



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 03:08 am GMT

PDB ID : 6ZXL
EMDB ID : EMD-11524
Title : Fully-loaded anthrax lethal toxin in its heptameric pre-pore state and PA7LF(2+1A) arrangement
Authors : Quentin, D.; Antoni, C.; Gatsogiannis, C.; Raunser, S.
Deposited on : 2020-07-29
Resolution : 4.20 Å(reported)
Based on initial model : 6ZXK

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

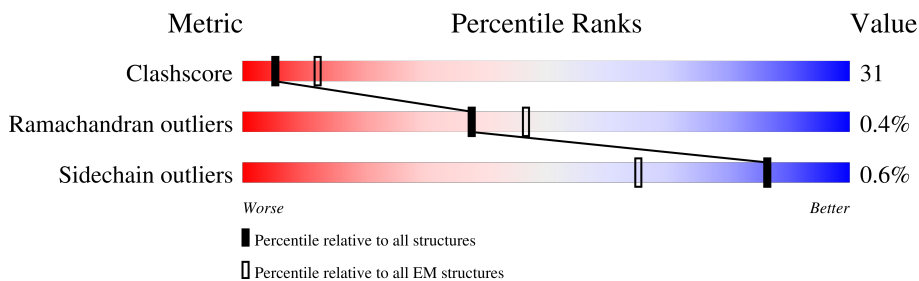
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	
1	B	759	
1	C	759	
1	D	759	
1	E	759	
1	F	759	
1	G	759	
2	H	809	

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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 42172 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	3961	2477	691	789	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

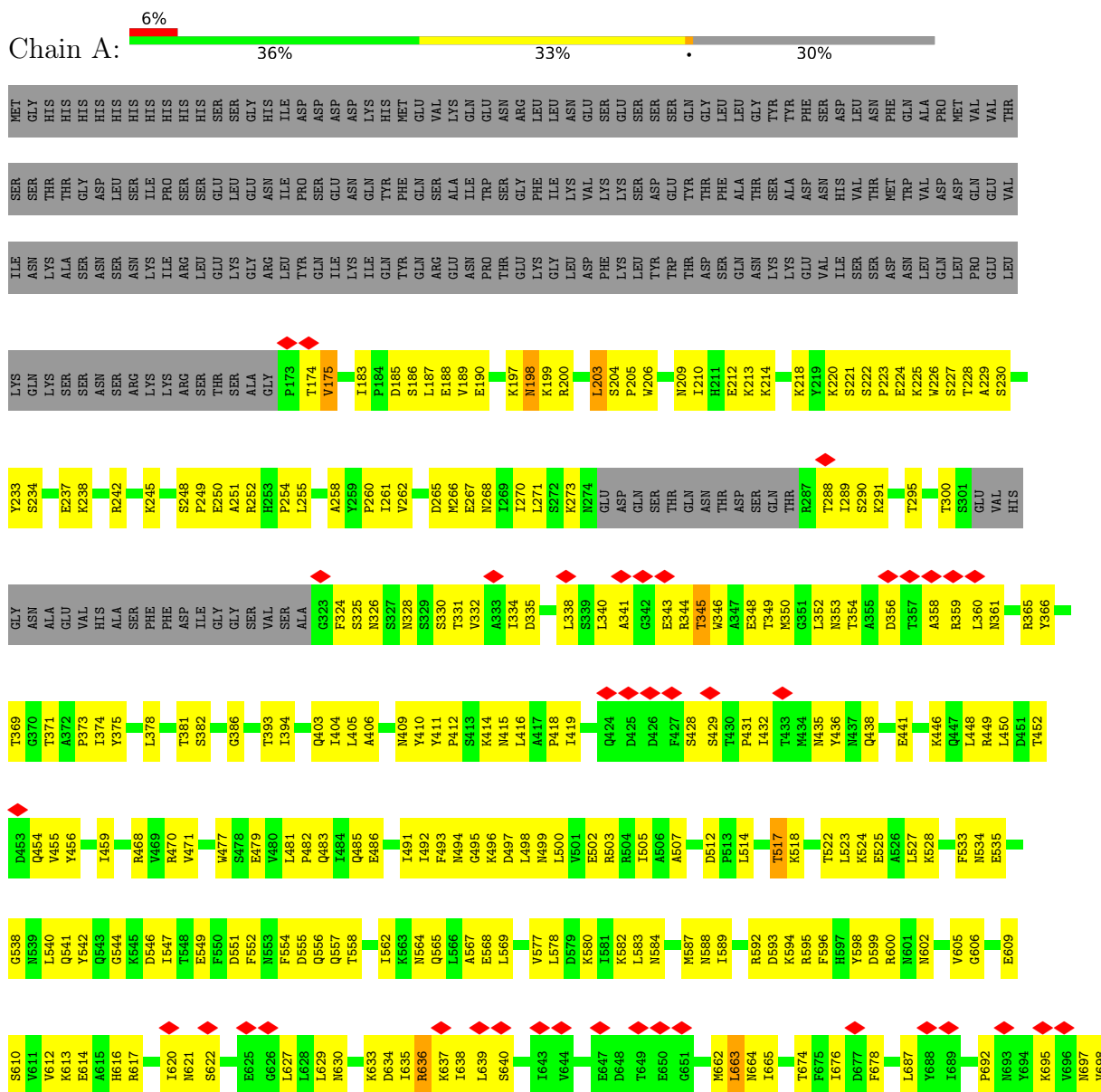
- Molecule 2 is a protein called Lethal factor.

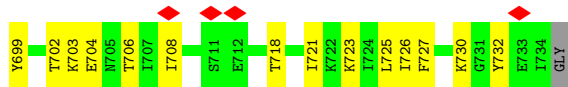
Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	699	Total	C	N	O	S	0	0
			5378	3404	913	1055	6		
2	I	710	Total	C	N	O	S	0	0
			4739	2982	841	912	4		
2	J	661	Total	C	N	O	S	0	0
			4239	2655	752	830	2		

3 Residue-property plots [i](#)

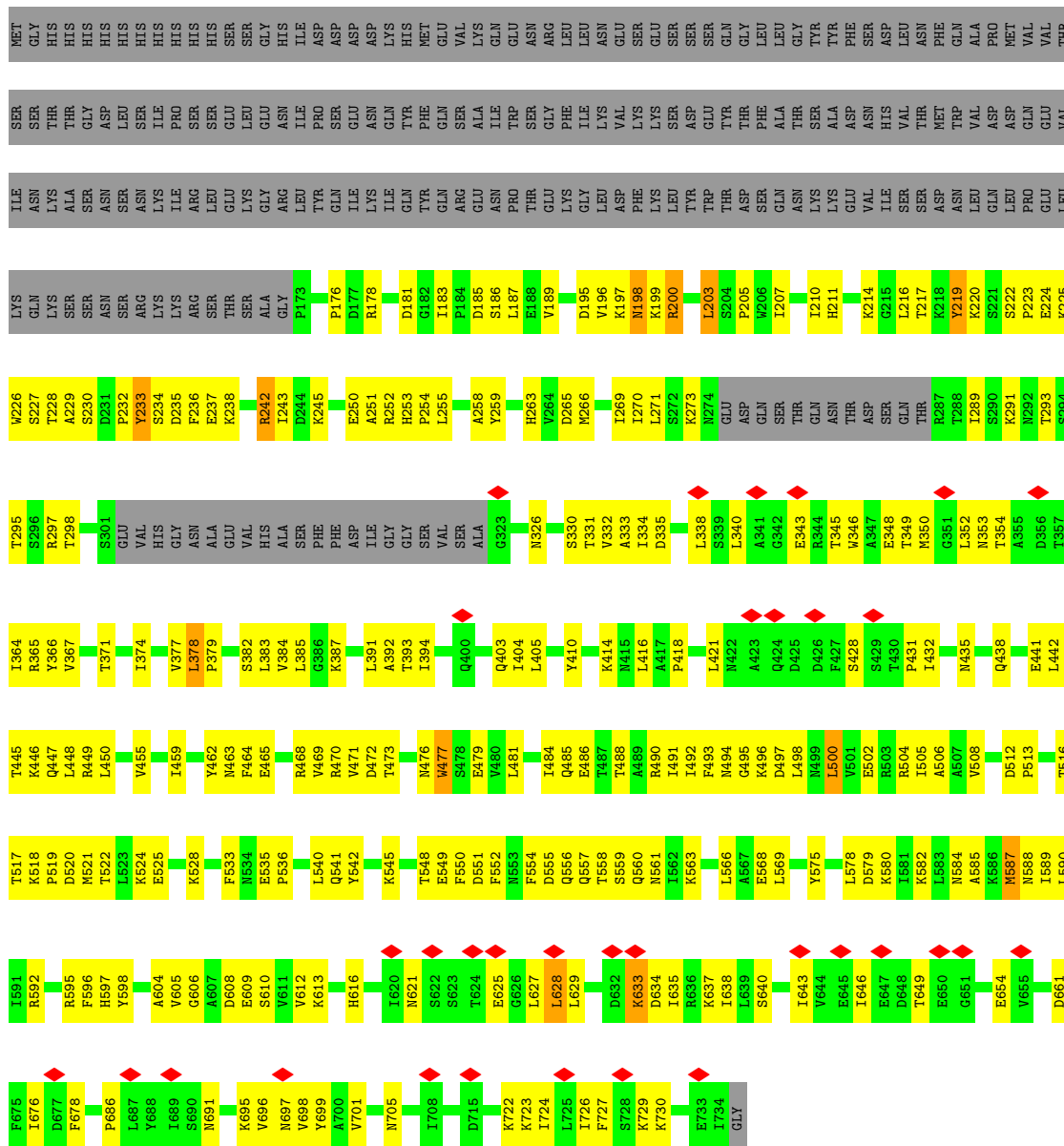
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Protective antigen

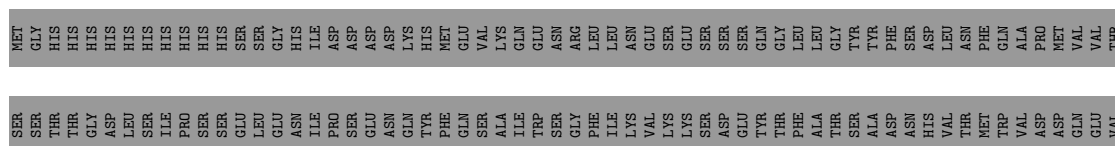


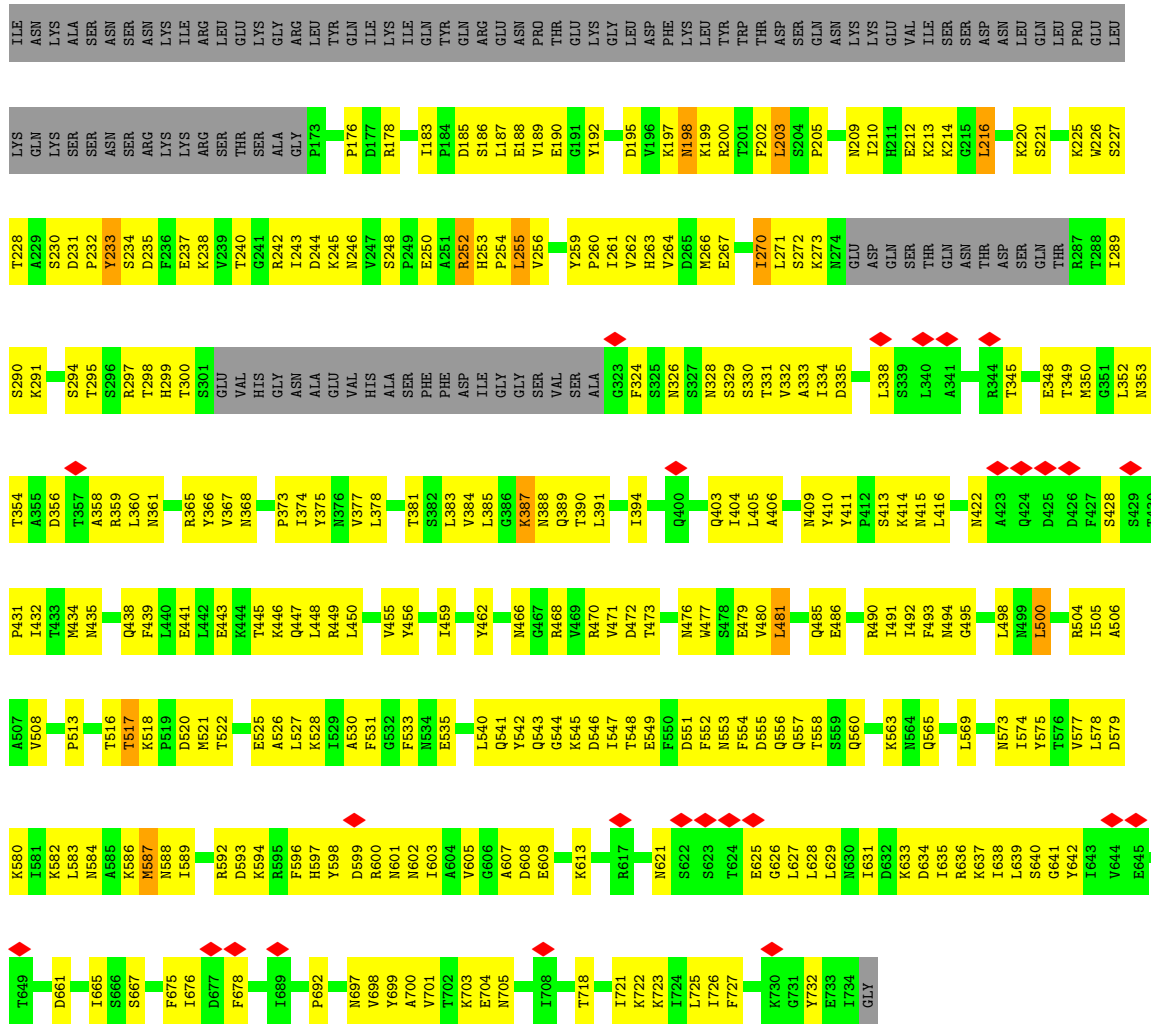


• Molecule 1: Protective antigen

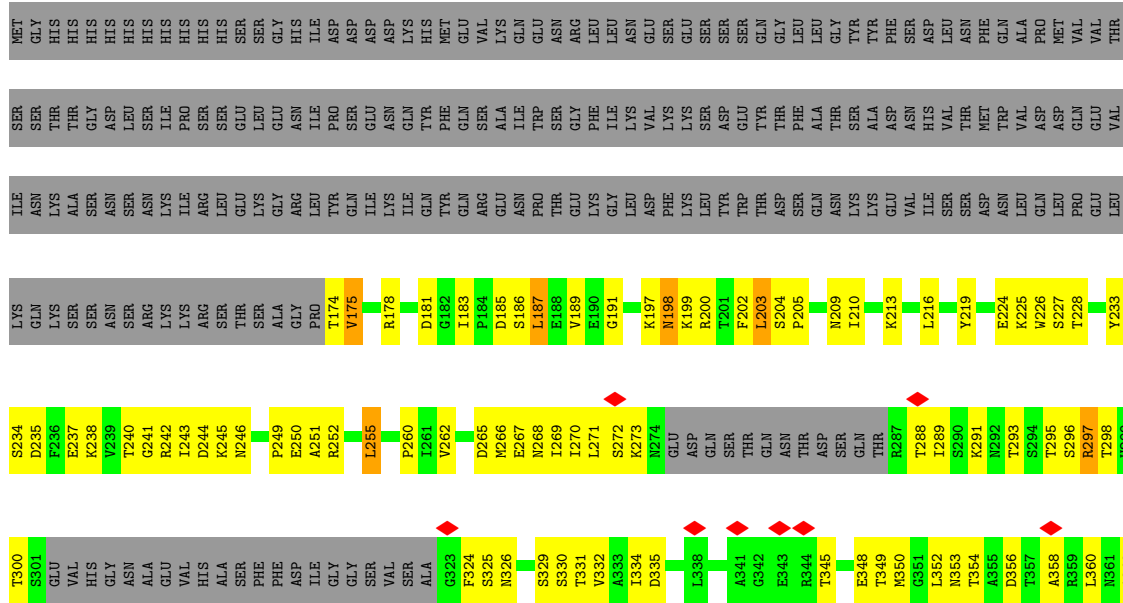


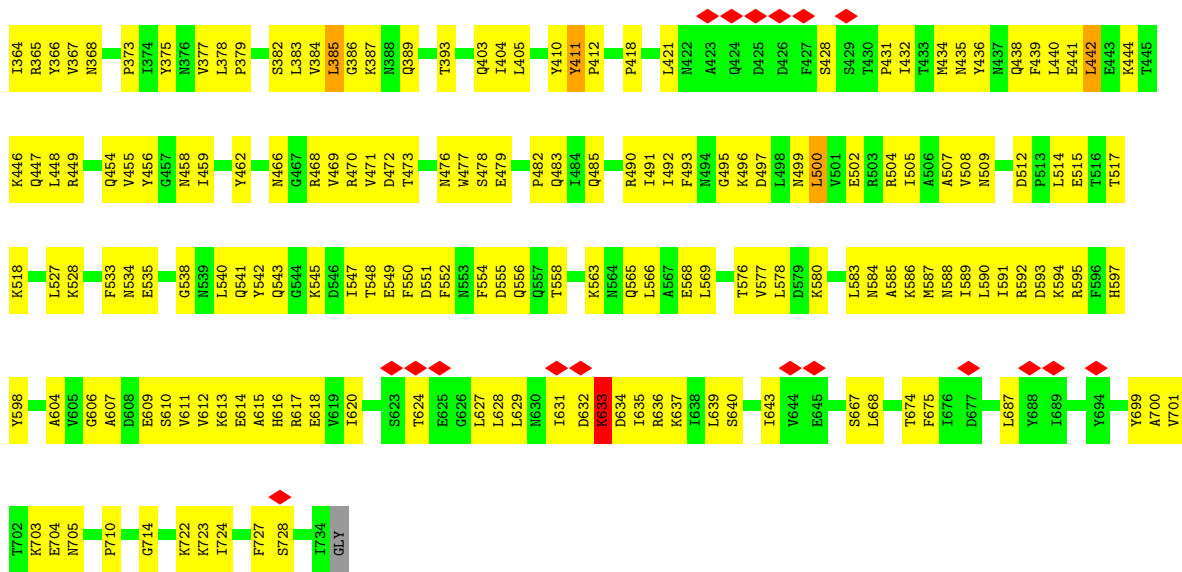
• Molecule 1: Protective antigen



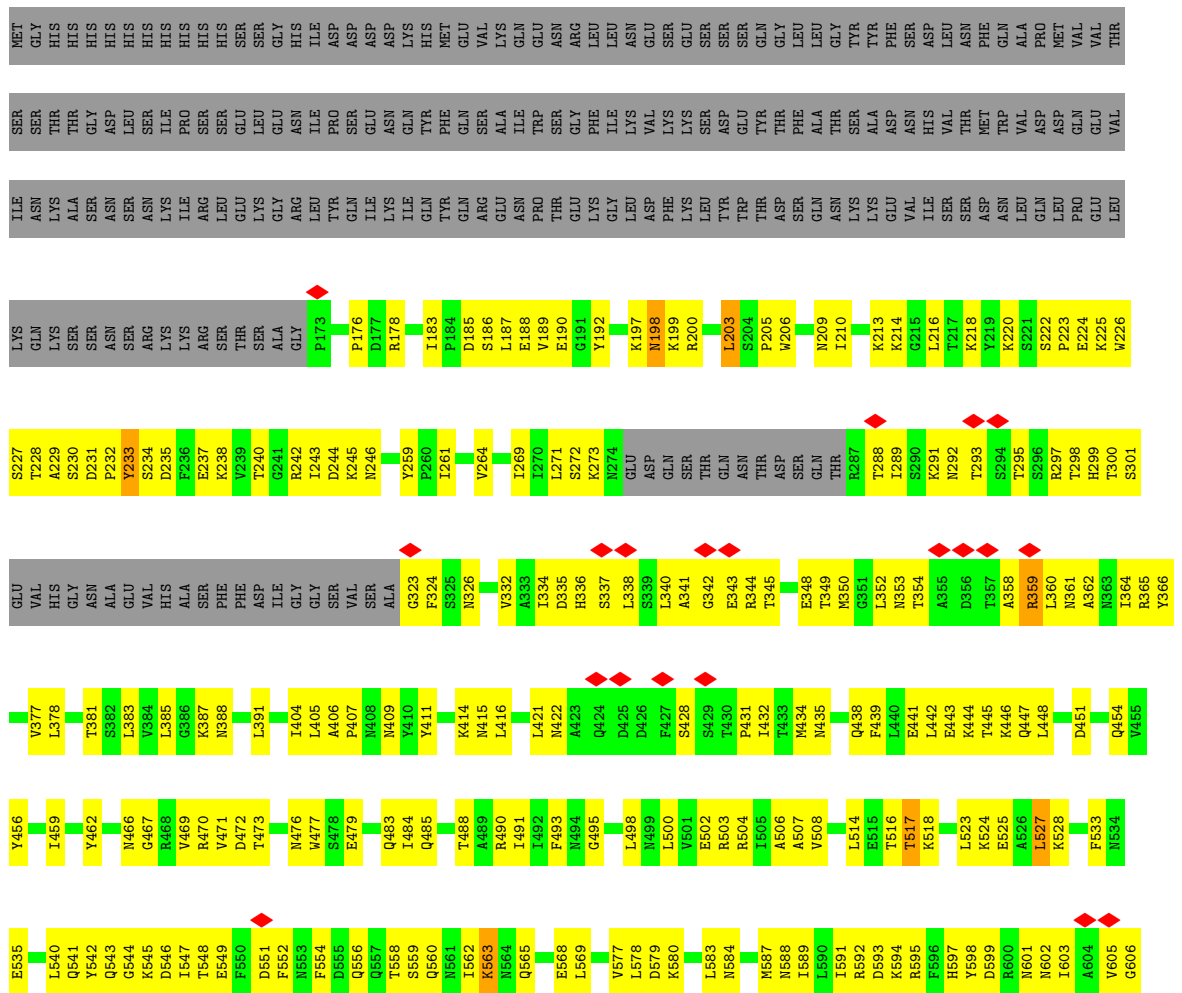


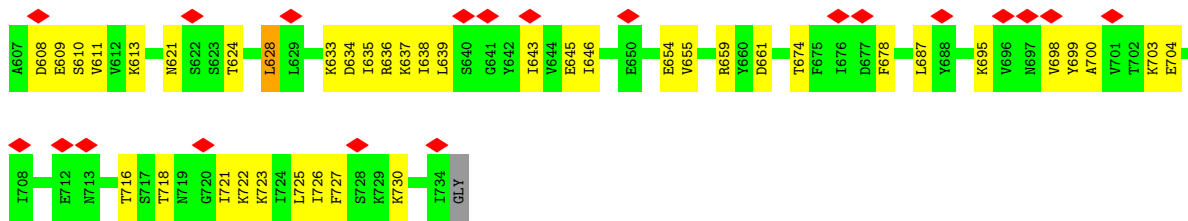
• Molecule 1: Protective antigen



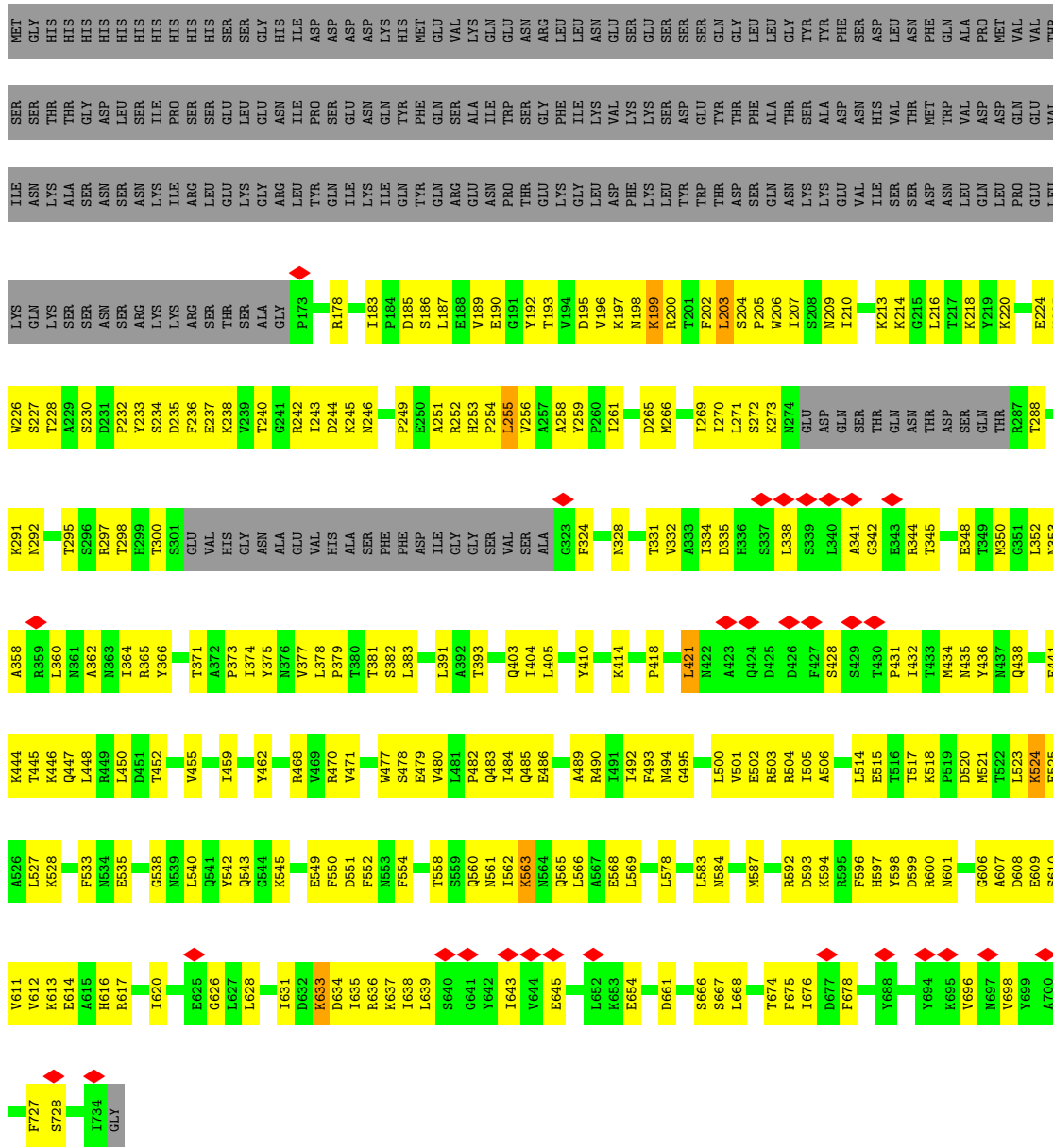
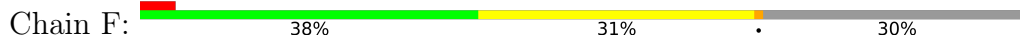


