



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 11:15 PM UTC

PDB ID : 5LCW / pdb_00005lcw
EMDB ID : EMD-4037
Title : Cryo-EM structure of the Anaphase-promoting complex/Cyclosome, in complex with the Mitotic checkpoint complex (APC/C-MCC) at 4.2 angstrom resolution
Authors : Alfieri, C.; Chang, L.; Zhang, Z.; Yang, J.; Maslen, S.; Skehel, M.; Barford, D.
Deposited on : 2016-06-22
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

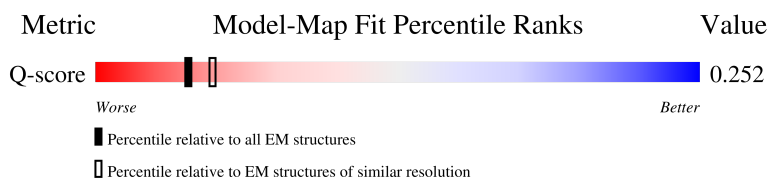
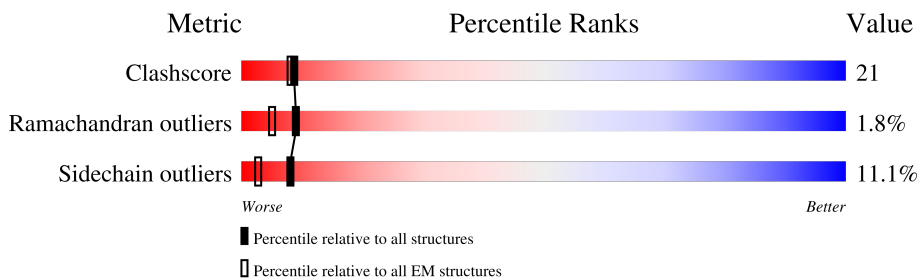
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	5410 (3.70 - 4.70)

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	1944	
2	B	84	
3	C	597	
3	P	597	

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Mol	Chain	Length	Quality of chain
4	D	121	
5	E	110	
6	F	824	
6	H	824	
7	G	85	
7	W	85	
8	I	808	
9	J	620	
9	K	620	
10	L	185	
11	M	74	
12	N	822	
13	O	755	
14	Q	374	
15	R	499	
16	S	342	
17	X	599	
17	Y	599	
18	Z	205	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 72075 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 Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1441	Total	C	N	O	S	0	0
			10949	7039	1853	1983	74		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	PHE	PRO	conflict	UNP Q9H1A4

- Molecule 2 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	79	Total	C	N	O	S	0	0
			643	411	116	100	16		

- Molecule 3 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	524	Total	C	N	O	S	0	0
			4306	2774	727	781	24		
3	P	491	Total	C	N	O	S	0	0
			4043	2611	679	729	24		

- Molecule 4 is a protein called Anaphase-promoting complex subunit 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	18	Total	C	N	O	0	0
			153	104	23	26		

- Molecule 5 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	56	Total	C	N	O	S	0	0
			450	290	74	85	1		

- Molecule 6 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	483	Total	C	N	O	S	0	0
			3849	2470	649	704	26		
6	H	483	Total	C	N	O	S	0	0
			3853	2473	650	704	26		

- Molecule 7 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	25	Total	C	N	O	S	0	0
			213	133	40	39	1		
7	W	25	Total	C	N	O	S	0	0
			213	133	40	39	1		

- Molecule 8 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	733	Total	C	N	O	S	0	0
			5716	3665	951	1067	33		

- Molecule 9 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	504	Total	C	N	O	S	0	0
			4047	2601	684	737	25		
9	K	493	Total	C	N	O	S	0	0
			3988	2563	672	729	24		

- Molecule 10 is a protein called Anaphase-promoting complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	182	Total	C	N	O	S	0	0
			1435	898	263	268	6		

- Molecule 11 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	59	Total	C	N	O	S	0	0
			493	310	79	102	2		

- Molecule 12 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	703	Total	C	N	O	S	0	0
			5403	3436	971	971	25		

- Molecule 13 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	685	Total	C	N	O	S	0	0
			5402	3446	940	988	28		

- Molecule 14 is a protein called Cell division cycle protein 20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	354	Total	C	N	O	S	0	0
			2671	1676	488	496	11		

- Molecule 15 is a protein called Cell division cycle protein 20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	383	Total	C	N	O	S	0	0
			2953	1855	538	548	12		

- Molecule 16 is a protein called Mitotic checkpoint serine/threonine-protein kinase BUB1 beta,Mitotic checkpoint serine/threonine-protein kinase BUB1 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	277	Total	C	N	O	S	0	0
			2077	1292	380	400	5		

- Molecule 17 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	484	Total	C	N	O	S	0	0
			3773	2393	652	704	24		
17	Y	496	Total	C	N	O	S	0	0
			3868	2449	669	724	26		

