984	0	3762	164	0
1	B	3977	0	3761	147	0
1	C	3977	0	3761	173	0
1	D	3970	0	3753	172	0
1	E	3977	0	3761	165	0
1	F	3977	0	3761	171	0
1	G	3977	0	3761	153	0
2	H	5401	0	5036	270	0
2	I	4734	0	3781	134	0
2	J	4318	0	3304	117	0
All	All	42292	0	38441	1610	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 20.

All (1610) 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:I:89:THR:CG2	2:I:115:HIS:HA	1.42	1.48
1:F:643:ILE:CD1	1:F:723:LYS:HD3	1.56	1.33
2:J:89:THR:CG2	2:J:115:HIS:HA	1.59	1.32
1:D:176:PRO:HG2	1:D:185:ASP:OD2	1.25	1.25
2:I:89:THR:HG21	2:I:115:HIS:CB	1.74	1.17
1:F:643:ILE:HD12	1:F:723:LYS:CD	1.73	1.17
2:I:89:THR:CG2	2:I:115:HIS:CA	2.26	1.14
2:J:89:THR:HG21	2:J:115:HIS:HA	1.32	1.12
1:D:176:PRO:CG	1:D:185:ASP:OD2	1.97	1.12
1:F:643:ILE:HD13	1:F:723:LYS:HD3	1.33	1.11
2:I:89:THR:HG21	2:I:115:HIS:CA	1.83	1.08
1:F:643:ILE:CD1	1:F:723:LYS:CD	2.29	1.08
2:I:89:THR:HG21	2:I:115:HIS:HA	1.36	1.05
1:E:721:ILE:HD11	1:E:723:LYS:HD3	1.32	1.05
1:C:643:ILE:CD1	1:C:723:LYS:HD3	1.87	1.05
2:H:578:LYS:CD	2:H:579:TYR:HE1	1.72	1.03
1:E:721:ILE:HG13	1:E:723:LYS:HG3	1.42	1.00
1:C:643:ILE:HD12	1:C:723:LYS:CD	1.91	1.00
1:F:291:LYS:HZ1	1:F:335:ASP:H	1.03	1.00
1:G:198:ASN:HB2	1:G:200:ARG:HH12	1.29	0.98
1:A:486:GLU:OE1	1:A:586:LYS:NZ	1.95	0.98
2:I:89:THR:HG21	2:I:115:HIS:HB3	1.48	0.96
2:I:89:THR:HG23	2:I:115:HIS:HA	1.44	0.96
1:C:643:ILE:HD12	1:C:723:LYS:HD3	1.43	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:89:THR:HG22	2:I:115:HIS:HA	1.49	0.95
2:H:578:LYS:HD3	2:H:579:TYR:HE1	1.28	0.95
1:E:291:LYS:HZ1	1:E:335:ASP:H	1.13	0.95
1:C:705:ASN:HD21	1:C:722:LYS:HB3	1.28	0.94
1:E:394:ILE:HD12	1:E:421:LEU:HD11	1.49	0.94
1:B:291:LYS:HZ1	1:B:335:ASP:H	1.15	0.93
1:A:210:ILE:O	1:A:214:LYS:NZ	2.03	0.92
1:D:176:PRO:HG2	1:D:185:ASP:CG	1.89	0.92
1:G:592:ARG:NH2	1:G:602:ASN:OD1	2.02	0.92
2:H:446:LEU:HD12	2:H:591:TYR:HB2	1.50	0.92
1:B:365:ARG:HE	1:B:418:PRO:HB3	1.37	0.90
1:B:428:SER:HB2	1:B:431:PRO:HG3	1.53	0.90
2:J:441:MET:HB3	2:J:499:LEU:HD22	1.54	0.90
1:A:225:LYS:HD3	1:A:514:LEU:HD21	1.53	0.89
1:D:643:ILE:HG13	1:D:723:LYS:HE2	1.52	0.89
2:J:278:TYR:CD1	2:J:513:TYR:HE2	1.90	0.88
1:C:490:ARG:HH21	1:C:504:ARG:HH22	1.17	0.88
2:J:499:LEU:HG	2:J:545:ILE:HD13	1.55	0.88
2:J:89:THR:HG21	2:J:115:HIS:CA	2.03	0.88
2:H:84:VAL:CG1	2:H:87:ASP:OD1	2.21	0.88
1:F:561:ASN:OD1	1:F:565:GLN:NE2	2.06	0.87
1:A:497:ASP:O	1:A:637:LYS:NZ	2.07	0.87
2:I:768:ASP:HA	2:I:771:LYS:HD2	1.56	0.87
2:H:639:ILE:HG13	2:H:640:ALA:H	1.38	0.86
2:J:89:THR:CG2	2:J:115:HIS:CA	2.51	0.86
1:A:189:VAL:O	1:A:220:LYS:NZ	2.08	0.86
1:B:497:ASP:O	1:B:637:LYS:NZ	2.08	0.86
1:B:394:ILE:HD12	1:B:421:LEU:HD11	1.57	0.86
2:H:578:LYS:HD3	2:H:579:TYR:CE1	2.10	0.85
2:H:739:GLU:HA	2:H:742:ARG:HH12	1.41	0.85
2:J:550:VAL:HG22	2:J:551:PRO:HD2	1.58	0.85
1:E:365:ARG:HH12	1:E:414:LYS:HA	1.39	0.84
1:F:386:GLY:O	1:F:449:ARG:NH1	2.09	0.84
2:I:451:GLY:HA2	2:I:454:LEU:HD23	1.59	0.84
1:E:225:LYS:HD3	1:E:514:LEU:HD21	1.59	0.84
2:J:278:TYR:CG	2:J:513:TYR:CE2	2.66	0.84
2:H:84:VAL:HG13	2:H:87:ASP:OD1	1.76	0.83
1:F:291:LYS:NZ	1:F:335:ASP:H	1.77	0.83
2:J:499:LEU:HD21	2:J:501:TRP:CD1	2.13	0.83
1:A:428:SER:HB2	1:A:431:PRO:HG3	1.61	0.83
1:G:515:GLU:OE1	1:G:518:LYS:NZ	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:226:GLU:OE2	2:I:229:HIS:ND1	2.09	0.83
1:A:291:LYS:HB2	1:A:334:ILE:HD11	1.61	0.82
1:A:599:ASP:OD1	1:A:600:ARG:N	2.10	0.82
2:H:578:LYS:NZ	2:H:579:TYR:CE1	2.47	0.82
2:H:424:HIS:O	2:H:510:ARG:NH2	2.12	0.82
2:J:768:ASP:HA	2:J:771:LYS:HD2	1.62	0.82
2:I:499:LEU:HD23	2:I:501:TRP:HE1	1.45	0.82
2:H:446:LEU:HD11	2:H:590:ARG:HB2	1.62	0.81
1:F:225:LYS:HD3	1:F:514:LEU:HD21	1.62	0.81
1:C:631:ILE:O	1:C:636:ARG:NH2	2.14	0.81
1:A:695:LYS:HA	1:A:730:LYS:HA	1.63	0.81
1:F:643:ILE:HD12	1:F:723:LYS:HD2	1.58	0.81
1:B:185:ASP:OD1	1:B:186:SER:N	2.14	0.81
2:J:621:TYR:O	2:J:664:ARG:NH2	2.14	0.81
2:H:81:ILE:HG22	2:H:129:LEU:HD21	1.61	0.81
2:H:578:LYS:HG2	2:H:579:TYR:CE1	2.16	0.81
1:E:721:ILE:CD1	1:E:723:LYS:HD3	2.10	0.80
1:F:428:SER:HB2	1:F:431:PRO:HG3	1.63	0.80
2:J:89:THR:HG22	2:J:115:HIS:HA	1.64	0.80
1:A:360:LEU:HB3	1:A:432:ILE:HG21	1.63	0.80
1:E:428:SER:HB2	1:E:431:PRO:HG3	1.64	0.80
1:F:365:ARG:HE	1:F:418:PRO:HB3	1.47	0.79
1:A:365:ARG:HE	1:A:418:PRO:HB3	1.47	0.78
1:B:695:LYS:HA	1:B:730:LYS:HA	1.65	0.78
2:I:81:ILE:HG22	2:I:129:LEU:HB3	1.65	0.78
1:E:592:ARG:NH2	1:E:602:ASN:OD1	2.17	0.78
1:G:428:SER:HB2	1:G:431:PRO:HG3	1.64	0.78
1:E:234:SER:N	1:E:237:GLU:OE2	2.16	0.78
1:B:374:ILE:HD11	1:B:405:LEU:HD12	1.65	0.77
1:F:631:ILE:H	1:F:636:ARG:HH22	1.33	0.77
1:C:428:SER:HB2	1:C:431:PRO:HG3	1.64	0.77
1:D:374:ILE:HD11	1:D:405:LEU:HD12	1.66	0.77
2:H:87:ASP:OD2	2:H:132:GLN:HB2	1.85	0.77
1:A:374:ILE:HD11	1:A:405:LEU:HD22	1.66	0.77
1:E:273:LYS:O	1:E:359:ARG:NH1	2.17	0.77
2:H:159:ILE:HG23	2:H:259:LEU:HD21	1.66	0.77
1:B:584:ASN:H	1:B:587:MET:HE3	1.49	0.76
1:F:250:GLU:OE2	1:F:503:ARG:NH2	2.18	0.76
2:I:169:LYS:HZ1	2:I:534:ILE:H	1.30	0.76
1:D:293:THR:HG22	1:D:334:ILE:HA	1.67	0.76
1:F:614:GLU:HA	1:F:617:ARG:HH12	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:278:TYR:CD1	2:J:513:TYR:CE2	2.73	0.76
2:J:622:LEU:HA	2:J:664:ARG:HH22	1.50	0.76
1:A:446:LYS:NZ	1:A:708:ILE:O	2.19	0.75
1:C:541:GLN:OE1	1:C:544:GLY:N	2.19	0.75
1:G:541:GLN:OE1	1:G:544:GLY:N	2.19	0.75
1:F:643:ILE:HD12	1:F:723:LYS:HD3	1.36	0.75
1:F:209:ASN:O	1:F:213:LYS:NZ	2.16	0.75
1:F:185:ASP:OD1	1:F:186:SER:N	2.19	0.75
1:D:428:SER:HB2	1:D:431:PRO:HG3	1.66	0.75
2:H:563:GLN:HE22	2:H:585:PHE:H	1.35	0.75
2:I:115:HIS:CE1	2:I:116:GLU:HG3	2.22	0.75
1:E:360:LEU:HB3	1:E:432:ILE:HG21	1.68	0.74
1:E:721:ILE:HG13	1:E:723:LYS:CG	2.16	0.74
1:F:524:LYS:NZ	1:F:525:GLU:OE2	2.14	0.74
1:F:562:ILE:HA	1:F:565:GLN:OE1	1.85	0.74
1:G:524:LYS:HG3	1:G:540:LEU:HD21	1.67	0.74
2:H:578:LYS:CD	2:H:579:TYR:CE1	2.64	0.74
1:F:595:ARG:HD2	1:F:611:VAL:HG11	1.68	0.74
1:E:185:ASP:OD1	1:E:186:SER:N	2.20	0.74
2:H:80:LYS:HB3	2:J:577:PRO:HB3	1.69	0.74
2:J:451:GLY:HA2	2:J:454:LEU:HD23	1.69	0.74
2:H:578:LYS:HG2	2:H:579:TYR:CD1	2.24	0.73
1:C:267:GLU:N	1:C:267:GLU:OE1	2.20	0.73
1:D:331:THR:HG23	1:D:447:GLN:HE21	1.53	0.73
1:D:468:ARG:HH12	1:D:470:ARG:HD2	1.54	0.73
2:I:583:ILE:HD13	2:I:629:PHE:HB2	1.71	0.73
1:D:365:ARG:HH12	1:D:414:LYS:HA	1.53	0.73
1:E:558:THR:HG21	1:E:588:ASN:H	1.53	0.73
1:G:209:ASN:O	1:G:213:LYS:NZ	2.20	0.73
2:J:499:LEU:HD21	2:J:501:TRP:HD1	1.54	0.73
1:E:541:GLN:HG2	1:E:546:ASP:HA	1.69	0.73
1:G:365:ARG:HE	1:G:418:PRO:HB3	1.54	0.73
2:H:578:LYS:CG	2:H:579:TYR:CE1	2.72	0.73
1:A:475:SER:OG	1:G:470:ARG:NH2	2.22	0.72
1:B:470:ARG:HA	1:C:479:GLU:OE1	1.89	0.72
1:A:185:ASP:OD1	1:A:186:SER:N	2.22	0.72
1:F:643:ILE:HD13	1:F:723:LYS:CD	2.11	0.72
1:A:187:LEU:HD11	1:A:205:PRO:HG3	1.72	0.72
1:D:471:VAL:HG12	1:E:479:GLU:OE2	1.89	0.72
1:C:558:THR:HG21	1:C:588:ASN:H	1.53	0.72
1:D:643:ILE:HG21	1:D:723:LYS:NZ	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:600:TYR:O	2:H:604:ASN:ND2	2.23	0.72
2:H:617:LYS:NZ	2:H:772:PHE:O	2.23	0.72
1:A:577:VAL:HG22	1:A:580:LYS:HB2	1.71	0.72
1:C:643:ILE:HD12	1:C:723:LYS:HD2	1.69	0.71
1:A:541:GLN:OE1	1:A:544:GLY:N	2.24	0.71
2:H:739:GLU:HA	2:H:742:ARG:NH1	2.06	0.71
1:F:592:ARG:HD2	1:F:598:TYR:CE2	2.26	0.71
1:G:583:LEU:HA	1:G:587:MET:HE1	1.71	0.71
1:E:695:LYS:HA	1:E:730:LYS:HA	1.72	0.71
1:E:698:VAL:HB	1:E:727:PHE:HB3	1.70	0.71
1:C:197:LYS:HB2	1:C:202:PHE:HE1	1.56	0.71
1:E:636:ARG:HG2	1:E:637:LYS:HZ3	1.55	0.71
1:G:225:LYS:HD3	1:G:514:LEU:HD21	1.72	0.71
1:C:584:ASN:H	1:C:587:MET:CE	2.03	0.70
1:D:434:MET:SD	1:D:438:GLN:HB2	2.31	0.70
1:D:558:THR:HG21	1:D:588:ASN:H	1.57	0.70
1:G:374:ILE:HD11	1:G:405:LEU:HD22	1.72	0.70
2:H:157:ARG:NH2	2:H:211:ASN:OD1	2.24	0.70
1:A:297:ARG:NH1	1:A:328:ASN:OD1	2.24	0.70
1:C:555:ASP:OD2	1:C:557:GLN:NE2	2.25	0.70
1:G:435:ASN:OD1	1:G:437:ASN:ND2	2.24	0.70
2:H:190:PHE:O	2:H:195:LYS:NZ	2.24	0.70
1:G:435:ASN:CG	1:G:438:GLN:HE22	1.95	0.70
1:E:561:ASN:C	1:E:561:ASN:HD22	1.92	0.70
1:F:443:GLU:HA	1:F:446:LYS:NZ	2.07	0.70
1:A:470:ARG:NH1	1:A:471:VAL:O	2.24	0.70
2:J:89:THR:HG21	2:J:115:HIS:CG	2.26	0.70
1:G:366:TYR:CZ	1:G:378:LEU:HD21	2.25	0.70
2:H:226:GLU:OE1	2:H:229:HIS:N	2.25	0.70
1:C:415:ASN:ND2	1:D:325:SER:OG	2.25	0.70
1:B:291:LYS:NZ	1:B:335:ASP:H	1.89	0.69
1:C:387:LYS:HD2	1:C:388:ASN:HB2	1.73	0.69
2:J:762:THR:HA	2:J:765:PHE:CE1	2.27	0.69
2:H:768:ASP:HA	2:H:771:LYS:HD2	1.74	0.69
2:H:579:TYR:N	2:H:579:TYR:HD1	1.90	0.69
1:B:471:VAL:HG12	1:C:479:GLU:OE2	1.92	0.69
1:F:190:GLU:O	1:F:220:LYS:NZ	2.25	0.69
1:F:584:ASN:H	1:F:587:MET:CE	2.05	0.69
2:H:434:LYS:HE2	2:H:436:TYR:CZ	2.28	0.69
2:J:437:LEU:HD22	2:J:488:ILE:HA	1.73	0.69
1:G:212:GLU:OE1	1:G:212:GLU:N	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:117:HIS:NE2	2:J:119:VAL:O	2.25	0.69
1:D:497:ASP:O	1:D:637:LYS:NZ	2.25	0.69
1:E:189:VAL:O	1:E:220:LYS:NZ	2.20	0.68
1:C:187:LEU:HD11	1:C:205:PRO:HG3	1.74	0.68
1:D:178:ARG:NE	1:D:224:GLU:OE2	2.27	0.68
1:D:643:ILE:HG13	1:D:723:LYS:CE	2.22	0.68
1:E:583:LEU:HA	1:E:587:MET:HE1	1.74	0.68
1:G:185:ASP:OD1	1:G:186:SER:N	2.23	0.68
2:I:221:PHE:HA	2:I:244:MET:HE1	1.76	0.68
1:C:185:ASP:OD1	1:C:186:SER:N	2.26	0.68
1:F:360:LEU:HB3	1:F:432:ILE:HG21	1.75	0.68
1:B:210:ILE:HD11	2:H:188:LEU:HB2	1.76	0.68
1:G:443:GLU:HA	1:G:446:LYS:HE2	1.74	0.68
2:H:504:GLN:NE2	2:H:505:LEU:O	2.27	0.68
2:H:578:LYS:CG	2:H:579:TYR:HE1	2.06	0.68
1:G:643:ILE:HB	1:G:699:TYR:HB2	1.76	0.67
1:B:698:VAL:HB	1:B:727:PHE:HB3	1.75	0.67
1:C:410:TYR:HD2	1:C:414:LYS:HD3	1.59	0.67
1:A:698:VAL:HB	1:A:727:PHE:HB3	1.76	0.67
1:C:584:ASN:H	1:C:587:MET:HE2	1.59	0.67
2:H:504:GLN:HB3	2:H:548:LYS:HD2	1.74	0.67
1:A:552:PHE:HB3	1:A:554:PHE:CZ	2.29	0.67
1:C:262:VAL:O	1:C:328:ASN:ND2	2.27	0.67
1:E:266:MET:H	1:E:295:THR:HG21	1.58	0.67
1:D:266:MET:H	1:D:295:THR:HG21	1.57	0.67
2:H:121:ALA:HA	2:H:129:LEU:HA	1.77	0.67
1:B:699:TYR:CE1	1:B:725:LEU:HD13	2.29	0.67
2:H:579:TYR:CD1	2:H:579:TYR:N	2.63	0.67
1:C:226:TRP:CZ2	1:C:234:SER:HB3	2.30	0.67
2:H:406:LEU:HG	2:H:410:LYS:HE2	1.76	0.67
1:A:558:THR:HG21	1:A:588:ASN:H	1.59	0.67
2:H:550:VAL:HG23	2:H:555:ILE:HD11	1.77	0.67
2:I:278:TYR:HB2	2:I:513:TYR:CE2	2.30	0.66
2:J:89:THR:HG23	2:J:115:HIS:HA	1.72	0.66
2:J:278:TYR:CG	2:J:513:TYR:HE2	2.08	0.66
1:D:508:VAL:HG23	1:D:516:THR:HA	1.77	0.66
2:H:119:VAL:HG11	2:H:147:VAL:HG22	1.76	0.66
2:H:526:GLY:HA3	2:H:555:ILE:HD13	1.77	0.66
2:H:563:GLN:NE2	2:H:585:PHE:O	2.29	0.66
2:J:550:VAL:CG2	2:J:551:PRO:HD2	2.25	0.66
1:B:584:ASN:H	1:B:587:MET:CE	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:183:SER:HB2	2:H:186:GLN:HE21	1.60	0.66
1:B:200:ARG:HG2	1:C:178:ARG:HH22	1.60	0.66
1:E:524:LYS:HE3	1:E:579:ASP:HB3	1.78	0.66
2:H:122:LYS:HB3	2:H:128:VAL:H	1.60	0.66
2:H:578:LYS:HE3	2:I:63:LEU:CD2	2.26	0.66
2:H:622:LEU:HD11	2:H:664:ARG:O	1.95	0.66
2:J:249:GLU:HG2	2:J:250:GLN:HG3	1.78	0.66
1:D:577:VAL:HG22	1:D:580:LYS:HB2	1.78	0.66
1:G:577:VAL:HG22	1:G:580:LYS:HB2	1.77	0.66
1:E:197:LYS:HB2	1:E:202:PHE:HE1	1.61	0.66
2:H:491:ARG:HG2	2:H:492:PRO:HD2	1.78	0.65
2:H:111:ASP:OD1	2:H:112:ALA:N	2.30	0.65
1:C:365:ARG:NH2	1:C:413:SER:O	2.30	0.65
1:C:643:ILE:CD1	1:C:723:LYS:CD	2.60	0.65
1:D:509:ASN:HB3	1:D:515:GLU:HG2	1.77	0.65
2:J:544:ARG:HD3	2:J:545:ILE:N	2.12	0.65
1:B:555:ASP:OD1	1:B:556:GLN:N	2.30	0.65
1:D:643:ILE:HG21	1:D:723:LYS:HZ2	1.62	0.65
1:C:410:TYR:CD2	1:C:414:LYS:HD3	2.30	0.65
1:C:521:MET:HE3	1:C:583:LEU:HB2	1.79	0.65
1:D:698:VAL:HB	1:D:727:PHE:HB3	1.79	0.65
1:G:187:LEU:HD11	1:G:205:PRO:HG3	1.79	0.65
2:I:118:TYR:OH	2:I:146:ASN:OD1	2.15	0.65
2:J:630:VAL:N	2:J:666:ILE:O	2.29	0.65
1:A:479:GLU:OE2	1:G:471:VAL:HG12	1.96	0.64
1:B:568:GLU:HG2	1:B:569:LEU:HD22	1.77	0.64
1:D:476:ASN:HB2	1:D:479:GLU:OE1	1.98	0.64
1:D:534:ASN:OD1	1:D:541:GLN:NE2	2.29	0.64
1:F:698:VAL:HB	1:F:727:PHE:HB3	1.78	0.64
2:I:589:ASN:OD1	2:I:590:ARG:N	2.28	0.64
1:E:291:LYS:NZ	1:E:335:ASP:H	1.92	0.64
1:C:577:VAL:HG22	1:C:580:LYS:HB2	1.78	0.64
2:H:118:TYR:HB2	2:H:132:GLN:HB3	1.80	0.64
2:I:762:THR:HA	2:I:765:PHE:CE1	2.32	0.64
1:C:705:ASN:ND2	1:C:722:LYS:O	2.31	0.64
1:D:584:ASN:H	1:D:587:MET:CE	2.10	0.64
2:H:171:LEU:O	2:H:175:ASN:ND2	2.30	0.64
1:C:508:VAL:HG23	1:C:516:THR:HA	1.79	0.64
1:F:555:ASP:OD1	1:F:556:GLN:N	2.29	0.64
2:H:129:LEU:HD23	2:H:129:LEU:H	1.60	0.64
2:H:727:SER:HA	2:H:730:ARG:HD3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:PRO:HG2	1:B:541:GLN:HE21	1.63	0.64
1:D:512:ASP:HB3	1:D:515:GLU:HB3	1.80	0.64
1:F:387:LYS:O	1:F:449:ARG:NH2	2.30	0.64
1:B:265:ASP:OD1	1:B:295:THR:OG1	2.11	0.63
1:D:202:PHE:HE2	1:D:204:SER:HB3	1.63	0.63
2:H:226:GLU:OE1	2:H:229:HIS:ND1	2.23	0.63
2:H:706:ASP:OD2	2:H:707:LEU:N	2.31	0.63
1:A:523:LEU:HD23	1:A:527:LEU:HD11	1.81	0.63
2:I:270:LYS:HZ3	2:I:488:ILE:HG22	1.62	0.63
2:H:434:LYS:HE2	2:H:436:TYR:CE2	2.33	0.63
1:A:336:HIS:HB2	1:A:446:LYS:HZ2	1.63	0.63
1:D:470:ARG:HA	1:E:479:GLU:OE1	1.98	0.63
1:E:560:GLN:O	1:E:563:LYS:HG3	1.99	0.63
1:G:638:ILE:HG13	1:G:639:LEU:HD12	1.80	0.63
2:H:207:GLU:OE2	2:H:536:LYS:HE3	1.99	0.63
1:B:626:GLY:HA2	1:B:678:PHE:CE2	2.34	0.63
1:C:380:THR:HG22	1:C:396:ALA:HB2	1.81	0.63
1:C:551:ASP:OD1	1:C:552:PHE:N	2.32	0.63
1:E:383:LEU:HD11	1:E:448:LEU:HD23	1.80	0.63
1:D:202:PHE:CE2	1:D:204:SER:HB3	2.34	0.63
1:D:568:GLU:HG2	1:D:569:LEU:HD22	1.81	0.63
2:J:502:ARG:NH2	2:J:544:ARG:HH12	1.96	0.63
2:H:83:ILE:HG22	2:H:131:ILE:HD11	1.81	0.62
1:C:291:LYS:HB3	1:C:335:ASP:OD1	1.99	0.62
1:E:291:LYS:HE2	1:E:335:ASP:HB3	1.80	0.62
2:H:255:SER:O	2:H:258:GLU:HG3	1.99	0.62
2:H:563:GLN:HE22	2:H:585:PHE:N	1.96	0.62
1:A:266:MET:H	1:A:295:THR:HG21	1.64	0.62
1:B:550:PHE:O	1:B:575:TYR:OH	2.17	0.62
1:B:558:THR:HG21	1:B:588:ASN:H	1.63	0.62
1:F:291:LYS:HZ2	1:F:334:ILE:HG23	1.63	0.62
1:G:234:SER:OG	1:G:237:GLU:HG2	1.99	0.62
1:F:722:LYS:NZ	1:F:723:LYS:O	2.33	0.62
2:J:581:LYS:C	2:J:583:ILE:H	2.02	0.62
1:D:584:ASN:H	1:D:587:MET:HE1	1.64	0.62
2:H:183:SER:CB	2:H:186:GLN:HE21	2.13	0.62
2:H:639:ILE:HG13	2:H:640:ALA:N	2.13	0.62
1:G:266:MET:H	1:G:295:THR:HG21	1.63	0.62
1:A:394:ILE:HD12	1:A:421:LEU:HD11	1.81	0.62
1:B:226:TRP:CZ2	1:B:234:SER:HB3	2.35	0.62
1:F:374:ILE:HD11	1:F:405:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:34:GLU:O	2:I:37:LYS:HG2	1.99	0.62
1:C:705:ASN:ND2	1:C:722:LYS:HB3	2.10	0.62
1:D:187:LEU:HD21	1:D:205:PRO:HG3	1.82	0.62
2:H:427:ILE:HG21	2:H:505:LEU:HD12	1.82	0.62
2:H:427:ILE:HG12	2:H:505:LEU:HD11	1.82	0.62
2:H:578:LYS:HE3	2:I:63:LEU:HD21	1.81	0.62
1:A:498:LEU:HB2	1:A:637:LYS:NZ	2.15	0.61
2:I:63:LEU:O	2:I:66:VAL:HG12	2.00	0.61
1:B:415:ASN:ND2	1:C:325:SER:OG	2.33	0.61
1:E:599:ASP:HB3	1:E:605:VAL:HG21	1.83	0.61
2:H:574:LEU:HD11	2:H:615:ILE:HG22	1.82	0.61
2:J:175:ASN:C	2:J:175:ASN:HD22	2.04	0.61
1:A:267:GLU:OE2	1:A:267:GLU:N	2.33	0.61
1:B:360:LEU:HB3	1:B:432:ILE:HG21	1.82	0.61
1:D:197:LYS:HD3	1:D:198:ASN:OD1	2.01	0.61
1:D:233:TYR:HB2	1:D:238:LYS:HZ2	1.64	0.61
1:D:705:ASN:ND2	1:D:722:LYS:O	2.33	0.61
1:E:291:LYS:HZ1	1:E:335:ASP:N	1.92	0.61
1:E:546:ASP:OD1	1:E:547:ILE:N	2.33	0.61
1:F:617:ARG:NH1	1:F:617:ARG:HB2	2.15	0.61
1:C:506:ALA:HB1	1:C:518:LYS:HE3	1.81	0.61
1:G:295:THR:HG22	1:G:332:VAL:HG23	1.82	0.61
2:H:55:LYS:HE2	2:H:134:SER:HA	1.82	0.61
1:A:336:HIS:CB	1:A:446:LYS:HZ2	2.13	0.61
1:C:326:ASN:HB3	1:C:490:ARG:HH22	1.65	0.61
1:C:595:ARG:HG3	1:C:596:PHE:CD1	2.35	0.61
1:D:176:PRO:HG3	1:D:185:ASP:OD2	1.97	0.61
1:C:265:ASP:OD1	1:C:295:THR:OG1	2.16	0.61
1:F:233:TYR:HB2	1:F:238:LYS:NZ	2.16	0.61
2:I:576:LEU:HD21	2:I:619:THR:HB	1.82	0.61
1:A:213:LYS:HG3	1:A:214:LYS:HD3	1.83	0.61
2:H:160:LEU:HB3	2:H:165:GLN:O	2.01	0.61
1:A:459:ILE:HD12	1:A:475:SER:HB3	1.83	0.60
1:A:555:ASP:OD1	1:A:556:GLN:N	2.33	0.60
2:H:459:ASP:OD1	2:H:461:THR:OG1	2.15	0.60
2:H:469:ASN:OD1	2:H:472:LYS:NZ	2.33	0.60
2:H:707:LEU:HD23	2:H:709:THR:HG22	1.82	0.60
2:J:89:THR:HG21	2:J:115:HIS:CB	2.30	0.60
1:C:599:ASP:OD1	1:C:600:ARG:N	2.31	0.60
2:J:278:TYR:CE1	2:J:513:TYR:HE2	2.19	0.60
1:G:270:ILE:HG13	1:G:361:ASN:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:63:LEU:O	2:J:66:VAL:HG22	2.01	0.60
1:B:195:ASP:OD2	2:H:236:TYR:OH	2.19	0.60
1:D:458:ASN:OD1	1:D:476:ASN:ND2	2.34	0.60
1:D:705:ASN:HD21	1:D:722:LYS:HB3	1.67	0.60
1:B:536:PRO:HG2	1:B:541:GLN:NE2	2.16	0.60
1:C:521:MET:SD	1:C:526:ALA:HB2	2.41	0.60
1:C:366:TYR:HD2	1:C:378:LEU:HD11	1.65	0.60
1:F:226:TRP:CZ2	1:F:234:SER:HB3	2.36	0.60
1:B:633:LYS:HA	1:B:636:ARG:NH1	2.17	0.60
1:E:197:LYS:O	1:E:200:ARG:N	2.33	0.60
1:F:272:SER:HB3	1:F:288:THR:HG22	1.83	0.60
1:F:584:ASN:H	1:F:587:MET:HE1	1.65	0.60
2:H:463:ILE:N	2:H:541:GLU:OE1	2.34	0.60
2:I:587:VAL:O	2:I:588:HIS:ND1	2.35	0.60
1:A:242:ARG:HB3	1:A:462:TYR:CE2	2.36	0.60
1:B:353:ASN:OD1	1:B:354:THR:N	2.34	0.60
1:D:233:TYR:HB2	1:D:238:LYS:NZ	2.17	0.60
1:F:266:MET:H	1:F:295:THR:HG21	1.65	0.60
1:C:490:ARG:NH2	1:C:504:ARG:HH22	1.96	0.60
1:F:200:ARG:HG2	1:G:178:ARG:NH1	2.17	0.60
1:G:505:ILE:HD13	1:G:526:ALA:HB1	1.82	0.60
2:H:478:SER:OG	2:H:590:ARG:NH2	2.35	0.60
1:C:353:ASN:OD1	1:C:354:THR:N	2.35	0.60
1:D:265:ASP:OD1	1:D:295:THR:OG1	2.14	0.60
2:H:124:GLY:N	2:H:127:PRO:HG3	2.16	0.60
1:C:300:THR:O	1:C:324:PHE:HB3	2.01	0.59
2:H:202:SER:OG	2:H:204:GLU:HG3	2.01	0.59
2:J:499:LEU:CD2	2:J:501:TRP:HD1	2.14	0.59
1:D:198:ASN:O	1:D:199:LYS:HD2	2.02	0.59
1:D:353:ASN:OD1	1:D:354:THR:N	2.35	0.59
1:E:226:TRP:CZ2	1:E:234:SER:HB3	2.37	0.59
1:F:443:GLU:HA	1:F:446:LYS:HZ1	1.66	0.59
1:F:444:LYS:HG3	1:F:445:THR:HG23	1.83	0.59
1:C:612:VAL:HG12	1:C:726:ILE:HD11	1.83	0.59
1:D:639:LEU:N	1:D:703:LYS:HZ3	2.00	0.59
1:E:183:ILE:HD11	1:E:236:PHE:HD1	1.66	0.59
1:B:634:ASP:O	1:B:637:LYS:HG2	2.03	0.59
1:E:626:GLY:HA2	1:E:678:PHE:HE2	1.68	0.59
1:C:705:ASN:HD21	1:C:722:LYS:CB	2.10	0.59
1:D:555:ASP:OD1	1:D:556:GLN:N	2.35	0.59
1:D:633:LYS:HA	1:D:636:ARG:NH2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:636:ARG:O	1:E:637:LYS:HD3	2.03	0.59
2:H:563:GLN:NE2	2:H:585:PHE:H	1.97	0.59
2:I:281:TRP:HH2	2:I:423:LEU:HD23	1.67	0.59
1:D:610:SER:HA	1:D:613:LYS:NZ	2.17	0.59
