



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 09:52 AM UTC

PDB ID : 3J99 / pdb_00003j99
EMDB ID : EMD-6209
Title : Structure of 20S supercomplex determined by single particle cryoelectron microscopy (State IIIb)
Authors : Zhao, M.; Wu, S.; Cheng, Y.; Brunger, A.T.
Deposited on : 2014-12-05
Resolution : 8.20 Å (reported)
Based on initial models : 1NSF, 1QCS, 1N7S

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

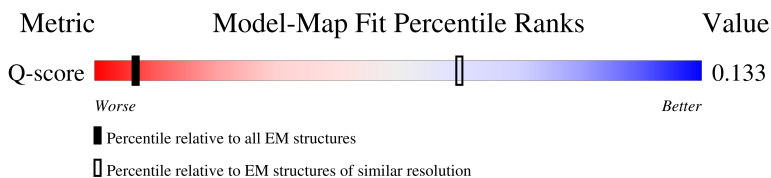
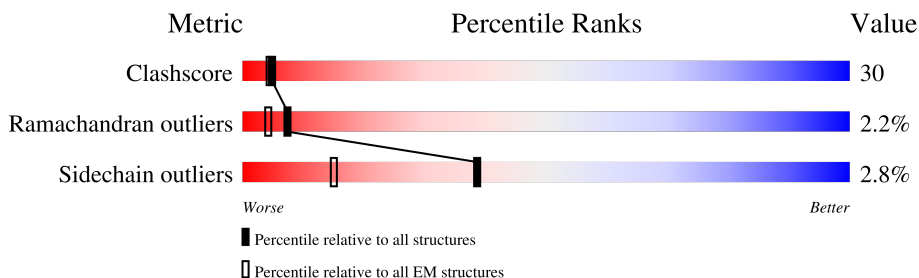
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.20 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.



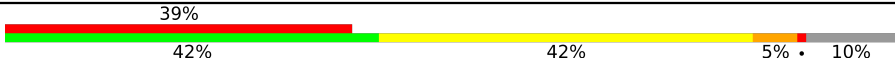
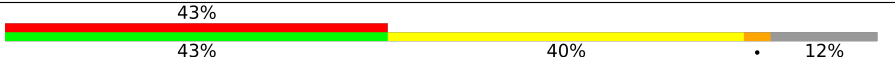
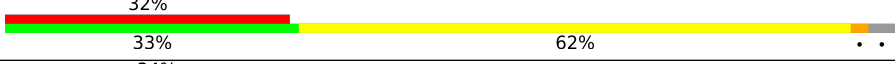
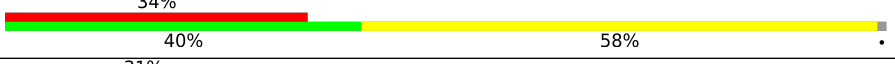
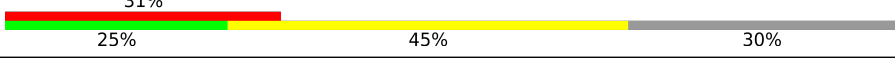
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	337 (7.70 - 8.70)

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	747	
1	B	747	
1	C	747	
1	D	747	

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Mol	Chain	Length	Quality of chain
1	E	747	
1	F	747	
2	G	297	
2	H	297	
2	I	297	
2	J	297	
3	K	63	
4	L	67	
5	M	188	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 40976 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 Vesicle-fusing ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	678	Total	C	N	O	S	0	0
			5039	3197	876	943	23		
1	B	672	Total	C	N	O	S	0	0
			4995	3168	863	940	24		
1	C	676	Total	C	N	O	S	0	0
			5027	3186	871	947	23		
1	D	673	Total	C	N	O	S	0	0
			4976	3157	856	939	24		
1	E	670	Total	C	N	O	S	0	0
			4992	3171	860	938	23		
1	F	654	Total	C	N	O	S	0	0
			4903	3112	849	918	24		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P18708
A	-1	ALA	-	expression tag	UNP P18708
A	0	HIS	-	expression tag	UNP P18708
B	-2	GLY	-	expression tag	UNP P18708
B	-1	ALA	-	expression tag	UNP P18708
B	0	HIS	-	expression tag	UNP P18708
C	-2	GLY	-	expression tag	UNP P18708
C	-1	ALA	-	expression tag	UNP P18708
C	0	HIS	-	expression tag	UNP P18708
D	-2	GLY	-	expression tag	UNP P18708
D	-1	ALA	-	expression tag	UNP P18708
D	0	HIS	-	expression tag	UNP P18708
E	-2	GLY	-	expression tag	UNP P18708
E	-1	ALA	-	expression tag	UNP P18708
E	0	HIS	-	expression tag	UNP P18708
F	-2	GLY	-	expression tag	UNP P18708
F	-1	ALA	-	expression tag	UNP P18708
F	0	HIS	-	expression tag	UNP P18708

- Molecule 2 is a protein called Alpha-soluble NSF attachment protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	286	Total	C	N	O	S	0	0
			2246	1415	373	441	17		
2	I	286	Total	C	N	O	S	0	0
			2249	1418	373	441	17		
2	J	286	Total	C	N	O	S	0	0
			2255	1424	373	441	17		
2	G	286	Total	C	N	O	S	0	0
			2249	1421	370	441	17		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	GLY	-	expression tag	UNP P54921
H	0	SER	-	expression tag	UNP P54921
I	-1	GLY	-	expression tag	UNP P54921
I	0	SER	-	expression tag	UNP P54921
J	-1	GLY	-	expression tag	UNP P54921
J	0	SER	-	expression tag	UNP P54921
G	-1	GLY	-	expression tag	UNP P54921
G	0	SER	-	expression tag	UNP P54921

- Molecule 3 is a protein called Vesicle-associated membrane protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	61	Total	C	N	O	S	0	0
			480	293	89	97	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	27	GLY	-	expression tag	UNP P63045

- Molecule 4 is a protein called Syntaxin-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	66	Total	C	N	O	S	0	0
			523	320	89	109	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	190	MET	-	expression tag	UNP P32851

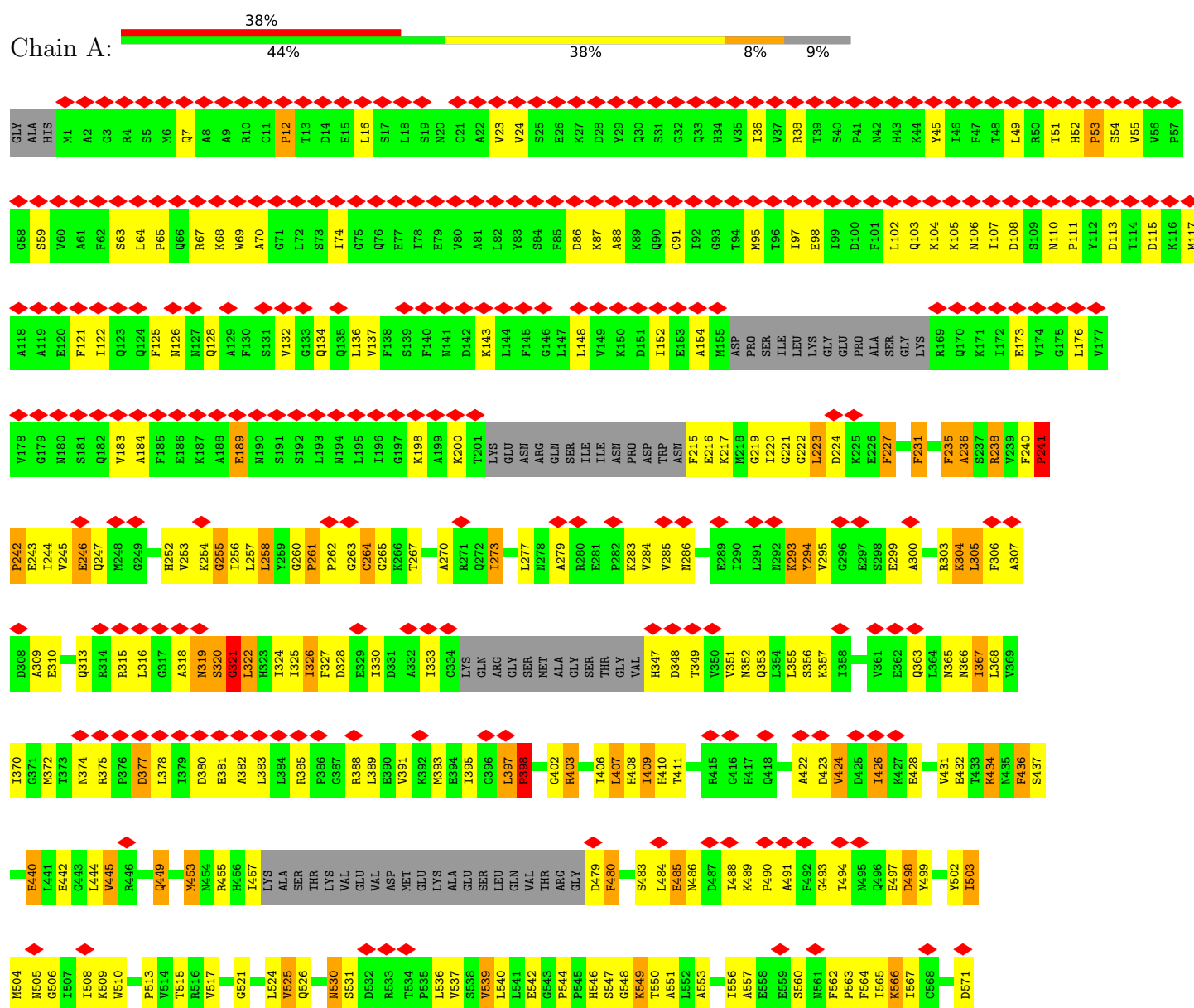
- Molecule 5 is a protein called Synaptosomal-associated protein 25.

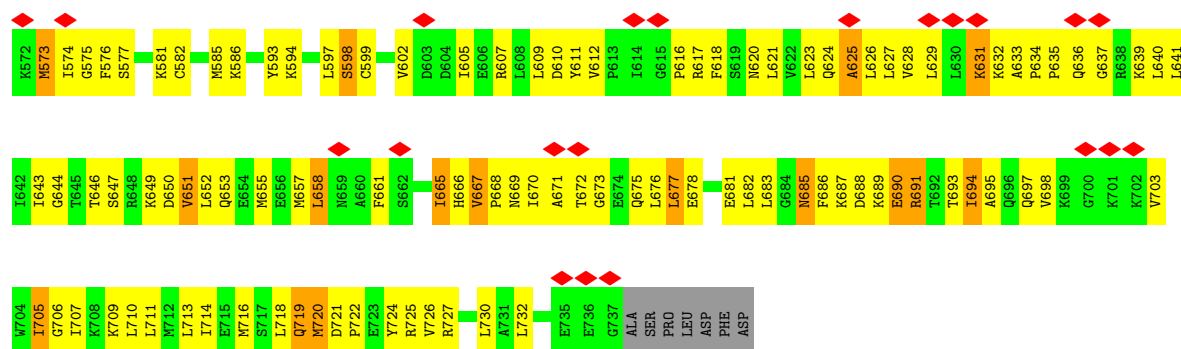
Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	131	Total	C	N	O	S	0	0
			1042	617	195	221	9		

3 Residue-property plots

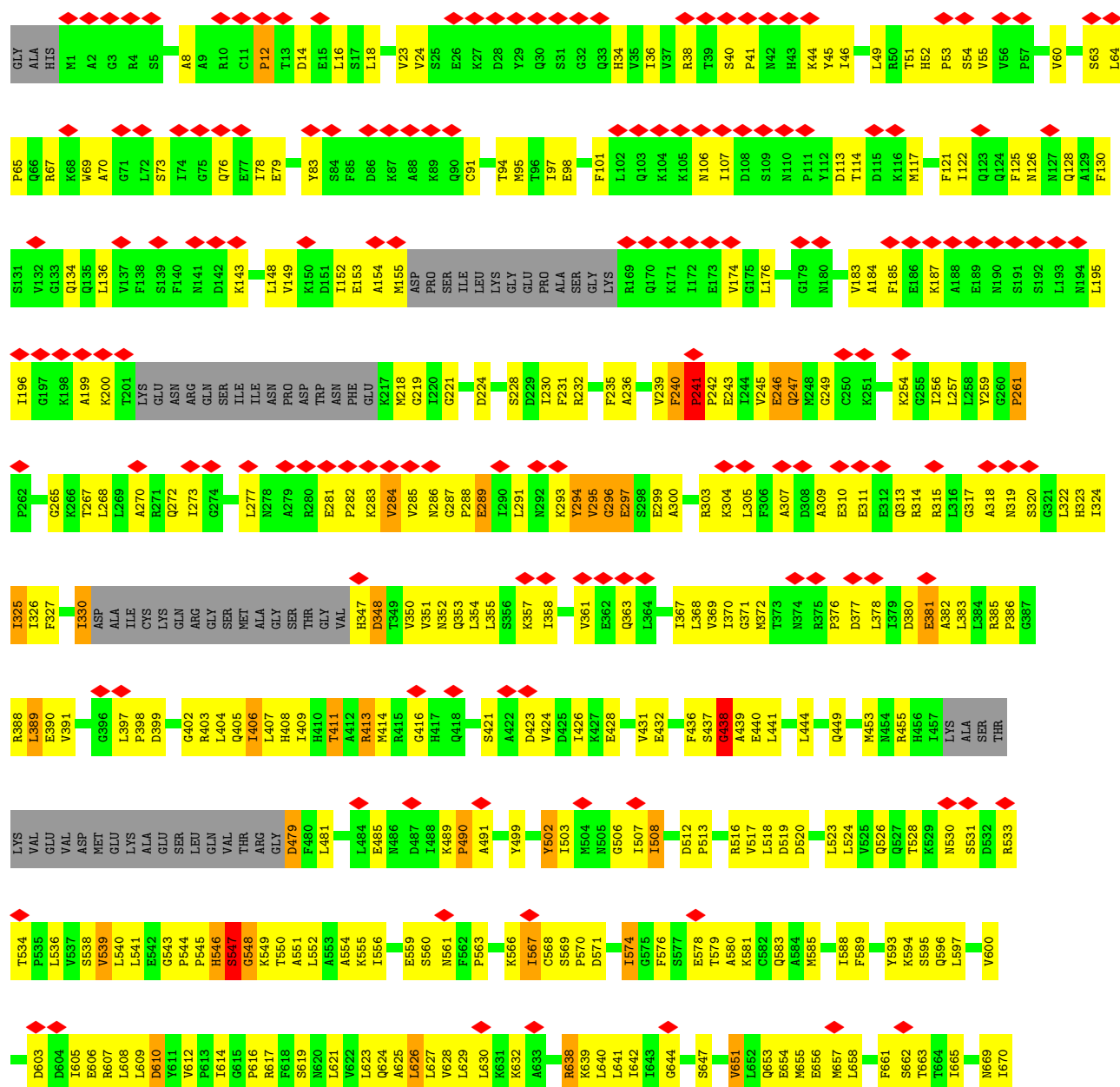
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

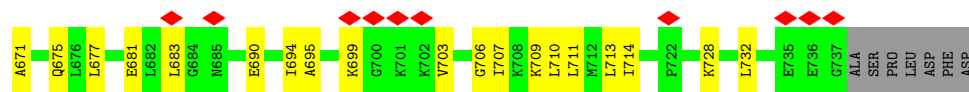
• Molecule 1: Vesicle-fusing ATPase



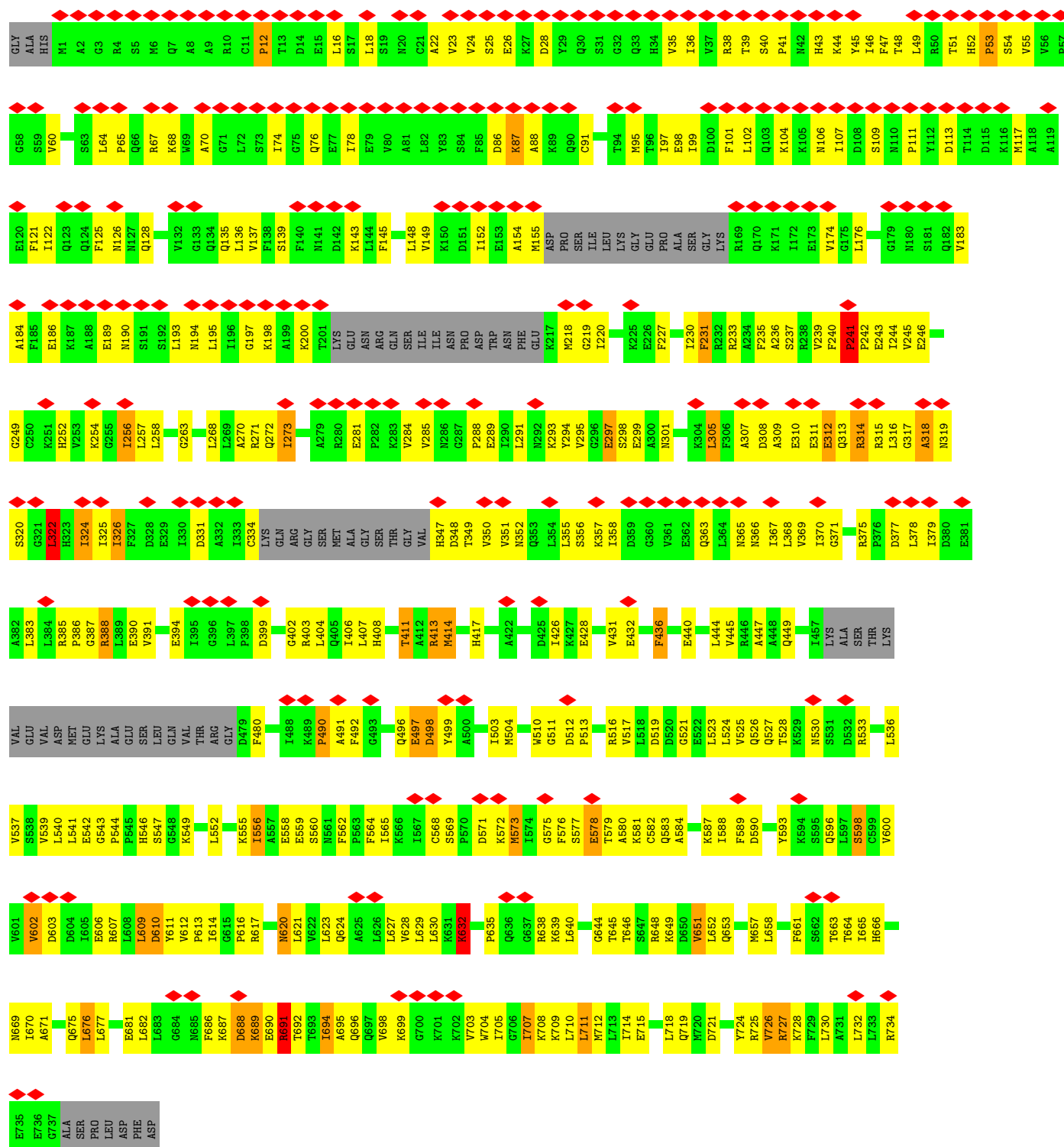
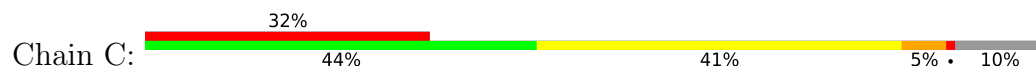


• Molecule 1: Vesicle-fusing ATPase

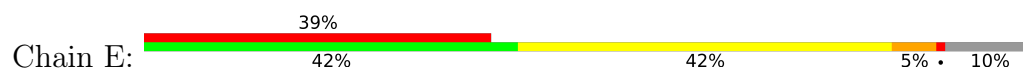




• Molecule 1: Vesicle-fusing ATPase

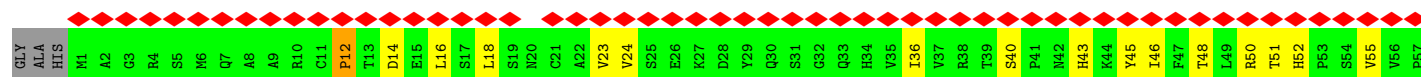


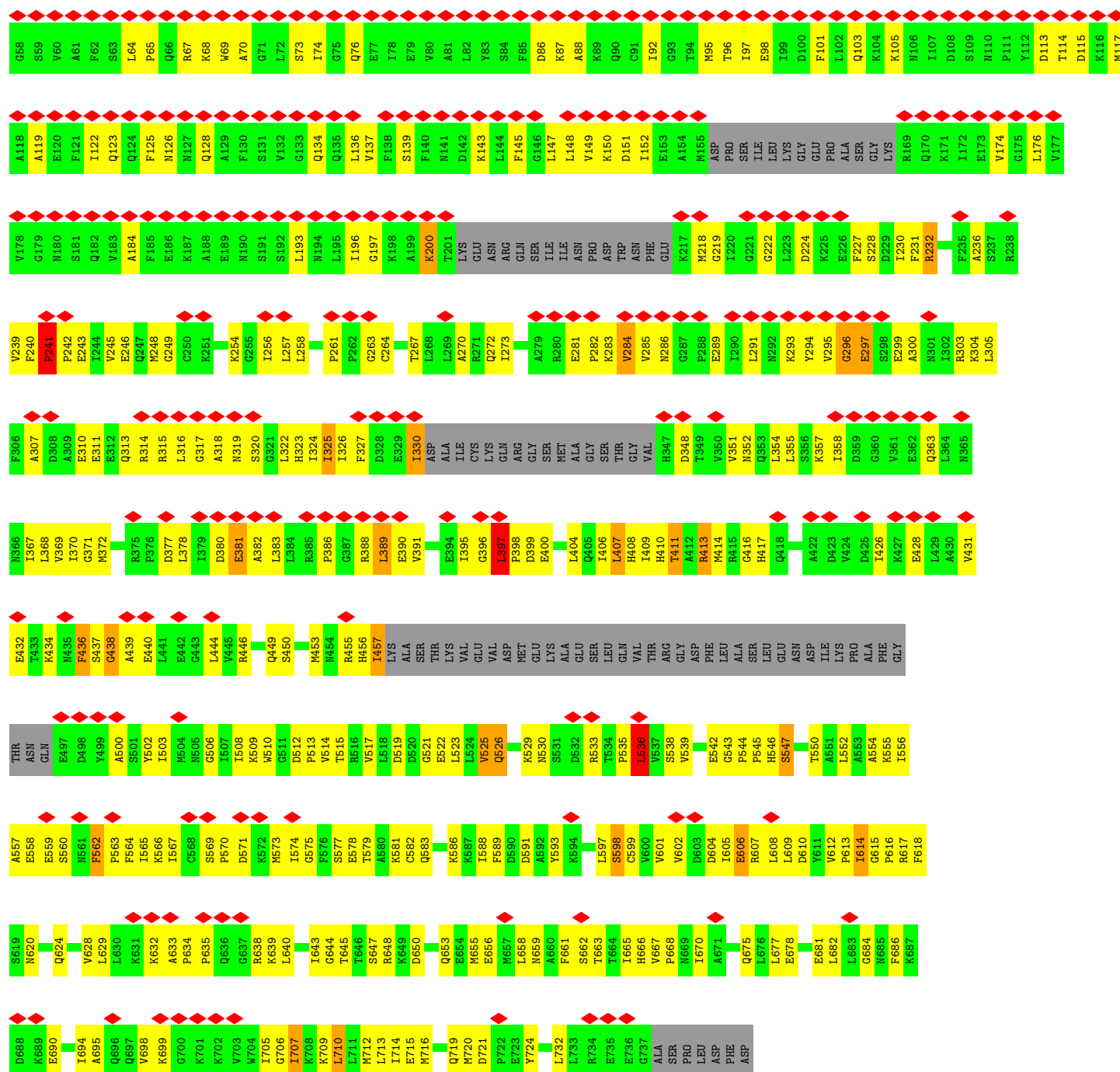
Chain D: 23% 44% 43% 10%



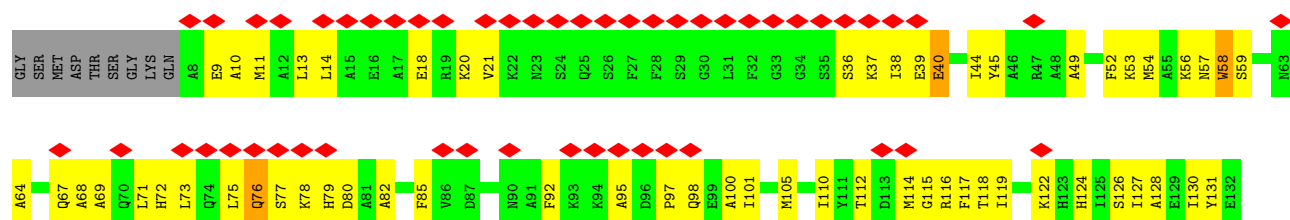
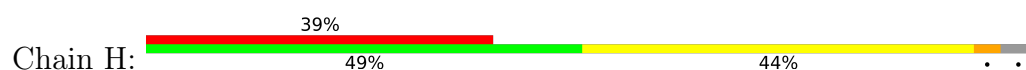


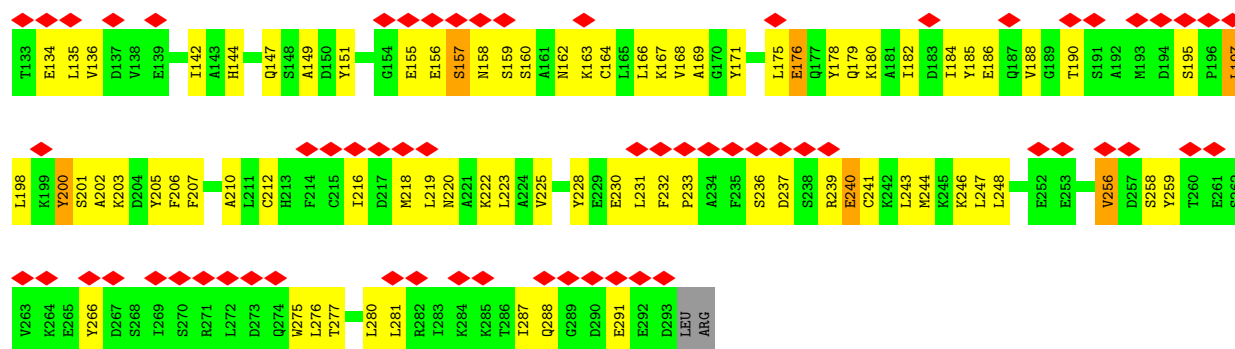
• Molecule 1: Vesicle-fusing ATPase



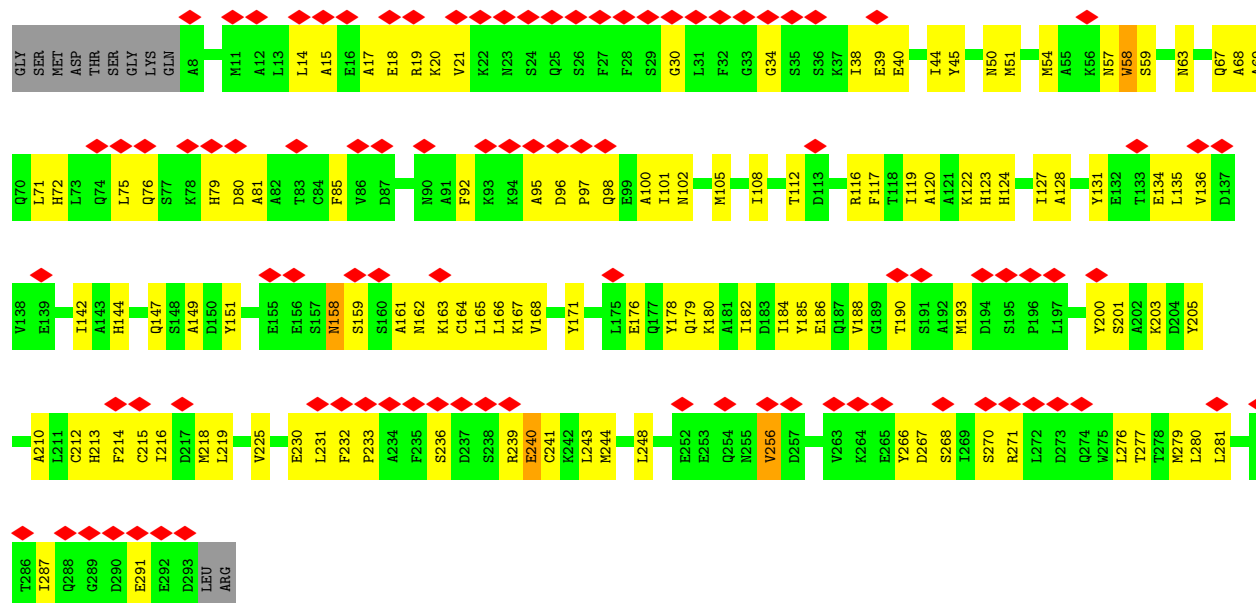


● Molecule 2: Alpha-soluble NSF attachment protein

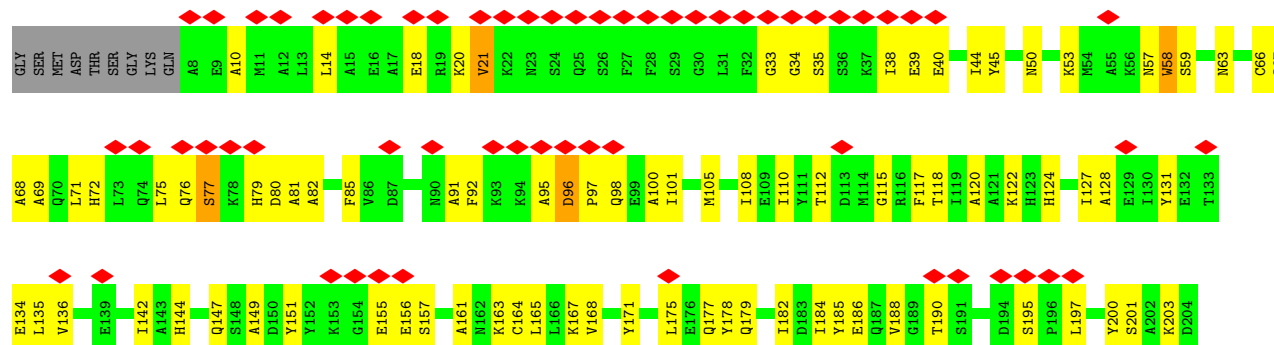


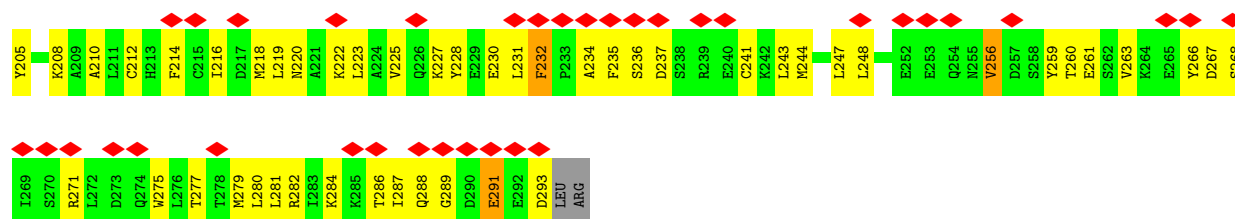


• Molecule 2: Alpha-soluble NSF attachment protein

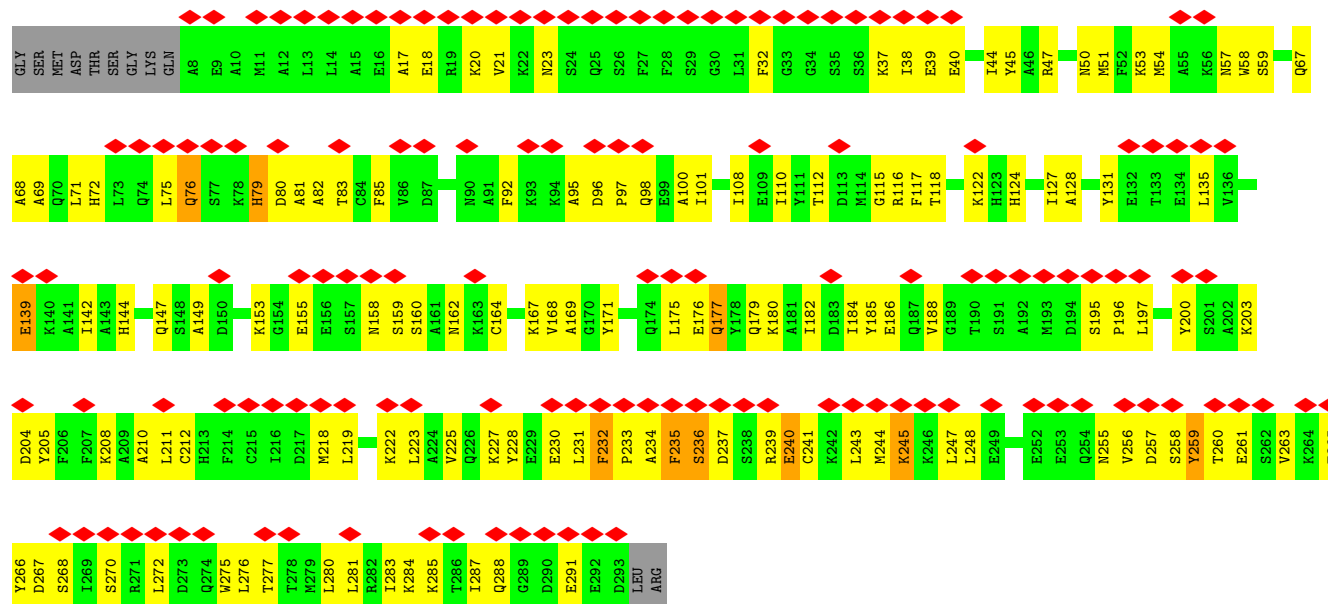


• Molecule 2: Alpha-soluble NSF attachment protein

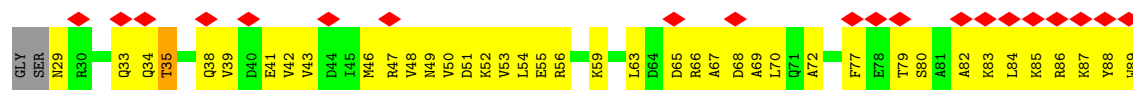




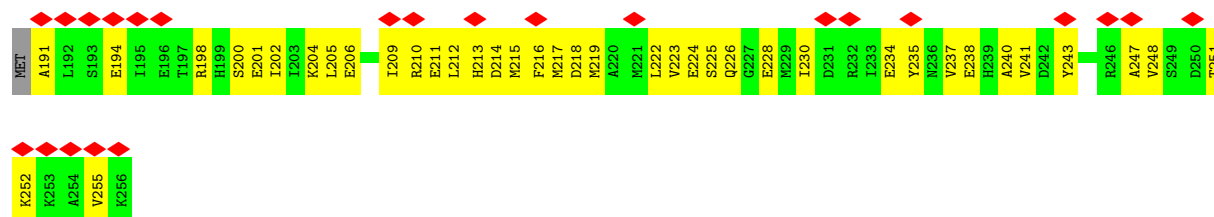
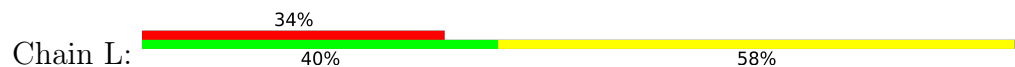
• Molecule 2: Alpha-soluble NSF attachment protein



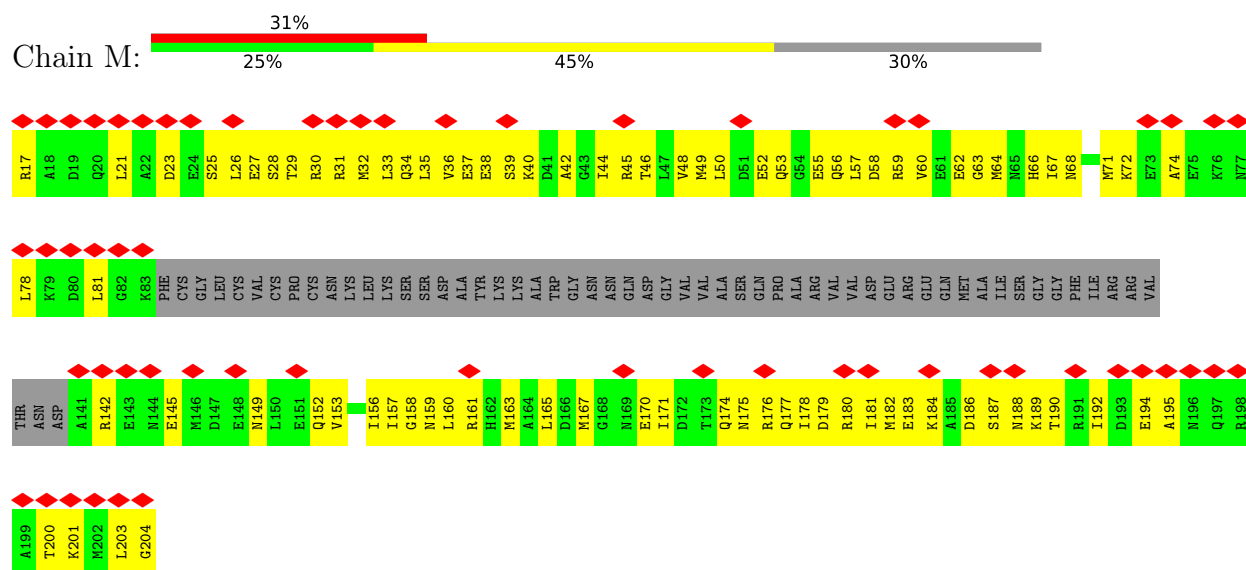
• Molecule 3: Vesicle-associated membrane protein 2