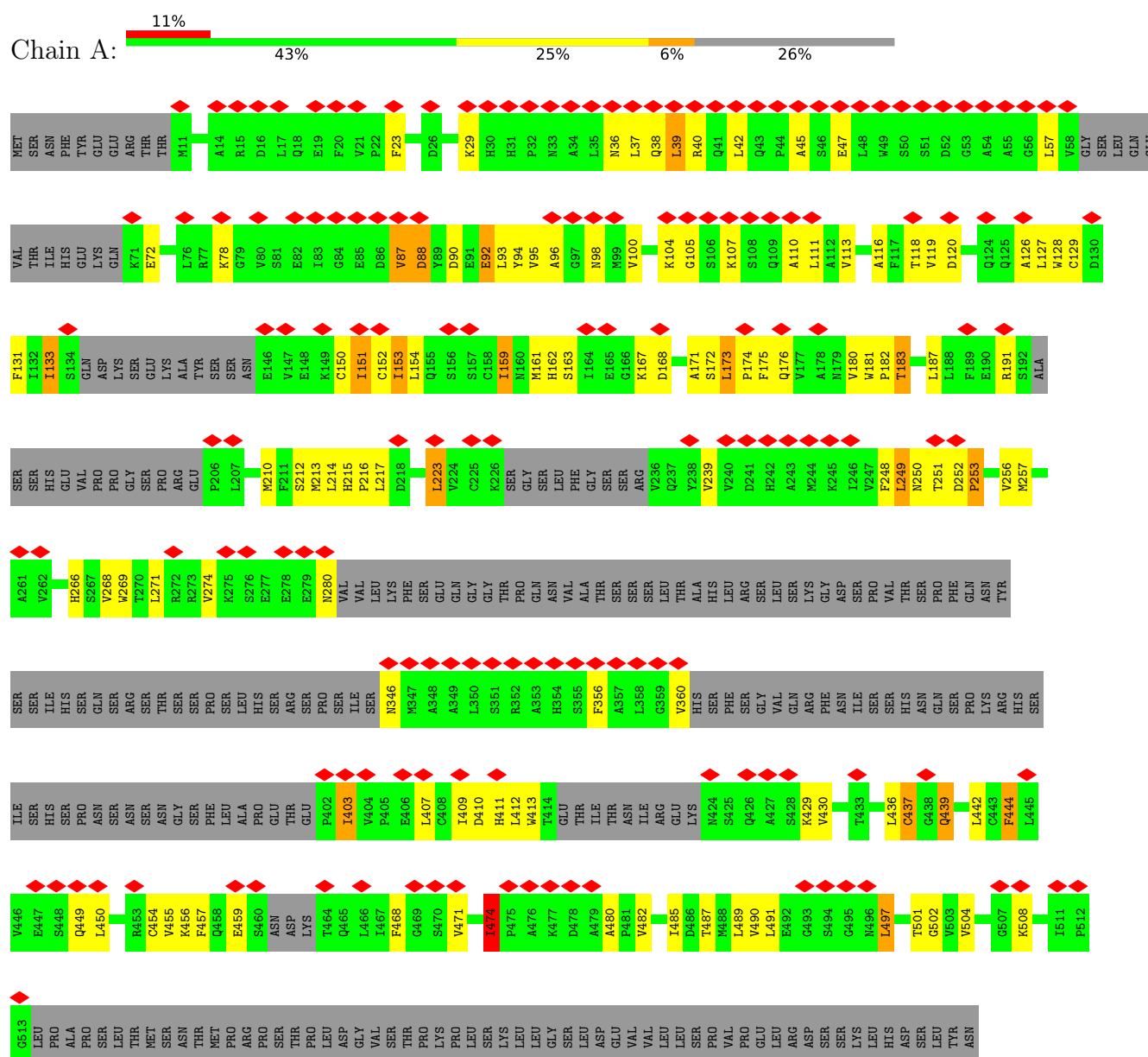
- Molecule 18 is a protein called Mitotic spindle assembly checkpoint protein MAD2A.