• Molecule 1: Protective antigen

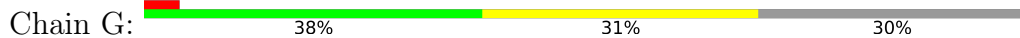


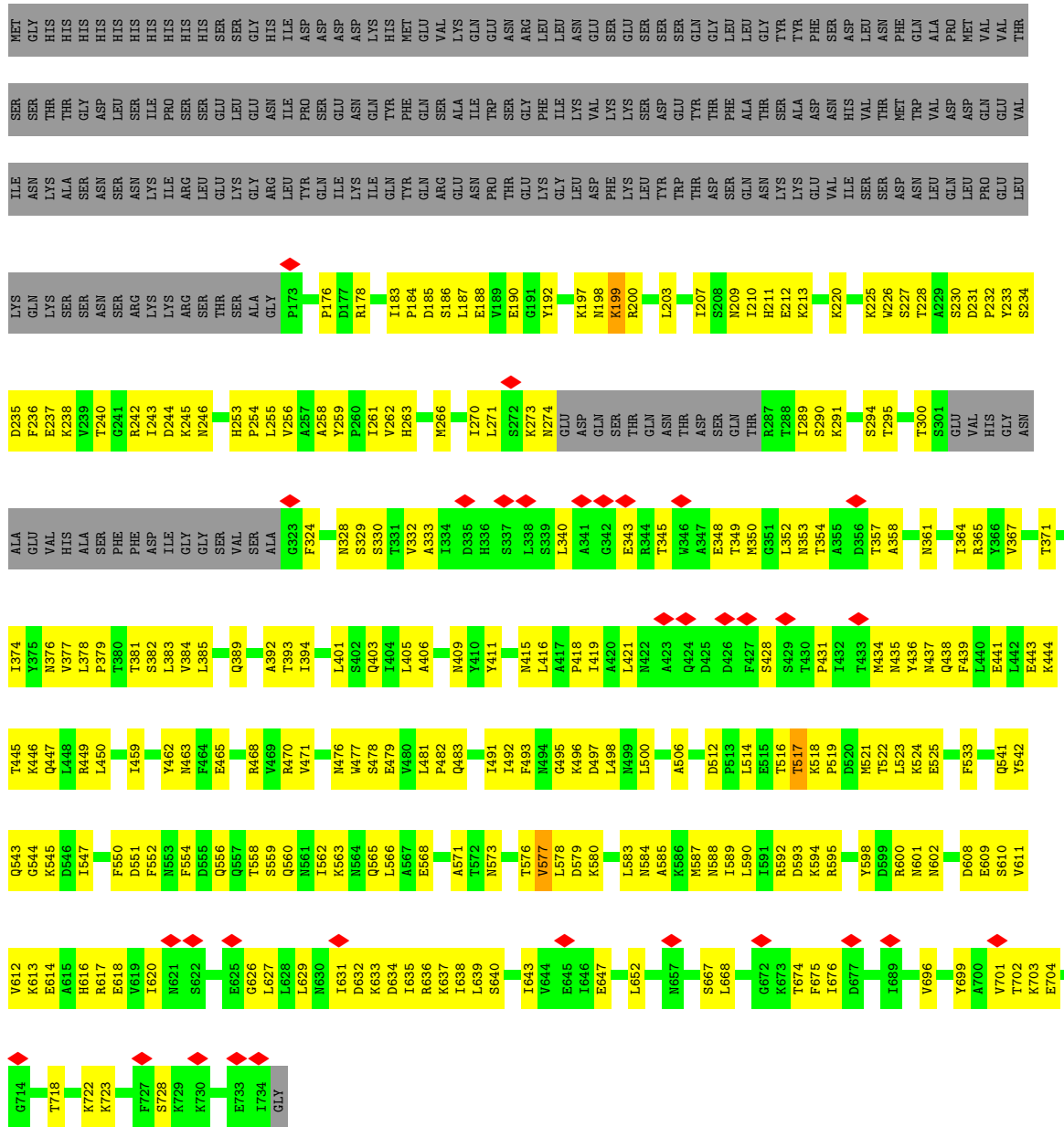


• Molecule 1: Protective antigen

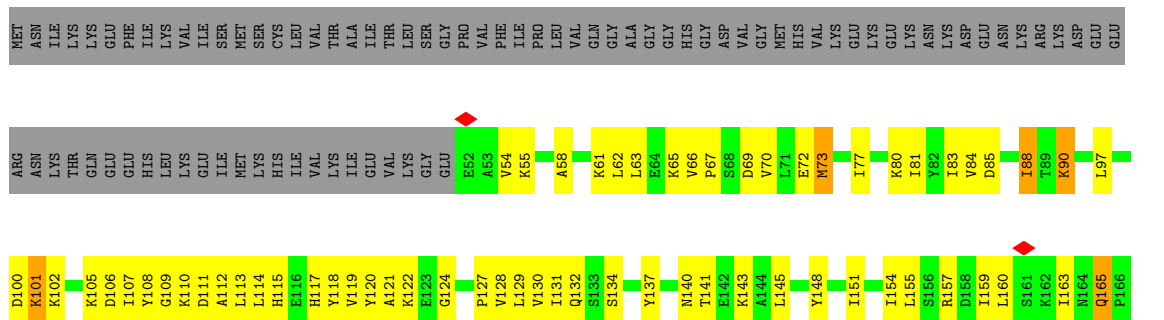


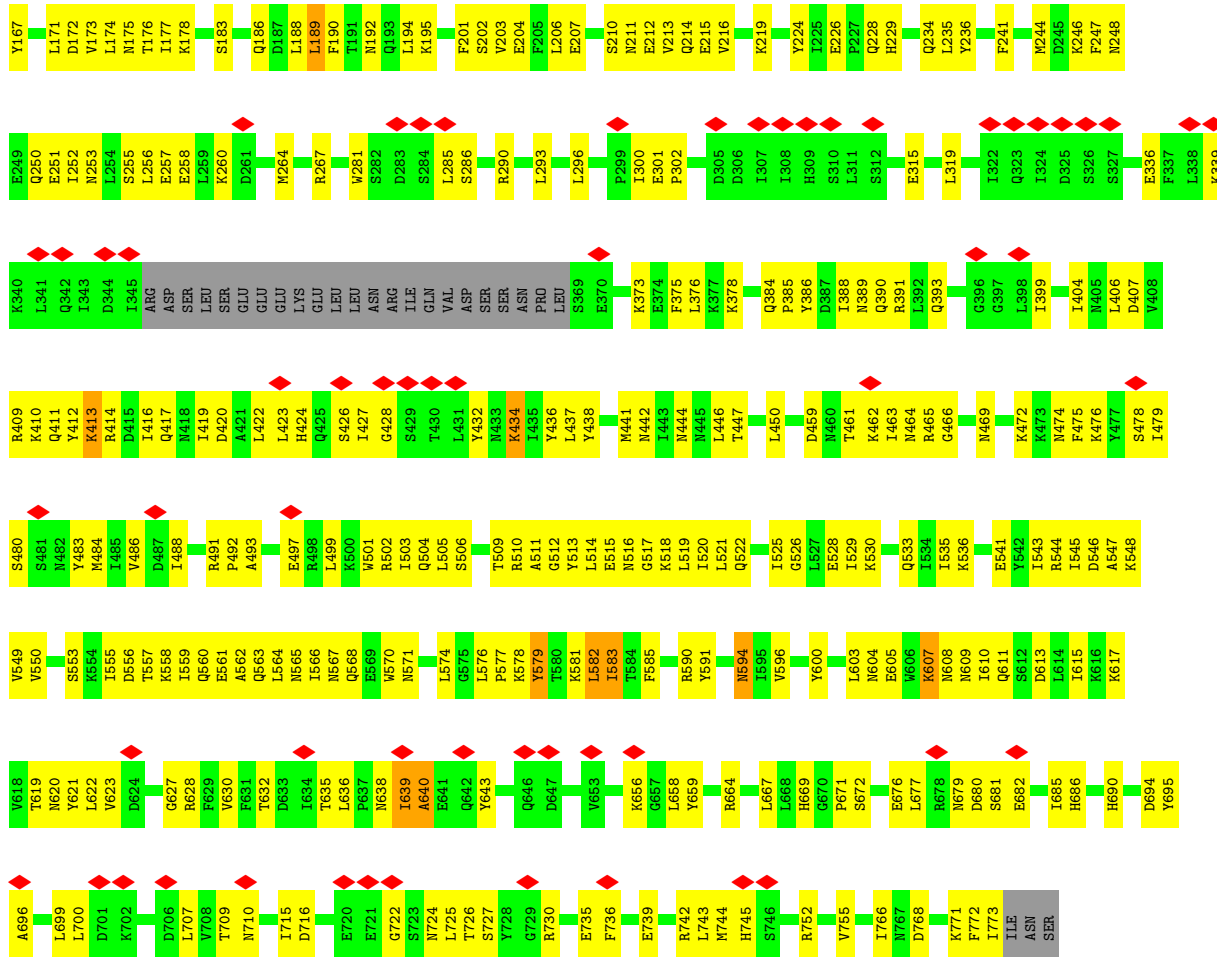
• Molecule 1: Protective antigen



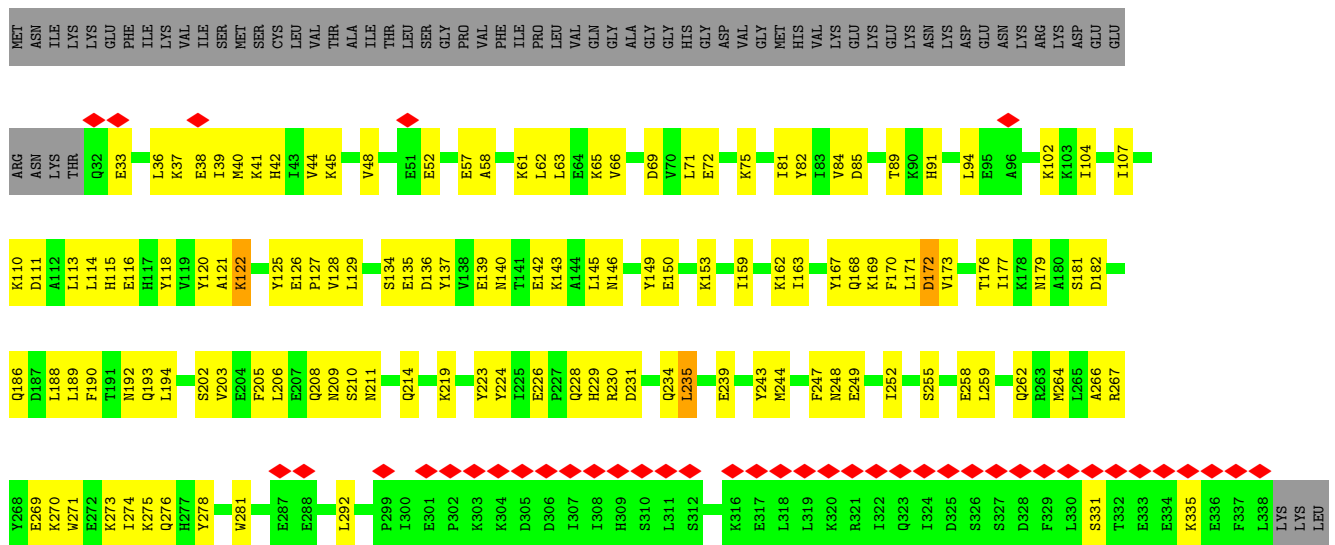


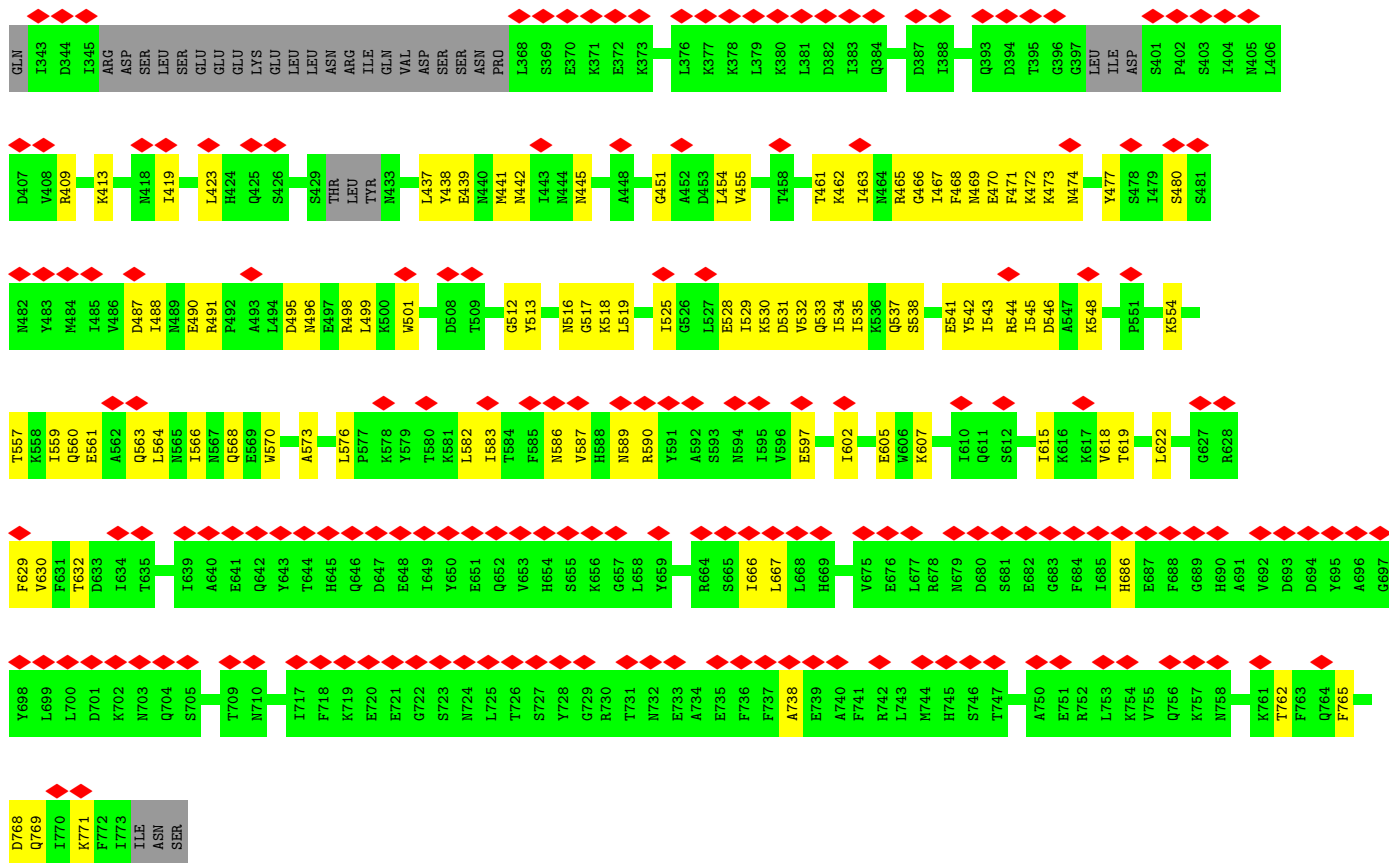
• Molecule 2: Lethal factor



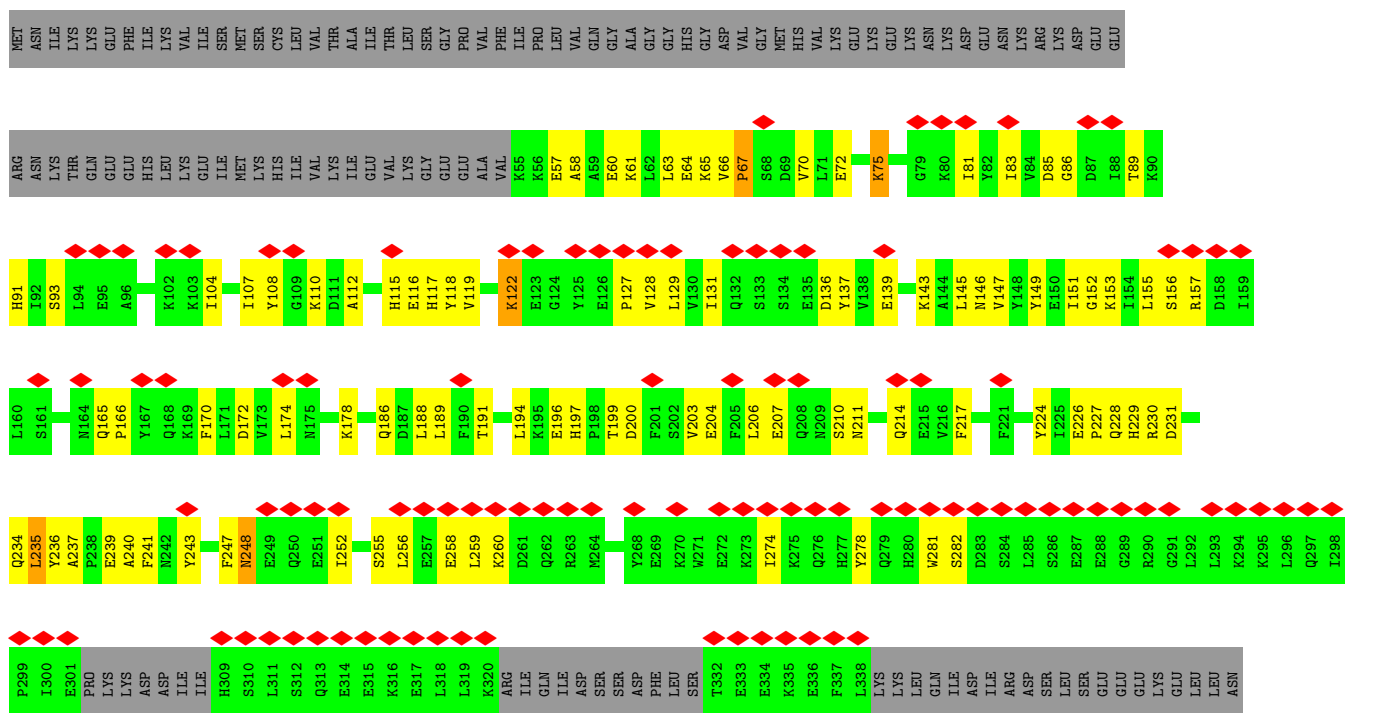


• Molecule 2: Lethal factor





• Molecule 2: Lethal factor



ARG	ILE	GLN	VAL	ASP	SER	ASN	PRO	L368	S369	E370	K371	E372	K373	E374	F375	L376	K377	L378	L379	K380	L381	L382	I383	Q384	P385	Y386	D387	I388	N389	Q390	R391	L392	Q393	D394	T395	G396	G397	LEU	ILE	ASP	SER	PRO	SER	SER	ILE	M405	L406	D407	V408	R409	K410	Q411	Y412	K413	R414	D415	I416	Q417	M418	
I419	D420	A421	L422	L423	H424	Q425	S426	I427	G428	SER	THR	LEU	TYR	M433	K434	I435	Y436	L437	Y438	E439	M440	M441	M442	I443	M444	M445	L446	T447	I448	A449	N516	T449	L450	C451	A452	D453	L454	V455	D456	S457	T458	D459	M460	T461	K462	I463	M464	M469	E470	F471	M474	F475	K476	Y477	S478	I479	S480	S481	M482	
Y483	M484	I485	V486	D487	I488	P492	A493	L494	D495	M496	E497	R498	L499	K500	M501	R502	I503	Q504	L505	S506	P507	D508	T509	G512	Y513	L514	E515	N516	G517	K518	L519	I520	L521	Q522	R523	N524	I525	G526	L527	E528	I529	K530	D531	V532	Q533	I534	I535	K536	Q537	S538	E539	K540	E541	Y542	I543	R544	I545			
D546	A547	K548	V549	V550	P551	K552	S553	K554	I555	D556	K558	I559	Q560	E561	A562	Q563	L564	N565	I566	N567	Q568	E569	M570	N571	K572	Y573	L574	G575	L576	P577	K578	Y579	T580	K581	L582	I583	T584	F585	N586	V587	H588	N589	R590	Y591	A592	S593	N594	I595	V596	E597	S598	A599	Y600	L601	I602	L603	N604	E605		
W606	K607	N608	N609	I610	Q611	S612	D613	K614	L614	I615	K616	K617	V618	T619	N620	Y621	L622	V623	D624	G625	N626	G627	R628	F629	V630	F631	T632	D633	I634	T635	L636	P637	N638	I639	A640	E641	Q642	Y643	T644	H645	Q646	D647	E648	I649	Y650	E651	Q652	V653	H654	S655	K656	G657	L658	Y659	V660	P661	E662	S663	R664	S665
I666	L667	L668	H669	G670	P671	S672	K673	G674	V675	E676	L677	R678	N679	D680	S681	R682	G683	F684	I685	H686	E687	F688	G689	H690	A691	V692	D693	D694	V695	A696	G697	Y698	L699	L700	D701	K702	N703	Q704	S705	D706	D707	L707	V708	T709	M710	S711	K712	K713	F714	I715	D716	I717	F718	K719	E720	T721	G722	S723	N724	L725
T726	S727	Y728	G729	R730	T731	M732	E733	A734	E735	F736	F737	A738	E739	A740	F741	R742	L743	M744	H745	S746	T747	D748	H749	A750	E751	R752	L753	K754	V755	Q756	K757	N758	A759	P760	K761	T762	F763	Q764	F765	I766	N767	D768	Q769	I770	K771	F772	I773	ILE	ASN	SER										

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44000	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	1.098	Depositor
Minimum map value	-0.772	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	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	0.67	1/4029 (0.0%)	0.73	3/5491 (0.1%)
1	B	0.73	3/4045 (0.1%)	0.77	5/5511 (0.1%)
1	C	0.75	2/4045 (0.0%)	0.78	8/5511 (0.1%)
1	D	0.74	1/4037 (0.0%)	0.82	10/5500 (0.2%)
1	E	0.69	1/4045 (0.0%)	0.78	6/5511 (0.1%)
1	F	0.70	1/4045 (0.0%)	0.75	3/5511 (0.1%)
1	G	0.68	1/4045 (0.0%)	0.71	0/5511
2	H	0.50	0/5476	0.71	5/7434 (0.1%)
2	I	0.47	0/4804	0.64	4/6565 (0.1%)
2	J	0.32	0/4294	0.58	8/5903 (0.1%)
All	All	0.63	10/42865 (0.0%)	0.73	52/58448 (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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	517	THR	C-N	-10.63	1.09	1.34
1	G	517	THR	C-N	-10.43	1.10	1.34
1	B	517	THR	C-N	-9.98	1.11	1.34
1	F	517	THR	C-N	-8.53	1.14	1.34
1	A	517	THR	C-N	-7.07	1.17	1.34
1	E	517	THR	C-N	-6.85	1.18	1.34
1	B	219	TYR	CD1-CE1	-5.94	1.30	1.39
1	B	477	TRP	CB-CG	-5.57	1.40	1.50
1	D	517	THR	C-N	-5.46	1.21	1.34
1	C	252	ARG	C-N	-5.35	1.21	1.34

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	582	LEU	CA-CB-CG	10.52	139.48	115.30
2	H	88	ILE	C-N-CA	8.96	144.10	121.70
1	D	297	ARG	NE-CZ-NH1	-8.65	115.98	120.30
1	A	203	LEU	CA-CB-CG	-8.57	95.59	115.30
1	A	450	LEU	CA-CB-CG	-7.98	96.95	115.30
1	D	500	LEU	CB-CG-CD2	7.51	123.77	111.00
1	D	385	LEU	CB-CG-CD2	-7.38	98.45	111.00
1	F	203	LEU	CA-CB-CG	-7.17	98.81	115.30
1	E	527	LEU	CA-CB-CG	-6.85	99.55	115.30
2	J	499	LEU	CB-CG-CD2	-6.70	99.61	111.00
1	C	481	LEU	CA-CB-CG	-6.70	99.90	115.30
2	I	235	LEU	CA-CB-CG	-6.53	100.29	115.30
1	F	255	LEU	CA-CB-CG	-6.49	100.38	115.30
2	H	583	ILE	CG1-CB-CG2	-6.48	97.15	111.40
2	J	127	PRO	N-CD-CG	-6.47	93.50	103.20
2	I	194	LEU	CA-CB-CG	-6.38	100.62	115.30
1	D	187	LEU	CA-CB-CG	-6.34	100.71	115.30
1	C	517	THR	C-N-CA	-6.34	105.85	121.70
1	D	517	THR	C-N-CA	-6.33	105.86	121.70
1	B	628	LEU	CA-CB-CG	6.30	129.79	115.30
1	D	255	LEU	CA-CB-CG	-6.20	101.04	115.30
1	C	203	LEU	CA-CB-CG	-6.12	101.22	115.30
1	E	517	THR	C-N-CA	-6.02	106.65	121.70
2	J	127	PRO	CA-N-CD	-5.95	103.17	111.50
1	B	500	LEU	CA-CB-CG	-5.93	101.66	115.30
1	C	216	LEU	CA-CB-CG	-5.90	101.73	115.30
1	C	587	MET	CG-SD-CE	-5.90	90.77	100.20
2	H	73	MET	CB-CG-SD	-5.87	94.80	112.40
1	E	203	LEU	CA-CB-CG	-5.72	102.14	115.30
1	B	378	LEU	CB-CG-CD2	-5.65	101.39	111.00
1	B	203	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	E	628	LEU	CA-CB-CG	5.59	128.16	115.30
2	I	189	LEU	CA-CB-CG	-5.54	102.56	115.30
1	E	500	LEU	CA-CB-CG	-5.54	102.56	115.30
2	H	189	LEU	CA-CB-CG	-5.53	102.58	115.30
1	C	255	LEU	CA-CB-CG	-5.49	102.68	115.30
1	F	421	LEU	CA-CB-CG	-5.40	102.89	115.30
1	C	500	LEU	CA-CB-CG	-5.39	102.90	115.30
1	E	216	LEU	CA-CB-CG	-5.35	102.99	115.30
1	B	587	MET	CG-SD-CE	-5.23	91.83	100.20
1	D	411	TYR	CA-CB-CG	-5.22	103.48	113.40
1	D	297	ARG	CA-CB-CG	-5.22	101.93	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	172	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	517	THR	C-N-CA	-5.17	108.77	121.70
2	J	235	LEU	CA-CB-CG	-5.14	103.47	115.30
2	J	172	ASP	CB-CG-OD2	5.14	122.93	118.30
1	D	442	LEU	CB-CG-CD2	-5.13	102.28	111.00
2	J	67	PRO	CA-N-CD	-5.12	104.33	111.50
1	C	270	ILE	CG1-CB-CG2	-5.11	100.16	111.40
2	J	544	ARG	CG-CD-NE	5.06	122.43	111.80
2	J	454	LEU	CA-CB-CG	5.06	126.94	115.30
1	D	203	LEU	CA-CB-CG	-5.03	103.74	115.30

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3961	0	3728	237	0
1	B	3977	0	3760	302	0
1	C	3977	0	3760	311	0
1	D	3970	0	3753	283	0
1	E	3977	0	3761	266	0
1	F	3977	0	3760	242	0
1	G	3977	0	3760	239	0
2	H	5378	0	5004	353	0
2	I	4739	0	3782	223	0
2	J	4239	0	3182	123	0
All	All	42172	0	38250	2526	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 31.