• Molecule 4: Syntaxin-1A



• Molecule 5: Synaptosomal-associated protein 25



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14991	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	-1800	Depositor
Maximum defocus (nm)	-2800	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	10.964	Depositor
Minimum map value	-5.319	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5	Depositor
Map size ($\text{\AA}$)	311.1936, 311.1936, 311.1936	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.4312, 2.4312, 2.4312	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.66	4/5116 (0.1%)	1.36	59/6925 (0.9%)
1	B	0.56	1/5069 (0.0%)	1.20	46/6863 (0.7%)
1	C	0.53	0/5102	1.18	35/6905 (0.5%)
1	D	0.57	0/5050	1.20	43/6840 (0.6%)
1	E	0.60	0/5068	1.23	50/6859 (0.7%)
1	F	0.58	1/4977 (0.0%)	1.21	40/6730 (0.6%)
2	G	0.46	0/2289	0.92	5/3079 (0.2%)
2	H	0.49	0/2285	0.93	2/3073 (0.1%)
2	I	0.44	0/2288	0.90	0/3077
2	J	0.45	0/2295	0.91	3/3086 (0.1%)
3	K	0.28	0/483	0.83	0/648
4	L	0.28	0/527	0.78	0/704
5	M	0.27	0/1042	0.83	0/1385
All	All	0.55	6/41591 (0.0%)	1.15	283/56174 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	E	0	1
1	F	0	1
2	H	0	1
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	547	SER	C-O	8.08	1.34	1.24
1	A	503	ILE	C-O	6.28	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	514	VAL	CA-CB	5.64	1.61	1.54
1	A	485	GLU	C-O	-5.56	1.17	1.24
1	A	330	ILE	CA-CB	5.43	1.61	1.54
1	A	321	GLY	N-CA	5.09	1.50	1.45

All (283) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ASN	N-CA-C	-16.40	84.15	109.07
1	A	549	LYS	N-CA-C	-14.90	95.04	111.28
1	A	236	ALA	N-CA-C	-13.65	96.46	111.07
1	A	261	PRO	CA-C-N	13.54	136.77	119.84
1	A	261	PRO	C-N-CA	13.54	136.77	119.84
1	E	231	PHE	N-CA-C	-12.08	98.15	111.07
1	B	544	PRO	N-CA-C	-11.90	99.05	110.47
1	C	413	ARG	N-CA-C	-11.85	98.36	111.28
1	B	287	GLY	CA-C-N	10.58	130.79	119.05
1	B	287	GLY	C-N-CA	10.58	130.79	119.05
1	F	547	SER	N-CA-C	-10.58	96.27	110.55
1	F	294	TYR	N-CA-C	10.52	122.83	111.36
1	D	416	GLY	N-CA-C	-10.49	99.80	112.49
1	F	543	GLY	CA-C-N	-10.45	109.62	120.38
1	F	543	GLY	C-N-CA	-10.45	109.62	120.38
1	A	241	PRO	N-CA-C	10.22	123.17	110.70
1	D	547	SER	CA-C-N	-10.16	103.72	121.00
1	D	547	SER	C-N-CA	-10.16	103.72	121.00
1	D	314	ARG	N-CA-C	-9.96	100.51	111.36
1	C	241	PRO	N-CA-C	9.62	122.44	110.70
1	C	504	MET	CA-C-N	-9.53	106.82	122.54
1	C	504	MET	C-N-CA	-9.53	106.82	122.54
1	F	241	PRO	N-CA-C	9.49	122.27	110.70
1	B	241	PRO	N-CA-C	9.44	122.22	110.70
1	A	238	ARG	N-CA-C	9.34	121.23	111.14
1	A	484	LEU	N-CA-C	-9.12	101.34	111.28
1	B	231	PHE	N-CA-C	-9.01	101.44	111.07
1	F	514	VAL	N-CA-C	-8.96	101.82	110.42
1	C	543	GLY	CA-C-N	8.95	126.19	119.66
1	C	543	GLY	C-N-CA	8.95	126.19	119.66
1	A	216	GLU	N-CA-C	-8.85	96.34	109.62
1	F	396	GLY	N-CA-C	8.77	123.26	112.73
1	E	241	PRO	N-CA-C	8.75	121.37	110.70
1	A	273	ILE	N-CA-C	-8.72	102.33	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	PHE	N-CA-C	-8.61	101.89	111.28
1	D	544	PRO	CA-C-N	8.55	130.52	119.84
1	D	544	PRO	C-N-CA	8.55	130.52	119.84
1	A	260	GLY	CA-C-N	8.45	129.08	120.38
1	A	260	GLY	C-N-CA	8.45	129.08	120.38
1	C	620	ASN	N-CA-C	8.44	120.48	111.28
1	C	231	PHE	N-CA-C	-8.31	102.22	111.28
1	A	625	ALA	N-CA-C	-8.20	102.34	111.28
1	A	277	LEU	N-CA-C	8.19	120.29	111.36
1	B	544	PRO	CB-CA-C	8.07	118.98	111.39
1	F	416	GLY	N-CA-C	-7.98	102.84	112.49
1	C	314	ARG	N-CA-C	-7.95	102.61	111.28
1	D	241	PRO	N-CA-C	7.85	120.28	110.70
1	A	455	ARG	N-CA-C	7.72	119.70	111.28
1	B	295	VAL	N-CA-C	7.66	117.77	110.42
1	A	304	LYS	N-CA-C	7.61	119.21	111.07
1	C	688	ASP	N-CA-C	7.55	119.14	111.07
1	E	413	ARG	N-CA-C	-7.49	103.12	111.28
1	E	649	LYS	N-CA-C	7.48	119.22	111.14
1	E	295	VAL	N-CA-C	7.48	119.14	110.62
1	A	488	ILE	N-CA-C	7.38	121.28	112.80
1	F	525	VAL	CB-CA-C	-7.30	102.62	111.97
1	A	694	ILE	N-CA-C	-7.28	103.37	110.72
1	C	691	ARG	N-CA-C	-7.25	103.38	111.28
1	D	643	ILE	CB-CA-C	-7.25	99.91	110.63
1	E	294	TYR	N-CA-C	7.24	119.25	111.36
1	B	413	ARG	N-CA-C	-7.22	103.41	111.28
1	E	287	GLY	CA-C-N	7.22	127.06	119.05
1	E	287	GLY	C-N-CA	7.22	127.06	119.05
1	D	312	GLU	N-CA-C	7.21	118.78	111.07
1	E	416	GLY	N-CA-C	-7.21	103.77	112.49
1	B	294	TYR	N-CA-C	7.18	119.18	111.36
1	B	530	ASN	N-CA-C	7.17	119.09	111.28
1	C	632	LYS	N-CA-C	7.10	120.52	110.50
1	E	603	ASP	N-CA-C	7.04	120.99	109.72
1	A	422	ALA	N-CA-C	6.98	118.97	111.36
1	B	543	GLY	N-CA-C	-6.97	98.13	112.34
1	F	231	PHE	N-CA-C	-6.94	103.64	111.07
1	C	394	GLU	CA-C-N	-6.93	114.60	123.19
1	C	394	GLU	C-N-CA	-6.93	114.60	123.19
1	D	512	ASP	N-CA-C	-6.86	103.42	113.16
1	F	413	ARG	N-CA-C	-6.83	103.83	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	512	ASP	N-CA-C	-6.83	103.46	113.16
1	A	436	PHE	N-CA-C	6.82	120.37	110.28
1	A	598	SER	N-CA-C	6.81	120.27	108.76
1	A	685	ASN	N-CA-C	6.81	118.78	111.36
1	C	598	SER	N-CA-C	6.72	118.42	108.60
1	D	609	LEU	CA-C-N	6.70	131.87	122.36
1	D	609	LEU	C-N-CA	6.70	131.87	122.36
1	F	563	PRO	N-CA-C	-6.70	104.42	113.40
1	B	539	VAL	N-CA-C	6.64	117.68	108.12
1	B	651	VAL	CB-CA-C	-6.59	103.24	112.14
1	C	387	GLY	N-CA-C	-6.58	97.58	113.18
1	A	551	ALA	CA-C-N	6.55	129.59	120.29
1	A	551	ALA	C-N-CA	6.55	129.59	120.29
1	A	258	LEU	CA-C-N	-6.55	113.76	122.99
1	A	258	LEU	C-N-CA	-6.55	113.76	122.99
1	A	434	LYS	N-CA-C	-6.41	106.05	114.31
1	F	515	THR	N-CA-C	6.40	118.34	111.36
1	B	406	ILE	CB-CA-C	-6.38	103.41	112.22
1	C	726	VAL	N-CA-C	6.34	117.09	110.62
1	A	530	ASN	N-CA-C	6.33	121.14	113.17
1	E	548	GLY	CA-C-N	6.32	128.74	120.28
1	E	548	GLY	C-N-CA	6.32	128.74	120.28
1	C	436	PHE	N-CA-C	6.31	119.38	110.23
1	C	689	LYS	N-CA-C	6.30	118.14	111.28
1	D	238	ARG	N-CA-C	6.28	118.20	111.36
1	C	239	VAL	N-CA-C	6.26	117.05	110.72
1	C	694	ILE	N-CA-C	-6.25	104.25	110.62
1	D	642	ILE	N-CA-C	6.22	116.82	108.11
1	B	348	ASP	CB-CA-C	-6.21	109.42	116.63
1	F	598	SER	N-CA-C	6.21	118.29	108.79
1	A	480	PHE	CB-CA-C	-6.20	109.41	116.54
1	C	363	GLN	CB-CA-C	-6.17	109.47	116.63
1	B	610	ASP	N-CA-CB	-6.14	102.86	112.13
1	B	574	ILE	N-CA-C	6.14	117.34	109.30
1	A	391	VAL	N-CA-C	6.13	116.69	108.11
1	A	330	ILE	N-CA-C	-6.13	104.37	110.62
1	A	363	GLN	CB-CA-C	-6.12	109.53	116.63
1	E	235	PHE	N-CA-C	6.11	118.02	111.36
1	A	279	ALA	N-CA-C	-6.10	100.06	109.52
1	B	543	GLY	CA-C-N	6.09	124.10	119.66
1	B	543	GLY	C-N-CA	6.09	124.10	119.66
2	G	235	PHE	N-CA-CB	-6.08	102.21	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	363	GLN	CB-CA-C	-6.06	109.60	116.63
1	B	299	GLU	N-CA-C	-6.05	104.68	111.28
1	E	670	ILE	CB-CA-C	-6.04	101.75	111.59
1	B	550	THR	N-CA-C	-6.03	104.79	111.36
2	G	236	SER	N-CA-C	-6.01	104.07	111.40
1	F	363	GLN	CB-CA-C	-6.01	109.66	116.63
2	H	197	LEU	N-CA-C	-6.00	105.27	113.30
1	F	348	ASP	CB-CA-C	-5.99	109.68	116.63
1	B	544	PRO	CA-C-O	-5.99	116.59	120.90
1	A	398	PRO	CA-N-CD	-5.97	103.65	112.00
1	B	416	GLY	N-CA-C	-5.94	105.31	112.49
1	D	312	GLU	CA-C-N	5.93	128.51	120.38
1	D	312	GLU	C-N-CA	5.93	128.51	120.38
1	E	625	ALA	N-CA-C	-5.91	104.84	111.28
1	A	403	ARG	N-CA-C	-5.88	104.87	111.28
1	E	348	ASP	CB-CA-C	-5.87	109.83	116.63
1	A	503	ILE	O-C-N	5.86	127.86	121.83
1	B	240	PHE	CA-C-N	5.86	126.41	120.38
1	B	240	PHE	C-N-CA	5.86	126.41	120.38
1	B	547	SER	O-C-N	5.85	130.37	122.59
1	B	289	GLU	N-CA-C	-5.85	104.81	111.07
1	D	546	HIS	N-CA-C	-5.84	104.77	112.24
1	A	453	MET	N-CA-C	-5.83	104.93	111.28
1	D	493	GLY	N-CA-C	-5.83	107.64	115.21
1	A	426	ILE	N-CA-C	5.82	116.01	110.42
1	D	294	TYR	N-CA-C	5.82	119.48	112.38
1	B	544	PRO	O-C-N	5.81	123.98	121.31
1	D	599	CYS	N-CA-C	5.79	118.34	108.90
1	B	548	GLY	N-CA-C	-5.77	99.50	113.18
1	E	550	THR	N-CA-C	5.77	117.65	111.36
1	D	403	ARG	N-CA-C	-5.75	105.01	111.28
1	E	363	GLN	CB-CA-C	-5.75	109.96	116.63
1	D	394	GLU	CA-C-N	-5.75	116.07	123.19
1	D	394	GLU	C-N-CA	-5.75	116.07	123.19
1	F	526	GLN	N-CA-C	-5.75	104.92	111.07
1	E	718	LEU	N-CA-C	5.73	117.52	111.28
1	A	349	THR	N-CA-C	5.71	117.51	111.28
1	A	407	LEU	N-CA-C	-5.70	105.07	111.28
2	G	258	SER	N-CA-C	-5.70	106.17	113.23
1	E	227	PHE	N-CA-C	-5.69	105.08	111.28
1	E	349	THR	N-CA-C	5.67	117.46	111.28
1	F	397	LEU	CA-CB-CG	5.67	136.15	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	709	LYS	N-CA-C	-5.67	105.10	111.28
1	B	363	GLN	CB-CA-C	-5.66	110.06	116.63
1	D	598	SER	N-CA-C	5.66	117.88	108.99
1	C	480	PHE	CB-CA-C	-5.66	110.06	116.63
1	C	406	ILE	CB-CA-C	-5.63	104.65	112.02
1	D	647	SER	N-CA-C	5.62	117.41	111.28
1	E	629	LEU	N-CA-C	5.62	117.40	111.28
1	C	230	ILE	CA-C-N	5.61	127.80	120.28
1	C	230	ILE	C-N-CA	5.61	127.80	120.28
1	E	714	ILE	CB-CA-C	-5.61	104.78	111.97
1	A	241	PRO	C-N-CD	5.57	132.86	120.60
1	E	480	PHE	CB-CA-C	-5.57	110.17	116.63
1	F	241	PRO	C-N-CD	5.57	132.85	120.60
1	F	299	GLU	N-CA-C	-5.57	105.21	111.28
1	F	455	ARG	N-CA-C	-5.56	105.22	111.28
1	C	727	ARG	N-CA-C	-5.54	105.24	111.28
1	B	405	GLN	N-CA-C	5.54	117.00	111.07
1	E	570	PRO	N-CA-C	-5.54	105.83	113.53
1	B	235	PHE	N-CA-C	5.53	118.49	111.69
1	F	562	PHE	CA-C-N	5.52	124.87	118.85
1	F	562	PHE	C-N-CA	5.52	124.87	118.85
1	F	533	ARG	N-CA-C	5.52	117.30	111.28
1	E	438	GLY	N-CA-C	5.50	126.22	113.18
1	E	585	MET	N-CA-C	-5.48	105.31	111.28
2	G	272	LEU	N-CA-C	5.45	118.18	110.50
1	A	235	PHE	CA-CB-CG	-5.44	108.36	113.80
1	A	227	PHE	N-CA-C	-5.43	105.36	111.28
1	C	348	ASP	CB-CA-C	-5.41	110.35	116.63
1	D	276	MET	N-CA-C	5.40	117.25	111.36
1	E	522	GLU	CA-CB-CG	5.39	124.89	114.10
1	B	638	ARG	N-CA-C	5.39	118.24	109.24
1	A	577	SER	N-CA-C	-5.39	103.42	110.53
1	B	560	SER	N-CA-C	5.38	117.14	111.28
1	E	505	ASN	CA-C-N	5.37	125.08	119.92
1	E	505	ASN	C-N-CA	5.37	125.08	119.92
1	E	247	GLN	CA-C-N	5.37	127.48	120.28
1	E	247	GLN	C-N-CA	5.37	127.48	120.28
1	F	227	PHE	N-CA-C	-5.37	105.42	111.28
1	A	255	GLY	N-CA-C	5.37	119.12	110.90
1	A	503	ILE	CA-C-N	5.36	131.77	121.54
1	A	503	ILE	C-N-CA	5.36	131.77	121.54
1	B	247	GLN	CA-C-N	5.36	127.46	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	GLN	C-N-CA	5.36	127.46	120.28
1	F	232	ARG	N-CA-C	-5.36	105.34	111.07
1	B	574	ILE	CB-CA-C	-5.35	103.26	111.71
1	C	388	ARG	N-CA-C	5.33	117.09	111.28
1	D	547	SER	N-CA-C	-5.32	106.46	113.17
1	F	500	ALA	N-CA-C	5.32	117.16	111.36
1	A	525	VAL	CB-CA-C	-5.32	105.17	111.97
1	D	569	SER	CA-C-N	5.31	125.12	119.28
1	D	569	SER	C-N-CA	5.31	125.12	119.28
1	B	518	LEU	N-CA-C	5.31	117.06	111.28
1	A	691	ARG	CA-C-N	5.30	127.38	120.28
1	A	691	ARG	C-N-CA	5.30	127.38	120.28
1	A	273	ILE	N-CA-CB	5.29	117.34	110.57
1	F	547	SER	O-C-N	-5.29	116.82	122.85
1	A	377	ASP	N-CA-C	5.29	117.12	111.36
2	G	259	TYR	N-CA-C	-5.28	105.19	111.69
1	C	447	ALA	N-CA-C	-5.28	105.60	111.36
1	C	414	MET	N-CA-C	5.28	117.78	111.71
1	C	556	ILE	N-CA-C	-5.27	105.36	110.42
1	D	414	MET	CA-C-N	5.26	127.76	120.29
1	D	414	MET	C-N-CA	5.26	127.76	120.29
1	D	643	ILE	CA-C-N	-5.26	117.56	121.61
1	D	643	ILE	C-N-CA	-5.26	117.56	121.61
1	D	508	ILE	CA-C-N	-5.25	116.01	122.84
1	D	508	ILE	C-N-CA	-5.25	116.01	122.84
1	E	435	ASN	N-CA-C	5.25	117.08	111.36
1	E	640	LEU	N-CA-C	5.25	117.23	108.99
1	D	546	HIS	CA-C-N	-5.24	113.89	122.54
1	D	546	HIS	C-N-CA	-5.24	113.89	122.54
1	E	230	ILE	CA-C-N	5.24	127.25	120.44
1	E	230	ILE	C-N-CA	5.24	127.25	120.44
1	D	233	ARG	N-CA-C	5.24	118.13	111.69
1	C	312	GLU	N-CA-C	-5.23	105.47	111.07
1	D	227	PHE	N-CA-C	-5.22	105.59	111.28
1	F	436	PHE	N-CA-C	5.22	117.80	110.23
1	E	624	GLN	N-CA-C	5.19	116.94	111.28
1	E	629	LEU	CB-CA-C	-5.19	102.18	110.79
1	E	727	ARG	N-CA-C	-5.19	105.31	111.69
1	C	707	ILE	N-CA-C	5.18	115.39	110.42
2	J	291	GLU	N-CA-C	5.17	116.77	111.03
1	D	390	GLU	N-CA-C	5.17	116.92	111.28
1	E	519	ASP	N-CA-CB	5.17	117.72	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	709	LYS	N-CA-C	-5.16	105.78	111.71
1	D	648	ARG	N-CA-C	5.14	116.78	108.41
1	F	628	VAL	CB-CA-C	-5.13	105.30	112.02
1	B	438	GLY	N-CA-C	5.12	125.32	113.18
1	B	479	ASP	N-CA-C	-5.12	96.66	111.00
1	F	295	VAL	N-CA-C	5.12	116.46	110.62
1	A	720	MET	N-CA-C	5.12	117.29	110.53
2	H	40	GLU	N-CA-C	-5.12	105.78	111.36
1	E	381	GLU	N-CA-C	5.10	116.92	111.36
1	C	322	LEU	CA-CB-CG	5.10	134.15	116.30
1	A	321	GLY	N-CA-C	-5.10	101.18	110.97
1	E	296	GLY	CA-C-N	5.10	130.87	121.70
1	E	296	GLY	C-N-CA	5.10	130.87	121.70
1	F	710	LEU	N-CA-C	-5.09	105.63	111.07
1	F	536	LEU	N-CA-C	5.08	117.73	109.24
1	A	547	SER	N-CA-C	-5.08	105.74	111.28
1	F	381	GLU	N-CA-C	5.08	116.89	111.36
2	J	33	GLY	N-CA-C	-5.08	106.64	112.73
1	B	296	GLY	CA-C-N	5.07	130.83	121.70
1	B	296	GLY	C-N-CA	5.07	130.83	121.70
1	A	719	GLN	N-CA-C	5.07	117.46	111.33
1	D	537	VAL	N-CA-C	5.07	115.20	108.11
1	A	424	VAL	CB-CA-C	-5.07	103.33	111.59
1	F	296	GLY	CA-C-N	5.06	130.80	121.70
1	F	296	GLY	C-N-CA	5.06	130.80	121.70
1	F	707	ILE	N-CA-C	5.06	115.28	110.42
2	J	261	GLU	N-CA-C	-5.06	106.80	113.12
1	E	261	PRO	O-C-N	5.05	123.52	121.15
1	E	643	ILE	CA-C-N	-5.05	118.65	122.33
1	E	643	ILE	C-N-CA	-5.05	118.65	122.33
1	E	407	LEU	N-CA-C	-5.04	105.79	111.28
1	A	440	GLU	N-CA-C	-5.04	105.68	111.07
1	E	415	ARG	CA-C-N	5.02	125.42	119.94
1	E	415	ARG	C-N-CA	5.02	125.42	119.94
1	B	381	GLU	N-CA-C	5.02	116.83	111.36
1	B	277	LEU	N-CA-C	5.02	116.75	111.28
1	B	261	PRO	O-C-N	5.01	123.50	121.15
1	F	407	LEU	N-CA-C	-5.01	105.82	111.28
1	F	640	LEU	N-CA-C	5.00	116.99	109.23

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	PRO	Peptide
1	A	321	GLY	Peptide
1	B	438	GLY	Peptide
1	E	438	GLY	Peptide
1	F	438	GLY	Peptide
2	H	200	TYR	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5039	0	4945	325	0
1	B	4995	0	4920	284	0
1	C	5027	0	4945	339	0
1	D	4976	0	4880	333	0
1	E	4992	0	4910	329	0
1	F	4903	0	4853	312	0
2	G	2249	0	2188	119	0
2	H	2246	0	2183	135	0
2	I	2249	0	2192	108	0
2	J	2255	0	2199	132	0
3	K	480	0	465	78	0
4	L	523	0	497	54	0
5	M	1042	0	1022	126	0
All	All	40976	0	40199	2416	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 30.