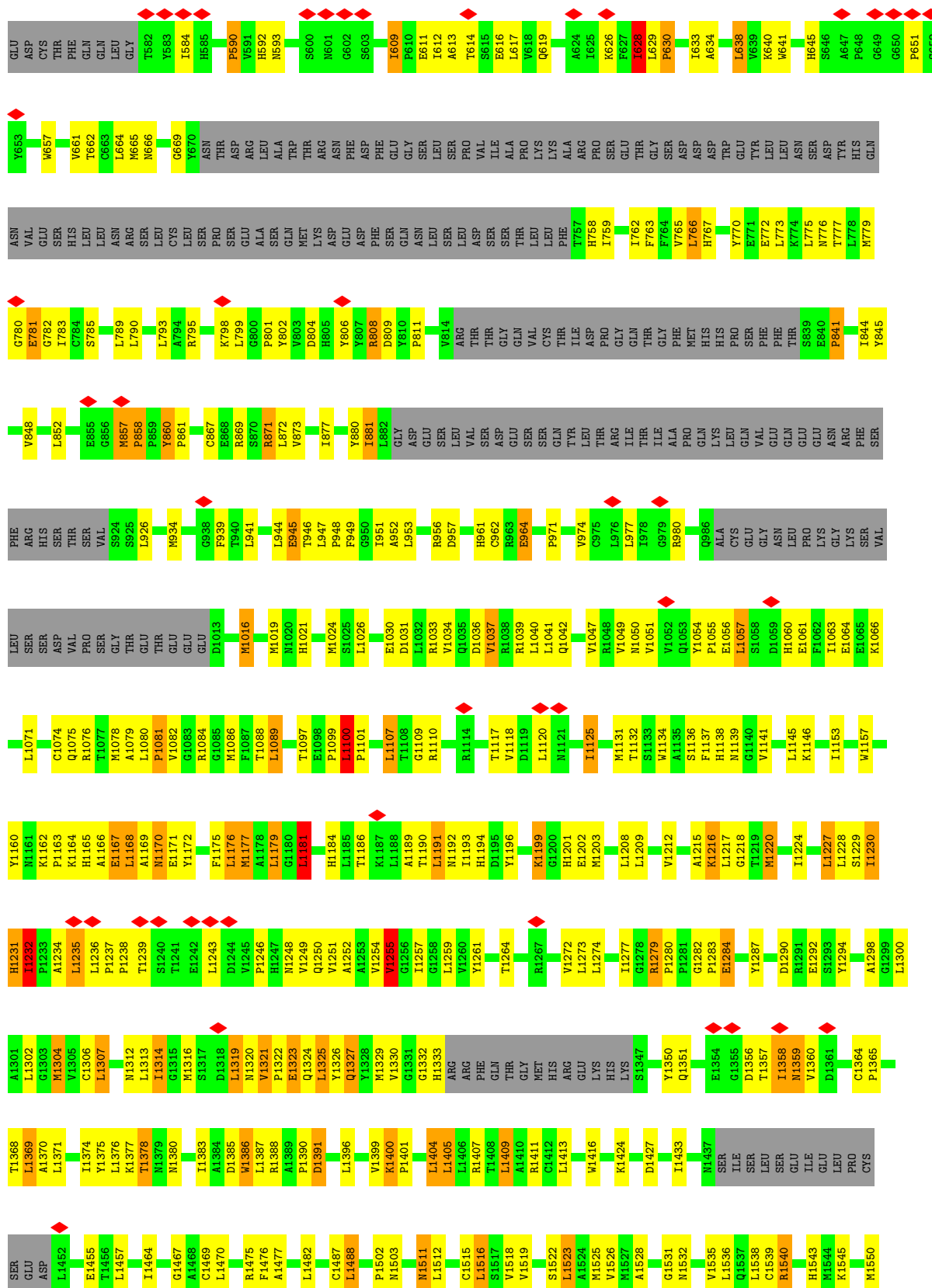
Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	195	Total	C	N	O	S	0	0
			1577	1012	256	305	4		

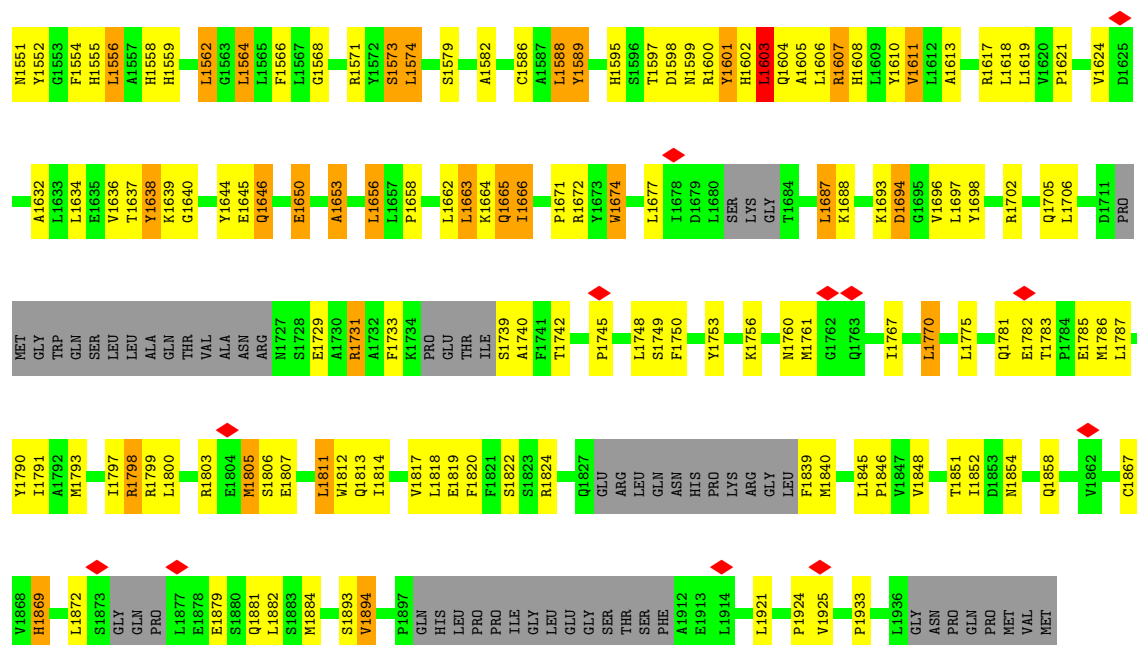
3 Residue-property plots

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.