All (2526) 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	1.55	1.35
1:C:233:TYR:CD1	1:C:243:ILE:HD11	1.74	1.23
2:H:117:HIS:NE2	2:H:119:VAL:HG23	1.56	1.21
2:I:89:THR:HG21	2:I:115:HIS:CB	1.72	1.19
2:H:578:LYS:HD3	2:H:579:TYR:HE1	1.04	1.16
1:B:233:TYR:HD2	1:B:243:ILE:HD11	1.01	1.14
2:H:578:LYS:CD	2:H:579:TYR:HE1	1.63	1.11
2:I:89:THR:HG22	2:I:115:HIS:HA	1.23	1.10
2:H:117:HIS:NE2	2:H:119:VAL:CG2	2.13	1.10
1:C:233:TYR:HD1	1:C:243:ILE:CD1	1.65	1.09
1:C:232:PRO:HD2	1:C:233:TYR:CD2	1.88	1.09
1:B:233:TYR:CD2	1:B:243:ILE:HD11	1.86	1.08
1:E:721:ILE:HD11	1:E:723:LYS:HD2	1.29	1.07
1:G:643:ILE:HG12	1:G:723:LYS:HE2	1.35	1.05
2:I:89:THR:CG2	2:I:115:HIS:CA	2.34	1.05
1:E:721:ILE:HG13	1:E:723:LYS:HG3	1.38	1.04
1:E:643:ILE:HG21	1:E:723:LYS:NZ	1.71	1.03
2:J:89:THR:CG2	2:J:115:HIS:HA	1.86	1.03
1:E:643:ILE:HG21	1:E:723:LYS:HZ2	1.20	1.02
2:H:578:LYS:HD3	2:H:579:TYR:CE1	1.94	1.02
1:A:210:ILE:O	1:A:214:LYS:NZ	1.95	1.00
1:G:643:ILE:HG12	1:G:723:LYS:CE	1.94	0.98
1:B:428:SER:HB2	1:B:431:PRO:HG3	1.46	0.97
2:H:446:LEU:HD11	2:H:590:ARG:HB2	1.47	0.97
1:E:232:PRO:HD2	1:E:233:TYR:CE1	2.00	0.95
2:H:563:GLN:HE22	2:H:585:PHE:H	1.08	0.95
1:E:428:SER:HB2	1:E:431:PRO:HG3	1.49	0.94
1:E:232:PRO:HD2	1:E:233:TYR:CD1	2.02	0.94
1:C:721:ILE:HB	1:C:723:LYS:HE2	1.50	0.93
1:E:524:LYS:HD2	1:E:579:ASP:HB3	1.48	0.92
1:E:524:LYS:HE3	1:E:578:LEU:HB3	1.51	0.92
2:H:157:ARG:NH2	2:H:211:ASN:OD1	2.02	0.92
1:E:721:ILE:CD1	1:E:723:LYS:HD2	1.98	0.92
1:E:176:PRO:HB2	1:E:178:ARG:HH12	1.33	0.92
1:A:428:SER:HB2	1:A:431:PRO:HG3	1.51	0.92
1:C:233:TYR:CD1	1:C:243:ILE:CD1	2.45	0.91
2:H:578:LYS:CD	2:H:579:TYR:CE1	2.53	0.91
1:G:273:LYS:HA	1:G:358:ALA:HA	1.53	0.91
1:B:238:LYS:HZ3	1:B:254:PRO:HA	1.35	0.91
2:I:81:ILE:HG22	2:I:129:LEU:HB3	1.51	0.90
2:H:639:ILE:HG13	2:H:640:ALA:H	1.35	0.90
1:C:232:PRO:HD2	1:C:233:TYR:CE2	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:TYR:HE1	1:B:378:LEU:CG	1.85	0.89
1:A:265:ASP:OD1	1:A:295:THR:OG1	1.90	0.89
1:B:233:TYR:HD2	1:B:243:ILE:CD1	1.85	0.89
1:G:428:SER:HB2	1:G:431:PRO:HG3	1.53	0.89
2:I:89:THR:HG21	2:I:115:HIS:HB2	1.54	0.89
2:H:117:HIS:CE1	2:H:119:VAL:HG22	2.08	0.89
1:C:233:TYR:CE1	1:C:243:ILE:HD11	2.08	0.88
2:J:502:ARG:HH22	2:J:544:ARG:HB3	1.38	0.88
1:C:232:PRO:HD2	1:C:233:TYR:HD2	1.37	0.88
1:B:394:ILE:HD12	1:B:421:LEU:HD11	1.54	0.87
1:E:291:LYS:HZ1	1:E:335:ASP:H	1.19	0.87
1:B:185:ASP:OD1	1:B:186:SER:N	2.06	0.87
1:E:502:GLU:O	1:E:503:ARG:NH1	2.07	0.87
1:B:291:LYS:HZ1	1:B:335:ASP:H	1.19	0.87
2:I:89:THR:CG2	2:I:115:HIS:CB	2.53	0.87
1:A:365:ARG:HE	1:A:418:PRO:HB3	1.39	0.87
1:B:643:ILE:HB	1:B:699:TYR:HB2	1.55	0.86
1:B:497:ASP:O	1:B:637:LYS:NZ	2.08	0.86
2:I:226:GLU:OE2	2:I:229:HIS:ND1	2.09	0.86
1:F:297:ARG:HH12	1:F:328:ASN:HB3	1.41	0.86
1:C:705:ASN:ND2	1:C:722:LYS:O	2.08	0.86
1:E:234:SER:N	1:E:237:GLU:OE2	2.08	0.85
2:H:117:HIS:CD2	2:H:119:VAL:O	2.30	0.85
1:F:185:ASP:OD1	1:F:186:SER:N	2.09	0.85
1:E:721:ILE:HG13	1:E:723:LYS:CG	2.07	0.85
1:B:365:ARG:HH21	1:B:418:PRO:HD3	1.42	0.85
1:E:189:VAL:O	1:E:220:LYS:NZ	2.10	0.85
2:I:768:ASP:HA	2:I:771:LYS:HD2	1.59	0.85
1:G:541:GLN:OE1	1:G:544:GLY:N	2.09	0.84
1:F:249:PRO:HA	1:F:252:ARG:HH11	1.43	0.84
1:G:523:LEU:HD22	1:G:578:LEU:HD11	1.60	0.84
1:G:198:ASN:HB2	1:G:200:ARG:HH12	1.41	0.84
2:J:89:THR:HG22	2:J:115:HIS:HA	1.56	0.83
1:A:599:ASP:OD1	1:A:600:ARG:N	2.08	0.83
1:D:365:ARG:NH1	1:D:412:PRO:O	2.11	0.83
1:C:234:SER:OG	1:C:237:GLU:OE1	1.96	0.83
1:C:262:VAL:O	1:C:328:ASN:ND2	2.11	0.83
2:I:89:THR:HG22	2:I:115:HIS:CA	2.04	0.83
1:A:497:ASP:O	1:A:637:LYS:NZ	2.11	0.83
1:A:189:VAL:O	1:A:220:LYS:NZ	2.10	0.83
1:D:326:ASN:OD1	1:D:490:ARG:NH2	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:578:LYS:CG	2:H:579:TYR:CE1	2.63	0.82
2:H:707:LEU:HD23	2:H:709:THR:HG22	1.62	0.82
2:I:451:GLY:HA2	2:I:454:LEU:HD23	1.61	0.82
1:D:331:THR:HG23	1:D:447:GLN:HE21	1.45	0.82
1:G:718:THR:CB	1:G:723:LYS:NZ	2.43	0.82
1:B:297:ARG:NH1	1:B:298:THR:O	2.12	0.82
1:G:718:THR:CB	1:G:723:LYS:HZ1	1.92	0.81
2:J:197:HIS:HE2	2:J:199:THR:HG1	1.29	0.81
2:H:117:HIS:CE1	2:H:119:VAL:CG2	2.63	0.81
2:H:578:LYS:HG2	2:H:579:TYR:CE1	2.15	0.81
1:C:447:GLN:HB3	1:C:449:ARG:HH22	1.46	0.81
2:H:424:HIS:O	2:H:510:ARG:NH2	2.13	0.81
2:H:635:THR:OG1	2:H:638:ASN:ND2	2.14	0.80
1:C:259:TYR:HE2	1:C:261:ILE:HD11	1.46	0.80
1:D:202:PHE:HE2	1:D:204:SER:HB2	1.45	0.80
1:A:262:VAL:O	1:A:328:ASN:ND2	2.14	0.80
1:B:366:TYR:HE1	1:B:378:LEU:HD21	1.47	0.80
1:B:522:THR:OG1	1:B:525:GLU:OE1	1.98	0.80
1:C:490:ARG:HH21	1:C:504:ARG:HH22	1.29	0.79
1:D:459:ILE:HG13	1:D:477:TRP:NE1	1.96	0.79
1:B:584:ASN:H	1:B:587:MET:HE3	1.47	0.79
1:B:552:PHE:HD2	1:B:554:PHE:HE2	1.30	0.79
1:G:492:ILE:HB	1:G:590:LEU:HD13	1.64	0.79
1:G:643:ILE:HB	1:G:699:TYR:HB2	1.63	0.79
2:J:81:ILE:HG22	2:J:129:LEU:HB3	1.65	0.79
2:I:570:TRP:CZ3	2:I:607:LYS:HE2	2.18	0.79
1:B:346:TRP:HZ3	1:B:446:LYS:HZ1	1.25	0.79
1:C:584:ASN:H	1:C:587:MET:HE3	1.48	0.79
2:H:446:LEU:HD12	2:H:591:TYR:HB2	1.64	0.79
1:B:210:ILE:O	1:B:214:LYS:NZ	2.14	0.79
1:A:386:GLY:O	1:A:449:ARG:NH2	2.15	0.78
2:H:406:LEU:HG	2:H:410:LYS:HE2	1.64	0.78
2:I:278:TYR:HB2	2:I:513:TYR:CZ	2.19	0.78
1:F:643:ILE:CD1	1:F:723:LYS:HE2	2.13	0.78
2:H:190:PHE:O	2:H:195:LYS:NZ	2.17	0.78
2:I:169:LYS:HZ1	2:I:534:ILE:H	1.29	0.78
1:B:366:TYR:HE1	1:B:378:LEU:CD2	1.96	0.78
1:E:599:ASP:HB3	1:E:605:VAL:HG21	1.65	0.78
1:G:253:HIS:CE1	1:G:255:LEU:HD13	2.18	0.78
1:F:360:LEU:HB3	1:F:432:ILE:HG21	1.66	0.77
1:C:428:SER:HB2	1:C:431:PRO:HG3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:428:SER:HB2	1:F:431:PRO:HG3	1.66	0.77
1:B:391:LEU:HB3	1:B:432:ILE:HD11	1.65	0.77
1:G:212:GLU:OE1	1:G:212:GLU:N	2.17	0.77
2:I:89:THR:HG21	2:I:115:HIS:CA	2.07	0.77
2:H:117:HIS:NE2	2:H:119:VAL:HG22	1.97	0.77
1:C:721:ILE:CG2	1:C:723:LYS:HE2	2.15	0.77
2:I:115:HIS:CE1	2:I:116:GLU:HG3	2.20	0.77
1:C:721:ILE:CB	1:C:723:LYS:HE2	2.15	0.77
2:H:768:ASP:HA	2:H:771:LYS:HD2	1.66	0.77
1:C:267:GLU:N	1:C:267:GLU:OE1	2.17	0.77
1:C:384:VAL:HG12	1:C:390:THR:HA	1.67	0.77
2:I:89:THR:HG21	2:I:115:HIS:HB3	1.61	0.77
1:G:435:ASN:OD1	1:G:437:ASN:ND2	2.18	0.77
1:C:248:SER:OG	1:C:250:GLU:OE1	2.02	0.77
1:D:297:ARG:HH21	1:D:499:ASN:HA	1.49	0.77
1:G:176:PRO:HB3	1:G:178:ARG:HH12	1.50	0.77
2:H:186:GLN:HB2	2:H:190:PHE:CZ	2.20	0.77
2:J:768:ASP:HA	2:J:771:LYS:HD2	1.66	0.77
1:F:291:LYS:HZ1	1:F:335:ASP:H	1.31	0.76
1:G:435:ASN:CG	1:G:438:GLN:HE22	1.87	0.76
1:E:185:ASP:OD1	1:E:186:SER:N	2.17	0.76
1:A:185:ASP:OD1	1:A:186:SER:N	2.18	0.76
1:F:643:ILE:HD12	1:F:723:LYS:HE2	1.65	0.76
1:G:263:HIS:HB3	1:G:328:ASN:HD21	1.51	0.76
1:B:365:ARG:HE	1:B:418:PRO:HB3	1.50	0.76
1:F:225:LYS:HD3	1:F:514:LEU:HD21	1.69	0.75
1:F:470:ARG:NH1	1:F:471:VAL:O	2.19	0.75
1:G:584:ASN:H	1:G:587:MET:CE	1.99	0.75
1:C:387:LYS:HD2	1:C:388:ASN:HB2	1.67	0.75
1:F:233:TYR:CD2	1:F:243:ILE:HD11	2.22	0.75
1:B:366:TYR:CE1	1:B:378:LEU:CG	2.68	0.75
1:A:341:ALA:O	1:A:344:ARG:NH1	2.19	0.75
1:B:238:LYS:NZ	1:B:254:PRO:HA	2.01	0.75
1:A:541:GLN:OE1	1:A:544:GLY:N	2.20	0.75
1:F:198:ASN:HB2	1:F:200:ARG:HH22	1.51	0.75
1:D:297:ARG:NH2	1:D:499:ASN:HA	2.01	0.75
1:D:548:THR:O	1:D:594:LYS:NZ	2.15	0.75
1:B:470:ARG:HA	1:C:479:GLU:OE1	1.87	0.75
1:D:439:PHE:HA	1:D:442:LEU:HD12	1.69	0.75
1:G:506:ALA:HB1	1:G:518:LYS:HZ2	1.51	0.75
2:H:579:TYR:N	2:H:579:TYR:HD1	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:GLU:HB2	1:B:724:ILE:HG21	1.69	0.74
1:C:541:GLN:OE1	1:C:544:GLY:N	2.20	0.74
1:B:568:GLU:HG2	1:B:569:LEU:HD12	1.67	0.74
1:F:592:ARG:HD2	1:F:598:TYR:CE2	2.21	0.74
1:D:633:LYS:O	1:D:637:LYS:NZ	2.17	0.74
1:E:326:ASN:HD22	1:E:485:GLN:HG3	1.52	0.74
1:E:541:GLN:HG2	1:E:546:ASP:HA	1.69	0.74
1:B:225:LYS:HD3	1:B:228:THR:HA	1.68	0.74
1:F:374:ILE:HD11	1:F:405:LEU:HD22	1.69	0.74
1:B:236:PHE:HE2	1:B:242:ARG:HH21	1.33	0.74
1:F:443:GLU:HA	1:F:446:LYS:NZ	2.02	0.74
1:B:198:ASN:HD21	1:B:200:ARG:HH22	1.35	0.74
2:H:483:TYR:HB3	2:H:520:ILE:HD11	1.69	0.74
1:A:270:ILE:HD13	1:A:290:SER:HB3	1.69	0.74
1:B:229:ALA:O	1:B:230:SER:OG	2.05	0.74
2:H:427:ILE:O	2:H:432:TYR:OH	2.06	0.74
1:G:443:GLU:HA	1:G:446:LYS:HE2	1.69	0.74
1:F:445:THR:O	1:F:447:GLN:NE2	2.20	0.73
2:H:578:LYS:CG	2:H:579:TYR:HE1	2.01	0.73
1:C:698:VAL:HB	1:C:727:PHE:HB3	1.70	0.73
1:A:525:GLU:OE1	1:A:525:GLU:N	2.17	0.73
1:D:363:ASN:ND2	1:D:418:PRO:HG2	2.03	0.73
1:E:362:ALA:HB3	1:E:421:LEU:HD12	1.71	0.73
2:I:271:TRP:HE1	2:I:275:LYS:HE2	1.53	0.73
1:G:584:ASN:OD1	1:G:585:ALA:N	2.20	0.73
2:J:441:MET:HB3	2:J:499:LEU:HD22	1.70	0.73
1:A:374:ILE:HD11	1:A:405:LEU:HD22	1.68	0.73
1:C:326:ASN:HB3	1:C:490:ARG:HH22	1.54	0.73
1:C:490:ARG:HH21	1:C:504:ARG:NH2	1.86	0.73
2:H:253:ASN:O	2:H:256:LEU:HG	1.89	0.73
2:J:153:LYS:O	2:J:157:ARG:HG2	1.89	0.73
1:B:226:TRP:CZ2	1:B:234:SER:HB2	2.24	0.73
2:H:563:GLN:HE22	2:H:585:PHE:N	1.85	0.73
2:H:264:MET:HA	2:H:267:ARG:HD3	1.71	0.73
1:D:296:SER:O	1:D:331:THR:N	2.22	0.72
1:E:233:TYR:CD2	1:E:243:ILE:HD11	2.25	0.72
2:H:579:TYR:N	2:H:579:TYR:CD1	2.57	0.72
1:G:478:SER:OG	1:G:479:GLU:OE1	2.07	0.72
1:C:197:LYS:HB2	1:C:202:PHE:HE1	1.53	0.72
1:C:226:TRP:CZ2	1:C:234:SER:HB3	2.25	0.72
1:A:223:PRO:HG2	1:A:224:GLU:OE1	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:226:GLU:OE1	2:J:229:HIS:N	2.22	0.72
1:C:533:PHE:CE2	1:C:542:TYR:HB2	2.24	0.72
1:D:643:ILE:HB	1:D:699:TYR:HB2	1.71	0.72
1:B:548:THR:HA	1:B:575:TYR:CE1	2.25	0.72
1:B:498:LEU:HB2	1:B:637:LYS:HZ1	1.53	0.72
1:C:555:ASP:OD1	1:C:556:GLN:N	2.22	0.72
2:H:563:GLN:NE2	2:H:585:PHE:H	1.87	0.72
1:E:721:ILE:HD11	1:E:723:LYS:CD	2.16	0.71
1:F:240:THR:HG21	1:F:242:ARG:HH22	1.55	0.71
1:A:522:THR:OG1	1:A:525:GLU:OE1	2.08	0.71
1:A:695:LYS:HA	1:A:730:LYS:HA	1.72	0.71
1:B:366:TYR:CE1	1:B:378:LEU:HD11	2.25	0.71
1:E:592:ARG:HD3	1:E:598:TYR:CE2	2.25	0.71
2:J:226:GLU:OE1	2:J:229:HIS:ND1	2.20	0.71
1:G:209:ASN:O	1:G:213:LYS:NZ	2.23	0.71
1:G:185:ASP:OD1	1:G:186:SER:N	2.24	0.71
2:I:142:GLU:N	2:I:142:GLU:OE2	2.23	0.71
1:B:298:THR:HB	1:B:331:THR:HG22	1.73	0.71
2:H:160:LEU:HB3	2:H:165:GLN:O	1.91	0.71
2:J:500:LYS:O	2:J:502:ARG:NH1	2.22	0.71
1:C:200:ARG:HH22	1:D:189:VAL:HG11	1.56	0.71
2:H:73:MET:SD	2:H:73:MET:N	2.58	0.71
1:B:366:TYR:CE1	1:B:378:LEU:HG	2.26	0.71
1:C:189:VAL:HG13	1:C:190:GLU:HG3	1.71	0.71
1:E:466:ASN:HB2	1:F:226:TRP:CE3	2.26	0.71
1:B:232:PRO:C	1:B:233:TYR:HD1	1.94	0.70
1:D:568:GLU:HG2	1:D:569:LEU:HD22	1.73	0.70
1:C:272:SER:O	1:C:359:ARG:N	2.18	0.70
1:E:297:ARG:NH1	1:E:298:THR:O	2.23	0.70
1:F:341:ALA:O	1:F:344:ARG:NH1	2.23	0.70
1:F:560:GLN:O	1:F:563:LYS:HG3	1.92	0.70
2:I:281:TRP:HH2	2:I:423:LEU:HA	1.56	0.70
1:A:552:PHE:HB3	1:A:554:PHE:CZ	2.25	0.70
1:D:643:ILE:HG13	1:D:723:LYS:HE2	1.72	0.70
1:F:291:LYS:NZ	1:F:335:ASP:H	1.87	0.70
2:H:183:SER:HB2	2:H:186:GLN:HE22	1.56	0.70
1:G:234:SER:N	1:G:237:GLU:OE2	2.22	0.70
1:D:265:ASP:OD1	1:D:295:THR:OG1	2.08	0.70
1:D:490:ARG:NH2	1:D:504:ARG:HH22	1.90	0.70
1:C:631:ILE:O	1:C:636:ARG:NH2	2.23	0.70
1:F:200:ARG:HH11	1:F:200:ARG:HG3	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:530:LYS:HE3	2:I:548:LYS:HE3	1.73	0.70
1:B:366:TYR:CE1	1:B:378:LEU:HD21	2.25	0.70
1:D:297:ARG:HD2	1:D:297:ARG:O	1.91	0.70
1:G:365:ARG:NH2	1:G:418:PRO:HD3	2.07	0.70
1:D:610:SER:HA	1:D:613:LYS:NZ	2.06	0.69
2:H:514:LEU:HD23	2:H:518:LYS:HB2	1.75	0.69
2:I:278:TYR:HB2	2:I:513:TYR:CE2	2.27	0.69
1:C:584:ASN:H	1:C:587:MET:CE	2.05	0.69
1:C:185:ASP:OD1	1:C:186:SER:N	2.24	0.69
1:B:234:SER:N	1:B:237:GLU:OE2	2.21	0.69
1:B:340:LEU:O	1:B:343:GLU:HG2	1.92	0.69
1:C:705:ASN:HD21	1:C:722:LYS:HB3	1.56	0.69
1:D:534:ASN:OD1	1:D:541:GLN:NE2	2.26	0.69
1:E:225:LYS:HD3	1:E:514:LEU:HD21	1.75	0.69
1:E:377:VAL:O	1:E:378:LEU:HD12	1.93	0.69
2:H:578:LYS:HG2	2:H:579:TYR:CD1	2.27	0.69
1:B:238:LYS:HE2	1:B:252:ARG:O	1.91	0.69
1:E:291:LYS:HZ1	1:E:335:ASP:N	1.89	0.69
1:D:174:THR:O	1:D:175:VAL:HG22	1.93	0.69
1:E:360:LEU:HB3	1:E:432:ILE:HG21	1.75	0.69
1:G:198:ASN:HB2	1:G:200:ARG:NH1	2.07	0.69
1:B:552:PHE:HD2	1:B:554:PHE:CE2	2.10	0.68
1:E:490:ARG:HD3	1:E:504:ARG:NH2	2.08	0.68
1:C:527:LEU:HB3	1:C:533:PHE:HD1	1.58	0.68
1:F:562:ILE:HA	1:F:565:GLN:OE1	1.93	0.68
1:D:458:ASN:OD1	1:D:476:ASN:ND2	2.27	0.68
2:H:117:HIS:HD2	2:H:119:VAL:O	1.75	0.68
2:I:192:ASN:OD1	2:I:193:GLN:N	2.26	0.68
2:J:118:TYR:OH	2:J:146:ASN:HB2	1.93	0.68
1:A:583:LEU:HB3	1:A:587:MET:HE1	1.75	0.68
1:B:232:PRO:C	1:B:233:TYR:CD1	2.67	0.68
1:E:198:ASN:HD21	1:E:200:ARG:HH22	1.40	0.68
1:G:524:LYS:HB2	1:G:578:LEU:HG	1.75	0.68
1:D:428:SER:HB2	1:D:431:PRO:HG3	1.75	0.68
1:A:528:LYS:NZ	1:A:535:GLU:HG2	2.08	0.68
1:C:198:ASN:ND2	2:I:139:GLU:OE2	2.24	0.68
1:F:273:LYS:HA	1:F:358:ALA:HA	1.75	0.68
2:H:600:TYR:O	2:H:604:ASN:ND2	2.27	0.68
1:B:273:LYS:HA	1:B:358:ALA:HA	1.76	0.68
1:C:233:TYR:HD1	1:C:243:ILE:HD12	1.57	0.68
1:A:551:ASP:OD1	1:A:552:PHE:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:556:ASP:O	2:H:559:ILE:HG12	1.94	0.68
1:C:187:LEU:HD11	1:C:205:PRO:HG3	1.76	0.68
1:D:612:VAL:O	1:D:616:HIS:ND1	2.24	0.67
1:A:527:LEU:HB3	1:A:533:PHE:HD2	1.60	0.67
1:C:197:LYS:O	1:C:200:ARG:N	2.26	0.67
1:C:415:ASN:ND2	1:D:325:SER:OG	2.27	0.67
1:F:533:PHE:CE2	1:F:542:TYR:HB2	2.28	0.67
1:G:262:VAL:O	1:G:328:ASN:ND2	2.28	0.67
2:I:468:PHE:HA	2:I:471:PHE:HD1	1.59	0.67
1:G:226:TRP:CZ2	1:G:234:SER:HB3	2.30	0.67
1:A:527:LEU:HB3	1:A:533:PHE:CD2	2.30	0.67
1:A:718:THR:O	1:A:723:LYS:HE3	1.94	0.67
1:D:200:ARG:HG3	1:D:200:ARG:HH11	1.60	0.67
1:F:183:ILE:HD11	1:F:236:PHE:HD1	1.59	0.67
2:H:437:LEU:HD22	2:H:488:ILE:HA	1.76	0.67
2:H:514:LEU:HG	2:H:516:ASN:H	1.59	0.67
2:I:252:ILE:O	2:I:255:SER:OG	2.13	0.67
1:G:382:SER:HA	1:G:393:THR:HA	1.76	0.67
1:A:267:GLU:N	1:A:267:GLU:OE2	2.26	0.67
1:E:490:ARG:HH21	1:E:588:ASN:CG	1.98	0.67
2:H:427:ILE:HD11	2:H:506:SER:O	1.95	0.67
1:A:524:LYS:HG3	1:A:540:LEU:HD21	1.77	0.67
1:E:552:PHE:HB3	1:E:554:PHE:CZ	2.30	0.67
1:F:202:PHE:HE2	1:F:204:SER:HB2	1.60	0.67
1:G:374:ILE:HD11	1:G:405:LEU:HD22	1.77	0.67
2:J:451:GLY:HA2	2:J:454:LEU:HD23	1.77	0.67
1:A:502:GLU:O	1:A:503:ARG:NH1	2.24	0.67
1:C:493:PHE:CE2	1:C:495:GLY:HA3	2.30	0.67
1:E:365:ARG:NH1	1:E:414:LYS:HA	2.10	0.67
1:A:555:ASP:OD1	1:A:556:GLN:N	2.27	0.66
1:G:577:VAL:HG12	1:G:580:LYS:HB2	1.77	0.66
1:C:565:GLN:HE22	1:C:582:LYS:HB2	1.60	0.66
2:I:168:GLN:O	2:I:172:ASP:N	2.28	0.66
1:C:546:ASP:OD1	1:C:547:ILE:N	2.29	0.66
1:G:584:ASN:H	1:G:587:MET:HE3	1.60	0.66
2:H:420:ASP:OD1	2:H:483:TYR:OH	2.13	0.66
1:C:270:ILE:HG12	1:C:361:ASN:O	1.95	0.66
2:J:762:THR:HA	2:J:765:PHE:CE1	2.29	0.66
1:D:262:VAL:HG21	1:D:379:PRO:HG2	1.78	0.66
1:D:297:ARG:HH22	1:D:500:LEU:HD23	1.60	0.66
1:G:552:PHE:HB3	1:G:554:PHE:CZ	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:111:ASP:OD1	2:H:112:ALA:N	2.25	0.66
2:I:583:ILE:HD13	2:I:629:PHE:HB2	1.78	0.66
1:B:485:GLN:HA	1:B:504:ARG:HH12	1.59	0.66
1:C:231:ASP:HB2	1:C:232:PRO:HD3	1.75	0.66
1:C:244:ASP:OD1	1:C:246:ASN:ND2	2.28	0.66
2:H:106:ASP:OD1	2:H:108:TYR:N	2.27	0.66
2:H:226:GLU:OE1	2:H:229:HIS:N	2.29	0.66
1:F:561:ASN:OD1	1:F:565:GLN:NE2	2.29	0.66
1:C:273:LYS:HA	1:C:358:ALA:HA	1.78	0.66
1:D:226:TRP:CH2	1:D:234:SER:HB3	2.31	0.66
2:I:619:THR:HA	2:I:622:LEU:HG	1.76	0.66
1:D:293:THR:HG22	1:D:334:ILE:HD12	1.78	0.66
1:E:176:PRO:HB2	1:E:178:ARG:NH1	2.08	0.66
1:E:546:ASP:OD1	1:E:547:ILE:N	2.29	0.66
1:G:345:THR:O	1:G:348:GLU:HG3	1.95	0.66
2:I:42:HIS:O	2:I:45:LYS:NZ	2.25	0.66
1:E:295:THR:HA	1:E:332:VAL:HA	1.78	0.66
1:E:721:ILE:CG1	1:E:723:LYS:HD2	2.24	0.66
2:H:535:ILE:HD13	2:H:544:ARG:HD3	1.77	0.66
2:I:122:LYS:HE3	2:I:128:VAL:HB	1.77	0.66
1:A:614:GLU:OE2	1:A:617:ARG:HD3	1.96	0.65
1:E:540:LEU:HB3	1:E:547:ILE:HG21	1.76	0.65
1:F:636:ARG:HG3	1:F:637:LYS:NZ	2.11	0.65
2:I:274:ILE:O	2:I:513:TYR:OH	2.05	0.65
1:F:249:PRO:HA	1:F:252:ARG:NH1	2.11	0.65
1:G:226:TRP:CH2	1:G:234:SER:HB3	2.31	0.65
2:H:190:PHE:HB2	2:H:194:LEU:HD12	1.77	0.65
2:H:574:LEU:HD11	2:H:615:ILE:HG22	1.79	0.65
1:C:553:ASN:OD1	1:C:554:PHE:N	2.29	0.65
1:F:490:ARG:HB2	1:F:504:ARG:NH1	2.12	0.65
1:G:627:LEU:HB2	1:G:676:ILE:HD13	1.77	0.65
1:B:187:LEU:HD11	1:B:205:PRO:HG3	1.79	0.65
1:C:718:THR:HA	1:C:721:ILE:HD13	1.77	0.65
1:G:383:LEU:N	1:G:392:ALA:O	2.30	0.65
2:H:226:GLU:OE1	2:H:229:HIS:ND1	2.26	0.65
1:C:297:ARG:NH1	1:C:329:SER:H	1.95	0.65
1:F:373:PRO:HB2	1:F:375:TYR:HE1	1.62	0.65
2:J:478:SER:OG	2:J:590:ARG:NE	2.26	0.65
1:F:568:GLU:HG2	1:F:569:LEU:HD22	1.79	0.65
1:B:471:VAL:HG12	1:C:479:GLU:OE2	1.96	0.65
1:C:558:THR:HG21	1:C:588:ASN:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:568:GLU:HG2	1:E:569:LEU:HD22	1.79	0.65
1:F:244:ASP:OD1	1:G:483:GLN:NE2	2.30	0.65
1:D:273:LYS:HA	1:D:358:ALA:HA	1.79	0.65
1:D:512:ASP:HB3	1:D:515:GLU:HB3	1.79	0.65
1:D:585:ALA:O	1:D:586:LYS:HG2	1.96	0.65
2:H:639:ILE:HG13	2:H:640:ALA:N	2.11	0.65
1:D:249:PRO:HA	1:D:252:ARG:NH1	2.12	0.65
1:G:253:HIS:HE1	1:G:255:LEU:HD13	1.59	0.65
2:H:528:GLU:OE2	2:H:548:LYS:HB3	1.97	0.65
2:J:89:THR:CG2	2:J:115:HIS:CA	2.72	0.65
1:A:340:LEU:O	1:A:343:GLU:HG2	1.96	0.64
1:A:692:PRO:O	1:A:732:TYR:N	2.30	0.64
1:C:260:PRO:HD3	1:C:477:TRP:CH2	2.32	0.64
1:D:383:LEU:HD21	1:D:448:LEU:HD23	1.79	0.64
2:H:635:THR:HG1	2:H:638:ASN:ND2	1.95	0.64
1:B:266:MET:SD	1:B:269:ILE:HD11	2.37	0.64
1:B:269:ILE:HG22	1:B:270:ILE:N	2.12	0.64
2:J:89:THR:HG21	2:J:115:HIS:CB	2.27	0.64
1:B:485:GLN:HA	1:B:504:ARG:HH22	1.61	0.64
1:D:438:GLN:O	1:D:441:GLU:HG3	1.98	0.64
1:E:643:ILE:HG21	1:E:723:LYS:HZ1	1.61	0.64
2:I:441:MET:SD	2:I:445:ASN:HB3	2.37	0.64
2:H:505:LEU:H	2:H:505:LEU:HD23	1.62	0.64
2:J:118:TYR:OH	2:J:143:LYS:O	2.15	0.64
1:A:248:SER:OG	1:A:250:GLU:OE1	2.14	0.64
1:F:240:THR:HG21	1:F:242:ARG:NH2	2.12	0.64
1:F:722:LYS:NZ	1:F:723:LYS:O	2.31	0.64
2:H:727:SER:HA	2:H:730:ARG:HD3	1.80	0.64
1:B:366:TYR:CD1	1:B:378:LEU:HD11	2.32	0.64
1:C:226:TRP:CE2	1:C:234:SER:HB3	2.32	0.64
1:E:405:LEU:HD11	1:E:411:TYR:HB2	1.78	0.64
2:J:137:TYR:HE1	2:J:143:LYS:HE3	1.62	0.64
2:H:121:ALA:HA	2:H:129:LEU:HA	1.79	0.64
1:A:270:ILE:HD11	1:A:288:THR:HB	1.79	0.64
1:C:270:ILE:HA	1:C:290:SER:HA	1.80	0.64
1:E:345:THR:O	1:E:348:GLU:HG3	1.97	0.64
1:F:612:VAL:O	1:F:616:HIS:ND1	2.30	0.64
1:G:643:ILE:HG21	1:G:723:LYS:HZ2	1.62	0.64
2:I:89:THR:HG23	2:I:115:HIS:HA	1.71	0.64
2:I:535:ILE:HD13	2:I:544:ARG:HB2	1.78	0.64
1:C:552:PHE:HB3	1:C:554:PHE:CZ	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:547:ILE:HD12	1:G:550:PHE:HD2	1.62	0.64
1:A:234:SER:N	1:A:237:GLU:OE2	2.26	0.64
1:D:297:ARG:HH12	1:D:500:LEU:HD23	1.63	0.64
1:E:643:ILE:CG2	1:E:723:LYS:NZ	2.54	0.64
1:B:225:LYS:NZ	1:B:228:THR:O	2.26	0.63
1:C:345:THR:O	1:C:348:GLU:HG3	1.97	0.63
1:G:381:THR:HG23	1:G:394:ILE:HD13	1.79	0.63
2:I:226:GLU:OE1	2:I:228:GLN:N	2.30	0.63
1:D:491:ILE:HD13	1:D:589:ILE:HB	1.79	0.63
1:D:633:LYS:HA	1:D:636:ARG:NH2	2.13	0.63
1:G:551:ASP:OD1	1:G:552:PHE:N	2.31	0.63
2:I:501:TRP:HD1	2:I:545:ILE:HB	1.63	0.63
1:C:639:LEU:N	1:C:703:LYS:HZ3	1.96	0.63
1:G:340:LEU:O	1:G:343:GLU:HG2	1.98	0.63
1:G:403:GLN:OE1	1:G:403:GLN:N	2.32	0.63
2:H:710:ASN:HA	2:H:715:ILE:HD11	1.81	0.63
1:D:490:ARG:HH21	1:D:504:ARG:HH22	1.46	0.63
2:H:463:ILE:N	2:H:541:GLU:OE2	2.31	0.63
2:H:739:GLU:HA	2:H:742:ARG:NH1	2.14	0.63
2:I:107:ILE:HA	2:I:219:LYS:HZ2	1.62	0.63
1:A:197:LYS:O	1:A:200:ARG:N	2.32	0.63
2:I:167:TYR:HE2	2:I:534:ILE:HG12	1.62	0.63
1:E:583:LEU:HA	1:E:587:MET:HE1	1.81	0.63
1:E:695:LYS:HA	1:E:730:LYS:HA	1.79	0.63
1:G:523:LEU:HA	1:G:583:LEU:HD11	1.81	0.63
1:B:365:ARG:NH2	1:B:416:LEU:O	2.31	0.63
1:B:410:TYR:CE2	1:B:414:LYS:HE3	2.34	0.63
1:C:197:LYS:HB2	1:C:202:PHE:CE1	2.34	0.63
1:E:232:PRO:HD2	1:E:233:TYR:HE1	1.60	0.63
1:C:226:TRP:CH2	1:C:234:SER:HB3	2.33	0.63
1:C:508:VAL:HA	1:C:518:LYS:HD3	1.81	0.63
1:E:541:GLN:NE2	1:E:544:GLY:O	2.32	0.63
1:F:480:VAL:HG12	1:F:484:ILE:HD11	1.80	0.63
1:A:183:ILE:HD12	1:A:183:ILE:H	1.64	0.63
1:A:187:LEU:HD11	1:A:205:PRO:HG3	1.79	0.63
1:F:626:GLY:HA2	1:F:678:PHE:CZ	2.34	0.62
1:C:459:ILE:HG12	1:C:477:TRP:NE1	2.14	0.62
1:E:273:LYS:O	1:E:359:ARG:NH1	2.32	0.62
2:J:104:ILE:O	2:J:112:ALA:N	2.32	0.62
1:C:527:LEU:HD12	1:C:533:PHE:CE1	2.34	0.62
1:F:240:THR:O	1:G:514:LEU:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:366:TYR:HD2	1:F:378:LEU:HD11	1.64	0.62
1:F:631:ILE:O	1:F:636:ARG:NH1	2.22	0.62
2:J:170:PHE:CE1	2:J:217:PHE:HD1	2.16	0.62
2:J:689:GLY:HA3	2:J:738:ALA:HA	1.81	0.62
1:A:373:PRO:HB2	1:A:375:TYR:HE1	1.62	0.62
1:C:260:PRO:HB2	1:C:456:TYR:CE2	2.34	0.62
1:E:523:LEU:HD22	1:E:578:LEU:HD11	1.82	0.62
1:D:326:ASN:HD22	1:D:485:GLN:HE21	1.47	0.62
2:H:407:ASP:HA	2:H:410:LYS:HE3	1.82	0.62
2:H:504:GLN:NE2	2:H:505:LEU:O	2.32	0.62
1:B:250:GLU:OE1	1:B:250:GLU:N	2.27	0.62
2:H:578:LYS:NZ	2:H:579:TYR:CE1	2.67	0.62
2:I:226:GLU:OE2	2:I:229:HIS:N	2.33	0.62
1:C:721:ILE:HG21	1:C:723:LYS:NZ	2.14	0.62
1:D:345:THR:O	1:D:348:GLU:HG3	1.99	0.62
1:G:345:THR:O	1:G:349:THR:HG23	1.99	0.62
1:G:522:THR:O	1:G:525:GLU:HG3	1.98	0.62
1:B:627:LEU:H	1:B:676:ILE:HG22	1.64	0.62
1:D:178:ARG:NE	1:D:224:GLU:OE1	2.33	0.62
1:D:552:PHE:HB3	1:D:554:PHE:CZ	2.34	0.62
1:D:705:ASN:HD21	1:D:722:LYS:HB3	1.65	0.62
1:E:231:ASP:HA	1:E:484:ILE:HD11	1.81	0.62
1:F:345:THR:O	1:F:348:GLU:HG3	2.00	0.62
1:A:496:LYS:HE2	1:A:542:TYR:OH	2.00	0.62
1:D:295:THR:HG22	1:D:332:VAL:HG23	1.80	0.62
1:E:232:PRO:HD2	1:E:233:TYR:HD1	1.64	0.62
1:F:298:THR:HG21	1:F:331:THR:HB	1.79	0.62
1:F:524:LYS:NZ	1:F:525:GLU:OE2	2.21	0.62
2:J:231:ASP:O	2:J:234:GLN:HG3	1.99	0.62
1:B:226:TRP:CH2	1:B:234:SER:HB2	2.35	0.62
1:D:478:SER:OG	1:D:479:GLU:OE1	2.16	0.62
1:E:525:GLU:HA	1:E:528:LYS:HD2	1.81	0.62
2:H:255:SER:O	2:H:258:GLU:HG3	1.99	0.62
1:G:207:ILE:HB	1:G:210:ILE:HG12	1.82	0.61
2:J:542:TYR:CB	2:J:544:ARG:HH12	2.13	0.61
1:C:493:PHE:CZ	1:C:495:GLY:HA3	2.35	0.61
1:E:560:GLN:O	1:E:563:LYS:HG3	1.99	0.61
1:G:403:GLN:H	1:G:403:GLN:CD	2.03	0.61
1:G:468:ARG:CZ	1:G:470:ARG:HE	2.13	0.61
1:G:254:PRO:HB2	1:G:255:LEU:HD12	1.82	0.61
1:G:638:ILE:HG13	1:G:639:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:157:ARG:NH1	2:H:214:GLN:HG3	2.15	0.61
2:H:617:LYS:NZ	2:H:772:PHE:O	2.32	0.61
2:I:58:ALA:O	2:I:61:LYS:HG2	2.01	0.61
2:I:576:LEU:HD21	2:I:619:THR:HB	1.83	0.61
2:J:57:GLU:O	2:J:61:LYS:HG2	2.00	0.61
1:A:507:ALA:O	1:A:518:LYS:NZ	2.31	0.61
1:C:466:ASN:ND2	1:C:468:ARG:HE	1.97	0.61
1:D:490:ARG:HG3	1:D:502:GLU:OE1	2.01	0.61
1:A:698:VAL:HB	1:A:727:PHE:HB3	1.82	0.61
1:B:612:VAL:O	1:B:616:HIS:ND1	2.34	0.61
1:E:459:ILE:HG12	1:E:477:TRP:NE1	2.15	0.61
1:E:476:ASN:N	1:E:476:ASN:OD1	2.30	0.61
1:G:643:ILE:CG1	1:G:723:LYS:HE2	2.23	0.61
2:H:491:ARG:HG2	2:H:492:PRO:HD2	1.83	0.61
1:A:250:GLU:H	1:A:250:GLU:CD	2.04	0.61
2:H:479:ILE:O	2:H:590:ARG:NH1	2.34	0.61
1:D:634:ASP:OD1	1:D:635:ILE:N	2.34	0.61
1:F:698:VAL:HB	1:F:727:PHE:HB3	1.83	0.61
1:B:449:ARG:HB3	1:B:449:ARG:HH11	1.66	0.61
1:C:368:ASN:ND2	1:C:405:LEU:O	2.34	0.61
1:D:471:VAL:HG12	1:E:479:GLU:OE2	2.00	0.61
2:H:285:LEU:O	2:H:290:ARG:NH2	2.34	0.61
1:A:493:PHE:CE2	1:A:495:GLY:HA3	2.36	0.61
1:F:265:ASP:OD2	1:F:295:THR:OG1	2.15	0.61
1:B:298:THR:HG22	1:B:330:SER:HA	1.83	0.60
1:D:436:TYR:CE2	1:D:440:LEU:HD11	2.35	0.60
2:H:427:ILE:CD1	2:H:505:LEU:HD12	2.29	0.60
1:C:627:LEU:H	1:C:676:ILE:HG22	1.66	0.60
1:E:233:TYR:HB2	1:E:238:LYS:HZ2	1.66	0.60
1:E:491:ILE:HD12	1:E:589:ILE:HB	1.82	0.60
2:H:173:VAL:O	2:H:176:THR:OG1	2.17	0.60
2:H:388:ILE:HD11	2:H:416:ILE:HG13	1.82	0.60
2:I:63:LEU:O	2:I:66:VAL:HG12	2.02	0.60
1:C:233:TYR:CD2	1:C:233:TYR:N	2.69	0.60
1:C:295:THR:HG22	1:C:332:VAL:HG23	1.83	0.60
1:E:387:LYS:HG2	1:E:388:ASN:OD1	2.02	0.60
1:E:445:THR:HG22	1:E:447:GLN:OE1	2.01	0.60
1:F:209:ASN:O	1:F:213:LYS:NZ	2.25	0.60
1:F:297:ARG:NH2	1:F:328:ASN:OD1	2.34	0.60
1:F:551:ASP:OD1	1:F:552:PHE:N	2.34	0.60
2:I:188:LEU:HD11	2:I:223:TYR:HE2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:60:GLU:O	2:J:64:GLU:HG3	2.01	0.60
2:J:252:ILE:O	2:J:255:SER:OG	2.17	0.60
1:A:270:ILE:HG22	1:A:361:ASN:O	2.01	0.60
1:A:353:ASN:OD1	1:A:354:THR:N	2.33	0.60
1:B:253:HIS:CE1	1:B:254:PRO:HD2	2.37	0.60
1:G:449:ARG:O	1:G:450:LEU:HD23	2.01	0.60
2:H:183:SER:CB	2:H:186:GLN:HE22	2.15	0.60
1:C:535:GLU:OE1	1:C:540:LEU:HD13	2.00	0.60
1:F:617:ARG:NH1	1:F:617:ARG:HB2	2.16	0.60
1:G:233:TYR:HB2	1:G:238:LYS:HE2	1.82	0.60
2:H:514:LEU:HB3	2:H:518:LYS:O	2.01	0.60
1:A:524:LYS:O	1:A:528:LYS:HG2	2.02	0.60
1:D:584:ASN:OD1	1:D:585:ALA:N	2.33	0.60
2:H:578:LYS:C	2:H:579:TYR:HD1	2.04	0.60
2:J:571:ASN:HA	2:J:576:LEU:HB2	1.84	0.60
1:A:365:ARG:HH21	1:A:418:PRO:HD3	1.66	0.60
1:B:625:GLU:HA	1:B:678:PHE:CE1	2.37	0.60
1:C:200:ARG:NH1	2:I:139:GLU:OE1	2.35	0.60
1:B:269:ILE:HG22	1:B:270:ILE:H	1.67	0.60
1:D:266:MET:CE	1:D:364:ILE:HG22	2.31	0.60
1:F:353:ASN:OD1	1:F:354:THR:N	2.33	0.60
1:F:552:PHE:HB3	1:F:554:PHE:CZ	2.36	0.60
1:C:521:MET:HG2	1:C:525:GLU:OE2	2.02	0.60
1:E:233:TYR:HB2	1:E:238:LYS:NZ	2.17	0.60
1:G:295:THR:HG22	1:G:332:VAL:HG23	1.83	0.60
2:H:286:SER:O	2:H:290:ARG:HG3	2.01	0.60
1:A:558:THR:HG21	1:A:588:ASN:H	1.67	0.59
1:B:266:MET:HE1	1:B:332:VAL:HG21	1.84	0.59
2:H:427:ILE:HD12	2:H:505:LEU:HD12	1.83	0.59
1:B:271:LEU:HB2	1:B:289:ILE:HB	1.84	0.59
1:E:634:ASP:OD1	1:E:635:ILE:N	2.34	0.59
1:E:639:LEU:N	1:E:703:LYS:HZ3	2.00	0.59
1:F:633:LYS:HA	1:F:636:ARG:HH11	1.66	0.59
2:J:170:PHE:O	2:J:174:LEU:HD23	2.02	0.59
1:A:533:PHE:CE1	1:A:542:TYR:HB2	2.38	0.59
1:B:233:TYR:CD1	1:B:233:TYR:N	2.69	0.59
1:B:333:ALA:HB2	1:B:447:GLN:HE22	1.67	0.59
1:D:493:PHE:CZ	1:D:495:GLY:HA3	2.37	0.59
1:F:444:LYS:HG3	1:F:445:THR:HG23	1.83	0.59
1:F:599:ASP:OD1	1:F:600:ARG:N	2.32	0.59
1:G:411:TYR:C	1:G:411:TYR:CD2	2.76	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:577:PRO:HA	2:I:82:TYR:HB3	1.84	0.59
1:B:225:LYS:HZ1	1:B:230:SER:HB3	1.67	0.59
1:C:242:ARG:HG3	1:C:242:ARG:HH11	1.68	0.59
1:D:242:ARG:HB3	1:D:462:TYR:CZ	2.38	0.59
1:E:678:PHE:HB3	1:E:687:LEU:HD11	1.83	0.59
1:F:193:THR:HG21	1:F:216:LEU:HB3	1.84	0.59
1:A:221:SER:OG	1:A:222:SER:N	2.34	0.59
1:F:366:TYR:CD2	1:F:378:LEU:HD11	2.37	0.59
1:F:443:GLU:HA	1:F:446:LYS:HZ1	1.68	0.59
1:G:225:LYS:HD3	1:G:514:LEU:HD21	1.85	0.59
2:H:465:ARG:HH11	2:H:465:ARG:HG2	1.67	0.59
1:A:289:ILE:HG21	1:A:346:TRP:CH2	2.37	0.59
1:A:718:THR:HA	1:A:721:ILE:HD13	1.83	0.59
1:B:266:MET:HB2	1:B:364:ILE:HG22	1.85	0.59
1:D:250:GLU:OE1	1:D:250:GLU:N	2.31	0.59
1:F:189:VAL:O	1:F:220:LYS:NZ	2.24	0.59
1:G:190:GLU:O	1:G:220:LYS:NZ	2.29	0.59
1:D:226:TRP:CZ2	1:D:234:SER:HB3	2.38	0.59
1:E:233:TYR:CD1	1:E:233:TYR:N	2.70	0.59
1:E:605:VAL:HG12	1:E:704:GLU:HB3	1.84	0.59
1:F:373:PRO:HB2	1:F:375:TYR:CE1	2.37	0.59
2:H:167:TYR:CZ	2:H:536:LYS:HE2	2.38	0.59
2:H:419:ILE:HD13	2:H:422:LEU:HD12	1.84	0.59
2:H:469:ASN:HA	2:H:472:LYS:NZ	2.18	0.59
1:C:466:ASN:HD21	1:C:468:ARG:HE	1.49	0.59
1:C:642:TYR:HD1	1:C:700:ALA:HA	1.66	0.59
1:G:403:GLN:HG3	1:G:411:TYR:HE1	1.68	0.59
1:B:695:LYS:HA	1:B:730:LYS:HA	1.83	0.59
1:E:580:LYS:HA	1:E:580:LYS:HE3	1.84	0.59
2:I:203:VAL:O	2:I:206:LEU:HG	2.02	0.59
2:I:467:ILE:HG22	2:I:471:PHE:CE1	2.37	0.59
1:A:238:LYS:NZ	1:A:254:PRO:HA	2.18	0.59
1:B:536:PRO:HG2	1:B:541:GLN:HE21	1.67	0.59
1:D:266:MET:H	1:D:295:THR:HG21	1.66	0.59
1:F:489:ALA:N	1:F:505:ILE:O	2.33	0.59
2:H:203:VAL:O	2:H:206:LEU:HG	2.03	0.59
1:A:261:ILE:HG13	1:A:261:ILE:O	2.03	0.58
1:D:459:ILE:HG13	1:D:477:TRP:CD1	2.38	0.58
2:H:300:ILE:HD13	2:H:386:TYR:HD2	1.65	0.58
1:A:468:ARG:CZ	1:A:468:ARG:HB2	2.32	0.58
1:A:568:GLU:HG2	1:A:569:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:TYR:HD1	1:B:233:TYR:N	2.01	0.58
1:C:486:GLU:HA	1:C:586:LYS:NZ	2.18	0.58
1:C:721:ILE:CG2	1:C:723:LYS:CE	2.81	0.58
1:D:643:ILE:N	1:D:699:TYR:O	2.29	0.58
1:E:699:TYR:CE1	1:E:725:LEU:HD13	2.39	0.58
1:G:633:LYS:HA	1:G:636:ARG:HH21	1.66	0.58
1:B:253:HIS:ND1	1:B:254:PRO:HD2	2.18	0.58
1:B:476:ASN:N	1:B:479:GLU:OE2	2.25	0.58
1:D:238:LYS:NZ	1:D:251:ALA:O	2.34	0.58
1:D:300:THR:O	1:D:324:PHE:HB3	2.04	0.58
1:F:238:LYS:NZ	1:F:252:ARG:HA	2.18	0.58
2:H:478:SER:OG	2:H:590:ARG:NH2	2.35	0.58
1:E:353:ASN:OD1	1:E:354:THR:N	2.36	0.58
1:F:443:GLU:HA	1:F:446:LYS:HZ3	1.68	0.58
1:E:721:ILE:CD1	1:E:723:LYS:CD	2.79	0.58