1:D:634:ASP:OD2	1:D:635:ILE:N	2.36	0.59
2:I:435:ILE:O	2:I:505:LEU:HD22	2.03	0.59
2:J:502:ARG:HH21	2:J:544:ARG:HH12	1.50	0.59
1:G:631:ILE:O	1:G:636:ARG:NH1	2.35	0.59
2:H:190:PHE:HB2	2:H:194:LEU:HD12	1.84	0.59
2:H:506:SER:O	2:H:509:THR:HG22	2.03	0.59
1:B:334:ILE:CG1	1:B:446:LYS:HB2	2.33	0.59
1:C:605:VAL:HG22	1:C:704:GLU:HB3	1.85	0.59
2:H:465:ARG:HG2	2:H:465:ARG:HH11	1.67	0.59
2:H:480:SER:HA	2:H:590:ARG:HH12	1.68	0.59
2:H:678:ARG:HD2	2:H:678:ARG:N	2.18	0.59
2:J:571:ASN:HA	2:J:576:LEU:HB2	1.83	0.58
1:D:174:THR:O	1:D:174:THR:OG1	2.20	0.58
1:F:647:GLU:N	1:F:695:LYS:O	2.25	0.58
1:C:535:GLU:OE1	1:C:540:LEU:HD13	2.03	0.58
1:A:638:ILE:HG13	1:A:639:LEU:HD12	1.86	0.58
1:B:446:LYS:HZ1	1:B:708:ILE:HG21	1.68	0.58
1:E:626:GLY:HA2	1:E:678:PHE:CE2	2.39	0.58
1:F:560:GLN:O	1:F:563:LYS:HG3	2.03	0.58
2:H:610:ILE:HB	2:H:615:ILE:HD11	1.85	0.58
2:J:118:TYR:OH	2:J:146:ASN:HB2	2.04	0.58
1:B:269:ILE:HG22	1:B:362:ALA:HB2	1.85	0.58
2:H:80:LYS:H	2:H:128:VAL:HG12	1.69	0.58
2:I:169:LYS:HZ3	2:I:533:GLN:HB2	1.69	0.58
1:A:359:ARG:NH2	1:A:429:SER:O	2.37	0.58
1:B:626:GLY:HA2	1:B:678:PHE:HE2	1.68	0.58
1:A:479:GLU:OE1	1:G:470:ARG:HA	2.04	0.58
1:B:522:THR:OG1	1:B:525:GLU:OE1	2.16	0.58
1:C:340:LEU:O	1:C:343:GLU:HG2	2.03	0.58
2:J:89:THR:HG21	2:J:115:HIS:CD2	2.39	0.58
1:A:353:ASN:OD1	1:A:354:THR:N	2.36	0.57
2:J:392:LEU:HD23	2:J:482:ASN:HA	1.86	0.57
1:D:365:ARG:NH1	1:D:414:LYS:HA	2.18	0.57
1:E:700:ALA:HB3	1:E:726:ILE:HG13	1.86	0.57
1:F:353:ASN:OD1	1:F:354:THR:N	2.36	0.57
1:D:244:ASP:OD2	1:D:246:ASN:HB2	2.04	0.57
1:G:330:SER:OG	1:G:450:LEU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:345:THR:O	1:G:348:GLU:HG3	2.04	0.57
1:G:403:GLN:N	1:G:403:GLN:OE1	2.37	0.57
2:H:578:LYS:C	2:H:579:TYR:HD1	2.07	0.57
1:A:506:ALA:HB1	1:A:518:LYS:HE3	1.86	0.57
1:E:365:ARG:NH1	1:E:414:LYS:HA	2.17	0.57
2:H:253:ASN:O	2:H:256:LEU:HG	2.03	0.57
1:A:300:THR:O	1:A:324:PHE:HB3	2.04	0.57
1:A:438:GLN:HA	1:A:441:GLU:OE1	2.04	0.57
1:D:628:LEU:HA	1:D:674:THR:O	2.04	0.57
1:E:443:GLU:O	1:E:446:LYS:NZ	2.35	0.57
1:G:551:ASP:OD1	1:G:552:PHE:N	2.37	0.57
2:H:656:LYS:HD2	2:H:672:SER:OG	2.05	0.57
1:E:187:LEU:HD11	1:E:205:PRO:HG3	1.85	0.57
2:H:80:LYS:HE2	2:J:577:PRO:HB2	1.86	0.57
2:H:578:LYS:NZ	2:H:579:TYR:CZ	2.72	0.57
2:H:686:HIS:HB2	2:H:742:ARG:HD3	1.86	0.57
1:B:449:ARG:HB3	1:B:449:ARG:HH11	1.69	0.57
1:D:360:LEU:HB3	1:D:432:ILE:HG21	1.87	0.57
1:E:634:ASP:OD1	1:E:635:ILE:N	2.38	0.57
1:G:403:GLN:NE2	1:G:411:TYR:OH	2.38	0.57
2:H:161:SER:OG	2:H:214:GLN:NE2	2.38	0.57
1:C:643:ILE:HD13	1:C:723:LYS:HD3	1.81	0.56
1:E:550:PHE:O	1:E:575:TYR:OH	2.18	0.56
1:A:403:GLN:HE21	1:B:453:ASP:HB2	1.69	0.56
1:A:633:LYS:HA	1:A:636:ARG:CZ	2.36	0.56
1:B:438:GLN:HA	1:B:441:GLU:OE2	2.05	0.56
1:B:638:ILE:HG13	1:B:639:LEU:HD12	1.86	0.56
1:D:438:GLN:O	1:D:441:GLU:HG3	2.04	0.56
1:E:584:ASN:O	1:E:587:MET:HE2	2.05	0.56
1:G:558:THR:HG21	1:G:588:ASN:H	1.70	0.56
2:I:516:ASN:OD1	2:I:518:LYS:HD3	2.06	0.56
2:H:469:ASN:HA	2:H:472:LYS:NZ	2.20	0.56
1:A:554:PHE:HB3	1:A:558:THR:OG1	2.04	0.56
1:A:627:LEU:O	1:A:675:PHE:HA	2.06	0.56
1:F:568:GLU:HG2	1:F:569:LEU:HD22	1.87	0.56
1:F:621:ASN:HB3	1:F:628:LEU:HG	1.88	0.56
1:G:382:SER:HA	1:G:393:THR:HA	1.88	0.56
2:H:77:ILE:O	2:H:126:GLU:HG3	2.06	0.56
2:H:530:LYS:HE2	2:H:546:ASP:OD2	2.06	0.56
2:I:762:THR:HA	2:I:765:PHE:HE1	1.70	0.56
2:J:657:GLY:HA3	2:J:667:LEU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:LYS:O	1:G:517:THR:HG23	2.05	0.56
1:A:493:PHE:CE2	1:A:495:GLY:HA3	2.40	0.56
1:D:334:ILE:O	1:D:446:LYS:HE3	2.05	0.56
1:E:345:THR:O	1:E:348:GLU:HG3	2.06	0.56
2:H:411:GLN:OE1	2:H:414:ARG:NH1	2.38	0.56
2:I:40:MET:O	2:I:44:VAL:HG12	2.05	0.56
1:A:224:GLU:OE2	1:G:242:ARG:NH1	2.36	0.56
1:A:336:HIS:HB2	1:A:446:LYS:NZ	2.21	0.56
1:F:345:THR:O	1:F:348:GLU:HG3	2.06	0.56
1:G:198:ASN:HB2	1:G:200:ARG:NH1	2.10	0.56
1:G:340:LEU:O	1:G:343:GLU:HG2	2.05	0.56
2:J:622:LEU:HA	2:J:664:ARG:NH2	2.21	0.56
1:A:233:TYR:HA	1:A:237:GLU:OE2	2.06	0.56
1:B:200:ARG:HG2	1:C:178:ARG:NH2	2.21	0.56
1:B:699:TYR:HE1	1:B:725:LEU:HD13	1.69	0.56
1:C:546:ASP:OD1	1:C:547:ILE:N	2.38	0.56
1:E:334:ILE:HD11	1:E:446:LYS:HD2	1.88	0.56
1:D:226:TRP:CZ2	1:D:234:SER:HB3	2.41	0.56
1:G:231:ASP:N	1:G:231:ASP:OD1	2.38	0.56
1:C:345:THR:O	1:C:348:GLU:HG3	2.07	0.55
1:E:183:ILE:HD12	1:E:203:LEU:HD22	1.88	0.55
1:G:453:ASP:OD2	1:G:455:VAL:HG12	2.05	0.55
1:C:270:ILE:HG12	1:C:361:ASN:O	2.06	0.55
1:E:353:ASN:OD1	1:E:354:THR:N	2.39	0.55
1:G:521:MET:SD	1:G:525:GLU:HG3	2.46	0.55
2:H:437:LEU:HD22	2:H:488:ILE:HA	1.88	0.55
1:F:542:TYR:O	1:F:545:LYS:NZ	2.25	0.55
1:F:634:ASP:OD1	1:F:635:ILE:N	2.40	0.55
1:A:183:ILE:H	1:A:183:ILE:HD12	1.71	0.55
1:A:234:SER:OG	1:A:237:GLU:HG2	2.07	0.55
1:F:200:ARG:HB3	1:G:178:ARG:HH22	1.71	0.55
2:H:74:TYR:CE1	2:H:79:GLY:HA3	2.42	0.55
1:A:434:MET:HE1	1:A:438:GLN:HB3	1.88	0.55
1:E:365:ARG:NH1	1:E:414:LYS:HD2	2.21	0.55
1:E:633:LYS:O	1:E:636:ARG:NH1	2.40	0.55
2:H:501:TRP:HB3	2:H:503:ILE:HD11	1.87	0.55
2:J:64:GLU:OE1	2:J:65:LYS:HD2	2.07	0.55
1:C:293:THR:HG22	1:C:334:ILE:HA	1.89	0.55
2:I:281:TRP:CH2	2:I:423:LEU:HD23	2.42	0.55
2:I:686:HIS:O	2:I:738:ALA:HB1	2.06	0.55
1:C:606:GLY:HA3	1:C:704:GLU:CD	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:ILE:HD11	1:F:236:PHE:HD1	1.71	0.55
1:F:599:ASP:OD1	1:F:600:ARG:N	2.35	0.55
2:J:443:ILE:HG21	2:J:454:LEU:HD21	1.89	0.55
1:A:568:GLU:HG2	1:A:569:LEU:HD22	1.88	0.54
1:C:493:PHE:CZ	1:C:495:GLY:HA3	2.42	0.54
1:E:552:PHE:HB3	1:E:554:PHE:CZ	2.42	0.54
2:H:286:SER:O	2:H:290:ARG:HG3	2.07	0.54
2:J:171:LEU:HD22	2:J:206:LEU:HD23	1.89	0.54
1:B:340:LEU:O	1:B:343:GLU:HG2	2.07	0.54
1:C:226:TRP:CH2	1:C:234:SER:HB3	2.42	0.54
1:D:621:ASN:HB3	1:D:628:LEU:HG	1.89	0.54
1:C:626:GLY:HA2	1:C:678:PHE:CE2	2.42	0.54
1:E:459:ILE:HD12	1:E:475:SER:HB3	1.88	0.54
2:H:122:LYS:N	2:H:128:VAL:O	2.37	0.54
2:H:478:SER:OG	2:H:590:ARG:HA	2.07	0.54
1:A:270:ILE:HG12	1:A:361:ASN:O	2.08	0.54
1:A:634:ASP:OD1	1:A:635:ILE:N	2.41	0.54
1:B:498:LEU:HB2	1:B:637:LYS:NZ	2.22	0.54
1:D:340:LEU:O	1:D:343:GLU:HG2	2.07	0.54
1:E:608:ASP:O	1:E:611:VAL:HG22	2.06	0.54
2:H:407:ASP:HA	2:H:410:LYS:HE3	1.90	0.54
2:I:115:HIS:ND1	2:I:116:GLU:HG3	2.21	0.54
2:J:454:LEU:HD12	2:J:455:VAL:HG13	1.88	0.54
1:A:377:VAL:O	1:A:378:LEU:HD12	2.08	0.54
1:D:565:GLN:HA	1:D:568:GLU:OE1	2.08	0.54
1:F:200:ARG:HG2	1:G:178:ARG:HH12	1.72	0.54
1:F:291:LYS:HZ1	1:F:335:ASP:N	1.88	0.54
1:F:480:VAL:HG12	1:F:484:ILE:HD11	1.89	0.54
2:H:113:LEU:HD22	2:H:115:HIS:HE1	1.72	0.54
2:H:528:GLU:OE2	2:H:548:LYS:HB2	2.07	0.54
1:A:226:TRP:CZ2	1:A:234:SER:HB3	2.42	0.54
1:A:535:GLU:OE2	1:A:540:LEU:HD12	2.08	0.54
2:H:285:LEU:O	2:H:290:ARG:NH2	2.40	0.54
1:E:524:LYS:CE	1:E:579:ASP:HB3	2.38	0.54
1:F:178:ARG:NE	1:F:224:GLU:OE2	2.41	0.54
1:G:634:ASP:OD1	1:G:635:ILE:N	2.41	0.54
2:I:528:GLU:O	2:I:548:LYS:HG2	2.07	0.54
1:A:524:LYS:HE2	1:A:540:LEU:HD11	1.90	0.54
1:D:365:ARG:HE	1:D:418:PRO:HB3	1.73	0.54
1:G:353:ASN:OD1	1:G:354:THR:N	2.38	0.54
2:H:250:GLN:N	2:H:250:GLN:OE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:584:ASN:H	1:F:587:MET:HE3	1.73	0.54
2:H:614:LEU:HD23	2:H:773:ILE:HD11	1.90	0.54
1:A:556:GLN:OE1	1:A:557:GLN:NE2	2.40	0.53
1:A:634:ASP:O	1:A:637:LYS:HG2	2.07	0.53
1:A:699:TYR:CD1	1:A:725:LEU:HA	2.43	0.53
2:H:555:ILE:HD12	2:H:555:ILE:H	1.73	0.53
1:B:441:GLU:HA	1:B:444:LYS:NZ	2.24	0.53
1:C:197:LYS:HB2	1:C:202:PHE:CE1	2.41	0.53
1:C:554:PHE:HB3	1:C:558:THR:OG1	2.09	0.53
1:D:441:GLU:O	1:D:444:LYS:HG2	2.09	0.53
1:D:524:LYS:HE3	1:D:579:ASP:CG	2.29	0.53
1:E:633:LYS:HA	1:E:636:ARG:NE	2.24	0.53
1:F:244:ASP:OD2	1:F:246:ASN:HB2	2.08	0.53
2:H:122:LYS:CB	2:H:128:VAL:H	2.21	0.53
2:H:535:ILE:HD13	2:H:544:ARG:HD3	1.89	0.53
2:H:656:LYS:HG3	2:H:674:GLY:HA2	1.90	0.53
2:J:67:PRO:O	2:J:70:VAL:HG22	2.08	0.53
1:A:718:THR:O	1:A:723:LYS:HE3	2.07	0.53
1:B:610:SER:HA	1:B:613:LYS:NZ	2.24	0.53
1:B:643:ILE:HG12	1:B:723:LYS:HE2	1.91	0.53
1:C:638:ILE:HG13	1:C:639:LEU:HD12	1.90	0.53
1:E:335:ASP:OD1	1:E:337:SER:N	2.40	0.53
1:E:561:ASN:C	1:E:561:ASN:ND2	2.61	0.53
1:F:577:VAL:HG22	1:F:580:LYS:HB2	1.90	0.53
1:G:293:THR:HG22	1:G:334:ILE:HD12	1.89	0.53
1:C:627:LEU:H	1:C:676:ILE:HG22	1.74	0.53
1:E:609:GLU:HG2	1:E:613:LYS:HZ1	1.73	0.53
1:G:381:THR:HG23	1:G:394:ILE:HD13	1.89	0.53
1:G:438:GLN:HA	1:G:441:GLU:OE2	2.09	0.53
2:H:419:ILE:HD13	2:H:422:LEU:HD12	1.91	0.53
2:I:531:ASP:OD1	2:I:532:VAL:N	2.41	0.53
1:D:234:SER:OG	1:D:237:GLU:HG2	2.09	0.53
1:B:187:LEU:HD11	1:B:205:PRO:HG3	1.89	0.53
1:C:637:LYS:HE2	1:C:637:LYS:HA	1.90	0.53
1:G:610:SER:O	1:G:613:LYS:HG2	2.09	0.53
1:C:366:TYR:CD2	1:C:378:LEU:HD11	2.43	0.53
1:F:269:ILE:HG22	1:F:270:ILE:N	2.23	0.53
1:G:493:PHE:CE2	1:G:495:GLY:HA3	2.44	0.53
2:I:122:LYS:HE3	2:I:128:VAL:HB	1.90	0.53
2:I:247:PHE:CE2	2:I:252:ILE:HD11	2.44	0.53
2:J:589:ASN:OD1	2:J:590:ARG:N	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:MET:O	1:A:352:LEU:N	2.42	0.53
1:C:238:LYS:HB3	1:C:252:ARG:O	2.09	0.53
1:C:634:ASP:OD1	1:C:635:ILE:N	2.42	0.53
1:F:209:ASN:OD1	1:F:210:ILE:HG12	2.09	0.53
1:F:291:LYS:NZ	1:F:292:ASN:O	2.39	0.53
2:H:73:MET:HB2	2:H:259:LEU:HD22	1.91	0.53
1:A:616:HIS:CD2	1:A:726:ILE:HD12	2.44	0.53
1:B:365:ARG:HH12	1:B:414:LYS:HA	1.74	0.53
1:G:722:LYS:NZ	1:G:723:LYS:O	2.42	0.53
1:A:237:GLU:HB2	1:A:242:ARG:O	2.08	0.53
1:E:508:VAL:HG23	1:E:516:THR:HA	1.89	0.53
2:H:676:GLU:HG2	2:H:677:LEU:N	2.24	0.53
2:H:707:LEU:HD23	2:H:709:THR:CG2	2.38	0.53
1:A:324:PHE:CZ	1:A:588:ASN:HB3	2.44	0.52
1:G:435:ASN:ND2	1:G:438:GLN:HE22	2.07	0.52
1:B:210:ILE:HD11	2:H:188:LEU:HD13	1.91	0.52
1:B:445:THR:O	1:B:446:LYS:HG2	2.09	0.52
1:C:435:ASN:ND2	1:C:438:GLN:HE22	2.07	0.52
1:D:643:ILE:HB	1:D:699:TYR:HB2	1.92	0.52
1:F:410:TYR:CE1	1:F:414:LYS:HE2	2.44	0.52
1:F:535:GLU:OE2	1:F:540:LEU:HD12	2.08	0.52
1:G:617:ARG:HG2	1:G:617:ARG:HH11	1.75	0.52
1:A:197:LYS:O	1:A:200:ARG:N	2.38	0.52
1:A:403:GLN:N	1:A:403:GLN:OE1	2.43	0.52
1:E:468:ARG:NH1	1:F:475:SER:OG	2.42	0.52
1:C:295:THR:HG22	1:C:332:VAL:HG23	1.91	0.52
1:G:242:ARG:HG2	1:G:462:TYR:CZ	2.44	0.52
2:I:586:ASN:OD1	2:I:630:VAL:HG13	2.09	0.52
1:B:266:MET:H	1:B:295:THR:HG21	1.75	0.52
1:B:558:THR:HG22	1:B:587:MET:HA	1.92	0.52
1:E:524:LYS:HE2	1:E:540:LEU:HD11	1.91	0.52
1:G:290:SER:O	1:G:291:LYS:HE2	2.08	0.52
1:C:197:LYS:O	1:C:200:ARG:N	2.40	0.52
1:E:533:PHE:CE1	1:E:542:TYR:HB2	2.44	0.52
1:F:291:LYS:HD3	1:F:291:LYS:C	2.30	0.52
1:F:628:LEU:HD12	1:F:628:LEU:O	2.10	0.52
2:J:118:TYR:OH	2:J:143:LYS:O	2.21	0.52
1:C:639:LEU:N	1:C:703:LYS:HZ3	2.07	0.52
1:F:552:PHE:HB3	1:F:554:PHE:CZ	2.44	0.52
2:I:274:ILE:O	2:I:513:TYR:OH	2.18	0.52
2:I:469:ASN:HA	2:I:472:LYS:HZ2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:581:LYS:C	2:J:583:ILE:N	2.64	0.52
2:H:578:LYS:CG	2:H:579:TYR:CD1	2.92	0.52
2:I:110:LYS:HD3	2:I:110:LYS:N	2.25	0.52
1:A:365:ARG:HH21	1:A:418:PRO:HD3	1.75	0.52
1:A:394:ILE:CD1	1:A:421:LEU:HD11	2.40	0.52
1:C:692:PRO:O	1:C:732:TYR:N	2.43	0.52
1:F:486:GLU:CG	1:F:486:GLU:O	2.58	0.52
1:D:552:PHE:HB3	1:D:554:PHE:CZ	2.44	0.51
1:D:610:SER:HA	1:D:613:LYS:HZ3	1.73	0.51
1:F:192:TYR:HD1	1:F:203:LEU:HD11	1.75	0.51
1:F:385:LEU:HD11	1:F:442:LEU:HB2	1.92	0.51
1:G:632:ASP:O	1:G:635:ILE:HG22	2.10	0.51
2:H:566:ILE:HG12	2:H:600:TYR:CZ	2.45	0.51
2:J:437:LEU:O	2:J:502:ARG:HA	2.09	0.51
1:C:188:GLU:OE2	1:C:223:PRO:HA	2.10	0.51
1:E:200:ARG:HG2	1:F:178:ARG:HH12	1.75	0.51
1:E:639:LEU:N	1:E:703:LYS:HZ3	2.08	0.51
1:G:522:THR:O	1:G:525:GLU:HG2	2.10	0.51
1:B:634:ASP:OD1	1:B:635:ILE:N	2.43	0.51
1:B:705:ASN:HB3	1:B:722:LYS:HB2	1.93	0.51
1:F:610:SER:O	1:F:613:LYS:HG2	2.09	0.51
1:A:610:SER:O	1:A:613:LYS:HG2	2.11	0.51
1:C:702:THR:O	1:C:706:THR:HG23	2.11	0.51
1:E:541:GLN:NE2	1:E:544:GLY:O	2.43	0.51
1:F:198:ASN:O	1:F:199:LYS:HG2	2.10	0.51
1:E:523:LEU:HD22	1:E:578:LEU:HD11	1.93	0.51
1:G:592:ARG:HD3	1:G:598:TYR:CE2	2.46	0.51
2:H:148:TYR:HA	2:H:151:ILE:HG22	1.92	0.51
2:I:52:GLU:O	2:I:52:GLU:HG3	2.10	0.51
1:A:523:LEU:O	1:A:527:LEU:HD12	2.11	0.51
1:A:524:LYS:HG3	1:A:540:LEU:HD21	1.91	0.51
1:E:699:TYR:CD1	1:E:725:LEU:HA	2.46	0.51
1:F:197:LYS:O	1:F:199:LYS:N	2.43	0.51
1:F:533:PHE:CE2	1:F:542:TYR:HB2	2.46	0.51
1:F:628:LEU:HA	1:F:674:THR:O	2.11	0.51
2:H:572:LYS:NZ	2:I:85:ASP:OD2	2.43	0.51
2:J:762:THR:HA	2:J:765:PHE:HE1	1.74	0.51
1:B:498:LEU:HB2	1:B:637:LYS:HZ2	1.76	0.51
1:E:628:LEU:O	1:E:628:LEU:HD12	2.11	0.51
1:F:459:ILE:HD12	1:F:475:SER:HB3	1.93	0.51
1:G:492:ILE:HB	1:G:590:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:633:LYS:HA	1:G:636:ARG:NH2	2.25	0.51
2:H:226:GLU:CD	2:H:229:HIS:HD1	2.11	0.51
2:H:583:ILE:HG22	2:H:583:ILE:O	2.11	0.51
2:H:612:SER:O	2:H:616:LYS:HD3	2.11	0.51
2:I:469:ASN:HA	2:I:472:LYS:NZ	2.25	0.51
1:A:435:ASN:ND2	1:A:438:GLN:HG2	2.26	0.51
1:C:366:TYR:HE2	1:C:378:LEU:HG	1.74	0.51
1:C:609:GLU:OE1	1:C:609:GLU:N	2.43	0.51
1:E:659:ARG:HA	1:E:716:THR:O	2.11	0.51
1:F:365:ARG:HH21	1:F:418:PRO:HD3	1.75	0.51
2:H:410:LYS:O	2:H:413:LYS:HG3	2.10	0.51
2:H:739:GLU:CD	2:H:742:ARG:HH22	2.15	0.51
1:B:365:ARG:HH21	1:B:418:PRO:HD3	1.76	0.51
1:B:380:THR:HG22	1:B:396:ALA:HB2	1.93	0.51
1:C:385:LEU:HD11	1:C:442:LEU:HB2	1.93	0.51
1:D:584:ASN:OD1	1:D:585:ALA:N	2.44	0.51
1:E:270:ILE:HG12	1:E:361:ASN:O	2.11	0.51
2:H:100:ASP:C	2:H:102:LYS:H	2.15	0.51
1:B:527:LEU:HD23	1:B:533:PHE:CE1	2.45	0.51
1:C:496:LYS:HG3	1:C:497:ASP:H	1.76	0.51
1:D:193:THR:HG21	1:D:216:LEU:HB3	1.93	0.51
1:D:615:ALA:O	1:D:631:ILE:HD12	2.11	0.51
1:E:497:ASP:HB2	1:E:633:LYS:HZ3	1.76	0.51
1:G:226:TRP:CZ2	1:G:234:SER:HB3	2.45	0.51
2:I:273:LYS:O	2:I:276:GLN:HG3	2.11	0.51
1:A:558:THR:O	1:A:562:ILE:HG23	2.11	0.50
1:E:610:SER:HA	1:E:613:LYS:NZ	2.26	0.50
2:H:411:GLN:HA	2:H:414:ARG:NH1	2.27	0.50
2:H:479:ILE:O	2:H:590:ARG:NH1	2.44	0.50
1:B:524:LYS:HE2	1:B:540:LEU:HD11	1.92	0.50
1:C:242:ARG:HB3	1:C:462:TYR:CE2	2.45	0.50
1:D:366:TYR:CD1	1:D:378:LEU:HD11	2.46	0.50
1:E:621:ASN:HB3	1:E:628:LEU:HG	1.93	0.50
1:F:632:ASP:O	1:F:635:ILE:HG22	2.10	0.50
2:H:171:LEU:HD22	2:H:206:LEU:HD23	1.93	0.50
1:C:381:THR:O	1:C:394:ILE:HG22	2.12	0.50
1:C:695:LYS:HA	1:C:730:LYS:HA	1.92	0.50
1:E:197:LYS:HB2	1:E:202:PHE:CE1	2.43	0.50
1:E:345:THR:O	1:E:349:THR:HG23	2.12	0.50
1:E:350:MET:O	1:E:352:LEU:N	2.43	0.50
2:H:544:ARG:HG3	2:H:544:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:169:LYS:HZ1	2:I:534:ILE:HG22	1.76	0.50
2:I:175:ASN:OD1	2:I:201:PHE:HB2	2.11	0.50
2:J:83:ILE:HG22	2:J:131:ILE:HB	1.92	0.50
1:A:359:ARG:HB2	1:A:430:THR:HG23	1.92	0.50
1:C:435:ASN:N	1:C:438:GLN:OE1	2.44	0.50
1:E:579:ASP:OD1	1:E:580:LYS:HG2	2.11	0.50
2:H:188:LEU:HD11	2:H:223:TYR:HE2	1.76	0.50
2:H:710:ASN:HA	2:H:715:ILE:HD11	1.93	0.50
1:B:193:THR:HG21	1:B:216:LEU:HB3	1.93	0.50
1:C:183:ILE:HB	1:C:188:GLU:OE1	2.11	0.50
1:D:554:PHE:HE1	1:D:589:ILE:HG23	1.77	0.50
1:F:434:MET:SD	1:F:438:GLN:HB2	2.50	0.50
1:F:443:GLU:HA	1:F:446:LYS:HZ3	1.77	0.50
2:J:278:TYR:CD2	2:J:513:TYR:CE2	2.98	0.50
1:B:365:ARG:NH1	1:B:414:LYS:HA	2.26	0.50
1:B:479:GLU:N	1:B:479:GLU:OE1	2.44	0.50
1:B:552:PHE:HB3	1:B:554:PHE:CZ	2.47	0.50
1:C:291:LYS:NZ	1:C:337:SER:O	2.41	0.50
1:D:439:PHE:O	1:D:443:GLU:HG2	2.12	0.50
1:D:558:THR:HG22	1:D:587:MET:HA	1.93	0.50
1:E:273:LYS:C	1:E:359:ARG:HH11	2.15	0.50
1:E:324:PHE:CZ	1:E:588:ASN:HB3	2.47	0.50
1:G:237:GLU:HB2	1:G:242:ARG:O	2.12	0.50
1:G:350:MET:O	1:G:352:LEU:N	2.43	0.50
2:H:118:TYR:HA	2:H:132:GLN:OE1	2.12	0.50
2:H:478:SER:HG	2:H:590:ARG:HA	1.76	0.50
2:I:221:PHE:HA	2:I:244:MET:CE	2.42	0.50
1:G:617:ARG:O	1:G:617:ARG:NH1	2.45	0.50
2:H:696:ALA:O	2:H:699:LEU:HG	2.11	0.50
2:I:44:VAL:HG13	2:I:44:VAL:O	2.12	0.50
2:J:248:ASN:O	2:J:248:ASN:ND2	2.43	0.50
1:A:496:LYS:HE2	1:A:542:TYR:OH	2.12	0.50
1:A:523:LEU:HD23	1:A:527:LEU:CD1	2.41	0.50
1:B:198:ASN:ND2	1:B:200:ARG:HH12	2.10	0.50
2:H:105:LYS:HD2	2:H:109:GLY:O	2.12	0.50
2:H:479:ILE:C	2:H:590:ARG:HH22	2.14	0.50
1:A:521:MET:SD	1:A:525:GLU:HB2	2.52	0.50
1:B:449:ARG:HB3	1:B:449:ARG:NH1	2.27	0.50
1:A:558:THR:HG22	1:A:587:MET:HA	1.94	0.49
1:C:599:ASP:CG	1:C:600:ARG:H	2.16	0.49
1:F:554:PHE:HB3	1:F:558:THR:OG1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:584:ASN:O	1:F:587:MET:HE3	2.12	0.49
1:G:384:VAL:HG13	1:G:449:ARG:HB2	1.94	0.49
1:G:640:SER:OG	1:G:701:VAL:HG13	2.12	0.49
2:H:487:ASP:OD1	2:H:518:LYS:NZ	2.45	0.49
2:H:602:ILE:HD11	2:H:680:ASP:CG	2.32	0.49
1:A:434:MET:CE	1:A:438:GLN:HB3	2.42	0.49
1:C:496:LYS:HG3	1:C:497:ASP:N	2.27	0.49
1:D:233:TYR:HA	1:D:237:GLU:OE2	2.13	0.49
1:F:410:TYR:CD1	1:F:414:LYS:HE2	2.47	0.49
1:F:558:THR:HG21	1:F:588:ASN:H	1.77	0.49
1:G:584:ASN:O	1:G:587:MET:HE2	2.12	0.49
2:H:118:TYR:CD2	2:H:119:VAL:HG13	2.46	0.49
2:H:635:THR:OG1	2:H:638:ASN:ND2	2.43	0.49
1:A:340:LEU:O	1:A:343:GLU:HG2	2.11	0.49
1:A:609:GLU:OE1	1:A:609:GLU:N	2.42	0.49
1:F:631:ILE:H	1:F:636:ARG:NH2	2.05	0.49
1:G:403:GLN:O	1:G:404:ILE:HD13	2.12	0.49
1:G:439:PHE:O	1:G:443:GLU:HG2	2.11	0.49
1:G:595:ARG:HD2	1:G:611:VAL:HG11	1.93	0.49
2:H:505:LEU:HD23	2:H:505:LEU:H	1.77	0.49
1:D:383:LEU:HD21	1:D:448:LEU:HD23	1.94	0.49
1:F:438:GLN:HA	1:F:441:GLU:OE1	2.13	0.49
2:I:137:TYR:HE2	2:I:143:LYS:HE3	1.77	0.49
2:I:274:ILE:HG13	2:I:275:LYS:N	2.27	0.49
1:A:566:LEU:HD21	1:A:574:ILE:HG22	1.94	0.49
1:B:197:LYS:NZ	2:H:184:ASP:OD2	2.45	0.49
1:C:628:LEU:HD12	1:C:628:LEU:O	2.13	0.49
2:J:456:ASP:HB2	2:J:459:ASP:O	2.13	0.49
1:D:631:ILE:O	1:D:636:ARG:NH1	2.46	0.49
1:G:403:GLN:CD	1:G:403:GLN:H	2.16	0.49
1:G:628:LEU:O	1:G:628:LEU:HD12	2.11	0.49
1:B:291:LYS:C	1:B:291:LYS:HD3	2.33	0.49
1:G:198:ASN:O	1:G:199:LYS:HG2	2.13	0.49
1:G:205:PRO:HD2	2:J:232:VAL:HG21	1.95	0.49
1:G:620:ILE:HD12	1:G:620:ILE:H	1.77	0.49
2:H:257:GLU:OE1	2:H:438:TYR:OH	2.30	0.49
2:I:226:GLU:OE2	2:I:229:HIS:N	2.46	0.49
1:B:252:ARG:NH1	1:C:512:ASP:OD1	2.37	0.49
1:C:522:THR:O	1:C:525:GLU:HG2	2.12	0.49
1:C:660:TYR:N	1:C:716:THR:O	2.45	0.49
1:D:628:LEU:HD12	1:D:628:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:ASN:OD1	1:E:210:ILE:HG12	2.12	0.49
1:F:242:ARG:HB3	1:F:462:TYR:CE2	2.47	0.49