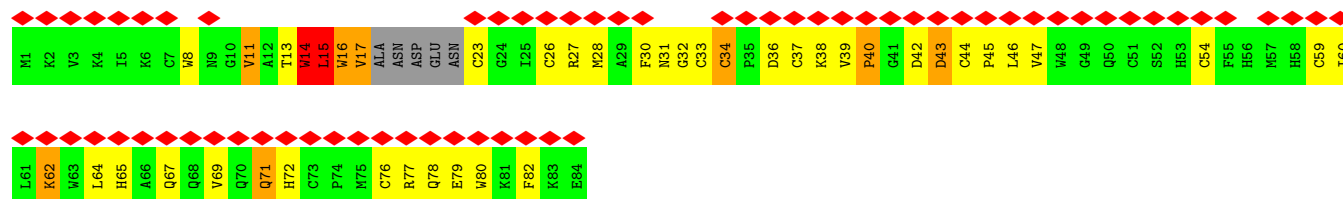
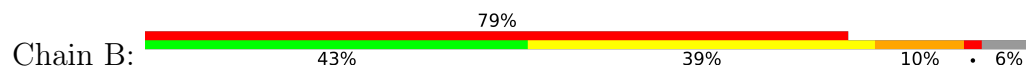
• Molecule 1: Anaphase-promoting complex subunit 1