1:G:543:GLN:HG2	1:G:545:LYS:NZ	2.18	0.58
2:H:739:GLU:HA	2:H:742:ARG:HH12	1.67	0.58
2:I:173:VAL:HG23	2:I:239:GLU:HG3	1.85	0.58
1:A:565:GLN:NE2	1:A:582:LYS:O	2.36	0.58
1:C:508:VAL:HG23	1:C:516:THR:HA	1.85	0.58
1:C:573:ASN:ND2	1:C:575:TYR:HB2	2.18	0.58
1:G:496:LYS:HE2	1:G:496:LYS:HA	1.86	0.58
1:A:494:ASN:HB2	1:A:498:LEU:HA	1.84	0.58
1:C:551:ASP:OD1	1:C:552:PHE:N	2.37	0.58
1:D:360:LEU:HB3	1:D:432:ILE:CG2	2.33	0.58
1:E:246:ASN:HD21	1:E:406:ALA:HB1	1.68	0.58
1:E:366:TYR:CE1	1:E:378:LEU:HD23	2.39	0.58
2:H:55:LYS:HE2	2:H:134:SER:HA	1.84	0.58
2:H:441:MET:HE3	2:H:499:LEU:HD22	1.86	0.58
2:I:530:LYS:HB3	2:I:548:LYS:NZ	2.19	0.58
1:D:549:GLU:HB3	1:D:595:ARG:NH1	2.18	0.58
2:H:62:LEU:HD21	2:H:137:TYR:HB3	1.86	0.58
1:A:366:TYR:CZ	1:A:378:LEU:HD12	2.39	0.58
1:A:438:GLN:HA	1:A:441:GLU:OE1	2.04	0.58
1:B:291:LYS:HZ1	1:B:335:ASP:N	1.97	0.58
1:D:332:VAL:O	1:D:447:GLN:HG2	2.04	0.58
1:D:382:SER:HA	1:D:393:THR:HA	1.86	0.58
1:F:636:ARG:HG3	1:F:637:LYS:HZ3	1.67	0.58
1:B:353:ASN:OD1	1:B:354:THR:N	2.37	0.57
1:C:233:TYR:HD2	1:C:233:TYR:N	2.02	0.57
1:E:291:LYS:HE3	1:E:335:ASP:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:454:LEU:HD12	2:J:455:VAL:HG13	1.86	0.57
1:B:326:ASN:ND2	1:B:485:GLN:HE21	2.02	0.57
1:G:234:SER:OG	1:G:237:GLU:HG2	2.04	0.57
2:H:578:LYS:NZ	2:H:579:TYR:CZ	2.72	0.57
2:I:113:LEU:HD23	2:I:115:HIS:NE2	2.18	0.57
2:J:91:HIS:CD2	2:J:93:SER:H	2.22	0.57
1:C:353:ASN:OD1	1:C:354:THR:N	2.37	0.57
1:C:634:ASP:OD1	1:C:635:ILE:N	2.37	0.57
1:E:300:THR:O	1:E:324:PHE:HB3	2.03	0.57
1:F:667:SER:O	1:F:675:PHE:N	2.32	0.57
2:J:226:GLU:HB3	2:J:229:HIS:HB2	1.86	0.57
1:A:338:LEU:CD1	1:A:344:ARG:HH21	2.17	0.57
2:H:157:ARG:HD3	2:H:214:GLN:HG3	1.86	0.57
2:I:38:GLU:HG2	2:I:39:ILE:HD12	1.85	0.57
2:I:167:TYR:CE2	2:I:168:GLN:NE2	2.73	0.57
2:J:63:LEU:O	2:J:66:VAL:HG12	2.04	0.57
1:A:226:TRP:CZ2	1:A:234:SER:HB3	2.39	0.57
1:A:249:PRO:HA	1:A:252:ARG:HG2	1.87	0.57
1:B:366:TYR:CE1	1:B:378:LEU:CD1	2.87	0.57
1:B:468:ARG:HB3	1:B:470:ARG:NH2	2.19	0.57
1:C:225:LYS:HG2	1:C:228:THR:HA	1.86	0.57
1:C:334:ILE:CG2	1:C:446:LYS:HB3	2.34	0.57
1:C:403:GLN:O	1:C:404:ILE:HD13	2.04	0.57
1:C:513:PRO:O	1:C:516:THR:HG22	2.04	0.57
1:D:202:PHE:CE2	1:D:204:SER:HB2	2.35	0.57
1:E:524:LYS:HG2	1:E:540:LEU:HD21	1.87	0.57
1:F:202:PHE:CE2	1:F:204:SER:HB2	2.38	0.57
1:G:584:ASN:H	1:G:587:MET:HE1	1.68	0.57
2:H:55:LYS:HG3	2:H:134:SER:O	2.05	0.57
2:H:194:LEU:HD11	2:H:212:GLU:HB3	1.85	0.57
1:A:210:ILE:HA	1:A:213:LYS:NZ	2.20	0.57
1:B:492:ILE:CG2	1:B:500:LEU:HD12	2.34	0.57
1:D:535:GLU:OE1	1:D:540:LEU:HD13	2.03	0.57
1:E:385:LEU:HD23	1:E:391:LEU:HD21	1.85	0.57
1:F:233:TYR:HA	1:F:237:GLU:OE2	2.05	0.57
1:F:269:ILE:HG22	1:F:270:ILE:N	2.19	0.57
1:B:443:GLU:HA	1:B:446:LYS:NZ	2.20	0.57
1:D:266:MET:HE1	1:D:364:ILE:HG22	1.86	0.57
1:F:485:GLN:HE22	1:F:504:ARG:CZ	2.18	0.57
2:H:202:SER:OG	2:H:204:GLU:HG3	2.04	0.57
2:I:159:ILE:O	2:I:162:LYS:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:LEU:N	1:B:392:ALA:O	2.36	0.57
1:D:643:ILE:HG13	1:D:723:LYS:CE	2.34	0.57
1:E:234:SER:O	1:E:237:GLU:HG2	2.05	0.57
1:F:253:HIS:O	1:F:256:VAL:HG22	2.04	0.57
1:F:350:MET:O	1:F:352:LEU:N	2.38	0.57
1:F:468:ARG:NH2	1:G:232:PRO:HB3	2.20	0.57
1:B:609:GLU:HB2	1:B:724:ILE:CG2	2.35	0.57
1:C:384:VAL:HG23	1:C:449:ARG:HB2	1.87	0.57
1:D:492:ILE:HD13	1:D:502:GLU:OE2	2.05	0.57
1:D:554:PHE:CE1	1:D:589:ILE:HD12	2.40	0.57
2:J:227:PRO:HB2	2:J:228:GLN:NE2	2.19	0.57
1:C:250:GLU:H	1:C:250:GLU:CD	2.08	0.57
1:C:374:ILE:HG12	1:C:405:LEU:HB2	1.86	0.57
1:G:639:LEU:N	1:G:703:LYS:HZ2	2.03	0.57
2:H:426:SER:HB3	2:H:510:ARG:CZ	2.35	0.57
2:I:409:ARG:O	2:I:413:LYS:HG3	2.05	0.57
1:B:463:ASN:ND2	1:B:465:GLU:OE2	2.37	0.56
1:B:555:ASP:OD1	1:B:556:GLN:N	2.36	0.56
1:D:197:LYS:HD3	1:D:198:ASN:OD1	2.05	0.56
1:D:628:LEU:HD12	1:D:628:LEU:O	2.05	0.56
1:G:233:TYR:HA	1:G:237:GLU:OE2	2.05	0.56
1:B:223:PRO:HG2	1:B:224:GLU:OE1	2.05	0.56
2:H:124:GLY:N	2:H:127:PRO:HG3	2.20	0.56
1:B:627:LEU:HB3	1:B:629:LEU:HD23	1.87	0.56
1:D:483:GLN:OE1	1:D:483:GLN:N	2.39	0.56
1:D:535:GLU:OE2	1:D:540:LEU:HD22	2.05	0.56
1:D:577:VAL:HG12	1:D:580:LYS:HB2	1.87	0.56
1:E:271:LEU:HB2	1:E:289:ILE:HG13	1.88	0.56
1:E:301:SER:O	1:E:323:GLY:N	2.38	0.56
1:F:295:THR:HG22	1:F:332:VAL:HG23	1.88	0.56
1:F:634:ASP:OD1	1:F:635:ILE:N	2.38	0.56
1:G:271:LEU:HB2	1:G:289:ILE:HG23	1.86	0.56
2:I:150:GLU:CD	2:I:153:LYS:HZ3	2.08	0.56
2:J:589:ASN:OD1	2:J:590:ARG:N	2.34	0.56
1:B:488:THR:OG1	1:B:504:ARG:NH2	2.38	0.56
1:B:533:PHE:CZ	1:B:542:TYR:HB2	2.40	0.56
1:C:350:MET:O	1:C:352:LEU:N	2.38	0.56
1:D:362:ALA:HB3	1:D:421:LEU:HD13	1.86	0.56
1:E:721:ILE:HG13	1:E:723:LYS:CD	2.34	0.56
1:F:187:LEU:HD11	1:F:205:PRO:HG3	1.86	0.56
1:F:297:ARG:HD2	1:F:298:THR:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:365:ARG:HE	1:F:418:PRO:HB3	1.70	0.56
2:H:155:LEU:HD13	2:H:159:ILE:HG13	1.88	0.56
2:H:183:SER:HB2	2:H:186:GLN:NE2	2.20	0.56
2:H:676:GLU:HG2	2:H:677:LEU:N	2.21	0.56
2:H:743:LEU:HB3	2:H:755:VAL:HG11	1.87	0.56
1:A:612:VAL:O	1:A:616:HIS:NE2	2.38	0.56
1:B:234:SER:HB3	1:B:237:GLU:HG2	1.87	0.56
1:C:203:LEU:HB3	2:I:44:VAL:HA	1.87	0.56
1:D:326:ASN:ND2	1:D:485:GLN:HB2	2.20	0.56
1:E:609:GLU:HG2	1:E:613:LYS:HZ1	1.69	0.56
1:F:484:ILE:H	1:F:484:ILE:HD12	1.69	0.56
1:A:234:SER:OG	1:A:237:GLU:HG2	2.06	0.56
1:B:345:THR:O	1:B:348:GLU:HG3	2.06	0.56
1:F:468:ARG:HH21	1:G:232:PRO:HB3	1.70	0.56
1:B:291:LYS:NZ	1:B:335:ASP:H	1.97	0.56
1:B:550:PHE:O	1:B:575:TYR:OH	2.23	0.56
1:B:634:ASP:OD1	1:B:635:ILE:N	2.38	0.56
1:C:333:ALA:HA	1:C:447:GLN:HE22	1.71	0.56
1:F:198:ASN:O	1:F:199:LYS:HG2	2.06	0.56
1:G:353:ASN:OD1	1:G:354:THR:N	2.37	0.56
1:B:445:THR:O	1:B:447:GLN:HG2	2.05	0.56
1:B:552:PHE:HB2	1:B:554:PHE:CZ	2.41	0.56
1:C:264:VAL:HG21	1:C:381:THR:HG21	1.88	0.56
1:D:492:ILE:HG22	1:D:500:LEU:HD12	1.88	0.56
1:F:523:LEU:HD22	1:F:578:LEU:HD11	1.87	0.56
1:E:345:THR:O	1:E:349:THR:HG23	2.05	0.56
1:G:207:ILE:H	1:G:211:HIS:CE1	2.23	0.56
2:H:165:GLN:OE1	2:H:165:GLN:N	2.29	0.56
2:H:247:PHE:HA	2:H:251:GLU:CD	2.25	0.56
2:H:479:ILE:C	2:H:590:ARG:HH22	2.08	0.56
1:A:338:LEU:HD13	1:A:344:ARG:HH21	1.71	0.56
1:A:638:ILE:HG13	1:A:639:LEU:HD12	1.88	0.56
1:B:245:LYS:HB3	1:C:486:GLU:OE2	2.05	0.56
1:B:584:ASN:H	1:B:587:MET:CE	2.18	0.56
1:C:560:GLN:HA	1:C:563:LYS:HE3	1.88	0.56
1:D:434:MET:SD	1:D:438:GLN:HB2	2.45	0.56
1:E:459:ILE:HG12	1:E:477:TRP:CE2	2.40	0.56
1:G:560:GLN:HA	1:G:563:LYS:HE3	1.88	0.56
1:B:365:ARG:HH12	1:B:414:LYS:HA	1.71	0.55
1:D:183:ILE:HD12	1:D:183:ILE:H	1.71	0.55
1:D:373:PRO:HB2	1:D:375:TYR:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:ALA:O	1:E:344:ARG:NH1	2.34	0.55
1:E:593:ASP:OD1	1:E:595:ARG:NH2	2.39	0.55
2:H:63:LEU:O	2:H:66:VAL:HG12	2.06	0.55
1:B:441:GLU:HA	1:B:444:LYS:NZ	2.21	0.55
1:B:584:ASN:OD1	1:B:585:ALA:N	2.38	0.55
1:C:250:GLU:OE1	1:C:250:GLU:N	2.24	0.55
1:C:573:ASN:HD21	1:C:575:TYR:HB2	1.70	0.55
1:D:508:VAL:HA	1:D:515:GLU:OE2	2.07	0.55
1:E:493:PHE:CZ	1:E:495:GLY:HA3	2.41	0.55
1:F:266:MET:H	1:F:295:THR:HG21	1.71	0.55
1:G:403:GLN:HG3	1:G:411:TYR:CE1	2.41	0.55
1:G:667:SER:N	1:G:675:PHE:O	2.26	0.55
1:A:556:GLN:OE1	1:A:557:GLN:NE2	2.40	0.55
1:B:634:ASP:O	1:B:637:LYS:HG2	2.06	0.55
1:C:577:VAL:HG22	1:C:580:LYS:HB2	1.88	0.55
1:G:493:PHE:CE2	1:G:495:GLY:HA3	2.41	0.55
1:G:722:LYS:NZ	1:G:723:LYS:O	2.40	0.55
2:H:83:ILE:HG22	2:H:131:ILE:HD11	1.87	0.55
2:I:531:ASP:OD1	2:I:532:VAL:N	2.40	0.55
2:I:533:GLN:OE1	2:I:533:GLN:N	2.39	0.55
1:A:325:SER:OG	1:G:415:ASN:ND2	2.39	0.55
1:C:565:GLN:NE2	1:C:582:LYS:HB2	2.21	0.55
1:E:233:TYR:O	1:E:238:LYS:NZ	2.39	0.55
1:E:645:GLU:HA	1:E:655:VAL:HA	1.89	0.55
1:F:468:ARG:NH1	1:F:468:ARG:HB2	2.21	0.55
2:H:550:VAL:HG23	2:H:555:ILE:HD11	1.89	0.55
2:I:480:SER:CB	2:I:590:ARG:HE	2.19	0.55
2:J:248:ASN:ND2	2:J:248:ASN:O	2.38	0.55
1:A:634:ASP:OD1	1:A:635:ILE:N	2.40	0.55
1:C:485:GLN:HG2	1:C:504:ARG:NH2	2.22	0.55
1:D:242:ARG:HB3	1:D:462:TYR:CE2	2.41	0.55
1:D:610:SER:HA	1:D:613:LYS:HZ2	1.70	0.55
2:I:498:ARG:NH2	2:I:541:GLU:O	2.37	0.55
1:A:266:MET:H	1:A:295:THR:HG21	1.69	0.55
1:A:328:ASN:HD21	1:A:452:THR:HB	1.72	0.55
1:A:359:ARG:NH2	1:A:429:SER:O	2.40	0.55
1:A:620:ILE:HG13	1:A:630:ASN:HD22	1.72	0.55
1:C:260:PRO:HB2	1:C:456:TYR:HE2	1.70	0.55
1:E:442:LEU:O	1:E:446:LYS:HD2	2.06	0.55
2:H:696:ALA:O	2:H:699:LEU:HG	2.06	0.55
2:I:463:ILE:HB	2:I:465:ARG:HH22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:477:TYR:HA	2:I:529:ILE:H	1.71	0.55
1:A:233:TYR:HA	1:A:237:GLU:OE2	2.06	0.55
1:A:350:MET:O	1:A:352:LEU:N	2.37	0.55
1:A:629:LEU:O	1:A:674:THR:N	2.40	0.55
1:B:698:VAL:HB	1:B:727:PHE:HB3	1.88	0.55
1:C:190:GLU:O	1:C:220:LYS:HE2	2.07	0.55
1:C:266:MET:H	1:C:295:THR:HG21	1.70	0.55
1:C:447:GLN:HB3	1:C:449:ARG:NH2	2.18	0.55
1:C:520:ASP:OD1	1:C:521:MET:N	2.39	0.55
1:C:639:LEU:HD12	1:C:639:LEU:O	2.07	0.55
1:D:636:ARG:HG3	1:D:639:LEU:HD21	1.89	0.55
2:H:264:MET:N	2:H:264:MET:SD	2.79	0.55
2:I:211:ASN:O	2:I:214:GLN:HG2	2.06	0.55
2:J:594:ASN:OD1	2:J:595:ILE:N	2.39	0.55
1:D:297:ARG:NH2	1:D:500:LEU:HD23	2.21	0.55
1:E:540:LEU:HB2	1:E:547:ILE:HD13	1.89	0.55
1:F:297:ARG:HD2	1:F:298:THR:H	1.72	0.55
2:H:605:GLU:O	2:H:609:ASN:ND2	2.38	0.55
1:A:260:PRO:HB2	1:A:456:TYR:CE2	2.42	0.55
1:C:560:GLN:O	1:C:563:LYS:HG2	2.05	0.55
1:D:667:SER:O	1:D:675:PHE:N	2.33	0.55
1:F:242:ARG:HB3	1:F:462:TYR:CE2	2.42	0.55
1:F:643:ILE:HD13	1:F:723:LYS:HE2	1.89	0.55
2:H:108:TYR:O	2:H:110:LYS:HE2	2.07	0.55
2:I:40:MET:O	2:I:44:VAL:HG12	2.07	0.55
2:I:170:PHE:HD1	2:I:243:TYR:CE2	2.24	0.55
2:I:487:ASP:HA	2:I:518:LYS:HG3	1.88	0.55
1:C:228:THR:HG23	1:C:235:ASP:OD1	2.07	0.55
1:D:198:ASN:O	1:D:199:LYS:HD2	2.05	0.55
1:D:668:LEU:HA	1:D:674:THR:HA	1.89	0.55
2:H:171:LEU:O	2:H:175:ASN:ND2	2.38	0.55
2:H:386:TYR:CE1	2:H:412:TYR:HE1	2.25	0.55
2:J:136:ASP:OD1	2:J:136:ASP:N	2.39	0.55
1:A:546:ASP:OD1	1:A:547:ILE:N	2.40	0.54
1:A:610:SER:O	1:A:613:LYS:HG2	2.07	0.54
1:B:506:ALA:HB1	1:B:518:LYS:HZ1	1.71	0.54
1:B:558:THR:HG21	1:B:588:ASN:H	1.72	0.54
2:H:296:LEU:HD23	2:H:388:ILE:HG21	1.88	0.54
1:A:634:ASP:O	1:A:637:LYS:HG2	2.06	0.54
1:B:382:SER:HA	1:B:393:THR:HA	1.90	0.54
1:C:383:LEU:HD11	1:C:448:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:ASP:HB3	1:C:548:THR:HG22	1.89	0.54
1:D:233:TYR:HA	1:D:237:GLU:OE2	2.07	0.54
1:D:411:TYR:CD1	1:D:412:PRO:HA	2.42	0.54
1:D:471:VAL:N	1:E:479:GLU:OE1	2.39	0.54
1:G:620:ILE:HD12	1:G:620:ILE:H	1.72	0.54
2:H:247:PHE:HA	2:H:251:GLU:OE2	2.07	0.54
2:H:480:SER:HA	2:H:590:ARG:HH12	1.72	0.54
2:I:136:ASP:OD1	2:I:136:ASP:N	2.34	0.54
1:C:245:LYS:HE2	1:C:245:LYS:HA	1.89	0.54
1:D:209:ASN:OD1	1:D:210:ILE:HG12	2.08	0.54
1:G:212:GLU:OE2	1:G:213:LYS:NZ	2.38	0.54
2:H:129:LEU:HD23	2:H:129:LEU:H	1.71	0.54
2:J:203:VAL:O	2:J:206:LEU:HG	2.06	0.54
1:B:582:LYS:HE2	1:B:582:LYS:HA	1.88	0.54
1:C:221:SER:HB2	1:C:228:THR:HG21	1.89	0.54
1:D:542:TYR:O	1:D:545:LYS:HE2	2.07	0.54
1:E:209:ASN:OD1	1:E:210:ILE:HG12	2.06	0.54
1:F:542:TYR:O	1:F:545:LYS:HE2	2.08	0.54
1:G:543:GLN:HG2	1:G:545:LYS:HZ3	1.72	0.54
1:G:634:ASP:OD1	1:G:635:ILE:N	2.40	0.54
2:H:478:SER:OG	2:H:590:ARG:HA	2.07	0.54
1:C:291:LYS:HE2	1:C:335:ASP:O	2.07	0.54
1:E:659:ARG:HA	1:E:716:THR:O	2.07	0.54
1:F:234:SER:N	1:F:237:GLU:OE2	2.38	0.54
1:G:200:ARG:HG3	1:G:200:ARG:HH11	1.72	0.54
1:B:224:GLU:OE1	1:B:224:GLU:N	2.40	0.54
1:B:295:THR:HG22	1:B:332:VAL:HG23	1.90	0.54
1:G:573:ASN:ND2	1:G:576:THR:OG1	2.41	0.54
2:I:176:THR:HB	2:I:239:GLU:OE2	2.07	0.54
2:I:264:MET:HA	2:I:267:ARG:NH2	2.23	0.54
2:I:533:GLN:HE21	2:I:544:ARG:HG3	1.73	0.54
1:D:590:LEU:HD21	1:D:592:ARG:HG3	1.89	0.54
1:E:326:ASN:OD1	1:E:490:ARG:NH1	2.41	0.54
1:E:562:ILE:HD13	1:E:565:GLN:OE1	2.07	0.54
1:G:258:ALA:HA	1:G:371:THR:OG1	2.07	0.54
2:H:469:ASN:HA	2:H:472:LYS:HZ3	1.72	0.54
2:H:656:LYS:HD2	2:H:672:SER:OG	2.08	0.54
1:A:446:LYS:NZ	1:A:708:ILE:O	2.30	0.54
1:E:231:ASP:HB2	1:E:232:PRO:HD3	1.90	0.54
1:E:350:MET:O	1:E:352:LEU:N	2.40	0.54
1:F:291:LYS:HZ2	1:F:334:ILE:HG23	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:411:GLN:HA	2:H:414:ARG:NH1	2.21	0.54
1:A:261:ILE:HD11	1:A:369:THR:HG23	1.90	0.54
1:D:552:PHE:HB3	1:D:554:PHE:CE2	2.43	0.54
1:E:447:GLN:C	1:E:448:LEU:HD22	2.28	0.54
1:F:485:GLN:OE1	1:F:504:ARG:NH1	2.41	0.54
1:G:245:LYS:HA	1:G:245:LYS:HE3	1.89	0.54
1:G:266:MET:H	1:G:295:THR:HG21	1.73	0.54
2:H:190:PHE:CD1	2:H:194:LEU:HB2	2.42	0.54
2:H:301:GLU:HG2	2:H:302:PRO:HD2	1.90	0.54
2:J:107:ILE:HD13	2:J:149:TYR:CD2	2.42	0.54
1:A:291:LYS:HB3	1:A:335:ASP:OD1	2.07	0.54
1:B:195:ASP:OD2	2:H:236:TYR:OH	2.25	0.54
1:E:646:ILE:N	1:E:654:GLU:O	2.37	0.54
1:G:198:ASN:H	1:G:200:ARG:HH22	1.56	0.54
1:G:593:ASP:OD2	1:G:595:ARG:HB3	2.08	0.54
1:G:617:ARG:HH11	1:G:617:ARG:HG2	1.73	0.54
2:H:434:LYS:HD3	2:H:436:TYR:CZ	2.43	0.54
1:C:244:ASP:CG	1:C:246:ASN:HD22	2.12	0.53
1:E:490:ARG:HB2	1:E:504:ARG:NH1	2.23	0.53
2:H:447:THR:HG23	2:H:450:LEU:HB2	1.89	0.53
1:B:197:LYS:HZ1	2:H:236:TYR:HD1	1.53	0.53
1:D:267:GLU:OE1	1:D:267:GLU:N	2.40	0.53
1:D:297:ARG:NH1	1:D:500:LEU:HD23	2.23	0.53
1:E:462:TYR:CZ	1:E:467:GLY:HA2	2.43	0.53
1:E:565:GLN:HA	1:E:568:GLU:OE2	2.08	0.53
1:F:197:LYS:O	1:F:199:LYS:N	2.39	0.53
2:H:192:ASN:HA	2:H:195:LYS:HD2	1.90	0.53
2:H:447:THR:HG21	2:H:450:LEU:HD12	1.90	0.53
2:H:669:HIS:CE1	2:H:671:PRO:HB2	2.43	0.53
2:I:61:LYS:C	2:I:65:LYS:HZ3	2.11	0.53
1:A:498:LEU:HB2	1:A:637:LYS:NZ	2.23	0.53
1:A:512:ASP:OD2	1:G:245:LYS:NZ	2.30	0.53
1:B:178:ARG:HA	1:B:178:ARG:NE	2.22	0.53
1:C:697:ASN:HA	1:C:727:PHE:O	2.09	0.53
1:D:459:ILE:HG13	1:D:477:TRP:CE2	2.44	0.53
1:E:187:LEU:HD11	1:E:205:PRO:HG3	1.89	0.53
1:E:490:ARG:HD3	1:E:504:ARG:HH22	1.72	0.53
1:F:200:ARG:HG3	1:F:200:ARG:NH1	2.22	0.53
1:F:610:SER:O	1:F:613:LYS:HG2	2.08	0.53
1:G:667:SER:O	1:G:675:PHE:N	2.35	0.53
2:I:89:THR:HG22	2:I:114:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:115:HIS:CD2	2:J:116:GLU:HG3	2.43	0.53
1:A:678:PHE:CZ	1:A:687:LEU:HD23	2.43	0.53
1:E:435:ASN:OD1	1:E:438:GLN:N	2.31	0.53
2:H:250:GLN:OE1	2:H:250:GLN:N	2.42	0.53
2:H:404:ILE:O	2:H:409:ARG:NH2	2.37	0.53
2:I:82:TYR:OH	2:I:91:HIS:CE1	2.62	0.53
2:I:273:LYS:O	2:I:276:GLN:HG3	2.08	0.53
2:J:502:ARG:NH1	2:J:544:ARG:HD3	2.23	0.53
1:A:174:THR:O	1:A:175:VAL:HB	2.08	0.53
1:C:202:PHE:HB2	2:I:45:LYS:HD3	1.91	0.53
1:D:353:ASN:OD1	1:D:354:THR:N	2.38	0.53
1:E:608:ASP:O	1:E:611:VAL:HG22	2.09	0.53
1:F:259:TYR:CE2	1:F:261:ILE:HD11	2.44	0.53
1:F:584:ASN:O	1:F:587:MET:HE2	2.09	0.53
1:G:617:ARG:NH1	1:G:617:ARG:O	2.41	0.53
2:H:105:LYS:HD2	2:H:109:GLY:O	2.07	0.53
1:D:297:ARG:CZ	1:D:500:LEU:H	2.21	0.53
1:D:385:LEU:HD13	1:D:448:LEU:HG	1.90	0.53
1:E:233:TYR:CD2	1:E:243:ILE:CD1	2.91	0.53
1:G:610:SER:O	1:G:613:LYS:HG2	2.08	0.53
2:I:469:ASN:HA	2:I:472:LYS:NZ	2.24	0.53
2:I:762:THR:HA	2:I:765:PHE:CE1	2.44	0.53
1:A:227:SER:O	1:A:230:SER:N	2.41	0.53
1:A:455:VAL:O	1:A:455:VAL:HG13	2.08	0.53
1:B:443:GLU:HA	1:B:446:LYS:HZ2	1.74	0.53
1:B:533:PHE:CE2	1:B:542:TYR:HB2	2.44	0.53
1:C:297:ARG:NH1	1:C:329:SER:O	2.40	0.53
1:C:506:ALA:HB1	1:C:518:LYS:HZ1	1.74	0.53
1:D:297:ARG:NH1	1:D:500:LEU:HB2	2.23	0.53
2:I:589:ASN:OD1	2:I:590:ARG:N	2.34	0.53
2:J:503:ILE:HG13	2:J:549:VAL:HG23	1.91	0.53
1:A:435:ASN:ND2	1:A:438:GLN:HG2	2.24	0.53
1:B:266:MET:CE	1:B:332:VAL:HG21	2.39	0.53
1:C:705:ASN:ND2	1:C:722:LYS:HB3	2.24	0.53
1:D:269:ILE:HG22	1:D:270:ILE:N	2.24	0.53
1:E:385:LEU:CD2	1:E:391:LEU:HD21	2.38	0.53
1:E:584:ASN:O	1:E:587:MET:HE2	2.08	0.53
1:F:187:LEU:HD12	1:F:192:TYR:HB3	1.91	0.53
1:F:209:ASN:OD1	1:F:210:ILE:HG12	2.09	0.53
1:F:535:GLU:OE2	1:F:540:LEU:HD12	2.09	0.53
2:H:155:LEU:O	2:H:159:ILE:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:HE2	1:A:245:LYS:HA	1.89	0.53
1:C:291:LYS:HE2	1:C:335:ASP:OD1	2.09	0.53
1:C:385:LEU:HG	1:C:391:LEU:HD21	1.91	0.53
1:G:263:HIS:CE1	1:G:367:VAL:HB	2.43	0.53
2:I:114:LEU:HD12	2:I:115:HIS:N	2.24	0.53
1:B:217:THR:HG1	1:B:219:TYR:HE1	1.57	0.53
1:B:536:PRO:HG2	1:B:541:GLN:NE2	2.24	0.53
1:D:620:ILE:HD13	1:D:629:LEU:HA	1.91	0.53
1:E:226:TRP:CZ2	1:E:234:SER:HB3	2.44	0.53
1:E:406:ALA:HB1	1:E:407:PRO:HD2	1.90	0.53
1:G:438:GLN:HA	1:G:441:GLU:OE2	2.09	0.53
1:G:559:SER:HA	1:G:562:ILE:HG22	1.90	0.53
2:I:607:LYS:HA	2:I:615:ILE:HD11	1.91	0.53
2:J:89:THR:HG21	2:J:115:HIS:HA	1.82	0.53
1:A:470:ARG:HD3	1:A:471:VAL:H	1.73	0.52
1:B:392:ALA:HB2	1:B:432:ILE:HD13	1.91	0.52
1:C:405:LEU:HD21	1:C:411:TYR:HB2	1.92	0.52
1:E:610:SER:HA	1:E:613:LYS:NZ	2.24	0.52
1:E:721:ILE:CG1	1:E:723:LYS:CD	2.88	0.52
2:I:137:TYR:CE2	2:I:143:LYS:HE3	2.44	0.52
2:J:110:LYS:HD3	2:J:110:LYS:N	2.23	0.52
2:J:145:LEU:HD21	2:J:226:GLU:HG3	1.91	0.52
2:J:204:GLU:O	2:J:207:GLU:HG2	2.08	0.52
1:A:190:GLU:C	1:A:220:LYS:HZ2	2.13	0.52
1:A:415:ASN:C	1:A:416:LEU:HD22	2.30	0.52
1:B:183:ILE:HG13	1:B:236:PHE:HD1	1.75	0.52
1:B:449:ARG:HB3	1:B:449:ARG:NH1	2.23	0.52
1:D:635:ILE:HG23	1:D:636:ARG:HD3	1.91	0.52
1:F:515:GLU:CD	1:F:515:GLU:N	2.63	0.52
2:H:80:LYS:H	2:H:128:VAL:HG12	1.74	0.52
2:H:567:ASN:OD1	2:H:568:GLN:N	2.42	0.52
2:I:115:HIS:ND1	2:I:116:GLU:HG3	2.23	0.52
2:J:443:ILE:HG21	2:J:454:LEU:HD21	1.91	0.52
1:A:360:LEU:HD12	1:A:361:ASN:H	1.74	0.52
1:C:459:ILE:HG12	1:C:477:TRP:CE2	2.44	0.52
1:E:470:ARG:HD2	1:E:471:VAL:N	2.24	0.52
1:E:628:LEU:HA	1:E:674:THR:O	2.10	0.52
1:G:459:ILE:HG13	1:G:477:TRP:NE1	2.24	0.52
1:B:263:HIS:CG	1:B:297:ARG:HG3	2.44	0.52
1:E:488:THR:HG22	1:E:506:ALA:HA	1.91	0.52
2:H:475:PHE:O	2:H:476:LYS:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:658:LEU:HD22	2:H:667:LEU:HD12	1.91	0.52
2:J:577:PRO:O	2:J:580:THR:HG22	2.09	0.52
1:A:360:LEU:HD12	1:A:361:ASN:N	2.24	0.52
1:D:705:ASN:ND2	1:D:722:LYS:O	2.42	0.52
1:E:240:THR:O	1:F:514:LEU:HB2	2.09	0.52
1:F:364:ILE:HG23	1:F:421:LEU:HD11	1.91	0.52
2:H:100:ASP:C	2:H:102:LYS:H	2.13	0.52
1:B:508:VAL:HA	1:B:518:LYS:HD3	1.92	0.52
1:C:435:ASN:N	1:C:438:GLN:OE1	2.42	0.52
1:D:234:SER:OG	1:D:237:GLU:HG2	2.10	0.52
1:G:270:ILE:HG13	1:G:361:ASN:OD1	2.10	0.52
1:G:696:VAL:O	1:G:728:SER:HA	2.08	0.52
2:H:591:TYR:CE2	2:H:594:ASN:HB3	2.45	0.52
2:H:640:ALA:HA	2:H:643:TYR:CE1	2.44	0.52
2:H:707:LEU:HD23	2:H:709:THR:CG2	2.37	0.52
2:I:686:HIS:O	2:I:738:ALA:HB1	2.10	0.52
2:J:237:ALA:HB1	2:J:240:ALA:HB3	1.90	0.52
1:A:697:ASN:HA	1:A:727:PHE:O	2.10	0.52
1:C:366:TYR:CD2	1:C:378:LEU:HD11	2.45	0.52
1:E:183:ILE:HD12	1:E:203:LEU:HD22	1.92	0.52
2:H:257:GLU:HA	2:H:260:LYS:HZ3	1.74	0.52
2:I:586:ASN:OD1	2:I:630:VAL:HG13	2.10	0.52
2:J:278:TYR:HB3	2:J:513:TYR:CE2	2.44	0.52
1:A:238:LYS:HD2	1:A:251:ALA:O	2.10	0.52
1:A:300:THR:O	1:A:324:PHE:HB3	2.09	0.52
1:A:528:LYS:HZ1	1:A:534:ASN:HA	1.75	0.52
1:D:535:GLU:HB3	1:D:538:GLY:HA2	1.91	0.52
1:E:508:VAL:HG23	1:E:516:THR:HA	1.92	0.52
1:E:562:ILE:HA	1:E:565:GLN:OE1	2.10	0.52
1:F:198:ASN:HB2	1:F:200:ARG:NH2	2.22	0.52
1:F:234:SER:OG	1:F:237:GLU:HG2	2.09	0.52
2:H:427:ILE:HG12	2:H:509:THR:O	2.09	0.52
2:H:427:ILE:HG13	2:H:428:GLY:N	2.25	0.52
2:I:118:TYR:OH	2:I:146:ASN:OD1	2.27	0.52
2:J:392:LEU:HD23	2:J:482:ASN:HA	1.91	0.52
2:J:513:TYR:HA	2:J:519:LEU:HD13	1.92	0.52
1:A:609:GLU:OE1	1:A:609:GLU:N	2.40	0.52
1:C:260:PRO:HD3	1:C:477:TRP:CZ3	2.45	0.52
1:C:578:LEU:HD12	1:C:579:ASP:N	2.25	0.52
1:E:365:ARG:HH12	1:E:414:LYS:HA	1.74	0.52
1:F:226:TRP:CZ2	1:F:234:SER:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:251:ALA:HA	1:F:256:VAL:HG21	1.92	0.52
2:H:204:GLU:O	2:H:207:GLU:HG3	2.10	0.52
2:H:555:ILE:H	2:H:555:ILE:HD12	1.74	0.52
1:B:435:ASN:OD1	1:B:438:GLN:N	2.31	0.52
1:B:485:GLN:HA	1:B:504:ARG:NH1	2.25	0.52
1:B:524:LYS:NZ	1:B:528:LYS:HE3	2.24	0.52
1:B:552:PHE:HB2	1:B:554:PHE:HZ	1.75	0.52
1:B:610:SER:HA	1:B:613:LYS:NZ	2.25	0.52
1:C:360:LEU:HD12	1:C:361:ASN:H	1.75	0.52
1:D:527:LEU:HD23	1:D:533:PHE:CE1	2.44	0.52
1:E:599:ASP:OD2	1:E:601:ASN:ND2	2.43	0.52
1:G:558:THR:HG21	1:G:588:ASN:H	1.75	0.52
2:H:171:LEU:HD22	2:H:206:LEU:HD23	1.92	0.52
2:I:615:ILE:O	2:I:619:THR:HG23	2.10	0.52
2:J:274:ILE:HD11	2:J:488:ILE:HD13	1.92	0.52
1:A:454:GLN:OE1	1:A:454:GLN:N	2.42	0.51
1:A:459:ILE:HG13	1:A:477:TRP:CE2	2.45	0.51
1:A:491:ILE:HG12	1:A:589:ILE:HB	1.93	0.51
1:A:528:LYS:NZ	1:A:534:ASN:HA	2.24	0.51
1:C:721:ILE:O	1:C:723:LYS:HG2	2.09	0.51
1:F:232:PRO:O	1:F:233:TYR:HD1	1.92	0.51
1:F:549:GLU:C	1:F:594:LYS:HE3	2.30	0.51
2:I:271:TRP:CD1	2:I:275:LYS:HG2	2.44	0.51
2:J:72:GLU:O	2:J:75:LYS:HG3	2.11	0.51
1:B:345:THR:O	1:B:349:THR:HG23	2.10	0.51
1:B:621:ASN:OD1	1:B:628:LEU:HG	2.09	0.51
1:C:345:THR:O	1:C:349:THR:HG23	2.11	0.51
1:D:550:PHE:CD1	1:D:593:ASP:HA	2.45	0.51
1:E:624:THR:O	1:E:687:LEU:HD13	2.10	0.51
1:F:362:ALA:HB3	1:F:421:LEU:HD12	1.92	0.51
1:F:668:LEU:HA	1:F:674:THR:HA	1.93	0.51
1:G:199:LYS:H	1:G:200:ARG:NH1	2.08	0.51
2:H:526:GLY:HA3	2:H:555:ILE:HD13	1.92	0.51
2:I:72:GLU:HG3	2:I:75:LYS:HZ3	1.75	0.51
2:J:502:ARG:HH12	2:J:544:ARG:HD3	1.75	0.51
1:A:226:TRP:CH2	1:A:234:SER:HB3	2.46	0.51
1:B:334:ILE:HD11	1:B:446:LYS:HE3	1.92	0.51
1:B:365:ARG:NH1	1:B:414:LYS:HA	2.26	0.51
1:C:210:ILE:O	1:C:213:LYS:NZ	2.43	0.51
1:G:242:ARG:HD3	1:G:462:TYR:CE2	2.45	0.51
1:B:485:GLN:HA	1:B:504:ARG:NH2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:LEU:HB3	1:D:432:ILE:HG21	1.91	0.51
1:D:378:LEU:HD12	1:D:379:PRO:HD3	1.91	0.51
2:H:578:LYS:CG	2:H:579:TYR:CD1	2.91	0.51
2:J:58:ALA:HA	2:J:61:LYS:HE2	1.93	0.51
1:B:259:TYR:N	1:B:371:THR:OG1	2.42	0.51
1:B:438:GLN:HA	1:B:441:GLU:OE2	2.10	0.51
1:C:244:ASP:C	1:C:246:ASN:H	2.14	0.51
1:C:259:TYR:CE2	1:C:261:ILE:HD11	2.36	0.51
1:D:639:LEU:HD12	1:D:639:LEU:O	2.11	0.51
1:F:192:TYR:N	1:F:192:TYR:CD2	2.78	0.51
1:F:626:GLY:HA3	1:F:676:ILE:O	2.10	0.51
2:H:188:LEU:O	2:H:188:LEU:HG	2.10	0.51
2:H:516:ASN:O	2:H:518:LYS:NZ	2.32	0.51
2:I:107:ILE:HD11	2:I:146:ASN:HA	1.93	0.51
2:I:110:LYS:HD3	2:I:110:LYS:N	2.25	0.51
1:D:509:ASN:N	1:D:515:GLU:OE1	2.39	0.51
1:D:549:GLU:O	1:D:595:ARG:NH1	2.44	0.51
2:H:582:LEU:HD12	2:H:583:ILE:CD1	2.41	0.51
2:H:686:HIS:CE1	2:H:690:HIS:CE1	2.99	0.51
2:I:454:LEU:HD12	2:I:455:VAL:N	2.25	0.51
2:J:170:PHE:HB2	2:J:243:TYR:OH	2.10	0.51
1:A:419:ILE:O	1:A:419:ILE:HG13	2.10	0.51
1:A:584:ASN:O	1:A:587:MET:HG3	2.10	0.51
1:C:298:THR:HG23	1:C:603:ILE:HD11	1.92	0.51
1:C:500:LEU:N	1:C:500:LEU:HD22	2.26	0.51
1:D:297:ARG:HA	1:D:330:SER:HA	1.93	0.51
1:E:342:GLY:HA2	1:E:344:ARG:NH1	2.25	0.51
1:G:330:SER:OG	1:G:450:LEU:HB2	2.11	0.51
2:H:257:GLU:HA	2:H:260:LYS:NZ	2.25	0.51
2:H:434:LYS:HG2	2:H:504:GLN:OE1	2.10	0.51
1:B:181:ASP:O	1:B:236:PHE:HB2	2.10	0.51
1:B:198:ASN:ND2	1:B:200:ARG:HH22	2.06	0.51
1:B:443:GLU:OE2	1:B:446:LYS:NZ	2.44	0.51
1:C:410:TYR:CD1	1:C:414:LYS:HE3	2.45	0.51
1:D:185:ASP:OD1	1:D:186:SER:N	2.43	0.51
1:D:554:PHE:HE1	1:D:589:ILE:HD12	1.76	0.51
1:G:255:LEU:HD12	1:G:255:LEU:N	2.26	0.51
1:G:600:ARG:HD2	1:G:601:ASN:N	2.25	0.51
2:H:154:ILE:HG23	2:H:155:LEU:HD22	1.93	0.51
2:I:528:GLU:O	2:I:548:LYS:HG2	2.11	0.51
1:A:345:THR:O	1:A:349:THR:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:GLN:CD	1:A:403:GLN:H	2.13	0.51
1:B:627:LEU:H	1:B:676:ILE:CG2	2.24	0.51
1:C:227:SER:O	1:C:230:SER:N	2.42	0.51
1:C:447:GLN:O	1:C:448:LEU:HD22	2.10	0.51
1:C:628:LEU:HD12	1:C:628:LEU:O	2.11	0.51
1:E:340:LEU:HD23	1:E:343:GLU:HG2	1.92	0.51
1:E:454:GLN:HA	1:E:456:TYR:CZ	2.45	0.51
1:F:468:ARG:HB2	1:F:468:ARG:HH11	1.75	0.51
1:G:350:MET:O	1:G:352:LEU:N	2.42	0.51
2:H:215:GLU:OE2	2:H:219:LYS:HD2	2.11	0.51
1:B:223:PRO:HG2	1:B:224:GLU:OE2	2.10	0.51
1:G:445:THR:O	1:G:447:GLN:HG2	2.10	0.51
2:H:557:THR:HA	2:H:560:GLN:NE2	2.26	0.51
1:A:634:ASP:OD1	1:A:635:ILE:HG12	2.11	0.50
1:B:442:LEU:HD23	1:B:446:LYS:HZ2	1.76	0.50
1:B:597:HIS:N	1:B:606:GLY:O	2.45	0.50
1:D:435:ASN:OD1	1:D:438:GLN:OE1	2.29	0.50
1:E:224:GLU:HB2	1:E:517:THR:HG21	1.93	0.50
1:E:439:PHE:O	1:E:443:GLU:HG2	2.11	0.50
1:F:207:ILE:HG23	2:J:108:TYR:HE2	1.75	0.50
1:F:238:LYS:HZ1	1:F:252:ARG:HA	1.76	0.50
1:F:492:ILE:HD12	1:F:501:VAL:O	2.12	0.50
1:G:176:PRO:HB3	1:G:178:ARG:NH1	2.23	0.50
1:G:290:SER:O	1:G:291:LYS:HE2	2.11	0.50
2:H:388:ILE:O	2:H:391:ARG:HG3	2.10	0.50
2:H:571:ASN:ND2	2:H:578:LYS:O	2.44	0.50
2:H:583:ILE:HG22	2:H:583:ILE:O	2.11	0.50
1:A:435:ASN:OD1	1:A:438:GLN:N	2.34	0.50
1:B:385:LEU:HB3	1:B:391:LEU:HD21	1.93	0.50
1:E:597:HIS:N	1:E:606:GLY:O	2.42	0.50
1:G:497:ASP:O	1:G:637:LYS:NZ	2.40	0.50
2:I:162:LYS:HD3	2:I:259:LEU:HD22	1.91	0.50
2:I:516:ASN:OD1	2:I:518:LYS:HD3	2.11	0.50
1:A:200:ARG:HH22	1:B:186:SER:HA	1.75	0.50
1:A:238:LYS:CE	1:A:254:PRO:HA	2.41	0.50
1:B:560:GLN:HA	1:B:563:LYS:HZ2	1.76	0.50
1:D:210:ILE:HD11	2:I:188:LEU:HA	1.92	0.50
1:E:524:LYS:O	1:E:528:LYS:HG3	2.11	0.50
1:F:459:ILE:HG12	1:F:477:TRP:NE1	2.25	0.50
1:G:365:ARG:HH22	1:G:418:PRO:HD3	1.77	0.50
1:G:592:ARG:HD3	1:G:598:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TYR:CG	1:A:414:LYS:HD3	2.47	0.50
1:C:480:VAL:HG13	1:C:481:LEU:N	2.27	0.50
1:D:331:THR:HG23	1:D:447:GLN:NE2	2.20	0.50
1:D:441:GLU:HA	1:D:444:LYS:NZ	2.26	0.50
1:D:540:LEU:HB3	1:D:547:ILE:HB	1.94	0.50
1:E:609:GLU:HG2	1:E:613:LYS:NZ	2.26	0.50
1:E:628:LEU:O	1:E:628:LEU:HD12	2.10	0.50
1:E:638:ILE:HG22	1:E:638:ILE:O	2.11	0.50
1:F:493:PHE:CE2	1:F:495:GLY:HA3	2.46	0.50
1:F:597:HIS:N	1:F:606:GLY:O	2.43	0.50
1:G:401:LEU:HA	1:G:403:GLN:NE2	2.26	0.50
2:H:148:TYR:HA	2:H:151:ILE:HG22	1.93	0.50
2:H:502:ARG:CB	2:H:544:ARG:HH12	2.25	0.50
2:H:562:ALA:O	2:H:566:ILE:HG13	2.10	0.50
2:I:137:TYR:HE2	2:I:143:LYS:HE3	1.76	0.50
2:I:247:PHE:CE2	2:I:252:ILE:HD11	2.46	0.50
1:B:223:PRO:HG2	1:B:224:GLU:CD	2.32	0.50
1:B:493:PHE:CE2	1:B:495:GLY:HA3	2.46	0.50
1:D:636:ARG:HA	1:D:639:LEU:HG	1.93	0.50
1:E:435:ASN:ND2	1:E:438:GLN:HG3	2.27	0.50
1:E:678:PHE:CB	1:E:687:LEU:HD11	2.42	0.50
1:F:291:LYS:NZ	1:F:292:ASN:O	2.43	0.50
1:G:592:ARG:NH1	1:G:598:TYR:CG	2.80	0.50
2:H:250:GLN:O	2:H:253:ASN:ND2	2.44	0.50
2:J:89:THR:HG21	2:J:115:HIS:CA	2.40	0.50
2:J:502:ARG:NH2	2:J:544:ARG:HB3	2.19	0.50
1:C:209:ASN:HA	1:C:212:GLU:OE1	2.10	0.50
1:C:300:THR:O	1:C:324:PHE:HB3	2.12	0.50
1:E:197:LYS:O	1:E:200:ARG:N	2.35	0.50
1:E:326:ASN:ND2	1:E:485:GLN:HG3	2.24	0.50
2:H:118:TYR:CZ	2:H:143:LYS:HD2	2.46	0.50
1:C:381:THR:O	1:C:394:ILE:HG22	2.11	0.50
1:C:548:THR:HA	1:C:575:TYR:HE2	1.77	0.50
1:C:548:THR:HA	1:C:575:TYR:CE2	2.47	0.50
1:C:597:HIS:NE2	1:C:608:ASP:OD1	2.38	0.50
1:C:625:GLU:N	1:C:625:GLU:OE1	2.45	0.50
1:F:599:ASP:CG	1:F:600:ARG:H	2.15	0.50
2:H:186:GLN:HB2	2:H:190:PHE:HZ	1.74	0.50
2:I:224:TYR:CZ	2:I:230:ARG:NH1	2.80	0.50
2:I:441:MET:SD	2:I:442:ASN:O	2.69	0.50
2:J:278:TYR:CE1	2:J:425:GLN:HG2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ILE:HG13	1:A:477:TRP:NE1	2.26	0.50
1:B:263:HIS:CE1	1:B:297:ARG:HG3	2.47	0.50
1:B:578:LEU:HD12	1:B:579:ASP:N	2.27	0.50
1:C:330:SER:OG	1:C:331:THR:N	2.45	0.50
1:C:575:TYR:O	1:C:578:LEU:HD23	2.11	0.50
1:D:507:ALA:C	1:D:518:LYS:HD2	2.32	0.50
1:D:639:LEU:N	1:D:703:LYS:HZ3	2.09	0.50
1:E:476:ASN:OD1	1:E:479:GLU:HG3	2.12	0.50
1:F:242:ARG:HB3	1:F:462:TYR:CZ	2.47	0.50
1:F:382:SER:HA	1:F:393:THR:HA	1.94	0.50
2:H:459:ASP:OD1	2:H:461:THR:OG1	2.25	0.50
2:H:530:LYS:HE2	2:H:546:ASP:OD2	2.12	0.50
2:I:437:LEU:HD23	2:I:438:TYR:N	2.27	0.50
2:J:239:GLU:OE1	2:J:239:GLU:N	2.44	0.50
1:A:381:THR:O	1:A:394:ILE:HG22	2.12	0.50
1:A:577:VAL:HG22	1:A:580:LYS:HB2	1.93	0.50
1:B:459:ILE:HG12	1:B:477:TRP:CE2	2.46	0.50
1:C:599:ASP:OD1	1:C:600:ARG:N	2.41	0.50
2:H:66:VAL:HG21	2:H:70:VAL:HG22	1.93	0.50
2:H:410:LYS:HB3	2:H:414:ARG:NH2	2.26	0.50
2:I:89:THR:CG2	2:I:115:HIS:HB3	2.34	0.50
2:J:197:HIS:HE1	2:J:200:ASP:O	1.95	0.50
2:J:762:THR:HA	2:J:765:PHE:HE1	1.76	0.50
1:A:206:TRP:CH2	1:A:218:LYS:HB2	2.47	0.49
1:B:199:LYS:H	1:B:200:ARG:NH1	2.10	0.49
1:C:360:LEU:HB3	1:C:432:ILE:HG21	1.92	0.49
1:C:470:ARG:HG2	1:C:470:ARG:HH11	1.77	0.49
1:C:521:MET:SD	1:C:526:ALA:HB2	2.52	0.49
1:D:187:LEU:HD21	1:D:205:PRO:HG3	1.93	0.49
1:D:640:SER:OG	1:D:701:VAL:O	2.19	0.49
1:E:549:GLU:C	1:E:594:LYS:HE3	2.33	0.49
1:F:269:ILE:HG22	1:F:270:ILE:H	1.76	0.49
1:G:227:SER:O	1:G:230:SER:N	2.44	0.49
2:I:135:GLU:CD	2:I:135:GLU:H	2.15	0.49
1:A:332:VAL:CG1	1:A:448:LEU:HB2	2.42	0.49
1:B:563:LYS:O	1:B:566:LEU:HG	2.13	0.49
1:C:635:ILE:C	1:C:637:LYS:H	2.15	0.49