All (2416) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:MET:HE3	1:F:97:ILE:HD11	1.44	0.99
1:B:490:PRO:HA	1:B:491:ALA:HB3	1.46	0.93
1:A:490:PRO:HA	1:A:491:ALA:HB3	1.50	0.92
1:C:386:PRO:HA	1:C:390:GLU:HA	1.54	0.90
1:C:490:PRO:HA	1:C:491:ALA:HB3	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:545:PRO:HA	1:F:547:SER:H	1.38	0.89
1:F:105:LYS:HZ3	2:G:257:ASP:HB2	1.39	0.87
1:C:240:PHE:HD2	1:C:244:ILE:HG21	1.37	0.86
2:I:38:ILE:HD11	2:I:71:LEU:HB3	1.57	0.86
1:D:628:VAL:HG11	1:E:574:ILE:HG21	1.57	0.86
2:H:219:LEU:HB2	2:H:222:LYS:HB3	1.57	0.86
1:B:256:ILE:HG13	1:B:370:ILE:HG22	1.57	0.86
2:I:80:ASP:OD1	5:M:187:SER:OG	1.93	0.86
3:K:56:ARG:HD2	5:M:171:ILE:HG23	1.58	0.85
2:J:235:PHE:HB3	3:K:38:GLN:HE21	1.38	0.85
1:F:539:VAL:HB	1:F:643:ILE:HG12	1.59	0.85
1:B:327:PHE:HB2	1:B:330:ILE:HG22	1.59	0.85
1:E:386:PRO:HA	1:E:390:GLU:HA	1.59	0.84
1:A:264:CYS:SG	1:A:265:GLY:N	2.48	0.84
1:A:542:GLU:HG2	1:A:649:LYS:HD2	1.59	0.84
1:C:497:GLU:O	1:C:499:TYR:N	2.09	0.84
1:E:256:ILE:HG13	1:E:370:ILE:HG22	1.58	0.84
2:I:38:ILE:HG23	2:I:75:LEU:HD12	1.59	0.84
1:A:305:LEU:HD23	1:A:325:ILE:HG21	1.59	0.84
1:E:526:GLN:NE2	1:F:719:GLN:O	2.10	0.83
1:E:585:MET:HG3	1:E:589:PHE:CZ	2.13	0.83
1:A:562:PHE:CD2	1:A:597:LEU:HD21	2.14	0.83
1:E:327:PHE:HB2	1:E:330:ILE:HG22	1.58	0.83
1:E:527:GLN:O	1:E:531:SER:OG	1.97	0.83
1:F:570:PRO:HG2	1:F:604:ASP:HB2	1.61	0.83
1:B:651:VAL:CG1	1:B:655:MET:HE3	2.08	0.83
2:G:159:SER:OG	5:M:48:VAL:HG13	1.79	0.83
1:C:111:PRO:HG3	1:C:194:ASN:ND2	1.94	0.83
1:F:386:PRO:HA	1:F:390:GLU:HA	1.60	0.83
1:B:249:GLY:HA3	1:C:414:MET:HE3	1.59	0.83
1:D:67:ARG:HD2	2:J:218:MET:HE2	1.59	0.83
1:D:518:LEU:HD21	1:D:552:LEU:HD22	1.61	0.83
2:G:219:LEU:HB2	2:G:222:LYS:HB3	1.58	0.83
2:H:157:SER:HA	4:L:228:GLU:OE1	1.79	0.82
1:D:606:GLU:HA	1:D:609:LEU:HG	1.59	0.82
1:D:95:MET:HE3	1:D:97:ILE:HD11	1.61	0.82
1:A:398:PRO:HG3	1:A:436:PHE:O	1.78	0.82
1:F:327:PHE:HB2	1:F:330:ILE:HG22	1.59	0.82
1:C:256:ILE:HG13	1:C:370:ILE:HG22	1.61	0.82
3:K:54:LEU:HD21	4:L:222:LEU:HD13	1.61	0.81
1:B:566:LYS:HD2	1:B:588:ILE:HG23	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:ILE:HD13	1:A:710:LEU:HD12	1.61	0.81
1:B:662:SER:HB3	1:C:712:MET:HE3	1.61	0.81
1:D:510:TRP:HE3	1:D:675:GLN:HG2	1.45	0.81
1:E:490:PRO:HA	1:E:491:ALA:HB3	1.61	0.81
2:H:116:ARG:NH2	3:K:68:ASP:OD2	2.13	0.81
2:J:201:SER:HB2	5:M:165:LEU:HD11	1.60	0.81
1:A:502:TYR:HE2	1:A:567:ILE:HG21	1.45	0.80
1:D:313:GLN:HE22	1:D:364:LEU:HA	1.45	0.80
1:B:386:PRO:HA	1:B:390:GLU:HA	1.62	0.80
1:C:687:LYS:N	1:C:690:GLU:OE2	2.14	0.80
1:F:256:ILE:HG13	1:F:370:ILE:HG22	1.63	0.80
2:J:235:PHE:CZ	3:K:34:GLN:HG2	2.17	0.80
1:D:510:TRP:CD2	1:D:670:ILE:HG22	2.16	0.80
4:L:212:LEU:HA	4:L:215:MET:HE3	1.63	0.80
1:E:240:PHE:HD2	1:E:244:ILE:HG21	1.46	0.80
1:A:497:GLU:O	1:A:499:TYR:N	2.15	0.79
5:M:32:MET:HA	5:M:35:LEU:HD12	1.65	0.79
1:B:407:LEU:HD11	1:B:426:ILE:HG23	1.64	0.79
2:I:72:HIS:HE1	2:I:80:ASP:HB2	1.47	0.79
1:E:720:MET:HG3	1:E:728:LYS:HE3	1.65	0.79
2:J:219:LEU:HB2	2:J:222:LYS:HB3	1.62	0.79
1:E:527:GLN:HE22	1:F:716:MET:HG2	1.48	0.79
1:C:627:LEU:HD12	1:D:607:ARG:HH12	1.47	0.79
1:E:407:LEU:HD11	1:E:426:ILE:HG23	1.65	0.79
1:E:686:PHE:HE1	1:E:714:ILE:HG23	1.47	0.79
1:B:589:PHE:HE1	1:B:600:VAL:HG11	1.48	0.78
1:C:313:GLN:O	1:C:317:GLY:N	2.17	0.78
1:C:690:GLU:HB2	1:C:726:VAL:HG21	1.65	0.78
1:E:589:PHE:CZ	1:E:629:LEU:HD11	2.19	0.78
1:E:618:PHE:HZ	1:F:612:VAL:HG11	1.48	0.78
1:F:525:VAL:HG13	1:F:562:PHE:CE1	2.18	0.78
1:F:545:PRO:HA	1:F:547:SER:N	1.99	0.78
1:A:557:ALA:O	1:A:560:SER:OG	2.01	0.78
1:B:526:GLN:HE21	1:C:719:GLN:HB3	1.48	0.78
5:M:49:MET:HB3	5:M:53:GLN:NE2	1.99	0.78
1:A:316:LEU:HB3	1:A:320:SER:HB2	1.65	0.77
1:A:713:LEU:HD21	1:A:732:LEU:HB3	1.67	0.77
1:F:105:LYS:NZ	2:G:257:ASP:HB2	1.99	0.77
1:D:627:LEU:HD21	1:D:657:MET:HG3	1.67	0.77
2:H:119:ILE:HD11	3:K:65:ASP:OD2	1.85	0.77
1:C:676:LEU:HD12	1:C:705:ILE:HG21	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:PHE:HE2	1:A:714:ILE:HG12	1.49	0.77
1:D:106:ASN:HB3	1:D:143:LYS:HZ1	1.49	0.77
1:E:587:LYS:NZ	1:E:587:LYS:O	2.15	0.77
1:A:285:VAL:HG13	1:A:326:ILE:HD11	1.65	0.77
1:A:353:GLN:HA	1:B:288:PRO:HG3	1.65	0.77
1:F:407:LEU:HD11	1:F:426:ILE:HG23	1.65	0.77
1:E:246:GLU:O	1:F:413:ARG:NH1	2.14	0.76
1:B:621:LEU:HD11	1:C:575:GLY:HA2	1.66	0.76
5:M:50:LEU:HB3	5:M:170:GLU:HG2	1.67	0.76
1:D:399:ASP:O	1:D:403:ARG:N	2.19	0.76
1:A:115:ASP:CB	1:A:242:PRO:HG3	2.16	0.76
1:D:605:ILE:HD11	1:D:644:GLY:HA3	1.67	0.76
1:C:496:GLN:O	1:C:498:ASP:N	2.19	0.76
1:C:540:LEU:HB3	1:C:664:THR:HG22	1.68	0.76
1:D:568:CYS:SG	1:D:585:MET:HE1	2.26	0.76
1:A:353:GLN:HE21	1:A:357:LYS:HG2	1.50	0.75
1:A:316:LEU:HB3	1:A:320:SER:CB	2.17	0.75
1:C:407:LEU:HD11	1:C:426:ILE:HG23	1.66	0.75
1:E:585:MET:HA	1:E:588:ILE:HD12	1.68	0.75
1:C:524:LEU:HD21	1:C:537:VAL:CG1	2.16	0.75
1:A:525:VAL:HG13	1:A:562:PHE:CZ	2.21	0.75
4:L:209:ILE:HG21	5:M:32:MET:HG3	1.68	0.75
1:D:386:PRO:HA	1:D:390:GLU:HA	1.69	0.75
1:D:728:LYS:HE3	1:D:732:LEU:HD11	1.69	0.75
1:F:536:LEU:HD11	1:F:634:PRO:HD3	1.66	0.75
1:B:651:VAL:HG12	1:B:655:MET:HE3	1.67	0.75
1:F:98:GLU:HB3	1:F:148:LEU:HB3	1.69	0.75
1:C:331:ASP:HA	1:C:379:ILE:HD11	1.69	0.74
1:D:720:MET:HE3	1:D:724:TYR:HE1	1.52	0.74
1:E:627:LEU:HG	1:E:657:MET:HE1	1.67	0.74
2:J:53:LYS:HE3	2:G:117:PHE:HD2	1.52	0.74
1:A:221:GLY:HA3	1:A:406:ILE:HD11	1.70	0.74
1:E:300:ALA:O	1:E:304:LYS:HG2	1.87	0.74
2:H:149:ALA:HB2	2:H:164:CYS:HB2	1.67	0.74
1:D:711:LEU:HA	1:D:714:ILE:HD12	1.70	0.74
1:E:653:GLN:HA	1:E:658:LEU:HB2	1.67	0.74
1:E:625:ALA:HA	1:F:574:ILE:HD11	1.70	0.74
1:F:564:PHE:O	1:F:598:SER:OG	2.04	0.74
1:C:544:PRO:O	1:C:547:SER:OG	2.06	0.73
1:E:606:GLU:OE2	1:E:646:THR:OG1	2.06	0.73
2:H:239:ARG:NH1	4:L:214:ASP:OD1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:178:ILE:HG22	5:M:182:MET:HE2	1.69	0.73
1:E:624:GLN:NE2	1:F:610:ASP:OD1	2.20	0.73
1:C:98:GLU:HB3	1:C:148:LEU:HB3	1.70	0.73
1:C:724:TYR:HD2	1:C:727:ARG:HH21	1.36	0.73
1:F:300:ALA:O	1:F:304:LYS:HG2	1.87	0.73
1:B:540:LEU:HD23	1:B:661:PHE:CD1	2.23	0.73
1:F:303:ARG:HG3	1:F:357:LYS:HE2	1.70	0.73
2:I:21:VAL:HG21	2:I:71:LEU:HD22	1.71	0.73
1:C:524:LEU:HD21	1:C:537:VAL:HG11	1.70	0.73
1:E:240:PHE:CD2	1:E:244:ILE:HG21	2.23	0.73
1:B:300:ALA:O	1:B:304:LYS:HG2	1.89	0.73
1:C:611:TYR:CE1	1:C:616:PRO:HB2	2.23	0.73
1:A:115:ASP:HB2	1:A:242:PRO:HG3	1.70	0.73
1:E:563:PRO:HG2	1:E:595:SER:OG	1.88	0.73
2:I:200:TYR:HB3	3:K:47:ARG:HH22	1.54	0.73
1:C:318:ALA:O	1:C:319:ASN:ND2	2.21	0.73
1:C:109:SER:OG	1:C:315:ARG:HB3	1.88	0.72
1:E:553:ALA:HA	1:E:556:ILE:HD12	1.70	0.72
2:H:115:GLY:HA2	2:G:50:ASN:ND2	2.04	0.72
3:K:53:VAL:HG22	4:L:226:GLN:HE22	1.54	0.72
1:A:309:ALA:HB1	1:A:367:ILE:HG21	1.71	0.72
1:F:569:SER:OG	1:F:571:ASP:OD2	2.06	0.72
1:A:549:LYS:NZ	1:A:647:SER:OG	2.19	0.72
1:A:602:VAL:HG12	1:A:605:ILE:HG12	1.71	0.72
1:D:106:ASN:HB3	1:D:143:LYS:NZ	2.04	0.72
2:G:175:LEU:HD23	2:G:177:GLN:HE21	1.55	0.72
1:A:626:LEU:HD21	1:A:657:MET:HE1	1.70	0.72
1:C:533:ARG:O	1:D:505:ASN:ND2	2.22	0.72
1:D:527:GLN:HE21	1:E:715:GLU:HG3	1.54	0.72
1:F:606:GLU:OE1	1:F:606:GLU:N	2.22	0.72
2:G:72:HIS:HE1	2:G:80:ASP:HB2	1.55	0.72
1:A:677:LEU:HD21	1:A:695:ALA:HA	1.70	0.72
1:C:691:ARG:HA	1:C:694:ILE:HD12	1.72	0.72
1:E:686:PHE:HB3	1:E:690:GLU:HB2	1.71	0.72
1:F:105:LYS:NZ	2:G:255:ASN:OD1	2.21	0.72
1:F:555:LYS:NZ	1:F:559:GLU:OE2	2.14	0.72
3:K:63:LEU:HD22	5:M:178:ILE:HG23	1.71	0.72
1:B:95:MET:HE3	1:B:97:ILE:HD11	1.72	0.71
1:D:654:GLU:HB3	1:E:614:ILE:HD11	1.72	0.71
1:A:125:PHE:HA	1:A:128:GLN:NE2	2.05	0.71
1:D:544:PRO:O	1:D:547:SER:HB3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:42:VAL:HG11	5:M:160:LEU:HD13	1.71	0.71
2:I:72:HIS:CE1	2:I:80:ASP:HB2	2.25	0.71
1:A:553:ALA:HA	1:A:556:ILE:HD12	1.73	0.71
1:F:634:PRO:HB2	1:F:638:ARG:HG3	1.70	0.71
1:A:562:PHE:HD2	1:A:597:LEU:HD21	1.55	0.71
1:B:303:ARG:HG3	1:B:357:LYS:HE2	1.73	0.71
1:D:527:GLN:HE22	1:E:715:GLU:C	1.99	0.71
2:G:228:TYR:OH	2:G:237:ASP:OD1	2.05	0.71
1:A:351:VAL:O	1:A:355:LEU:HG	1.90	0.71
1:F:125:PHE:HA	1:F:128:GLN:NE2	2.06	0.71
1:C:718:LEU:O	1:C:725:ARG:NH1	2.24	0.71
1:E:538:SER:OG	1:E:661:PHE:HA	1.91	0.71
1:D:301:ASN:HA	1:D:304:LYS:HD3	1.71	0.71
2:G:235:PHE:CG	5:M:152:GLN:HG2	2.25	0.71
5:M:49:MET:HB3	5:M:53:GLN:HE21	1.54	0.70
1:C:630:LEU:HD11	1:C:661:PHE:CE1	2.25	0.70
1:C:652:LEU:HD22	1:C:657:MET:HG2	1.73	0.70
1:F:517:VAL:HG13	1:F:665:ILE:HG21	1.73	0.70
1:A:326:ILE:HG22	1:A:370:ILE:HG12	1.73	0.70
1:E:125:PHE:HA	1:E:128:GLN:NE2	2.07	0.70
1:F:264:CYS:SG	1:F:395:ILE:HG22	2.32	0.70
1:C:564:PHE:O	1:C:598:SER:OG	2.10	0.70
1:E:303:ARG:HG3	1:E:357:LYS:HE2	1.73	0.70
1:E:680:LEU:HD13	1:E:694:ILE:HD13	1.73	0.70
2:J:235:PHE:CE2	3:K:34:GLN:HG2	2.26	0.70
1:E:253:VAL:N	1:F:446:ARG:HH12	1.89	0.70
1:E:586:LYS:NZ	1:F:574:ILE:O	2.24	0.70
3:K:83:LYS:HD2	5:M:203:LEU:HD11	1.73	0.70
1:D:620:ASN:O	1:D:624:GLN:HG2	1.92	0.70
1:E:513:PRO:HA	1:E:516:ARG:HG2	1.72	0.70
1:A:564:PHE:CE1	1:A:566:LYS:HB2	2.27	0.70
1:B:627:LEU:HD21	1:B:657:MET:HG3	1.74	0.70
1:D:513:PRO:HA	1:D:516:ARG:HG2	1.73	0.70
1:E:510:TRP:CZ3	1:E:670:ILE:HG13	2.27	0.70
3:K:52:LYS:HB3	5:M:171:ILE:HD13	1.74	0.70
1:E:397:LEU:HD22	1:E:398:PRO:HD2	1.73	0.69
2:H:155:GLU:C	2:H:157:SER:H	1.99	0.69
2:H:228:TYR:OH	2:H:237:ASP:OD1	2.05	0.69
1:C:513:PRO:O	1:C:516:ARG:HG2	1.91	0.69
2:H:18:GLU:HA	2:H:21:VAL:HG12	1.74	0.69
1:E:706:GLY:O	1:E:710:LEU:N	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:549:LYS:HA	1:E:552:LEU:HD12	1.75	0.69
1:C:111:PRO:HG3	1:C:194:ASN:HD22	1.55	0.69
1:F:96:THR:HB	1:F:151:ASP:H	1.57	0.69
3:K:63:LEU:HD13	5:M:182:MET:HG2	1.75	0.69
1:E:603:ASP:OD2	1:E:645:THR:OG1	2.09	0.69
1:B:581:LYS:NZ	1:B:608:LEU:O	2.25	0.69
1:B:713:LEU:HD22	1:B:732:LEU:HB3	1.74	0.69
1:A:502:TYR:CE2	1:A:567:ILE:HG21	2.26	0.69
1:D:353:GLN:HE22	1:E:288:PRO:HG2	1.56	0.69
1:B:533:ARG:HG3	1:B:534:THR:H	1.58	0.69
1:E:625:ALA:O	1:E:629:LEU:HG	1.93	0.69
1:E:670:ILE:HG22	1:E:672:THR:H	1.57	0.69
2:J:101:ILE:HG21	2:J:135:LEU:HD11	1.75	0.69
1:B:98:GLU:HB3	1:B:148:LEU:HB3	1.73	0.68
1:B:624:GLN:NE2	1:C:610:ASP:O	2.25	0.68
1:E:592:ALA:HB1	1:E:640:LEU:HD22	1.75	0.68
1:F:513:PRO:O	1:F:517:VAL:HG23	1.94	0.68
2:I:101:ILE:HG21	2:I:135:LEU:HD11	1.75	0.68
1:B:125:PHE:HA	1:B:128:GLN:NE2	2.08	0.68
1:C:542:GLU:CB	1:C:649:LYS:HD3	2.24	0.68
1:C:578:GLU:HB3	1:C:621:LEU:HB3	1.75	0.68
1:F:358:ILE:HD12	1:F:388:ARG:HB3	1.74	0.68
2:J:200:TYR:HE2	3:K:41:GLU:HG2	1.58	0.68
1:A:653:GLN:NE2	1:A:653:GLN:O	2.26	0.68
1:D:543:GLY:H	1:D:549:LYS:HD3	1.59	0.68
2:H:203:LYS:HD3	2:H:236:SER:HB3	1.74	0.68
2:J:50:ASN:ND2	2:G:115:GLY:HA2	2.07	0.68
1:A:111:PRO:HD2	1:A:320:SER:C	2.18	0.68
1:A:503:ILE:HG23	1:A:506:GLY:HA2	1.75	0.68
1:B:64:LEU:HA	1:B:67:ARG:HE	1.58	0.68
1:B:585:MET:HE1	1:B:626:LEU:HG	1.73	0.68
4:L:211:GLU:HA	4:L:214:ASP:OD2	1.92	0.68
1:A:258:LEU:HA	1:A:393:MET:O	1.94	0.68
1:D:67:ARG:HB3	2:J:218:MET:SD	2.34	0.68
1:D:404:LEU:HA	1:D:407:LEU:HD12	1.74	0.68
4:L:209:ILE:HG13	5:M:32:MET:HE2	1.76	0.68
1:F:589:PHE:HD2	1:F:629:LEU:HD13	1.57	0.68
1:C:596:GLN:HA	1:C:638:ARG:HD3	1.74	0.68
2:J:228:TYR:OH	2:J:237:ASP:OD1	2.10	0.68
1:A:262:PRO:HG2	1:A:374:ASN:OD1	1.94	0.68
1:B:538:SER:HB3	1:B:661:PHE:CD2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:PRO:HG2	1:B:23:VAL:HG11	1.75	0.67
1:F:92:ILE:HG21	1:F:95:MET:HB2	1.75	0.67
1:E:685:ASN:HB3	1:E:718:LEU:HD11	1.75	0.67
1:B:449:GLN:O	1:B:453:MET:HG2	1.94	0.67
1:D:628:VAL:HG13	1:E:571:ASP:OD1	1.93	0.67
4:L:216:PHE:CE2	5:M:39:SER:HB2	2.30	0.67
1:D:358:ILE:HD12	1:D:388:ARG:HB3	1.76	0.67
1:E:589:PHE:CD2	1:E:629:LEU:HD21	2.29	0.67
1:F:536:LEU:HD21	1:F:632:LYS:O	1.93	0.67
1:A:64:LEU:HB3	1:A:65:PRO:HD3	1.77	0.67
2:H:115:GLY:HA2	2:G:50:ASN:HD21	1.58	0.67
2:H:216:ILE:HG12	2:H:218:MET:H	1.59	0.67
1:E:12:PRO:HG2	1:E:23:VAL:HG11	1.77	0.67
2:J:271:ARG:NH2	2:G:234:ALA:HB2	2.10	0.67
1:C:106:ASN:HB3	1:C:143:LYS:NZ	2.10	0.67
1:D:546:HIS:ND1	1:D:709:LYS:HD3	2.10	0.67
1:E:449:GLN:O	1:E:453:MET:HG2	1.95	0.67
1:B:524:LEU:HD21	1:B:663:THR:HG21	1.75	0.67
1:D:510:TRP:CE3	1:D:670:ILE:HG22	2.30	0.67
1:E:311:GLU:OE1	1:E:314:ARG:NE	2.26	0.67
1:A:720:MET:O	1:A:725:ARG:NE	2.20	0.67
1:C:125:PHE:HA	1:C:128:GLN:NE2	2.10	0.67
1:F:311:GLU:OE1	1:F:314:ARG:NE	2.26	0.67
3:K:83:LYS:HG2	3:K:86:ARG:NH2	2.09	0.67
1:B:358:ILE:HD12	1:B:388:ARG:HB3	1.78	0.66
1:B:654:GLU:O	1:C:613:PRO:HG3	1.95	0.66
1:D:234:ALA:HA	1:D:253:VAL:HG11	1.77	0.66
2:J:230:GLU:HG2	2:J:231:LEU:N	2.09	0.66
1:F:258:LEU:HB3	1:F:395:ILE:HD11	1.75	0.66
1:F:535:PRO:HA	1:F:639:LYS:HG2	1.76	0.66
1:A:563:PRO:HD2	1:A:597:LEU:HD22	1.76	0.66
1:A:687:LYS:N	1:A:690:GLU:OE1	2.28	0.66
1:E:602:VAL:O	1:E:644:GLY:HA2	1.94	0.66
5:M:40:LYS:O	5:M:44:ILE:HG13	1.96	0.66
1:C:546:HIS:HA	1:C:708:LYS:HD3	1.78	0.66
1:F:605:ILE:HD11	1:F:644:GLY:HA3	1.76	0.66
1:F:612:VAL:HG12	1:F:617:ARG:HB2	1.77	0.66
2:H:197:LEU:HD12	5:M:45:ARG:HD3	1.78	0.66
4:L:240:ALA:HA	4:L:243:TYR:HD2	1.59	0.66
1:F:437:SER:OG	1:F:440:GLU:HG2	1.96	0.66
2:J:53:LYS:HE3	2:G:117:PHE:CD2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:21:VAL:HG21	2:G:71:LEU:HD22	1.78	0.66
1:A:231:PHE:CD1	1:A:235:PHE:HE2	2.13	0.66
1:F:635:PRO:O	1:F:638:ARG:HG2	1.96	0.66
1:E:64:LEU:HB3	1:E:65:PRO:HD3	1.78	0.66
1:C:236:ALA:HB1	1:D:453:MET:HB3	1.77	0.65
2:H:21:VAL:HG21	2:H:71:LEU:HD22	1.77	0.65
1:A:607:ARG:HD3	1:F:624:GLN:NE2	2.11	0.65
1:B:589:PHE:CE1	1:B:600:VAL:HG11	2.30	0.65
2:H:233:PRO:HB3	2:G:268:SER:O	1.95	0.65
1:B:224:ASP:O	1:B:228:SER:HB2	1.97	0.65
1:E:640:LEU:HD12	1:E:641:LEU:N	2.10	0.65
1:E:652:LEU:CD2	1:E:657:MET:HB3	2.27	0.65
1:F:570:PRO:HG2	1:F:604:ASP:CB	2.26	0.65
1:F:721:ASP:HB2	1:F:724:TYR:HD1	1.60	0.65
1:A:240:PHE:HE2	1:B:453:MET:HB3	1.61	0.65
1:A:562:PHE:HD2	1:A:597:LEU:CD2	2.10	0.65
1:D:223:LEU:HD11	1:D:395:ILE:HG12	1.77	0.65
1:E:534:THR:HG23	1:F:715:GLU:HG3	1.78	0.65
2:J:271:ARG:NH2	2:G:231:LEU:HB2	2.11	0.65
1:A:549:LYS:HE3	1:A:646:THR:C	2.21	0.65
1:B:40:SER:CB	1:B:41:PRO:HD2	2.27	0.65
1:A:710:LEU:O	1:A:714:ILE:HG13	1.96	0.65
1:C:614:ILE:C	1:C:616:PRO:HA	2.22	0.65
1:D:10:ARG:HG3	1:D:67:ARG:HH12	1.61	0.65
1:F:184:ALA:HB1	1:F:200:LYS:O	1.97	0.65
1:F:307:ALA:O	1:F:311:GLU:HG2	1.96	0.65
1:D:652:LEU:HB3	1:D:658:LEU:HB2	1.78	0.65
1:D:695:ALA:HB1	1:D:699:LYS:HE3	1.77	0.65
1:E:652:LEU:HD23	1:E:657:MET:HB3	1.79	0.65
1:A:612:VAL:HG11	1:F:618:PHE:HZ	1.60	0.65
1:C:711:LEU:HA	1:C:714:ILE:HD12	1.77	0.65
1:D:528:THR:OG1	1:D:641:LEU:HD12	1.96	0.65
1:E:358:ILE:HD12	1:E:388:ARG:HB3	1.77	0.65
5:M:153:VAL:O	5:M:157:ILE:HG12	1.97	0.65
1:A:624:GLN:HG3	1:B:610:ASP:OD2	1.96	0.65
1:B:538:SER:HB3	1:B:661:PHE:HD2	1.61	0.65
1:D:12:PRO:HG2	1:D:23:VAL:HG11	1.79	0.65
1:D:245:VAL:O	1:D:249:GLY:N	2.29	0.65
1:E:624:GLN:HA	1:E:624:GLN:OE1	1.95	0.65
1:A:95:MET:HE3	1:A:97:ILE:HD11	1.78	0.65
1:A:597:LEU:C	1:A:597:LEU:HD23	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ILE:O	2:J:214:PHE:HE2	1.79	0.65
1:D:573:MET:SD	1:D:581:LYS:HD3	2.37	0.65
1:E:14:ASP:O	1:E:18:LEU:HG	1.96	0.65
1:F:64:LEU:HB3	1:F:65:PRO:HD3	1.78	0.65
1:F:224:ASP:O	1:F:228:SER:HB2	1.97	0.65
1:A:671:ALA:HA	1:A:703:VAL:O	1.97	0.64
1:E:536:LEU:HD12	1:E:640:LEU:O	1.97	0.64
1:D:64:LEU:HB3	1:D:65:PRO:HD3	1.79	0.64
1:F:222:GLY:HA3	1:F:399:ASP:OD2	1.97	0.64
2:G:149:ALA:HB2	2:G:164:CYS:HB2	1.79	0.64
4:L:234:GLU:O	4:L:238:GLU:HG2	1.97	0.64
1:A:521:GLY:O	1:A:525:VAL:HG23	1.97	0.64
1:B:64:LEU:HB3	1:B:65:PRO:HD3	1.79	0.64
1:C:649:LYS:HE2	1:C:658:LEU:HD13	1.78	0.64
2:G:158:ASN:OD1	2:G:162:ASN:ND2	2.30	0.64
3:K:83:LYS:HG2	3:K:86:ARG:HH22	1.62	0.64
1:B:326:ILE:HG22	1:B:370:ILE:HG13	1.79	0.64
1:B:36:ILE:HD11	1:B:44:LYS:HB3	1.79	0.64
1:F:695:ALA:HB1	1:F:699:LYS:HE3	1.80	0.64
2:H:210:ALA:HB3	2:H:244:MET:HE3	1.80	0.64
1:F:670:ILE:HG23	1:F:675:GLN:HB2	1.79	0.64
4:L:223:VAL:HG21	5:M:46:THR:HG23	1.79	0.64
5:M:57:LEU:HA	5:M:60:VAL:HB	1.79	0.64
1:A:189:GLU:CD	1:A:189:GLU:H	2.06	0.64
2:G:256:VAL:HG21	2:G:288:GLN:HG3	1.79	0.64
1:E:640:LEU:HD12	1:E:641:LEU:H	1.63	0.64
1:F:713:LEU:HD22	1:F:732:LEU:HB3	1.80	0.64
5:M:68:ASN:HA	5:M:188:ASN:OD1	1.98	0.64
2:J:128:ALA:HB2	2:J:144:HIS:HB2	1.80	0.63
1:F:105:LYS:HZ3	2:G:257:ASP:CB	2.11	0.63
2:H:72:HIS:HE1	2:H:80:ASP:HB2	1.62	0.63
1:B:528:THR:O	1:B:639:LYS:HD2	1.98	0.63
1:D:284:VAL:HG23	1:D:324:ILE:O	1.97	0.63
1:E:604:ASP:HB3	1:E:607:ARG:HB3	1.80	0.63
1:D:632:LYS:NZ	1:E:571:ASP:HB3	2.13	0.63
2:H:101:ILE:HG21	2:H:135:LEU:HD11	1.80	0.63
2:H:128:ALA:HB2	2:H:144:HIS:HB2	1.80	0.63
5:M:42:ALA:HA	5:M:45:ARG:NH2	2.13	0.63
1:A:256:ILE:HG13	1:A:370:ILE:HG22	1.79	0.63
1:A:672:THR:OG1	1:A:675:GLN:OE1	2.12	0.63
1:E:710:LEU:O	1:E:714:ILE:HG13	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:THR:CG2	1:F:150:LYS:HB2	2.28	0.63
1:F:550:THR:HA	1:F:645:THR:HG21	1.80	0.63
2:G:72:HIS:CE1	2:G:80:ASP:HB2	2.34	0.63
1:A:508:ILE:HB	1:A:682:LEU:HD22	1.80	0.63
1:C:245:VAL:O	1:C:249:GLY:N	2.32	0.63
1:E:681:GLU:HA	1:E:691:ARG:HE	1.63	0.63
2:H:216:ILE:HD13	2:H:220:ASN:HB2	1.79	0.63
2:H:230:GLU:HG3	2:H:237:ASP:HB3	1.79	0.63
1:C:358:ILE:CB	1:C:388:ARG:HG3	2.28	0.63
1:E:224:ASP:O	1:E:228:SER:HB2	1.98	0.63
2:I:116:ARG:HH21	3:K:66:ARG:NH1	1.97	0.63
1:B:596:GLN:HA	1:B:638:ARG:HG2	1.79	0.62
1:C:64:LEU:HA	1:C:67:ARG:HE	1.64	0.62
1:F:67:ARG:NH1	1:F:74:ILE:HD11	2.13	0.62
1:F:284:VAL:HG23	1:F:324:ILE:O	1.99	0.62
5:M:170:GLU:HG3	5:M:174:GLN:HE21	1.64	0.62
1:D:604:ASP:HB3	1:D:607:ARG:CB	2.29	0.62
1:E:404:LEU:O	1:E:408:HIS:HB2	1.98	0.62
1:F:48:THR:HG21	1:F:128:GLN:HG2	1.81	0.62
1:A:238:ARG:HA	1:A:252:HIS:CE1	2.35	0.62
1:C:590:ASP:HA	1:C:593:TYR:CD2	2.34	0.62
1:D:125:PHE:HA	1:D:128:GLN:NE2	2.14	0.62
1:E:628:VAL:O	1:E:632:LYS:N	2.33	0.62
1:F:404:LEU:O	1:F:408:HIS:HB2	1.99	0.62
2:J:235:PHE:CE2	3:K:35:THR:HA	2.34	0.62
1:D:521:GLY:O	1:D:525:VAL:HG23	1.98	0.62
1:E:289:GLU:C	1:E:291:LEU:H	2.07	0.62
1:E:586:LYS:HA	1:E:589:PHE:CD2	2.34	0.62
1:E:674:GLU:HA	1:E:677:LEU:HD12	1.81	0.62
1:D:319:ASN:HB3	1:D:320:SER:HB2	1.81	0.62
1:D:545:PRO:HD3	1:D:647:SER:OG	1.99	0.62
2:G:159:SER:HG	5:M:48:VAL:HG13	1.61	0.62
1:A:585:MET:HE1	1:A:626:LEU:HD12	1.81	0.62
2:G:101:ILE:HG21	2:G:135:LEU:HD11	1.80	0.62
1:A:397:LEU:CB	1:A:398:PRO:HD3	2.30	0.62
1:F:570:PRO:HA	1:F:573:MET:HE2	1.80	0.62
2:G:235:PHE:CD1	5:M:152:GLN:HG2	2.35	0.62
1:B:221:GLY:HA3	1:B:406:ILE:HG13	1.80	0.62
1:D:348:ASP:O	1:D:352:ASN:ND2	2.33	0.62
1:F:538:SER:O	1:F:663:THR:HG22	1.99	0.62
1:B:307:ALA:O	1:B:311:GLU:HG2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:GLU:OE1	1:B:314:ARG:NE	2.28	0.62
1:B:398:PRO:HG3	1:B:436:PHE:O	2.00	0.62
1:C:289:GLU:O	1:C:291:LEU:N	2.24	0.62
1:E:513:PRO:O	1:E:517:VAL:HG23	2.00	0.62
1:C:310:GLU:OE2	1:C:357:LYS:NZ	2.27	0.62
1:D:312:GLU:CG	1:D:313:GLN:H	2.13	0.62
1:D:651:VAL:O	1:D:655:MET:HG2	1.99	0.62
1:A:423:ASP:HB2	1:A:480:PHE:CB	2.30	0.61
1:A:610:ASP:HA	1:F:624:GLN:NE2	2.15	0.61
1:A:657:MET:HE3	1:A:661:PHE:CE1	2.35	0.61
1:D:554:ALA:O	1:D:558:GLU:HG2	2.00	0.61
1:A:678:GLU:O	1:A:682:LEU:HD12	1.99	0.61
1:C:542:GLU:HB3	1:C:649:LYS:HD3	1.83	0.61
1:C:624:GLN:O	1:C:628:VAL:HG23	1.99	0.61
1:A:270:ALA:O	1:A:273:ILE:HG22	2.00	0.61
1:A:353:GLN:HA	1:B:288:PRO:CG	2.30	0.61
1:B:540:LEU:HA	1:B:644:GLY:O	2.00	0.61
2:H:20:LYS:HE2	2:H:37:LYS:HA	1.83	0.61
1:A:449:GLN:NE2	1:F:248:MET:O	2.34	0.61
1:C:67:ARG:NH1	1:C:74:ILE:HD11	2.16	0.61
1:D:353:GLN:HE22	1:E:288:PRO:CG	2.12	0.61
1:E:697:GLN:HG3	1:E:730:LEU:HD11	1.82	0.61
1:F:566:LYS:HD2	1:F:567:ILE:N	2.16	0.61
4:L:205:LEU:O	4:L:209:ILE:HG12	2.01	0.61
5:M:167:MET:O	5:M:171:ILE:HG13	2.01	0.61
1:A:231:PHE:CE1	1:A:235:PHE:HE2	2.18	0.61
1:B:236:ALA:HA	1:B:239:VAL:HG12	1.83	0.61
1:C:540:LEU:HD12	1:C:644:GLY:O	2.01	0.61
1:E:95:MET:HE3	1:E:97:ILE:HD11	1.82	0.61
1:F:565:ILE:HG23	1:F:599:CYS:HB3	1.81	0.61
1:E:240:PHE:HB3	1:E:244:ILE:HB	1.83	0.61
1:D:585:MET:O	1:D:589:PHE:HD2	1.84	0.61
2:I:69:ALA:HB1	2:I:85:PHE:CE1	2.36	0.61
1:A:628:VAL:HG11	1:B:571:ASP:HA	1.82	0.61
1:B:548:GLY:O	1:B:552:LEU:HD23	2.00	0.61
1:C:64:LEU:HB3	1:C:65:PRO:HD3	1.81	0.61
1:C:436:PHE:HB3	1:C:440:GLU:OE1	2.00	0.61
1:D:606:GLU:O	1:D:610:ASP:N	2.34	0.61
1:E:284:VAL:HG23	1:E:324:ILE:O	2.00	0.61
1:A:627:LEU:HD13	1:B:607:ARG:HH12	1.66	0.61
1:B:295:VAL:HB	1:C:294:TYR:CG	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:PRO:HD2	1:B:597:LEU:HB2	1.83	0.61
1:A:382:ALA:O	1:A:385:ARG:HG2	2.02	0.60
1:C:576:PHE:HB2	1:C:581:LYS:HE3	1.83	0.60
1:C:579:THR:O	1:C:583:GLN:HG2	2.01	0.60
1:D:122:ILE:HD12	1:D:181:SER:HB2	1.83	0.60
1:D:312:GLU:OE1	1:D:323:HIS:ND1	2.33	0.60
1:D:436:PHE:HE2	1:D:444:LEU:HD12	1.66	0.60
1:A:184:ALA:HB1	1:A:200:LYS:O	2.01	0.60
1:B:106:ASN:HB3	1:B:143:LYS:NZ	2.16	0.60
1:C:695:ALA:HB1	1:C:699:LYS:HE3	1.83	0.60
1:F:96:THR:HG21	1:F:150:LYS:HB2	1.83	0.60
2:G:200:TYR:O	2:G:203:LYS:HE2	2.01	0.60
1:C:711:LEU:O	1:C:715:GLU:HG2	2.01	0.60
1:D:527:GLN:NE2	1:E:715:GLU:O	2.32	0.60
2:J:57:ASN:O	2:J:59:SER:N	2.34	0.60
2:J:200:TYR:O	2:J:203:LYS:HE2	2.01	0.60
1:A:536:LEU:HD23	1:A:633:ALA:HA	1.83	0.60
1:B:625:ALA:O	1:B:629:LEU:HG	2.02	0.60
1:C:375:ARG:HH12	1:C:378:LEU:HG	1.66	0.60
1:C:383:LEU:HD22	1:C:388:ARG:HD2	1.83	0.60
1:D:534:THR:OG1	1:E:715:GLU:HG2	2.01	0.60
1:E:266:LYS:HG2	1:E:395:ILE:HG12	1.83	0.60
3:K:87:LYS:HD2	5:M:204:GLY:OXT	2.02	0.60
1:B:95:MET:HG3	1:B:152:ILE:HG12	1.83	0.60
1:C:540:LEU:HB2	1:C:661:PHE:CD2	2.35	0.60
1:C:658:LEU:HD11	1:C:664:THR:HG21	1.83	0.60
1:D:171:LYS:NZ	1:D:171:LYS:HB3	2.16	0.60
1:D:256:ILE:O	1:D:370:ILE:HA	2.02	0.60
1:D:263:GLY:O	1:D:439:ALA:N	2.34	0.60
1:A:617:ARG:HH11	1:A:617:ARG:HG3	1.65	0.60
1:A:627:LEU:O	1:A:631:LYS:NZ	2.35	0.60
1:C:386:PRO:HD2	1:D:440:GLU:OE1	2.00	0.60
1:D:313:GLN:O	1:D:317:GLY:N	2.35	0.60
1:F:397:LEU:HB3	1:F:398:PRO:CD	2.32	0.60
2:H:232:PHE:HB2	2:H:233:PRO:HD3	1.84	0.60
2:I:96:ASP:OD1	2:I:97:PRO:HD3	2.02	0.60
5:M:174:GLN:O	5:M:178:ILE:HG13	2.01	0.60
1:A:513:PRO:O	1:A:517:VAL:HG23	2.01	0.60
2:I:51:MET:HA	2:I:54:MET:HG2	1.83	0.60
1:A:540:LEU:HD11	1:A:646:THR:HG22	1.83	0.60
1:B:245:VAL:O	1:B:249:GLY:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:ILE:HG22	1:E:370:ILE:HG13	1.83	0.60
1:D:404:LEU:HD11	1:D:427:LYS:HE3	1.83	0.60
2:I:34:GLY:O	2:I:38:ILE:HG22	2.02	0.60
2:J:67:GLN:O	2:J:71:LEU:HG	2.02	0.60
1:B:526:GLN:NE2	1:C:719:GLN:HB3	2.17	0.60
1:C:624:GLN:NE2	1:D:610:ASP:HB2	2.17	0.60
1:E:307:ALA:O	1:E:311:GLU:HG2	2.01	0.60
2:I:225:VAL:HG23	2:I:241:CYS:HB2	1.84	0.60
1:E:236:ALA:HA	1:E:239:VAL:HG12	1.84	0.59
5:M:58:ASP:O	5:M:62:GLU:HG3	2.01	0.59
5:M:74:ALA:O	5:M:78:LEU:HG	2.02	0.59
1:B:571:ASP:OD2	1:B:571:ASP:N	2.34	0.59
1:D:312:GLU:HG2	1:D:313:GLN:H	1.66	0.59
1:E:407:LEU:CD1	1:E:426:ILE:HG23	2.32	0.59
1:F:197:GLY:O	1:F:200:LYS:HE2	2.01	0.59
1:A:242:PRO:HD2	1:A:243:GLU:CD	2.27	0.59
1:B:354:LEU:O	1:B:358:ILE:HG12	2.03	0.59
1:D:528:THR:OG1	1:D:537:VAL:HG21	2.02	0.59
1:D:625:ALA:O	1:D:629:LEU:HG	2.02	0.59
2:J:112:THR:HG23	2:J:117:PHE:HE1	1.66	0.59
4:L:218:ASP:O	4:L:222:LEU:HG	2.01	0.59
1:B:289:GLU:C	1:B:291:LEU:H	2.09	0.59
1:C:577:SER:O	1:C:580:ALA:N	2.33	0.59
1:F:612:VAL:CG1	1:F:617:ARG:HB2	2.32	0.59
2:H:230:GLU:HG2	2:H:231:LEU:N	2.17	0.59
1:A:683:LEU:HB3	1:A:685:ASN:ND2	2.18	0.59
1:D:513:PRO:HB3	1:D:516:ARG:HE	1.65	0.59
1:E:380:ASP:OD1	1:E:382:ALA:N	2.35	0.59
1:F:242:PRO:HD2	1:F:243:GLU:H	1.67	0.59
1:F:354:LEU:O	1:F:358:ILE:HG12	2.02	0.59
3:K:88:TYR:CD2	5:M:81:LEU:HD11	2.37	0.59
1:E:721:ASP:O	1:E:725:ARG:HG3	2.02	0.59
3:K:39:VAL:HG11	4:L:209:ILE:HD13	1.84	0.59
1:A:582:CYS:SG	1:A:621:LEU:HG	2.43	0.59
1:B:490:PRO:HA	1:B:491:ALA:CB	2.22	0.59
1:C:46:ILE:HD12	1:C:174:VAL:HG21	1.84	0.59
1:C:256:ILE:HG22	1:C:391:VAL:HG11	1.84	0.59
1:D:315:ARG:C	1:D:316:LEU:HD12	2.27	0.59
1:D:512:ASP:O	1:D:515:THR:OG1	2.18	0.59
2:H:195:SER:C	2:H:197:LEU:H	2.10	0.59
1:A:560:SER:HB2	1:A:562:PHE:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LYS:HD2	1:C:198:LYS:N	2.17	0.59
1:C:377:ASP:OD2	1:C:377:ASP:N	2.35	0.59
1:D:286:ASN:HB2	1:D:327:PHE:HD1	1.67	0.59
1:D:604:ASP:HB3	1:D:607:ARG:HB3	1.85	0.59
2:I:210:ALA:HB3	2:I:244:MET:HE3	1.84	0.59
1:A:670:ILE:HG23	1:A:675:GLN:HB2	1.85	0.59
1:B:327:PHE:HB2	1:B:330:ILE:CG2	2.32	0.59
1:B:407:LEU:CD1	1:B:426:ILE:HG23	2.32	0.59
1:C:12:PRO:HG2	1:C:23:VAL:HG11	1.85	0.59
1:C:511:GLY:HA3	1:C:513:PRO:HD2	1.85	0.59
1:C:256:ILE:HA	1:C:391:VAL:HG13	1.84	0.59
1:D:299:GLU:OE1	1:D:350:VAL:HG13	2.03	0.59
1:D:513:PRO:O	1:D:516:ARG:HG2	2.03	0.59
1:A:111:PRO:HD2	1:A:321:GLY:N	2.18	0.58
1:A:562:PHE:CD2	1:A:597:LEU:CD2	2.85	0.58
1:C:311:GLU:HA	1:C:314:ARG:HG2	1.85	0.58
1:E:532:ASP:OD2	1:E:533:ARG:N	2.35	0.58
2:G:210:ALA:HB3	2:G:244:MET:HE3	1.84	0.58
1:E:573:MET:SD	1:E:581:LYS:HG2	2.43	0.58
1:F:380:ASP:OD1	1:F:382:ALA:N	2.34	0.58
1:A:67:ARG:NH1	1:A:74:ILE:HD11	2.18	0.58
1:A:726:VAL:O	1:A:730:LEU:HG	2.04	0.58
1:B:128:GLN:O	1:B:176:LEU:HD12	2.04	0.58
1:B:437:SER:O	1:B:440:GLU:HB2	2.03	0.58
1:B:545:PRO:O	1:B:546:HIS:HB2	2.03	0.58
1:A:687:LYS:HB2	1:A:690:GLU:HG3	1.85	0.58
1:B:296:GLY:H	1:B:297:GLU:CB	2.17	0.58
1:E:648:ARG:NE	1:E:650:ASP:OD1	2.31	0.58
2:J:225:VAL:HG23	2:J:241:CYS:HB2	1.84	0.58
2:G:142:ILE:HG23	2:G:168:VAL:HG13	1.84	0.58
1:A:598:SER:OG	1:A:640:LEU:HD12	2.02	0.58
1:C:533:ARG:HB2	1:D:715:GLU:OE1	2.03	0.58
1:D:267:THR:HA	1:D:372:MET:SD	2.44	0.58
1:D:383:LEU:O	1:D:389:LEU:HB2	2.03	0.58
1:F:383:LEU:O	1:F:389:LEU:HB2	2.03	0.58
1:F:604:ASP:HB3	1:F:607:ARG:HB2	1.85	0.58
5:M:176:ARG:HA	5:M:179:ASP:OD2	2.03	0.58
1:B:284:VAL:HG23	1:B:324:ILE:O	2.03	0.58
1:D:73:SER:O	1:D:76:GLN:HG2	2.03	0.58
1:D:114:THR:OG1	1:D:199:ALA:HB3	2.03	0.58
1:C:414:MET:HE2	1:C:414:MET:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:GLU:HG3	1:B:619:SER:HB2	1.86	0.58
1:B:605:ILE:HD11	1:B:644:GLY:HA3	1.84	0.58
1:E:296:GLY:H	1:E:297:GLU:CB	2.16	0.58
1:E:686:PHE:CE1	1:E:714:ILE:HG23	2.34	0.58
1:F:326:ILE:HG22	1:F:370:ILE:HG13	1.85	0.58
1:F:650:ASP:O	1:F:653:GLN:HG3	2.03	0.58
5:M:179:ASP:HA	5:M:182:MET:HE3	1.85	0.58
1:A:315:ARG:O	1:A:316:LEU:HD12	2.03	0.58
1:A:539:VAL:HG13	1:A:643:ILE:HA	1.84	0.58
1:B:380:ASP:OD1	1:B:382:ALA:N	2.36	0.58
1:E:587:LYS:HZ3	1:E:587:LYS:C	2.08	0.58
1:A:694:ILE:O	1:A:698:VAL:HG13	2.04	0.58
1:C:240:PHE:CD2	1:C:244:ILE:HG21	2.29	0.58
1:D:618:PHE:CE2	1:E:614:ILE:HD12	2.39	0.58
1:E:713:LEU:HD22	1:E:732:LEU:HD13	1.85	0.58
2:G:69:ALA:HB1	2:G:85:PHE:CE1	2.39	0.57
2:G:266:TYR:C	2:G:268:SER:H	2.10	0.57
2:J:266:TYR:C	2:J:268:SER:H	2.11	0.57
1:A:242:PRO:HD2	1:A:243:GLU:H	1.69	0.57
1:A:315:ARG:C	1:A:316:LEU:HD12	2.29	0.57
1:B:397:LEU:CD2	1:B:398:PRO:HD2	2.34	0.57
1:C:254:LYS:O	1:C:368:LEU:HA	2.04	0.57
1:C:404:LEU:O	1:C:408:HIS:HB2	2.03	0.57
1:C:728:LYS:O	1:C:732:LEU:HG	2.03	0.57
1:F:521:GLY:O	1:F:525:VAL:HG23	2.04	0.57
2:I:38:ILE:CD1	2:I:71:LEU:HB3	2.33	0.57
2:J:21:VAL:HG23	2:J:38:ILE:HD12	1.86	0.57
1:C:490:PRO:HA	1:C:491:ALA:CB	2.28	0.57
1:F:554:ALA:O	1:F:558:GLU:HG3	2.05	0.57
5:M:36:VAL:HG23	5:M:156:ILE:HG21	1.85	0.57
1:A:257:LEU:HG	1:A:389:LEU:HD12	1.86	0.57
1:B:589:PHE:HE2	1:B:629:LEU:HB3	1.68	0.57
1:D:284:VAL:HB	1:D:325:ILE:HA	1.86	0.57
1:E:399:ASP:HB2	1:E:402:GLY:H	1.69	0.57
1:F:407:LEU:CD1	1:F:426:ILE:HG23	2.34	0.57
1:B:385:ARG:NH1	1:C:263:GLY:HA2	2.19	0.57
1:C:95:MET:HE3	1:C:97:ILE:HD11	1.86	0.57
1:F:522:GLU:OE2	1:F:526:GLN:HG2	2.05	0.57
3:K:70:LEU:HD13	5:M:189:LYS:HB2	1.86	0.57
4:L:198:ARG:O	4:L:202:ILE:HG13	2.03	0.57
1:B:670:ILE:HG23	1:B:675:GLN:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:ALA:HB1	1:B:699:LYS:HE3	1.87	0.57
1:C:334:CYS:HA	1:C:351:VAL:HG22	1.86	0.57
1:E:437:SER:O	1:E:440:GLU:HB2	2.05	0.57
2:G:160:SER:OG	5:M:52:GLU:OE2	2.19	0.57
1:A:247:GLN:O	1:B:413:ARG:NH1	2.37	0.57
1:A:313:GLN:NE2	1:A:365:ASN:O	2.36	0.57
1:A:607:ARG:HD3	1:F:624:GLN:HE22	1.69	0.57
1:B:424:VAL:N	1:B:479:ASP:N	2.52	0.57
1:C:606:GLU:HG2	1:C:607:ARG:N	2.18	0.57
1:D:680:LEU:HB2	1:D:691:ARG:HH21	1.68	0.57
2:I:128:ALA:HB2	2:I:144:HIS:HB2	1.87	0.57
5:M:200:THR:O	5:M:203:LEU:HB2	2.05	0.57
1:A:322:LEU:HA	1:A:366:ASN:O	2.04	0.57
1:E:502:TYR:CZ	1:E:567:ILE:HG21	2.40	0.57
1:A:306:PHE:CD1	1:A:357:LYS:HB3	2.40	0.57
1:A:307:ALA:O	1:A:310:GLU:HG3	2.05	0.57
1:B:404:LEU:O	1:B:408:HIS:HB2	2.05	0.57
1:D:510:TRP:CE3	1:D:675:GLN:HG2	2.34	0.57
1:E:289:GLU:O	1:E:291:LEU:N	2.25	0.57
1:F:86:ASP:C	1:F:88:ALA:H	2.13	0.57
5:M:68:ASN:O	5:M:72:LYS:HG3	2.04	0.57
1:C:240:PHE:HZ	1:D:456:HIS:HB3	1.69	0.56
1:C:490:PRO:HB2	1:C:492:PHE:N	2.20	0.56
1:E:672:THR:OG1	1:E:675:GLN:HB2	2.04	0.56
2:I:75:LEU:O	2:I:76:GLN:HG2	2.04	0.56
1:B:267:THR:HA	1:B:372:MET:SD	2.46	0.56
1:C:407:LEU:CD1	1:C:426:ILE:HG23	2.32	0.56
1:D:312:GLU:CG	1:D:313:GLN:N	2.67	0.56
1:D:510:TRP:HB3	1:D:679:ALA:HB2	1.87	0.56
1:D:686:PHE:CE1	1:D:714:ILE:HG23	2.40	0.56
1:A:352:ASN:HA	1:A:355:LEU:HD12	1.87	0.56
1:A:449:GLN:O	1:A:453:MET:HG2	2.05	0.56
1:B:353:GLN:HA	1:C:288:PRO:HG3	1.88	0.56
1:C:411:THR:O	1:C:414:MET:HB2	2.06	0.56
1:C:540:LEU:HD23	1:C:649:LYS:HE3	1.88	0.56
1:D:592:ALA:HB1	1:D:640:LEU:HD13	1.86	0.56
1:E:240:PHE:HZ	1:F:456:HIS:HB2	1.69	0.56
1:F:562:PHE:HE2	1:F:597:LEU:HD12	1.69	0.56
2:H:117:PHE:CD2	2:G:53:LYS:HE3	2.40	0.56
3:K:39:VAL:O	3:K:43:VAL:HG23	2.05	0.56
1:A:267:THR:OG1	1:A:328:ASP:OD2	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:ARG:HG3	1:B:534:THR:HG23	1.87	0.56
1:C:694:ILE:O	1:C:698:VAL:HG22	2.06	0.56
1:E:502:TYR:OH	1:E:569:SER:OG	2.20	0.56
2:H:38:ILE:HD11	2:H:71:LEU:HB3	1.88	0.56
5:M:55:GLU:HA	5:M:58:ASP:OD2	2.06	0.56
1:B:361:VAL:O	1:C:271:ARG:HD2	2.05	0.56
1:B:552:LEU:O	1:B:556:ILE:HG13	2.06	0.56
1:D:648:ARG:HG3	1:D:651:VAL:HG23	1.87	0.56
1:F:196:ILE:CA	1:F:200:LYS:HD3	2.35	0.56
1:B:73:SER:O	1:B:76:GLN:HG2	2.05	0.56
1:C:95:MET:HG3	1:C:152:ILE:HG12	1.86	0.56
1:E:664:THR:C	1:E:665:ILE:HD13	2.29	0.56
1:E:684:GLY:HA2	1:E:691:ARG:HH21	1.70	0.56
1:A:408:HIS:HA	1:A:426:ILE:HD12	1.88	0.56
1:B:383:LEU:O	1:B:389:LEU:HB2	2.06	0.56
1:B:404:LEU:HG	1:B:426:ILE:HG22	1.88	0.56
1:C:524:LEU:HD21	1:C:537:VAL:HG12	1.87	0.56
1:F:296:GLY:H	1:F:297:GLU:CB	2.19	0.56
1:F:327:PHE:HB2	1:F:330:ILE:CG2	2.35	0.56
2:H:155:GLU:C	2:H:157:SER:N	2.64	0.56
1:A:223:LEU:HD12	1:A:227:PHE:HB2	1.88	0.56
1:A:657:MET:HE3	1:A:661:PHE:HE1	1.71	0.56
1:B:114:THR:OG1	1:B:199:ALA:HB3	2.06	0.56
1:B:289:GLU:O	1:B:291:LEU:N	2.29	0.56
1:C:690:GLU:CB	1:C:726:VAL:HG21	2.36	0.56
2:I:200:TYR:C	3:K:47:ARG:HH12	2.14	0.56
3:K:80:SER:O	3:K:84:LEU:HG	2.06	0.56
1:B:559:GLU:O	1:B:561:ASN:ND2	2.38	0.56
1:C:106:ASN:HB3	1:C:143:LYS:HZ1	1.70	0.56
1:C:555:LYS:HA	1:C:558:GLU:OE1	2.05	0.56
1:D:242:PRO:HD2	1:D:243:GLU:H	1.69	0.56
1:A:111:PRO:O	1:A:319:ASN:ND2	2.39	0.55
1:C:542:GLU:HB2	1:C:649:LYS:HD3	1.88	0.55
1:D:303:ARG:HD3	1:D:353:GLN:CG	2.36	0.55
1:D:527:GLN:HE22	1:E:716:MET:HA	1.71	0.55
1:F:96:THR:HB	1:F:151:ASP:N	2.19	0.55
2:G:128:ALA:HB2	2:G:144:HIS:HB2	1.87	0.55
1:A:676:LEU:CD1	1:A:710:LEU:HD11	2.36	0.55
1:C:527:GLN:HB2	1:D:719:GLN:HG3	1.88	0.55
1:D:731:ALA:HA	1:D:734:ARG:NH1	2.21	0.55
1:E:573:MET:O	1:E:576:PHE:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:LEU:O	1:E:358:ILE:HG12	2.06	0.55
1:F:437:SER:O	1:F:440:GLU:HB2	2.05	0.55
2:I:116:ARG:HH11	2:I:116:ARG:HG3	1.71	0.55
2:I:127:ILE:HG23	2:I:131:TYR:CE1	2.41	0.55
2:G:232:PHE:H	2:G:233:PRO:HD2	1.71	0.55
3:K:77:PHE:HE1	5:M:78:LEU:HD11	1.70	0.55
5:M:180:ARG:O	5:M:184:LYS:HD3	2.07	0.55
1:A:678:GLU:O	1:A:681:GLU:HG2	2.05	0.55
1:C:40:SER:OG	1:C:41:PRO:HD2	2.07	0.55
1:D:593:TYR:O	1:D:638:ARG:HG2	2.07	0.55
1:F:67:ARG:HH12	1:F:74:ILE:HD11	1.71	0.55
2:H:233:PRO:HG2	2:G:268:SER:HA	1.87	0.55
5:M:177:GLN:HA	5:M:180:ARG:NH1	2.21	0.55
1:A:121:PHE:CD2	1:A:183:VAL:HG21	2.40	0.55
1:B:503:ILE:HG12	1:B:551:ALA:HA	1.88	0.55
1:B:576:PHE:HB2	1:B:581:LYS:HG3	1.89	0.55
1:D:527:GLN:NE2	1:E:716:MET:HA	2.21	0.55
1:E:242:PRO:HD2	1:E:243:GLU:H	1.71	0.55
1:F:18:LEU:HA	1:F:137:VAL:HG23	1.89	0.55
1:F:196:ILE:HA	1:F:200:LYS:HD3	1.89	0.55
1:F:503:ILE:HG22	1:F:506:GLY:H	1.71	0.55
1:F:529:LYS:HG3	1:F:597:LEU:HD11	1.89	0.55
2:H:40:GLU:O	2:H:44:ILE:HG12	2.07	0.55
1:A:411:THR:OG1	1:A:426:ILE:HD11	2.07	0.55
1:A:688:ASP:OD1	1:A:689:LYS:N	2.39	0.55
1:A:690:GLU:O	1:A:694:ILE:HG13	2.05	0.55
1:A:709:LYS:HE2	1:A:709:LYS:HA	1.88	0.55
1:B:295:VAL:C	1:C:294:TYR:HB2	2.31	0.55
1:D:67:ARG:HB3	2:J:218:MET:CG	2.37	0.55
1:E:652:LEU:HD22	1:E:658:LEU:HD13	1.89	0.55
1:F:715:GLU:O	1:F:719:GLN:HG2	2.07	0.55
2:I:149:ALA:HB2	2:I:164:CYS:HB2	1.89	0.55
5:M:56:GLN:O	5:M:60:VAL:HG23	2.06	0.55
1:A:223:LEU:CD1	1:A:227:PHE:HB2	2.36	0.55
1:A:531:SER:O	1:A:639:LYS:HE2	2.05	0.55
1:D:547:SER:OG	1:D:549:LYS:HG3	2.06	0.55
1:E:587:LYS:HZ1	1:E:591:ASP:CG	2.15	0.55
1:F:632:LYS:HD2	1:F:633:ALA:H	1.71	0.55
2:J:39:GLU:HB2	2:J:75:LEU:HD13	1.89	0.55
1:B:414:MET:HE2	1:B:414:MET:HA	1.88	0.55
1:C:533:ARG:HD2	1:D:505:ASN:OD1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:686:PHE:HB2	1:D:691:ARG:HG2	1.89	0.55
1:E:654:GLU:CD	1:F:614:ILE:HD11	2.32	0.55
1:E:671:ALA:HA	1:E:703:VAL:O	2.07	0.55
1:F:542:GLU:O	1:F:666:HIS:ND1	2.39	0.55
2:H:39:GLU:HB2	2:H:75:LEU:HD11	1.88	0.55
2:H:124:HIS:HE1	2:H:147:GLN:HB3	1.71	0.55
2:I:179:GLN:O	2:I:182:ILE:HG12	2.07	0.55
2:G:80:ASP:O	2:G:83:THR:OG1	2.24	0.55
4:L:206:GLU:HG3	5:M:28:SER:OG	2.06	0.55
1:A:542:GLU:OE2	1:A:666:HIS:NE2	2.40	0.55
1:B:242:PRO:HD2	1:B:243:GLU:H	1.71	0.55
1:B:589:PHE:CE2	1:B:629:LEU:HB3	2.41	0.55
1:C:533:ARG:C	1:D:505:ASN:HD21	2.14	0.55
1:E:383:LEU:O	1:E:389:LEU:HB2	2.07	0.55
1:F:613:PRO:HD3	1:F:648:ARG:HH12	1.72	0.55
2:I:39:GLU:HB2	2:I:75:LEU:HD11	1.89	0.55
2:I:108:ILE:HD12	2:I:127:ILE:HD12	1.89	0.55
2:J:35:SER:HB3	2:J:75:LEU:HD12	1.88	0.55
3:K:46:MET:O	3:K:50:VAL:HG23	2.07	0.55
4:L:200:SER:O	4:L:204:LYS:HG3	2.07	0.55
1:D:10:ARG:HA	1:D:67:ARG:NH1	2.22	0.55
1:E:516:ARG:O	1:E:519:ASP:OD1	2.24	0.55
1:E:527:GLN:HG3	1:F:719:GLN:HG3	1.87	0.55
1:F:410:HIS:O	1:F:414:MET:HG2	2.06	0.55
1:A:571:ASP:HA	1:A:574:ILE:HG23	1.89	0.54
1:A:677:LEU:HG	1:A:695:ALA:HB2	1.88	0.54
1:B:310:GLU:OE2	1:B:357:LYS:NZ	2.40	0.54
1:C:536:LEU:HD12	1:C:640:LEU:HB3	1.89	0.54
1:D:67:ARG:HB3	2:J:218:MET:HG2	1.88	0.54
1:E:673:GLY:HA3	1:E:698:VAL:HB	1.89	0.54
1:A:383:LEU:O	1:A:389:LEU:HB2	2.07	0.54
1:C:577:SER:O	1:C:579:THR:N	2.40	0.54
1:C:688:ASP:O	1:C:692:THR:HG23	2.07	0.54
1:C:689:LYS:O	1:C:692:THR:OG1	2.21	0.54
1:F:635:PRO:HD2	1:F:638:ARG:HD2	1.89	0.54
2:H:98:GLN:H	2:H:98:GLN:CD	2.15	0.54
1:A:300:ALA:O	1:A:304:LYS:HG3	2.08	0.54
1:A:503:ILE:CG2	1:A:506:GLY:HA2	2.37	0.54
1:A:563:PRO:HG2	1:A:597:LEU:O	2.07	0.54
1:D:663:THR:HG22	1:D:664:THR:N	2.21	0.54
1:F:508:ILE:C	1:F:509:LYS:HD3	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:230:GLU:HG2	2:G:231:LEU:N	2.23	0.54
1:A:625:ALA:O	1:A:629:LEU:HG	2.07	0.54
1:C:653:GLN:HG3	1:C:658:LEU:HD23	1.89	0.54
1:E:552:LEU:HD11	1:E:667:VAL:HG11	1.88	0.54
1:E:581:LYS:NZ	1:E:610:ASP:OD1	2.35	0.54
4:L:248:VAL:O	4:L:252:LYS:HG3	2.07	0.54
5:M:71:MET:HE2	5:M:192:ILE:HG12	1.90	0.54
1:C:227:PHE:O	1:C:231:PHE:HB2	2.08	0.54
1:E:604:ASP:O	1:E:608:LEU:N	2.38	0.54
1:F:602:VAL:N	1:F:643:ILE:O	2.26	0.54
2:G:57:ASN:O	2:G:59:SER:N	2.41	0.54
2:G:67:GLN:O	2:G:71:LEU:HG	2.08	0.54
1:A:293:LYS:O	1:A:294:TYR:CG	2.61	0.54
1:C:18:LEU:HA	1:C:137:VAL:HG23	1.90	0.54
1:C:307:ALA:O	1:C:310:GLU:HG2	2.07	0.54
1:D:380:ASP:OD1	1:D:382:ALA:N	2.37	0.54
1:E:95:MET:HG3	1:E:152:ILE:HG12	1.90	0.54
1:F:103:GLN:C	1:F:105:LYS:H	2.15	0.54
1:B:270:ALA:O	1:B:273:ILE:HG22	2.08	0.54
1:C:64:LEU:O	1:C:68:LYS:HG3	2.07	0.54
1:D:687:LYS:O	1:D:691:ARG:HG3	2.07	0.54