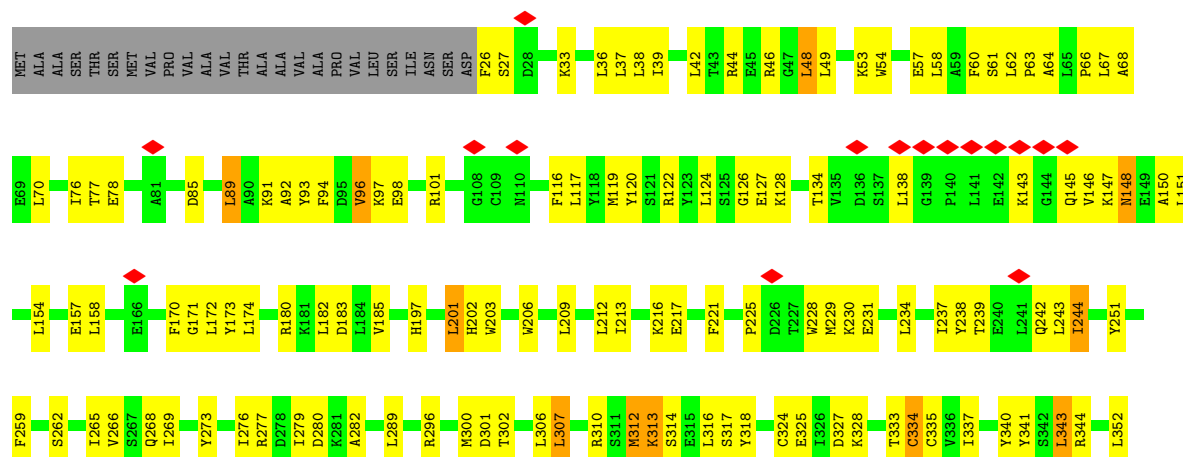


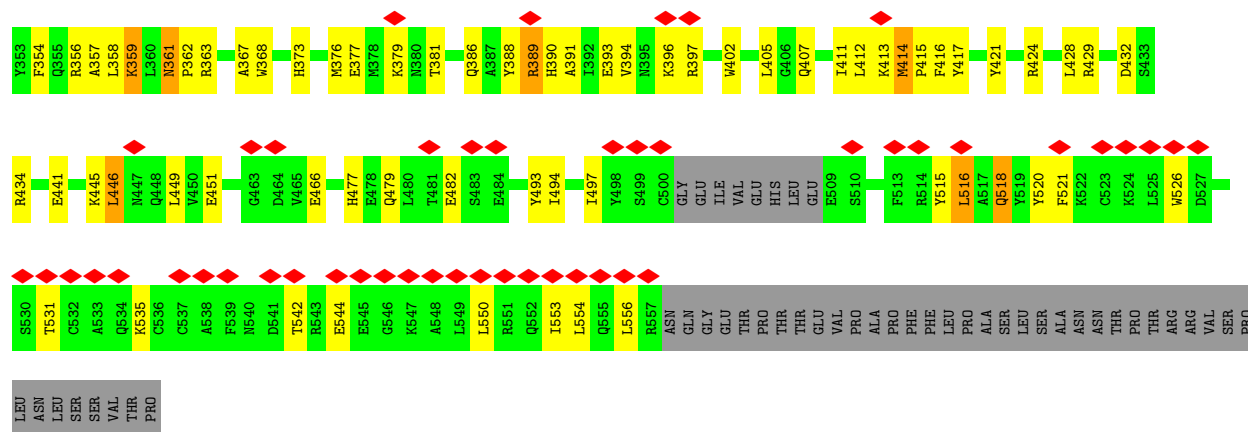


• Molecule 2: Anaphase-promoting complex subunit 11

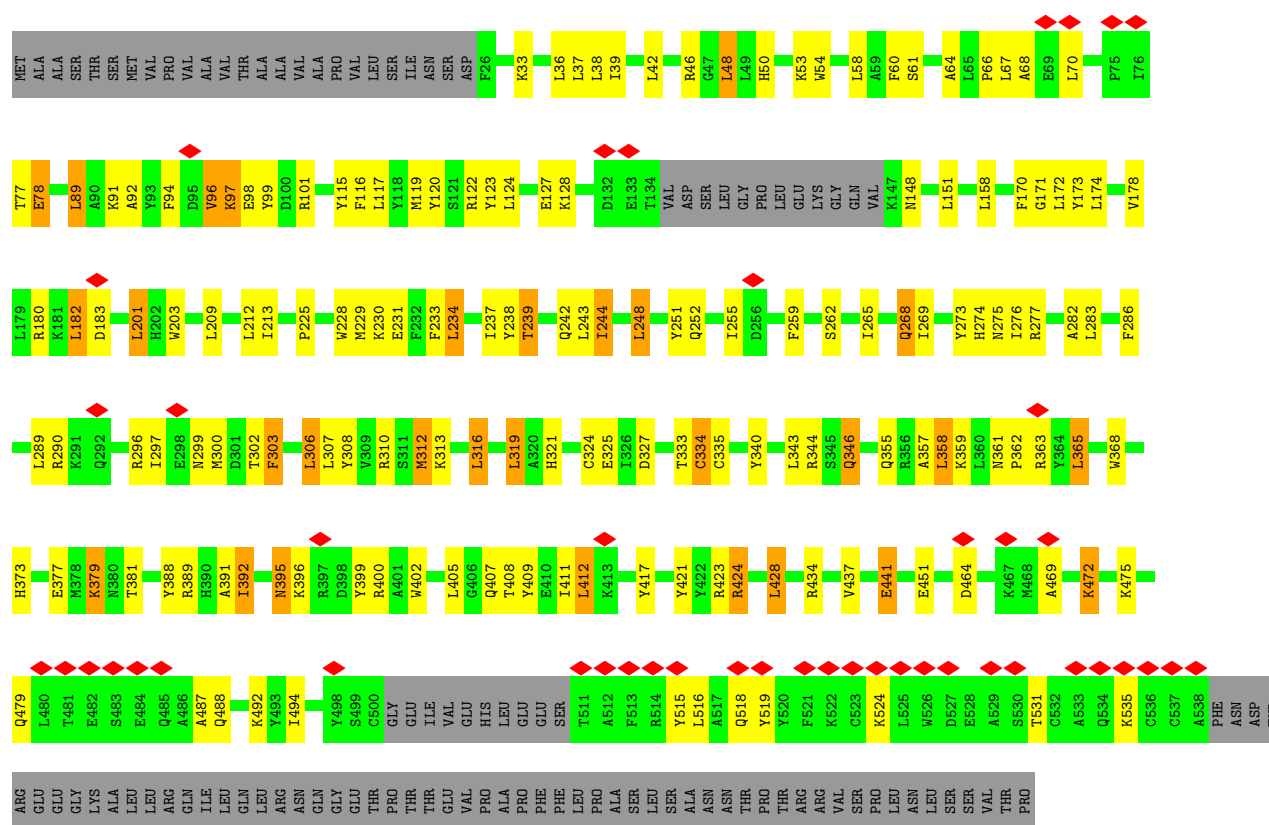


• Molecule 3: Cell division cycle protein 23 homolog

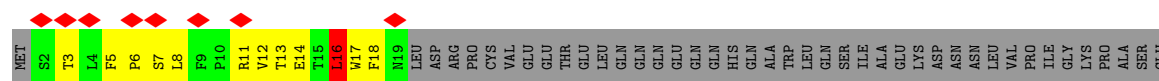




• Molecule 3: Cell division cycle protein 23 homolog



• Molecule 4: Anaphase-promoting complex subunit 15



- Molecule 5: Anaphase-promoting complex subunit 16

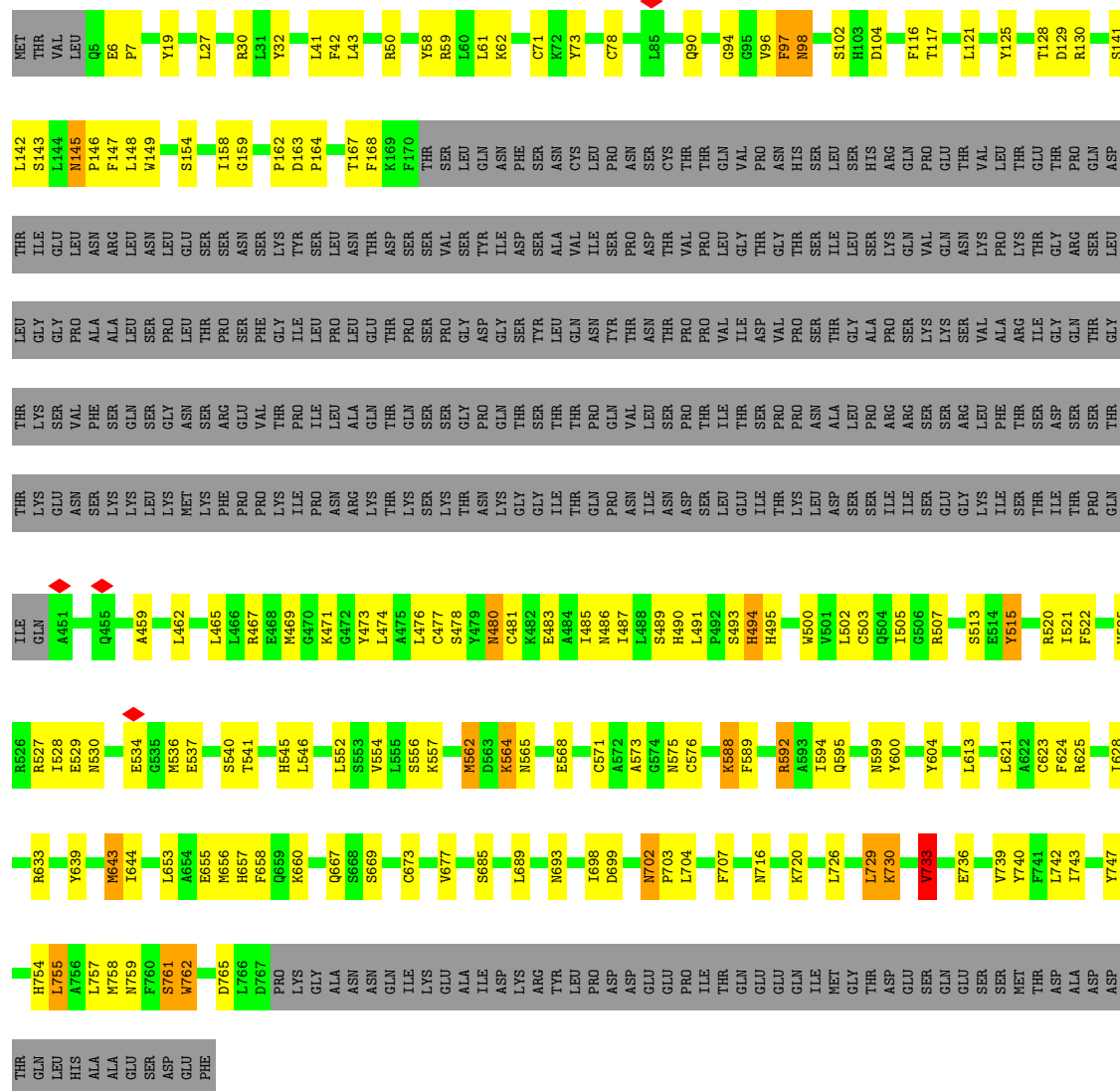
Sequence logo for the 100th position of the protein. The y-axis represents information content in bits, ranging from 0 to 0.62. The x-axis shows amino acids: MET, ALA, SER, VAL, GLY, THR, PHE, VAL, ASP, LEU, PRO, ARG, LYS, LEU, PHE, THR, PRO, LYS, GLY, ALA, GLY, MET, LEU, GLU, ASP, GLY, SER, GLU, and RG2. The 'RG2' label is highlighted in red. A red diamond is placed above the 'E90' label, which is also highlighted in red. The 'RG2' label is also highlighted in red. The 'E90' label is also highlighted in red. The 'RG2' label is also highlighted in red.

K720	Y600	B507	LEU	ASN	SER	SER	THR	T117	MET
S721	A601	L512	ASP	ALA	THR	ILE	LEU	L118	THR
L726	Y602	L512	SER	LEU	GLY	LEU	SER	L121	VAL
L729	A603	R520	SER	PRO	ALA	SER	HIS	L121	LEU
K730	T605	I521	ILE	ARG	PRO	LYS	ARG	Y125	Q5
	L606	F522	ILE	ARG	SER	GLN	GLN	Y125	E6
			SER	SER	VAL	VAL	PRO		P7
	V612	V525	GLU	SER	LYS	GLN	GLU	D129	
P734	L613	R526	GLY	ARG	ASN	ASN	THR	R130	A15
K735	T614	R527	LYS	LEU	VAL	LYS	VAL	L131	Y19
	E615	I528	ILE	PHE	ALA	PRO	LEU	A132	
V739	E616	F529	SER	THR	ALA	LYS	THR	K133	
Y740		N530	THR	SER	ILE	THR	GLU	G134	R22
F741	L621		ILE	ASP	GLY	GLY	THR	S135	
L742		V533	THR	SER	GLN	ARG	PRO	E136	F26