1:G:556:GLN:HG2	1:G:557:GLN:N	2.28	0.49
1:G:696:VAL:O	1:G:728:SER:HA	2.12	0.49
2:H:188:LEU:HD11	2:H:223:TYR:CE2	2.48	0.49
2:H:590:ARG:HG2	2:H:590:ARG:HH11	1.78	0.49
2:H:717:ILE:HD12	2:H:765:PHE:HE2	1.77	0.49
2:I:530:LYS:HE3	2:I:548:LYS:HE3	1.95	0.49
2:J:121:ALA:HB2	2:J:129:LEU:HD13	1.94	0.49
1:A:528:LYS:HB2	1:A:528:LYS:HE2	1.50	0.49
1:D:483:GLN:N	1:D:483:GLN:OE1	2.46	0.49
1:G:366:TYR:CE2	1:G:378:LEU:HD21	2.48	0.49
2:H:491:ARG:HG2	2:H:492:PRO:CD	2.43	0.49
1:B:548:THR:HA	1:B:575:TYR:CE1	2.47	0.49
1:D:535:GLU:OE2	1:D:540:LEU:HD22	2.13	0.49
1:E:245:LYS:O	1:F:486:GLU:OE2	2.30	0.49
2:H:475:PHE:O	2:H:476:LYS:HD3	2.13	0.49
2:H:553:SER:O	2:H:557:THR:HG23	2.12	0.49
2:I:553:SER:O	2:I:557:THR:HG23	2.13	0.49
2:J:65:LYS:HE3	2:J:65:LYS:HA	1.94	0.49
1:A:697:ASN:HA	1:A:727:PHE:O	2.12	0.48
1:B:385:LEU:HB3	1:B:391:LEU:HD21	1.95	0.48
1:B:506:ALA:HB1	1:B:518:LYS:HE3	1.94	0.48
1:C:627:LEU:H	1:C:676:ILE:CG2	2.25	0.48
2:H:102:LYS:HB2	2:H:114:LEU:HD23	1.95	0.48
1:B:494:ASN:OD1	1:B:592:ARG:HA	2.13	0.48
1:B:599:ASP:OD1	1:B:600:ARG:N	2.39	0.48
1:C:387:LYS:HD2	1:C:388:ASN:CB	2.41	0.48
1:D:554:PHE:CE1	1:D:589:ILE:HG23	2.48	0.48
1:D:702:THR:O	1:D:706:THR:HG23	2.13	0.48
1:E:291:LYS:CE	1:E:335:ASP:HB3	2.43	0.48
1:G:365:ARG:HH21	1:G:418:PRO:HD3	1.78	0.48
2:H:446:LEU:HD11	2:H:590:ARG:CB	2.39	0.48
2:H:594:ASN:ND2	2:H:594:ASN:O	2.46	0.48
2:I:455:VAL:HA	2:I:463:ILE:HD13	1.95	0.48
1:A:455:VAL:O	1:A:455:VAL:HG13	2.12	0.48
1:A:517:THR:HG23	1:G:199:LYS:O	2.13	0.48
1:A:546:ASP:OD1	1:A:547:ILE:N	2.46	0.48
1:B:291:LYS:HZ1	1:B:335:ASP:N	1.96	0.48
1:G:212:GLU:OE2	1:G:213:LYS:NZ	2.44	0.48
1:G:345:THR:O	1:G:349:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:594:LYS:HB2	1:G:594:LYS:HE3	1.63	0.48
2:H:257:GLU:OE1	2:H:436:TYR:HD2	1.96	0.48
2:H:426:SER:HB3	2:H:510:ARG:CZ	2.43	0.48
2:H:669:HIS:CE1	2:H:671:PRO:HB2	2.49	0.48
2:I:718:PHE:HA	2:I:722:GLY:HA3	1.95	0.48
2:J:142:GLU:OE2	2:J:142:GLU:N	2.44	0.48
1:C:633:LYS:HD2	1:C:636:ARG:NH1	2.28	0.48
1:E:507:ALA:O	1:E:518:LYS:NZ	2.29	0.48
2:H:558:LYS:O	2:H:561:GLU:HG3	2.14	0.48
2:J:81:ILE:HG22	2:J:129:LEU:HD23	1.94	0.48
1:A:250:GLU:CD	1:A:250:GLU:H	2.17	0.48
1:C:250:GLU:H	1:C:250:GLU:CD	2.16	0.48
1:C:578:LEU:HD12	1:C:578:LEU:HA	1.68	0.48
1:F:200:ARG:NH2	2:J:139:GLU:HB3	2.28	0.48
2:H:607:LYS:HD2	2:H:608:ASN:N	2.29	0.48
2:J:511:ALA:HB1	2:J:519:LEU:HD12	1.96	0.48
1:C:228:THR:HG23	1:C:235:ASP:OD2	2.13	0.48
1:D:696:VAL:O	1:D:728:SER:HA	2.13	0.48
2:J:500:LYS:O	2:J:544:ARG:NE	2.47	0.48
1:B:524:LYS:HG2	1:B:540:LEU:HD21	1.94	0.48
1:E:470:ARG:HD2	1:E:471:VAL:N	2.29	0.48
1:F:508:VAL:HG23	1:F:516:THR:HA	1.96	0.48
1:G:643:ILE:HG13	1:G:723:LYS:HE2	1.96	0.48
2:H:709:THR:HB	2:H:737:PHE:CE2	2.48	0.48
2:I:82:TYR:HH	2:I:91:HIS:CE1	2.31	0.48
2:J:72:GLU:O	2:J:75:LYS:HG3	2.14	0.48
2:J:231:ASP:O	2:J:234:GLN:HG3	2.13	0.48
1:C:621:ASN:HB3	1:C:628:LEU:HG	1.95	0.48
1:D:365:ARG:NH1	1:D:414:LYS:HD2	2.28	0.48
1:D:635:ILE:HG23	1:D:636:ARG:HD3	1.95	0.48
2:H:530:LYS:NZ	2:H:548:LYS:HG2	2.28	0.48
2:I:169:LYS:NZ	2:I:533:GLN:HB2	2.28	0.48
1:B:554:PHE:HB3	1:B:558:THR:OG1	2.14	0.48
1:C:345:THR:O	1:C:349:THR:HG23	2.14	0.48
1:D:250:GLU:OE1	1:D:250:GLU:N	2.35	0.48
1:D:267:GLU:OE1	1:D:267:GLU:N	2.46	0.48
1:F:291:LYS:NZ	1:F:335:ASP:N	2.55	0.48
2:H:110:LYS:HA	2:H:110:LYS:HD3	1.67	0.48
1:A:330:SER:OG	1:A:450:LEU:HB2	2.14	0.48
1:A:365:ARG:NH1	1:A:414:LYS:HA	2.29	0.48
1:A:523:LEU:CD2	1:A:527:LEU:HD11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:ASP:CG	1:B:600:ARG:H	2.17	0.48
2:J:594:ASN:OD1	2:J:595:ILE:N	2.47	0.48
1:B:197:LYS:HZ1	2:H:236:TYR:HD1	1.62	0.47
1:D:345:THR:O	1:D:348:GLU:HG3	2.13	0.47
1:D:554:PHE:HB3	1:D:558:THR:OG1	2.14	0.47
1:F:234:SER:OG	1:F:237:GLU:HG2	2.14	0.47
1:F:340:LEU:O	1:F:343:GLU:HG2	2.13	0.47
2:J:224:TYR:CZ	2:J:230:ARG:NH1	2.80	0.47
1:A:512:ASP:HB3	1:A:515:GLU:HB2	1.95	0.47
1:B:403:GLN:O	1:B:404:ILE:HD13	2.14	0.47
1:F:599:ASP:CG	1:F:600:ARG:H	2.16	0.47
2:H:80:LYS:CE	2:J:577:PRO:HB2	2.44	0.47
2:H:124:GLY:CA	2:H:127:PRO:HG3	2.44	0.47
2:H:420:ASP:OD1	2:H:483:TYR:OH	2.30	0.47
2:H:557:THR:HA	2:H:560:GLN:NE2	2.28	0.47
2:H:744:MET:SD	2:H:766:ILE:HG12	2.54	0.47
2:I:142:GLU:OE2	2:I:142:GLU:N	2.47	0.47
2:J:60:GLU:OE2	2:J:61:LYS:HE3	2.14	0.47
1:A:454:GLN:OE1	1:A:454:GLN:N	2.47	0.47
1:D:216:LEU:HD23	1:D:216:LEU:HA	1.72	0.47
1:D:403:GLN:O	1:D:404:ILE:HD13	2.14	0.47
1:F:493:PHE:CE2	1:F:495:GLY:HA3	2.48	0.47
1:G:297:ARG:NH1	1:G:328:ASN:OD1	2.46	0.47
1:G:406:ALA:O	1:G:409:ASN:HB2	2.14	0.47
2:H:264:MET:HA	2:H:267:ARG:HD3	1.96	0.47
2:I:60:GLU:OE2	2:I:61:LYS:HE3	2.14	0.47
2:I:167:TYR:CD2	2:I:168:GLN:HG2	2.49	0.47
2:I:437:LEU:HD21	2:I:486:VAL:CB	2.44	0.47
2:I:465:ARG:H	2:I:465:ARG:HD3	1.80	0.47
1:D:643:ILE:N	1:D:699:TYR:O	2.36	0.47
1:F:350:MET:O	1:F:352:LEU:N	2.47	0.47
1:G:207:ILE:HB	1:G:210:ILE:HG22	1.97	0.47
2:H:113:LEU:HD13	2:H:115:HIS:CE1	2.50	0.47
2:H:605:GLU:O	2:H:609:ASN:ND2	2.47	0.47
2:J:625:GLY:HA3	2:J:664:ARG:NH1	2.29	0.47
1:A:481:LEU:HB3	1:A:482:PRO:HD3	1.97	0.47
1:C:494:ASN:OD1	1:C:592:ARG:HA	2.15	0.47
2:I:135:GLU:CD	2:I:135:GLU:H	2.18	0.47
1:B:493:PHE:CE2	1:B:495:GLY:HA3	2.50	0.47
1:D:185:ASP:OD1	1:D:185:ASP:N	2.47	0.47
2:H:70:VAL:HA	2:H:73:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:331:SER:O	2:I:335:LYS:N	2.43	0.47
1:A:583:LEU:HA	1:A:587:MET:HE1	1.96	0.47
1:B:187:LEU:HD21	2:H:228:GLN:HE21	1.80	0.47
1:B:493:PHE:CZ	1:B:495:GLY:HA3	2.50	0.47
1:C:367:VAL:HG22	1:C:410:TYR:CE1	2.50	0.47
1:D:678:PHE:HB2	1:D:687:LEU:HD11	1.97	0.47
1:E:186:SER:O	1:E:190:GLU:HG2	2.15	0.47
1:E:636:ARG:HG2	1:E:637:LYS:NZ	2.26	0.47
1:F:365:ARG:HH12	1:F:414:LYS:HA	1.79	0.47
1:F:592:ARG:HG3	1:F:592:ARG:HH11	1.78	0.47
2:H:80:LYS:NZ	2:J:577:PRO:HB2	2.29	0.47
2:I:82:TYR:OH	2:I:93:SER:HB2	2.15	0.47
2:I:274:ILE:HD12	2:I:488:ILE:HD13	1.97	0.47
2:I:576:LEU:HB3	2:I:580:THR:HG21	1.96	0.47
2:J:193:GLN:OE1	2:J:212:GLU:OE2	2.33	0.47
1:B:345:THR:O	1:B:348:GLU:HG3	2.15	0.47
1:C:503:ARG:HG3	1:C:531:PHE:HE2	1.79	0.47
1:C:628:LEU:HA	1:C:674:THR:O	2.15	0.47
1:D:385:LEU:HD13	1:D:448:LEU:HG	1.96	0.47
1:D:540:LEU:HB3	1:D:547:ILE:HB	1.96	0.47
1:F:270:ILE:CG1	1:F:361:ASN:HB2	2.45	0.47
2:H:163:ILE:O	2:H:163:ILE:HG22	2.15	0.47
1:A:605:VAL:HG22	1:A:704:GLU:HB3	1.96	0.47
1:D:185:ASP:OD1	1:D:186:SER:N	2.47	0.47
1:D:364:ILE:O	1:D:419:ILE:HG22	2.15	0.47
1:D:629:LEU:HB3	1:D:631:ILE:HD11	1.97	0.47
1:E:358:ALA:O	1:E:434:MET:HG3	2.15	0.47
1:G:212:GLU:HG2	1:G:213:LYS:HD3	1.96	0.47
2:H:210:SER:HA	2:H:213:VAL:HG12	1.97	0.47
1:A:486:GLU:HA	1:A:586:LYS:CE	2.45	0.47
1:A:600:ARG:HA	1:A:600:ARG:NE	2.30	0.47
1:C:535:GLU:OE2	1:C:540:LEU:HD22	2.15	0.47
1:C:626:GLY:HA2	1:C:678:PHE:HE2	1.80	0.47
1:E:449:ARG:O	1:E:450:LEU:HD23	2.15	0.47
1:E:554:PHE:HB3	1:E:558:THR:OG1	2.15	0.47
1:F:523:LEU:HD22	1:F:578:LEU:HD11	1.97	0.47
2:H:375:PHE:HA	2:H:378:LYS:HE2	1.97	0.47
2:H:475:PHE:CE2	2:H:529:ILE:HG13	2.50	0.47
2:H:617:LYS:HE3	2:H:695:TYR:CE2	2.49	0.47
2:H:621:TYR:CG	2:H:695:TYR:CD1	3.03	0.47
1:A:197:LYS:HB2	1:A:202:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ILE:HG12	1:B:361:ASN:O	2.15	0.46
1:E:197:LYS:O	1:E:198:ASN:C	2.54	0.46
1:F:269:ILE:HG22	1:F:270:ILE:H	1.80	0.46
1:G:491:ILE:HD12	1:G:505:ILE:HD12	1.97	0.46
2:J:252:ILE:O	2:J:255:SER:OG	2.27	0.46
1:A:224:GLU:O	1:A:224:GLU:HG3	2.15	0.46
1:A:295:THR:HG22	1:A:332:VAL:HG23	1.97	0.46
1:B:702:THR:O	1:B:706:THR:HG23	2.16	0.46
1:E:300:THR:O	1:E:324:PHE:HB3	2.15	0.46
1:E:406:ALA:HB3	1:E:409:ASN:HD22	1.79	0.46
1:E:524:LYS:HG3	1:E:540:LEU:HD21	1.96	0.46
2:H:100:ASP:O	2:H:102:LYS:N	2.48	0.46
2:H:699:LEU:HD12	2:H:700:LEU:HD22	1.98	0.46
2:I:461:THR:HG23	2:I:540:LYS:HA	1.97	0.46
1:D:705:ASN:HD21	1:D:722:LYS:CB	2.27	0.46
1:E:358:ALA:HB3	1:E:434:MET:SD	2.55	0.46
1:G:659:ARG:HA	1:G:716:THR:O	2.16	0.46
1:G:718:THR:CB	1:G:723:LYS:NZ	2.78	0.46
2:H:162:LYS:HZ2	2:H:163:ILE:HD11	1.81	0.46
2:H:446:LEU:CD1	2:H:591:TYR:HB2	2.34	0.46
2:I:211:ASN:O	2:I:214:GLN:HG2	2.15	0.46
1:A:241:GLY:O	1:A:245:LYS:NZ	2.39	0.46
1:B:324:PHE:CZ	1:B:588:ASN:HB3	2.50	0.46
1:B:387:LYS:HA	1:B:387:LYS:HE2	1.97	0.46
1:F:696:VAL:O	1:F:728:SER:HA	2.16	0.46
1:G:300:THR:O	1:G:324:PHE:HB3	2.16	0.46
2:H:555:ILE:O	2:H:559:ILE:HD12	2.15	0.46
2:H:744:MET:HG3	2:H:745:HIS:CE1	2.50	0.46
2:I:89:THR:HG22	2:I:115:HIS:CA	2.24	0.46
2:J:239:GLU:OE1	2:J:239:GLU:N	2.49	0.46
1:A:190:GLU:C	1:A:220:LYS:HZ2	2.18	0.46
1:B:595:ARG:HG3	1:B:596:PHE:CD1	2.51	0.46
1:E:200:ARG:HB3	1:F:178:ARG:HH22	1.80	0.46
2:H:567:ASN:OD1	2:H:568:GLN:N	2.48	0.46
2:H:709:THR:HG21	2:H:733:GLU:HG3	1.98	0.46
1:A:197:LYS:O	1:A:198:ASN:C	2.54	0.46
1:B:263:HIS:CE1	1:B:297:ARG:HB2	2.50	0.46
1:C:490:ARG:HH21	1:C:504:ARG:NH2	1.98	0.46
1:G:273:LYS:HA	1:G:358:ALA:HA	1.97	0.46
1:G:441:GLU:HA	1:G:444:LYS:NZ	2.31	0.46
2:H:65:LYS:HE2	2:H:65:LYS:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:680:ASP:N	2:H:680:ASP:OD1	2.47	0.46
2:I:36:LEU:HD12	2:I:37:LYS:N	2.31	0.46
1:A:188:GLU:OE1	1:A:223:PRO:HA	2.15	0.46
1:D:272:SER:HB3	1:D:288:THR:HG22	1.98	0.46
1:D:535:GLU:HB3	1:D:538:GLY:HA2	1.97	0.46
1:F:416:LEU:HD23	1:F:416:LEU:HA	1.61	0.46
1:G:291:LYS:HB2	1:G:334:ILE:HD11	1.98	0.46
1:G:512:ASP:HB3	1:G:515:GLU:HB2	1.98	0.46
2:H:155:LEU:HD12	2:H:159:ILE:HB	1.98	0.46
2:H:578:LYS:CE	2:H:579:TYR:HE1	2.27	0.46
2:I:82:TYR:OH	2:I:91:HIS:CE1	2.69	0.46
2:I:136:ASP:OD1	2:I:136:ASP:N	2.38	0.46
1:A:240:THR:HG21	1:A:242:ARG:NH1	2.30	0.46
1:E:213:LYS:HE2	1:E:214:LYS:HZ1	1.81	0.46
1:G:524:LYS:HE3	1:G:579:ASP:HB3	1.97	0.46
1:G:702:THR:O	1:G:706:THR:HG23	2.16	0.46
2:H:427:ILE:HG12	2:H:505:LEU:CD1	2.46	0.46
1:D:415:ASN:OD1	1:E:325:SER:OG	2.21	0.46
1:E:700:ALA:CB	1:E:726:ILE:HG13	2.45	0.46
1:F:381:THR:HG23	1:F:394:ILE:HD13	1.96	0.46
2:H:617:LYS:HD3	2:H:773:ILE:HD13	1.97	0.46
2:I:113:LEU:HD12	2:I:113:LEU:HA	1.72	0.46
2:J:211:ASN:O	2:J:214:GLN:HG2	2.16	0.46
1:A:298:THR:OG1	1:A:601:ASN:HB2	2.15	0.46
1:A:508:VAL:HG23	1:A:516:THR:HA	1.98	0.46
1:A:522:THR:OG1	1:A:525:GLU:HG2	2.16	0.46
1:B:291:LYS:HE2	1:B:335:ASP:HB3	1.98	0.46
1:C:521:MET:HA	1:C:525:GLU:OE1	2.16	0.46
1:D:632:ASP:O	1:D:635:ILE:HG22	2.16	0.46
1:E:183:ILE:HD12	1:E:203:LEU:CD2	2.45	0.46
1:G:334:ILE:HG22	1:G:446:LYS:HB3	1.98	0.46
1:G:359:ARG:NH2	1:G:430:THR:OG1	2.48	0.46
2:I:443:ILE:HG21	2:I:454:LEU:HD21	1.97	0.46
2:I:530:LYS:HB3	2:I:548:LYS:NZ	2.31	0.46
2:J:136:ASP:HB2	2:J:140:ASN:ND2	2.31	0.46
1:A:200:ARG:HB3	1:B:178:ARG:HH22	1.82	0.45
1:B:205:PRO:HD2	2:H:232:VAL:HG21	1.97	0.45
1:B:330:SER:OG	1:B:450:LEU:HB2	2.16	0.45
1:D:345:THR:O	1:D:349:THR:HG23	2.16	0.45
1:D:576:THR:C	1:D:578:LEU:H	2.20	0.45
2:H:533:GLN:N	2:H:533:GLN:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LEU:HD12	1:B:421:LEU:HA	1.65	0.45
1:B:616:HIS:CE1	1:B:726:ILE:HD12	2.51	0.45
1:B:629:LEU:HD23	1:B:631:ILE:HD11	1.98	0.45
1:D:191:GLY:HA2	1:D:219:TYR:O	2.17	0.45
1:G:578:LEU:HD12	1:G:578:LEU:HA	1.70	0.45
2:H:52:GLU:N	2:H:55:LYS:HB3	2.32	0.45
2:H:576:LEU:HD22	2:H:623:VAL:HG11	1.96	0.45
2:H:622:LEU:HD12	2:H:622:LEU:HA	1.69	0.45
1:A:324:PHE:HZ	1:A:588:ASN:HB3	1.81	0.45
1:A:583:LEU:CA	1:A:587:MET:HE1	2.46	0.45
1:B:406:ALA:HB3	1:B:409:ASN:OD1	2.17	0.45
1:C:271:LEU:HB2	1:C:289:ILE:CG2	2.47	0.45
1:C:350:MET:O	1:C:352:LEU:N	2.49	0.45
1:C:455:VAL:O	1:C:455:VAL:HG13	2.16	0.45
1:F:187:LEU:HD11	1:F:205:PRO:HG3	1.98	0.45
1:F:535:GLU:HB3	1:F:538:GLY:HA2	1.97	0.45
2:H:659:TYR:HE2	2:H:694:ASP:OD2	1.99	0.45
1:A:492:ILE:HG21	1:A:500:LEU:HD12	1.98	0.45
1:B:463:ASN:ND2	1:B:465:GLU:OE2	2.46	0.45
1:B:528:LYS:HE2	1:B:528:LYS:HB2	1.61	0.45
1:C:266:MET:H	1:C:295:THR:HG21	1.81	0.45
1:C:468:ARG:HG2	1:C:468:ARG:HH11	1.81	0.45
1:D:350:MET:O	1:D:352:LEU:N	2.46	0.45
1:E:535:GLU:OE2	1:E:540:LEU:HD12	2.16	0.45
1:G:271:LEU:HB2	1:G:289:ILE:CG2	2.47	0.45
1:G:626:GLY:HA2	1:G:678:PHE:CE1	2.50	0.45
2:H:84:VAL:O	2:H:132:GLN:HA	2.15	0.45
2:I:414:ARG:O	2:I:418:ASN:N	2.34	0.45
1:A:700:ALA:CB	1:A:726:ILE:HG13	2.47	0.45
1:C:465:GLU:OE1	2:I:35:HIS:CE1	2.70	0.45
1:D:262:VAL:O	1:D:328:ASN:ND2	2.49	0.45
1:E:291:LYS:HE3	1:E:335:ASP:O	2.16	0.45
1:E:385:LEU:HD11	1:E:448:LEU:HG	1.97	0.45
1:E:500:LEU:HA	1:E:500:LEU:HD23	1.61	0.45
1:G:324:PHE:HZ	1:G:588:ASN:HB3	1.81	0.45
1:G:584:ASN:H	1:G:587:MET:CE	2.29	0.45
2:H:435:ILE:HB	2:H:505:LEU:HD21	1.97	0.45
2:J:88:ILE:HD11	2:J:130:VAL:HG23	1.98	0.45
1:A:445:THR:HG22	1:A:447:GLN:HB3	1.98	0.45
1:B:593:ASP:OD1	1:B:595:ARG:HG2	2.16	0.45
1:C:640:SER:OG	1:C:701:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:THR:HG23	1:D:447:GLN:NE2	2.26	0.45
1:E:405:LEU:HD13	1:E:405:LEU:HA	1.84	0.45
1:G:324:PHE:CZ	1:G:588:ASN:HB3	2.52	0.45
2:H:67:PRO:HB2	2:H:68:SER:H	1.52	0.45
2:H:578:LYS:NZ	2:H:579:TYR:HE1	2.02	0.45
1:E:468:ARG:NH2	1:F:475:SER:OG	2.50	0.45
1:E:497:ASP:HB2	1:E:633:LYS:NZ	2.31	0.45
1:E:595:ARG:CZ	1:E:596:PHE:HE1	2.30	0.45
1:F:643:ILE:CD1	1:F:723:LYS:HD2	2.26	0.45
1:G:593:ASP:OD2	1:G:595:ARG:HB3	2.16	0.45
2:J:117:HIS:CD2	2:J:119:VAL:O	2.69	0.45
1:A:449:ARG:NH2	1:A:451:ASP:OD2	2.49	0.45
1:C:374:ILE:HG12	1:C:405:LEU:HB2	1.98	0.45
1:C:438:GLN:HA	1:C:441:GLU:OE1	2.16	0.45
1:D:609:GLU:HB2	1:D:724:ILE:HG12	1.98	0.45
1:D:632:ASP:C	1:D:636:ARG:HH12	2.21	0.45
2:H:107:ILE:HD12	2:H:107:ILE:H	1.81	0.45
2:H:656:LYS:HE3	2:H:656:LYS:HB3	1.75	0.45
2:I:466:GLY:O	2:I:470:GLU:HG2	2.16	0.45
2:I:577:PRO:O	2:I:580:THR:HG22	2.17	0.45
2:J:235:LEU:HD12	2:J:235:LEU:HA	1.66	0.45
1:C:605:VAL:HG13	1:C:704:GLU:OE1	2.16	0.45
1:D:493:PHE:CZ	1:D:495:GLY:HA3	2.52	0.45
1:D:535:GLU:OE1	1:D:540:LEU:HD13	2.17	0.45
1:E:528:LYS:HB2	1:E:528:LYS:HE2	1.54	0.45
1:G:360:LEU:HB3	1:G:432:ILE:HG21	1.99	0.45
2:H:74:TYR:OH	2:H:154:ILE:HG12	2.17	0.45
2:H:197:HIS:ND1	2:H:199:THR:O	2.44	0.45
2:H:709:THR:HB	2:H:737:PHE:HE2	1.82	0.45
2:I:33:GLU:O	2:I:36:LEU:HG	2.16	0.45
2:I:498:ARG:NH2	2:I:540:LYS:HE2	2.32	0.45
2:J:125:TYR:O	2:J:127:PRO:HD3	2.16	0.45
1:D:247:VAL:HG23	1:D:252:ARG:HE	1.82	0.45
1:E:291:LYS:HD3	1:E:291:LYS:C	2.37	0.45
1:E:627:LEU:O	1:E:675:PHE:HA	2.17	0.45
2:I:168:GLN:O	2:I:172:ASP:N	2.49	0.45
1:A:345:THR:O	1:A:349:THR:HG23	2.17	0.44
1:A:639:LEU:N	1:A:703:LYS:HZ2	2.15	0.44
1:B:361:ASN:OD1	1:B:422:ASN:HB3	2.16	0.44
1:B:494:ASN:HD21	1:B:592:ARG:HB3	1.82	0.44
1:C:549:GLU:O	1:C:594:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:365:ARG:NH1	1:F:414:LYS:HA	2.33	0.44
1:F:471:VAL:HG13	1:G:479:GLU:CD	2.37	0.44
1:F:505:ILE:HD12	1:F:526:ALA:HB1	1.99	0.44
2:H:105:LYS:NZ	2:H:110:LYS:O	2.49	0.44
2:H:388:ILE:HG23	2:H:416:ILE:HD11	1.99	0.44
2:J:77:ILE:HD13	2:J:159:ILE:HD13	1.98	0.44
1:A:242:ARG:HB3	1:A:462:TYR:CD2	2.53	0.44
1:A:618:GLU:O	1:A:618:GLU:HG2	2.17	0.44
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.76	0.44
1:B:486:GLU:O	1:B:486:GLU:HG3	2.17	0.44
1:D:210:ILE:HD11	2:I:188:LEU:HA	1.99	0.44
1:D:354:THR:HA	1:D:436:TYR:CD1	2.52	0.44
1:D:606:GLY:HA3	1:D:704:GLU:OE1	2.17	0.44
1:E:200:ARG:CB	1:F:178:ARG:HH22	2.31	0.44
1:A:360:LEU:HD12	1:A:361:ASN:N	2.31	0.44
1:C:696:VAL:O	1:C:728:SER:HA	2.17	0.44
1:D:187:LEU:HA	1:D:187:LEU:HD23	1.68	0.44
1:E:234:SER:O	1:E:237:GLU:HG2	2.18	0.44
1:F:528:LYS:HB2	1:F:528:LYS:HE2	1.57	0.44
1:G:542:TYR:CE2	1:G:543:GLN:NE2	2.85	0.44
2:H:188:LEU:O	2:H:188:LEU:HG	2.17	0.44
2:H:469:ASN:HA	2:H:472:LYS:HZ3	1.81	0.44
1:E:234:SER:OG	1:E:237:GLU:HG2	2.16	0.44
1:E:506:ALA:HB1	1:E:518:LYS:HE3	1.98	0.44
1:E:609:GLU:HG2	1:E:613:LYS:NZ	2.33	0.44
1:F:486:GLU:HG3	1:F:586:LYS:NZ	2.33	0.44
1:F:668:LEU:HA	1:F:674:THR:HA	2.00	0.44
1:G:563:LYS:HA	1:G:566:LEU:HG	1.99	0.44
2:H:171:LEU:HD11	2:H:201:PHE:HB3	1.99	0.44
2:H:197:HIS:CG	2:H:201:PHE:HE1	2.35	0.44
2:I:226:GLU:OE1	2:I:228:GLN:N	2.43	0.44
2:I:463:ILE:HG12	2:I:541:GLU:OE1	2.18	0.44
2:I:554:LYS:O	2:I:557:THR:OG1	2.33	0.44
1:A:178:ARG:HH22	1:G:200:ARG:HB3	1.80	0.44
1:B:384:VAL:HG13	1:B:449:ARG:HB2	2.00	0.44
1:D:486:GLU:HG3	1:D:486:GLU:O	2.18	0.44
1:D:626:GLY:HA2	1:D:678:PHE:HE2	1.82	0.44
1:F:233:TYR:HB2	1:F:238:LYS:HZ3	1.82	0.44
1:G:450:LEU:HA	1:G:450:LEU:HD23	1.74	0.44
2:J:503:ILE:HG13	2:J:549:VAL:HG23	2.00	0.44
1:A:468:ARG:CZ	1:A:468:ARG:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ASN:OD1	1:C:210:ILE:HG12	2.18	0.44
1:E:271:LEU:HB2	1:E:289:ILE:HG22	1.98	0.44
1:E:603:ILE:O	1:E:605:VAL:HG23	2.17	0.44
1:F:203:LEU:HD12	1:F:203:LEU:HA	1.74	0.44
1:G:543:GLN:HG2	1:G:545:LYS:NZ	2.32	0.44
2:H:165:GLN:OE1	2:H:165:GLN:N	2.43	0.44
2:I:34:GLU:HA	2:I:37:LYS:NZ	2.33	0.44
2:I:235:LEU:HA	2:I:235:LEU:HD12	1.55	0.44
2:J:256:LEU:O	2:J:259:LEU:HG	2.17	0.44
1:B:468:ARG:CZ	1:B:468:ARG:HB3	2.47	0.44
1:D:203:LEU:HD12	1:D:203:LEU:HA	1.71	0.44
1:E:569:LEU:HD23	1:E:569:LEU:HA	1.83	0.44
1:F:291:LYS:HE2	1:F:335:ASP:HB3	2.00	0.44
1:F:435:ASN:OD1	1:F:438:GLN:HG3	2.17	0.44
1:F:627:LEU:O	1:F:675:PHE:HA	2.18	0.44
1:F:701:VAL:HG22	1:F:706:THR:HG22	1.98	0.44
1:G:233:TYR:HA	1:G:237:GLU:OE2	2.18	0.44
2:J:136:ASP:HA	2:J:139:GLU:OE1	2.18	0.44
2:J:247:PHE:CE2	2:J:252:ILE:HD11	2.53	0.44
1:A:209:ASN:OD1	1:A:210:ILE:HG12	2.17	0.44
1:A:299:HIS:NE2	1:A:324:PHE:CG	2.85	0.44
1:A:382:SER:HA	1:A:393:THR:HA	1.99	0.44
1:B:405:LEU:HD23	1:B:405:LEU:HA	1.74	0.44
1:C:627:LEU:HB3	1:C:629:LEU:CD2	2.47	0.44
1:D:240:THR:O	1:E:514:LEU:HB2	2.17	0.44
1:D:406:ALA:O	1:D:409:ASN:HB2	2.18	0.44
1:D:512:ASP:HB3	1:D:515:GLU:CB	2.47	0.44
1:G:449:ARG:HG3	1:G:449:ARG:HH11	1.83	0.44
2:I:115:HIS:ND1	2:I:116:GLU:N	2.65	0.44
1:B:291:LYS:NZ	1:B:335:ASP:N	2.61	0.44
1:D:237:GLU:HB2	1:D:242:ARG:O	2.17	0.44
1:D:468:ARG:HH12	1:D:470:ARG:CD	2.28	0.44
1:D:591:ILE:O	1:D:591:ILE:HG13	2.18	0.44
1:D:638:ILE:HG13	1:D:639:LEU:HD12	2.00	0.44
1:E:272:SER:HB3	1:E:288:THR:HG22	1.99	0.44
2:H:83:ILE:HB	2:H:133:SER:HB3	1.99	0.44
1:C:250:GLU:OE1	1:C:250:GLU:N	2.29	0.43
1:C:326:ASN:HB3	1:C:490:ARG:NH2	2.30	0.43
1:D:524:LYS:HB2	1:D:578:LEU:HD23	2.00	0.43
2:H:434:LYS:O	2:H:434:LYS:HD3	2.17	0.43
2:I:454:LEU:HD12	2:I:455:VAL:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LEU:HD11	1:A:434:MET:SD	2.58	0.43