1:E:466:ASN:HB2	1:F:226:TRP:CD2	2.46	0.49
2:H:561:GLU:O	2:H:564:LEU:HG	2.12	0.49
2:I:231:ASP:O	2:I:234:GLN:HG3	2.12	0.49
1:D:185:ASP:OD1	1:D:185:ASP:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:TYR:CE2	1:D:543:GLN:NE2	2.80	0.49
1:D:633:LYS:HA	1:D:636:ARG:CZ	2.42	0.49
1:E:244:ASP:C	1:E:246:ASN:H	2.15	0.49
2:H:436:TYR:CE1	2:H:504:GLN:HB2	2.47	0.49
2:H:553:SER:O	2:H:557:THR:HG23	2.12	0.49
2:H:558:LYS:O	2:H:561:GLU:HG3	2.13	0.49
1:C:443:GLU:O	1:C:446:LYS:NZ	2.40	0.49
1:E:438:GLN:HA	1:E:441:GLU:OE1	2.12	0.49
1:F:195:ASP:OD2	1:F:196:VAL:N	2.44	0.49
1:F:410:TYR:CD2	1:F:414:LYS:HE2	2.47	0.49
2:H:257:GLU:O	2:H:260:LYS:HG2	2.12	0.49
2:I:531:ASP:HB3	2:I:546:ASP:OD2	2.12	0.49
2:I:554:LYS:O	2:I:557:THR:OG1	2.30	0.49
1:A:188:GLU:OE2	1:A:223:PRO:HA	2.13	0.49
1:A:479:GLU:N	1:A:479:GLU:CD	2.66	0.49
1:A:535:GLU:OE2	1:A:540:LEU:HD12	2.12	0.49
1:A:662:MET:O	1:A:664:ASN:N	2.46	0.49
1:B:340:LEU:HB2	1:B:343:GLU:HB3	1.93	0.49
1:C:554:PHE:HB3	1:C:558:THR:OG1	2.12	0.49
1:C:609:GLU:OE2	1:C:613:LYS:HE2	2.12	0.49
1:D:198:ASN:OD1	1:D:200:ARG:NH2	2.45	0.49
1:F:298:THR:HG21	1:F:331:THR:CB	2.43	0.49
1:F:608:ASP:O	1:F:611:VAL:HG22	2.12	0.49
1:G:491:ILE:CD1	1:G:589:ILE:HB	2.42	0.49
2:I:206:LEU:O	2:I:210:SER:OG	2.20	0.49
2:J:147:VAL:O	2:J:151:ILE:HG12	2.12	0.49
1:A:326:ASN:ND2	1:A:485:GLN:OE1	2.45	0.49
1:A:558:THR:HG22	1:A:587:MET:HA	1.94	0.49
1:B:330:SER:OG	1:B:331:THR:N	2.46	0.49
1:C:183:ILE:O	1:C:183:ILE:HG13	2.11	0.49
1:C:533:PHE:HE2	1:C:542:TYR:HB2	1.75	0.49
1:C:546:ASP:N	1:C:549:GLU:OE1	2.45	0.49
1:D:200:ARG:HG3	1:D:200:ARG:NH1	2.26	0.49
1:D:497:ASP:OD2	1:D:499:ASN:HB2	2.11	0.49
1:D:502:GLU:OE2	1:D:502:GLU:HA	2.11	0.49
1:D:628:LEU:HA	1:D:674:THR:O	2.13	0.49
1:F:210:ILE:HA	1:F:213:LYS:NZ	2.27	0.49
1:G:439:PHE:O	1:G:443:GLU:HG2	2.13	0.49
2:H:499:LEU:HG	2:H:543:ILE:CG2	2.42	0.49
2:I:44:VAL:O	2:I:44:VAL:HG13	2.13	0.49
2:J:152:GLY:O	2:J:155:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:255:SER:O	2:J:258:GLU:HG3	2.12	0.49
2:J:469:ASN:OD1	2:J:470:GLU:N	2.45	0.49
1:C:192:TYR:CD1	1:C:192:TYR:C	2.86	0.49
1:F:300:THR:O	1:F:324:PHE:HB3	2.13	0.49
2:J:557:THR:O	2:J:560:GLN:HG3	2.12	0.49
1:A:593:ASP:OD2	1:A:595:ARG:HB2	2.12	0.49
1:C:522:THR:O	1:C:525:GLU:HG3	2.12	0.49
1:D:297:ARG:NH2	1:D:500:LEU:H	2.11	0.49
1:E:226:TRP:CH2	1:E:234:SER:HB3	2.48	0.49
1:F:434:MET:SD	1:F:438:GLN:HB2	2.52	0.49
2:I:292:LEU:HD13	2:I:419:ILE:HB	1.94	0.49
2:I:469:ASN:HD22	2:I:472:LYS:HZ3	1.61	0.49
2:J:153:LYS:HG2	2:J:157:ARG:HE	1.77	0.49
1:C:633:LYS:HA	1:C:636:ARG:CZ	2.43	0.49
1:D:629:LEU:HB3	1:D:631:ILE:HD11	1.95	0.49
1:E:542:TYR:CE2	1:E:543:GLN:NE2	2.81	0.49
1:F:614:GLU:O	1:F:617:ARG:NE	2.46	0.49
2:H:141:THR:O	2:H:145:LEU:HG	2.13	0.49
2:H:525:ILE:HG23	2:H:549:VAL:HG23	1.94	0.49
2:H:607:LYS:HD2	2:H:608:ASN:N	2.28	0.49
1:A:528:LYS:HZ2	1:A:535:GLU:HG2	1.75	0.49
1:A:639:LEU:N	1:A:703:LYS:HZ2	2.11	0.49
1:C:435:ASN:ND2	1:C:438:GLN:HE22	2.11	0.49
1:C:574:ILE:H	1:C:574:ILE:HD12	1.77	0.49
1:D:224:GLU:OE2	1:D:224:GLU:HA	2.12	0.49
1:D:366:TYR:CD2	1:D:378:LEU:HD11	2.47	0.49
1:D:366:TYR:HD2	1:D:378:LEU:HD11	1.78	0.49
1:E:338:LEU:HG	1:E:661:ASP:CB	2.43	0.49
1:E:643:ILE:CG2	1:E:723:LYS:HZ1	2.20	0.49
2:I:271:TRP:NE1	2:I:275:LYS:HE2	2.24	0.49
2:I:561:GLU:O	2:I:564:LEU:HG	2.13	0.49
1:A:200:ARG:HH21	1:B:185:ASP:HB2	1.78	0.48
1:D:482:PRO:HA	1:D:485:GLN:HG2	1.95	0.48
1:D:509:ASN:H	1:D:515:GLU:CD	2.15	0.48
1:E:178:ARG:HB2	1:E:224:GLU:OE2	2.13	0.48
1:E:240:THR:HG22	1:E:242:ARG:NH1	2.28	0.48
1:E:621:ASN:HB3	1:E:628:LEU:HG	1.95	0.48
1:G:231:ASP:N	1:G:231:ASP:OD1	2.41	0.48
2:I:573:ALA:HB1	2:I:607:LYS:HE3	1.95	0.48
1:A:528:LYS:HZ3	1:A:535:GLU:HG2	1.75	0.48
1:B:462:TYR:HE1	1:B:464:PHE:HA	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:TYR:HE2	1:D:378:LEU:HG	1.78	0.48
1:D:385:LEU:HD21	1:D:442:LEU:HD21	1.94	0.48
1:E:271:LEU:HB2	1:E:289:ILE:CG1	2.43	0.48
1:E:597:HIS:H	1:E:606:GLY:C	2.16	0.48
1:F:631:ILE:C	1:F:636:ARG:HH12	2.13	0.48
1:G:647:GLU:HA	1:G:652:LEU:O	2.13	0.48
2:H:54:VAL:O	2:H:58:ALA:N	2.41	0.48
1:B:350:MET:O	1:B:352:LEU:N	2.42	0.48
1:B:528:LYS:HB2	1:B:528:LYS:HE2	1.57	0.48
1:B:724:ILE:O	1:B:726:ILE:HG12	2.13	0.48
1:C:197:LYS:O	1:C:198:ASN:C	2.51	0.48
1:C:240:THR:O	1:D:514:LEU:HB2	2.13	0.48
1:C:244:ASP:O	1:C:246:ASN:N	2.47	0.48
1:D:555:ASP:OD2	1:D:556:GLN:N	2.46	0.48
1:F:198:ASN:HB2	1:F:200:ARG:HH12	1.78	0.48
1:F:227:SER:HA	1:F:235:ASP:OD2	2.13	0.48
1:F:600:ARG:HD2	1:F:601:ASN:N	2.28	0.48
1:G:640:SER:HB3	1:G:703:LYS:HD3	1.94	0.48
2:H:410:LYS:O	2:H:413:LYS:HG3	2.12	0.48
2:I:186:GLN:HA	2:I:190:PHE:HD2	1.79	0.48
2:I:495:ASP:OD1	2:I:496:ASN:N	2.46	0.48
2:J:536:LYS:HE3	2:J:539:GLU:HA	1.95	0.48
1:A:620:ILE:HG13	1:A:630:ASN:ND2	2.28	0.48
1:B:222:SER:H	1:B:228:THR:CG2	2.27	0.48
1:B:441:GLU:HA	1:B:444:LYS:HZ3	1.77	0.48
1:C:298:THR:CG2	1:C:601:ASN:HB2	2.43	0.48
1:C:492:ILE:CG2	1:C:500:LEU:HD12	2.43	0.48
1:E:178:ARG:HA	1:E:178:ARG:NE	2.27	0.48
1:G:198:ASN:HB2	1:G:200:ARG:HH22	1.78	0.48
1:G:563:LYS:O	1:G:566:LEU:HG	2.13	0.48
2:H:293:LEU:HA	2:H:296:LEU:HD12	1.94	0.48
2:H:590:ARG:HG2	2:H:590:ARG:HH11	1.78	0.48
2:I:107:ILE:HD13	2:I:145:LEU:HG	1.94	0.48
2:I:274:ILE:HG13	2:I:275:LYS:N	2.28	0.48
1:B:207:ILE:HB	1:B:210:ILE:HG22	1.95	0.48
1:B:555:ASP:N	1:B:558:THR:OG1	2.47	0.48
1:F:442:LEU:HD23	1:F:446:LYS:NZ	2.27	0.48
2:H:151:ILE:O	2:H:155:LEU:HD23	2.12	0.48
2:H:744:MET:HG3	2:H:745:HIS:CE1	2.48	0.48
2:I:169:LYS:HZ3	2:I:533:GLN:HB2	1.79	0.48
1:A:403:GLN:O	1:A:404:ILE:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LEU:HB2	1:G:240:THR:O	2.14	0.48
1:C:543:GLN:OE1	1:C:543:GLN:N	2.46	0.48
1:C:596:PHE:CD1	1:C:607:ALA:HB2	2.48	0.48
1:C:621:ASN:HB3	1:C:628:LEU:HG	1.96	0.48
1:D:234:SER:N	1:D:237:GLU:OE2	2.44	0.48
1:D:568:GLU:HG2	1:D:569:LEU:CD2	2.41	0.48
1:G:270:ILE:O	1:G:271:LEU:HD22	2.13	0.48
2:I:162:LYS:NZ	2:I:262:GLN:OE1	2.47	0.48
2:I:630:VAL:O	2:I:667:LEU:HA	2.13	0.48
2:I:762:THR:HA	2:I:765:PHE:HE1	1.79	0.48
2:J:211:ASN:O	2:J:214:GLN:HG2	2.13	0.48
1:A:365:ARG:NH2	1:A:418:PRO:HD3	2.28	0.48
1:B:638:ILE:HG22	1:B:638:ILE:O	2.13	0.48
1:C:271:LEU:HB2	1:C:289:ILE:HG23	1.94	0.48
1:C:377:VAL:HG22	1:C:378:LEU:N	2.28	0.48
1:C:626:GLY:HA2	1:C:678:PHE:CE2	2.48	0.48
1:D:466:ASN:HD21	1:D:468:ARG:NH1	2.12	0.48
1:F:515:GLU:O	1:F:518:LYS:HG2	2.12	0.48
1:G:244:ASP:C	1:G:246:ASN:H	2.16	0.48
2:H:300:ILE:HB	2:H:386:TYR:HB3	1.94	0.48
2:I:72:GLU:HA	2:I:75:LYS:NZ	2.29	0.48
2:I:439:GLU:OE1	2:I:501:TRP:CE3	2.66	0.48
2:I:533:GLN:NE2	2:I:544:ARG:HG3	2.28	0.48
1:C:383:LEU:HD12	1:C:384:VAL:H	1.77	0.48
1:D:551:ASP:C	1:D:552:PHE:HD1	2.17	0.48
1:E:721:ILE:CG1	1:E:723:LYS:CG	2.87	0.48
1:F:364:ILE:HG12	1:F:421:LEU:HD21	1.95	0.48
1:G:640:SER:OG	1:G:701:VAL:HG13	2.14	0.48
2:H:118:TYR:CD2	2:H:119:VAL:HG13	2.49	0.48
1:B:492:ILE:HG22	1:B:500:LEU:HD12	1.95	0.48
1:B:579:ASP:OD1	1:B:580:LYS:HG2	2.14	0.48
1:C:387:LYS:HD2	1:C:388:ASN:CB	2.42	0.48
1:D:198:ASN:HD21	1:D:200:ARG:HH22	1.62	0.48
1:D:618:GLU:N	1:D:618:GLU:OE1	2.47	0.48
1:E:491:ILE:CD1	1:E:589:ILE:HB	2.44	0.48
1:G:270:ILE:C	1:G:271:LEU:HD22	2.33	0.48
1:G:533:PHE:CE2	1:G:542:TYR:HB2	2.49	0.48
2:H:252:ILE:O	2:H:255:SER:OG	2.26	0.48
2:H:441:MET:CE	2:H:499:LEU:HD22	2.42	0.48
2:H:491:ARG:HG2	2:H:492:PRO:CD	2.43	0.48
1:A:197:LYS:O	1:A:198:ASN:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:TYR:CD1	1:B:219:TYR:N	2.78	0.48
1:C:447:GLN:C	1:C:448:LEU:HD22	2.35	0.48
1:C:721:ILE:HG21	1:C:723:LYS:CE	2.44	0.48
1:E:447:GLN:O	1:E:448:LEU:HD22	2.13	0.48
1:E:558:THR:O	1:E:562:ILE:HG12	2.14	0.48
1:E:700:ALA:CB	1:E:726:ILE:HG13	2.44	0.48
1:F:494:ASN:OD1	1:F:592:ARG:HA	2.13	0.48
1:G:262:VAL:HG11	1:G:379:PRO:HG2	1.96	0.48
2:H:423:LEU:HD22	2:H:512:GLY:HA3	1.95	0.48
2:H:566:ILE:HG12	2:H:600:TYR:CE1	2.48	0.48
2:I:33:GLU:O	2:I:36:LEU:HG	2.13	0.48
1:A:565:GLN:HA	1:A:568:GLU:OE2	2.14	0.47
1:A:640:SER:HA	1:A:703:LYS:HE3	1.96	0.47
1:B:238:LYS:HE3	1:B:251:ALA:O	2.14	0.47
1:B:255:LEU:HD12	1:B:255:LEU:N	2.29	0.47
1:B:558:THR:HG22	1:B:587:MET:HA	1.94	0.47
1:C:203:LEU:HD12	1:C:203:LEU:HA	1.66	0.47
1:D:266:MET:HB3	1:D:295:THR:HG21	1.95	0.47
1:D:610:SER:HA	1:D:613:LYS:HZ3	1.77	0.47
1:E:533:PHE:CZ	1:E:542:TYR:HB2	2.49	0.47
1:F:635:ILE:C	1:F:637:LYS:H	2.17	0.47
2:H:69:ASP:O	2:H:72:GLU:HG2	2.14	0.47
2:H:163:ILE:O	2:H:163:ILE:HG22	2.14	0.47
2:H:257:GLU:OE1	2:H:436:TYR:HD2	1.97	0.47
2:I:455:VAL:HA	2:I:463:ILE:HD13	1.95	0.47
1:B:332:VAL:HG12	1:B:448:LEU:HB2	1.96	0.47
1:B:403:GLN:O	1:B:404:ILE:HD13	2.15	0.47
1:C:334:ILE:HG22	1:C:446:LYS:HB3	1.95	0.47
1:C:605:VAL:HG22	1:C:704:GLU:HB3	1.96	0.47
1:D:606:GLY:HA3	1:D:704:GLU:OE1	2.14	0.47
1:E:291:LYS:HZ2	1:E:334:ILE:HB	1.78	0.47
1:F:442:LEU:HD23	1:F:446:LYS:HZ2	1.77	0.47
1:F:492:ILE:HD11	1:F:500:LEU:HB3	1.94	0.47
1:F:563:LYS:O	1:F:566:LEU:HG	2.14	0.47
2:H:81:ILE:HG22	2:H:129:LEU:HD21	1.96	0.47
1:A:225:LYS:HD2	1:A:228:THR:HA	1.96	0.47
1:B:496:LYS:HE2	1:B:496:LYS:HA	1.95	0.47
1:B:598:TYR:CD2	1:B:604:ALA:HA	2.49	0.47
1:D:260:PRO:HD3	1:D:477:TRP:CZ3	2.49	0.47
1:D:491:ILE:CD1	1:D:589:ILE:HB	2.45	0.47
1:F:245:LYS:NZ	1:G:512:ASP:OD2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:256:LEU:O	2:J:259:LEU:HG	2.14	0.47
1:A:523:LEU:HD23	1:A:527:LEU:HD13	1.96	0.47
1:B:502:GLU:OE2	1:B:504:ARG:HG2	2.15	0.47
1:B:549:GLU:HB3	1:B:595:ARG:NH1	2.29	0.47
1:C:360:LEU:HD12	1:C:361:ASN:N	2.28	0.47
1:C:476:ASN:N	1:C:476:ASN:OD1	2.47	0.47
1:D:558:THR:HG21	1:D:588:ASN:H	1.80	0.47
1:D:629:LEU:HD23	1:D:631:ILE:HD11	1.96	0.47
1:E:232:PRO:CD	1:E:233:TYR:CE1	2.88	0.47
1:G:212:GLU:HG2	1:G:213:LYS:HD3	1.96	0.47
2:H:163:ILE:HB	2:H:165:GLN:OE1	2.14	0.47
2:H:469:ASN:OD1	2:H:472:LYS:NZ	2.47	0.47
2:H:699:LEU:HD11	2:H:772:PHE:CD2	2.49	0.47
1:B:610:SER:HA	1:B:613:LYS:HZ3	1.79	0.47
1:C:456:TYR:N	1:C:456:TYR:CD1	2.82	0.47
1:C:521:MET:HE3	1:C:583:LEU:HB2	1.96	0.47
1:D:244:ASP:OD1	1:E:483:GLN:NE2	2.46	0.47
1:E:225:LYS:HD2	1:E:225:LYS:HA	1.74	0.47
1:E:231:ASP:HB2	1:E:232:PRO:CD	2.44	0.47
1:F:504:ARG:O	1:F:505:ILE:HD13	2.13	0.47
1:G:560:GLN:OE1	1:G:563:LYS:NZ	2.34	0.47
1:G:584:ASN:O	1:G:587:MET:HE3	2.14	0.47
1:G:629:LEU:O	1:G:674:THR:N	2.47	0.47
1:G:635:ILE:HG23	1:G:636:ARG:HD3	1.95	0.47
2:H:533:GLN:O	2:H:543:ILE:HD12	2.14	0.47
1:A:702:THR:O	1:A:706:THR:HG23	2.15	0.47
1:E:197:LYS:O	1:E:198:ASN:C	2.53	0.47
1:E:227:SER:O	1:E:230:SER:N	2.47	0.47
2:H:114:LEU:HD12	2:H:115:HIS:N	2.29	0.47
2:J:83:ILE:HG13	2:J:131:ILE:O	2.15	0.47
1:A:199:LYS:HG3	1:B:189:VAL:HG23	1.96	0.47
1:A:273:LYS:HA	1:A:358:ALA:HA	1.96	0.47
1:A:554:PHE:HB3	1:A:558:THR:OG1	2.13	0.47
1:B:197:LYS:O	1:B:198:ASN:C	2.53	0.47
1:B:367:VAL:HG12	1:B:410:TYR:CD1	2.50	0.47
1:B:625:GLU:HA	1:B:678:PHE:HE1	1.78	0.47
1:C:253:HIS:O	1:C:256:VAL:HG22	2.15	0.47
1:C:527:LEU:HB3	1:C:533:PHE:CD1	2.43	0.47
1:C:631:ILE:C	1:C:636:ARG:HH12	2.18	0.47
1:D:496:LYS:HZ2	1:D:497:ASP:CG	2.17	0.47
1:D:563:LYS:O	1:D:566:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:565:GLN:HA	1:D:568:GLU:OE1	2.14	0.47
1:D:592:ARG:HB3	1:D:598:TYR:HE2	1.79	0.47
1:D:640:SER:OG	1:D:701:VAL:HG13	2.15	0.47
1:E:264:VAL:HG12	1:E:366:TYR:CE2	2.50	0.47
1:E:533:PHE:CE1	1:E:542:TYR:HB2	2.50	0.47
1:E:545:LYS:N	1:E:545:LYS:HD3	2.30	0.47
1:G:519:PRO:O	1:G:521:MET:HE2	2.14	0.47
2:H:157:ARG:HH11	2:H:214:GLN:HG3	1.76	0.47
2:H:564:LEU:O	2:H:568:GLN:HG3	2.15	0.47
2:H:685:ILE:CG2	2:H:742:ARG:HG2	2.45	0.47
2:I:331:SER:O	2:I:335:LYS:N	2.45	0.47
2:I:469:ASN:HB3	2:I:473:LYS:NZ	2.30	0.47
2:J:67:PRO:O	2:J:70:VAL:HG22	2.14	0.47
1:C:439:PHE:O	1:C:443:GLU:HG2	2.14	0.47
1:D:249:PRO:HA	1:D:252:ARG:HH11	1.78	0.47
1:E:434:MET:SD	1:E:439:PHE:N	2.88	0.47
1:E:507:ALA:C	1:E:518:LYS:HD2	2.35	0.47
1:E:610:SER:HA	1:E:613:LYS:HZ2	1.79	0.47
1:F:506:ALA:C	1:F:518:LYS:HE3	2.35	0.47
1:F:549:GLU:O	1:F:594:LYS:HG2	2.15	0.47
1:G:498:LEU:HB2	1:G:637:LYS:NZ	2.30	0.47
2:H:373:LYS:HA	2:H:376:LEU:HD12	1.97	0.47
2:H:414:ARG:HA	2:H:417:GLN:HE21	1.80	0.47
2:H:514:LEU:HD12	2:H:515:GLU:H	1.80	0.47
2:H:724:ASN:O	2:H:725:LEU:HD22	2.15	0.47
2:I:557:THR:O	2:I:560:GLN:HG3	2.15	0.47
2:J:178:LYS:HA	2:J:186:GLN:OE1	2.14	0.47
2:J:188:LEU:HG	2:J:189:LEU:HD22	1.97	0.47
2:J:542:TYR:CB	2:J:544:ARG:HH22	2.27	0.47
1:A:373:PRO:HB2	1:A:375:TYR:CE1	2.46	0.47
1:A:517:THR:HG23	1:G:199:LYS:O	2.15	0.47
1:A:564:ASN:O	1:A:567:ALA:N	2.46	0.47
1:B:269:ILE:HD12	1:B:269:ILE:N	2.30	0.47
1:B:497:ASP:OD1	1:B:633:LYS:NZ	2.37	0.47
1:C:242:ARG:HD3	1:C:462:TYR:CE2	2.50	0.47
1:C:385:LEU:O	1:C:389:GLN:HB2	2.15	0.47
1:D:353:ASN:H	1:D:356:ASP:CG	2.19	0.47
1:F:255:LEU:HD23	1:F:255:LEU:HA	1.52	0.47
1:F:528:LYS:NZ	1:F:535:GLU:HG2	2.30	0.47
1:G:253:HIS:O	1:G:256:VAL:HG22	2.15	0.47
2:H:81:ILE:HG13	2:H:81:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:235:LEU:HD23	2:J:236:TYR:CZ	2.50	0.47
2:J:461:THR:HG23	2:J:540:LYS:HA	1.97	0.47
1:A:198:ASN:O	1:A:199:LYS:HD2	2.15	0.47
1:A:360:LEU:O	1:A:432:ILE:HG21	2.14	0.47
1:B:442:LEU:O	1:B:446:LYS:HD2	2.15	0.47
1:C:446:LYS:O	1:C:447:GLN:NE2	2.47	0.47
1:D:614:GLU:O	1:D:617:ARG:HG2	2.15	0.47
1:E:535:GLU:OE1	1:E:540:LEU:HA	2.15	0.47
1:F:203:LEU:HD12	1:F:203:LEU:HA	1.54	0.47
1:F:592:ARG:HH11	1:F:592:ARG:HG3	1.80	0.47
1:F:628:LEU:HA	1:F:674:THR:O	2.15	0.47
1:G:468:ARG:NH2	1:G:470:ARG:HE	2.12	0.47
2:H:722:GLY:HA2	2:H:736:PHE:CE1	2.50	0.47
1:C:188:GLU:HG3	1:C:221:SER:OG	2.15	0.46
1:G:234:SER:O	1:G:237:GLU:HG2	2.15	0.46
1:G:626:GLY:HA3	1:G:676:ILE:O	2.15	0.46
2:H:100:ASP:O	2:H:102:LYS:N	2.48	0.46
2:H:163:ILE:HB	2:H:165:GLN:HE22	1.81	0.46
1:B:498:LEU:HA	1:B:498:LEU:HD23	1.76	0.46
1:B:628:LEU:O	1:B:628:LEU:HD12	2.15	0.46
1:C:297:ARG:NH1	1:C:298:THR:O	2.48	0.46
1:C:592:ARG:CZ	1:C:598:TYR:CD2	2.99	0.46
1:D:245:LYS:HE3	1:D:245:LYS:HB2	1.67	0.46
1:D:442:LEU:O	1:D:446:LYS:HD2	2.14	0.46
1:D:446:LYS:HA	1:D:446:LYS:HE3	1.97	0.46
1:F:190:GLU:C	1:F:220:LYS:HZ2	2.19	0.46
1:F:198:ASN:CB	1:F:200:ARG:HH12	2.28	0.46
1:G:600:ARG:NH1	1:G:601:ASN:HB3	2.30	0.46
2:H:474:ASN:HA	2:H:476:LYS:NZ	2.31	0.46
2:H:501:TRP:HB3	2:H:503:ILE:HD11	1.98	0.46
2:I:113:LEU:HD23	2:I:115:HIS:HE2	1.80	0.46
1:A:270:ILE:CG2	1:A:361:ASN:HB3	2.45	0.46
1:C:486:GLU:HA	1:C:586:LYS:HZ3	1.79	0.46
1:E:415:ASN:C	1:E:416:LEU:HD12	2.36	0.46
1:E:698:VAL:HB	1:E:727:PHE:HB3	1.97	0.46
1:E:700:ALA:HB3	1:E:726:ILE:HG13	1.96	0.46
1:F:206:TRP:CH2	1:F:218:LYS:HB2	2.49	0.46
1:F:214:LYS:HE2	1:F:214:LYS:HA	1.96	0.46
1:F:354:THR:HA	1:F:436:TYR:CD2	2.50	0.46
1:G:643:ILE:HD11	1:G:701:VAL:HB	1.98	0.46
2:H:83:ILE:HG13	2:H:83:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:140:ASN:ND2	2:H:143:LYS:HB2	2.30	0.46
2:H:578:LYS:C	2:H:579:TYR:CD1	2.85	0.46
2:H:621:TYR:CE1	2:H:664:ARG:CZ	2.98	0.46
2:I:134:SER:HB2	2:I:137:TYR:CE2	2.50	0.46
2:J:657:GLY:HA3	2:J:667:LEU:O	2.16	0.46
1:C:545:LYS:HD3	1:C:545:LYS:N	2.30	0.46
1:C:640:SER:OG	1:C:701:VAL:HG13	2.15	0.46
1:D:244:ASP:C	1:D:246:ASN:H	2.19	0.46
1:D:543:GLN:HG2	1:D:545:LYS:NZ	2.31	0.46
1:E:176:PRO:CB	1:E:178:ARG:HH12	2.15	0.46
1:E:377:VAL:C	1:E:378:LEU:HD12	2.36	0.46
1:E:543:GLN:HG2	1:E:545:LYS:NZ	2.31	0.46
1:F:258:ALA:HA	1:F:371:THR:OG1	2.15	0.46
1:G:635:ILE:CG2	1:G:636:ARG:HD3	2.45	0.46
2:H:390:GLN:HA	2:H:393:GLN:HE22	1.80	0.46
2:H:474:ASN:HA	2:H:476:LYS:HZ2	1.81	0.46
2:J:428:GLY:N	2:J:507:PRO:O	2.42	0.46
1:A:198:ASN:OD1	1:A:198:ASN:N	2.48	0.46
1:B:291:LYS:HZ2	1:B:334:ILE:HB	1.81	0.46
1:B:493:PHE:CZ	1:B:495:GLY:HA3	2.50	0.46
1:C:256:VAL:HG12	1:C:505:ILE:CD1	2.45	0.46
1:C:626:GLY:HA2	1:C:678:PHE:HE2	1.80	0.46
1:E:245:LYS:HE2	1:E:245:LYS:HA	1.97	0.46
1:E:269:ILE:HG22	1:E:362:ALA:HB2	1.97	0.46
1:E:527:LEU:HD23	1:E:527:LEU:HA	1.53	0.46
1:F:568:GLU:HG2	1:F:569:LEU:CD2	2.46	0.46
1:G:459:ILE:HG13	1:G:477:TRP:CD1	2.51	0.46
1:G:476:ASN:HB3	1:G:479:GLU:OE2	2.16	0.46
2:H:511:ALA:HB2	2:H:521:LEU:HD13	1.97	0.46
2:H:679:ASN:HD21	2:H:682:GLU:HG3	1.80	0.46
1:A:627:LEU:H	1:A:676:ILE:CG2	2.27	0.46
1:B:291:LYS:NZ	1:B:293:THR:HG22	2.31	0.46
1:B:551:ASP:OD1	1:B:592:ARG:N	2.38	0.46
1:D:291:LYS:HE2	1:D:335:ASP:HB3	1.97	0.46
1:D:403:GLN:O	1:D:404:ILE:HD13	2.16	0.46
1:F:377:VAL:HG12	1:F:378:LEU:N	2.31	0.46
1:G:384:VAL:HG13	1:G:449:ARG:HB2	1.98	0.46
2:H:514:LEU:HD12	2:H:515:GLU:N	2.30	0.46
1:B:449:ARG:O	1:B:450:LEU:HD23	2.15	0.46
1:C:410:TYR:CG	1:C:414:LYS:HE3	2.51	0.46
1:D:271:LEU:HB2	1:D:289:ILE:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:VAL:HG21	1:E:483:GLN:HG3	1.98	0.46
1:D:705:ASN:HD21	1:D:722:LYS:CB	2.28	0.46
1:E:289:ILE:HG13	1:E:289:ILE:O	2.16	0.46
1:F:410:TYR:CE2	1:F:414:LYS:HE2	2.50	0.46
1:G:498:LEU:HB2	1:G:637:LYS:HZ1	1.79	0.46
2:H:244:MET:HE3	2:H:248:ASN:HB3	1.97	0.46
2:H:504:GLN:NE2	2:H:505:LEU:HD23	2.31	0.46
2:H:739:GLU:HA	2:H:742:ARG:CZ	2.46	0.46
2:I:140:ASN:ND2	2:I:142:GLU:OE1	2.49	0.46
2:J:91:HIS:HD2	2:J:93:SER:HB2	1.81	0.46
1:A:200:ARG:HH12	1:B:189:VAL:HG11	1.80	0.46
1:B:197:LYS:O	1:B:200:ARG:N	2.46	0.46
1:D:632:ASP:O	1:D:635:ILE:HG22	2.16	0.46
1:D:710:PRO:HB2	1:D:714:GLY:HA2	1.98	0.46
1:E:358:ALA:HB3	1:E:434:MET:CE	2.46	0.46
2:H:615:ILE:O	2:H:619:THR:HG23	2.16	0.46
2:I:168:GLN:HA	2:I:171:LEU:HB3	1.98	0.46
2:I:468:PHE:HA	2:I:471:PHE:CD1	2.45	0.46
1:D:297:ARG:H	1:D:297:ARG:HG3	1.49	0.46
1:D:386:GLY:HA3	1:D:389:GLN:NE2	2.31	0.46
1:D:493:PHE:O	1:D:500:LEU:HD13	2.16	0.46
1:F:234:SER:O	1:F:237:GLU:HG2	2.16	0.46
2:H:620:ASN:HA	2:H:623:VAL:HG22	1.98	0.46
2:I:107:ILE:HA	2:I:219:LYS:NZ	2.30	0.46
1:A:203:LEU:HG	1:A:204:SER:N	2.30	0.46
1:C:198:ASN:HD21	2:I:139:GLU:CD	2.17	0.46
1:D:255:LEU:HD23	1:D:255:LEU:HA	1.52	0.46
1:E:197:LYS:O	1:E:199:LYS:N	2.49	0.46
1:F:381:THR:HG23	1:F:452:THR:HG22	1.99	0.46
1:G:608:ASP:OD1	1:G:609:GLU:N	2.49	0.46
1:G:618:GLU:O	1:G:618:GLU:HG2	2.16	0.46
2:I:564:LEU:O	2:I:568:GLN:N	2.31	0.46
1:A:496:LYS:HE2	1:A:496:LYS:HA	1.98	0.45
1:A:500:LEU:HD23	1:A:500:LEU:HA	1.76	0.45
1:A:605:VAL:HG22	1:A:704:GLU:HB3	1.97	0.45
1:D:558:THR:HG22	1:D:587:MET:HA	1.98	0.45
1:E:334:ILE:HD11	1:E:446:LYS:HE3	1.97	0.45
1:F:244:ASP:OD2	1:F:246:ASN:HB3	2.15	0.45
1:G:592:ARG:HH22	1:G:602:ASN:C	2.19	0.45
2:H:160:LEU:HD22	2:H:165:GLN:HG2	1.98	0.45
2:H:502:ARG:CB	2:H:544:ARG:HH22	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:248:ASN:OD1	2:I:249:GLU:N	2.49	0.45
1:C:216:LEU:HA	1:C:216:LEU:HD23	1.73	0.45
1:D:326:ASN:HD22	1:D:485:GLN:HB2	1.81	0.45
1:D:386:GLY:HA3	1:D:389:GLN:HE22	1.81	0.45
1:D:476:ASN:HB2	1:D:479:GLU:OE2	2.16	0.45
1:F:332:VAL:CG1	1:F:448:LEU:HB2	2.47	0.45
1:G:340:LEU:HB2	1:G:343:GLU:HB3	1.98	0.45
1:G:668:LEU:HA	1:G:674:THR:HA	1.97	0.45
2:H:681:SER:O	2:H:685:ILE:HG12	2.16	0.45
2:J:191:THR:HG22	2:J:194:LEU:HG	1.99	0.45
1:A:523:LEU:HA	1:A:583:LEU:HD11	1.98	0.45
1:B:198:ASN:N	1:B:198:ASN:OD1	2.48	0.45
1:B:705:ASN:CG	1:B:722:LYS:HB3	2.35	0.45
1:C:263:HIS:NE2	1:C:367:VAL:HB	2.31	0.45
1:D:387:LYS:HE2	1:D:387:LYS:HA	1.98	0.45
1:D:615:ALA:O	1:D:631:ILE:HD12	2.16	0.45
1:E:186:SER:O	1:E:190:GLU:HG2	2.16	0.45
1:F:291:LYS:NZ	1:F:335:ASP:N	2.62	0.45
1:F:535:GLU:HB3	1:F:538:GLY:HA2	1.98	0.45
2:H:533:GLN:OE1	2:H:533:GLN:N	2.49	0.45
2:H:560:GLN:HG2	2:H:561:GLU:N	2.32	0.45
2:H:594:ASN:O	2:H:594:ASN:ND2	2.48	0.45
2:I:563:GLN:O	2:I:566:ILE:HG22	2.16	0.45
1:C:298:THR:HG22	1:C:299:HIS:N	2.31	0.45
1:C:527:LEU:HD12	1:C:533:PHE:HE1	1.81	0.45
1:C:558:THR:HG22	1:C:587:MET:HA	1.97	0.45
1:D:216:LEU:HD12	1:D:216:LEU:N	2.31	0.45
1:F:206:TRP:CD1	1:F:218:LYS:NZ	2.80	0.45
1:F:403:GLN:O	1:F:404:ILE:HD13	2.16	0.45
2:H:113:LEU:HD22	2:H:115:HIS:HE1	1.81	0.45
2:H:122:LYS:HB3	2:H:128:VAL:H	1.81	0.45
2:H:544:ARG:HH11	2:H:544:ARG:HG3	1.80	0.45
2:I:208:GLN:NE2	2:I:209:ASN:OD1	2.49	0.45
2:I:274:ILE:HD12	2:I:488:ILE:HD13	1.99	0.45
1:A:209:ASN:HA	1:A:212:GLU:OE1	2.16	0.45
1:A:435:ASN:CG	1:A:438:GLN:HG2	2.37	0.45
1:B:238:LYS:HE2	1:B:252:ARG:C	2.36	0.45
1:B:491:ILE:CD1	1:B:589:ILE:HB	2.46	0.45
1:E:366:TYR:HE1	1:E:378:LEU:HD23	1.80	0.45
2:H:578:LYS:HB3	2:H:579:TYR:CD1	2.52	0.45
2:I:62:LEU:HD12	2:I:137:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:115:HIS:ND1	2:I:116:GLU:N	2.64	0.45
2:I:466:GLY:O	2:I:470:GLU:HG2	2.17	0.45
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.54	0.45
1:A:606:GLY:HA3	1:A:704:GLU:OE1	2.17	0.45
1:B:640:SER:OG	1:B:701:VAL:HG13	2.17	0.45
1:D:471:VAL:HG12	1:E:479:GLU:CD	2.37	0.45
1:D:500:LEU:HD13	1:D:500:LEU:HA	1.53	0.45
1:F:272:SER:HB3	1:F:288:THR:HG22	1.98	0.45
1:F:441:GLU:HA	1:F:444:LYS:NZ	2.31	0.45
1:F:479:GLU:OE1	1:F:479:GLU:N	2.49	0.45
2:H:190:PHE:HB3	2:H:216:VAL:HG12	1.98	0.45
2:H:579:TYR:C	2:H:581:LYS:HZ1	2.20	0.45
2:H:622:LEU:HD23	2:H:622:LEU:HA	1.73	0.45
2:I:150:GLU:OE1	2:I:153:LYS:HD2	2.17	0.45
2:J:155:LEU:HD12	2:J:156:SER:N	2.31	0.45
1:A:291:LYS:HB2	1:A:334:ILE:HD11	1.98	0.45
1:A:330:SER:OG	1:A:331:THR:N	2.49	0.45
1:B:263:HIS:ND1	1:B:297:ARG:HG3	2.31	0.45
1:C:195:ASP:O	1:C:195:ASP:OD1	2.34	0.45
1:D:271:LEU:N	1:D:289:ILE:O	2.49	0.45
1:D:384:VAL:O	1:D:449:ARG:HG2	2.16	0.45
1:E:490:ARG:HH21	1:E:588:ASN:ND2	2.15	0.45
1:F:183:ILE:CD1	1:F:236:PHE:HD1	2.28	0.45
1:G:376:ASN:OD1	1:G:377:VAL:N	2.48	0.45
2:H:62:LEU:HD11	2:H:137:TYR:CB	2.47	0.45
2:H:375:PHE:HA	2:H:378:LYS:HE2	1.97	0.45
2:H:513:TYR:HD1	2:H:519:LEU:HD22	1.82	0.45
2:H:630:VAL:HG12	2:H:632:THR:HG23	1.98	0.45
2:H:735:GLU:O	2:H:739:GLU:OE1	2.34	0.45
2:I:247:PHE:CZ	2:I:252:ILE:HD11	2.52	0.45
1:B:518:LYS:HB2	1:B:519:PRO:HD2	1.99	0.45
1:B:542:TYR:O	1:B:545:LYS:HE2	2.17	0.45
1:C:294:SER:O	1:C:333:ALA:N	2.34	0.45
1:D:528:LYS:NZ	1:D:534:ASN:HA	2.32	0.45
1:E:335:ASP:OD1	1:E:336:HIS:N	2.50	0.45
1:E:634:ASP:O	1:E:637:LYS:HG2	2.17	0.45
1:G:584:ASN:N	1:G:587:MET:HE3	2.30	0.45
2:H:566:ILE:HG12	2:H:600:TYR:CZ	2.52	0.45
1:A:406:ALA:O	1:A:409:ASN:HB2	2.17	0.45
1:A:665:ILE:O	1:A:676:ILE:HD12	2.17	0.45
1:B:227:SER:O	1:B:230:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ALA:HA	1:B:371:THR:OG1	2.16	0.45
1:C:331:THR:HG22	1:C:449:ARG:NE	2.31	0.45
1:C:627:LEU:H	1:C:676:ILE:CG2	2.27	0.45
1:E:206:TRP:CH2	1:E:218:LYS:HB2	2.52	0.45
1:E:524:LYS:HG3	1:E:578:LEU:HG	1.98	0.45
1:E:568:GLU:HG2	1:E:569:LEU:CD2	2.46	0.45
1:G:434:MET:SD	1:G:438:GLN:HB2	2.56	0.45
2:H:530:LYS:HZ1	2:H:547:ALA:C	2.21	0.45
2:I:255:SER:O	2:I:259:LEU:HG	2.16	0.45
2:J:239:GLU:HG2	2:J:240:ALA:N	2.32	0.45
2:J:485:ILE:HA	2:J:519:LEU:O	2.17	0.45
1:B:233:TYR:HA	1:B:237:GLU:OE2	2.17	0.45
1:B:269:ILE:CG2	1:B:270:ILE:N	2.80	0.45
1:C:176:PRO:HB3	1:C:178:ARG:HH12	1.82	0.45
1:C:197:LYS:O	1:C:199:LYS:N	2.50	0.45
1:D:363:ASN:HD21	1:D:418:PRO:HG2	1.78	0.45
1:D:624:THR:O	1:D:687:LEU:HD13	2.17	0.45
1:E:299:HIS:O	1:E:602:ASN:HB2	2.17	0.45
1:F:527:LEU:HA	1:F:527:LEU:HD23	1.70	0.45
1:G:365:ARG:NH1	1:G:416:LEU:O	2.37	0.45
2:H:336:GLU:HA	2:H:339:LYS:HE2	1.99	0.45
2:H:414:ARG:O	2:H:417:GLN:NE2	2.50	0.45
2:H:548:LYS:NZ	2:H:549:VAL:HG12	2.32	0.45
2:I:186:GLN:HA	2:I:190:PHE:CD2	2.53	0.45
2:I:587:VAL:HA	2:I:632:THR:HA	1.99	0.45
2:J:478:SER:C	2:J:590:ARG:HH21	2.21	0.45
1:A:471:VAL:HG13	1:A:471:VAL:O	2.17	0.44
1:B:678:PHE:HZ	1:B:686:PRO:HA	1.82	0.44
1:C:383:LEU:HD12	1:C:384:VAL:N	2.32	0.44
1:C:528:LYS:HE2	1:C:528:LYS:HB2	1.52	0.44
1:D:197:LYS:HZ2	1:D:200:ARG:NH2	2.15	0.44
1:D:459:ILE:HD11	1:D:477:TRP:N	2.32	0.44
1:E:293:THR:HG22	1:E:334:ILE:HG22	1.99	0.44
1:E:445:THR:O	1:E:447:GLN:OE1	2.35	0.44
1:F:609:GLU:OE1	1:F:609:GLU:N	2.39	0.44
1:G:542:TYR:CE2	1:G:543:GLN:NE2	2.85	0.44
2:I:120:TYR:CG	2:I:121:ALA:N	2.85	0.44
2:J:194:LEU:C	2:J:196:GLU:H	2.21	0.44
1:A:183:ILE:HD12	1:A:183:ILE:N	2.32	0.44
1:B:197:LYS:O	1:B:199:LYS:N	2.51	0.44
1:B:332:VAL:CG1	1:B:448:LEU:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:THR:HG22	1:C:449:ARG:CD	2.46	0.44
1:C:367:VAL:HG22	1:C:410:TYR:CE1	2.52	0.44
1:C:490:ARG:O	1:C:491:ILE:HD13	2.17	0.44
1:C:699:TYR:CD1	1:C:725:LEU:HA	2.52	0.44
1:D:492:ILE:HD12	1:D:492:ILE:HG23	1.80	0.44
1:F:558:THR:O	1:F:562:ILE:HG12	2.16	0.44
2:H:73:MET:O	2:H:77:ILE:HG12	2.17	0.44
2:H:484:MET:N	2:H:484:MET:SD	2.90	0.44
2:J:117:HIS:NE2	2:J:119:VAL:O	2.50	0.44
2:J:281:TRP:CH2	2:J:423:LEU:HA	2.52	0.44
1:A:229:ALA:O	1:A:230:SER:HB2	2.18	0.44
1:D:378:LEU:HD12	1:D:379:PRO:CD	2.47	0.44
1:D:533:PHE:N	1:D:533:PHE:CD2	2.86	0.44
1:D:591:ILE:O	1:D:591:ILE:HG13	2.17	0.44
1:E:242:ARG:HG2	1:E:462:TYR:CZ	2.52	0.44
1:F:435:ASN:OD1	1:F:438:GLN:HG3	2.17	0.44
1:F:480:VAL:HG12	1:F:484:ILE:CD1	2.45	0.44
1:G:627:LEU:HB3	1:G:629:LEU:CD2	2.48	0.44
2:H:438:TYR:HE1	2:H:544:ARG:NH2	2.15	0.44
2:H:676:GLU:OE1	2:H:676:GLU:N	2.50	0.44
1:A:470:ARG:HD3	1:A:471:VAL:N	2.31	0.44
1:B:643:ILE:HG12	1:B:723:LYS:HE2	1.99	0.44
1:C:200:ARG:HH22	1:D:189:VAL:CG1	2.27	0.44
1:C:415:ASN:OD1	1:C:416:LEU:HD23	2.18	0.44
1:D:354:THR:HA	1:D:436:TYR:CD1	2.52	0.44
1:E:213:LYS:HE2	1:E:214:LYS:HZ1	1.81	0.44
1:E:335:ASP:OD1	1:E:337:SER:N	2.44	0.44
1:F:378:LEU:HD12	1:F:379:PRO:HD3	2.00	0.44
1:G:192:TYR:CD2	1:G:192:TYR:N	2.85	0.44
1:G:259:TYR:CE1	1:G:261:ILE:HD11	2.52	0.44
2:H:224:TYR:CE2	2:H:248:ASN:ND2	2.86	0.44
2:I:281:TRP:CH2	2:I:423:LEU:HA	2.45	0.44
2:I:438:TYR:HD2	2:I:490:GLU:N	2.15	0.44
2:I:615:ILE:HA	2:I:618:VAL:HG22	1.99	0.44
2:J:243:TYR:O	2:J:247:PHE:HD2	2.01	0.44
1:A:245:LYS:HB3	1:B:486:GLU:OE1	2.18	0.44
1:A:432:ILE:HG23	1:A:432:ILE:O	2.17	0.44
1:A:470:ARG:HA	1:A:470:ARG:HE	1.82	0.44
1:B:490:ARG:HH11	1:B:502:GLU:HG3	1.80	0.44
1:B:678:PHE:CZ	1:B:686:PRO:HA	2.53	0.44
1:D:245:LYS:HD3	1:D:245:LYS:HA	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:592:ARG:HB3	1:D:598:TYR:CE2	2.52	0.44
1:D:597:HIS:N	1:D:606:GLY:O	2.51	0.44
2:H:636:LEU:HD23	2:H:636:LEU:HA	1.85	0.44
2:J:122:LYS:HE3	2:J:128:VAL:HB	1.99	0.44
2:J:136:ASP:HA	2:J:139:GLU:OE1	2.18	0.44
1:A:354:THR:HA	1:A:436:TYR:CD2	2.52	0.44
1:A:699:TYR:CD1	1:A:725:LEU:HA	2.53	0.44
1:B:491:ILE:HD13	1:B:589:ILE:HB	2.00	0.44
1:B:500:LEU:HA	1:B:500:LEU:HD13	1.68	0.44
1:C:178:ARG:NE	1:C:178:ARG:HA	2.32	0.44
1:D:203:LEU:HD12	1:D:203:LEU:HA	1.64	0.44
1:D:609:GLU:OE1	1:D:609:GLU:N	2.44	0.44
1:D:631:ILE:O	1:D:636:ARG:NH1	2.47	0.44
1:E:244:ASP:OD1	1:F:483:GLN:NE2	2.50	0.44
1:E:300:THR:HG22	1:E:601:ASN:HA	1.99	0.44
1:F:596:PHE:CD1	1:F:607:ALA:HB2	2.53	0.44
1:F:722:LYS:HZ1	1:F:724:ILE:HD13	1.83	0.44
2:H:210:SER:HA	2:H:213:VAL:HG12	1.97	0.44
2:H:413:LYS:O	2:H:417:GLN:HG3	2.18	0.44
2:H:686:HIS:CE1	2:H:690:HIS:HE1	2.35	0.44
2:I:107:ILE:HG12	2:I:219:LYS:HZ3	1.83	0.44
2:I:162:LYS:HG3	2:I:163:ILE:HG12	1.99	0.44
2:I:437:LEU:HG	2:I:488:ILE:HA	2.00	0.44
2:J:115:HIS:NE2	2:J:116:GLU:HG3	2.32	0.44
1:A:353:ASN:HB3	1:A:356:ASP:CG	2.38	0.44
1:B:203:LEU:HA	1:B:203:LEU:HD13	1.80	0.44
1:B:266:MET:HA	1:B:364:ILE:HA	2.00	0.44
1:B:490:ARG:HD3	1:B:492:ILE:HD11	2.00	0.44
1:C:267:GLU:H	1:C:267:GLU:CD	2.17	0.44
1:C:299:HIS:O	1:C:602:ASN:HB2	2.17	0.44
1:D:700:ALA:O	1:D:724:ILE:HG22	2.18	0.44
1:E:524:LYS:HZ2	1:E:579:ASP:H	1.65	0.44
1:E:718:THR:O	1:E:721:ILE:HG12	2.18	0.44
1:F:338:LEU:HG	1:F:661:ASP:CB	2.48	0.44
1:G:200:ARG:NH1	1:G:200:ARG:HG3	2.33	0.44
1:G:471:VAL:HG13	1:G:471:VAL:O	2.18	0.44
2:H:446:LEU:HA	2:H:446:LEU:HD13	1.68	0.44
2:H:679:ASN:OD1	2:H:681:SER:N	2.51	0.44
2:I:36:LEU:HD12	2:I:37:LYS:N	2.32	0.44
2:I:235:LEU:HD12	2:I:235:LEU:HA	1.60	0.44
1:A:558:THR:O	1:A:562:ILE:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:VAL:O	1:A:616:HIS:CD2	2.70	0.44
1:B:377:VAL:HG12	1:B:378:LEU:N	2.33	0.44
1:B:476:ASN:O	1:B:479:GLU:CD	2.56	0.44
1:C:200:ARG:HB3	1:D:178:ARG:HH22	1.82	0.44
1:F:253:HIS:CE1	1:F:254:PRO:HD2	2.53	0.44
1:F:447:GLN:C	1:F:448:LEU:HD22	2.38	0.44
1:F:550:PHE:CD2	1:F:593:ASP:HA	2.52	0.44
1:G:633:LYS:HD2	1:G:636:ARG:HH21	1.83	0.44
2:H:172:ASP:O	2:H:176:THR:HG23	2.18	0.44
2:H:300:ILE:HD13	2:H:386:TYR:CD2	2.49	0.44
2:H:611:GLN:HG3	2:H:613:ASP:OD1	2.18	0.44
2:I:162:LYS:NZ	2:I:163:ILE:HD11	2.33	0.44
2:I:179:ASN:ND2	2:I:179:ASN:O	2.51	0.44
1:B:295:THR:HG22	1:B:332:VAL:CG2	2.47	0.44
1:B:468:ARG:HG2	1:B:468:ARG:HH11	1.83	0.44
1:B:528:LYS:NZ	1:B:535:GLU:HG2	2.33	0.44
1:B:559:SER:O	1:B:563:LYS:HG3	2.17	0.44