I743	G623	E534	PRO	SER	GLN	LEU	GLN	C137	L27
F624	R625	M536	ILE	THR	GLY	SER	ASP		
K748		G535	GLN	THR	LYS	GLY	THR	S141	R30
		E537	GLN	GLU	SER	GLY	GLU	L142	L31
I628	I628	I538	A451	ASN	VAL	PRO	LEU	S143	Y32
L755		F539	Q455	SER	PHE	ALA	ASN	L144	
A756	Y639	S540	K456	LYS	ALA	ARG	ARG	R145	L41
L757	T541	T541	A457	LYS	GLN	LEU	LEU	F147	F42
			A458	LEU	SER	SER	ASN	L148	L43
W643	M643		A459	LYS	GLY	PRO	LEU		L44
I644		W544	E460	MET	ASN	LEU	GLU	F152	A45
			L461	LYS	SER	THR	SER		R50
L653		D549	G461	PHE	GLU	PRO	SER	E160	
A654	E655	V550	O462	THR	VAL	SER	ASN	K161	Y58
M656		A551		PRO	GLU	PHE	SER	P162	R59
			L465	LYS	THR	GLY	LYS	D163	L60
	V554		L466	ILE	THR	ILE	TVR	P164	L61
I664	L555		A467	LYS	THR	LEU	SER	D165	K62
R665	S556		E468	PRO	ILE	LEU	LEU	Q166	
P666			M469	ASN	LEU	PRO	LEU		T67
Q667		L559	G470	ARG	ALA	LEU	ASN	T167	
			K471	LYS	GLN	GLU	THR	F168	
	T560			THR	GLN	THR	ASP	K169	Q70
C673	D561		L476	LYS	GLN	PRO	SER	F170	C71
	O562		C477	SER	SER	SER	SER	THR	K72
V677	D563			LYS	SER	PRO	VAL	SER	Y73
L689	K564		M480	THR	GLY	GLY	SER	LEU	K74
	N565		C481	ASN	PRO	ASP	TYR	GLN	L75
			L482	LYS	GLN	GLY	ILE	ASN	L76
N653	E568		E483	GLY	THR	THR	ASP	PHE	C78
				ILE	SER	TYR	SER	SER	
I686	C571		I487	ILE	THR	LEU	ALA	ASN	
V697	A572			THR	THR	GLN	VAL	CYS	E87
I698	A573		L491	GLN	PRO	ASN	ILE	LEU	G88
D699	G574		P492	PRO	GLN	TYR	SER	PRO	E89
ASP	N575		S493	ASN	VAL	THR	PRO	ASN	Q90
ASP	C576		H494	ILE	LEU	ASN	ASP	SER	I91
K701	F577		H495	ASN	THR	THR	THR	CYS	
N702	S578			ASP	SER	PRO	VAL		G95
GLU	F577			ASP	THR	PRO	VAL		
GLU				SER	THR	PRO	PRO	THR	V96
P703			W500	LEU	ILE	VAL	LEU	GLN	N98
L704	K588		V501	GLU	ILE	ILE	GLY	VAL	F97
P705			L502	LEU	THR	ASP	THR	GLY	
THR				ILE					