1:A:725:LEU:O	1:A:725:LEU:HD12	2.18	0.43
1:B:291:LYS:HZ2	1:B:334:ILE:HB	1.83	0.43
1:B:628:LEU:O	1:B:628:LEU:HD12	2.18	0.43
1:C:447:GLN:C	1:C:448:LEU:HD12	2.38	0.43
1:E:583:LEU:CA	1:E:587:MET:HE1	2.46	0.43
1:G:382:SER:OG	1:G:451:ASP:OD2	2.29	0.43
1:G:700:ALA:HB2	1:G:726:ILE:HG13	2.00	0.43
2:H:106:ASP:OD1	2:H:108:TYR:N	2.45	0.43
2:H:191:THR:OG1	2:H:192:ASN:N	2.51	0.43
2:H:693:ASP:OD1	2:H:708:VAL:HG12	2.18	0.43
2:J:88:ILE:HD11	2:J:130:VAL:CG2	2.47	0.43
1:A:338:LEU:HG	1:A:661:ASP:CB	2.48	0.43
1:A:490:ARG:HE	1:A:502:GLU:CD	2.21	0.43
1:B:270:ILE:C	1:B:271:LEU:HD22	2.39	0.43
1:C:330:SER:OG	1:C:331:THR:N	2.50	0.43
1:C:378:LEU:HA	1:C:379:PRO:HD3	1.88	0.43
1:D:263:HIS:NE2	1:D:367:VAL:HB	2.33	0.43
1:E:365:ARG:HH12	1:E:414:LYS:HD2	1.81	0.43
1:E:415:ASN:C	1:E:416:LEU:HD12	2.38	0.43
1:F:377:VAL:HG12	1:F:378:LEU:N	2.33	0.43
1:G:621:ASN:HB3	1:G:628:LEU:HG	2.00	0.43
2:H:384:GLN:HA	2:H:384:GLN:OE1	2.18	0.43
2:H:656:LYS:HD3	2:H:673:LYS:C	2.38	0.43
2:I:227:PRO:HB2	2:I:228:GLN:NE2	2.32	0.43
1:C:195:ASP:O	1:C:195:ASP:OD1	2.36	0.43
1:D:701:VAL:HG22	1:D:706:THR:HG22	2.00	0.43
1:G:299:HIS:O	1:G:602:ASN:HB2	2.18	0.43
1:G:332:VAL:CG1	1:G:448:LEU:HB2	2.48	0.43
1:G:633:LYS:HA	1:G:636:ARG:CZ	2.47	0.43
2:H:108:TYR:O	2:H:110:LYS:HE2	2.19	0.43
2:H:289:GLY:O	2:H:293:LEU:HG	2.17	0.43
2:I:221:PHE:CA	2:I:244:MET:HE1	2.47	0.43
2:J:581:LYS:O	2:J:583:ILE:N	2.51	0.43
1:B:520:ASP:N	1:B:520:ASP:OD1	2.52	0.43
1:B:621:ASN:OD1	1:B:628:LEU:HG	2.18	0.43
1:E:245:LYS:HE2	1:E:245:LYS:HA	1.99	0.43
1:E:250:GLU:H	1:E:250:GLU:CD	2.22	0.43
1:F:255:LEU:HD23	1:F:255:LEU:HA	1.77	0.43
1:F:403:GLN:O	1:F:404:ILE:HD13	2.19	0.43
1:F:524:LYS:HG2	1:F:579:ASP:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:561:GLU:O	2:H:564:LEU:HG	2.19	0.43
2:I:81:ILE:HG13	2:I:81:ILE:O	2.17	0.43
2:J:160:LEU:HD22	2:J:165:GLN:CB	2.48	0.43
1:A:406:ALA:O	1:A:409:ASN:HB2	2.18	0.43
1:B:258:ALA:HA	1:B:371:THR:OG1	2.18	0.43
1:B:267:GLU:C	1:B:293:THR:HG1	2.22	0.43
1:C:445:THR:HG22	1:C:447:GLN:HB2	1.99	0.43
1:C:543:GLN:N	1:C:543:GLN:OE1	2.52	0.43
1:D:332:VAL:O	1:D:447:GLN:HG2	2.18	0.43
1:E:271:LEU:HB2	1:E:289:ILE:CG2	2.48	0.43
1:E:471:VAL:HG13	1:E:471:VAL:O	2.19	0.43
1:G:271:LEU:HB2	1:G:289:ILE:HG23	1.99	0.43
1:G:359:ARG:HB2	1:G:430:THR:HG21	2.00	0.43
1:G:384:VAL:CG1	1:G:449:ARG:HB2	2.49	0.43
2:H:118:TYR:CZ	2:H:143:LYS:HG3	2.54	0.43
2:I:278:TYR:CE1	2:I:425:GLN:HG2	2.54	0.43
2:J:203:VAL:O	2:J:206:LEU:HG	2.18	0.43
1:A:199:LYS:HD2	1:A:199:LYS:HA	1.85	0.43
1:C:226:TRP:CE2	1:C:234:SER:HB3	2.54	0.43
1:C:521:MET:CE	1:C:583:LEU:HD12	2.49	0.43
2:H:80:LYS:N	2:H:128:VAL:HG12	2.32	0.43
2:H:83:ILE:HG13	2:H:83:ILE:O	2.19	0.43
2:H:116:GLU:OE2	2:H:117:HIS:ND1	2.51	0.43
2:H:578:LYS:HE3	2:I:63:LEU:HD22	1.98	0.43
2:I:72:GLU:HA	2:I:75:LYS:HG2	2.00	0.43
2:J:108:TYR:HB3	2:J:110:LYS:NZ	2.34	0.43
1:D:438:GLN:HA	1:D:441:GLU:HG3	2.01	0.43
1:E:245:LYS:HB3	1:F:486:GLU:OE2	2.19	0.43
1:E:326:ASN:ND2	1:E:485:GLN:HG2	2.34	0.43
1:F:291:LYS:CE	1:F:335:ASP:HB3	2.49	0.43
1:F:466:ASN:ND2	1:F:468:ARG:HG3	2.33	0.43
1:F:500:LEU:HD23	1:F:500:LEU:HA	1.61	0.43
1:G:200:ARG:HH11	1:G:200:ARG:HG3	1.83	0.43
2:H:80:LYS:HZ1	2:J:577:PRO:HB2	1.84	0.43
2:H:94:LEU:HD12	2:H:94:LEU:HA	1.90	0.43
2:J:278:TYR:CE1	2:J:425:GLN:HG2	2.54	0.43
2:J:469:ASN:OD1	2:J:470:GLU:N	2.51	0.43
2:J:576:LEU:HD21	2:J:619:THR:HB	2.01	0.43
1:B:176:PRO:HB2	1:B:185:ASP:OD2	2.19	0.43
1:B:334:ILE:HG12	1:B:446:LYS:HB2	2.00	0.43
1:D:563:LYS:O	1:D:566:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:469:VAL:HG23	1:E:469:VAL:O	2.19	0.43
1:E:551:ASP:OD1	1:E:594:LYS:HB3	2.19	0.43
2:H:410:LYS:HE3	2:H:410:LYS:HB2	1.85	0.43
2:H:518:LYS:O	2:H:519:LEU:HD23	2.18	0.43
2:H:630:VAL:HG12	2:H:632:THR:HG23	2.00	0.43
2:I:81:ILE:HA	2:I:129:LEU:O	2.19	0.43
2:I:134:SER:HB3	2:I:136:ASP:OD1	2.19	0.43
1:B:450:LEU:HD23	1:B:450:LEU:HA	1.85	0.43
1:C:377:VAL:HG22	1:C:378:LEU:N	2.33	0.43
1:D:214:LYS:O	1:D:214:LYS:HG3	2.19	0.43
1:D:270:ILE:C	1:D:271:LEU:HD22	2.40	0.43
1:D:590:LEU:HD21	1:D:592:ARG:HG3	2.01	0.43
1:G:596:PHE:CE2	1:G:638:ILE:HD13	2.53	0.43
2:H:494:LEU:HD13	2:H:494:LEU:HA	1.91	0.43
2:I:442:ASN:HB2	2:I:497:GLU:OE1	2.19	0.43
2:I:465:ARG:HD3	2:I:465:ARG:N	2.33	0.43
2:I:771:LYS:O	2:I:773:ILE:HG12	2.18	0.43
1:A:549:GLU:N	1:A:549:GLU:OE1	2.52	0.42
1:C:522:THR:N	1:C:525:GLU:OE1	2.43	0.42
1:F:199:LYS:HA	1:F:199:LYS:HD3	1.83	0.42
1:G:554:PHE:HB3	1:G:558:THR:OG1	2.19	0.42
2:H:627:GLY:HA3	2:H:664:ARG:O	2.18	0.42
2:H:722:GLY:HA2	2:H:736:PHE:CE2	2.54	0.42
2:J:110:LYS:N	2:J:110:LYS:HD3	2.33	0.42
2:J:630:VAL:O	2:J:667:LEU:HA	2.18	0.42
1:A:564:ASN:O	1:A:567:ALA:N	2.51	0.42
1:B:507:ALA:O	1:B:518:LYS:NZ	2.33	0.42
1:C:446:LYS:NZ	1:C:709:ASN:HD21	2.17	0.42
1:C:486:GLU:O	1:C:486:GLU:HG3	2.18	0.42
1:D:524:LYS:HB2	1:D:578:LEU:CD2	2.49	0.42
1:F:360:LEU:HB3	1:F:432:ILE:CG2	2.47	0.42
1:F:366:TYR:CE1	1:F:378:LEU:HD21	2.54	0.42
1:B:528:LYS:NZ	1:B:535:GLU:HG2	2.34	0.42
1:C:493:PHE:HB2	1:C:531:PHE:CE1	2.53	0.42
1:D:599:ASP:HB3	1:D:605:VAL:HG11	2.02	0.42
1:F:666:SER:OG	1:F:676:ILE:HG12	2.19	0.42
2:H:726:THR:HG23	2:H:729:GLY:H	1.85	0.42
1:B:360:LEU:HD12	1:B:361:ASN:H	1.84	0.42
1:B:434:MET:SD	1:B:439:PHE:N	2.92	0.42
1:D:255:LEU:HA	1:D:255:LEU:HD23	1.72	0.42
1:F:442:LEU:HD23	1:F:446:LYS:HZ2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:490:ARG:HB2	1:F:504:ARG:NH1	2.35	0.42
2:H:235:LEU:HA	2:H:235:LEU:HD13	1.79	0.42
2:H:468:PHE:CE2	2:H:472:LYS:HD3	2.55	0.42
2:H:564:LEU:O	2:H:568:GLN:HG3	2.20	0.42
2:I:203:VAL:O	2:I:206:LEU:HG	2.20	0.42
1:A:403:GLN:O	1:A:404:ILE:HD13	2.19	0.42
1:C:326:ASN:ND2	1:C:485:GLN:OE1	2.53	0.42
1:D:494:ASN:ND2	1:D:592:ARG:HG2	2.35	0.42
1:E:403:GLN:O	1:E:404:ILE:HD13	2.18	0.42
1:F:346:TRP:CD1	1:F:346:TRP:N	2.88	0.42
2:H:81:ILE:HG22	2:H:129:LEU:CD2	2.41	0.42
2:H:304:LYS:HE3	2:H:304:LYS:HB2	1.72	0.42
2:H:442:ASN:ND2	2:H:444:ASN:HB2	2.35	0.42
2:H:480:SER:HA	2:H:590:ARG:NH1	2.34	0.42
1:A:721:ILE:O	1:A:723:LYS:HG3	2.20	0.42
1:B:174:THR:O	1:B:175:VAL:C	2.56	0.42
1:B:535:GLU:OE2	1:B:540:LEU:HD12	2.19	0.42
1:D:535:GLU:CD	1:D:540:LEU:HD22	2.39	0.42
1:E:377:VAL:HG12	1:E:378:LEU:N	2.34	0.42
1:E:458:ASN:HD22	1:E:473:THR:HA	1.85	0.42
1:E:636:ARG:NH1	1:E:637:LYS:NZ	2.67	0.42
1:F:558:THR:O	1:F:562:ILE:HG13	2.20	0.42
2:I:171:LEU:HD11	2:I:201:PHE:HB3	2.01	0.42
2:J:140:ASN:HD21	2:J:143:LYS:HD3	1.84	0.42
2:J:171:LEU:HD11	2:J:201:PHE:HB3	2.02	0.42
2:J:258:GLU:O	2:J:262:GLN:NE2	2.44	0.42
1:A:592:ARG:HD2	1:A:598:TYR:CE2	2.55	0.42
1:C:596:PHE:CD2	1:C:638:ILE:HD13	2.54	0.42
1:C:633:LYS:HA	1:C:636:ARG:NH1	2.35	0.42
1:E:197:LYS:O	1:E:199:LYS:N	2.52	0.42
1:E:237:GLU:HB2	1:E:242:ARG:O	2.19	0.42
1:G:175:VAL:CG2	1:G:184:PRO:HB3	2.50	0.42
2:I:72:GLU:HG3	2:I:75:LYS:HZ3	1.85	0.42
2:J:136:ASP:OD1	2:J:136:ASP:N	2.46	0.42
1:A:360:LEU:HD12	1:A:361:ASN:H	1.84	0.42
1:B:300:THR:HG22	1:B:601:ASN:HA	2.00	0.42
1:B:627:LEU:O	1:B:675:PHE:HA	2.19	0.42
1:C:197:LYS:O	1:C:198:ASN:C	2.58	0.42
1:D:637:LYS:HB2	1:D:637:LYS:HE3	1.86	0.42
1:E:628:LEU:HA	1:E:674:THR:O	2.19	0.42
1:G:293:THR:HG22	1:G:334:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:73:MET:O	2:H:77:ILE:HG12	2.19	0.42
2:H:114:LEU:HD12	2:H:115:HIS:N	2.34	0.42
2:I:84:VAL:HG22	2:I:85:ASP:H	1.84	0.42
2:I:266:ALA:O	2:I:269:GLU:HG3	2.20	0.42
2:I:541:GLU:O	2:I:542:TYR:HD1	2.02	0.42
2:J:439:GLU:OE2	2:J:441:MET:HB2	2.19	0.42
2:J:771:LYS:O	2:J:773:ILE:HG12	2.20	0.42
1:C:471:VAL:HG13	1:C:471:VAL:O	2.20	0.42
1:D:481:LEU:HD23	1:D:481:LEU:HA	1.90	0.42
1:E:385:LEU:HD23	1:E:391:LEU:HD23	2.02	0.42
1:F:492:ILE:HB	1:F:590:LEU:CD1	2.50	0.42
1:G:359:ARG:HB2	1:G:430:THR:CG2	2.50	0.42
1:G:403:GLN:HG3	1:G:411:TYR:HE1	1.85	0.42
2:H:189:LEU:O	2:H:216:VAL:HG13	2.20	0.42
2:I:169:LYS:HA	2:I:169:LYS:HD3	1.85	0.42
2:I:555:ILE:HD12	2:I:555:ILE:HA	1.89	0.42
1:B:358:ALA:HB3	1:B:434:MET:CE	2.50	0.42
1:B:469:VAL:O	1:B:469:VAL:HG23	2.19	0.42
1:C:377:VAL:HG12	1:C:457:GLY:CA	2.50	0.42
1:D:360:LEU:HB3	1:D:432:ILE:CG2	2.49	0.42
1:D:528:LYS:HE2	1:D:528:LYS:HB2	1.55	0.42
1:D:640:SER:OG	1:D:701:VAL:HG13	2.19	0.42
1:F:192:TYR:CD1	1:F:203:LEU:HD11	2.54	0.42
1:G:415:ASN:OD1	1:G:415:ASN:N	2.50	0.42
2:H:163:ILE:HG13	2:H:258:GLU:OE2	2.20	0.42
2:H:219:LYS:HE3	2:H:219:LYS:HB2	1.80	0.42
2:H:685:ILE:HB	2:H:742:ARG:HG2	2.01	0.42
1:C:210:ILE:HA	1:C:213:LYS:NZ	2.34	0.41
1:C:632:ASP:O	1:C:635:ILE:HG22	2.20	0.41
1:D:378:LEU:HD12	1:D:379:PRO:CD	2.50	0.41
1:D:678:PHE:CB	1:D:687:LEU:HD11	2.50	0.41
1:G:500:LEU:HD13	1:G:500:LEU:HA	1.87	0.41
1:G:559:SER:HA	1:G:562:ILE:HG22	2.00	0.41
2:H:122:LYS:HD2	2:H:127:PRO:HA	2.02	0.41
2:H:212:GLU:O	2:H:216:VAL:HG23	2.20	0.41
2:I:38:GLU:HA	2:I:41:LYS:HE3	2.01	0.41
2:J:585:PHE:CE2	2:J:596:VAL:HG13	2.55	0.41
1:A:197:LYS:HB2	1:A:202:PHE:HE2	1.85	0.41
1:A:505:ILE:N	1:A:505:ILE:HD12	2.35	0.41
1:A:612:VAL:O	1:A:616:HIS:CD2	2.72	0.41
1:B:498:LEU:HD23	1:B:498:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:PHE:CE2	1:B:542:TYR:HB2	2.55	0.41
1:C:242:ARG:HD3	1:C:462:TYR:CE2	2.54	0.41
1:C:505:ILE:HD12	1:C:505:ILE:HG23	1.74	0.41
1:E:636:ARG:C	1:E:637:LYS:HD3	2.41	0.41
1:F:404:ILE:HD13	1:F:404:ILE:HA	1.80	0.41
2:H:88:ILE:C	2:H:90:LYS:H	2.22	0.41
2:J:175:ASN:HA	2:J:201:PHE:HD2	1.85	0.41
2:J:477:TYR:HA	2:J:529:ILE:H	1.85	0.41
1:A:332:VAL:CG1	1:A:448:LEU:HB2	2.49	0.41
1:C:520:ASP:OD1	1:C:521:MET:N	2.53	0.41
1:C:541:GLN:CD	1:C:544:GLY:H	2.24	0.41
1:D:176:PRO:HG2	1:D:176:PRO:O	2.20	0.41
1:D:338:LEU:HG	1:D:661:ASP:CB	2.50	0.41
1:D:551:ASP:C	1:D:552:PHE:HD1	2.23	0.41
1:E:295:THR:HG22	1:E:332:VAL:HG23	2.02	0.41
1:E:549:GLU:C	1:E:594:LYS:HE3	2.41	0.41
1:F:183:ILE:HD12	1:F:183:ILE:HG23	1.78	0.41
1:F:270:ILE:HG22	1:F:290:SER:HA	2.02	0.41
1:F:434:MET:CE	1:F:439:PHE:HB2	2.50	0.41
1:F:614:GLU:HA	1:F:617:ARG:NH1	2.28	0.41
2:H:145:LEU:HA	2:H:145:LEU:HD12	1.75	0.41
2:H:162:LYS:NZ	2:H:163:ILE:HD11	2.34	0.41
2:H:491:ARG:CG	2:H:492:PRO:HD2	2.48	0.41
2:H:615:ILE:HD12	2:H:615:ILE:H	1.86	0.41
2:I:194:LEU:HA	2:I:194:LEU:HD23	1.82	0.41
2:J:259:LEU:HD12	2:J:260:LYS:N	2.36	0.41
1:C:267:GLU:H	1:C:267:GLU:CD	2.20	0.41
1:D:346:TRP:HH2	1:D:446:LYS:NZ	2.17	0.41
1:D:624:THR:O	1:D:687:LEU:HD13	2.21	0.41
1:E:338:LEU:HG	1:E:661:ASP:CB	2.50	0.41
1:E:543:GLN:HG2	1:E:545:LYS:NZ	2.36	0.41
1:F:242:ARG:NH2	1:G:224:GLU:OE1	2.53	0.41
1:F:298:THR:HG21	1:F:331:THR:HB	2.01	0.41
1:G:234:SER:N	1:G:237:GLU:OE2	2.48	0.41
2:H:447:THR:HG21	2:H:450:LEU:HD12	2.02	0.41
1:B:497:ASP:OD1	1:B:633:LYS:NZ	2.44	0.41
1:B:514:LEU:HD12	1:B:514:LEU:HA	1.80	0.41
1:C:366:TYR:CE2	1:C:378:LEU:HG	2.53	0.41
1:E:183:ILE:HD11	1:E:236:PHE:CD1	2.52	0.41
1:E:203:LEU:HD12	1:E:203:LEU:HA	1.87	0.41
1:E:548:THR:HA	1:E:575:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:245:LYS:HA	1:F:245:LYS:HE2	2.01	0.41
1:F:558:THR:H	1:F:558:THR:HG23	1.66	0.41
1:G:455:VAL:HG13	1:G:455:VAL:O	2.20	0.41
2:H:724:ASN:O	2:H:725:LEU:HD22	2.20	0.41
2:J:435:ILE:O	2:J:505:LEU:HD22	2.20	0.41
1:A:471:VAL:O	1:A:471:VAL:HG13	2.20	0.41
1:B:226:TRP:CH2	1:B:234:SER:HB3	2.55	0.41
1:B:471:VAL:O	1:B:471:VAL:HG13	2.21	0.41
1:C:264:VAL:HG21	1:C:381:THR:HG21	2.03	0.41
1:C:545:LYS:HD3	1:C:545:LYS:N	2.35	0.41
1:C:592:ARG:H	1:C:592:ARG:HG2	1.63	0.41
1:C:697:ASN:HA	1:C:727:PHE:O	2.19	0.41
1:D:222:SER:H	1:D:228:THR:CG2	2.34	0.41
1:D:493:PHE:HD1	1:D:591:ILE:HG13	1.86	0.41
1:E:199:LYS:HG2	1:F:189:VAL:HG23	2.01	0.41
1:E:291:LYS:NZ	1:E:293:THR:HG22	2.35	0.41
1:E:512:ASP:OD2	1:E:512:ASP:C	2.59	0.41
1:F:442:LEU:HD23	1:F:446:LYS:NZ	2.35	0.41
1:F:566:LEU:HD21	1:F:574:ILE:HG22	2.03	0.41
1:F:617:ARG:HB2	1:F:617:ARG:CZ	2.50	0.41
1:G:377:VAL:HG12	1:G:378:LEU:N	2.35	0.41
1:A:507:ALA:O	1:A:518:LYS:NZ	2.37	0.41
1:C:244:ASP:O	1:C:246:ASN:N	2.53	0.41
1:C:264:VAL:HG22	1:C:366:TYR:CE1	2.55	0.41
1:D:406:ALA:HB3	1:D:409:ASN:HD22	1.84	0.41
1:F:291:LYS:HD3	1:F:292:ASN:N	2.35	0.41
1:F:557:GLN:OE1	1:F:557:GLN:N	2.44	0.41
1:G:469:VAL:O	1:G:469:VAL:HG23	2.19	0.41
2:H:203:VAL:O	2:H:206:LEU:HG	2.21	0.41
2:H:611:GLN:HG3	2:H:613:ASP:OD1	2.20	0.41
2:I:233:LEU:HA	2:I:233:LEU:HD12	1.86	0.41
2:I:434:LYS:HA	2:I:505:LEU:HD21	2.03	0.41
2:I:437:LEU:HD23	2:I:438:TYR:N	2.35	0.41
2:I:557:THR:O	2:I:560:GLN:HG3	2.20	0.41
2:J:466:GLY:O	2:J:469:ASN:OD1	2.39	0.41
1:C:383:LEU:HD21	1:C:448:LEU:HD23	2.02	0.41
1:G:631:ILE:CG2	1:G:635:ILE:HG21	2.51	0.41
1:G:640:SER:HG	1:G:701:VAL:HG13	1.86	0.41
2:H:557:THR:HA	2:H:560:GLN:CD	2.41	0.41
2:I:70:VAL:HG13	2:I:155:LEU:HD12	2.02	0.41
2:I:108:TYR:CD2	2:I:108:TYR:N	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASN:ND2	1:A:485:GLN:OE1	2.53	0.41
1:A:377:VAL:C	1:A:378:LEU:HD12	2.40	0.41
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.84	0.41
1:A:624:THR:OG1	1:A:687:LEU:HB3	2.21	0.41
1:A:702:THR:O	1:A:706:THR:HG23	2.20	0.41
1:B:291:LYS:NZ	1:B:293:THR:HG22	2.36	0.41
1:B:459:ILE:HB	1:B:475:SER:OG	2.21	0.41
1:C:200:ARG:HH22	1:D:189:VAL:HG11	1.86	0.41
1:C:404:ILE:HD12	1:C:404:ILE:N	2.36	0.41
1:C:627:LEU:O	1:C:675:PHE:HA	2.20	0.41
1:C:639:LEU:C	1:C:703:LYS:HZ2	2.23	0.41
1:D:618:GLU:N	1:D:618:GLU:OE1	2.54	0.41
1:E:406:ALA:HB1	1:E:407:PRO:HD2	2.03	0.41
1:E:444:LYS:HE2	1:E:444:LYS:HA	2.03	0.41
1:E:542:TYR:CE2	1:E:543:GLN:NE2	2.88	0.41
1:E:697:ASN:HB3	1:E:699:TYR:CE2	2.56	0.41
1:F:338:LEU:HG	1:F:661:ASP:CB	2.51	0.41
1:F:383:LEU:HD13	1:F:450:LEU:HD21	2.01	0.41
1:F:496:LYS:HA	1:F:496:LYS:HD3	1.89	0.41
1:F:702:THR:O	1:F:706:THR:HG23	2.21	0.41
1:G:366:TYR:CE2	1:G:378:LEU:HD11	2.56	0.41
1:G:494:ASN:OD1	1:G:592:ARG:HA	2.20	0.41
1:G:603:ILE:HD12	1:G:603:ILE:HA	1.91	0.41
2:H:239:GLU:H	2:H:239:GLU:CD	2.24	0.41
2:H:474:ASN:HA	2:H:476:LYS:HZ2	1.85	0.41
2:H:565:ASN:O	2:H:568:GLN:NE2	2.53	0.41
2:H:566:ILE:HG12	2:H:600:TYR:CE1	2.55	0.41
2:I:401:SER:O	2:I:401:SER:OG	2.36	0.41
2:J:239:GLU:HG2	2:J:240:ALA:N	2.34	0.41
2:J:582:LEU:C	2:J:583:ILE:HG13	2.41	0.41
1:B:242:ARG:HB3	1:B:462:TYR:CZ	2.56	0.41
1:B:404:ILE:HD13	1:B:404:ILE:HA	1.79	0.41
1:D:226:TRP:CH2	1:D:234:SER:HB3	2.55	0.41
1:D:366:TYR:CE1	1:D:378:LEU:HD21	2.56	0.41
1:E:295:THR:HG22	1:E:332:VAL:HB	2.03	0.41
1:F:381:THR:OG1	1:F:452:THR:HG22	2.20	0.41
1:F:387:LYS:HA	1:F:387:LYS:HE2	2.03	0.41
2:H:591:TYR:CE2	2:H:594:ASN:HB3	2.56	0.41
2:I:292:LEU:HD13	2:I:419:ILE:HB	2.02	0.41
2:I:517:GLY:C	2:I:518:LYS:HD2	2.41	0.41
2:J:503:ILE:CG1	2:J:549:VAL:HG23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:LYS:CE	1:A:579:ASP:HB3	2.51	0.40
1:B:240:THR:O	1:C:514:LEU:HB2	2.21	0.40
1:B:441:GLU:HA	1:B:444:LYS:HZ2	1.86	0.40
1:B:462:TYR:CD1	1:B:462:TYR:C	2.95	0.40
1:C:298:THR:OG1	1:C:601:ASN:HB2	2.21	0.40
1:C:340:LEU:HB2	1:C:343:GLU:HB3	2.04	0.40
1:D:584:ASN:H	1:D:587:MET:HE3	1.85	0.40
1:E:335:ASP:OD1	1:E:336:HIS:N	2.54	0.40
1:E:368:ASN:ND2	1:E:405:LEU:O	2.53	0.40
1:E:527:LEU:HD23	1:E:527:LEU:HA	1.71	0.40
1:E:577:VAL:HG22	1:E:577:VAL:O	2.21	0.40
1:G:468:ARG:NH2	1:G:470:ARG:HH21	2.19	0.40
2:H:113:LEU:HD22	2:H:115:HIS:CE1	2.54	0.40
2:I:544:ARG:HH11	2:I:544:ARG:HG3	1.85	0.40
2:J:81:ILE:HG22	2:J:129:LEU:HB3	2.03	0.40
1:A:411:TYR:HA	1:A:412:PRO:HA	1.94	0.40
1:A:599:ASP:CG	1:A:600:ARG:N	2.73	0.40
1:A:632:ASP:O	1:A:635:ILE:HG22	2.20	0.40
1:B:524:LYS:NZ	1:B:528:LYS:HE3	2.36	0.40
1:D:610:SER:O	1:D:614:GLU:OE1	2.38	0.40
1:D:631:ILE:C	1:D:636:ARG:HH12	2.25	0.40
1:E:443:GLU:O	1:E:709:ASN:ND2	2.53	0.40
1:E:558:THR:HG22	1:E:587:MET:HA	2.03	0.40
1:F:480:VAL:HG12	1:F:484:ILE:CD1	2.51	0.40
1:F:565:GLN:HA	1:F:568:GLU:OE2	2.21	0.40
1:G:404:ILE:HD13	1:G:404:ILE:HA	1.82	0.40
1:G:563:LYS:O	1:G:566:LEU:HG	2.20	0.40
2:H:113:LEU:HB3	2:H:115:HIS:CE1	2.57	0.40
2:H:473:LYS:O	2:H:476:LYS:NZ	2.51	0.40
1:C:202:PHE:HA	2:I:43:ILE:HG23	2.02	0.40
1:C:297:ARG:HG2	1:C:297:ARG:NH1	2.36	0.40
1:D:198:ASN:C	1:D:199:LYS:HD2	2.42	0.40
1:D:498:LEU:HB2	1:D:637:LYS:NZ	2.36	0.40
1:D:595:ARG:CZ	1:D:596:PHE:HE1	2.34	0.40
1:F:270:ILE:HG12	1:F:361:ASN:O	2.21	0.40
1:F:583:LEU:HD23	1:F:583:LEU:HA	1.76	0.40
1:F:643:ILE:HD12	1:F:723:LYS:CG	2.43	0.40
2:H:226:GLU:OE2	2:H:228:GLN:HB2	2.21	0.40
2:J:221:PHE:CZ	2:J:225:ILE:HD11	2.56	0.40
1:A:198:ASN:OD1	1:A:198:ASN:N	2.54	0.40
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ASN:OD1	1:A:592:ARG:HA	2.21	0.40
1:A:583:LEU:HD22	1:A:587:MET:CE	2.51	0.40
1:A:640:SER:HA	1:A:703:LYS:HE3	2.03	0.40
1:B:405:LEU:HD21	1:B:411:TYR:HB2	2.03	0.40
1:B:505:ILE:HD12	1:B:505:ILE:N	2.37	0.40
1:C:187:LEU:HD13	1:C:187:LEU:HA	1.86	0.40
1:C:297:ARG:HG2	1:C:297:ARG:HH11	1.85	0.40
1:C:698:VAL:HB	1:C:727:PHE:HB3	2.04	0.40
1:D:328:ASN:N	1:D:328:ASN:OD1	2.51	0.40
1:D:514:LEU:HA	1:D:514:LEU:HD12	1.78	0.40
1:D:517:THR:O	1:D:517:THR:HG22	2.22	0.40
2:I:65:LYS:N	2:I:65:LYS:HD2	2.36	0.40
2:I:134:SER:HB2	2:I:137:TYR:CE2	2.57	0.40
2:I:467:ILE:HD12	2:I:467:ILE:H	1.86	0.40
2:I:593:SER:O	2:I:597:GLU:OE1	2.38	0.40
2:J:408:VAL:HG12	2:J:412:TYR:CE2	2.57	0.40
1:A:225:LYS:HE2	1:A:225:LYS:HB3	1.86	0.40
1:A:364:ILE:O	1:A:419:ILE:HG22	2.21	0.40
1:B:628:LEU:HA	1:B:674:THR:O	2.21	0.40
1:C:500:LEU:HD13	1:C:500:LEU:HA	1.88	0.40
1:C:500:LEU:HD22	1:C:500:LEU:N	2.37	0.40
1:D:610:SER:O	1:D:613:LYS:HG2	2.22	0.40
1:E:261:ILE:HG23	1:E:328:ASN:HD21	1.87	0.40
1:F:250:GLU:CD	1:F:503:ARG:HE	2.24	0.40
1:G:383:LEU:N	1:G:392:ALA:O	2.53	0.40
2:I:84:VAL:HG22	2:I:85:ASP:N	2.36	0.40
2:I:91:HIS:HB3	2:I:94:LEU:HG	2.03	0.40
2:J:718:PHE:HA	2:J:722:GLY:HA3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/759 (69%)	479 (92%)	40 (8%)	4 (1%)	19	57
1	B	523/759 (69%)	477 (91%)	44 (8%)	2 (0%)	34	70
1	C	523/759 (69%)	477 (91%)	44 (8%)	2 (0%)	34	70
1	D	522/759 (69%)	474 (91%)	46 (9%)	2 (0%)	34	70
1	E	523/759 (69%)	477 (91%)	45 (9%)	1 (0%)	47	79
1	F	523/759 (69%)	474 (91%)	47 (9%)	2 (0%)	34	70
1	G	523/759 (69%)	478 (91%)	42 (8%)	3 (1%)	25	62
2	H	695/809 (86%)	638 (92%)	53 (8%)	4 (1%)	25	62
2	I	700/809 (86%)	648 (93%)	51 (7%)	1 (0%)	51	83
2	J	649/809 (80%)	606 (93%)	41 (6%)	2 (0%)	41	74
All	All	5704/7740 (74%)	5228 (92%)	453 (8%)	23 (0%)	38	70