1:E:670:ILE:H	1:E:670:ILE:HD12	1.73	0.54
2:H:239:ARG:NH2	4:L:217:MET:HG3	2.23	0.54
2:H:256:VAL:HG11	2:H:288:GLN:HG2	1.90	0.54
5:M:17:ARG:CZ	5:M:21:LEU:HD21	2.38	0.54
1:A:111:PRO:HD2	1:A:320:SER:HA	1.89	0.54
1:E:104:LYS:HA	1:E:107:ILE:HD11	1.90	0.54
1:E:240:PHE:HZ	1:F:456:HIS:CB	2.21	0.54
1:E:550:THR:HA	1:E:645:THR:HG21	1.89	0.54
1:F:105:LYS:CE	2:G:257:ASP:HB2	2.37	0.54
1:F:270:ALA:O	1:F:273:ILE:HG22	2.08	0.54
1:F:544:PRO:HD2	1:F:547:SER:OG	2.08	0.54
5:M:59:ARG:HA	5:M:62:GLU:OE1	2.08	0.54
1:E:284:VAL:O	1:E:326:ILE:HG12	2.06	0.54
1:F:542:GLU:HB2	1:F:666:HIS:HA	1.90	0.54
1:F:555:LYS:HE2	1:F:555:LYS:HA	1.90	0.54
2:J:210:ALA:HB3	2:J:244:MET:HE3	1.88	0.54
2:J:212:CYS:SG	2:J:279:MET:HE1	2.48	0.54
4:L:198:ARG:HG2	4:L:202:ILE:HD11	1.89	0.54
1:B:187:LYS:HZ1	1:B:315:ARG:NH1	2.06	0.54
1:B:570:PRO:HG3	1:B:608:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:LYS:HE3	1:B:732:LEU:HD21	1.89	0.54
1:D:98:GLU:HB3	1:D:148:LEU:HB3	1.90	0.54
1:E:508:ILE:HB	1:E:682:LEU:HD13	1.90	0.54
1:F:525:VAL:HG13	1:F:562:PHE:HE1	1.72	0.54
1:A:247:GLN:O	1:B:414:MET:HE3	2.08	0.53
1:A:424:VAL:HG22	1:A:479:ASP:O	2.08	0.53
1:C:589:PHE:CD2	1:C:629:LEU:HD13	2.43	0.53
1:D:257:LEU:HG	1:D:371:GLY:O	2.07	0.53
1:D:681:GLU:HG2	1:D:691:ARG:NH1	2.23	0.53
1:A:12:PRO:HG2	1:A:23:VAL:HG11	1.90	0.53
1:B:669:ASN:CG	1:B:706:GLY:HA2	2.33	0.53
1:F:606:GLU:OE2	1:F:647:SER:HB2	2.07	0.53
1:F:710:LEU:O	1:F:714:ILE:HG13	2.08	0.53
3:K:51:ASP:O	3:K:55:GLU:HG3	2.07	0.53
1:B:261:PRO:HB3	1:B:594:LYS:NZ	2.23	0.53
1:B:397:LEU:HD11	1:B:595:SER:HA	1.89	0.53
1:C:18:LEU:HD13	1:C:139:SER:HB2	1.90	0.53
1:C:40:SER:HB3	1:C:43:HIS:HB2	1.88	0.53
1:C:308:ASP:OD1	1:C:309:ALA:N	2.41	0.53
1:C:728:LYS:HE3	1:C:732:LEU:HD21	1.91	0.53
1:D:657:MET:HG2	1:D:661:PHE:CE2	2.44	0.53
1:E:310:GLU:OE2	1:E:357:LYS:NZ	2.41	0.53
2:H:95:ALA:HB1	2:H:97:PRO:HD2	1.90	0.53
2:I:120:ALA:O	2:I:124:HIS:HB2	2.08	0.53
3:K:56:ARG:NH1	3:K:56:ARG:HB3	2.23	0.53
1:B:626:LEU:O	1:B:630:LEU:HG	2.09	0.53
1:C:285:VAL:HG13	1:C:326:ILE:HD11	1.89	0.53
1:D:64:LEU:N	1:D:67:ARG:HH21	2.06	0.53
1:D:95:MET:HG3	1:D:152:ILE:HG12	1.91	0.53
1:D:677:LEU:O	1:D:691:ARG:NH2	2.41	0.53
1:E:399:ASP:O	1:E:403:ARG:N	2.34	0.53
1:F:245:VAL:O	1:F:249:GLY:N	2.37	0.53
2:J:188:VAL:HG13	2:J:205:TYR:HD2	1.73	0.53
4:L:230:ILE:HD12	5:M:53:GLN:OE1	2.08	0.53
1:A:406:ILE:O	1:A:409:ILE:HG22	2.09	0.53
1:B:284:VAL:O	1:B:326:ILE:HG12	2.09	0.53
1:D:23:VAL:HG12	1:D:55:VAL:HG21	1.90	0.53
1:D:524:LEU:O	1:D:527:GLN:HB3	2.08	0.53
1:D:686:PHE:HE1	1:D:714:ILE:HG23	1.74	0.53
2:I:116:ARG:HH21	3:K:66:ARG:HH12	1.57	0.53
1:B:546:HIS:O	1:B:549:LYS:HE3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ILE:HD11	1:D:44:LYS:HB3	1.91	0.53
1:E:684:GLY:HA2	1:E:691:ARG:NH2	2.24	0.53
5:M:171:ILE:HG22	5:M:175:ASN:HD21	1.73	0.53
1:A:724:TYR:HD1	1:A:727:ARG:HH12	1.56	0.53
1:C:584:ALA:O	1:C:588:ILE:HG13	2.09	0.53
1:C:613:PRO:HD3	1:C:648:ARG:NH2	2.24	0.53
1:D:539:VAL:HG13	1:D:643:ILE:HG13	1.91	0.53
1:E:595:SER:HB3	1:E:598:SER:HB3	1.90	0.53
1:E:666:HIS:CD2	1:E:668:PRO:HD3	2.44	0.53
1:F:562:PHE:CD1	1:F:599:CYS:HB2	2.44	0.53
2:H:203:LYS:NZ	2:H:239:ARG:HH21	2.05	0.53
3:K:33:GLN:HG2	4:L:201:GLU:HG3	1.89	0.53
3:K:42:VAL:HG21	5:M:157:ILE:HD12	1.91	0.53
1:A:121:PHE:HD2	1:A:183:VAL:HG21	1.73	0.53
1:F:236:ALA:HA	1:F:239:VAL:HG12	1.91	0.53
1:F:263:GLY:HA3	1:F:437:SER:HA	1.89	0.53
1:F:617:ARG:HH11	1:F:617:ARG:HG3	1.73	0.53
2:H:72:HIS:CE1	2:H:80:ASP:HB2	2.44	0.53
2:H:239:ARG:HH22	4:L:217:MET:HG3	1.73	0.53
3:K:67:ALA:O	3:K:70:LEU:HB3	2.09	0.53
1:A:64:LEU:HA	1:A:67:ARG:HE	1.74	0.53
1:A:113:ASP:O	1:A:117:MET:HG3	2.09	0.53
1:A:544:PRO:HB2	1:A:669:ASN:ND2	2.24	0.53
1:C:122:ILE:O	1:C:126:ASN:HB3	2.08	0.53
2:G:38:ILE:HD11	2:G:71:LEU:HB3	1.91	0.53
1:A:136:LEU:N	1:A:136:LEU:HD23	2.24	0.53
1:C:135:GLN:HG2	1:C:148:LEU:HD13	1.91	0.53
1:D:599:CYS:SG	1:D:641:LEU:HD22	2.49	0.53
1:E:267:THR:HA	1:E:372:MET:SD	2.48	0.53
1:F:559:GLU:HA	1:F:559:GLU:OE1	2.08	0.53
1:F:720:MET:HB3	1:F:724:TYR:HB2	1.91	0.53
2:H:57:ASN:O	2:H:59:SER:N	2.42	0.53
2:J:201:SER:OG	2:J:205:TYR:HE1	1.92	0.53
2:J:219:LEU:CB	2:J:222:LYS:HB3	2.36	0.53
1:A:64:LEU:HA	1:A:67:ARG:HH21	1.75	0.52
1:A:286:ASN:HB2	1:A:327:PHE:CB	2.39	0.52
1:E:506:GLY:O	1:E:508:ILE:N	2.40	0.52
1:A:536:LEU:HD23	1:A:634:PRO:HD3	1.91	0.52
1:A:719:GLN:HG2	1:F:523:LEU:HG	1.91	0.52
1:C:388:ARG:NH1	1:C:388:ARG:HB2	2.24	0.52
1:D:113:ASP:O	1:D:117:MET:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:GLY:O	1:D:268:LEU:HG	2.09	0.52
1:E:122:ILE:O	1:E:126:ASN:HB3	2.09	0.52
2:H:116:ARG:HH21	3:K:68:ASP:CG	2.17	0.52
2:I:119:ILE:O	2:I:122:LYS:HB2	2.09	0.52
1:F:512:ASP:OD1	1:F:513:PRO:HD3	2.09	0.52
2:H:207:PHE:HB2	2:H:240:GLU:HG2	1.91	0.52
2:J:45:TYR:HB2	2:J:68:ALA:HB2	1.89	0.52
2:G:182:ILE:O	2:G:186:GLU:HG2	2.10	0.52
1:C:242:PRO:HD2	1:C:243:GLU:H	1.74	0.52
1:C:444:LEU:HD12	1:C:445:VAL:HG23	1.91	0.52
1:C:688:ASP:OD1	1:C:691:ARG:NH2	2.31	0.52
1:D:64:LEU:O	1:D:68:LYS:HG3	2.09	0.52
1:D:300:ALA:O	1:D:303:ARG:HB3	2.09	0.52
1:E:313:GLN:O	1:E:317:GLY:N	2.42	0.52
2:I:147:GLN:HG2	2:I:151:TYR:CE2	2.44	0.52
2:I:158:ASN:O	2:I:162:ASN:ND2	2.39	0.52
1:A:428:GLU:O	1:A:432:GLU:HG2	2.10	0.52
1:A:525:VAL:HG13	1:A:562:PHE:CE1	2.43	0.52
1:B:421:SER:HB3	1:B:424:VAL:HG23	1.91	0.52
1:C:281:GLU:CB	1:C:324:ILE:HD13	2.40	0.52
1:C:521:GLY:HA3	1:C:556:ILE:HD13	1.92	0.52
1:D:632:LYS:HZ3	1:E:571:ASP:HB3	1.75	0.52
1:E:36:ILE:HD11	1:E:44:LYS:HB3	1.91	0.52
1:E:549:LYS:O	1:E:552:LEU:HB2	2.10	0.52
1:E:666:HIS:HD2	1:E:668:PRO:HD3	1.75	0.52
1:F:289:GLU:O	1:F:291:LEU:N	2.32	0.52
2:H:179:GLN:O	2:H:182:ILE:HG12	2.10	0.52
2:J:175:LEU:HD23	2:J:177:GLN:HE21	1.74	0.52
2:G:239:ARG:NH2	5:M:37:GLU:OE1	2.42	0.52
1:B:34:HIS:HB2	1:B:83:TYR:O	2.10	0.52
1:B:113:ASP:O	1:B:117:MET:HG3	2.09	0.52
1:B:606:GLU:OE1	1:B:606:GLU:N	2.43	0.52
1:C:399:ASP:O	1:C:403:ARG:N	2.36	0.52
1:C:703:VAL:O	1:C:704:TRP:HD1	1.93	0.52
1:D:94:THR:HA	1:D:182:GLN:O	2.09	0.52
1:D:128:GLN:O	1:D:176:LEU:HD12	2.09	0.52
1:F:128:GLN:O	1:F:176:LEU:HD12	2.09	0.52
1:F:450:SER:O	1:F:453:MET:HB2	2.09	0.52
1:F:635:PRO:HB2	1:F:638:ARG:NH1	2.25	0.52
2:H:9:GLU:O	2:H:13:LEU:HG	2.10	0.52
2:H:243:LEU:HD13	2:H:266:TYR:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLY:O	1:A:224:ASP:N	2.42	0.52
1:A:716:MET:HG2	1:A:732:LEU:HD11	1.92	0.52
1:B:106:ASN:HB3	1:B:143:LYS:HZ1	1.75	0.52
1:D:312:GLU:O	1:D:316:LEU:N	2.38	0.52
1:E:18:LEU:HD13	1:E:139:SER:OG	2.10	0.52
1:E:270:ALA:O	1:E:273:ILE:HG22	2.09	0.52
5:M:52:GLU:O	5:M:56:GLN:HG3	2.10	0.52
1:A:227:PHE:CE1	1:A:273:ILE:HD13	2.45	0.52
1:D:104:LYS:HA	1:D:107:ILE:HD11	1.92	0.52
1:D:528:THR:CB	1:D:641:LEU:HD12	2.40	0.52
1:F:14:ASP:O	1:F:18:LEU:HG	2.09	0.52
2:H:244:MET:O	2:H:248:LEU:HG	2.09	0.52
2:J:149:ALA:HB2	2:J:164:CYS:HB2	1.92	0.52
2:G:40:GLU:O	2:G:44:ILE:HG12	2.09	0.52
2:G:203:LYS:HZ2	2:G:236:SER:C	2.17	0.52
5:M:171:ILE:HG22	5:M:175:ASN:ND2	2.24	0.52
1:A:355:LEU:HB3	1:A:388:ARG:NH1	2.25	0.52
1:B:576:PHE:HB3	1:B:580:ALA:HB3	1.90	0.52
1:C:231:PHE:O	1:C:235:PHE:HB2	2.09	0.52
1:C:525:VAL:HG13	1:C:562:PHE:CZ	2.45	0.52
1:D:527:GLN:NE2	1:E:715:GLU:HG3	2.23	0.52
1:F:96:THR:O	1:F:149:VAL:HA	2.10	0.52
1:F:562:PHE:HB2	1:F:565:ILE:HG12	1.92	0.52
2:H:219:LEU:HD12	2:H:223:LEU:HB2	1.91	0.52
1:C:326:ILE:HB	1:C:370:ILE:HD11	1.92	0.52
1:C:611:TYR:CZ	1:C:651:VAL:HG11	2.45	0.52
1:D:604:ASP:HB3	1:D:607:ARG:HB2	1.91	0.52
1:D:720:MET:HE3	1:D:724:TYR:CE1	2.40	0.52
1:F:655:MET:O	1:F:656:GLU:CB	2.58	0.52
2:I:271:ARG:NH2	2:J:231:LEU:HB2	2.25	0.52
2:G:127:ILE:HG23	2:G:131:TYR:CE1	2.44	0.52
1:A:300:ALA:HA	1:A:303:ARG:HG2	1.92	0.51
1:A:407:LEU:HD12	1:A:426:ILE:HG23	1.92	0.51
1:A:607:ARG:NH1	1:F:624:GLN:OE1	2.42	0.51
1:E:705:ILE:HD13	1:E:710:LEU:HD13	1.91	0.51
1:A:565:ILE:HA	1:A:599:CYS:O	2.09	0.51
1:A:646:THR:HG21	1:A:652:LEU:HD22	1.93	0.51
1:E:527:GLN:NE2	1:F:716:MET:HG2	2.20	0.51
2:I:116:ARG:NH1	5:M:186:ASP:OD2	2.43	0.51
2:G:51:MET:HA	2:G:54:MET:HG2	1.93	0.51
1:A:598:SER:O	1:A:640:LEU:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:VAL:CG1	1:C:617:ARG:HB3	2.40	0.51
1:D:43:HIS:HB3	1:D:45:TYR:HE1	1.74	0.51
1:D:260:GLY:N	1:D:266:LYS:HD3	2.25	0.51
1:E:611:TYR:CE1	1:E:616:PRO:HB2	2.44	0.51
1:F:313:GLN:O	1:F:317:GLY:N	2.43	0.51
2:H:112:THR:HG23	2:H:117:PHE:CE1	2.45	0.51
2:J:167:LYS:HE2	2:J:171:TYR:HE2	1.75	0.51
2:G:266:TYR:CZ	2:G:270:SER:HB2	2.44	0.51
5:M:25:SER:O	5:M:29:THR:HG23	2.11	0.51
1:A:102:LEU:HD22	1:A:137:VAL:HG12	1.91	0.51
1:A:546:HIS:NE2	1:F:659:ASN:OD1	2.43	0.51
1:D:512:ASP:N	1:D:513:PRO:CD	2.74	0.51
1:D:560:SER:HB2	1:D:562:PHE:CD1	2.45	0.51
1:D:657:MET:HG2	1:D:661:PHE:HE2	1.76	0.51
1:E:428:GLU:O	1:E:432:GLU:HG2	2.10	0.51
1:E:612:VAL:HG22	1:E:613:PRO:HD2	1.92	0.51
1:F:517:VAL:HG13	1:F:665:ILE:CG2	2.40	0.51
1:F:544:PRO:O	1:F:547:SER:OG	2.25	0.51
2:H:69:ALA:HB1	2:H:85:PHE:CE1	2.45	0.51
2:J:243:LEU:HD13	2:J:266:TYR:HB2	1.92	0.51
1:A:283:LYS:HA	1:A:324:ILE:O	2.11	0.51
1:A:326:ILE:HG22	1:A:370:ILE:CG1	2.41	0.51
1:D:618:PHE:HE1	1:E:612:VAL:HG21	1.76	0.51
1:E:247:GLN:HA	1:F:417:HIS:ND1	2.26	0.51
2:H:49:ALA:HB2	2:H:64:ALA:HB3	1.93	0.51
2:J:195:SER:C	2:J:197:LEU:H	2.19	0.51
2:J:243:LEU:HD22	2:J:266:TYR:CD2	2.45	0.51
5:M:179:ASP:O	5:M:183:GLU:HG2	2.11	0.51
1:B:570:PRO:HD3	1:B:603:ASP:HB3	1.93	0.51
1:D:67:ARG:CD	2:J:218:MET:HE2	2.35	0.51
1:D:221:GLY:HA3	1:D:406:ILE:HD13	1.93	0.51
1:D:313:GLN:OE1	1:D:365:ASN:O	2.29	0.51
2:I:124:HIS:HE1	2:I:147:GLN:HB3	1.76	0.51
2:J:69:ALA:HB1	2:J:85:PHE:CE1	2.46	0.51
2:G:260:THR:HG21	2:G:284:LYS:HE3	1.93	0.51
5:M:44:ILE:O	5:M:48:VAL:HG23	2.11	0.51
5:M:177:GLN:O	5:M:181:ILE:HG13	2.11	0.51
1:A:198:LYS:O	1:A:198:LYS:HD3	2.10	0.51
1:A:521:GLY:HA2	1:A:524:LEU:HD12	1.93	0.51
1:C:136:LEU:N	1:C:136:LEU:HD23	2.26	0.51
1:C:573:MET:HB3	1:C:576:PHE:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:GLU:OE2	1:D:556:ILE:HA	2.10	0.51
1:D:656:GLU:OE1	1:E:613:PRO:HB3	2.10	0.51
1:E:46:ILE:HD12	1:E:174:VAL:HG21	1.92	0.51
1:E:188:ALA:O	1:E:189:GLU:C	2.53	0.51
1:E:674:GLU:O	1:E:677:LEU:HB2	2.11	0.51
1:F:289:GLU:C	1:F:291:LEU:H	2.14	0.51
1:F:653:GLN:HB3	1:F:658:LEU:HD23	1.93	0.51
2:H:67:GLN:O	2:H:71:LEU:HG	2.10	0.51
1:A:686:PHE:CE2	1:A:714:ILE:HG12	2.37	0.51
1:B:136:LEU:N	1:B:136:LEU:HD23	2.26	0.51
1:C:236:ALA:HB1	1:D:453:MET:CB	2.41	0.51
1:D:527:GLN:NE2	1:E:715:GLU:C	2.69	0.51
1:E:327:PHE:CZ	1:E:369:VAL:HG21	2.46	0.51
2:H:45:TYR:HE2	2:H:71:LEU:HD11	1.75	0.51
2:I:122:LYS:HZ3	3:K:59:LYS:HZ3	1.57	0.51
2:I:163:LYS:O	2:I:167:LYS:HG2	2.10	0.51
2:J:235:PHE:CB	3:K:38:GLN:HE21	2.17	0.51
2:G:98:GLN:C	2:G:100:ALA:H	2.19	0.51
1:C:91:CYS:HB3	1:C:155:MET:HE2	1.92	0.51
1:C:404:LEU:HG	1:C:426:ILE:HG22	1.93	0.51
1:C:596:GLN:HA	1:C:638:ARG:CD	2.40	0.51
2:I:67:GLN:O	2:I:71:LEU:HG	2.11	0.51
2:J:230:GLU:HG3	2:J:237:ASP:CB	2.41	0.51
1:A:673:GLY:O	1:A:677:LEU:HD22	2.11	0.51
1:C:295:VAL:O	1:D:294:TYR:HB2	2.10	0.51
1:C:375:ARG:NH1	1:C:378:LEU:HG	2.26	0.51
1:E:230:ILE:HD11	1:E:391:VAL:HG11	1.93	0.51
1:E:303:ARG:CG	1:E:357:LYS:HE2	2.41	0.51
1:F:113:ASP:O	1:F:117:MET:HG3	2.11	0.51
1:F:538:SER:H	1:F:662:SER:CB	2.24	0.51
2:G:153:LYS:HE2	2:G:158:ASN:HD22	1.76	0.51
2:G:185:TYR:HA	2:G:188:VAL:HG12	1.92	0.51
1:A:546:HIS:CE1	1:A:709:LYS:HE3	2.46	0.50
1:B:24:VAL:HG12	1:B:60:VAL:HG13	1.92	0.50
1:B:539:VAL:HG21	1:B:665:ILE:HD12	1.93	0.50
1:D:528:THR:HG22	1:D:597:LEU:HD11	1.93	0.50
1:E:64:LEU:HA	1:E:67:ARG:HE	1.75	0.50
1:E:590:ASP:O	1:E:593:TYR:HB2	2.11	0.50
1:F:258:LEU:CB	1:F:395:ILE:HD11	2.40	0.50
1:F:721:ASP:HB2	1:F:724:TYR:CD1	2.44	0.50
5:M:26:LEU:HG	5:M:30:ARG:HH12	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:PRO:HG3	1:A:436:PHE:C	2.36	0.50
1:B:303:ARG:CG	1:B:357:LYS:HE2	2.41	0.50
1:C:399:ASP:O	1:C:402:GLY:N	2.45	0.50
1:C:524:LEU:CD2	1:C:537:VAL:HG11	2.37	0.50
1:C:730:LEU:O	1:C:734:ARG:HG3	2.11	0.50
1:D:136:LEU:N	1:D:136:LEU:HD23	2.26	0.50
1:D:618:PHE:CE1	1:E:612:VAL:HG21	2.47	0.50
1:E:245:VAL:O	1:E:249:GLY:N	2.39	0.50
1:F:281:GLU:N	1:F:282:PRO:HA	2.26	0.50
2:H:197:LEU:HD12	5:M:45:ARG:CD	2.41	0.50
1:A:315:ARG:HG2	1:A:316:LEU:CD1	2.40	0.50
1:A:347:HIS:N	1:A:348:ASP:HA	2.25	0.50
1:A:565:ILE:HG13	1:A:599:CYS:HB3	1.92	0.50
1:B:571:ASP:O	1:B:574:ILE:HG13	2.11	0.50
1:C:233:ARG:CZ	1:C:233:ARG:HB2	2.41	0.50
1:C:612:VAL:HG12	1:C:617:ARG:HB3	1.93	0.50
1:C:691:ARG:HH11	1:C:691:ARG:HB2	1.76	0.50
1:F:284:VAL:O	1:F:326:ILE:HG12	2.12	0.50
2:H:158:ASN:N	4:L:228:GLU:OE1	2.43	0.50
2:G:20:LYS:HE2	2:G:37:LYS:HA	1.93	0.50
5:M:171:ILE:CG2	5:M:175:ASN:HD21	2.24	0.50
1:C:24:VAL:O	1:C:51:THR:HA	2.12	0.50
1:C:284:VAL:HG11	1:C:305:LEU:HD11	1.93	0.50
1:C:677:LEU:HD21	1:C:695:ALA:CB	2.42	0.50
1:C:686:PHE:HE1	1:C:714:ILE:HG23	1.76	0.50
1:D:89:LYS:NZ	1:D:170:GLN:HE22	2.10	0.50
1:D:593:TYR:OH	1:D:632:LYS:HD2	2.11	0.50
1:E:136:LEU:N	1:E:136:LEU:HD23	2.25	0.50
1:F:267:THR:HA	1:F:372:MET:SD	2.52	0.50
2:J:200:TYR:HE2	3:K:41:GLU:CG	2.23	0.50
2:G:235:PHE:CD2	5:M:152:GLN:HG2	2.46	0.50
1:A:95:MET:HG3	1:A:152:ILE:HG12	1.92	0.50
1:B:499:TYR:HA	1:B:502:TYR:CD2	2.46	0.50
1:B:589:PHE:HD2	1:B:629:LEU:HD22	1.76	0.50
1:C:560:SER:HB2	1:C:562:PHE:CE1	2.46	0.50
1:E:585:MET:HG3	1:E:589:PHE:HZ	1.69	0.50
1:E:593:TYR:CD2	1:E:635:PRO:HD3	2.47	0.50
1:F:436:PHE:HB3	1:F:440:GLU:CB	2.41	0.50
1:F:589:PHE:CD2	1:F:629:LEU:HD22	2.47	0.50
2:G:244:MET:O	2:G:248:LEU:HG	2.12	0.50
5:M:142:ARG:HG2	5:M:142:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:GLU:O	1:C:432:GLU:HG2	2.12	0.50
1:D:298:SER:O	1:D:301:ASN:HB3	2.12	0.50
1:D:331:ASP:HA	1:D:379:ILE:HD11	1.92	0.50
1:D:690:GLU:O	1:D:693:THR:OG1	2.22	0.50
1:E:327:PHE:HB2	1:E:330:ILE:CG2	2.35	0.50
2:I:200:TYR:CB	3:K:47:ARG:HH12	2.25	0.50
5:M:149:ASN:HA	5:M:152:GLN:NE2	2.27	0.50
1:A:258:LEU:O	1:A:372:MET:HA	2.11	0.50
1:A:398:PRO:HD2	1:A:434:LYS:O	2.12	0.50
1:B:249:GLY:HA2	1:C:413:ARG:NH1	2.26	0.50
1:B:533:ARG:HG3	1:B:534:THR:N	2.26	0.50
1:C:375:ARG:NH2	1:C:377:ASP:OD1	2.44	0.50
1:C:614:ILE:O	1:C:616:PRO:HA	2.10	0.50
1:D:114:THR:HG21	1:D:200:LYS:HG2	1.94	0.50
1:F:64:LEU:HA	1:F:67:ARG:HE	1.77	0.50
2:H:20:LYS:HG2	2:H:37:LYS:HB3	1.92	0.50
2:H:38:ILE:HG23	2:H:75:LEU:HD12	1.94	0.50
2:J:18:GLU:HA	2:J:21:VAL:HG12	1.94	0.50
3:K:46:MET:SD	3:K:49:ASN:ND2	2.85	0.50
1:A:286:ASN:HB2	1:A:327:PHE:HB3	1.93	0.50
1:B:195:LEU:HB2	1:B:200:LYS:HE3	1.94	0.50
1:B:353:GLN:HE21	1:B:357:LYS:HG2	1.77	0.50
1:B:428:GLU:O	1:B:432:GLU:HG2	2.11	0.50
1:B:485:GLU:O	1:B:490:PRO:HD3	2.11	0.50
1:B:503:ILE:HD11	1:B:554:ALA:HB3	1.94	0.50
1:B:628:VAL:CG1	1:C:571:ASP:HA	2.42	0.50
1:C:299:GLU:OE2	1:C:349:THR:OG1	2.23	0.50
1:D:310:GLU:O	1:D:313:GLN:NE2	2.45	0.50
1:D:589:PHE:CE2	1:D:629:LEU:HD13	2.46	0.50
1:D:616:PRO:HG2	1:E:614:ILE:HG21	1.93	0.50
1:E:258:LEU:HB3	1:E:395:ILE:HD11	1.94	0.50
1:F:114:THR:HG21	1:F:200:LYS:HA	1.93	0.50
1:F:136:LEU:N	1:F:136:LEU:HD23	2.26	0.50
1:F:570:PRO:CG	1:F:604:ASP:HB2	2.39	0.50
2:G:256:VAL:HG22	2:G:256:VAL:O	2.12	0.50
1:C:36:ILE:HD11	1:C:44:LYS:HB3	1.92	0.50
1:C:113:ASP:O	1:C:117:MET:HG3	2.12	0.50
3:K:48:VAL:CG1	3:K:52:LYS:HZ1	2.25	0.50
1:A:132:VAL:HG23	1:A:173:GLU:O	2.12	0.49
1:A:540:LEU:HD12	1:A:644:GLY:O	2.12	0.49
1:A:650:ASP:OD1	1:A:650:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:ARG:HD3	1:D:353:GLN:CD	2.37	0.49
1:D:330:ILE:HD12	1:D:331:ASP:N	2.27	0.49
1:D:581:LYS:O	1:D:585:MET:HG2	2.12	0.49
2:H:112:THR:HG23	2:H:117:PHE:HE1	1.76	0.49
2:H:243:LEU:HD22	2:H:266:TYR:CD2	2.47	0.49
2:G:243:LEU:HD13	2:G:266:TYR:HB2	1.94	0.49
5:M:46:THR:O	5:M:50:LEU:HG	2.11	0.49
1:A:397:LEU:CB	1:A:398:PRO:CD	2.89	0.49
1:A:493:GLY:HA2	1:A:494:THR:CB	2.41	0.49
1:B:230:ILE:HD11	1:B:391:VAL:HG11	1.93	0.49
1:B:614:ILE:O	1:B:616:PRO:HA	2.12	0.49
1:C:510:TRP:CE3	1:C:670:ILE:HG12	2.46	0.49
1:D:508:ILE:HG12	1:D:683:LEU:HD21	1.93	0.49
1:D:540:LEU:HD12	1:D:661:PHE:CE1	2.47	0.49
1:D:657:MET:HE2	1:D:661:PHE:CZ	2.47	0.49
1:F:64:LEU:O	1:F:68:LYS:HG2	2.12	0.49
1:F:327:PHE:CZ	1:F:369:VAL:HG21	2.47	0.49
2:H:239:ARG:HH22	4:L:213:HIS:CE1	2.30	0.49
2:I:214:PHE:CE1	2:I:216:ILE:HB	2.47	0.49
3:K:85:LYS:HG3	3:K:89:TRP:HE3	1.77	0.49
4:L:240:ALA:HA	4:L:243:TYR:CD2	2.44	0.49
1:A:411:THR:HG21	1:A:426:ILE:HD11	1.93	0.49
1:A:683:LEU:HB3	1:A:685:ASN:HD22	1.75	0.49
1:B:14:ASP:O	1:B:18:LEU:HD13	2.11	0.49
1:B:63:SER:O	1:B:67:ARG:HG3	2.12	0.49
1:B:569:SER:HA	1:B:603:ASP:HB3	1.95	0.49
1:C:331:ASP:HA	1:C:379:ILE:CD1	2.39	0.49
1:C:544:PRO:HG2	1:C:669:ASN:CG	2.37	0.49
1:D:26:GLU:HG2	1:D:51:THR:HB	1.93	0.49
1:D:48:THR:HG21	1:D:128:GLN:HG2	1.95	0.49
1:D:627:LEU:HD13	1:E:607:ARG:HH12	1.78	0.49
1:F:712:MET:O	1:F:716:MET:HG3	2.11	0.49
5:M:190:THR:HG22	5:M:194:GLU:OE2	2.12	0.49
1:A:445:VAL:O	1:A:449:GLN:HG2	2.12	0.49
1:B:568:CYS:SG	1:B:588:ILE:HD12	2.53	0.49
1:C:511:GLY:C	1:C:513:PRO:HD2	2.36	0.49
1:C:589:PHE:CE1	1:C:600:VAL:HG11	2.48	0.49
1:E:653:GLN:OE1	1:E:658:LEU:HD23	2.13	0.49
5:M:31:ARG:O	5:M:35:LEU:HG	2.13	0.49
5:M:159:ASN:OD1	5:M:163:MET:HE2	2.12	0.49
1:A:299:GLU:HG3	1:B:289:GLU:CB	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:VAL:HG12	1:B:655:MET:CE	2.42	0.49
1:D:602:VAL:O	1:D:644:GLY:HA2	2.13	0.49
1:E:697:GLN:HG3	1:E:730:LEU:CD1	2.41	0.49
2:H:142:ILE:HG23	2:H:168:VAL:HG13	1.94	0.49
2:I:92:PHE:HD1	2:I:97:PRO:HG2	1.77	0.49
2:G:17:ALA:O	2:G:21:VAL:HG12	2.11	0.49
1:A:505:ASN:OD1	1:A:711:LEU:HD13	2.13	0.49
1:D:721:ASP:O	1:D:725:ARG:HG3	2.13	0.49
1:E:352:ASN:HA	1:E:355:LEU:HD12	1.95	0.49
1:F:352:ASN:HA	1:F:355:LEU:HD12	1.93	0.49
2:I:20:LYS:NZ	2:I:40:GLU:HG2	2.28	0.49
2:G:162:ASN:OD1	2:G:188:VAL:HG23	2.13	0.49
5:M:149:ASN:HA	5:M:152:GLN:HE21	1.77	0.49
1:A:295:VAL:HB	1:B:294:TYR:CB	2.43	0.49
1:B:272:GLN:OE1	1:B:272:GLN:HA	2.13	0.49
1:B:499:TYR:HA	1:B:502:TYR:CE2	2.47	0.49
1:C:347:HIS:O	1:C:350:VAL:HG22	2.13	0.49
1:D:325:ILE:O	1:D:369:VAL:HA	2.13	0.49
1:D:681:GLU:HG2	1:D:691:ARG:CZ	2.43	0.49
1:F:411:THR:O	1:F:414:MET:HB2	2.13	0.49
2:I:18:GLU:HA	2:I:21:VAL:HG12	1.94	0.49
2:J:40:GLU:O	2:J:44:ILE:HG12	2.13	0.49
2:J:120:ALA:O	2:J:124:HIS:HB2	2.12	0.49
2:G:95:ALA:HB1	2:G:97:PRO:HD2	1.95	0.49
1:C:101:PHE:CD2	1:C:107:ILE:HA	2.48	0.49
1:C:609:LEU:O	1:C:610:ASP:HB2	2.11	0.49
1:E:256:ILE:O	1:E:370:ILE:HA	2.13	0.49
2:H:203:LYS:O	2:H:206:PHE:N	2.46	0.49
2:I:50:ASN:ND2	2:J:115:GLY:HA2	2.27	0.49
2:I:142:ILE:HG23	2:I:168:VAL:HG13	1.95	0.49
2:J:118:THR:O	2:J:122:LYS:HG2	2.13	0.49
2:J:124:HIS:HE1	2:J:147:GLN:HB3	1.77	0.49
1:D:268:LEU:HA	1:D:271:ARG:HD2	1.95	0.49
1:D:284:VAL:HG21	1:D:325:ILE:HG22	1.95	0.49
1:D:564:PHE:HD2	1:D:598:SER:HB2	1.78	0.49
1:E:510:TRP:CE3	1:E:670:ILE:HG13	2.47	0.49
3:K:66:ARG:NH2	5:M:182:MET:HB3	2.26	0.49
3:K:69:ALA:O	3:K:72:ALA:HB3	2.12	0.49
5:M:178:ILE:O	5:M:182:MET:HG3	2.12	0.49
1:A:128:GLN:O	1:A:176:LEU:HD12	2.11	0.49
1:A:624:GLN:HG3	1:B:610:ASP:CG	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:705:ILE:HD11	1:C:710:LEU:HA	1.94	0.49
1:E:236:ALA:O	1:E:239:VAL:HG12	2.13	0.49
1:F:45:TYR:CE2	1:F:70:ALA:HA	2.48	0.49
1:F:105:LYS:HE2	2:G:257:ASP:HB2	1.95	0.49
1:F:535:PRO:HB2	1:F:536:LEU:HD13	1.93	0.49
2:H:243:LEU:HD22	2:H:266:TYR:CG	2.48	0.49
2:I:17:ALA:O	2:I:21:VAL:HG12	2.12	0.49
2:I:45:TYR:HB2	2:I:68:ALA:HB2	1.94	0.49
2:I:266:TYR:CZ	2:I:270:SER:HB2	2.48	0.49
2:J:127:ILE:HG23	2:J:131:TYR:CE1	2.48	0.49
2:G:223:LEU:O	2:G:227:LYS:HG3	2.13	0.49
1:B:256:ILE:O	1:B:370:ILE:HA	2.13	0.48
1:C:349:THR:O	1:C:352:ASN:HB3	2.13	0.48
1:C:677:LEU:HD11	1:C:698:VAL:CG2	2.42	0.48
1:E:696:GLN:HB3	1:E:697:GLN:NE2	2.28	0.48
1:F:95:MET:HG3	1:F:152:ILE:HG12	1.95	0.48
1:F:428:GLU:O	1:F:432:GLU:HG2	2.13	0.48
2:H:36:SER:OG	5:M:201:LYS:HE2	2.13	0.48
2:H:185:TYR:HA	2:H:188:VAL:HG12	1.94	0.48
1:A:262:PRO:HA	1:A:263:GLY:HA2	1.71	0.48
1:B:45:TYR:CE2	1:B:70:ALA:HA	2.48	0.48
1:D:242:PRO:HD2	1:D:243:GLU:N	2.28	0.48
1:D:254:LYS:O	1:D:368:LEU:HA	2.13	0.48
1:E:596:GLN:O	1:E:638:ARG:HA	2.13	0.48
2:H:45:TYR:HB2	2:H:68:ALA:HB2	1.94	0.48
5:M:170:GLU:HG3	5:M:174:GLN:NE2	2.27	0.48
1:A:609:LEU:O	1:A:610:ASP:HB3	2.13	0.48
1:C:193:LEU:HD21	1:C:195:LEU:HD21	1.95	0.48
1:C:603:ASP:HA	1:C:645:THR:HG1	1.77	0.48
1:C:611:TYR:HE1	1:C:616:PRO:HB2	1.76	0.48
1:D:310:GLU:O	1:D:313:GLN:HG2	2.13	0.48
1:D:663:THR:CG2	1:D:664:THR:N	2.76	0.48
1:D:670:ILE:HD11	1:D:705:ILE:HG23	1.94	0.48
1:E:257:LEU:HG	1:E:371:GLY:O	2.13	0.48
1:E:538:SER:OG	1:E:662:SER:N	2.43	0.48
3:K:56:ARG:HD2	5:M:171:ILE:HG12	1.95	0.48
1:A:490:PRO:HA	1:A:491:ALA:CB	2.23	0.48
1:A:548:GLY:C	1:A:550:THR:N	2.65	0.48
1:A:611:TYR:CE2	1:A:651:VAL:HG11	2.48	0.48
1:B:38:ARG:HB3	1:B:79:GLU:HB2	1.95	0.48
1:B:265:GLY:O	1:B:268:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:LEU:O	1:B:714:ILE:HG13	2.12	0.48
1:C:436:PHE:CD1	1:C:436:PHE:N	2.81	0.48
1:E:404:LEU:HG	1:E:426:ILE:HG22	1.96	0.48
1:F:114:THR:HG21	1:F:200:LYS:HG2	1.94	0.48
1:F:404:LEU:HG	1:F:426:ILE:HG22	1.96	0.48
2:J:72:HIS:CE1	2:J:80:ASP:HB2	2.49	0.48
1:A:612:VAL:HG12	1:A:617:ARG:HB2	1.94	0.48
1:B:236:ALA:O	1:B:239:VAL:HG12	2.14	0.48
1:C:616:PRO:HG2	1:D:614:ILE:HD13	1.95	0.48
1:D:304:LYS:HA	1:D:307:ALA:HB3	1.95	0.48
1:D:652:LEU:HD13	1:D:657:MET:HB3	1.96	0.48
2:H:182:ILE:O	2:H:186:GLU:HG2	2.14	0.48
1:A:388:ARG:O	1:A:389:LEU:HD22	2.13	0.48
1:A:620:ASN:ND2	1:B:610:ASP:OD1	2.46	0.48
1:B:578:GLU:CG	1:B:619:SER:HB2	2.44	0.48
1:C:184:ALA:HB1	1:C:200:LYS:O	2.14	0.48
1:C:289:GLU:C	1:C:291:LEU:H	2.16	0.48
1:D:326:ILE:HG22	1:D:370:ILE:HG13	1.95	0.48
1:D:618:PHE:HE2	1:E:614:ILE:HD12	1.78	0.48
1:E:281:GLU:N	1:E:282:PRO:HA	2.28	0.48
1:E:598:SER:OG	1:E:639:LYS:O	2.16	0.48
1:E:654:GLU:CG	1:F:614:ILE:HD11	2.43	0.48
1:E:714:ILE:O	1:E:718:LEU:HG	2.12	0.48
1:F:236:ALA:O	1:F:239:VAL:HG12	2.13	0.48
2:J:235:PHE:CD2	3:K:38:GLN:HB2	2.49	0.48
2:G:98:GLN:H	2:G:98:GLN:CD	2.22	0.48
3:K:33:GLN:HG2	4:L:201:GLU:CB	2.44	0.48
3:K:43:VAL:HG13	4:L:215:MET:HE1	1.95	0.48
1:A:299:GLU:HG2	1:A:353:GLN:HG2	1.95	0.48
1:A:428:GLU:O	1:A:431:VAL:HG12	2.14	0.48
1:B:531:SER:HA	1:B:639:LYS:HD3	1.96	0.48
1:C:318:ALA:C	1:C:319:ASN:HD22	2.21	0.48
1:D:375:ARG:NH2	1:D:377:ASP:OD2	2.47	0.48
1:E:658:LEU:HD12	1:E:658:LEU:HA	1.62	0.48
1:E:670:ILE:HG22	1:E:672:THR:N	2.27	0.48
1:F:136:LEU:HD23	1:F:136:LEU:H	1.79	0.48
2:J:182:ILE:O	2:J:186:GLU:HG2	2.13	0.48
2:J:201:SER:CB	5:M:165:LEU:HD11	2.37	0.48
1:A:403:ARG:O	1:A:407:LEU:HG	2.14	0.48
1:B:352:ASN:HA	1:B:355:LEU:HD12	1.95	0.48
1:B:516:ARG:O	1:B:519:ASP:OD1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:628:VAL:HG13	1:C:571:ASP:HA	1.95	0.48
1:C:677:LEU:HD11	1:C:698:VAL:HG21	1.96	0.48
1:D:184:ALA:HA	1:D:199:ALA:O	2.14	0.48
1:D:315:ARG:O	1:D:316:LEU:HD12	2.14	0.48
1:E:705:ILE:HG13	1:E:709:LYS:HG3	1.95	0.48
2:I:201:SER:N	3:K:47:ARG:NH1	2.61	0.48
1:A:104:LYS:HA	1:A:107:ILE:HD11	1.96	0.48
1:A:423:ASP:HB2	1:A:480:PHE:N	2.29	0.48
1:A:485:GLU:O	1:A:489:LYS:CB	2.62	0.48
1:A:593:TYR:HB3	1:A:635:PRO:HD3	1.96	0.48
1:B:399:ASP:O	1:B:403:ARG:N	2.42	0.48
1:C:322:LEU:HD22	1:C:366:ASN:O	2.14	0.48
1:D:63:SER:C	1:D:67:ARG:HE	2.22	0.48
1:D:402:GLY:HA2	1:D:405:GLN:OE1	2.12	0.48
1:D:570:PRO:HA	1:D:573:MET:HB3	1.96	0.48
1:D:578:GLU:OE1	1:D:621:LEU:HD13	2.13	0.48
1:E:526:GLN:HA	1:E:529:LYS:HG2	1.96	0.48
1:E:527:GLN:HA	1:F:719:GLN:CD	2.39	0.48
1:E:693:THR:O	1:E:697:GLN:NE2	2.22	0.48
1:F:18:LEU:HD13	1:F:139:SER:OG	2.13	0.48
2:H:201:SER:O	2:H:203:LYS:N	2.47	0.48
2:H:230:GLU:HG3	2:H:237:ASP:CB	2.41	0.48
2:I:57:ASN:O	2:I:59:SER:N	2.46	0.48
2:G:256:VAL:HG11	2:G:288:GLN:HG2	1.96	0.48
1:A:222:GLY:HA3	1:A:402:GLY:HA3	1.94	0.48
1:B:325:ILE:HG13	1:B:369:VAL:HB	1.95	0.48
1:C:270:ALA:O	1:C:273:ILE:HG22	2.14	0.48
1:C:612:VAL:CG2	1:C:613:PRO:HD2	2.44	0.48
1:E:605:ILE:HA	1:E:608:LEU:HB3	1.96	0.48
2:G:177:GLN:HB3	2:G:180:LYS:HB2	1.96	0.48
3:K:29:ASN:CB	4:L:198:ARG:HH12	2.26	0.48
3:K:42:VAL:HG11	5:M:160:LEU:CD1	2.41	0.48
3:K:83:LYS:HD2	5:M:203:LEU:CD1	2.43	0.48
1:A:255:GLY:HA3	1:A:389:LEU:HD13	1.96	0.47
1:B:91:CYS:O	1:B:154:ALA:HA	2.14	0.47
1:B:185:PHE:O	1:B:200:LYS:HA	2.14	0.47
1:B:327:PHE:CZ	1:B:369:VAL:HG21	2.50	0.47
1:C:576:PHE:HB3	1:C:580:ALA:HB3	1.96	0.47
1:E:428:GLU:O	1:E:431:VAL:HG12	2.13	0.47
1:F:579:THR:O	1:F:583:GLN:HG2	2.13	0.47
2:H:127:ILE:HG23	2:H:131:TYR:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:ASN:HB3	1:B:320:SER:HB2	1.96	0.47
1:B:406:ILE:HB	1:B:441:LEU:HD13	1.96	0.47
1:C:26:GLU:HG2	1:C:51:THR:HB	1.95	0.47
1:C:36:ILE:O	1:C:36:ILE:HG23	2.13	0.47
1:D:531:SER:OG	1:D:534:THR:OG1	2.29	0.47
1:E:319:ASN:HB3	1:E:320:SER:HB2	1.95	0.47
1:F:257:LEU:HG	1:F:371:GLY:O	2.12	0.47
1:F:286:ASN:OD1	1:F:327:PHE:HD1	1.97	0.47
1:F:303:ARG:CG	1:F:357:LYS:HE2	2.39	0.47
2:H:167:LYS:HE2	2:H:171:TYR:HE2	1.80	0.47
2:I:200:TYR:C	3:K:47:ARG:NH1	2.72	0.47
5:M:26:LEU:HG	5:M:30:ARG:NH1	2.29	0.47
5:M:45:ARG:O	5:M:49:MET:HG3	2.14	0.47
1:B:36:ILE:HG23	1:B:36:ILE:O	2.14	0.47
1:B:428:GLU:O	1:B:431:VAL:HG12	2.14	0.47
1:C:18:LEU:HA	1:C:137:VAL:CG2	2.44	0.47
1:C:91:CYS:O	1:C:154:ALA:HA	2.14	0.47
1:E:104:LYS:HA	1:E:107:ILE:CD1	2.44	0.47
1:E:153:GLU:OE1	1:E:169:ARG:HD3	2.14	0.47
1:E:315:ARG:HG3	1:E:316:LEU:HD12	1.94	0.47
1:F:653:GLN:HA	1:F:658:LEU:HB3	1.94	0.47
2:H:203:LYS:HZ1	2:H:239:ARG:HH21	1.63	0.47
2:I:14:LEU:O	2:I:17:ALA:HB3	2.14	0.47
1:B:436:PHE:HB3	1:B:440:GLU:CB	2.44	0.47
1:D:257:LEU:HB2	1:D:389:LEU:HD13	1.96	0.47
1:E:286:ASN:OD1	1:E:327:PHE:HD1	1.97	0.47
2:J:256:VAL:HG21	2:J:288:GLN:HG3	1.95	0.47
2:G:179:GLN:O	2:G:182:ILE:HG12	2.13	0.47
2:G:243:LEU:HD22	2:G:266:TYR:CG	2.49	0.47
2:G:243:LEU:HD22	2:G:266:TYR:CD2	2.49	0.47
1:A:115:ASP:CG	1:A:242:PRO:HG3	2.40	0.47
1:B:579:THR:O	1:B:583:GLN:HG2	2.14	0.47
1:C:681:GLU:HG3	1:C:691:ARG:HD2	1.97	0.47
1:C:686:PHE:CE1	1:C:714:ILE:HG23	2.49	0.47
1:F:256:ILE:O	1:F:370:ILE:HA	2.14	0.47
4:L:216:PHE:CD2	5:M:39:SER:HB2	2.49	0.47
5:M:64:MET:HG3	5:M:181:ILE:HG23	1.95	0.47
1:A:52:HIS:C	1:A:54:SER:H	2.23	0.47
1:A:489:LYS:H	1:A:490:PRO:HD2	1.80	0.47
1:B:297:GLU:O	1:B:300:ALA:HB3	2.14	0.47
1:C:18:LEU:HD23	1:C:137:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:ASP:N	1:C:513:PRO:CD	2.77	0.47
1:D:281:GLU:N	1:D:282:PRO:HA	2.29	0.47
1:E:128:GLN:O	1:E:176:LEU:HD12	2.14	0.47
1:E:257:LEU:HB2	1:E:389:LEU:HD13	1.96	0.47
1:E:585:MET:HE1	1:E:602:VAL:HG13	1.96	0.47
1:F:615:GLY:HA3	1:F:616:PRO:C	2.39	0.47
2:H:162:ASN:ND2	2:H:188:VAL:HG23	2.29	0.47
2:I:162:ASN:O	2:I:166:LEU:HG	2.14	0.47
2:I:167:LYS:HE2	2:I:171:TYR:HE2	1.79	0.47
2:J:96:ASP:H	2:J:97:PRO:HD2	1.80	0.47
4:L:222:LEU:O	4:L:226:GLN:HG3	2.15	0.47
1:B:455:ARG:HH21	1:B:481:LEU:CB	2.28	0.47
1:C:40:SER:HB3	1:C:43:HIS:CG	2.49	0.47
1:C:325:ILE:HG13	1:C:369:VAL:HG23	1.96	0.47
1:C:445:VAL:HG12	1:C:449:GLN:HE22	1.79	0.47
1:C:562:PHE:O	1:C:565:ILE:HD11	2.15	0.47
1:C:593:TYR:CE2	1:C:632:LYS:NZ	2.83	0.47
1:D:91:CYS:CB	1:D:155:MET:HE2	2.44	0.47
1:D:564:PHE:HB3	1:D:598:SER:HB3	1.95	0.47
1:D:632:LYS:HZ1	1:E:571:ASP:HB3	1.80	0.47
1:D:635:PRO:O	1:D:638:ARG:HB2	2.14	0.47
1:D:655:MET:O	1:D:656:GLU:HB2	2.14	0.47
1:D:694:ILE:O	1:D:698:VAL:HG22	2.15	0.47
1:E:26:GLU:HG2	1:E:51:THR:HB	1.95	0.47
1:E:612:VAL:CG2	1:E:613:PRO:HD2	2.45	0.47
2:H:276:LEU:O	2:H:280:LEU:HG	2.14	0.47
2:J:219:LEU:HD23	2:J:219:LEU:H	1.80	0.47
2:J:263:VAL:HG23	2:J:280:LEU:HD13	1.96	0.47
2:G:82:ALA:HB2	2:G:110:ILE:HG21	1.95	0.47
1:A:687:LYS:NZ	1:A:722:PRO:HB3	2.29	0.47
1:B:257:LEU:HG	1:B:371:GLY:O	2.15	0.47
1:B:640:LEU:CD2	1:B:642:ILE:HG13	2.44	0.47
1:C:356:SER:HB3	1:D:288:PRO:HG3	1.97	0.47
1:C:721:ASP:O	1:C:725:ARG:HG3	2.14	0.47
1:E:106:ASN:HB3	1:E:143:LYS:NZ	2.29	0.47
1:F:323:HIS:HB2	1:F:367:ILE:HG22	1.97	0.47
3:K:46:MET:HA	3:K:49:ASN:HB2	1.95	0.47
1:A:242:PRO:HD2	1:A:243:GLU:N	2.29	0.47
1:A:510:TRP:CE3	1:A:675:GLN:HG2	2.50	0.47
1:C:311:GLU:O	1:C:314:ARG:HG2	2.15	0.47
1:C:322:LEU:HD12	1:C:324:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:632:LYS:HG3	1:D:571:ASP:CG	2.40	0.47
1:D:246:GLU:HG2	1:D:247:GLN:N	2.30	0.47
1:D:611:TYR:CE2	1:D:613:PRO:HA	2.50	0.47
1:D:688:ASP:O	1:D:692:THR:HG23	2.15	0.47
1:E:240:PHE:HE1	1:F:457:ILE:CD1	2.28	0.47
2:J:98:GLN:C	2:J:100:ALA:H	2.23	0.47
1:A:111:PRO:CD	1:A:320:SER:HA	2.45	0.47
1:A:256:ILE:CG1	1:A:370:ILE:HG22	2.44	0.47
1:B:323:HIS:HB2	1:B:367:ILE:HG22	1.97	0.47
1:B:397:LEU:HD22	1:B:398:PRO:HD2	1.97	0.47
1:B:627:LEU:HB3	1:C:607:ARG:NH2	2.29	0.47
1:D:453:MET:O	1:D:457:ILE:HG13	2.15	0.47
1:E:16:LEU:HD11	1:E:52:HIS:CD2	2.50	0.47
1:E:113:ASP:O	1:E:117:MET:HG3	2.15	0.47
2:J:147:GLN:HG2	2:J:151:TYR:CE2	2.50	0.47
3:K:50:VAL:O	3:K:54:LEU:HG	2.15	0.47
1:A:564:PHE:CZ	1:A:566:LYS:HB2	2.50	0.46
1:B:307:ALA:HA	1:B:310:GLU:HG2	1.97	0.46
1:C:197:GLY:C	1:C:198:LYS:HD2	2.40	0.46
1:C:707:ILE:O	1:C:711:LEU:HG	2.15	0.46
1:D:45:TYR:CE2	1:D:70:ALA:HA	2.49	0.46
1:D:89:LYS:NZ	1:D:89:LYS:HB3	2.29	0.46
1:E:40:SER:OG	1:E:43:HIS:HB2	2.15	0.46
1:F:40:SER:HB3	1:F:43:HIS:ND1	2.30	0.46
1:F:686:PHE:HE1	1:F:714:ILE:HG23	1.79	0.46
2:H:180:LYS:O	2:H:184:ILE:HG13	2.15	0.46
2:I:230:GLU:HG2	2:I:231:LEU:N	2.30	0.46
2:I:244:MET:O	2:I:248:LEU:HG	2.15	0.46
2:G:188:VAL:HG13	2:G:205:TYR:HD2	1.80	0.46
2:G:195:SER:C	2:G:197:LEU:H	2.23	0.46
2:G:260:THR:HA	2:G:263:VAL:HG12	1.96	0.46
5:M:28:SER:O	5:M:32:MET:HB2	2.15	0.46
1:A:542:GLU:HA	1:A:646:THR:O	2.15	0.46
1:A:562:PHE:CE1	1:A:641:LEU:HD21	2.50	0.46
1:A:611:TYR:CE1	1:A:616:PRO:HB2	2.51	0.46
1:B:653:GLN:OE1	1:B:658:LEU:HD22	2.15	0.46
1:C:657:MET:HE3	1:C:661:PHE:CZ	2.51	0.46
1:D:536:LEU:HD21	1:D:630:LEU:O	2.15	0.46
1:E:669:ASN:CG	1:E:706:GLY:HA2	2.40	0.46
2:H:11:MET:HA	2:H:14:LEU:HD12	1.97	0.46
5:M:34:GLN:HA	5:M:37:GLU:HB2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:42:ALA:HA	5:M:45:ARG:CZ	2.44	0.46
1:A:111:PRO:HG3	1:A:321:GLY:O	2.16	0.46
1:A:319:ASN:O	1:A:320:SER:HB2	2.15	0.46
1:B:64:LEU:CA	1:B:67:ARG:HH21	2.28	0.46
1:B:149:VAL:HG11	1:B:152:ILE:HD11	1.98	0.46
1:E:46:ILE:HD12	1:E:174:VAL:HG11	1.96	0.46
1:E:562:PHE:CD1	1:E:597:LEU:HG	2.50	0.46
2:I:200:TYR:HB2	3:K:47:ARG:HH12	1.79	0.46
2:J:63:ASN:O	2:J:67:GLN:HG3	2.15	0.46
2:G:45:TYR:HB2	2:G:68:ALA:HB2	1.98	0.46
2:G:51:MET:HA	2:G:54:MET:HE3	1.96	0.46
1:C:45:TYR:CE2	1:C:70:ALA:HA	2.50	0.46
1:C:355:LEU:O	1:C:388:ARG:NH2	2.42	0.46
1:D:312:GLU:HG3	1:D:313:GLN:N	2.31	0.46
1:D:542:GLU:OE2	1:D:649:LYS:HD2	2.16	0.46
1:D:571:ASP:O	1:D:574:ILE:HG13	2.15	0.46
1:D:627:LEU:HA	1:D:627:LEU:HD23	1.56	0.46
1:E:111:PRO:HB2	1:E:196:ILE:HD13	1.98	0.46
1:E:250:CYS:SG	1:F:446:ARG:HD2	2.55	0.46
2:I:81:ALA:O	2:I:85:PHE:HD1	1.99	0.46
2:I:102:ASN:HA	2:I:105:MET:HE3	1.96	0.46
2:I:213:HIS:C	2:I:215:CYS:H	2.23	0.46
4:L:210:ARG:HH21	5:M:31:ARG:HH21	1.63	0.46
1:B:246:GLU:O	1:C:414:MET:HE1	2.15	0.46
1:B:628:VAL:HG13	1:C:571:ASP:OD1	2.16	0.46
1:C:240:PHE:HE2	1:D:456:HIS:HD1	1.62	0.46
1:C:536:LEU:CD1	1:C:640:LEU:HB3	2.46	0.46
1:C:568:CYS:HB2	1:C:602:VAL:HA	1.97	0.46
2:I:21:VAL:HG23	2:I:38:ILE:HD13	1.96	0.46
2:J:155:GLU:C	2:J:157:SER:H	2.23	0.46
4:L:252:LYS:O	4:L:255:VAL:HG22	2.15	0.46
5:M:67:ILE:O	5:M:71:MET:HG2	2.15	0.46
1:B:46:ILE:HD12	1:B:174:VAL:HG21	1.97	0.46
1:C:106:ASN:HB3	1:C:143:LYS:HZ2	1.79	0.46
1:C:428:GLU:O	1:C:431:VAL:HG12	2.15	0.46
1:D:171:LYS:HB3	1:D:171:LYS:HZ3	1.80	0.46
1:E:510:TRP:CE3	1:E:511:GLY:HA3	2.50	0.46
1:F:325:ILE:HG13	1:F:369:VAL:HB	1.96	0.46
1:F:503:ILE:HD11	1:F:554:ALA:HB3	1.98	0.46
2:G:118:THR:O	2:G:122:LYS:HG2	2.15	0.46
1:C:64:LEU:HA	1:C:67:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:GLU:O	1:D:313:GLN:CG	2.64	0.46
1:D:407:LEU:O	1:D:411:THR:HG23	2.16	0.46
1:D:519:ASP:O	1:D:523:LEU:HG	2.15	0.46
1:E:236:ALA:HA	1:E:239:VAL:CG1	2.46	0.46
1:E:272:GLN:OE1	1:E:272:GLN:HA	2.14	0.46
1:E:440:GLU:O	1:E:444:LEU:HG	2.16	0.46
2:J:203:LYS:HD3	2:J:236:SER:HB3	1.97	0.46
2:G:235:PHE:CD2	5:M:152:GLN:HA	2.50	0.46
1:A:546:HIS:CE1	1:F:659:ASN:OD1	2.69	0.46
1:B:76:GLN:HE21	1:B:78:ILE:CG2	2.29	0.46
1:B:281:GLU:N	1:B:282:PRO:HA	2.31	0.46
1:D:608:LEU:C	1:D:622:VAL:HG11	2.41	0.46
1:E:618:PHE:C	1:E:618:PHE:CD1	2.93	0.46
2:H:166:LEU:HD21	2:H:205:TYR:CE2	2.51	0.46
2:G:182:ILE:CG2	2:G:212:CYS:HB2	2.46	0.46
5:M:62:GLU:O	5:M:66:HIS:HB2	2.16	0.46
1:B:52:HIS:C	1:B:54:SER:H	2.24	0.46
1:C:23:VAL:HG12	1:C:55:VAL:CG2	2.46	0.46
1:C:513:PRO:HA	1:C:516:ARG:HG2	1.98	0.46
1:E:248:MET:C	1:F:414:MET:HE1	2.40	0.46
1:E:307:ALA:HA	1:E:310:GLU:HG2	1.98	0.46
1:F:23:VAL:HG12	1:F:55:VAL:HG21	1.98	0.46
2:J:287:ILE:O	2:J:291:GLU:HG3	2.15	0.46
2:G:79:HIS:O	2:G:83:THR:HG23	2.15	0.46
2:G:203:LYS:HB3	2:G:240:GLU:HG3	1.98	0.46
4:L:210:ARG:NH2	5:M:31:ARG:HH21	2.13	0.46
1:A:23:VAL:HG12	1:A:55:VAL:HG21	1.98	0.46
1:A:86:ASP:C	1:A:88:ALA:H	2.22	0.46
1:A:242:PRO:O	1:A:245:VAL:HG12	2.16	0.46
1:B:402:GLY:O	1:B:406:ILE:HD12	2.15	0.46
1:B:523:LEU:HA	1:B:526:GLN:HG2	1.98	0.46
1:C:540:LEU:HD22	1:C:661:PHE:CD2	2.51	0.46
1:D:72:LEU:C	2:J:218:MET:SD	2.99	0.46
1:E:531:SER:HB3	1:E:534:THR:O	2.16	0.46
2:H:95:ALA:CB	2:H:97:PRO:HD2	2.46	0.46
3:K:29:ASN:HA	4:L:198:ARG:NH1	2.30	0.46
5:M:184:LYS:HD2	5:M:184:LYS:N	2.31	0.46
1:A:623:LEU:O	1:A:626:LEU:HB3	2.16	0.45
1:A:713:LEU:CD2	1:A:732:LEU:HB3	2.41	0.45
1:B:24:VAL:HG23	1:B:51:THR:HG22	1.97	0.45
1:B:236:ALA:HA	1:B:239:VAL:CG1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ILE:HD11	1:D:183:VAL:HG23	1.97	0.45
1:D:609:LEU:O	1:D:610:ASP:OD1	2.34	0.45
1:F:517:VAL:HG21	1:F:667:VAL:HG22	1.98	0.45
2:H:98:GLN:C	2:H:100:ALA:H	2.25	0.45
2:H:159:SER:OG	4:L:225:SER:HB2	2.15	0.45
2:H:237:ASP:C	2:H:239:ARG:H	2.23	0.45
2:I:200:TYR:O	2:I:203:LYS:HE2	2.16	0.45
2:G:20:LYS:HG2	2:G:37:LYS:HB3	1.98	0.45
5:M:27:GLU:O	5:M:31:ARG:HG3	2.16	0.45
1:A:91:CYS:O	1:A:154:ALA:HA	2.17	0.45
1:A:215:PHE:N	1:A:231:PHE:CE2	2.84	0.45
1:B:627:LEU:CD2	1:B:657:MET:HG3	2.44	0.45
1:C:52:HIS:C	1:C:54:SER:H	2.24	0.45
1:C:285:VAL:HA	1:C:326:ILE:HG13	1.97	0.45
1:D:122:ILE:HD11	1:D:183:VAL:CG2	2.46	0.45
1:D:608:LEU:O	1:D:622:VAL:HG11	2.16	0.45
1:E:519:ASP:O	1:E:522:GLU:HB2	2.17	0.45
1:E:589:PHE:CE2	1:E:629:LEU:HD21	2.52	0.45
1:E:677:LEU:HD11	1:E:695:ALA:HA	1.99	0.45
1:F:440:GLU:O	1:F:444:LEU:HG	2.16	0.45
1:F:545:PRO:CB	1:F:546:HIS:HA	2.44	0.45
1:F:707:ILE:O	1:F:710:LEU:HB3	2.15	0.45
2:J:81:ALA:O	2:J:85:PHE:HD1	1.98	0.45
1:B:121:PHE:CD2	1:B:183:VAL:HG21	2.52	0.45
1:B:423:ASP:HB2	1:B:479:ASP:N	2.31	0.45
1:C:620:ASN:O	1:C:624:GLN:HG2	2.15	0.45
1:F:242:PRO:HD2	1:F:243:GLU:N	2.32	0.45
2:H:45:TYR:CE2	2:H:71:LEU:HD11	2.51	0.45
2:I:164:CYS:O	2:I:168:VAL:HG23	2.16	0.45
2:I:212:CYS:SG	2:I:279:MET:HE1	2.56	0.45
2:I:214:PHE:H	2:I:214:PHE:HD1	1.64	0.45
2:I:232:PHE:HB2	2:I:233:PRO:HD3	1.97	0.45
2:J:161:ALA:O	2:J:165:LEU:HG	2.16	0.45
2:G:124:HIS:HE1	2:G:147:GLN:HB3	1.81	0.45
4:L:247:ALA:O	4:L:251:THR:HG23	2.17	0.45
5:M:17:ARG:NE	5:M:21:LEU:HD11	2.32	0.45
1:A:23:VAL:HG12	1:A:55:VAL:CG2	2.47	0.45
1:A:705:ILE:HD13	1:A:710:LEU:CD1	2.38	0.45
1:B:289:GLU:C	1:B:291:LEU:N	2.73	0.45
1:B:540:LEU:HD12	1:B:540:LEU:O	2.16	0.45
1:C:128:GLN:O	1:C:176:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ILE:O	1:D:126:ASN:HB3	2.16	0.45
1:D:533:ARG:HD2	1:E:505:ASN:ND2	2.32	0.45
1:D:564:PHE:HB3	1:D:598:SER:CB	2.46	0.45
1:D:567:ILE:HG23	1:D:601:VAL:HB	1.99	0.45
1:D:609:LEU:CD1	1:D:611:TYR:HB2	2.47	0.45
1:E:27:LYS:HD2	1:E:57:PRO:HG3	1.97	0.45
1:F:16:LEU:HD11	1:F:52:HIS:HD2	1.80	0.45
1:F:254:LYS:O	1:F:368:LEU:HA	2.16	0.45
3:K:56:ARG:HH21	5:M:174:GLN:CB	2.30	0.45
5:M:176:ARG:HD3	5:M:180:ARG:NH1	2.31	0.45
1:A:258:LEU:O	1:A:258:LEU:HD12	2.17	0.45
1:A:542:GLU:OE2	1:A:666:HIS:CD2	2.69	0.45
1:A:611:TYR:HA	1:A:618:PHE:HB3	1.99	0.45
1:A:624:GLN:OE1	1:A:624:GLN:HA	2.16	0.45