MET GLY THR ASP GLU SER GLN GLU SER MET MET THR ASP ALA ASP ASP THR GLN LEU HIS ALA ALA GLU SER SER ASP GLU PHE

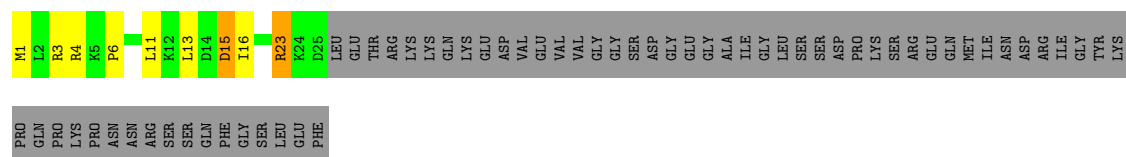
• Molecule 6: Cell division cycle protein 27 homolog

Chain H: 39% 17% . 41%



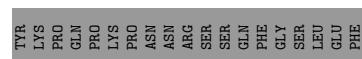
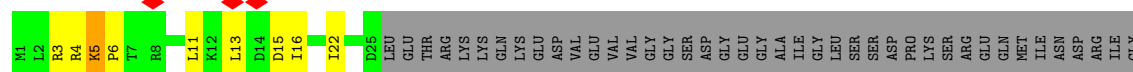
• Molecule 7: Anaphase-promoting complex subunit CDC26

Chain G: 19% 8% . 71%



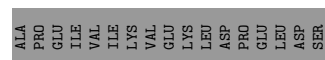
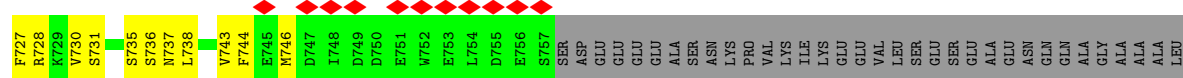
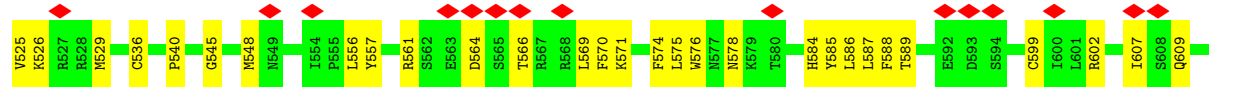
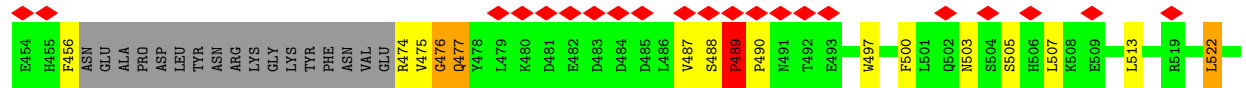
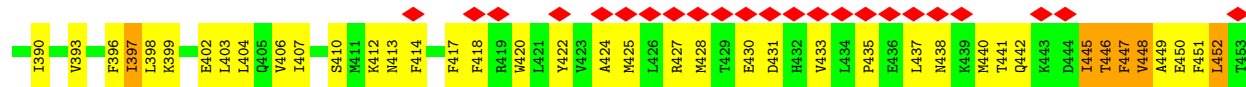
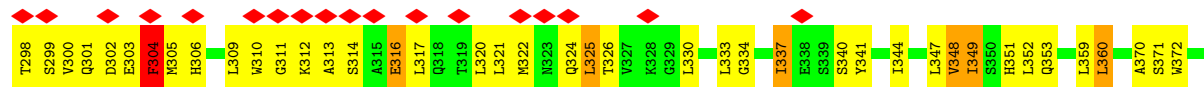
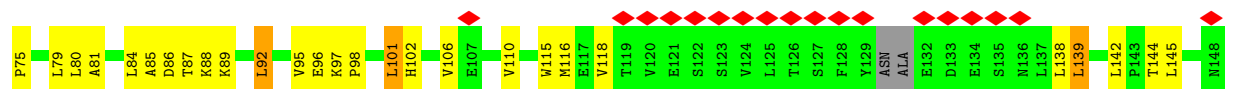
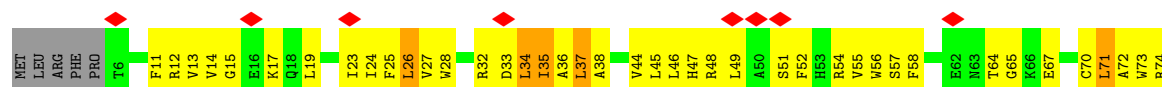
• Molecule 7: Anaphase-promoting complex subunit CDC26