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	663	LEU
1	B	198	ASN
1	C	198	ASN
1	D	198	ASN
1	E	198	ASN
1	F	199	LYS
2	H	67	PRO
2	H	90	LYS
2	J	582	LEU
2	H	101	LYS
1	G	199	LYS
1	A	345	THR
1	D	175	VAL
2	H	640	ALA
1	F	633	LYS
1	G	633	LYS
2	I	772	PHE
2	J	772	PHE
1	A	351	GLY
1	B	577	VAL
1	C	577	VAL
1	G	577	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	414/683 (61%)	410 (99%)	4 (1%)	76	86
1	B	415/683 (61%)	414 (100%)	1 (0%)	93	97
1	C	415/683 (61%)	414 (100%)	1 (0%)	93	97
1	D	414/683 (61%)	413 (100%)	1 (0%)	93	97
1	E	415/683 (61%)	409 (99%)	6 (1%)	67	81
1	F	415/683 (61%)	412 (99%)	3 (1%)	84	91
1	G	415/683 (61%)	415 (100%)	0	100	100
2	H	551/739 (75%)	542 (98%)	9 (2%)	62	79
2	I	338/739 (46%)	333 (98%)	5 (2%)	65	81
2	J	292/739 (40%)	285 (98%)	7 (2%)	49	71
All	All	4084/6998 (58%)	4047 (99%)	37 (1%)	79	88