1:B:122:ILE:O	1:B:126:ASN:HB3	2.17	0.45
1:C:121:PHE:HD2	1:C:183:VAL:HG21	1.81	0.45
1:D:36:ILE:HG23	1:D:36:ILE:O	2.16	0.45
1:D:89:LYS:HB3	1:D:89:LYS:HZ3	1.81	0.45
1:D:286:ASN:HB2	1:D:327:PHE:CD1	2.50	0.45
1:D:686:PHE:HB3	1:D:690:GLU:HG3	1.97	0.45
1:E:23:VAL:HG12	1:E:55:VAL:HG21	1.98	0.45
1:E:113:ASP:HA	1:E:196:ILE:HG13	1.98	0.45
1:F:12:PRO:HG2	1:F:23:VAL:HG11	1.98	0.45
1:F:113:ASP:OD1	1:F:115:ASP:HB2	2.17	0.45
1:F:597:LEU:HA	1:F:639:LYS:O	2.17	0.45
1:F:618:PHE:HE1	1:F:620:ASN:HA	1.82	0.45
2:I:63:ASN:O	2:I:67:GLN:HG3	2.15	0.45
2:I:122:LYS:HE3	5:M:182:MET:HE1	1.98	0.45
1:B:40:SER:CB	1:B:41:PRO:CD	2.94	0.45
1:B:125:PHE:HD2	1:B:130:PHE:HZ	1.65	0.45
1:B:247:GLN:O	1:C:414:MET:SD	2.75	0.45
1:C:220:ILE:HD11	1:C:272:GLN:HG3	1.97	0.45
1:C:540:LEU:HD11	1:C:646:THR:HG22	1.99	0.45
1:D:74:ILE:HG13	2:J:218:MET:HE3	1.99	0.45
1:D:326:ILE:HG22	1:D:370:ILE:CG1	2.47	0.45
1:E:45:TYR:CE2	1:E:70:ALA:HA	2.52	0.45
1:E:101:PHE:CD2	1:E:107:ILE:HA	2.51	0.45
1:E:436:PHE:HB3	1:E:440:GLU:CB	2.47	0.45
1:E:507:ILE:HD13	1:E:507:ILE:HA	1.75	0.45
1:E:527:GLN:HA	1:F:719:GLN:HG3	1.97	0.45
1:F:18:LEU:HA	1:F:137:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:414:MET:SD	1:F:449:GLN:NE2	2.88	0.45
1:F:705:ILE:HG12	1:F:706:GLY:O	2.15	0.45
2:H:201:SER:C	2:H:203:LYS:H	2.24	0.45
2:J:98:GLN:H	2:J:98:GLN:CD	2.25	0.45
2:J:188:VAL:HG13	2:J:205:TYR:CD2	2.51	0.45
2:J:197:LEU:HD13	3:K:52:LYS:HE3	1.99	0.45
1:A:45:TYR:CE2	1:A:70:ALA:HA	2.52	0.45
1:B:24:VAL:O	1:B:51:THR:HA	2.16	0.45
1:B:436:PHE:N	1:B:436:PHE:CD1	2.84	0.45
1:B:536:LEU:HD12	1:B:640:LEU:O	2.17	0.45
1:C:256:ILE:O	1:C:370:ILE:HA	2.17	0.45
1:D:710:LEU:HG	1:D:714:ILE:HD11	1.99	0.45
1:E:586:LYS:NZ	1:F:575:GLY:HA3	2.31	0.45
1:F:242:PRO:CD	1:F:243:GLU:H	2.28	0.45
1:F:327:PHE:CE2	1:F:369:VAL:HG21	2.52	0.45
1:F:605:ILE:O	1:F:608:LEU:HG	2.16	0.45
2:J:223:LEU:O	2:J:227:LYS:HG3	2.16	0.45
1:A:69:TRP:CE2	1:A:134:GLN:HA	2.52	0.45
1:A:489:LYS:N	1:A:490:PRO:HD2	2.31	0.45
1:A:509:LYS:HG2	1:A:515:THR:OG1	2.17	0.45
1:B:218:MET:HA	1:B:219:GLY:HA2	1.75	0.45
1:C:99:ILE:HG23	1:C:193:LEU:HD23	1.98	0.45
1:C:331:ASP:CA	1:C:379:ILE:HD11	2.44	0.45
1:C:414:MET:HA	1:C:414:MET:CE	2.45	0.45
1:C:552:LEU:HD23	1:C:552:LEU:HA	1.81	0.45
1:C:613:PRO:HD3	1:C:648:ARG:HH22	1.81	0.45
1:D:132:VAL:HG23	1:D:173:GLU:O	2.17	0.45
1:E:86:ASP:O	1:E:88:ALA:N	2.49	0.45
1:F:119:ALA:O	1:F:123:GLN:HB2	2.17	0.45
1:F:263:GLY:O	1:F:398:PRO:HG3	2.17	0.45
1:F:449:GLN:O	1:F:453:MET:HG2	2.17	0.45
1:F:552:LEU:O	1:F:556:ILE:HG13	2.16	0.45
1:F:612:VAL:HG13	1:F:614:ILE:O	2.16	0.45
2:H:78:LYS:HB2	2:H:114:MET:HE2	1.99	0.45
2:J:72:HIS:O	2:J:75:LEU:HB3	2.16	0.45
2:J:185:TYR:HA	2:J:188:VAL:HG12	1.97	0.45
1:A:36:ILE:HG23	1:A:36:ILE:O	2.15	0.45
1:A:122:ILE:O	1:A:126:ASN:HB3	2.17	0.45
1:A:436:PHE:CD2	1:A:444:LEU:HD11	2.51	0.45
1:A:457:ILE:CD1	1:F:236:ALA:HB1	2.47	0.45
1:A:483:SER:C	1:A:486:ASN:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:GLN:O	1:A:530:ASN:HB2	2.16	0.45
1:B:348:ASP:O	1:B:352:ASN:ND2	2.50	0.45
1:C:539:VAL:HG23	1:C:663:THR:HG23	1.98	0.45
1:D:589:PHE:CD2	1:D:629:LEU:HD13	2.52	0.45
1:E:299:GLU:HG3	1:E:349:THR:CB	2.47	0.45
1:E:713:LEU:CD2	1:E:732:LEU:HD13	2.47	0.45
1:F:319:ASN:HB3	1:F:320:SER:HB2	1.97	0.45
2:H:176:GLU:O	2:H:178:TYR:N	2.47	0.45
2:G:266:TYR:C	2:G:268:SER:N	2.75	0.45
3:K:82:ALA:O	3:K:85:LYS:HB3	2.17	0.45
4:L:210:ARG:HG2	4:L:210:ARG:HH11	1.82	0.45
1:A:610:ASP:OD1	1:F:620:ASN:ND2	2.50	0.45
1:A:617:ARG:HG3	1:A:617:ARG:NH1	2.30	0.45
1:B:677:LEU:O	1:B:681:GLU:HG3	2.17	0.45
1:C:555:LYS:O	1:C:559:GLU:HG2	2.17	0.45
1:D:303:ARG:HH11	1:D:357:LYS:CE	2.30	0.45
1:D:670:ILE:HG12	1:D:705:ILE:O	2.17	0.45
1:D:686:PHE:HB2	1:D:691:ARG:CG	2.47	0.45
1:E:149:VAL:HG11	1:E:152:ILE:HD11	1.97	0.45
1:E:721:ASP:HB2	1:E:724:TYR:CD2	2.52	0.45
1:F:36:ILE:HG23	1:F:36:ILE:O	2.17	0.45
2:H:53:LYS:HD2	2:I:117:PHE:CE2	2.51	0.45
2:H:78:LYS:HB3	2:H:110:ILE:HG23	1.98	0.45
2:H:116:ARG:NH1	2:H:116:ARG:HG3	2.32	0.45
2:H:203:LYS:HB2	2:H:203:LYS:HE3	1.52	0.45
2:I:236:SER:HA	2:I:239:ARG:NH1	2.32	0.45
2:I:243:LEU:HD13	2:I:266:TYR:HB2	1.99	0.45
2:J:230:GLU:HG3	2:J:237:ASP:HB3	1.98	0.45
2:G:139:GLU:CD	2:G:139:GLU:H	2.24	0.45
1:A:24:VAL:HG11	1:A:49:LEU:HD22	1.98	0.44
1:A:111:PRO:HG2	1:A:320:SER:HA	1.99	0.44
1:A:270:ALA:HA	1:A:273:ILE:HG22	1.98	0.44
1:A:502:TYR:N	1:A:502:TYR:HD1	2.15	0.44
1:A:573:MET:HA	1:A:576:PHE:CD2	2.53	0.44
1:A:636:GLN:HA	1:A:637:GLY:HA2	1.47	0.44
1:A:721:ASP:O	1:A:725:ARG:HG3	2.17	0.44
1:B:311:GLU:O	1:B:314:ARG:HG2	2.17	0.44
1:D:227:PHE:O	1:D:230:ILE:HG22	2.17	0.44
1:D:552:LEU:O	1:D:556:ILE:HG13	2.18	0.44
1:D:628:VAL:O	1:D:632:LYS:N	2.51	0.44
1:E:101:PHE:HE1	1:E:193:LEU:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:325:ILE:HG13	1:E:369:VAL:HB	1.98	0.44
1:E:377:ASP:OD1	1:E:378:LEU:N	2.50	0.44
1:F:307:ALA:O	1:F:310:GLU:HG2	2.17	0.44
1:F:428:GLU:O	1:F:431:VAL:HG12	2.16	0.44
2:J:38:ILE:HD11	2:J:71:LEU:HB3	1.98	0.44
5:M:142:ARG:HG2	5:M:142:ARG:NH1	2.33	0.44
1:A:16:LEU:HD11	1:A:52:HIS:HD2	1.81	0.44
1:A:103:GLN:C	1:A:105:LYS:H	2.25	0.44
1:A:242:PRO:HD2	1:A:243:GLU:OE1	2.17	0.44
1:B:528:THR:HG21	1:B:641:LEU:HD13	2.00	0.44
1:C:547:SER:HB2	1:C:549:LYS:HG3	2.00	0.44
1:C:635:PRO:HB2	1:C:638:ARG:NH1	2.31	0.44
1:D:263:GLY:C	1:D:437:SER:HB3	2.43	0.44
1:D:624:GLN:OE1	1:D:624:GLN:HA	2.18	0.44
1:D:731:ALA:HA	1:D:734:ARG:HH12	1.82	0.44
1:E:67:ARG:NH1	1:E:74:ILE:HD11	2.32	0.44
1:E:536:LEU:HD22	1:E:634:PRO:HD3	1.98	0.44
1:F:24:VAL:O	1:F:51:THR:HA	2.17	0.44
2:H:92:PHE:HB3	2:H:98:GLN:O	2.16	0.44
2:I:166:LEU:HD21	2:I:205:TYR:CE2	2.52	0.44
2:I:243:LEU:HD22	2:I:266:TYR:CG	2.51	0.44
2:J:20:LYS:NZ	2:J:40:GLU:HG2	2.31	0.44
2:G:47:ARG:O	2:G:50:ASN:HB3	2.17	0.44
2:G:283:ILE:O	2:G:287:ILE:HG13	2.17	0.44
2:G:287:ILE:O	2:G:291:GLU:HG3	2.17	0.44
3:K:55:GLU:O	3:K:59:LYS:HG3	2.18	0.44
1:A:410:HIS:NE2	1:A:442:GLU:HG2	2.32	0.44
1:B:246:GLU:HG3	1:C:417:HIS:CE1	2.53	0.44
1:D:510:TRP:NE1	1:D:514:VAL:HG21	2.33	0.44
1:E:563:PRO:HD2	1:E:597:LEU:O	2.18	0.44
1:E:691:ARG:HA	1:E:694:ILE:HD12	1.99	0.44
1:F:272:GLN:OE1	1:F:272:GLN:HA	2.17	0.44
2:H:101:ILE:O	2:H:105:MET:HG3	2.18	0.44
2:J:21:VAL:O	2:J:21:VAL:HG22	2.18	0.44
2:J:182:ILE:CG2	2:J:212:CYS:HB2	2.47	0.44
1:A:502:TYR:N	1:A:502:TYR:CD1	2.84	0.44
1:B:16:LEU:HD11	1:B:52:HIS:HD2	1.82	0.44
1:B:101:PHE:CD2	1:B:107:ILE:HA	2.52	0.44
1:B:651:VAL:CG1	1:B:655:MET:CE	2.90	0.44
1:C:499:TYR:HB3	1:C:558:GLU:OE2	2.18	0.44
1:E:36:ILE:HG23	1:E:36:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:TRP:NE1	1:E:134:GLN:HA	2.33	0.44
1:E:254:LYS:O	1:E:368:LEU:HA	2.17	0.44
1:E:507:ILE:O	1:E:507:ILE:HG22	2.17	0.44
1:F:525:VAL:HG11	1:F:560:SER:CB	2.47	0.44
1:F:588:ILE:O	1:F:591:ASP:HB2	2.18	0.44
2:I:276:LEU:O	2:I:280:LEU:HG	2.18	0.44
2:J:243:LEU:O	2:J:247:LEU:HG	2.18	0.44
2:G:32:PHE:HD1	2:G:32:PHE:H	1.65	0.44
1:B:569:SER:OG	1:B:571:ASP:OD2	2.34	0.44
1:C:104:LYS:HA	1:C:107:ILE:HD11	1.98	0.44
1:C:606:GLU:HB2	1:C:648:ARG:HD2	1.99	0.44
1:E:65:PRO:HG2	1:E:137:VAL:HG13	2.00	0.44
1:E:114:THR:CG2	1:E:195:LEU:HB3	2.47	0.44
1:E:327:PHE:CE2	1:E:369:VAL:HG21	2.52	0.44
1:E:539:VAL:HG13	1:E:643:ILE:HA	2.00	0.44
1:E:586:LYS:NZ	1:F:574:ILE:HG23	2.33	0.44
1:E:689:LYS:O	1:E:692:THR:OG1	2.25	0.44
1:F:560:SER:HB2	1:F:562:PHE:CD1	2.52	0.44
2:H:75:LEU:O	2:H:76:GLN:HB3	2.17	0.44
2:G:225:VAL:HG23	2:G:241:CYS:HB2	1.99	0.44
3:K:79:THR:O	3:K:83:LYS:HG3	2.18	0.44
5:M:71:MET:HE2	5:M:192:ILE:CG1	2.48	0.44
1:A:254:LYS:O	1:A:368:LEU:HA	2.17	0.44
1:D:527:GLN:HE22	1:E:716:MET:CA	2.31	0.44
1:D:626:LEU:O	1:D:630:LEU:HG	2.17	0.44
1:F:261:PRO:O	1:F:264:CYS:HB2	2.18	0.44
1:F:324:ILE:HG12	1:F:368:LEU:HD11	2.00	0.44
1:F:436:PHE:CD2	1:F:444:LEU:HD11	2.53	0.44
2:G:81:ALA:O	2:G:85:PHE:HD1	2.01	0.44
5:M:152:GLN:O	5:M:156:ILE:HG13	2.18	0.44
1:A:215:PHE:C	1:A:217:LYS:N	2.75	0.44
1:A:611:TYR:HD1	1:A:618:PHE:HB3	1.82	0.44
1:C:76:GLN:HE21	1:C:78:ILE:CG2	2.30	0.44
1:C:688:ASP:HA	1:C:691:ARG:NH1	2.32	0.44
1:C:721:ASP:HB2	1:C:724:TYR:CD1	2.52	0.44
1:F:218:MET:HA	1:F:219:GLY:HA2	1.74	0.44
2:I:180:LYS:O	2:I:184:ILE:HG13	2.18	0.44
2:J:216:ILE:HG12	2:J:220:ASN:HB2	1.98	0.44
2:G:75:LEU:O	2:G:76:GLN:HB3	2.18	0.44
1:B:246:GLU:HA	1:C:413:ARG:HH12	1.83	0.44
1:B:254:LYS:O	1:B:368:LEU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:GLN:HA	1:C:288:PRO:CG	2.47	0.44
1:B:609:LEU:HA	1:B:609:LEU:HD23	1.60	0.44
1:C:149:VAL:HG11	1:C:152:ILE:HD11	1.99	0.44
1:C:257:LEU:HG	1:C:371:GLY:O	2.18	0.44
1:D:388:ARG:O	1:D:389:LEU:HD23	2.18	0.44
1:D:627:LEU:CD2	1:D:657:MET:HG3	2.43	0.44
1:E:524:LEU:HD11	1:E:663:THR:HG21	1.99	0.44
1:F:69:TRP:CE2	1:F:134:GLN:HA	2.53	0.44
1:F:315:ARG:HG3	1:F:316:LEU:HD12	2.00	0.44
2:H:169:ALA:HB2	2:H:184:ILE:HB	2.00	0.44
2:G:116:ARG:HH21	4:L:238:GLU:CD	2.26	0.44
2:G:167:LYS:HE2	2:G:171:TYR:HE2	1.83	0.44
1:A:423:ASP:C	1:A:479:ASP:N	2.76	0.44
1:C:86:ASP:C	1:C:88:ALA:H	2.25	0.44
1:D:25:SER:HB3	1:D:28:ASP:OD2	2.18	0.44
1:D:91:CYS:HB3	1:D:155:MET:HE2	1.99	0.44
1:D:236:ALA:HB1	1:E:453:MET:HG3	2.00	0.44
1:D:709:LYS:HA	1:D:709:LYS:HD2	1.81	0.44
1:E:436:PHE:N	1:E:436:PHE:CD1	2.86	0.44
1:E:641:LEU:HD12	1:E:641:LEU:O	2.18	0.44
1:E:654:GLU:HG2	1:F:614:ILE:HD11	1.99	0.44
1:E:655:MET:C	1:E:656:GLU:HG3	2.43	0.44
1:F:257:LEU:HB2	1:F:389:LEU:HD13	1.99	0.44
2:J:101:ILE:HB	2:J:131:TYR:OH	2.18	0.44
4:L:213:HIS:NE2	5:M:38:GLU:OE1	2.51	0.44
1:C:320:SER:O	1:C:320:SER:OG	2.31	0.43
1:C:528:THR:O	1:C:639:LYS:HD3	2.18	0.43
1:C:582:CYS:SG	1:C:621:LEU:HG	2.58	0.43
1:C:671:ALA:HA	1:C:703:VAL:O	2.17	0.43
1:C:677:LEU:O	1:C:681:GLU:OE1	2.36	0.43
1:F:240:PHE:HA	1:F:241:PRO:HD3	1.75	0.43
1:F:307:ALA:HA	1:F:310:GLU:HG2	1.99	0.43
2:H:38:ILE:CD1	2:H:71:LEU:HB3	2.47	0.43
2:H:167:LYS:HE2	2:H:171:TYR:CE2	2.53	0.43
2:H:200:TYR:CE2	5:M:38:GLU:HG2	2.53	0.43
2:I:203:LYS:HB2	2:I:203:LYS:HE3	1.74	0.43
2:J:108:ILE:HD12	2:J:127:ILE:HD12	1.99	0.43
2:J:247:LEU:HD22	2:J:259:TYR:CD1	2.52	0.43
4:L:216:PHE:CZ	5:M:39:SER:HB2	2.53	0.43
1:A:355:LEU:HD22	1:A:388:ARG:NH1	2.33	0.43
1:B:531:SER:CB	1:B:639:LYS:HD3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ILE:HD11	1:D:145:PHE:CD2	2.53	0.43
1:E:246:GLU:HG2	1:E:247:GLN:N	2.33	0.43
1:E:696:GLN:OE1	1:E:696:GLN:HA	2.18	0.43
1:F:122:ILE:O	1:F:126:ASN:HB3	2.19	0.43
1:F:436:PHE:N	1:F:436:PHE:CD1	2.85	0.43
1:F:589:PHE:O	1:F:593:TYR:CD1	2.71	0.43
2:H:225:VAL:HG23	2:H:241:CYS:HB2	1.99	0.43
2:I:188:VAL:HG13	2:I:205:TYR:HD2	1.82	0.43
2:J:112:THR:HG23	2:J:117:PHE:CE1	2.48	0.43
2:G:204:ASP:OD2	2:G:208:LYS:HE2	2.18	0.43
1:A:609:LEU:HD23	1:A:609:LEU:HA	1.78	0.43
1:A:713:LEU:HD23	1:A:713:LEU:HA	1.74	0.43
1:B:257:LEU:HB2	1:B:389:LEU:HD13	2.00	0.43
1:B:508:ILE:HD13	1:B:683:LEU:HD21	2.00	0.43
1:B:669:ASN:OD1	1:B:706:GLY:HA2	2.17	0.43
1:D:149:VAL:HG11	1:D:152:ILE:HD11	2.00	0.43
1:D:543:GLY:O	1:D:647:SER:HA	2.18	0.43
1:E:91:CYS:O	1:E:154:ALA:HA	2.18	0.43
1:E:726:VAL:O	1:E:730:LEU:HG	2.19	0.43
2:H:58:TRP:HB3	2:H:95:ALA:HB2	2.00	0.43
2:J:178:TYR:OH	2:J:282:ARG:HG2	2.18	0.43
2:J:256:VAL:HG21	2:J:288:GLN:CG	2.48	0.43
2:G:83:THR:HB	4:L:235:TYR:OH	2.18	0.43
2:G:247:LEU:HB3	2:G:259:TYR:HE1	1.84	0.43
5:M:63:GLY:O	5:M:67:ILE:HG13	2.17	0.43
1:A:24:VAL:O	1:A:51:THR:HA	2.19	0.43
1:A:219:GLY:O	1:A:220:ILE:HG13	2.18	0.43
1:A:242:PRO:O	1:A:246:GLU:OE1	2.36	0.43
1:B:440:GLU:O	1:B:444:LEU:HG	2.19	0.43
1:C:48:THR:HG21	1:C:128:GLN:HG2	2.00	0.43
1:C:511:GLY:CA	1:C:513:PRO:HD2	2.48	0.43
1:C:569:SER:HB3	1:C:572:LYS:HG2	2.00	0.43
1:D:9:ALA:HA	1:D:74:ILE:HG23	2.00	0.43
1:E:299:GLU:HG3	1:E:349:THR:OG1	2.19	0.43
1:E:628:VAL:HB	1:F:574:ILE:HD12	2.00	0.43
1:E:705:ILE:CD1	1:E:713:LEU:HD12	2.49	0.43
1:F:289:GLU:C	1:F:291:LEU:N	2.76	0.43
2:I:161:ALA:O	2:I:165:LEU:HG	2.18	0.43
2:I:176:GLU:O	2:I:178:TYR:N	2.50	0.43
2:I:185:TYR:HA	2:I:188:VAL:HG12	1.99	0.43
2:G:112:THR:HG23	2:G:117:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:56:ARG:HH21	5:M:174:GLN:HB3	1.83	0.43
1:A:235:PHE:N	1:A:235:PHE:CD1	2.84	0.43
1:A:255:GLY:C	1:A:389:LEU:HD13	2.43	0.43
1:A:503:ILE:C	1:A:505:ASN:H	2.26	0.43
1:B:23:VAL:HG12	1:B:55:VAL:HG21	2.00	0.43
1:B:327:PHE:CE2	1:B:369:VAL:HG21	2.52	0.43
1:B:671:ALA:HA	1:B:703:VAL:O	2.18	0.43
1:C:39:THR:HG22	1:C:78:ILE:HG22	1.99	0.43
1:C:193:LEU:HG	1:C:195:LEU:HG	1.99	0.43
1:C:408:HIS:O	1:C:408:HIS:ND1	2.46	0.43
1:E:585:MET:HE2	1:E:626:LEU:HD21	2.00	0.43
2:H:186:GLU:O	2:H:190:THR:HG23	2.19	0.43
2:I:112:THR:HG23	2:I:117:PHE:HE1	1.83	0.43
2:J:230:GLU:HG2	2:J:231:LEU:H	1.81	0.43
5:M:46:THR:HG21	5:M:167:MET:HE2	2.00	0.43
5:M:188:ASN:O	5:M:192:ILE:HG13	2.19	0.43
1:A:222:GLY:CA	1:A:402:GLY:HA3	2.48	0.43
1:A:407:LEU:CD1	1:A:426:ILE:HG23	2.48	0.43
1:C:64:LEU:CA	1:C:67:ARG:HH21	2.31	0.43
1:C:378:LEU:HD23	1:C:378:LEU:HA	1.83	0.43
1:D:50:ARG:HG2	1:D:50:ARG:HH11	1.84	0.43
1:D:67:ARG:HH11	1:D:74:ILE:HD11	1.82	0.43
1:D:331:ASP:O	1:D:332:ALA:HB3	2.19	0.43
1:D:566:LYS:HA	1:D:566:LYS:HD3	1.81	0.43
1:E:717:SER:OG	1:E:729:PHE:HB2	2.19	0.43
1:F:310:GLU:OE2	1:F:357:LYS:NZ	2.50	0.43
1:F:589:PHE:N	1:F:589:PHE:CD1	2.85	0.43
2:H:163:LYS:O	2:H:167:LYS:HG2	2.19	0.43
2:I:134:GLU:O	2:I:136:VAL:HG23	2.18	0.43
2:I:182:ILE:O	2:I:186:GLU:HG2	2.17	0.43
2:J:59:SER:OG	2:J:97:PRO:HD3	2.18	0.43
2:J:134:GLU:O	2:J:136:VAL:HG23	2.19	0.43
2:G:211:LEU:HG	2:G:244:MET:HE1	2.01	0.43
2:G:256:VAL:HG21	2:G:288:GLN:CG	2.48	0.43
1:B:507:ILE:HG13	1:B:555:LYS:HD3	2.00	0.43
1:C:99:ILE:HD11	1:C:145:PHE:CD2	2.53	0.43
1:D:522:GLU:CD	1:D:559:GLU:HB2	2.43	0.43
1:E:311:GLU:O	1:E:314:ARG:HG2	2.18	0.43
1:E:388:ARG:O	1:E:389:LEU:HD23	2.18	0.43
1:F:96:THR:HG22	1:F:150:LYS:HB2	2.00	0.43
1:F:555:LYS:HD3	1:F:559:GLU:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:162:ASN:HD22	2:H:188:VAL:HG23	1.84	0.43
5:M:32:MET:O	5:M:36:VAL:HG22	2.18	0.43
1:B:240:PHE:HA	1:B:241:PRO:HD3	1.75	0.43
1:B:242:PRO:HD2	1:B:243:GLU:N	2.33	0.43
1:C:297:GLU:O	1:C:301:ASN:N	2.39	0.43
1:D:312:GLU:CD	1:D:323:HIS:ND1	2.77	0.43
1:E:259:TYR:C	1:E:395:ILE:HD13	2.43	0.43
1:E:585:MET:HG3	1:E:589:PHE:CE2	2.53	0.43
1:F:73:SER:O	1:F:76:GLN:HG2	2.18	0.43
2:H:21:VAL:O	2:H:21:VAL:HG13	2.19	0.43
2:H:118:THR:O	2:H:122:LYS:HG2	2.18	0.43
2:H:239:ARG:NH2	4:L:213:HIS:CE1	2.87	0.43
2:H:275:TRP:CE3	2:H:276:LEU:HD23	2.54	0.43
2:I:201:SER:N	3:K:47:ARG:HH12	2.16	0.43
5:M:23:ASP:O	5:M:26:LEU:HB3	2.18	0.43
1:A:106:ASN:HB3	1:A:143:LYS:NZ	2.34	0.43
1:B:8:ALA:HB3	1:B:73:SER:O	2.19	0.43
1:B:121:PHE:HD2	1:B:183:VAL:HG21	1.84	0.43
1:B:259:TYR:CD2	1:B:376:PRO:HD3	2.54	0.43
1:D:7:GLN:O	1:D:59:SER:HB2	2.19	0.43
1:D:541:LEU:HD12	1:D:541:LEU:O	2.19	0.43
1:D:573:MET:CE	1:D:585:MET:HE3	2.49	0.43
1:E:241:PRO:HA	1:E:242:PRO:HA	1.62	0.43
1:E:628:VAL:HB	1:F:574:ILE:CD1	2.48	0.43
1:F:536:LEU:HD11	1:F:633:ALA:HA	2.00	0.43
1:F:690:GLU:O	1:F:694:ILE:HG13	2.19	0.43
2:J:186:GLU:O	2:J:190:THR:HG23	2.18	0.43
2:G:261:GLU:O	2:G:265:GLU:HG3	2.18	0.43
1:A:235:PHE:O	1:A:236:ALA:C	2.62	0.43
1:A:437:SER:OG	1:A:440:GLU:HG2	2.19	0.43
1:A:632:LYS:HE3	1:A:633:ALA:O	2.19	0.43
1:A:686:PHE:CE2	1:A:714:ILE:HG23	2.54	0.43
1:A:690:GLU:HB3	1:A:726:VAL:HG22	2.01	0.43
1:B:576:PHE:HB2	1:B:581:LYS:CG	2.49	0.43
1:B:707:ILE:O	1:B:711:LEU:HG	2.19	0.43
1:C:284:VAL:HB	1:C:325:ILE:HA	2.01	0.43
1:D:356:SER:OG	1:E:288:PRO:HB3	2.18	0.43
1:D:539:VAL:CG1	1:D:643:ILE:HG13	2.49	0.43
1:D:562:PHE:CD2	1:D:597:LEU:HG	2.54	0.43
1:E:676:LEU:O	1:E:680:LEU:HG	2.19	0.43
2:J:244:MET:O	2:J:248:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:77:PHE:CE1	5:M:78:LEU:HD11	2.52	0.43
1:A:575:GLY:HA3	1:F:586:LYS:CE	2.49	0.42
1:A:653:GLN:HB2	1:A:658:LEU:HD23	2.01	0.42
1:B:324:ILE:HG12	1:B:368:LEU:HD11	2.01	0.42
1:C:218:MET:HA	1:C:219:GLY:HA2	1.82	0.42
1:C:258:LEU:HD12	1:C:258:LEU:O	2.19	0.42
1:C:540:LEU:HD22	1:C:661:PHE:CE2	2.54	0.42
1:C:542:GLU:HG2	1:C:666:HIS:HA	2.01	0.42
1:E:586:LYS:O	1:E:589:PHE:HB2	2.19	0.42
1:F:311:GLU:O	1:F:314:ARG:HG2	2.18	0.42
2:H:277:THR:O	2:H:281:LEU:HD13	2.19	0.42
2:I:40:GLU:O	2:I:44:ILE:HG13	2.19	0.42
2:J:21:VAL:HG21	2:J:71:LEU:HD22	2.01	0.42
2:J:243:LEU:HD22	2:J:266:TYR:CG	2.54	0.42
2:J:289:GLY:O	2:J:293:ASP:HB2	2.19	0.42
1:A:64:LEU:O	1:A:68:LYS:HG3	2.19	0.42
1:A:219:GLY:C	1:A:220:ILE:HG13	2.44	0.42
1:B:407:LEU:O	1:B:411:THR:OG1	2.28	0.42
1:B:536:LEU:HD22	1:B:632:LYS:O	2.19	0.42
1:B:541:LEU:HA	1:B:665:ILE:O	2.19	0.42
1:B:612:VAL:HG13	1:B:614:ILE:O	2.19	0.42
1:C:385:ARG:HA	1:C:386:PRO:HD3	1.92	0.42
1:D:331:ASP:CA	1:D:379:ILE:HD11	2.48	0.42
1:D:406:ILE:HD12	1:D:406:ILE:HG23	1.68	0.42
1:E:265:GLY:O	1:E:268:LEU:HG	2.19	0.42
1:E:648:ARG:NE	1:E:651:VAL:HG13	2.34	0.42
1:F:677:LEU:O	1:F:681:GLU:HG3	2.19	0.42
2:H:10:ALA:HB1	2:H:52:PHE:CZ	2.53	0.42
2:I:159:SER:OG	3:K:55:GLU:HG2	2.18	0.42
2:J:142:ILE:HG23	2:J:168:VAL:HG13	2.01	0.42
2:J:179:GLN:O	2:J:182:ILE:HG12	2.19	0.42
2:G:18:GLU:HA	2:G:21:VAL:HG12	2.01	0.42
1:A:108:ASP:OD2	1:A:315:ARG:NH1	2.43	0.42
1:A:503:ILE:O	1:A:505:ASN:N	2.40	0.42
1:B:397:LEU:CD1	1:B:596:GLN:HG3	2.50	0.42
1:C:603:ASP:HA	1:C:645:THR:OG1	2.19	0.42
1:D:74:ILE:HG13	2:J:218:MET:CE	2.49	0.42
1:D:268:LEU:HA	1:D:271:ARG:CD	2.49	0.42
1:D:510:TRP:CB	1:D:679:ALA:HB2	2.48	0.42
1:E:299:GLU:HG3	1:E:349:THR:HB	2.01	0.42
1:F:114:THR:CG2	1:F:200:LYS:HG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:525:VAL:HG11	1:F:560:SER:HA	2.01	0.42
1:F:526:GLN:O	1:F:530:ASN:HB2	2.19	0.42
1:F:552:LEU:HD12	1:F:667:VAL:HG21	2.01	0.42
1:F:686:PHE:HB3	1:F:690:GLU:HB2	2.00	0.42
2:I:58:TRP:HB3	2:I:95:ALA:CB	2.49	0.42
2:I:203:LYS:NZ	2:I:236:SER:HB3	2.34	0.42
1:C:256:ILE:HG22	1:C:391:VAL:CG1	2.49	0.42
1:C:510:TRP:CZ3	1:C:670:ILE:HG12	2.54	0.42
1:D:573:MET:SD	1:D:608:LEU:HD22	2.59	0.42
1:E:46:ILE:HG21	1:E:85:PHE:CZ	2.54	0.42
1:E:91:CYS:HB3	1:E:155:MET:HE2	2.00	0.42
1:F:232:ARG:O	1:F:236:ALA:HB3	2.18	0.42
1:F:270:ALA:HA	1:F:273:ILE:HG22	2.01	0.42
2:I:119:ILE:HD12	2:I:122:LYS:HG3	2.01	0.42
2:I:179:GLN:HG3	2:I:180:LYS:N	2.35	0.42
2:J:66:CYS:SG	2:J:92:PHE:HE2	2.43	0.42
2:G:39:GLU:HB2	2:G:75:LEU:HD11	2.01	0.42
3:K:48:VAL:HG11	3:K:52:LYS:HZ1	1.85	0.42
1:A:110:ASN:HD22	1:A:321:GLY:HA2	1.83	0.42
1:B:91:CYS:HB3	1:B:155:MET:HE2	2.00	0.42
1:D:498:ASP:O	1:D:501:SER:HB3	2.18	0.42
1:E:406:ILE:O	1:E:409:ILE:HG22	2.20	0.42
1:F:230:ILE:HD11	1:F:391:VAL:HG11	2.00	0.42
1:F:606:GLU:H	1:F:606:GLU:CD	2.22	0.42
2:H:198:LEU:C	2:H:200:TYR:N	2.73	0.42
2:H:247:LEU:HD22	2:H:259:TYR:CD1	2.54	0.42
2:I:45:TYR:HE2	2:I:71:LEU:HD11	1.85	0.42
5:M:17:ARG:HE	5:M:21:LEU:HD11	1.83	0.42
1:A:65:PRO:HG2	1:A:137:VAL:HG13	2.01	0.42
1:B:309:ALA:HB1	1:B:367:ILE:HG21	2.01	0.42
1:B:593:TYR:OH	1:B:632:LYS:HG2	2.19	0.42
1:C:23:VAL:HG12	1:C:55:VAL:HG21	2.00	0.42
1:C:519:ASP:O	1:C:523:LEU:HG	2.19	0.42
1:D:690:GLU:O	1:D:694:ILE:HG13	2.19	0.42
1:F:143:LYS:HB3	1:F:145:PHE:HE1	1.84	0.42
1:F:557:ALA:HB2	1:F:601:VAL:HG21	2.02	0.42
1:F:602:VAL:O	1:F:644:GLY:HA2	2.20	0.42
1:F:678:GLU:O	1:F:682:LEU:HG	2.20	0.42
2:H:182:ILE:CG2	2:H:212:CYS:HB2	2.50	0.42
2:I:203:LYS:HB3	2:I:240:GLU:HG3	2.00	0.42
2:J:21:VAL:HG23	2:J:38:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:211:GLU:O	4:L:214:ASP:HB2	2.19	0.42
1:A:52:HIS:HA	1:A:53:PRO:HD3	1.91	0.42
1:A:624:GLN:CG	1:B:610:ASP:OD2	2.66	0.42
1:A:686:PHE:O	1:A:691:ARG:NH2	2.53	0.42
1:B:507:ILE:CG1	1:B:555:LYS:HD3	2.50	0.42
1:B:541:LEU:HD12	1:B:541:LEU:O	2.20	0.42
1:B:555:LYS:O	1:B:559:GLU:HG2	2.20	0.42
1:C:101:PHE:CE1	1:C:193:LEU:HD13	2.54	0.42
1:C:121:PHE:CD2	1:C:183:VAL:HG21	2.54	0.42
1:C:686:PHE:HB3	1:C:690:GLU:OE2	2.20	0.42
1:D:114:THR:HG21	1:D:200:LYS:CG	2.49	0.42
1:D:657:MET:HE2	1:D:661:PHE:HZ	1.85	0.42
1:F:377:ASP:OD1	1:F:378:LEU:N	2.52	0.42
1:F:694:ILE:O	1:F:698:VAL:HG22	2.20	0.42
2:G:208:LYS:HG2	2:G:275:TRP:CZ3	2.55	0.42
2:G:245:LYS:HB2	2:G:245:LYS:NZ	2.35	0.42
3:K:46:MET:HG3	4:L:216:PHE:CE1	2.55	0.42
1:A:262:PRO:CG	1:A:374:ASN:OD1	2.66	0.42
1:A:299:GLU:OE1	1:A:303:ARG:NH2	2.51	0.42
1:A:316:LEU:O	1:A:320:SER:HB2	2.20	0.42
1:B:286:ASN:OD1	1:B:327:PHE:HD1	2.03	0.42
1:B:397:LEU:HD23	1:B:398:PRO:HD2	2.01	0.42
1:B:502:TYR:CE2	1:B:567:ILE:HD13	2.55	0.42
1:B:539:VAL:HA	1:B:663:THR:O	2.19	0.42
1:C:325:ILE:O	1:C:369:VAL:HA	2.19	0.42
1:D:313:GLN:HG3	1:D:314:ARG:N	2.34	0.42
1:D:511:GLY:CA	1:D:675:GLN:HE21	2.33	0.42
1:E:11:CYS:HA	1:E:12:PRO:HD3	1.97	0.42
1:E:534:THR:HG21	1:F:712:MET:HA	2.01	0.42
1:F:297:GLU:O	1:F:300:ALA:HB3	2.19	0.42
2:H:73:LEU:C	2:H:75:LEU:H	2.27	0.42
2:I:15:ALA:O	2:I:19:ARG:HG3	2.19	0.42
2:I:122:LYS:NZ	3:K:59:LYS:HZ3	2.18	0.42
2:I:190:THR:HA	2:I:193:MET:HE3	2.01	0.42
2:I:277:THR:O	2:I:281:LEU:HD13	2.20	0.42
2:J:98:GLN:H	2:J:98:GLN:NE2	2.18	0.42
2:J:260:THR:HG21	2:J:284:LYS:HE3	2.01	0.42
2:G:38:ILE:CD1	2:G:71:LEU:HB3	2.50	0.42
5:M:78:LEU:CD1	5:M:195:ALA:HB1	2.50	0.42
1:A:231:PHE:CE2	1:A:235:PHE:HD2	2.38	0.42
1:A:319:ASN:O	1:A:320:SER:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:LEU:O	1:A:725:ARG:NE	2.52	0.42
1:B:246:GLU:HG2	1:B:247:GLN:N	2.35	0.42
1:B:540:LEU:HD12	1:B:540:LEU:C	2.45	0.42
1:C:35:VAL:HG11	1:C:49:LEU:HD11	2.02	0.42
1:D:268:LEU:O	1:D:271:ARG:HG2	2.20	0.42
1:E:240:PHE:HD2	1:E:244:ILE:CG2	2.26	0.42
1:E:713:LEU:HD23	1:E:713:LEU:HA	1.79	0.42
1:F:582:CYS:SG	1:F:586:LYS:HE3	2.60	0.42
2:H:101:ILE:HB	2:H:131:TYR:OH	2.20	0.42
2:H:203:LYS:HD3	2:H:236:SER:CB	2.47	0.42
2:H:230:GLU:CD	2:H:241:CYS:SG	3.03	0.42
1:A:261:PRO:HD2	1:A:395:ILE:O	2.20	0.42
1:C:38:ARG:HH11	1:C:38:ARG:HG2	1.84	0.42
1:C:38:ARG:HG3	1:C:44:LYS:HE2	2.01	0.42
1:C:186:GLU:HG3	1:C:186:GLU:O	2.18	0.42
1:C:291:LEU:HA	1:C:298:SER:CB	2.50	0.42
1:D:23:VAL:HG12	1:D:55:VAL:CG2	2.50	0.42
1:D:659:ASN:OD1	1:E:546:HIS:HE1	2.03	0.42
1:E:268:LEU:HD12	1:E:269:LEU:N	2.35	0.42
1:E:307:ALA:O	1:E:310:GLU:HG2	2.20	0.42
1:F:242:PRO:O	1:F:245:VAL:HG12	2.20	0.42
2:H:246:LYS:NZ	2:H:258:SER:HB3	2.35	0.42
2:I:69:ALA:HB1	2:I:85:PHE:CD1	2.55	0.42
2:I:184:ILE:O	2:I:188:VAL:HG12	2.20	0.42
2:J:72:HIS:CE1	2:J:77:SER:HB2	2.55	0.42
2:J:282:ARG:O	2:J:286:THR:HG23	2.19	0.42
2:G:45:TYR:HE2	2:G:71:LEU:HD11	1.84	0.42
3:K:42:VAL:HG21	5:M:157:ILE:HG23	2.02	0.42
1:A:706:GLY:O	1:A:710:LEU:N	2.50	0.41
1:B:24:VAL:HG11	1:B:49:LEU:HD22	2.02	0.41
1:B:512:ASP:N	1:B:513:PRO:CD	2.83	0.41
1:C:95:MET:CG	1:C:152:ILE:HG12	2.49	0.41
1:C:355:LEU:HA	1:C:388:ARG:NE	2.34	0.41
1:C:590:ASP:HA	1:C:593:TYR:HD2	1.80	0.41
1:D:96:THR:HA	1:D:184:ALA:O	2.20	0.41
1:D:231:PHE:HA	1:D:235:PHE:CD2	2.55	0.41
1:D:319:ASN:HA	1:D:320:SER:HA	1.81	0.41
1:D:327:PHE:HB2	1:D:330:ILE:CG2	2.50	0.41
1:D:510:TRP:HZ2	1:D:668:PRO:O	2.03	0.41
1:E:512:ASP:N	1:E:513:PRO:CD	2.82	0.41
1:F:24:VAL:HA	1:F:55:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:605:ILE:N	1:F:606:GLU:OE1	2.53	0.41
1:F:658:LEU:HA	1:F:661:PHE:HD2	1.84	0.41
2:I:243:LEU:HD22	2:I:266:TYR:CD2	2.55	0.41
2:I:266:TYR:C	2:I:268:SER:H	2.27	0.41
2:I:287:ILE:O	2:I:291:GLU:HG3	2.20	0.41
2:J:53:LYS:HG3	2:J:58:TRP:CZ3	2.55	0.41
2:J:232:PHE:C	2:J:234:ALA:H	2.28	0.41
2:G:92:PHE:HD1	2:G:97:PRO:HG2	1.84	0.41
2:G:108:ILE:HD12	2:G:127:ILE:HD12	2.02	0.41
3:K:53:VAL:HG13	3:K:54:LEU:N	2.35	0.41
1:A:7:GLN:H	1:A:59:SER:HA	1.85	0.41
1:A:98:GLU:HB3	1:A:148:LEU:HB3	2.01	0.41
1:A:220:ILE:HG22	1:A:221:GLY:N	2.33	0.41
1:A:322:LEU:HD13	1:A:366:ASN:O	2.19	0.41
1:A:356:SER:CB	1:B:288:PRO:HD3	2.50	0.41
1:A:517:VAL:HG13	1:A:665:ILE:CG2	2.50	0.41
1:B:69:TRP:CE2	1:B:134:GLN:HA	2.54	0.41
1:B:388:ARG:O	1:B:389:LEU:HD23	2.20	0.41
1:B:406:ILE:O	1:B:409:ILE:HG22	2.19	0.41
1:B:513:PRO:O	1:B:517:VAL:HG23	2.20	0.41
1:B:549:LYS:NZ	1:B:647:SER:HA	2.35	0.41
1:C:503:ILE:O	1:C:503:ILE:HG22	2.19	0.41
1:F:236:ALA:HA	1:F:239:VAL:CG1	2.49	0.41
1:F:629:LEU:O	1:F:632:LYS:HB3	2.20	0.41
2:H:228:TYR:CE2	2:H:230:GLU:HB2	2.54	0.41
2:H:237:ASP:C	2:H:239:ARG:N	2.75	0.41
2:J:188:VAL:HG22	2:J:205:TYR:HE2	1.86	0.41
4:L:213:HIS:HD2	5:M:35:LEU:HA	1.85	0.41
1:A:357:LYS:HA	1:A:357:LYS:HE3	2.01	0.41
1:A:497:GLU:O	1:A:498:ASP:C	2.63	0.41
1:B:503:ILE:HG22	1:B:506:GLY:H	1.85	0.41
1:C:386:PRO:HA	1:C:390:GLU:CA	2.37	0.41
1:C:696:GLN:O	1:C:696:GLN:NE2	2.53	0.41
1:D:46:ILE:HD12	1:D:174:VAL:HG21	2.02	0.41
1:D:582:CYS:O	1:D:586:LYS:HG3	2.19	0.41
1:E:259:TYR:HA	1:E:373:THR:O	2.20	0.41
1:F:502:TYR:CD2	1:F:503:ILE:HG13	2.55	0.41
1:F:502:TYR:HD2	1:F:503:ILE:HG13	1.85	0.41
2:J:91:ALA:O	2:J:95:ALA:HB2	2.21	0.41
2:J:268:SER:HA	2:G:233:PRO:HG3	2.03	0.41
5:M:17:ARG:O	5:M:21:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:HG3	1:B:44:LYS:HE3	2.03	0.41
1:B:523:LEU:O	1:B:526:GLN:HG2	2.21	0.41
1:C:237:SER:OG	1:C:252:HIS:ND1	2.45	0.41
1:C:526:GLN:OE1	1:C:530:ASN:ND2	2.54	0.41
1:C:676:LEU:HD12	1:C:705:ILE:CG2	2.44	0.41
1:D:271:ARG:HG2	1:D:272:GLN:N	2.34	0.41
1:D:436:PHE:CE2	1:D:444:LEU:HD12	2.49	0.41
1:E:242:PRO:HD2	1:E:243:GLU:N	2.34	0.41
1:E:250:CYS:SG	1:F:446:ARG:HB2	2.60	0.41
1:E:451:THR:O	1:E:454:ASN:HB3	2.20	0.41
1:E:697:GLN:O	1:E:701:LYS:HD2	2.21	0.41
1:F:18:LEU:HD23	1:F:137:VAL:HG21	2.02	0.41
1:F:95:MET:CE	1:F:97:ILE:HD11	2.30	0.41
1:F:388:ARG:O	1:F:389:LEU:HD23	2.19	0.41
2:H:200:TYR:O	4:L:217:MET:CE	2.68	0.41
2:J:101:ILE:O	2:J:105:MET:HG3	2.20	0.41
2:G:281:LEU:O	2:G:285:LYS:HG3	2.20	0.41
1:A:380:ASP:OD1	1:A:381:GLU:N	2.54	0.41
1:B:232:ARG:O	1:B:236:ALA:HB3	2.20	0.41
1:C:91:CYS:CB	1:C:155:MET:HE2	2.49	0.41
1:C:621:LEU:HD11	1:D:575:GLY:HA2	2.01	0.41
1:D:543:GLY:N	1:D:549:LYS:HD3	2.30	0.41
1:D:669:ASN:OD1	1:D:669:ASN:N	2.46	0.41
1:E:289:GLU:C	1:E:291:LEU:N	2.70	0.41
1:E:686:PHE:O	1:E:691:ARG:NH1	2.53	0.41
1:E:721:ASP:HB2	1:E:724:TYR:HD2	1.85	0.41
1:F:46:ILE:HD12	1:F:174:VAL:HG21	2.02	0.41
1:F:319:ASN:HA	1:F:320:SER:HA	1.91	0.41
1:F:545:PRO:HB3	1:F:546:HIS:HA	2.02	0.41
2:I:119:ILE:HD11	2:I:123:HIS:HE1	1.85	0.41
2:I:182:ILE:HG22	2:I:212:CYS:HB2	2.01	0.41
2:J:184:ILE:O	2:J:188:VAL:HG12	2.21	0.41
2:J:277:THR:O	2:J:281:LEU:HD13	2.20	0.41
1:A:247:GLN:C	1:B:413:ARG:HH12	2.28	0.41
1:B:95:MET:CG	1:B:152:ILE:HG12	2.50	0.41
1:B:326:ILE:HG22	1:B:370:ILE:CG1	2.49	0.41
1:C:517:VAL:HG13	1:C:665:ILE:HG21	2.01	0.41
1:C:690:GLU:HB2	1:C:726:VAL:CG2	2.43	0.41
1:C:709:LYS:HD2	1:C:709:LYS:HA	1.82	0.41
1:C:711:LEU:N	1:C:711:LEU:HD23	2.36	0.41
1:D:313:GLN:O	1:D:317:GLY:CA	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:SER:HB2	1:E:41:PRO:HD2	2.02	0.41
1:E:533:ARG:HB2	1:F:715:GLU:CD	2.45	0.41
1:F:64:LEU:HA	1:F:67:ARG:HH21	1.84	0.41
1:F:242:PRO:CD	1:F:243:GLU:N	2.83	0.41
2:H:134:GLU:O	2:H:136:VAL:HG23	2.20	0.41
2:J:201:SER:HB2	5:M:165:LEU:CD1	2.43	0.41
2:G:277:THR:O	2:G:281:LEU:HD13	2.21	0.41
3:K:79:THR:HG22	3:K:83:LYS:HE3	2.02	0.41
1:A:517:VAL:HG13	1:A:665:ILE:HG21	2.02	0.41
1:A:620:ASN:O	1:A:624:GLN:HG2	2.21	0.41
1:A:652:LEU:HA	1:A:655:MET:SD	2.60	0.41
1:A:673:GLY:O	1:A:676:LEU:HB3	2.20	0.41
1:B:347:HIS:O	1:B:350:VAL:HG22	2.20	0.41
1:B:690:GLU:O	1:B:694:ILE:HG13	2.21	0.41
1:C:87:LYS:HA	1:C:91:CYS:SG	2.61	0.41
1:C:102:LEU:HD22	1:C:137:VAL:HG12	2.02	0.41
1:C:560:SER:HB2	1:C:562:PHE:CZ	2.56	0.41
1:D:92:ILE:HG21	1:D:95:MET:HB2	2.02	0.41
1:E:324:ILE:HG12	1:E:368:LEU:HD11	2.02	0.41
1:E:598:SER:O	1:E:640:LEU:HA	2.20	0.41
1:F:601:VAL:HG22	1:F:643:ILE:HD12	2.03	0.41
2:H:54:MET:C	2:H:56:LYS:H	2.29	0.41
2:H:156:GLU:O	2:H:158:ASN:N	2.53	0.41
2:H:175:LEU:O	2:H:176:GLU:HB3	2.20	0.41
2:J:208:LYS:HG2	2:J:275:TRP:CZ3	2.56	0.41
3:K:39:VAL:HG22	5:M:157:ILE:HD11	2.03	0.41
1:A:215:PHE:N	1:A:231:PHE:CZ	2.89	0.41
1:A:575:GLY:HA3	1:F:586:LYS:HZ1	1.85	0.41
1:A:610:ASP:OD1	1:F:624:GLN:HG3	2.20	0.41
1:A:707:ILE:HA	1:A:710:LEU:HB2	2.03	0.41
1:B:94:THR:HB	1:B:153:GLU:HB2	2.02	0.41
1:B:313:GLN:O	1:B:317:GLY:N	2.53	0.41
1:B:423:ASP:CB	1:B:479:ASP:N	2.84	0.41
1:C:241:PRO:HA	1:C:242:PRO:HA	1.65	0.41
1:E:297:GLU:O	1:E:300:ALA:HB3	2.21	0.41
1:E:643:ILE:N	1:E:643:ILE:HD12	2.35	0.41
2:H:82:ALA:HB2	2:H:110:ILE:HG21	2.02	0.41
2:G:169:ALA:HB2	2:G:184:ILE:HB	2.03	0.41
5:M:31:ARG:C	5:M:33:LEU:N	2.79	0.41
1:A:240:PHE:CG	1:A:244:ILE:HD11	2.56	0.41
1:A:261:PRO:HB3	1:A:594:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:VAL:CG1	1:A:617:ARG:HB2	2.50	0.41
1:A:626:LEU:CD2	1:A:657:MET:HE1	2.45	0.41
1:A:676:LEU:HD12	1:A:710:LEU:HD11	2.03	0.41
1:B:406:ILE:HD12	1:B:406:ILE:H	1.86	0.41
1:B:533:ARG:CG	1:B:534:THR:H	2.24	0.41
1:C:22:ALA:HB3	1:C:49:LEU:HD23	2.03	0.41
1:C:499:TYR:OH	1:C:565:ILE:HB	2.20	0.41
1:C:624:GLN:CD	1:D:610:ASP:HB2	2.46	0.41
1:C:648:ARG:HD3	1:C:651:VAL:HG21	2.02	0.41
1:C:726:VAL:H	1:C:726:VAL:HG23	1.64	0.41
1:D:249:GLY:HA3	1:E:413:ARG:NH1	2.36	0.41
1:D:258:LEU:HD12	1:D:258:LEU:O	2.21	0.41
1:D:303:ARG:HH11	1:D:357:LYS:HE3	1.85	0.41
1:D:331:ASP:HA	1:D:379:ILE:CD1	2.51	0.41
1:D:349:THR:HA	1:D:352:ASN:HD22	1.85	0.41
1:D:711:LEU:O	1:D:715:GLU:HG2	2.21	0.41
1:E:35:VAL:HG13	1:E:49:LEU:HD11	2.02	0.41
1:E:231:PHE:O	1:E:235:PHE:CD2	2.74	0.41
1:E:257:LEU:C	1:E:257:LEU:HD23	2.46	0.41
1:E:607:ARG:HD3	1:E:607:ARG:HA	1.82	0.41
1:F:400:GLU:OE2	1:F:434:LYS:HA	2.21	0.41
1:F:406:ILE:O	1:F:409:ILE:HG22	2.20	0.41
1:F:510:TRP:HZ3	1:F:675:GLN:NE2	2.19	0.41
2:H:18:GLU:HA	2:H:21:VAL:CG1	2.48	0.41
2:H:116:ARG:HG3	2:H:116:ARG:HH11	1.86	0.41
2:H:126:SER:O	2:H:130:ILE:HG13	2.21	0.41
2:H:160:SER:O	2:H:163:LYS:HB3	2.21	0.41
2:H:200:TYR:N	2:H:200:TYR:CD1	2.89	0.41
2:I:39:GLU:HB2	2:I:75:LEU:CD1	2.50	0.41
2:I:162:ASN:HD22	2:I:162:ASN:H	1.69	0.41
2:I:182:ILE:CG2	2:I:212:CYS:HB2	2.50	0.41
2:I:256:VAL:O	2:I:256:VAL:HG22	2.21	0.41
2:J:10:ALA:O	2:J:14:LEU:HG	2.21	0.41
2:J:163:LYS:O	2:J:167:LYS:HG2	2.20	0.41
2:J:167:LYS:HE2	2:J:171:TYR:CE2	2.55	0.41
2:J:203:LYS:HD2	2:J:236:SER:C	2.46	0.41
2:J:256:VAL:HG22	2:J:256:VAL:O	2.21	0.41
2:G:276:LEU:O	2:G:280:LEU:HG	2.20	0.41
3:K:48:VAL:HG12	3:K:52:LYS:NZ	2.36	0.41
3:K:56:ARG:CD	5:M:171:ILE:HG23	2.41	0.41
3:K:77:PHE:HZ	5:M:74:ALA:HB1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:194:GLU:O	4:L:198:ARG:HB2	2.21	0.41
4:L:216:PHE:O	4:L:219:MET:HB3	2.21	0.41
4:L:237:VAL:O	4:L:241:VAL:HG23	2.21	0.41
1:B:184:ALA:HB1	1:B:200:LYS:O	2.20	0.41
1:B:307:ALA:O	1:B:310:GLU:HG2	2.20	0.41
1:B:377:ASP:OD1	1:B:378:LEU:N	2.54	0.41
1:B:385:ARG:HH21	1:B:388:ARG:CZ	2.34	0.41
1:D:24:VAL:HG11	1:D:49:LEU:HD22	2.02	0.41
1:D:527:GLN:HA	1:E:719:GLN:HG3	2.02	0.41
1:D:570:PRO:O	1:D:573:MET:HB3	2.21	0.41
1:E:92:ILE:HG13	1:E:176:LEU:N	2.36	0.41
1:E:596:GLN:HA	1:E:638:ARG:HA	2.03	0.41
1:E:623:LEU:HD23	1:E:624:GLN:NE2	2.36	0.41
1:E:705:ILE:HD12	1:E:713:LEU:HD12	2.02	0.41
1:F:86:ASP:O	1:F:88:ALA:N	2.54	0.41
1:F:101:PHE:CE1	1:F:193:LEU:HD13	2.55	0.41
1:F:264:CYS:SG	1:F:395:ILE:CG2	3.06	0.41
1:F:542:GLU:N	1:F:665:ILE:O	2.52	0.41
2:H:179:GLN:HG3	2:H:180:LYS:N	2.35	0.41
2:J:235:PHE:CG	3:K:38:GLN:NE2	2.89	0.41
2:G:275:TRP:CE3	2:G:276:LEU:HD23	2.55	0.41
1:A:549:LYS:CB	1:A:667:VAL:HG21	2.51	0.40
1:B:612:VAL:HG12	1:B:617:ARG:O	2.21	0.40
1:C:16:LEU:HD11	1:C:52:HIS:HD2	1.86	0.40
1:C:313:GLN:NE2	1:C:365:ASN:O	2.52	0.40
1:C:379:ILE:HA	1:C:379:ILE:HD13	1.71	0.40
1:C:691:ARG:HB2	1:C:691:ARG:NH1	2.35	0.40
1:D:186:GLU:HG3	1:D:186:GLU:O	2.21	0.40
1:D:223:LEU:HD23	1:D:223:LEU:O	2.21	0.40
1:D:377:ASP:OD1	1:D:378:LEU:N	2.54	0.40
1:E:63:SER:O	1:E:67:ARG:HG3	2.21	0.40
1:E:587:LYS:NZ	1:E:591:ASP:CG	2.78	0.40
1:E:627:LEU:HD13	1:F:607:ARG:CZ	2.51	0.40
1:E:640:LEU:HG	1:E:642:ILE:CD1	2.51	0.40
1:F:50:ARG:HG2	1:F:50:ARG:HH11	1.86	0.40
1:F:97:ILE:HG21	1:F:147:LEU:HD22	2.04	0.40
1:F:436:PHE:HD2	1:F:444:LEU:HD11	1.86	0.40
1:F:658:LEU:HD12	1:F:658:LEU:O	2.21	0.40
2:J:82:ALA:HB2	2:J:110:ILE:HG21	2.03	0.40
2:J:256:VAL:HG11	2:J:288:GLN:HG2	2.03	0.40
5:M:25:SER:O	5:M:28:SER:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:SER:O	1:A:67:ARG:HG3	2.21	0.40
1:C:52:HIS:HA	1:C:53:PRO:HD3	1.93	0.40
1:C:86:ASP:C	1:C:88:ALA:N	2.80	0.40
1:C:189:GLU:O	1:C:190:ASN:HB2	2.20	0.40
1:C:388:ARG:HB2	1:C:388:ARG:CZ	2.52	0.40
1:C:407:LEU:O	1:C:411:THR:OG1	2.30	0.40
1:C:629:LEU:HA	1:C:629:LEU:HD23	1.76	0.40
1:D:40:SER:C	1:D:42:ASN:H	2.29	0.40
1:D:612:VAL:HG13	1:D:614:ILE:O	2.21	0.40
1:F:577:SER:O	1:F:581:LYS:HG3	2.22	0.40
1:F:609:LEU:HD23	1:F:609:LEU:HA	1.80	0.40
2:H:147:GLN:HG2	2:H:151:TYR:CE2	2.57	0.40
2:H:200:TYR:O	4:L:217:MET:HE1	2.22	0.40
2:H:256:VAL:HG22	2:H:256:VAL:O	2.21	0.40
2:I:98:GLN:C	2:I:100:ALA:H	2.30	0.40
2:I:240:GLU:OE1	2:I:241:CYS:HB3	2.21	0.40
2:G:118:THR:HG22	2:G:155:GLU:HG3	2.03	0.40
5:M:30:ARG:NH2	5:M:145:GLU:OE2	2.54	0.40
1:A:38:ARG:HG2	1:A:38:ARG:HH11	1.85	0.40
1:A:377:ASP:OD2	1:A:378:LEU:HD23	2.21	0.40
1:A:566:LYS:HD3	1:A:566:LYS:HA	1.68	0.40
1:B:519:ASP:OD1	1:B:520:ASP:N	2.55	0.40
1:C:25:SER:HB3	1:C:28:ASP:OD2	2.21	0.40
1:C:319:ASN:HA	1:C:320:SER:HA	1.87	0.40
1:C:324:ILE:HD12	1:C:324:ILE:N	2.36	0.40
1:C:627:LEU:HA	1:C:627:LEU:HD23	1.77	0.40
1:D:86:ASP:C	1:D:88:ALA:N	2.79	0.40
1:D:263:GLY:HA2	1:D:439:ALA:HB3	2.04	0.40
1:D:397:LEU:HD22	1:D:435:ASN:O	2.22	0.40
1:D:511:GLY:HA3	1:D:675:GLN:HE21	1.85	0.40
1:E:490:PRO:HA	1:E:491:ALA:CB	2.36	0.40
1:F:241:PRO:HA	1:F:242:PRO:HA	1.53	0.40
2:H:287:ILE:O	2:H:291:GLU:HG3	2.21	0.40
2:J:45:TYR:CB	2:J:68:ALA:HB2	2.51	0.40
2:J:175:LEU:C	2:J:177:GLN:H	2.29	0.40
2:G:232:PHE:C	2:G:234:ALA:H	2.28	0.40
3:K:56:ARG:HD2	5:M:171:ILE:CG2	2.41	0.40
5:M:158:GLY:O	5:M:161:ARG:HB3	2.22	0.40
1:A:240:PHE:HA	1:A:241:PRO:HD3	1.91	0.40
1:A:693:THR:O	1:A:697:GLN:OE1	2.40	0.40
1:B:546:HIS:HB3	1:B:547:SER:H	1.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:MET:C	1:B:656:GLU:HG3	2.46	0.40
1:C:47:PHE:HZ	1:C:70:ALA:HB2	1.86	0.40
1:C:408:HIS:HD1	1:C:408:HIS:C	2.29	0.40
1:C:510:TRP:O	1:C:675:GLN:HG3	2.21	0.40
1:C:577:SER:O	1:C:578:GLU:C	2.64	0.40
1:C:638:ARG:HH11	1:C:638:ARG:HG3	1.86	0.40
1:D:221:GLY:O	1:D:406:ILE:HD11	2.21	0.40
1:D:278:ASN:O	1:D:279:ALA:C	2.64	0.40
1:D:407:LEU:HB2	1:D:426:ILE:HG23	2.02	0.40
1:D:573:MET:HA	1:D:576:PHE:CD2	2.57	0.40
1:E:140:PHE:O	1:E:141:ASN:HB2	2.21	0.40
1:F:103:GLN:C	1:F:105:LYS:N	2.76	0.40
2:H:198:LEU:HD21	4:L:224:GLU:OE1	2.21	0.40
2:I:179:GLN:HB3	2:I:214:PHE:HB3	2.02	0.40
2:J:203:LYS:HD2	2:J:236:SER:O	2.21	0.40
2:G:96:ASP:H	2:G:97:PRO:HD2	1.86	0.40
4:L:191:ALA:HB3	4:L:194:GLU:HG2	2.03	0.40
1:A:231:PHE:CD1	1:A:235:PHE:CE2	3.01	0.40
1:A:300:ALA:O	1:A:303:ARG:HG2	2.21	0.40
1:A:732:LEU:HD23	1:A:732:LEU:HA	1.86	0.40
1:B:113:ASP:HA	1:B:196:ILE:HG13	2.04	0.40
1:B:242:PRO:CD	1:B:243:GLU:N	2.85	0.40
1:B:531:SER:CA	1:B:639:LYS:HD3	2.51	0.40
1:C:24:VAL:HG12	1:C:60:VAL:HG22	2.03	0.40
1:C:624:GLN:HA	1:C:624:GLN:OE1	2.21	0.40
1:E:441:LEU:O	1:E:445:VAL:HG23	2.22	0.40
1:F:101:PHE:HD1	1:F:101:PHE:H	1.68	0.40
2:H:195:SER:C	2:H:197:LEU:N	2.76	0.40
2:J:38:ILE:CD1	2:J:71:LEU:HB3	2.52	0.40
2:J:175:LEU:HD23	2:J:177:GLN:NE2	2.36	0.40
2:G:101:ILE:HB	2:G:131:TYR:OH	2.20	0.40
2:G:219:LEU:HD12	2:G:223:LEU:HB2	2.04	0.40
5:M:56:GLN:HA	5:M:59:ARG:NH2	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	668/747 (89%)	614 (92%)	37 (6%)	17 (2%)	4	26
1	B	662/747 (89%)	593 (90%)	55 (8%)	14 (2%)	5	30
1	C	666/747 (89%)	615 (92%)	39 (6%)	12 (2%)	6	34
1	D	663/747 (89%)	607 (92%)	47 (7%)	9 (1%)	9	40
1	E	658/747 (88%)	603 (92%)	41 (6%)	14 (2%)	5	30
1	F	644/747 (86%)	587 (91%)	44 (7%)	13 (2%)	6	31
2	G	284/297 (96%)	230 (81%)	43 (15%)	11 (4%)	2	19
2	H	284/297 (96%)	229 (81%)	46 (16%)	9 (3%)	3	21
2	I	284/297 (96%)	227 (80%)	48 (17%)	9 (3%)	3	21
2	J	284/297 (96%)	232 (82%)	41 (14%)	11 (4%)	2	19
3	K	59/63 (94%)	56 (95%)	2 (3%)	1 (2%)	7	36
4	L	64/67 (96%)	56 (88%)	8 (12%)	0	100	100
5	M	127/188 (68%)	124 (98%)	3 (2%)	0	100	100
All	All	5347/5988 (89%)	4773 (89%)	454 (8%)	120 (2%)	7	29