1:D:240:THR:O	1:E:514:LEU:HB2	2.18	0.44
1:D:492:ILE:CG2	1:D:500:LEU:HD12	2.48	0.44
1:E:493:PHE:HD1	1:E:591:ILE:HB	1.80	0.44
1:G:184:PRO:O	1:G:188:GLU:HG3	2.18	0.44
1:G:612:VAL:HG12	1:G:616:HIS:HE1	1.83	0.44
2:H:178:LYS:HD2	2:H:201:PHE:CZ	2.53	0.44
2:H:486:VAL:HG23	2:H:519:LEU:HB2	1.98	0.44
2:H:582:LEU:HD12	2:H:583:ILE:HD12	1.99	0.44
2:H:617:LYS:HE3	2:H:695:TYR:HE2	1.82	0.44
2:I:91:HIS:HB3	2:I:94:LEU:HG	1.99	0.44
1:A:224:GLU:OE1	1:A:224:GLU:N	2.51	0.43
1:A:332:VAL:HG12	1:A:448:LEU:HB2	2.00	0.43
1:A:505:ILE:N	1:A:505:ILE:HD12	2.33	0.43
1:B:508:VAL:HG23	1:B:516:THR:HA	2.00	0.43
1:C:406:ALA:O	1:C:409:ASN:HB2	2.18	0.43
1:C:449:ARG:C	1:C:450:LEU:HD12	2.38	0.43
1:C:455:VAL:HG13	1:C:455:VAL:O	2.18	0.43
1:F:666:SER:OG	1:F:676:ILE:HG12	2.17	0.43
1:G:295:THR:HA	1:G:332:VAL:HA	2.00	0.43
2:H:438:TYR:HA	2:H:501:TRP:O	2.18	0.43
2:H:680:ASP:OD1	2:H:680:ASP:N	2.49	0.43
2:I:264:MET:N	2:I:264:MET:SD	2.91	0.43
1:B:196:VAL:HG11	1:C:516:THR:HG21	2.01	0.43
1:B:627:LEU:HB2	1:B:676:ILE:HG22	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:596:PHE:CE1	1:C:638:ILE:HD13	2.54	0.43
1:D:454:GLN:HA	1:D:456:TYR:CZ	2.53	0.43
1:E:361:ASN:ND2	1:E:422:ASN:HB3	2.33	0.43
1:F:297:ARG:HH22	1:F:328:ASN:CG	2.21	0.43
1:F:421:LEU:HA	1:F:421:LEU:HD23	1.63	0.43
2:H:157:ARG:HA	2:H:214:GLN:NE2	2.33	0.43
2:H:442:ASN:HD21	2:H:444:ASN:HB2	1.83	0.43
2:H:462:LYS:HA	2:H:541:GLU:CD	2.38	0.43
2:H:565:ASN:O	2:H:568:GLN:NE2	2.50	0.43
2:I:188:LEU:O	2:I:188:LEU:HG	2.18	0.43
2:J:235:LEU:HA	2:J:235:LEU:HD12	1.75	0.43
1:A:552:PHE:HB3	1:A:554:PHE:HZ	1.82	0.43
1:A:578:LEU:HA	1:A:578:LEU:HD12	1.60	0.43
1:B:391:LEU:HB3	1:B:432:ILE:CD1	2.42	0.43
1:B:609:GLU:OE1	1:B:609:GLU:N	2.46	0.43
1:D:597:HIS:H	1:D:607:ALA:HA	1.83	0.43
1:E:291:LYS:HZ3	1:E:293:THR:HA	1.83	0.43
1:E:404:ILE:HD11	1:F:478:SER:O	2.19	0.43
1:F:565:GLN:HA	1:F:568:GLU:OE2	2.18	0.43
1:F:620:ILE:HB	1:F:628:LEU:O	2.18	0.43
1:G:233:TYR:HB2	1:G:238:LYS:CE	2.48	0.43
1:G:449:ARG:HG3	1:G:449:ARG:HH11	1.84	0.43
2:H:107:ILE:H	2:H:107:ILE:HD12	1.83	0.43
2:H:190:PHE:HD1	2:H:194:LEU:HB2	1.82	0.43
2:H:386:TYR:CE1	2:H:412:TYR:CE1	3.06	0.43
2:H:610:ILE:HB	2:H:615:ILE:HD11	2.01	0.43
2:H:744:MET:SD	2:H:766:ILE:HG12	2.58	0.43
2:I:104:ILE:O	2:I:111:ASP:HA	2.19	0.43
2:I:113:LEU:HD12	2:I:113:LEU:HA	1.59	0.43
2:I:461:THR:HG1	2:I:462:LYS:HZ3	1.66	0.43
2:J:57:GLU:O	2:J:60:GLU:HG3	2.18	0.43
1:B:592:ARG:NE	1:B:598:TYR:CD1	2.86	0.43
1:C:300:THR:HG22	1:C:601:ASN:HA	1.99	0.43
1:D:350:MET:O	1:D:352:LEU:N	2.48	0.43
1:D:368:ASN:HB2	1:D:405:LEU:HD21	2.01	0.43
1:D:610:SER:O	1:D:613:LYS:HG2	2.18	0.43
1:E:200:ARG:HH21	2:J:139:GLU:HB3	1.84	0.43
1:F:528:LYS:HE2	1:F:528:LYS:HB2	1.60	0.43
1:G:643:ILE:HD13	1:G:723:LYS:HG2	2.00	0.43
1:G:718:THR:CB	1:G:723:LYS:HZ3	2.29	0.43
2:H:77:ILE:HG13	2:H:159:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:84:VAL:HG22	2:H:85:ASP:H	1.82	0.43
2:H:315:GLU:O	2:H:319:LEU:N	2.42	0.43
2:H:407:ASP:N	2:H:407:ASP:OD1	2.50	0.43
2:H:739:GLU:HA	2:H:742:ARG:NH2	2.33	0.43
2:I:441:MET:HE3	2:I:499:LEU:HD22	2.01	0.43
1:C:244:ASP:C	1:C:246:ASN:N	2.71	0.43
1:D:270:ILE:C	1:D:271:LEU:HD22	2.39	0.43
1:F:596:PHE:HD1	1:F:607:ALA:HB2	1.83	0.43
1:G:256:VAL:HG23	1:G:256:VAL:O	2.18	0.43
1:B:226:TRP:CE2	1:B:234:SER:HB2	2.54	0.43
1:B:471:VAL:HG13	1:B:471:VAL:O	2.19	0.43
1:B:505:ILE:HD13	1:B:505:ILE:HA	1.73	0.43
1:B:697:ASN:HB2	1:B:699:TYR:HE1	1.84	0.43
1:C:255:LEU:HA	1:C:255:LEU:HD23	1.66	0.43
1:C:326:ASN:ND2	1:C:485:GLN:OE1	2.51	0.43
1:C:500:LEU:N	1:C:500:LEU:CD2	2.82	0.43
1:D:440:LEU:HD12	1:D:440:LEU:N	2.33	0.43
1:D:598:TYR:CD1	1:D:604:ALA:HA	2.54	0.43
1:E:200:ARG:NH2	2:J:139:GLU:HB3	2.34	0.43
1:E:377:VAL:HG12	1:E:378:LEU:N	2.34	0.43
1:E:498:LEU:HA	1:E:498:LEU:HD13	1.81	0.43
1:F:245:LYS:HD3	1:F:245:LYS:HA	1.80	0.43
1:F:583:LEU:HD12	1:F:587:MET:HE3	2.01	0.43
1:G:244:ASP:O	1:G:246:ASN:N	2.52	0.43
2:I:134:SER:HB3	2:I:136:ASP:OD1	2.19	0.43
2:I:602:ILE:O	2:I:605:GLU:HG2	2.18	0.43
2:J:259:LEU:HD12	2:J:260:LYS:N	2.34	0.43
2:J:718:PHE:HA	2:J:722:GLY:HA3	2.01	0.43
1:A:197:LYS:O	1:A:199:LYS:N	2.52	0.43
1:A:687:LEU:HD12	1:A:687:LEU:O	2.18	0.43
1:B:498:LEU:HB2	1:B:637:LYS:NZ	2.26	0.43
1:B:557:GLN:NE2	1:B:561:ASN:OD1	2.46	0.43
1:C:500:LEU:HA	1:C:500:LEU:HD13	1.53	0.43
1:D:640:SER:HG	1:D:701:VAL:HG13	1.84	0.43
1:E:206:TRP:CD1	1:E:218:LYS:NZ	2.83	0.43
1:G:632:ASP:O	1:G:635:ILE:HG22	2.19	0.43
2:H:70:VAL:HA	2:H:73:MET:SD	2.58	0.43
2:I:71:LEU:HD13	2:I:71:LEU:HA	1.83	0.43
2:I:120:TYR:CZ	2:I:121:ALA:O	2.71	0.43
1:A:494:ASN:OD1	1:A:592:ARG:HA	2.19	0.43
1:A:629:LEU:N	1:A:674:THR:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:VAL:O	1:B:220:LYS:NZ	2.21	0.43
1:B:216:LEU:N	1:B:216:LEU:HD12	2.34	0.43
1:B:217:THR:OG1	1:B:219:TYR:HE1	2.00	0.43
1:B:222:SER:H	1:B:228:THR:HG21	1.84	0.43
1:C:256:VAL:HG23	1:C:256:VAL:O	2.19	0.43
1:C:665:ILE:O	1:C:676:ILE:HD12	2.18	0.43
1:D:272:SER:HB3	1:D:288:THR:HG22	2.00	0.43
1:D:345:THR:O	1:D:349:THR:HG23	2.19	0.43
1:D:447:GLN:C	1:D:448:LEU:HD12	2.39	0.43
1:E:234:SER:OG	1:E:237:GLU:HG2	2.19	0.43
1:E:259:TYR:CZ	1:E:261:ILE:HD11	2.54	0.43
1:E:535:GLU:OE2	1:E:540:LEU:HD12	2.19	0.43
1:E:551:ASP:HB2	1:E:592:ARG:HG2	2.01	0.43
1:F:199:LYS:HE2	1:G:516:THR:O	2.18	0.43
2:H:189:LEU:HD23	2:H:219:LYS:HE2	2.01	0.43
2:I:57:GLU:O	2:I:61:LYS:NZ	2.49	0.43
2:I:102:LYS:HA	2:I:114:LEU:HD23	2.00	0.43
2:I:162:LYS:HZ3	2:I:163:ILE:HD11	1.83	0.43
2:J:206:LEU:O	2:J:210:SER:OG	2.24	0.43
1:A:225:LYS:HE3	1:A:228:THR:HA	2.00	0.43
1:B:481:LEU:HD23	1:B:481:LEU:HA	1.78	0.43
1:B:590:LEU:HA	1:B:590:LEU:HD12	1.69	0.43
1:C:705:ASN:HD21	1:C:722:LYS:CB	2.27	0.43
1:D:269:ILE:HG22	1:D:270:ILE:H	1.81	0.43
1:D:627:LEU:HB3	1:D:629:LEU:CD1	2.49	0.43
1:E:222:SER:HB3	1:E:228:THR:HG22	2.01	0.43
1:E:332:VAL:CG1	1:E:448:LEU:HB2	2.48	0.43
2:H:61:LYS:O	2:H:65:LYS:HD2	2.19	0.43
2:H:88:ILE:C	2:H:90:LYS:H	2.22	0.43
2:I:167:TYR:CE2	2:I:534:ILE:HG12	2.49	0.43
2:J:165:GLN:N	2:J:166:PRO:HD2	2.33	0.43
1:B:554:PHE:HB3	1:B:558:THR:OG1	2.18	0.43
1:C:361:ASN:HA	1:C:422:ASN:OD1	2.19	0.43
1:C:569:LEU:HD23	1:C:569:LEU:HA	1.90	0.43
1:E:187:LEU:HA	1:E:187:LEU:HD13	1.78	0.43
1:E:200:ARG:N	1:E:200:ARG:HD3	2.34	0.43
1:E:472:ASP:OD1	1:E:473:THR:N	2.51	0.43
1:G:643:ILE:N	1:G:699:TYR:O	2.47	0.43
2:H:617:LYS:HE3	2:H:695:TYR:CE2	2.54	0.43
2:H:659:TYR:HE2	2:H:694:ASP:OD2	2.02	0.43
2:H:739:GLU:HG3	2:H:742:ARG:HH22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:469:ASN:HA	2:I:472:LYS:HZ2	1.84	0.43
2:I:477:TYR:HE2	2:I:559:ILE:HD11	1.84	0.43
2:I:480:SER:O	2:I:525:ILE:N	2.49	0.43
1:A:527:LEU:HD23	1:A:533:PHE:HE2	1.84	0.42
1:A:599:ASP:CG	1:A:600:ARG:N	2.71	0.42
1:B:338:LEU:HG	1:B:661:ASP:CB	2.48	0.42
1:B:555:ASP:HB3	1:B:558:THR:HG23	2.01	0.42
1:B:640:SER:HG	1:B:701:VAL:HG13	1.83	0.42
1:C:498:LEU:HD23	1:C:498:LEU:HA	1.88	0.42
1:D:472:ASP:OD1	1:D:473:THR:N	2.52	0.42
1:E:244:ASP:C	1:E:246:ASN:N	2.71	0.42
1:F:178:ARG:HB2	1:F:224:GLU:OE2	2.19	0.42
1:F:269:ILE:HG13	1:F:362:ALA:HB2	2.01	0.42
1:F:334:ILE:H	1:F:334:ILE:HD12	1.83	0.42
1:F:459:ILE:HG12	1:F:477:TRP:CE2	2.54	0.42
1:F:543:GLN:OE1	1:F:543:GLN:N	2.52	0.42
2:H:412:TYR:O	2:H:416:ILE:HD12	2.18	0.42
2:H:576:LEU:HG	2:H:577:PRO:HD2	2.00	0.42
2:I:252:ILE:HD13	2:I:252:ILE:HA	1.90	0.42
2:I:582:LEU:O	2:I:629:PHE:N	2.45	0.42
2:J:405:ASN:OD1	2:J:405:ASN:N	2.51	0.42
1:B:387:LYS:HE2	1:B:387:LYS:HA	2.01	0.42
1:B:462:TYR:CD1	1:B:462:TYR:C	2.93	0.42
1:B:463:ASN:HB3	1:B:470:ARG:HH21	1.83	0.42
1:B:596:PHE:N	1:B:596:PHE:CD1	2.87	0.42
1:C:366:TYR:HD2	1:C:378:LEU:HD11	1.82	0.42
1:D:226:TRP:CZ3	1:D:234:SER:HB3	2.54	0.42
1:D:405:LEU:HD12	1:D:405:LEU:HA	1.83	0.42
1:D:411:TYR:CD2	1:D:411:TYR:C	2.89	0.42
1:E:364:ILE:CD1	1:E:421:LEU:HD21	2.49	0.42
1:E:381:THR:HG23	1:E:451:ASP:O	2.18	0.42
1:G:300:THR:O	1:G:324:PHE:HB3	2.18	0.42
2:H:384:GLN:OE1	2:H:384:GLN:HA	2.18	0.42
2:H:391:ARG:HH12	2:H:399:ILE:HG22	1.83	0.42
2:H:522:GLN:HG3	2:H:525:ILE:HD11	2.00	0.42
1:A:583:LEU:CB	1:A:587:MET:HE1	2.45	0.42
1:C:237:GLU:OE1	1:C:237:GLU:N	2.47	0.42
1:C:535:GLU:OE2	1:C:540:LEU:HD22	2.19	0.42
1:D:584:ASN:H	1:D:587:MET:HE1	1.84	0.42
1:G:377:VAL:HG12	1:G:378:LEU:N	2.35	0.42
1:G:506:ALA:HB1	1:G:518:LYS:NZ	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:643:ILE:HG12	1:G:723:LYS:NZ	2.34	0.42
2:H:120:TYR:O	2:H:130:VAL:N	2.42	0.42
2:H:521:LEU:HD13	2:H:521:LEU:HA	1.87	0.42
2:H:615:ILE:H	2:H:615:ILE:HD12	1.84	0.42
2:H:699:LEU:HD12	2:H:700:LEU:HD22	2.02	0.42
2:I:169:LYS:NZ	2:I:533:GLN:HB2	2.33	0.42
2:J:61:LYS:O	2:J:64:GLU:HB2	2.19	0.42
1:A:250:GLU:OE1	1:A:250:GLU:N	2.30	0.42
1:A:365:ARG:NH1	1:A:414:LYS:HA	2.35	0.42
1:B:228:THR:HG23	1:B:235:ASP:CG	2.40	0.42
1:B:228:THR:HG23	1:B:235:ASP:OD2	2.19	0.42
1:B:365:ARG:HE	1:B:418:PRO:CB	2.27	0.42
1:C:187:LEU:HA	1:C:187:LEU:HD13	1.79	0.42
1:C:353:ASN:HB3	1:C:356:ASP:OD1	2.20	0.42
1:C:383:LEU:HD11	1:C:448:LEU:HB3	2.01	0.42
1:C:629:LEU:HA	1:C:629:LEU:HD12	1.82	0.42
1:D:360:LEU:HA	1:D:360:LEU:HD12	1.73	0.42
1:F:203:LEU:HG	1:F:204:SER:N	2.33	0.42
2:I:39:ILE:HD12	2:I:39:ILE:H	1.85	0.42
2:I:125:TYR:O	2:I:127:PRO:HD3	2.18	0.42
2:J:527:LEU:HA	2:J:548:LYS:O	2.19	0.42
2:J:664:ARG:HG3	2:J:664:ARG:O	2.19	0.42
1:A:255:LEU:HA	1:A:255:LEU:HD23	1.69	0.42
1:A:633:LYS:HE2	1:A:636:ARG:NH2	2.33	0.42
1:B:535:GLU:OE2	1:B:540:LEU:HD22	2.20	0.42
1:B:549:GLU:HB3	1:B:595:ARG:HH11	1.85	0.42
1:D:389:GLN:O	1:D:389:GLN:HG2	2.19	0.42
1:E:228:THR:HG23	1:E:235:ASP:OD2	2.20	0.42
1:F:438:GLN:HA	1:F:441:GLU:OE1	2.19	0.42
1:F:645:GLU:HA	1:F:654:GLU:O	2.19	0.42
1:G:178:ARG:NE	1:G:178:ARG:HA	2.34	0.42
1:G:199:LYS:H	1:G:200:ARG:HH12	1.66	0.42
1:G:228:THR:N	1:G:235:ASP:OD2	2.38	0.42
1:G:463:ASN:OD1	1:G:465:GLU:OE1	2.38	0.42
1:G:533:PHE:CZ	1:G:542:TYR:HB2	2.54	0.42
1:G:618:GLU:N	1:G:618:GLU:OE2	2.52	0.42
1:G:702:THR:OG1	1:G:704:GLU:OE1	2.32	0.42
2:H:281:TRP:CE2	2:H:285:LEU:HD21	2.54	0.42
2:I:84:VAL:HG22	2:I:85:ASP:H	1.84	0.42
2:I:512:GLY:O	2:I:519:LEU:HA	2.20	0.42
2:I:543:ILE:HG22	2:I:545:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:566:ILE:HG21	2:I:583:ILE:HG21	2.01	0.42
2:J:85:ASP:OD1	2:J:86:GLY:N	2.52	0.42
1:A:224:GLU:OE1	1:A:517:THR:HG21	2.19	0.42
1:A:345:THR:O	1:A:348:GLU:HG3	2.19	0.42
1:B:253:HIS:CE1	1:B:255:LEU:HD13	2.55	0.42
1:B:270:ILE:C	1:B:271:LEU:HD22	2.39	0.42
1:B:484:ILE:HG22	1:B:504:ARG:CZ	2.50	0.42
1:B:524:LYS:HE2	1:B:540:LEU:HD21	2.01	0.42
1:C:270:ILE:HG22	1:C:290:SER:HB3	2.02	0.42
1:C:373:PRO:HB2	1:C:375:TYR:CE2	2.55	0.42
1:C:374:ILE:CG1	1:C:405:LEU:HB2	2.50	0.42
1:C:549:GLU:HA	1:C:594:LYS:CE	2.50	0.42
1:E:228:THR:HG23	1:E:235:ASP:CG	2.40	0.42
1:F:245:LYS:HB3	1:G:483:GLN:OE1	2.19	0.42
1:F:259:TYR:HE2	1:F:261:ILE:HD11	1.83	0.42
1:F:455:VAL:HG13	1:F:455:VAL:O	2.19	0.42
2:H:118:TYR:HA	2:H:132:GLN:OE1	2.19	0.42
2:H:296:LEU:HD11	2:H:419:ILE:HD12	2.02	0.42
2:H:434:LYS:HD3	2:H:436:TYR:CE1	2.53	0.42
2:I:107:ILE:HG12	2:I:219:LYS:NZ	2.35	0.42
2:I:226:GLU:OE1	2:I:228:GLN:OE1	2.38	0.42
1:A:621:ASN:OD1	1:A:622:SER:N	2.53	0.42
1:A:698:VAL:O	1:A:726:ILE:HB	2.20	0.42
1:B:195:ASP:OD1	1:B:195:ASP:O	2.38	0.42
1:B:455:VAL:O	1:B:455:VAL:HG13	2.20	0.42
1:B:494:ASN:OD1	1:B:592:ARG:HA	2.18	0.42
1:B:500:LEU:N	1:B:500:LEU:HD22	2.35	0.42
1:B:520:ASP:OD1	1:B:521:MET:N	2.52	0.42
1:B:588:ASN:O	1:B:589:ILE:HD13	2.20	0.42
1:B:646:ILE:N	1:B:654:GLU:O	2.43	0.42
1:C:226:TRP:CD2	1:C:234:SER:HB3	2.55	0.42
1:C:297:ARG:HD2	1:C:298:THR:N	2.34	0.42
1:C:365:ARG:NH2	1:C:413:SER:O	2.53	0.42
1:C:445:THR:HG22	1:C:447:GLN:HB2	2.01	0.42
1:D:191:GLY:HA2	1:D:219:TYR:O	2.20	0.42
1:E:540:LEU:HB3	1:E:547:ILE:CG2	2.47	0.42
1:E:548:THR:O	1:E:594:LYS:NZ	2.37	0.42
1:G:187:LEU:HD23	1:G:187:LEU:HA	1.69	0.42
1:G:385:LEU:O	1:G:389:GLN:HB2	2.20	0.42
1:G:416:LEU:HD13	1:G:416:LEU:HA	1.80	0.42
1:G:643:ILE:HG12	1:G:723:LYS:CD	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:VAL:O	2:H:73:MET:SD	2.78	0.42
2:H:235:LEU:HD13	2:H:235:LEU:HA	1.65	0.42
2:H:442:ASN:ND2	2:H:444:ASN:HB2	2.34	0.42
2:H:617:LYS:HD3	2:H:773:ILE:HD13	2.01	0.42
2:H:628:ARG:HH11	2:H:628:ARG:HG3	1.84	0.42
1:A:411:TYR:CD1	1:A:412:PRO:HA	2.54	0.42
1:B:269:ILE:CG2	1:B:270:ILE:H	2.31	0.42
1:C:226:TRP:CZ3	1:C:234:SER:HB3	2.54	0.42
1:C:466:ASN:OD1	1:C:466:ASN:N	2.52	0.42
1:D:175:VAL:HG12	2:I:228:GLN:HE21	1.85	0.42
1:D:225:LYS:HE2	1:D:225:LYS:HB3	1.85	0.42
1:D:334:ILE:CG2	1:D:446:LYS:HB3	2.49	0.42
1:E:192:TYR:CD1	1:E:192:TYR:N	2.87	0.42
1:F:291:LYS:HZ2	1:F:334:ILE:CG2	2.32	0.42
1:F:291:LYS:HD3	1:F:291:LYS:C	2.40	0.42
1:F:391:LEU:HD13	1:F:391:LEU:HA	1.90	0.42
1:F:583:LEU:HD22	1:F:583:LEU:N	2.34	0.42
1:G:198:ASN:HB2	1:G:200:ARG:NH2	2.34	0.42
1:G:468:ARG:NH1	1:G:470:ARG:HH21	2.18	0.42
2:H:77:ILE:HG13	2:H:159:ILE:CD1	2.50	0.42
2:H:137:TYR:HE1	2:H:143:LYS:HE3	1.85	0.42
2:H:186:GLN:HB2	2:H:190:PHE:CE2	2.53	0.42
2:H:390:GLN:OE1	2:H:390:GLN:N	2.52	0.42
2:H:570:TRP:CZ2	2:H:603:LEU:HB3	2.54	0.42
2:H:725:LEU:HB3	2:H:726:THR:H	1.71	0.42
2:I:41:LYS:HE3	2:I:41:LYS:HB3	1.78	0.42
1:A:565:GLN:O	1:A:569:LEU:HD23	2.19	0.42
1:B:649:THR:CB	1:B:691:ASN:HD22	2.31	0.42
1:C:270:ILE:CG1	1:C:361:ASN:HB3	2.50	0.42
1:C:366:TYR:CE2	1:C:378:LEU:HD21	2.54	0.42
1:C:552:PHE:HB3	1:C:554:PHE:HZ	1.82	0.42
1:C:579:ASP:OD1	1:C:580:LYS:HG2	2.20	0.42
1:D:183:ILE:HD12	1:D:183:ILE:N	2.33	0.42
1:D:267:GLU:HG2	1:D:268:ASN:N	2.34	0.42
1:D:297:ARG:CZ	1:D:500:LEU:HD23	2.49	0.42
1:D:366:TYR:HE2	1:D:378:LEU:CG	2.33	0.42
1:D:403:GLN:H	1:D:403:GLN:CD	2.23	0.42
1:D:640:SER:HB3	1:D:703:LYS:HA	2.01	0.42
1:E:229:ALA:O	1:E:230:SER:HB2	2.19	0.42
1:E:365:ARG:HH11	1:E:414:LYS:HD2	1.84	0.42
1:E:603:ILE:O	1:E:605:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:ILE:C	1:F:271:LEU:HD22	2.40	0.42
1:F:450:LEU:HA	1:F:450:LEU:HD23	1.69	0.42
1:F:482:PRO:O	1:F:486:GLU:HG2	2.20	0.42
1:G:353:ASN:O	1:G:436:TYR:HD2	2.02	0.42
1:G:364:ILE:HD11	1:G:421:LEU:HD12	2.02	0.42
2:H:475:PHE:CD2	2:H:529:ILE:HG13	2.55	0.42
2:H:475:PHE:CE2	2:H:529:ILE:HG13	2.54	0.42
2:H:578:LYS:CB	2:H:579:TYR:CD1	3.03	0.42
2:I:69:ASP:HA	2:I:72:GLU:OE1	2.20	0.42
2:I:150:GLU:HA	2:I:153:LYS:HZ2	1.85	0.42
2:I:630:VAL:N	2:I:666:ILE:O	2.47	0.42
2:J:234:GLN:HA	2:J:241:PHE:HB2	2.01	0.42
1:A:199:LYS:NZ	1:B:516:THR:O	2.53	0.42
1:A:324:PHE:HZ	1:A:588:ASN:HB3	1.85	0.42
1:A:324:PHE:CZ	1:A:588:ASN:HB3	2.55	0.42
1:B:374:ILE:CG1	1:B:405:LEU:HB2	2.50	0.42
1:B:385:LEU:HB3	1:B:391:LEU:CD2	2.50	0.42
1:C:338:LEU:HG	1:C:661:ASP:CB	2.50	0.42
1:C:506:ALA:HB1	1:C:518:LYS:NZ	2.35	0.42
1:D:187:LEU:HA	1:D:187:LEU:HD23	1.53	0.42
1:E:244:ASP:O	1:E:246:ASN:N	2.53	0.42
1:E:442:LEU:C	1:E:446:LYS:HZ2	2.23	0.42
1:E:592:ARG:NH1	1:E:598:TYR:CG	2.88	0.42
1:F:199:LYS:HD2	1:G:517:THR:HA	2.02	0.42
1:G:579:ASP:OD1	1:G:580:LYS:HG2	2.20	0.42
2:H:97:LEU:HB2	2:H:101:LYS:HE2	2.02	0.42
2:H:437:LEU:HD23	2:H:437:LEU:HA	1.83	0.42
2:I:63:LEU:N	2:I:63:LEU:HD22	2.35	0.42
2:I:490:GLU:O	2:I:491:ARG:CZ	2.68	0.42
1:A:270:ILE:C	1:A:271:LEU:HD22	2.41	0.41
1:A:382:SER:HA	1:A:393:THR:HA	2.02	0.41
1:A:527:LEU:HD12	1:A:527:LEU:N	2.35	0.41
1:A:555:ASP:O	1:A:558:THR:OG1	2.21	0.41
1:B:468:ARG:CZ	1:B:468:ARG:HB2	2.50	0.41
1:B:629:LEU:N	1:B:674:THR:O	2.52	0.41
1:B:696:VAL:N	1:B:729:LYS:O	2.36	0.41
1:C:471:VAL:O	1:C:471:VAL:HG13	2.20	0.41
1:C:527:LEU:HD13	1:C:527:LEU:HA	1.89	0.41
1:D:198:ASN:CG	1:D:199:LYS:H	2.22	0.41
1:D:639:LEU:H	1:D:703:LYS:HZ3	1.68	0.41
1:E:471:VAL:O	1:E:471:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:624:THR:O	1:E:687:LEU:HB2	2.21	0.41
1:E:722:LYS:HA	1:E:722:LYS:HD2	1.70	0.41
1:F:228:THR:HG23	1:F:235:ASP:OD1	2.20	0.41
1:G:183:ILE:HD11	1:G:236:PHE:HD1	1.84	0.41
2:H:65:LYS:HD2	2:H:65:LYS:H	1.85	0.41
2:H:155:LEU:HD13	2:H:155:LEU:HA	1.90	0.41
2:H:165:GLN:O	2:H:165:GLN:HG2	2.20	0.41
2:H:517:GLY:C	2:H:518:LYS:HD3	2.41	0.41
2:I:81:ILE:O	2:I:81:ILE:HG13	2.20	0.41
1:A:382:SER:CB	1:A:393:THR:HG22	2.49	0.41
1:A:497:ASP:OD1	1:A:499:ASN:HB2	2.20	0.41
1:A:594:LYS:HB2	1:A:594:LYS:HE2	1.78	0.41
1:B:211:HIS:HA	1:B:214:LYS:NZ	2.36	0.41
1:B:512:ASP:OD1	1:B:513:PRO:HD2	2.21	0.41
1:C:253:HIS:HE1	1:C:255:LEU:HD12	1.85	0.41
1:C:476:ASN:HD21	1:C:479:GLU:HG3	1.85	0.41
1:C:588:ASN:O	1:C:589:ILE:HD13	2.19	0.41
1:D:198:ASN:ND2	1:D:200:ARG:HH22	2.18	0.41
1:E:552:PHE:HB3	1:E:554:PHE:HZ	1.81	0.41
1:E:577:VAL:HG22	1:E:580:LYS:HB2	2.02	0.41
1:G:203:LEU:HD22	1:G:203:LEU:N	2.35	0.41
1:G:643:ILE:HG21	1:G:723:LYS:NZ	2.31	0.41
2:J:247:PHE:O	2:J:252:ILE:HG12	2.20	0.41
1:A:258:ALA:HA	1:A:371:THR:OG1	2.20	0.41
1:A:435:ASN:O	1:A:438:GLN:HB2	2.20	0.41
1:B:200:ARG:N	1:B:200:ARG:HD3	2.35	0.41
1:C:558:THR:HG22	1:C:587:MET:HG3	2.02	0.41
1:D:181:ASP:O	1:D:183:ILE:HD12	2.19	0.41
1:D:197:LYS:O	1:D:200:ARG:N	2.46	0.41
1:D:241:GLY:O	1:D:243:ILE:N	2.52	0.41
1:D:576:THR:C	1:D:578:LEU:H	2.22	0.41
1:D:635:ILE:C	1:D:637:LYS:H	2.24	0.41
1:F:404:ILE:C	1:F:405:LEU:HD12	2.41	0.41
1:F:520:ASP:OD2	1:F:521:MET:N	2.53	0.41
1:F:638:ILE:HG13	1:F:639:LEU:HD22	2.02	0.41
1:G:244:ASP:C	1:G:246:ASN:N	2.73	0.41
1:G:441:GLU:HA	1:G:444:LYS:NZ	2.35	0.41
2:H:171:LEU:O	2:H:174:LEU:HB2	2.19	0.41
2:I:38:GLU:O	2:I:41:LYS:HG2	2.20	0.41
2:I:126:GLU:O	2:I:128:VAL:HG23	2.20	0.41
2:I:202:SER:H	2:I:205:PHE:HD2	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:474:ASN:HD22	2:I:597:GLU:HB2	1.86	0.41
2:I:501:TRP:CZ3	2:I:590:ARG:NH1	2.87	0.41
1:A:535:GLU:HB3	1:A:538:GLY:HA2	2.03	0.41
1:A:592:ARG:HH22	1:A:602:ASN:HA	1.85	0.41
1:A:663:LEU:O	1:A:665:ILE:N	2.53	0.41
1:B:225:LYS:NZ	1:B:230:SER:HB3	2.34	0.41
1:D:527:LEU:HD12	1:D:527:LEU:N	2.35	0.41
1:D:590:LEU:CD2	1:D:592:ARG:HG3	2.50	0.41
1:G:481:LEU:HB2	1:G:482:PRO:HD3	2.02	0.41
2:H:97:LEU:HB2	2:H:101:LYS:CE	2.50	0.41
2:H:189:LEU:HD23	2:H:189:LEU:HA	1.71	0.41
2:I:243:TYR:CE2	2:I:244:MET:HE3	2.55	0.41
2:J:224:TYR:CZ	2:J:230:ARG:NH1	2.89	0.41
1:A:524:LYS:HE2	1:A:540:LEU:HD11	2.03	0.41
1:A:568:GLU:HG2	1:A:569:LEU:CD2	2.50	0.41
1:A:614:GLU:OE2	1:A:617:ARG:NH1	2.44	0.41
1:B:366:TYR:HE1	1:B:378:LEU:CD1	2.23	0.41
1:B:608:ASP:OD1	1:B:609:GLU:N	2.53	0.41
1:C:438:GLN:HA	1:C:441:GLU:OE1	2.21	0.41
1:C:517:THR:HG22	1:C:517:THR:O	2.19	0.41
1:D:635:ILE:O	1:D:637:LYS:N	2.53	0.41
1:F:271:LEU:HD13	1:F:360:LEU:HA	2.01	0.41
1:F:378:LEU:HD12	1:F:379:PRO:CD	2.50	0.41
1:F:502:GLU:O	1:F:503:ARG:NH1	2.50	0.41
1:F:515:GLU:N	1:F:515:GLU:OE2	2.54	0.41
1:G:364:ILE:O	1:G:419:ILE:HG22	2.20	0.41
1:G:500:LEU:HD23	1:G:500:LEU:HA	1.85	0.41
1:G:631:ILE:HB	1:G:636:ARG:HD2	2.02	0.41
2:H:100:ASP:C	2:H:102:LYS:N	2.74	0.41
2:I:52:GLU:O	2:I:52:GLU:HG3	2.20	0.41
2:I:149:TYR:CE1	2:I:219:LYS:HE2	2.55	0.41
2:I:541:GLU:O	2:I:542:TYR:HD1	2.04	0.41
2:I:541:GLU:O	2:I:542:TYR:CD1	2.73	0.41
2:J:243:TYR:CE1	2:J:247:PHE:HE2	2.38	0.41
1:B:481:LEU:HB3	1:B:485:GLN:OE1	2.20	0.41
1:C:199:LYS:HD2	1:C:199:LYS:HA	1.85	0.41
1:C:596:PHE:HD1	1:C:607:ALA:HB2	1.84	0.41
1:D:377:VAL:HG12	1:D:378:LEU:N	2.35	0.41
1:E:405:LEU:HD13	1:E:405:LEU:HA	1.64	0.41
1:F:383:LEU:HD13	1:F:450:LEU:HD21	2.02	0.41
1:G:406:ALA:HB3	1:G:409:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:506:ALA:CB	1:G:518:LYS:HZ2	2.26	0.41
2:H:203:VAL:HA	2:H:206:LEU:CD2	2.51	0.41
2:I:181:SER:O	2:I:182:ASP:C	2.58	0.41
2:I:602:ILE:HA	2:I:605:GLU:HG2	2.02	0.41
1:A:583:LEU:HD22	1:A:587:MET:HE3	2.03	0.41
1:B:220:LYS:O	1:B:255:LEU:HD11	2.21	0.41
1:B:378:LEU:HA	1:B:379:PRO:HD3	1.88	0.41
1:C:198:ASN:N	1:C:198:ASN:OD1	2.52	0.41
1:C:232:PRO:CD	1:C:233:TYR:HD2	2.21	0.41
1:C:238:LYS:HG2	1:C:252:ARG:O	2.19	0.41
1:C:270:ILE:C	1:C:271:LEU:HD22	2.41	0.41
1:C:481:LEU:HA	1:C:481:LEU:HD23	1.61	0.41
1:C:692:PRO:O	1:C:732:TYR:HD2	2.04	0.41
1:E:291:LYS:NZ	1:E:292:ASN:O	2.54	0.41
1:E:326:ASN:HD22	1:E:485:GLN:CG	2.26	0.41
1:E:383:LEU:HA	1:E:383:LEU:HD13	1.83	0.41
1:E:523:LEU:C	1:E:523:LEU:HD23	2.41	0.41
1:F:199:LYS:HD3	1:F:199:LYS:HA	1.63	0.41
1:F:554:PHE:HB3	1:F:558:THR:OG1	2.21	0.41
2:H:544:ARG:O	2:H:545:ILE:HD13	2.20	0.41
2:I:224:TYR:CE1	2:I:248:ASN:ND2	2.88	0.41
2:J:503:ILE:CG1	2:J:549:VAL:HG23	2.50	0.41
1:A:592:ARG:NH2	1:A:598:TYR:CG	2.89	0.41
1:D:197:LYS:HB2	2:I:235:LEU:HD21	2.02	0.41
1:D:298:THR:HG22	1:D:329:SER:C	2.40	0.41
1:D:367:VAL:HG22	1:D:410:TYR:CE2	2.54	0.41
1:E:188:GLU:OE1	1:E:223:PRO:HA	2.21	0.41
1:E:272:SER:HB3	1:E:288:THR:HG22	2.01	0.41
1:E:556:GLN:O	1:E:559:SER:OG	2.30	0.41
1:G:611:VAL:HA	1:G:614:GLU:OE1	2.20	0.41
2:H:226:GLU:OE2	2:H:228:GLN:HB2	2.21	0.41
2:H:585:PHE:CE1	2:H:596:VAL:HG12	2.56	0.41
2:I:84:VAL:HG22	2:I:85:ASP:N	2.35	0.41
2:I:255:SER:O	2:I:258:GLU:HG3	2.20	0.41
2:J:408:VAL:HG12	2:J:412:TYR:CE2	2.56	0.41
1:A:406:ALA:HB3	1:A:409:ASN:HD22	1.86	0.41
1:A:416:LEU:HA	1:A:416:LEU:HD13	1.76	0.41
1:A:596:PHE:CD1	1:A:596:PHE:N	2.88	0.41
1:B:384:VAL:HG13	1:B:449:ARG:HB2	2.02	0.41
1:B:469:VAL:HG23	1:B:469:VAL:O	2.20	0.41
1:C:232:PRO:C	1:C:233:TYR:CD2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:LEU:CG	1:C:391:LEU:HD21	2.50	0.41
1:D:492:ILE:HG22	1:D:500:LEU:CD1	2.50	0.41
1:D:549:GLU:HB3	1:D:595:ARG:HH11	1.86	0.41
1:D:583:LEU:HA	1:D:583:LEU:HD23	1.65	0.41
1:D:593:ASP:OD1	1:D:593:ASP:C	2.59	0.41
1:E:421:LEU:HA	1:E:421:LEU:HD23	1.56	0.41
1:F:226:TRP:CE2	1:F:234:SER:HB3	2.55	0.41
1:G:198:ASN:CB	1:G:200:ARG:HH22	2.33	0.41
1:G:207:ILE:HG22	1:G:209:ASN:OD1	2.21	0.41
1:G:354:THR:HA	1:G:436:TYR:CD2	2.56	0.41
1:G:481:LEU:H	1:G:481:LEU:HD12	1.86	0.41
1:G:556:GLN:O	1:G:559:SER:OG	2.27	0.41
1:G:595:ARG:HD2	1:G:611:VAL:HG11	2.02	0.41
2:H:234:GLN:HG2	2:H:241:PHE:CG	2.56	0.41
2:I:153:LYS:HE3	2:I:153:LYS:HB3	1.87	0.41
2:J:61:LYS:O	2:J:65:LYS:HD2	2.21	0.41
2:J:81:ILE:HG13	2:J:81:ILE:O	2.21	0.41
2:J:170:PHE:HE1	2:J:217:PHE:HD1	1.66	0.41
1:A:541:GLN:CD	1:A:544:GLY:H	2.23	0.41
1:B:377:VAL:CG1	1:B:378:LEU:N	2.84	0.41
1:B:421:LEU:HA	1:B:421:LEU:HD12	1.70	0.41
1:B:447:GLN:C	1:B:448:LEU:HD22	2.42	0.41
1:B:490:ARG:HG3	1:B:502:GLU:OE2	2.20	0.41
1:B:575:TYR:O	1:B:578:LEU:HD23	2.21	0.41
1:B:598:TYR:HA	1:B:605:VAL:HG12	2.03	0.41
1:C:530:ALA:O	1:C:531:PHE:HD2	2.04	0.41
1:D:727:PHE:CD2	1:D:728:SER:N	2.89	0.41
1:F:490:ARG:HG3	1:F:502:GLU:OE2	2.21	0.41
1:G:242:ARG:HB3	1:G:462:TYR:CZ	2.56	0.41
1:G:243:ILE:HD12	1:G:243:ILE:HA	1.89	0.41
1:G:294:SER:O	1:G:333:ALA:N	2.42	0.41
1:G:364:ILE:HG22	1:G:365:ARG:N	2.36	0.41
1:G:415:ASN:N	1:G:415:ASN:OD1	2.47	0.41
1:G:571:ALA:CB	1:G:577:VAL:HG21	2.51	0.41
1:G:577:VAL:HG12	1:G:577:VAL:O	2.21	0.41
2:H:246:LYS:HB3	2:H:250:GLN:NE2	2.36	0.41
2:I:517:GLY:C	2:I:518:LYS:HD2	2.41	0.41
2:J:83:ILE:HG13	2:J:131:ILE:HB	2.02	0.41
1:A:481:LEU:HB3	1:A:482:PRO:HD3	2.03	0.40
1:A:583:LEU:HD23	1:A:583:LEU:HA	1.83	0.40
1:B:176:PRO:HB3	1:B:178:ARG:HH12	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ASP:OD1	1:B:295:THR:OG1	2.30	0.40
1:B:628:LEU:HA	1:B:674:THR:O	2.20	0.40
1:C:214:LYS:HE2	1:C:214:LYS:HB3	1.85	0.40
1:C:227:SER:OG	1:C:230:SER:HA	2.21	0.40
1:C:541:GLN:CD	1:C:544:GLY:H	2.24	0.40
1:C:542:TYR:O	1:C:545:LYS:HE2	2.21	0.40
1:D:244:ASP:O	1:D:246:ASN:N	2.54	0.40
1:D:266:MET:SD	1:D:362:ALA:HB1	2.61	0.40
1:D:378:LEU:HD12	1:D:378:LEU:HA	1.78	0.40
1:D:470:ARG:HA	1:E:479:GLU:OE1	2.21	0.40
1:E:269:ILE:HB	1:E:360:LEU:HD11	2.03	0.40
1:F:227:SER:O	1:F:230:SER:N	2.49	0.40
1:F:256:VAL:HG23	1:F:256:VAL:O	2.21	0.40
1:F:342:GLY:HA2	1:F:344:ARG:NH1	2.35	0.40
1:F:503:ARG:HD3	1:F:503:ARG:HA	1.88	0.40
1:G:271:LEU:HB2	1:G:289:ILE:CG2	2.49	0.40
1:G:565:GLN:HA	1:G:568:GLU:OE2	2.21	0.40
1:G:588:ASN:O	1:G:589:ILE:HD13	2.20	0.40
1:G:594:LYS:HB2	1:G:594:LYS:HE3	1.71	0.40
2:H:124:GLY:CA	2:H:127:PRO:HG3	2.50	0.40
2:H:427:ILE:HD13	2:H:505:LEU:HD12	2.01	0.40
2:H:464:ASN:OD1	2:H:466:GLY:N	2.53	0.40
2:I:177:ILE:HD13	2:I:177:ILE:HA	1.83	0.40
2:I:537:GLN:NE2	2:I:538:SER:HB3	2.36	0.40
2:J:552:LYS:O	2:J:555:ILE:HG22	2.21	0.40
1:A:482:PRO:O	1:A:486:GLU:HG2	2.21	0.40
1:A:483:GLN:H	1:A:483:GLN:CD	2.23	0.40
1:B:291:LYS:HE3	1:B:335:ASP:O	2.20	0.40
1:B:404:ILE:C	1:B:405:LEU:HD22	2.41	0.40
1:B:592:ARG:NE	1:B:598:TYR:CE1	2.84	0.40
1:B:592:ARG:HE	1:B:598:TYR:HE1	1.60	0.40
1:C:494:ASN:HD21	1:C:593:ASP:H	1.69	0.40
1:C:575:TYR:CD1	1:C:575:TYR:N	2.89	0.40
1:C:584:ASN:O	1:C:587:MET:HE1	2.21	0.40
1:C:641:GLY:O	1:C:701:VAL:HG12	2.21	0.40
1:C:667:SER:N	1:C:675:PHE:O	2.52	0.40
1:E:233:TYR:HD2	1:E:243:ILE:CD1	2.33	0.40
1:E:583:LEU:HA	1:E:583:LEU:HD23	1.87	0.40
1:E:639:LEU:C	1:E:703:LYS:HZ2	2.25	0.40
1:F:251:ALA:HA	1:F:256:VAL:CG2	2.50	0.40
1:F:480:VAL:O	1:F:484:ILE:HD12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:415:ASN:C	1:G:416:LEU:HD22	2.42	0.40
1:G:558:THR:HG22	1:G:587:MET:HA	2.02	0.40
2:H:122:LYS:N	2:H:128:VAL:O	2.49	0.40
2:H:302:PRO:HD3	2:H:385:PRO:HA	2.02	0.40
2:H:480:SER:HA	2:H:590:ARG:NH1	2.35	0.40
2:H:513:TYR:CD1	2:H:519:LEU:HD22	2.56	0.40
2:H:627:GLY:HA3	2:H:664:ARG:O	2.21	0.40
2:H:722:GLY:HA2	2:H:736:PHE:CZ	2.56	0.40
2:H:752:ARG:O	2:H:755:VAL:HG22	2.21	0.40
2:I:765:PHE:O	2:I:769:GLN:HG2	2.22	0.40
1:A:237:GLU:HB2	1:A:242:ARG:O	2.20	0.40
1:A:267:GLU:HG2	1:A:268:ASN:N	2.36	0.40
1:A:492:ILE:CD1	1:A:502:GLU:HB2	2.52	0.40
1:B:238:LYS:NZ	1:B:254:PRO:CA	2.80	0.40
1:B:404:ILE:HD12	1:B:404:ILE:HG23	1.90	0.40
1:C:405:LEU:HD21	1:C:411:TYR:CB	2.51	0.40
1:C:434:MET:O	1:C:434:MET:SD	2.79	0.40
1:C:472:ASP:OD1	1:C:473:THR:N	2.54	0.40
1:C:557:GLN:CD	1:C:557:GLN:H	2.24	0.40
1:C:635:ILE:O	1:C:637:LYS:N	2.54	0.40
1:D:611:VAL:HA	1:D:614:GLU:OE2	2.20	0.40
1:E:441:GLU:HA	1:E:444:LYS:HE3	2.03	0.40
1:E:469:VAL:HG13	1:E:469:VAL:O	2.21	0.40
1:F:381:THR:CG2	1:F:452:THR:HG22	2.52	0.40
1:G:274:ASN:N	1:G:357:THR:O	2.54	0.40
1:G:328:ASN:OD1	1:G:329:SER:N	2.55	0.40
2:H:493:ALA:HB1	2:H:497:GLU:HB2	2.04	0.40
2:H:499:LEU:HG	2:H:543:ILE:HG21	2.03	0.40
2:I:63:LEU:HD13	2:I:63:LEU:HA	1.88	0.40
2:I:266:ALA:O	2:I:269:GLU:HG3	2.22	0.40
1:A:549:GLU:N	1:A:549:GLU:OE1	2.54	0.40
1:B:199:LYS:HD2	1:B:199:LYS:HA	1.81	0.40
1:B:238:LYS:HZ1	1:B:253:HIS:C	2.21	0.40
1:B:472:ASP:OD1	1:B:473:THR:N	2.54	0.40
1:C:242:ARG:HG3	1:C:242:ARG:NH1	2.36	0.40
1:D:227:SER:O	1:D:227:SER:OG	2.36	0.40
1:D:505:ILE:HA	1:D:505:ILE:HD13	1.83	0.40
1:E:226:TRP:O	1:E:234:SER:HA	2.22	0.40
1:E:326:ASN:HB2	1:E:485:GLN:HE21	1.86	0.40
1:E:404:ILE:C	1:E:405:LEU:HD22	2.41	0.40
1:F:297:ARG:NH1	1:F:328:ASN:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:366:TYR:HE2	1:F:378:LEU:HG	1.87	0.40
1:G:203:LEU:HD13	1:G:203:LEU:HA	1.79	0.40
2:H:173:VAL:O	2:H:177:ILE:HG12	2.21	0.40
2:H:388:ILE:HG23	2:H:389:ASN:N	2.37	0.40
2:H:530:LYS:HB2	2:H:546:ASP:OD2	2.21	0.40
2:I:264:MET:O	2:I:267:ARG:HG2	2.21	0.40
2:J:237:ALA:CB	2:J:240:ALA:HB3	2.51	0.40
2:J:282:SER:HB3	2:J:513:TYR:OH	2.21	0.40
2:J:581:LYS:C	2:J:583:ILE:H	2.25	0.40
1:A:238:LYS:HZ3	1:A:254:PRO:HA	1.83	0.40
1:C:238:LYS:HD2	1:C:254:PRO:HA	2.02	0.40
1:C:366:TYR:HE2	1:C:378:LEU:HG	1.86	0.40
1:C:698:VAL:O	1:C:726:ILE:HB	2.21	0.40
1:D:228:THR:HG23	1:D:235:ASP:OD1	2.21	0.40
1:D:386:GLY:O	1:D:449:ARG:NH1	2.55	0.40
1:D:455:VAL:O	1:D:455:VAL:HG13	2.22	0.40
1:E:406:ALA:HB3	1:E:409:ASN:HD22	1.86	0.40
1:E:551:ASP:HB2	1:E:592:ARG:CG	2.51	0.40
1:F:521:MET:O	1:F:583:LEU:HD23	2.20	0.40
1:F:696:VAL:O	1:F:728:SER:HA	2.22	0.40
1:G:197:LYS:HB3	1:G:198:ASN:H	1.73	0.40
2:H:716:ASP:OD1	2:H:716:ASP:N	2.54	0.40
2:I:48:VAL:O	2:I:48:VAL:HG13	2.22	0.40
2:I:467:ILE:H	2:I:467:ILE:HD12	1.86	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%)	480 (92%)	39 (8%)	4 (1%)	19 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	523/759 (69%)	480 (92%)	42 (8%)	1 (0%)	47	80
1	C	523/759 (69%)	478 (91%)	44 (8%)	1 (0%)	47	80
1	D	522/759 (69%)	474 (91%)	45 (9%)	3 (1%)	25	64
1	E	523/759 (69%)	473 (90%)	49 (9%)	1 (0%)	47	80
1	F	523/759 (69%)	471 (90%)	50 (10%)	2 (0%)	34	72
1	G	523/759 (69%)	479 (92%)	42 (8%)	2 (0%)	34	72
2	H	695/809 (86%)	638 (92%)	52 (8%)	5 (1%)	22	62
2	I	700/809 (86%)	649 (93%)	51 (7%)	0	100	100
2	J	649/809 (80%)	604 (93%)	44 (7%)	1 (0%)	47	80
All	All	5704/7740 (74%)	5226 (92%)	458 (8%)	20 (0%)	38	72