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	ARG
1	A	470	ARG
1	A	521	MET
1	A	678	PHE
1	B	633	LYS
1	C	387	LYS
1	D	213	LYS
1	E	175	VAL
1	E	359	ARG
1	E	561	ASN
1	E	563	LYS
1	E	633	LYS
1	E	636	ARG
1	F	524	LYS
1	F	563	LYS
1	F	633	LYS

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Mol	Chain	Res	Type
2	H	169	LYS
2	H	251	GLU
2	H	264	MET
2	H	265	LEU
2	H	273	LYS
2	H	413	LYS
2	H	579	TYR
2	H	594	ASN
2	H	607	LYS
2	I	113	LEU
2	I	122	LYS
2	I	270	LYS
2	I	465	ARG
2	I	607	LYS
2	J	75	LYS
2	J	122	LYS
2	J	175	ASN
2	J	248	ASN
2	J	579	TYR
2	J	581	LYS
2	J	698	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	ASN
1	A	557	GLN
1	B	541	GLN
1	C	557	GLN
1	C	705	ASN
1	D	422	ASN
1	D	447	GLN
1	D	485	GLN
1	D	705	ASN
1	E	541	GLN
1	E	561	ASN
1	F	458	ASN
1	G	438	GLN
2	H	115	HIS
2	H	186	GLN
2	H	228	GLN
2	H	417	GLN