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	LEU
1	A	293	LYS
1	A	294	TYR
1	A	318	ALA
1	A	320	SER
1	A	333	ILE
1	A	397	LEU
1	A	498	ASP
1	A	504	MET
1	B	12	PRO

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Mol	Chain	Res	Type
1	B	283	LYS
1	B	297	GLU
1	B	318	ALA
1	B	439	ALA
1	B	489	LYS
1	C	297	GLU
1	C	318	ALA
1	C	497	GLU
1	C	498	ASP
1	C	578	GLU
1	D	188	ALA
1	D	283	LYS
1	D	318	ALA
1	D	489	LYS
1	E	283	LYS
1	E	297	GLU
1	E	318	ALA
1	E	439	ALA
1	E	489	LYS
1	F	200	LYS
1	F	283	LYS
1	F	297	GLU
1	F	318	ALA
1	F	439	ALA
2	H	58	TRP
2	H	79	HIS
2	I	219	LEU
2	J	58	TRP
2	J	76	GLN
2	G	58	TRP
2	G	176	GLU
1	C	293	LYS
1	C	610	ASP
1	E	12	PRO
1	E	88	ALA
1	E	507	ILE
1	F	87	LYS
2	H	76	GLN
2	H	202	ALA
2	I	79	HIS
2	J	156	GLU
2	G	76	GLN