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	B	198	ASN
1	C	198	ASN
1	D	198	ASN
1	E	198	ASN
2	H	67	PRO
2	H	90	LYS
2	J	582	LEU
1	A	663	LEU
1	F	199	LYS
2	H	101	LYS
1	A	345	THR
1	D	175	VAL
1	G	199	LYS
2	H	640	ALA
1	A	175	VAL
1	F	633	LYS
1	D	633	LYS
1	G	577	VAL
2	H	639	ILE

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	410/683 (60%)	409 (100%)	1 (0%)	93	96
1	B	415/683 (61%)	411 (99%)	4 (1%)	76	86
1	C	415/683 (61%)	413 (100%)	2 (0%)	88	93
1	D	414/683 (61%)	412 (100%)	2 (0%)	88	93
1	E	415/683 (61%)	410 (99%)	5 (1%)	71	83
1	F	415/683 (61%)	413 (100%)	2 (0%)	88	93
1	G	415/683 (61%)	415 (100%)	0	100	100
2	H	544/739 (74%)	539 (99%)	5 (1%)	78	87
2	I	338/739 (46%)	336 (99%)	2 (1%)	86	92
2	J	274/739 (37%)	271 (99%)	3 (1%)	73	84
All	All	4055/6998 (58%)	4029 (99%)	26 (1%)	86	92