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Mol	Chain	Res	Type
2	H	563	GLN
2	I	228	GLN
2	I	496	ASN
2	J	690	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

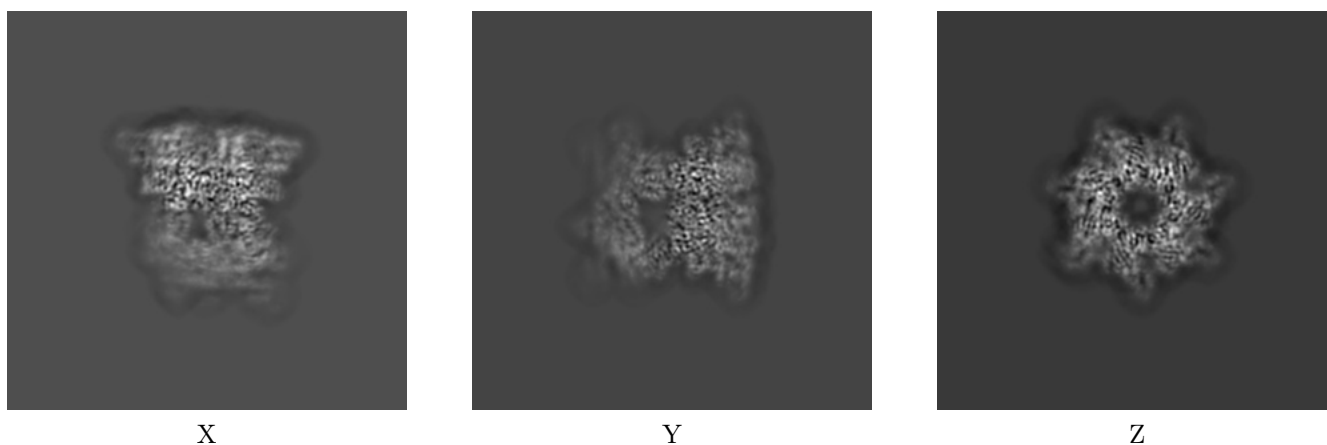
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11523. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

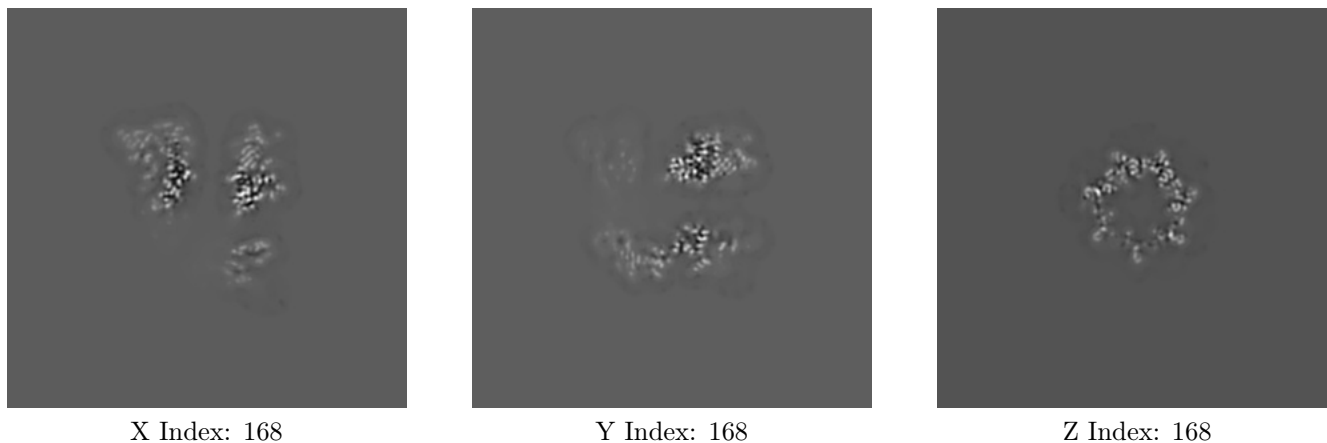
6.1.1 Primary map



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

6.2 Central slices [i](#)

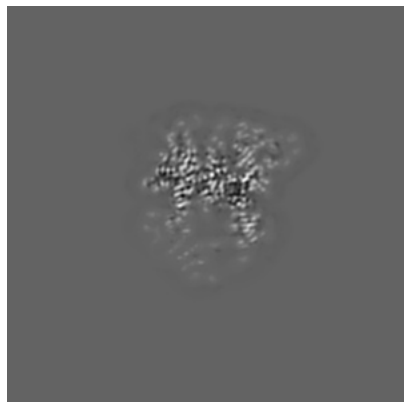
6.2.1 Primary map



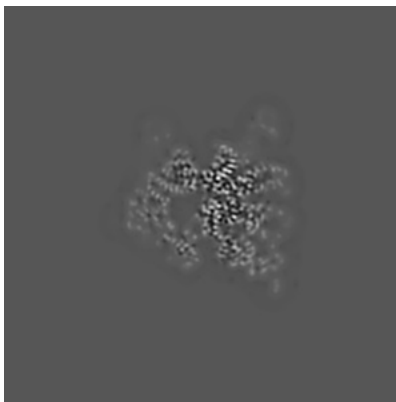
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

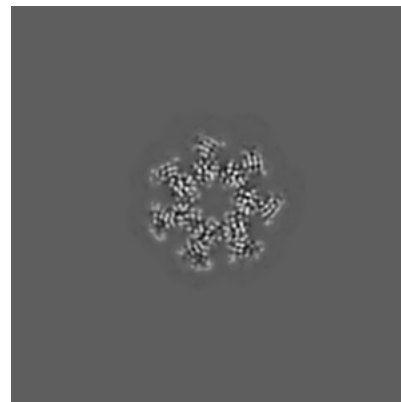
6.3.1 Primary map



X Index: 196



Y Index: 198

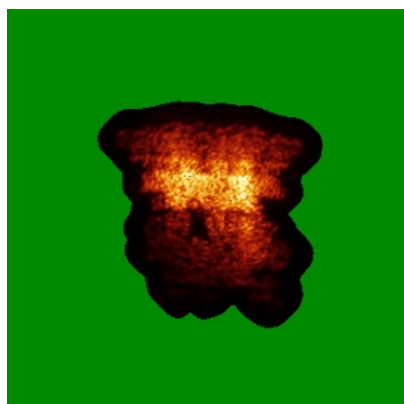


Z Index: 194

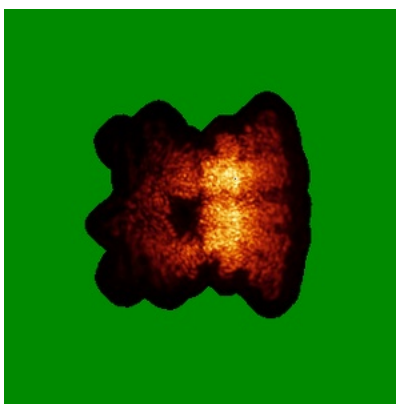
The images above show the largest variance slices of the map in three orthogonal directions.