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Mol	Chain	Res	Type
2	G	79	HIS
2	G	218	MET
1	A	12	PRO
1	A	241	PRO
1	A	242	PRO
1	A	264	CYS
1	B	241	PRO
1	B	293	LYS
1	B	502	TYR
1	C	241	PRO
1	D	293	LYS
1	E	241	PRO
1	E	293	LYS
1	F	12	PRO
1	F	241	PRO
1	F	293	LYS
2	H	240	GLU
2	H	256	VAL
2	I	58	TRP
2	J	34	GLY
2	J	77	SER
2	J	79	HIS
2	J	267	ASP
2	G	240	GLU
3	K	35	THR
1	B	546	HIS
1	C	87	LYS
1	D	12	PRO
1	E	87	LYS
1	E	189	GLU
1	F	397	LEU
2	H	157	SER
2	I	158	ASN
2	I	218	MET
2	I	240	GLU
2	I	256	VAL
2	G	267	ASP
1	A	53	PRO
1	A	398	PRO
1	A	668	PRO
1	B	53	PRO
1	B	547	SER

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Mol	Chain	Res	Type
1	C	53	PRO
1	D	241	PRO
2	H	77	SER
2	J	232	PHE
2	G	23	ASN
2	G	177	GLN
1	A	87	LYS
1	B	490	PRO
1	C	12	PRO
1	E	438	GLY
1	E	490	PRO
1	F	438	GLY
1	F	668	PRO
2	H	176	GLU
2	I	267	ASP
2	J	256	VAL
2	G	232	PHE
1	B	438	GLY
1	D	488	ILE
1	F	684	GLY
2	J	96	ASP
2	G	196	PRO
1	C	490	PRO
2	I	30	GLY
2	J	21	VAL
1	D	545	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	511/638 (80%)	485 (95%)	26 (5%)	21	42
1	B	512/638 (80%)	497 (97%)	15 (3%)	37	58
1	C	513/638 (80%)	489 (95%)	24 (5%)	23	45
1	D	506/638 (79%)	491 (97%)	15 (3%)	36	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	511/638 (80%)	491 (96%)	20 (4%)	28	49
1	F	505/638 (79%)	488 (97%)	17 (3%)	32	54
2	G	234/244 (96%)	232 (99%)	2 (1%)	70	79
2	H	233/244 (96%)	233 (100%)	0	100	100
2	I	234/244 (96%)	234 (100%)	0	100	100
2	J	235/244 (96%)	235 (100%)	0	100	100
3	K	49/54 (91%)	49 (100%)	0	100	100
4	L	56/61 (92%)	56 (100%)	0	100	100
5	M	114/161 (71%)	114 (100%)	0	100	100
All	All	4213/5080 (83%)	4094 (97%)	119 (3%)	38	60