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	636	ARG
1	B	200	ARG
1	B	233	TYR
1	B	242	ARG
1	B	633	LYS
1	C	233	TYR
1	C	387	LYS
1	D	213	LYS
1	D	633	LYS
1	E	233	TYR
1	E	359	ARG
1	E	563	LYS
1	E	633	LYS
1	E	636	ARG
1	F	524	LYS
1	F	563	LYS

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Mol	Chain	Res	Type
2	H	413	LYS
2	H	434	LYS
2	H	579	TYR
2	H	594	ASN
2	H	607	LYS
2	I	122	LYS
2	I	270	LYS
2	J	75	LYS
2	J	122	LYS
2	J	248	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	485	GLN
1	B	541	GLN
1	C	246	ASN
1	C	573	ASN
1	C	705	ASN
1	D	422	ASN
1	D	447	GLN
1	D	705	ASN
1	G	437	ASN
1	G	438	GLN
1	G	616	HIS
2	H	115	HIS
2	H	117	HIS
2	H	417	GLN
2	H	563	GLN
2	H	604	ASN
2	H	690	HIS
2	I	469	ASN
2	I	594	ASN
2	J	228	GLN

5.3.3 RNA

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](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	517:THR	C	518:LYS	N	1.18
1	A	517:THR	C	518:LYS	N	1.17
1	F	517:THR	C	518:LYS	N	1.14
1	B	517:THR	C	518:LYS	N	1.11
1	G	517:THR	C	518:LYS	N	1.10
1	C	517:THR	C	518:LYS	N	1.09

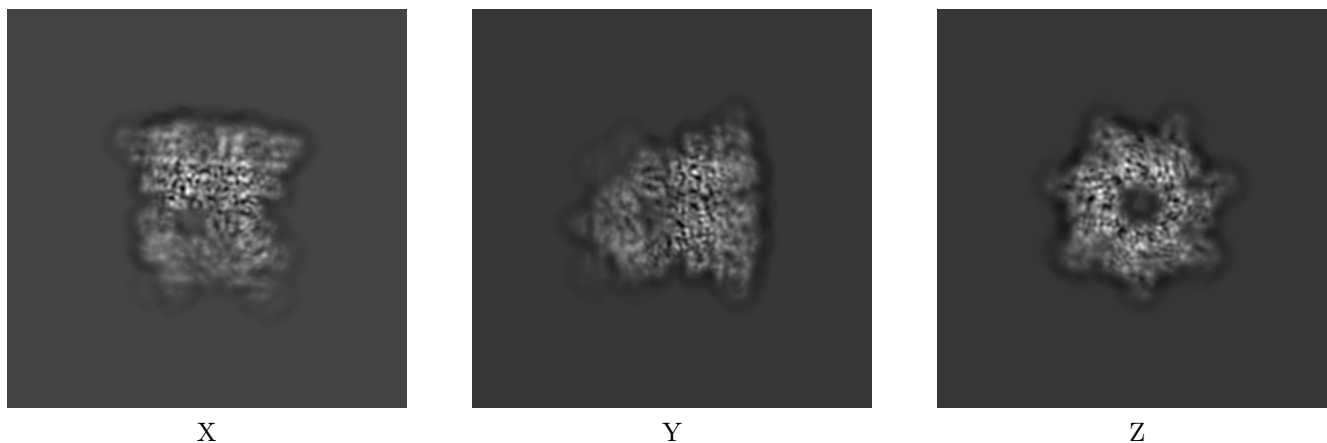
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11524. 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](#)

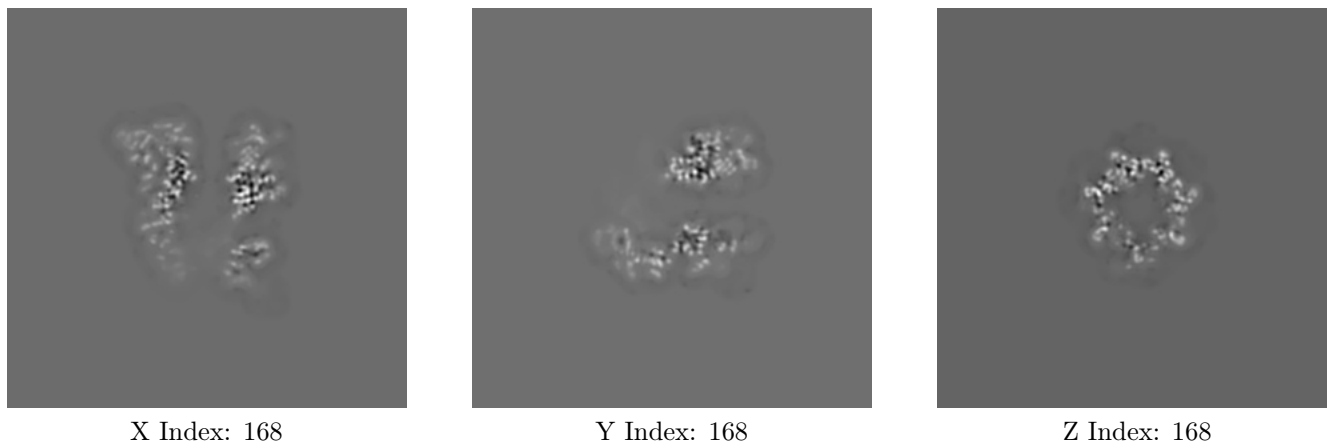
6.1.1 Primary map



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

6.2 Central slices [i](#)

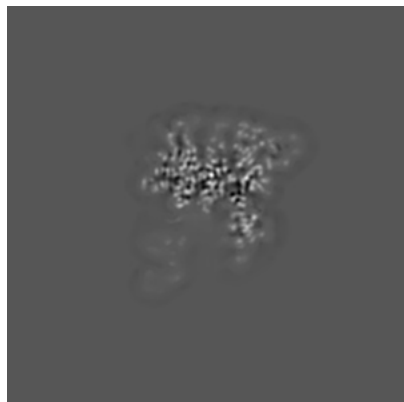
6.2.1 Primary map



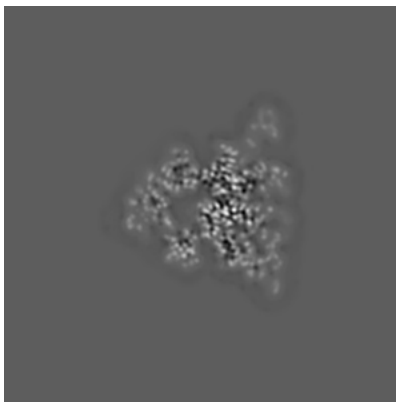
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

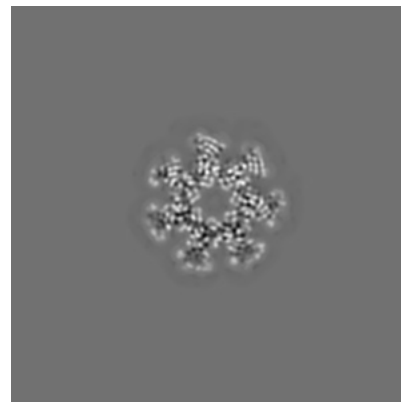
6.3.1 Primary map



X Index: 196



Y Index: 196

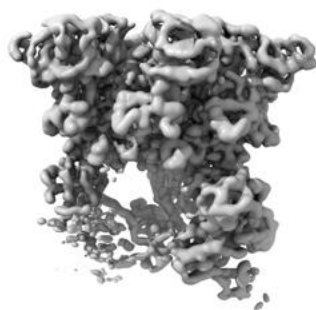


Z Index: 192

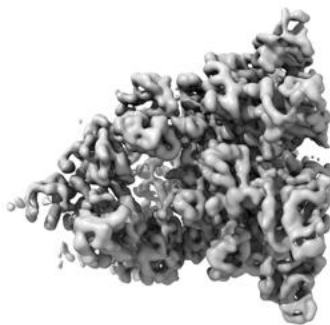
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

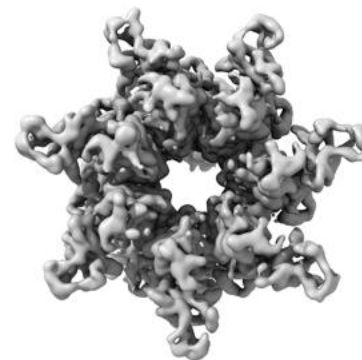
6.4.1 Primary map



X



Y



Z

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

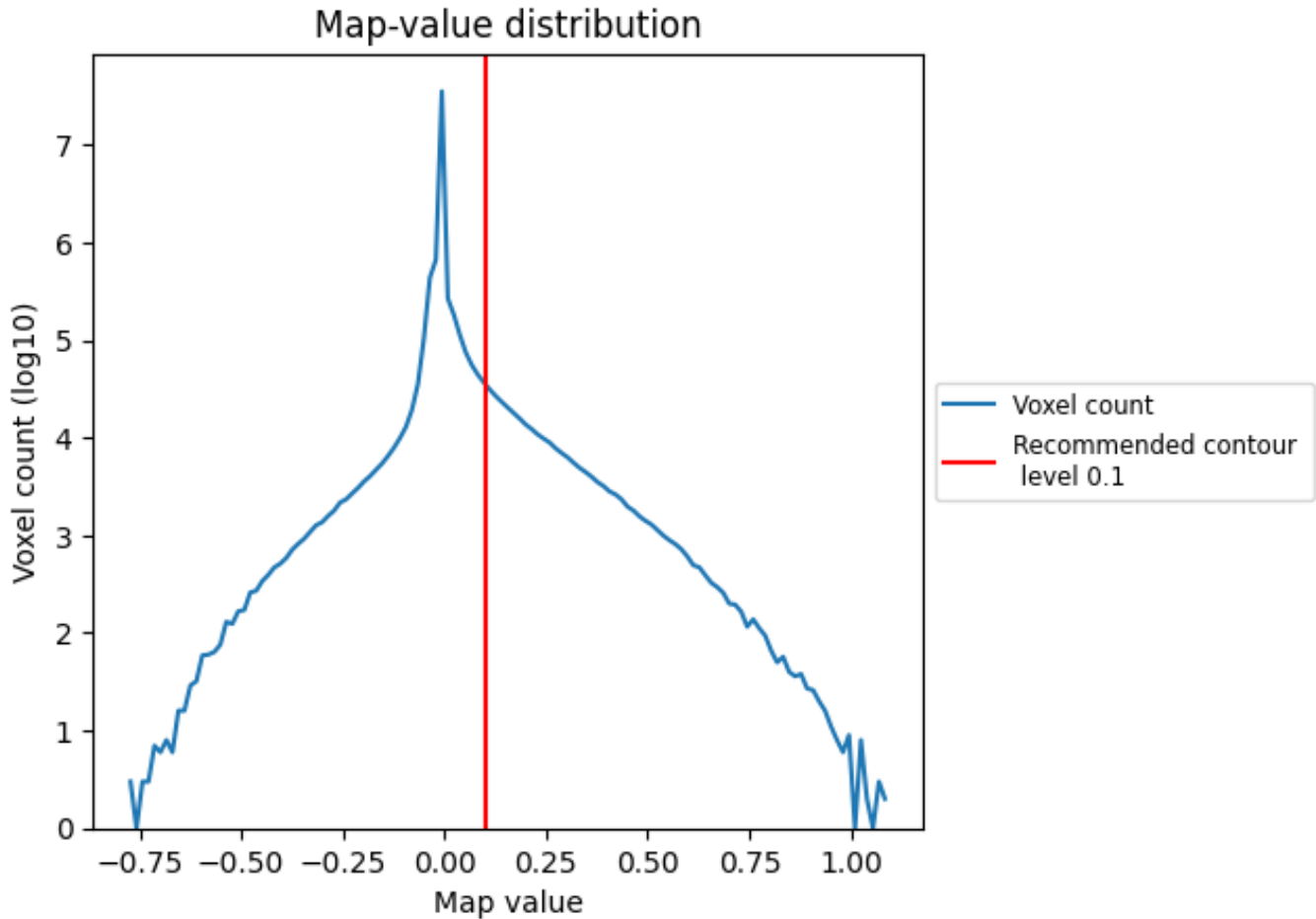
6.5 Mask visualisation

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

7 Map analysis [i](#)

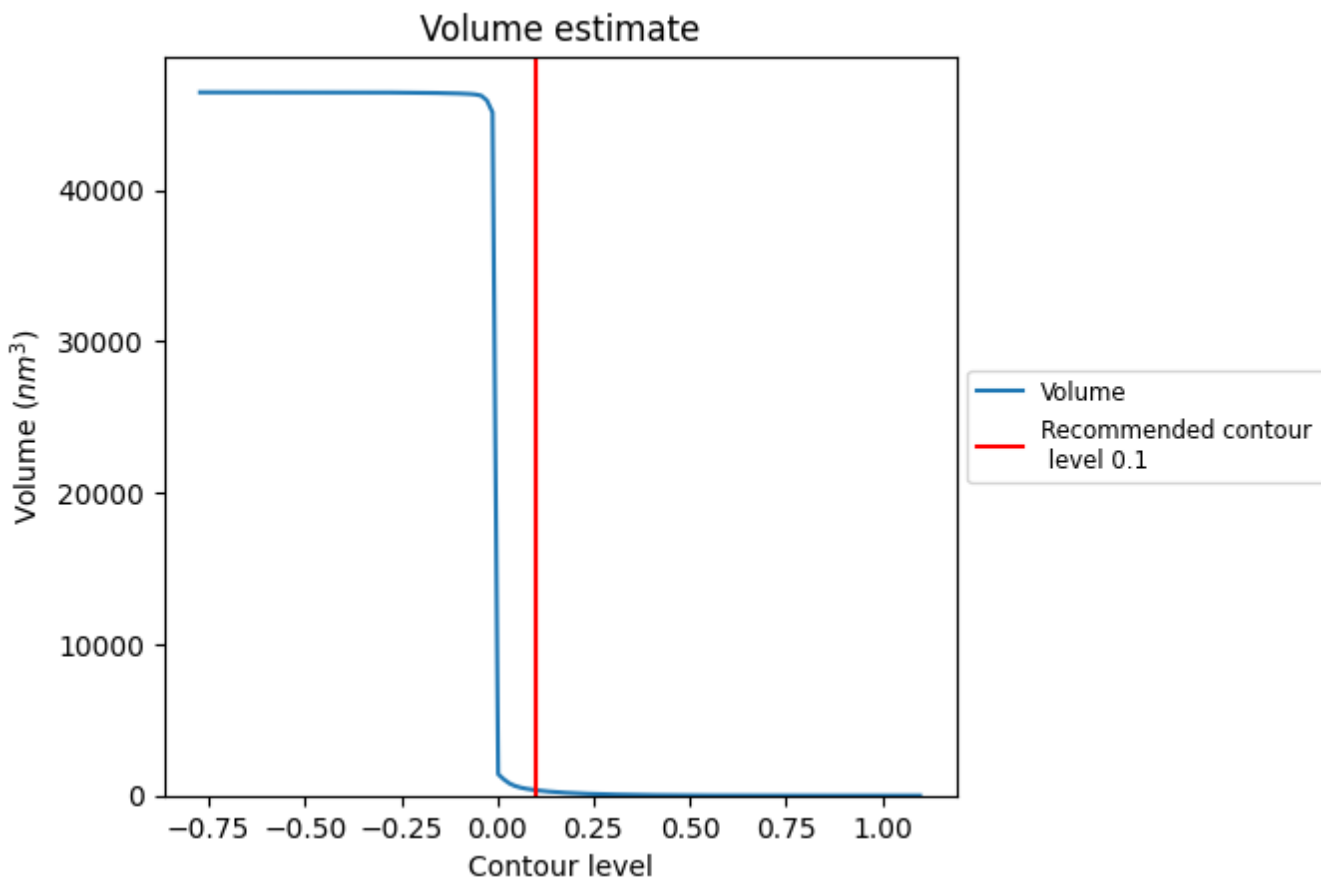
This section contains the results of statistical analysis of the map.

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.

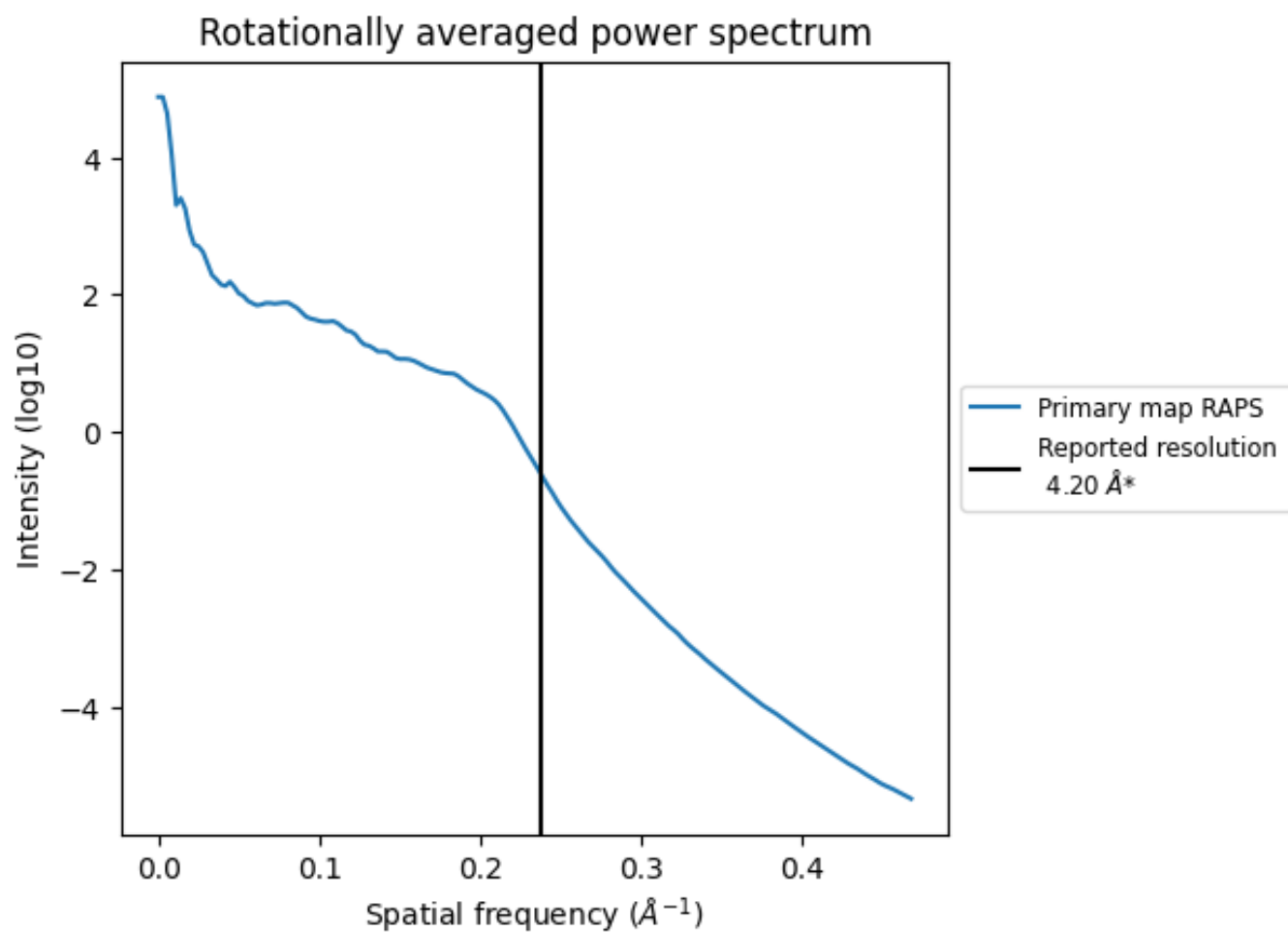
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 357 nm³; this corresponds to an approximate mass of 322 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 0.238\AA^{-1}

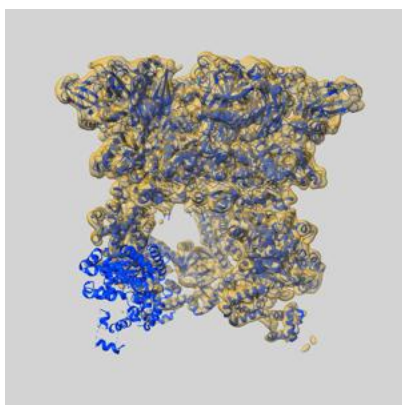
8 Fourier-Shell correlation

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

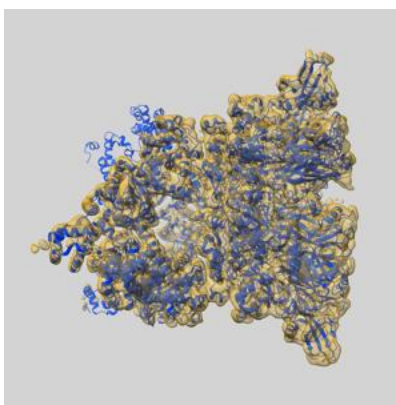
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11524 and PDB model 6ZXL. Per-residue inclusion information can be found in section 3 on page 9.

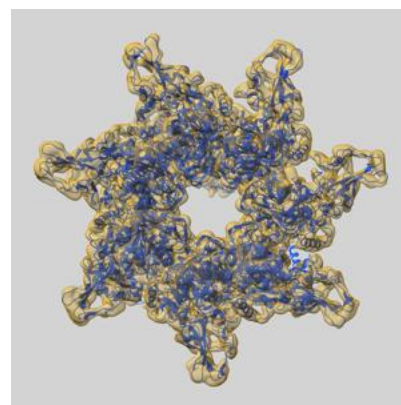
9.1 Map-model overlay [i](#)



X



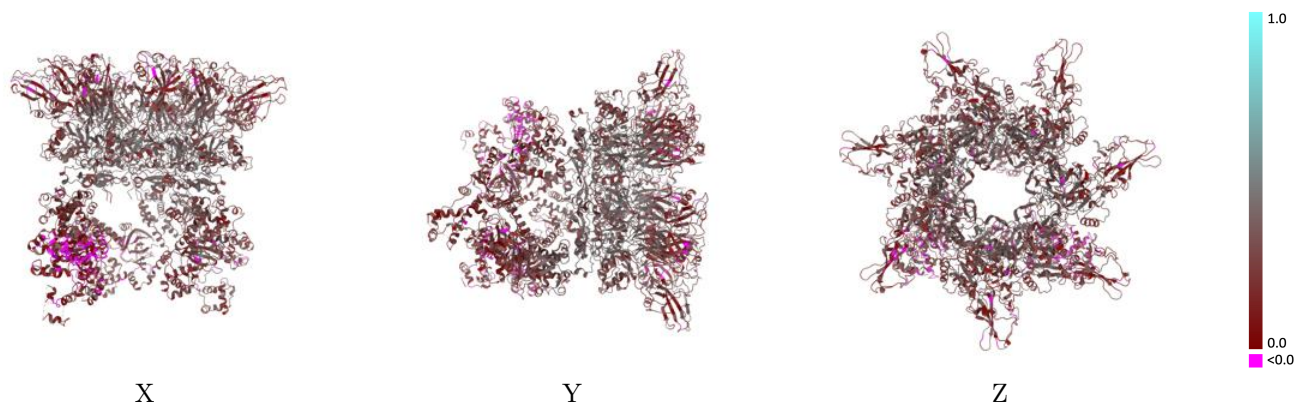
Y



Z

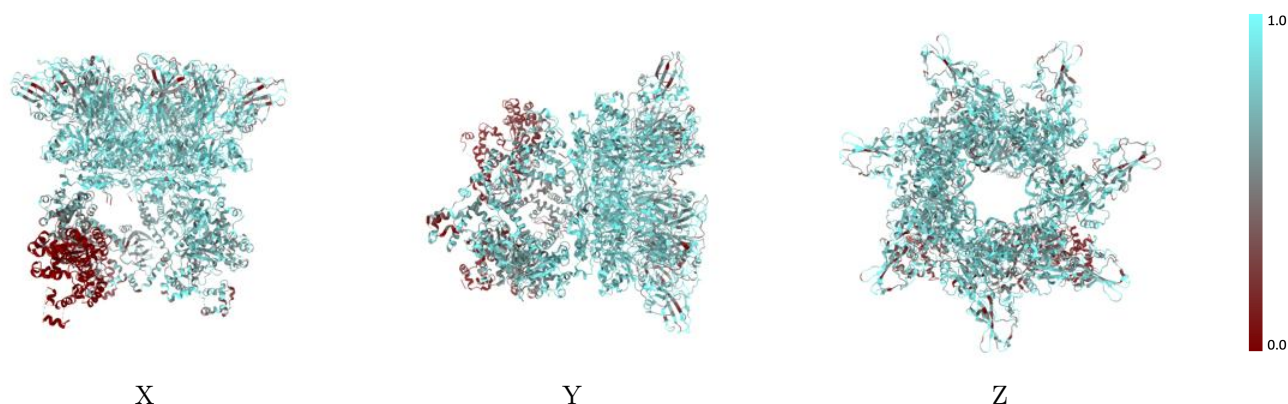
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



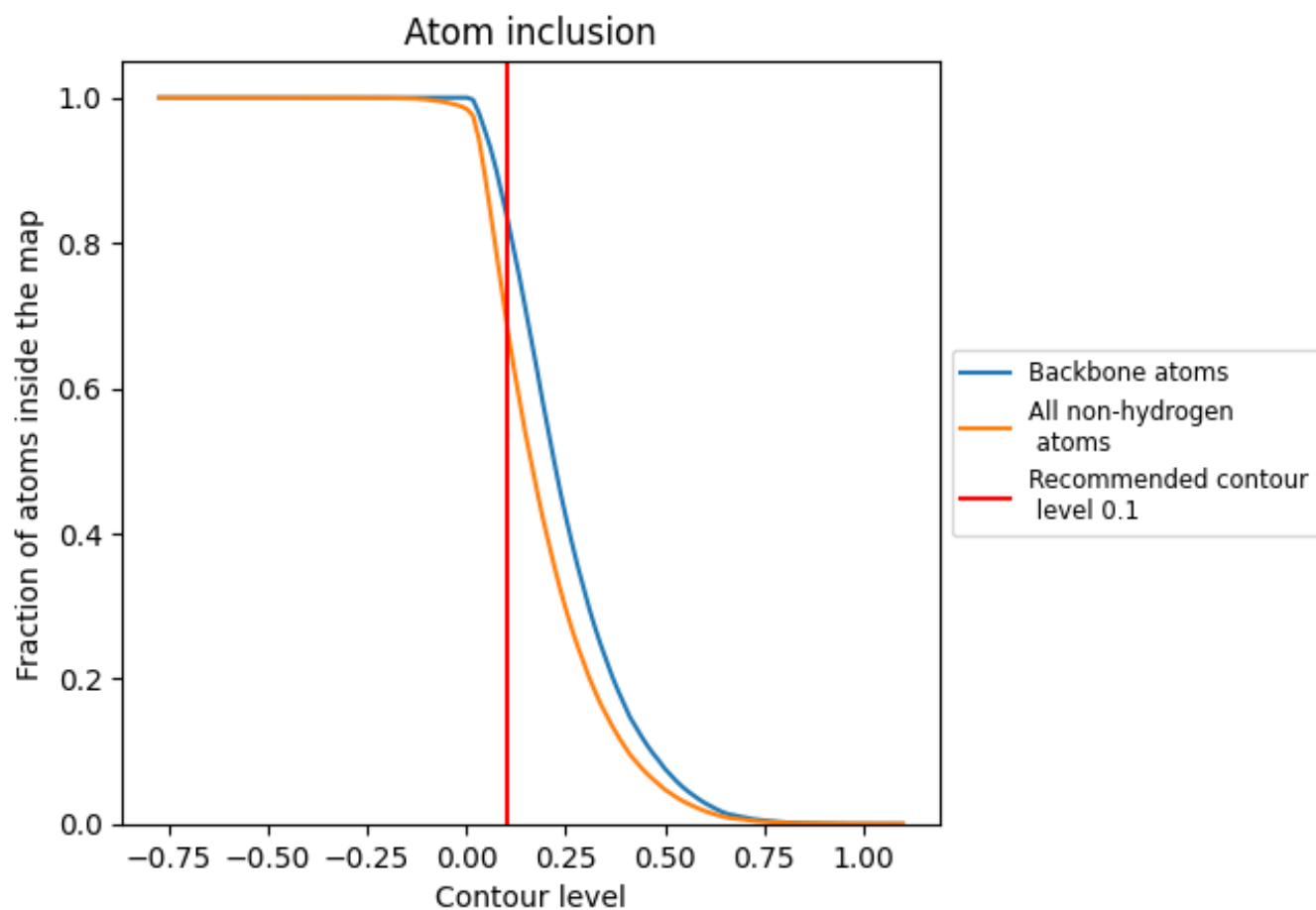
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 84% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.6953	 0.2870
A	 0.7667	 0.3190
B	 0.7815	 0.3230
C	 0.7853	 0.3270
D	 0.7852	 0.3280
E	 0.7728	 0.3160
F	 0.7848	 0.3240
G	 0.7697	 0.3130
H	 0.7001	 0.2540
I	 0.5939	 0.2320
J	 0.2631	 0.1620