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

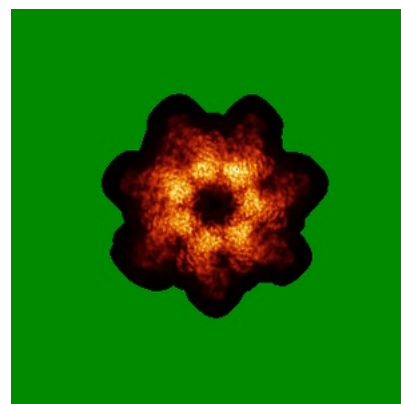
6.4.1 Primary map



X



Y

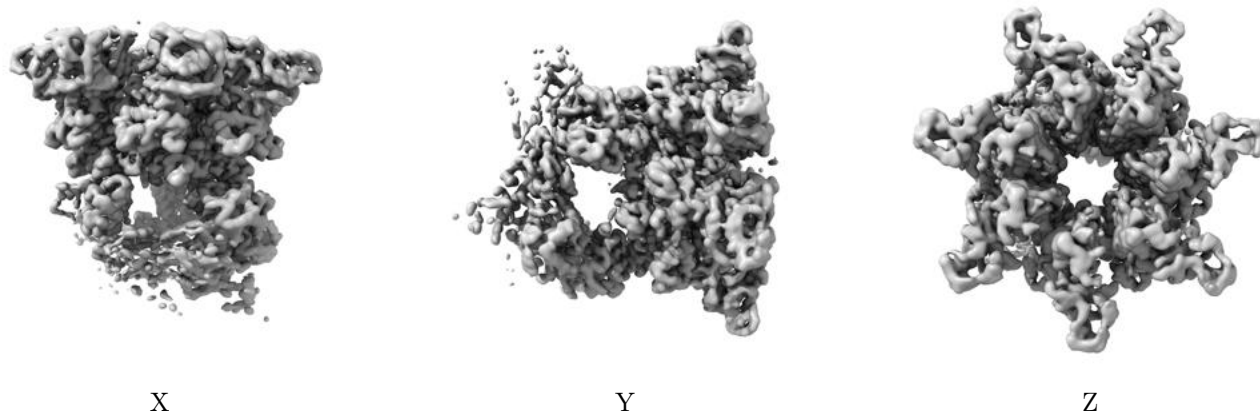


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

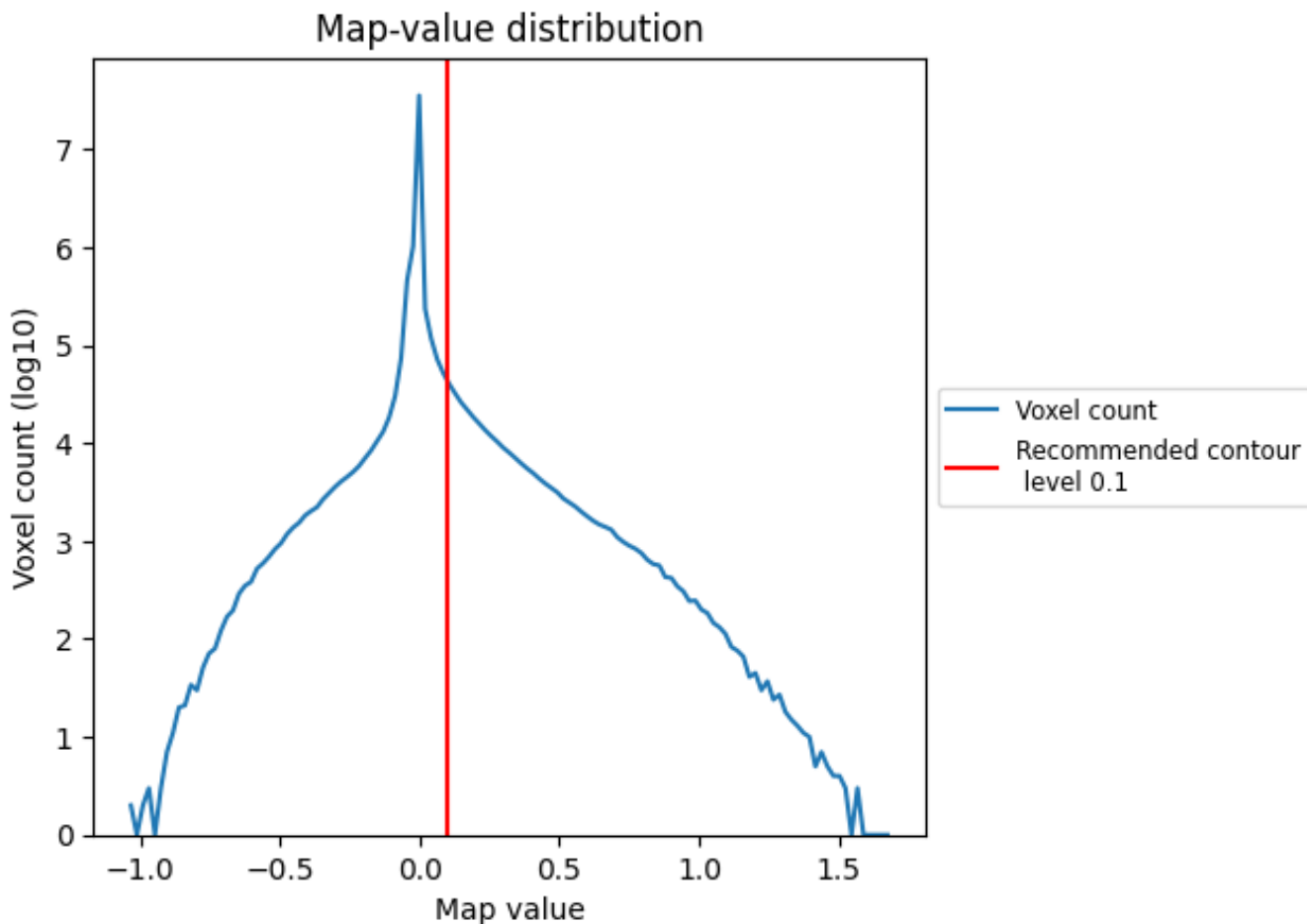
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

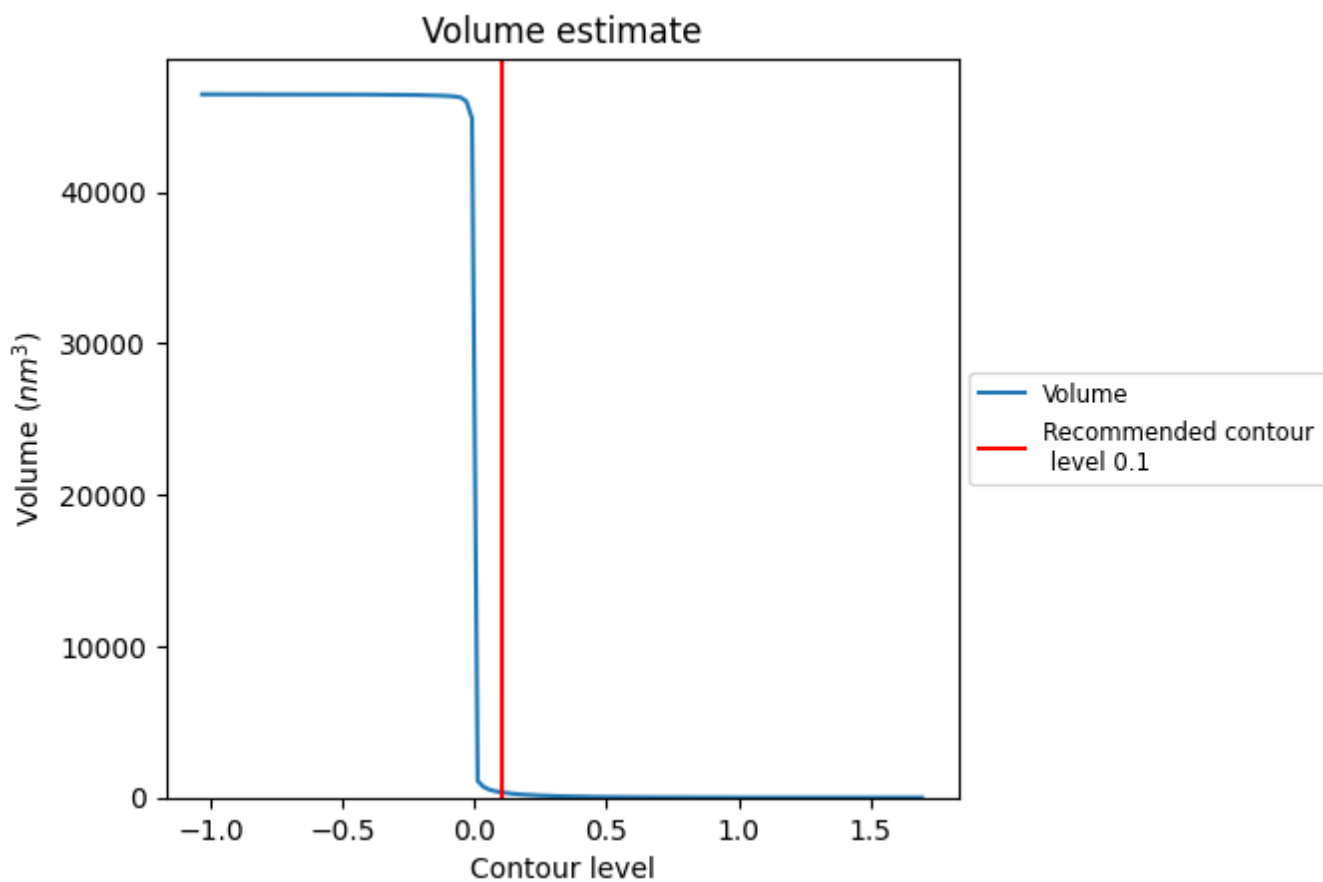
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

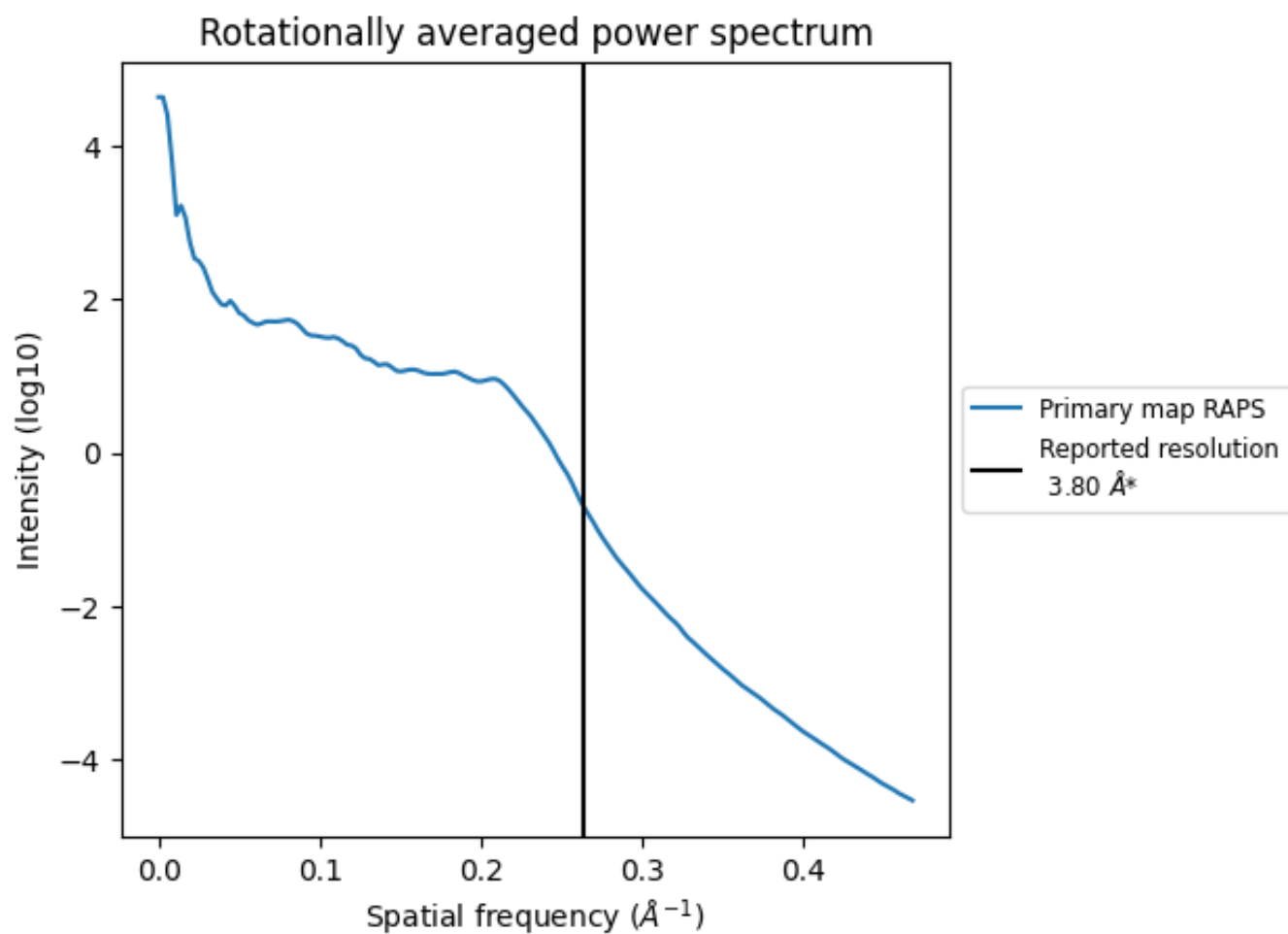
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 351 nm^3 ; this corresponds to an approximate mass of 317 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

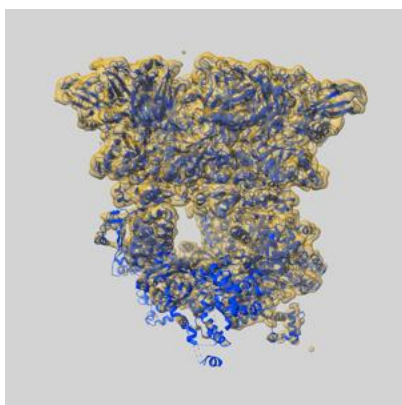
8 Fourier-Shell correlation

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

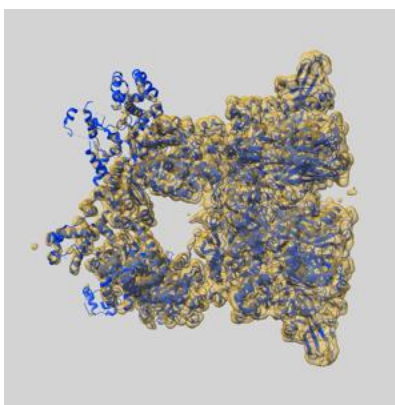
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11523 and PDB model 6ZXX. Per-residue inclusion information can be found in section 3 on page 9.

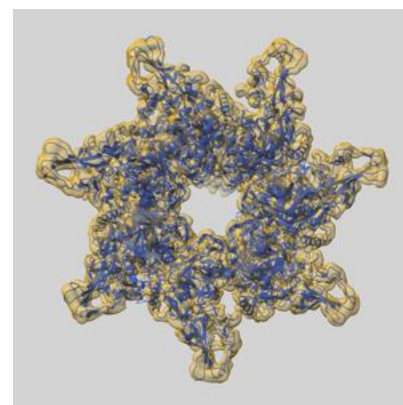
9.1 Map-model overlay [i](#)



X



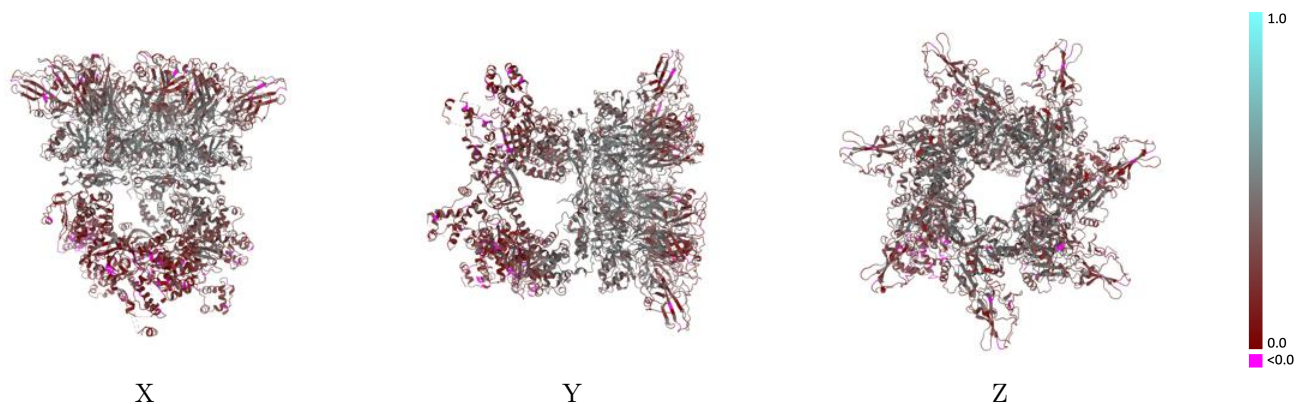
Y



Z

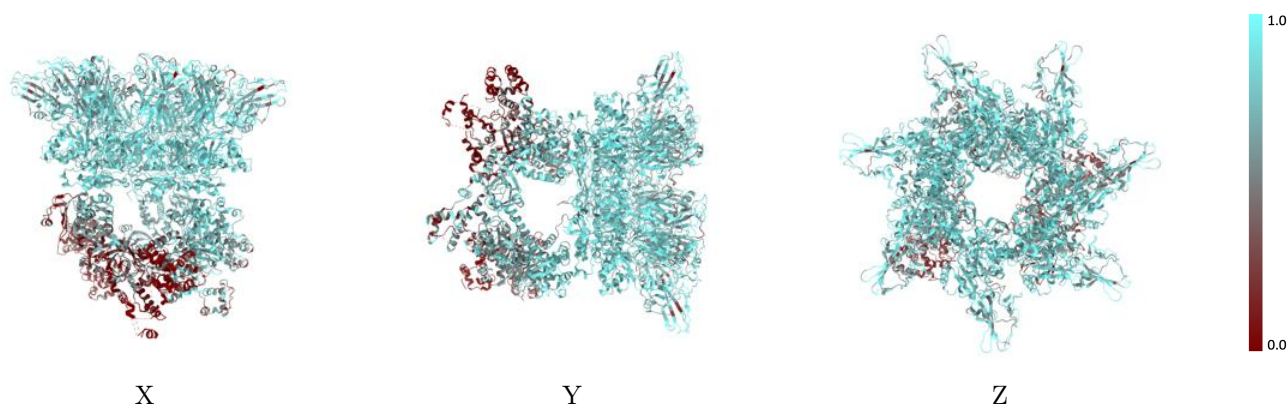
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



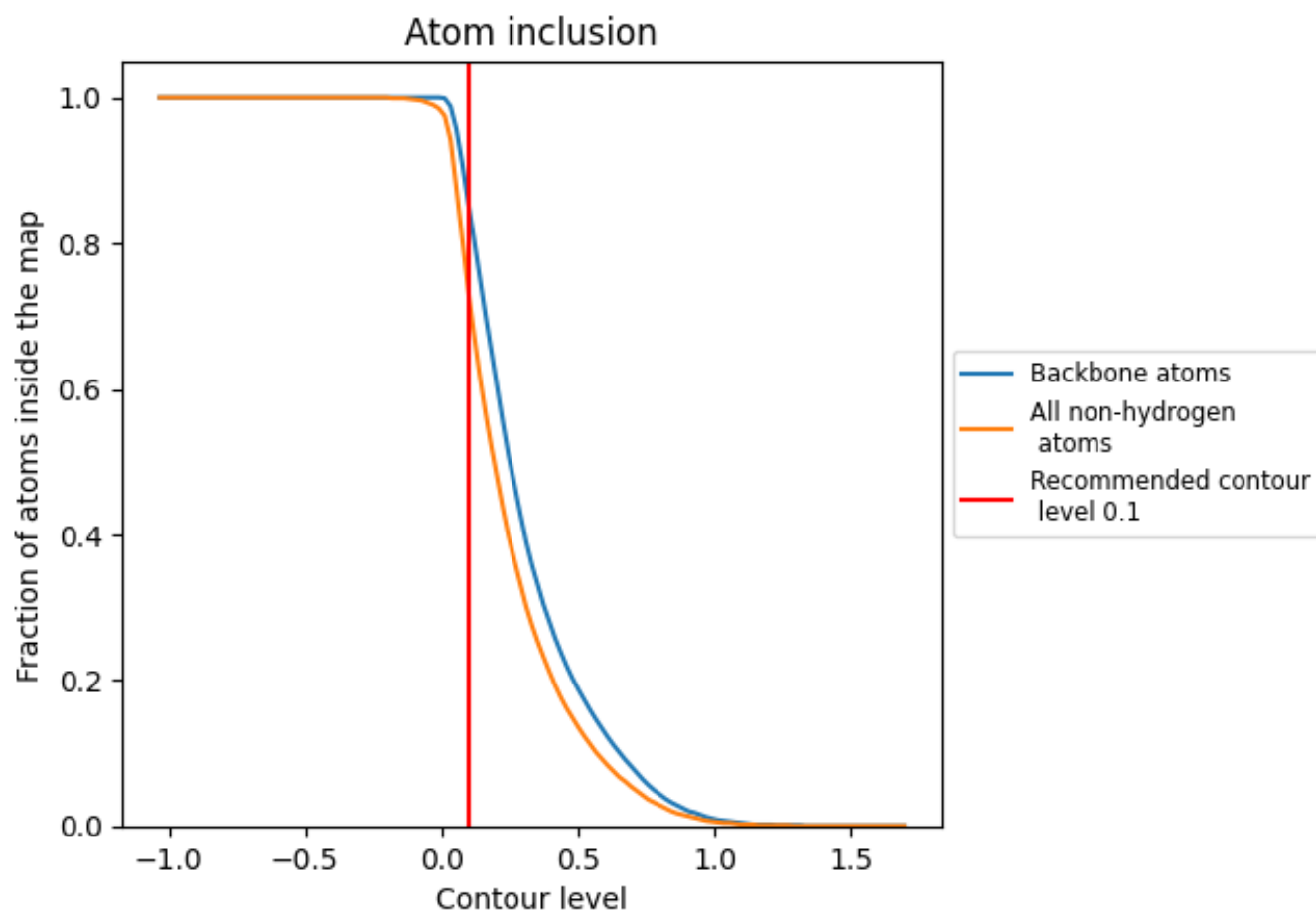
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).























9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7280	 0.3400
A	 0.8240	 0.3850
B	 0.8310	 0.3890
C	 0.8350	 0.3890
D	 0.8380	 0.3880
E	 0.8180	 0.3790
F	 0.8170	 0.3750
G	 0.8280	 0.3840
H	 0.6900	 0.2920
I	 0.5280	 0.2510
J	 0.3570	 0.2100