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	GLU
1	A	246	GLU
1	A	253	VAL
1	A	284	VAL
1	A	305	LEU
1	A	322	LEU
1	A	326	ILE
1	A	367	ILE
1	A	375	ARG
1	A	409	ILE
1	A	445	VAL
1	A	449	GLN
1	A	537	VAL
1	A	539	VAL
1	A	566	LYS
1	A	573	MET
1	A	581	LYS
1	A	586	LYS
1	A	631	LYS
1	A	651	VAL
1	A	658	LEU
1	A	665	ILE
1	A	667	VAL
1	A	677	LEU
1	A	690	GLU

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Mol	Chain	Res	Type
1	A	705	ILE
1	B	246	GLU
1	B	284	VAL
1	B	285	VAL
1	B	305	LEU
1	B	322	LEU
1	B	325	ILE
1	B	330	ILE
1	B	351	VAL
1	B	381	GLU
1	B	389	LEU
1	B	411	THR
1	B	508	ILE
1	B	567	ILE
1	B	623	LEU
1	B	626	LEU
1	C	246	GLU
1	C	256	ILE
1	C	268	LEU
1	C	273	ILE
1	C	305	LEU
1	C	312	GLU
1	C	316	LEU
1	C	322	LEU
1	C	324	ILE
1	C	326	ILE
1	C	367	ILE
1	C	411	THR
1	C	541	LEU
1	C	573	MET
1	C	587	LYS
1	C	602	VAL
1	C	609	LEU
1	C	623	LEU
1	C	632	LYS
1	C	651	VAL
1	C	676	LEU
1	C	682	LEU
1	C	691	ARG
1	C	711	LEU
1	D	198	LYS
1	D	246	GLU

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Mol	Chain	Res	Type
1	D	273	ILE
1	D	284	VAL
1	D	305	LEU
1	D	311	GLU
1	D	370	ILE
1	D	389	LEU
1	D	407	LEU
1	D	424	VAL
1	D	602	VAL
1	D	645	THR
1	D	666	HIS
1	D	681	GLU
1	D	716	MET
1	E	246	GLU
1	E	284	VAL
1	E	285	VAL
1	E	305	LEU
1	E	322	LEU
1	E	325	ILE
1	E	330	ILE
1	E	351	VAL
1	E	381	GLU
1	E	389	LEU
1	E	507	ILE
1	E	508	ILE
1	E	522	GLU
1	E	537	VAL
1	E	586	LYS
1	E	602	VAL
1	E	626	LEU
1	E	658	LEU
1	E	689	LYS
1	E	693	THR
1	F	246	GLU
1	F	284	VAL
1	F	285	VAL
1	F	305	LEU
1	F	322	LEU
1	F	325	ILE
1	F	330	ILE
1	F	351	VAL
1	F	381	GLU

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Mol	Chain	Res	Type
1	F	389	LEU
1	F	411	THR
1	F	457	ILE
1	F	519	ASP
1	F	536	LEU
1	F	578	GLU
1	F	606	GLU
1	F	614	ILE
2	G	139	GLU
2	G	245	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	110	ASN
1	A	124	GLN
1	A	194	ASN
1	A	272	GLN
1	A	319	ASN
1	A	408	HIS
1	A	418	GLN
1	A	583	GLN
1	A	653	GLN
1	A	685	ASN
1	B	103	GLN
1	B	141	ASN
1	B	313	GLN
1	B	352	ASN
1	B	374	ASN
1	B	405	GLN
1	B	418	GLN
1	B	505	ASN
1	B	526	GLN
1	B	527	GLN
1	B	620	ASN
1	B	675	GLN
1	C	141	ASN
1	C	194	ASN
1	C	319	ASN
1	C	405	GLN
1	C	418	GLN

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Mol	Chain	Res	Type
1	D	106	ASN
1	D	313	GLN
1	D	352	ASN
1	D	353	GLN
1	D	526	GLN
1	D	527	GLN
1	D	596	GLN
1	D	675	GLN
1	E	33	GLN
1	E	34	HIS
1	E	43	HIS
1	E	405	GLN
1	E	418	GLN
1	E	505	ASN
1	E	527	GLN
1	E	546	HIS
1	E	666	HIS
1	F	141	ASN
1	F	252	HIS
1	F	374	ASN
1	F	405	GLN
1	F	418	GLN
2	H	72	HIS
2	H	162	ASN
2	H	179	GLN
2	I	50	ASN
2	I	72	HIS
2	I	187	GLN
2	I	226	GLN
2	I	251	HIS
2	J	50	ASN
2	J	98	GLN
2	J	187	GLN
2	J	288	GLN
2	G	50	ASN
2	G	72	HIS
2	G	177	GLN
2	G	187	GLN
2	G	288	GLN
3	K	38	GLN
4	L	226	GLN
5	M	53	GLN

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Mol	Chain	Res	Type
5	M	196	ASN
5	M	197	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

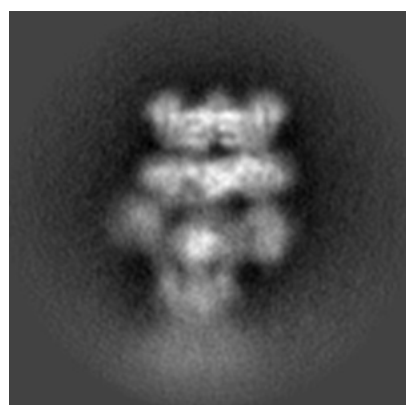
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6209. These allow visual inspection of the internal detail of the map and identification of artifacts.

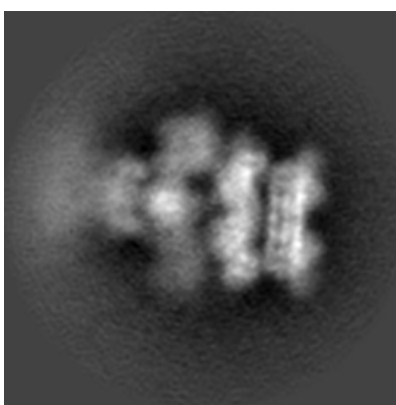
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

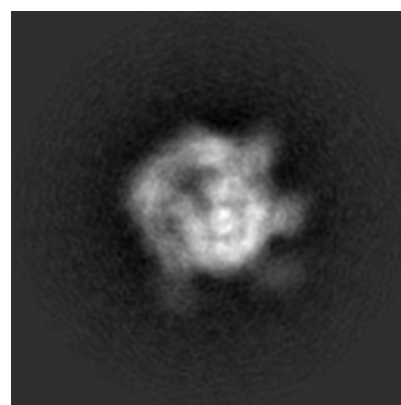
6.1.1 Primary map



X



Y

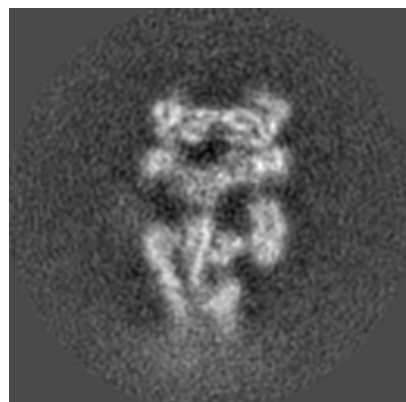


Z

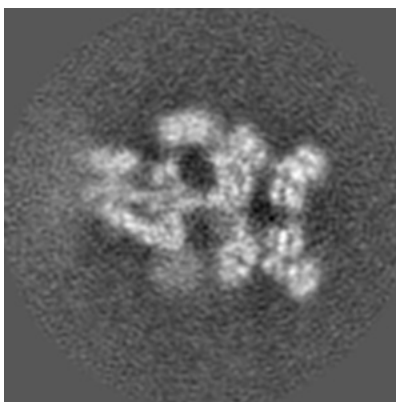
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

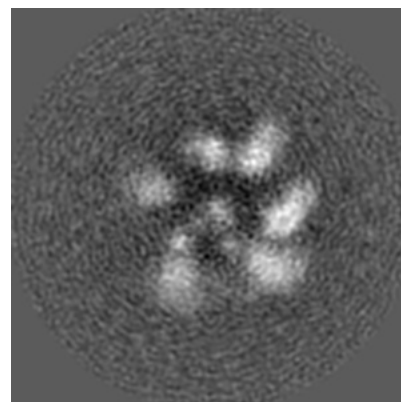
6.2.1 Primary map



X Index: 64



Y Index: 64

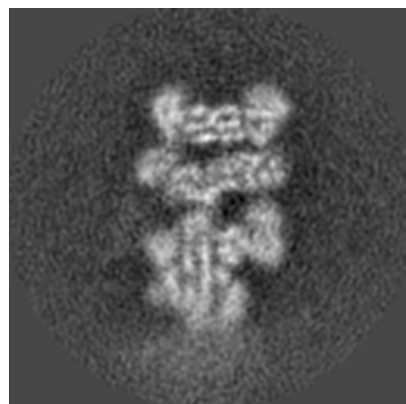


Z Index: 64

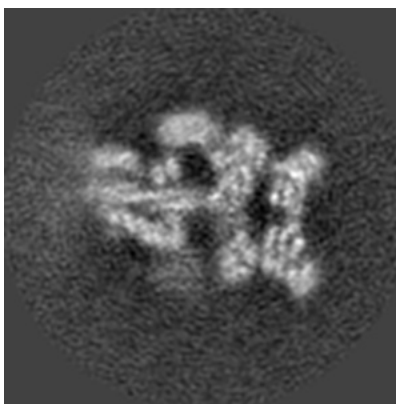
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

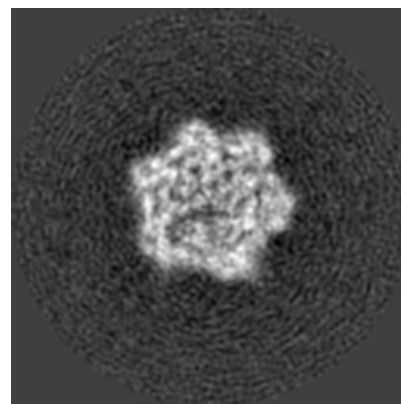
6.3.1 Primary map



X Index: 67



Y Index: 63

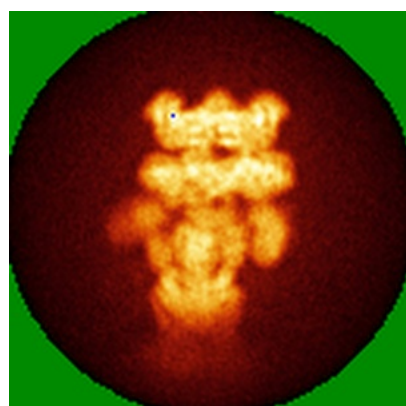


Z Index: 76

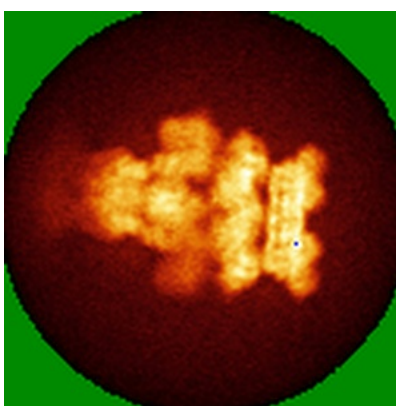
The images above show the largest variance slices of the map in three orthogonal directions.

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

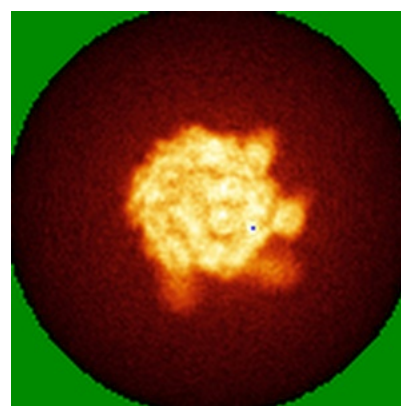
6.4.1 Primary map



X



Y

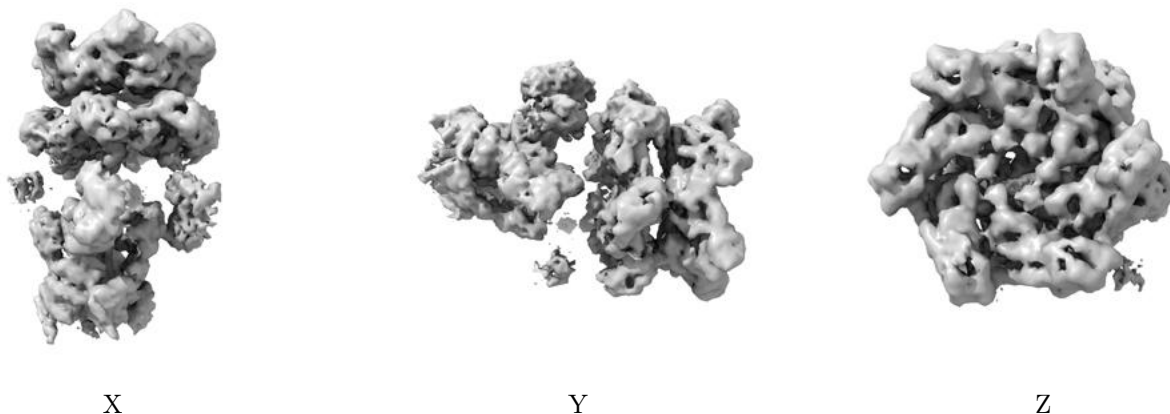


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

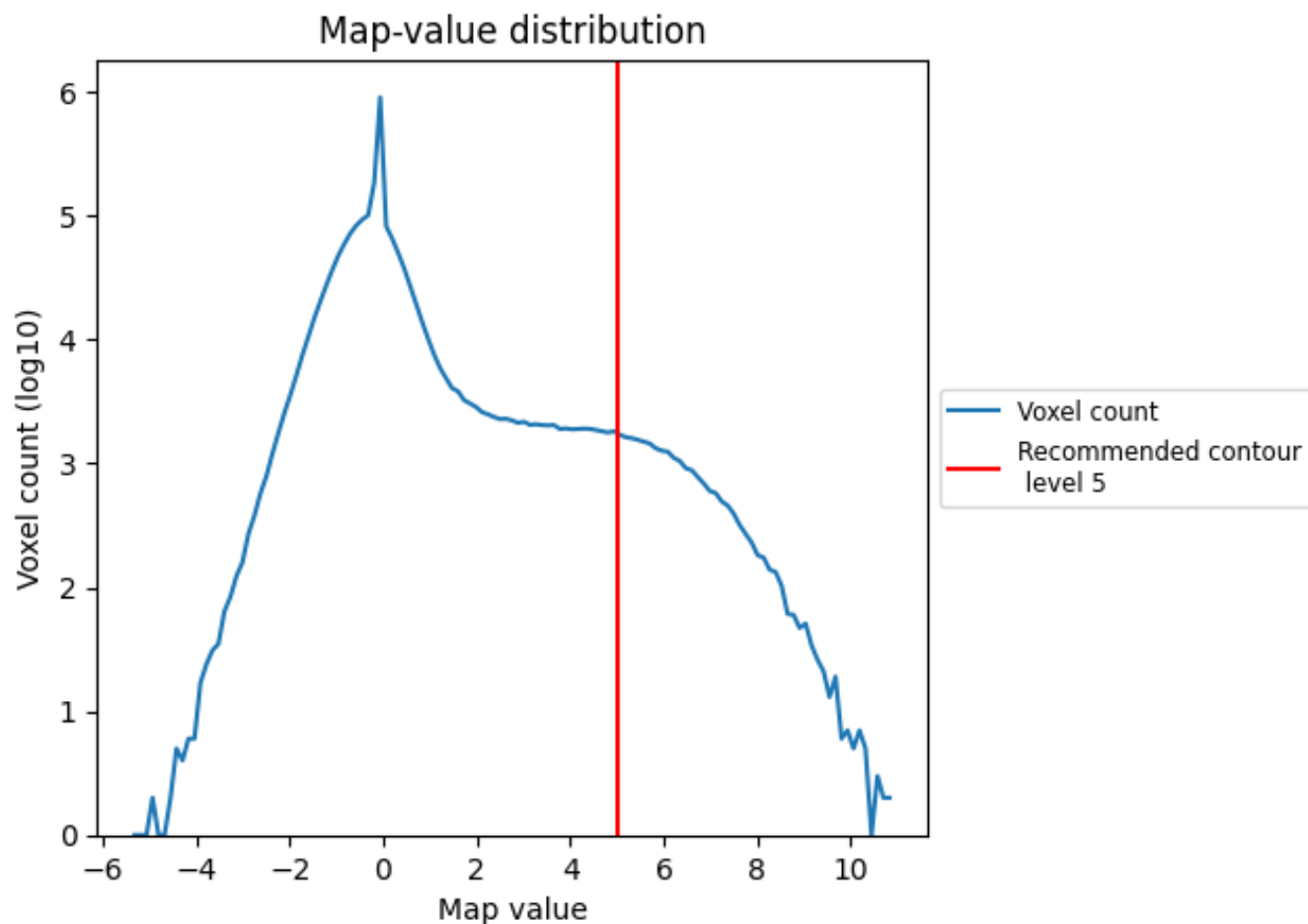
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

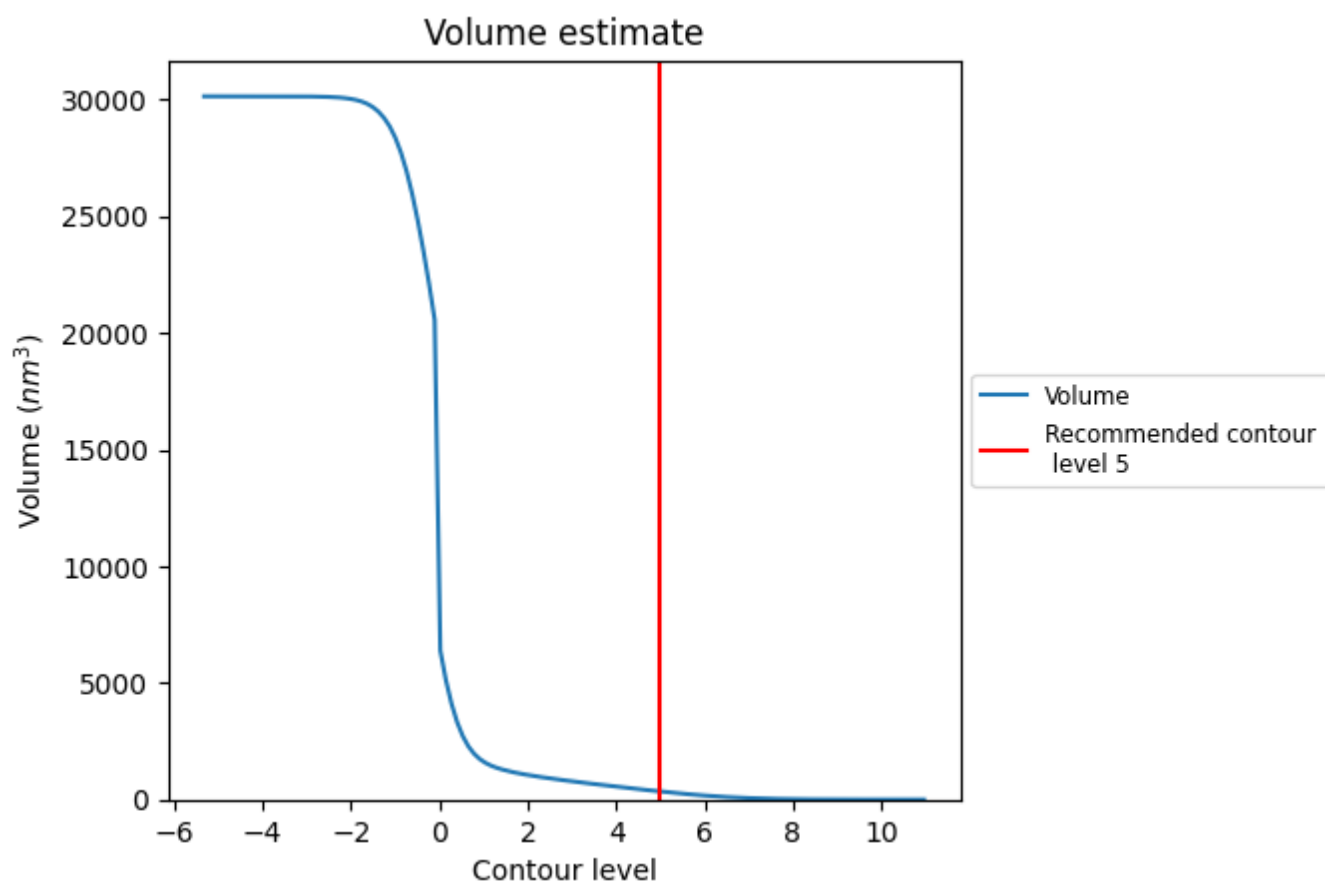
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

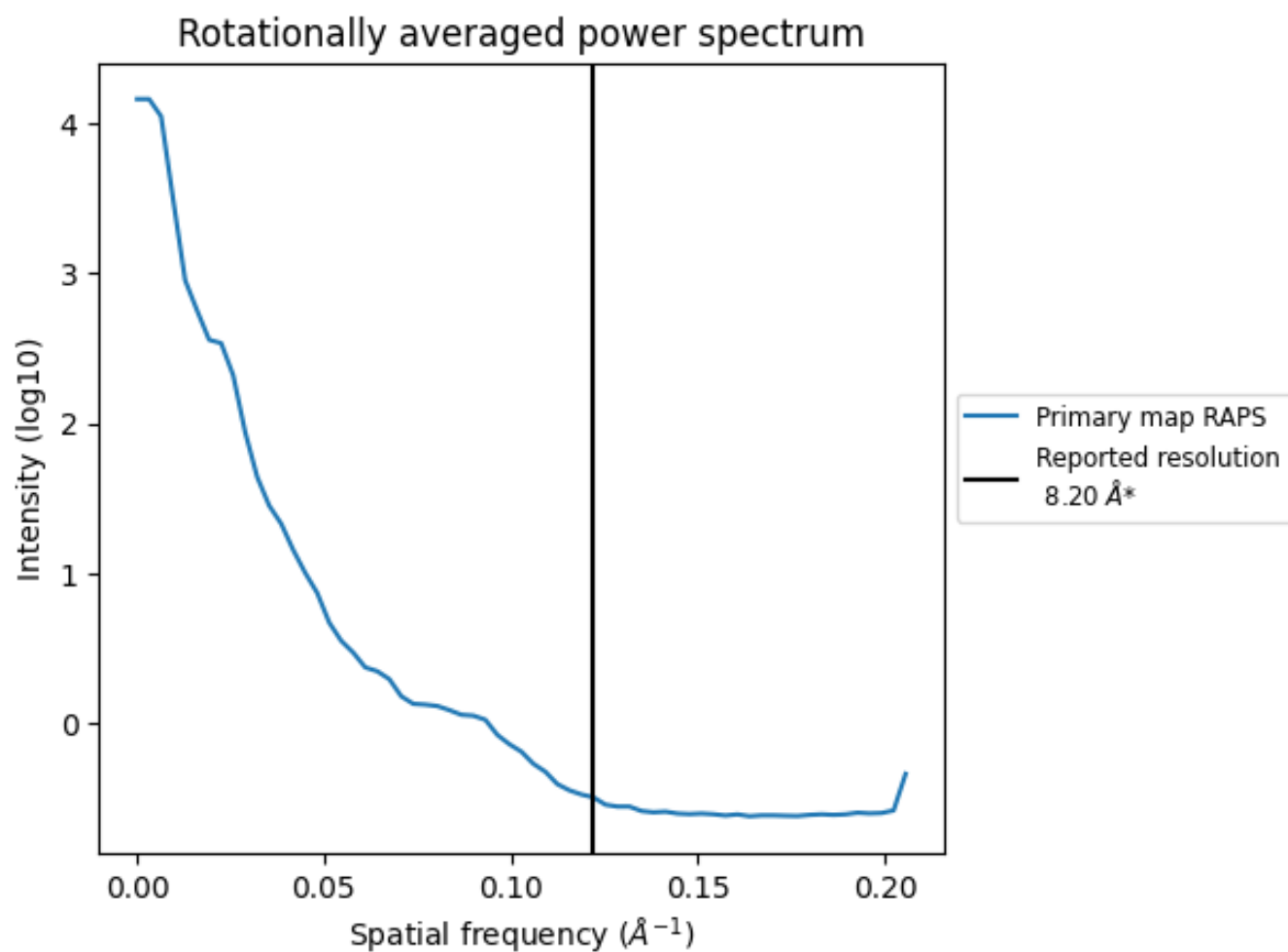
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 346 nm³; this corresponds to an approximate mass of 313 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.122 Å⁻¹

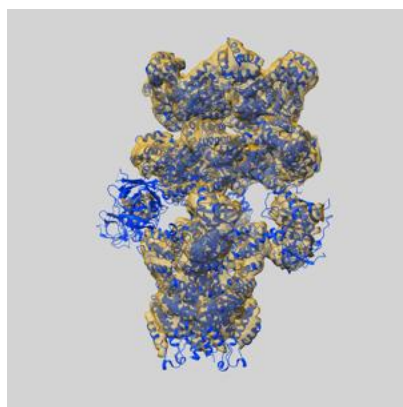
8 Fourier-Shell correlation

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

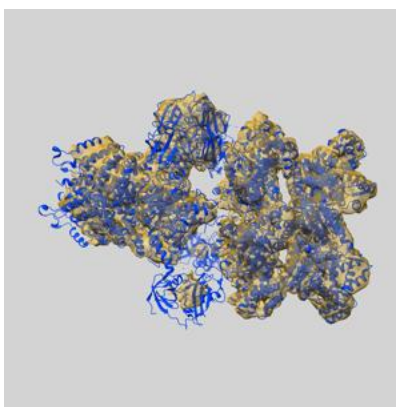
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6209 and PDB model 3J99. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

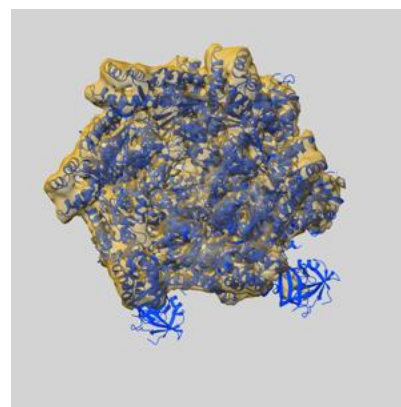
9.1 Map-model overlay [i](#)



X



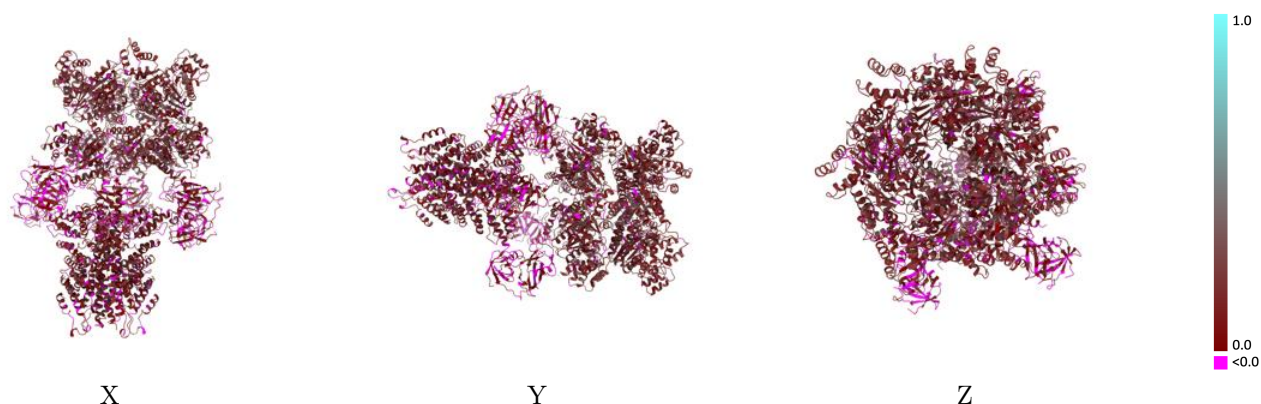
Y



Z

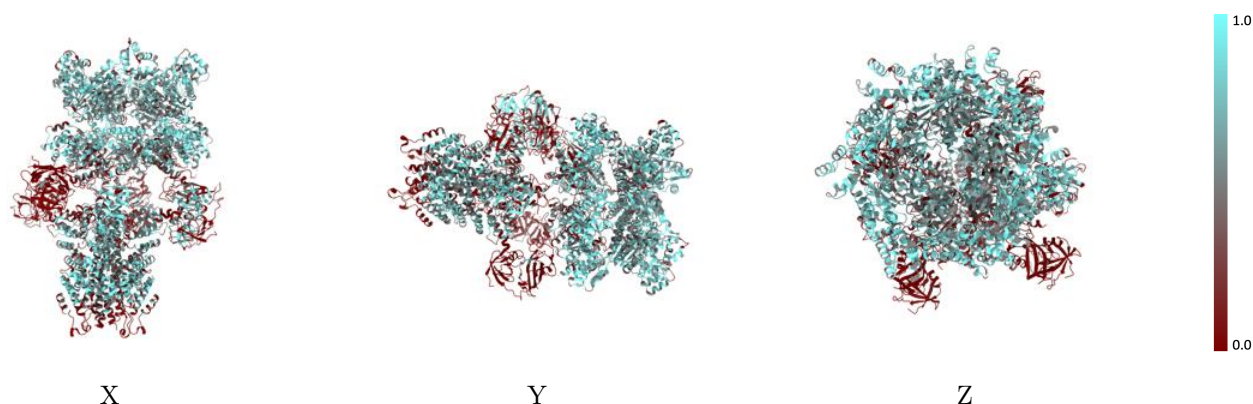
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



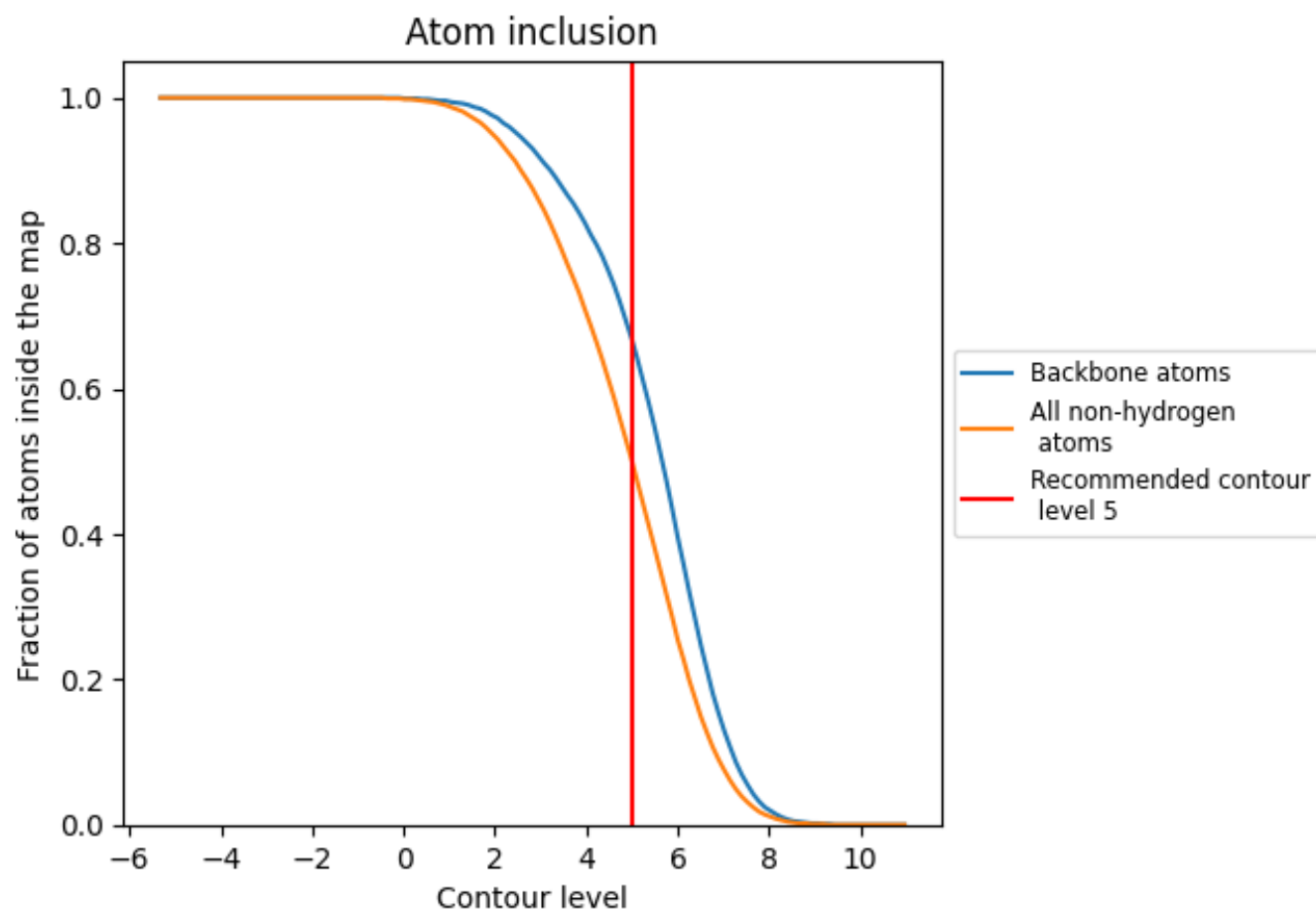
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5000	0.1330
A	0.4580	0.1250
B	0.5980	0.1550
C	0.5120	0.1420
D	0.6030	0.1590
E	0.4490	0.1270
F	0.4060	0.1150
G	0.4300	0.1110
H	0.4870	0.1190
I	0.5260	0.1270
J	0.5350	0.1230
K	0.4870	0.1240
L	0.4870	0.1580
M	0.4190	0.1200