Chain W:  19% 9% 71%

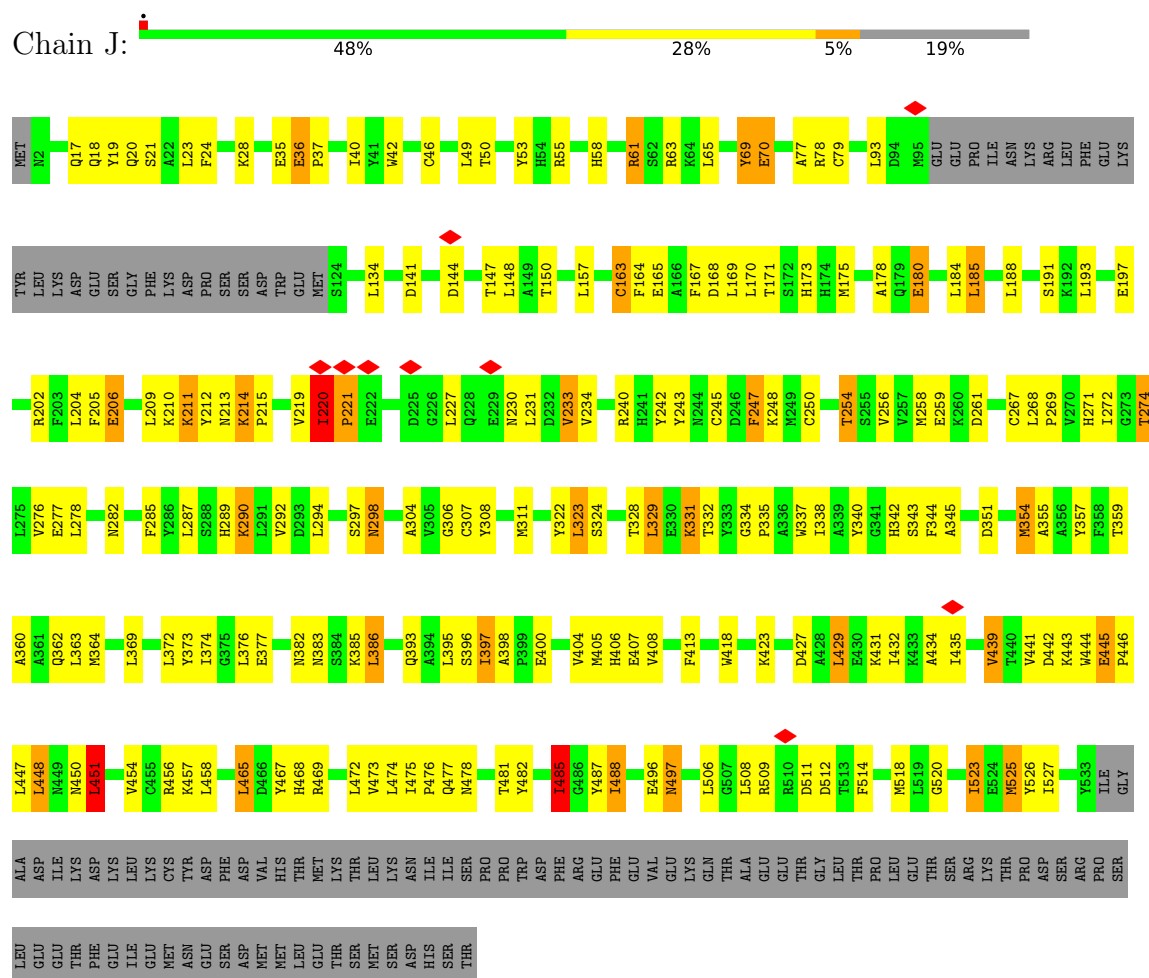


• Molecule 8: Anaphase-promoting complex subunit 4

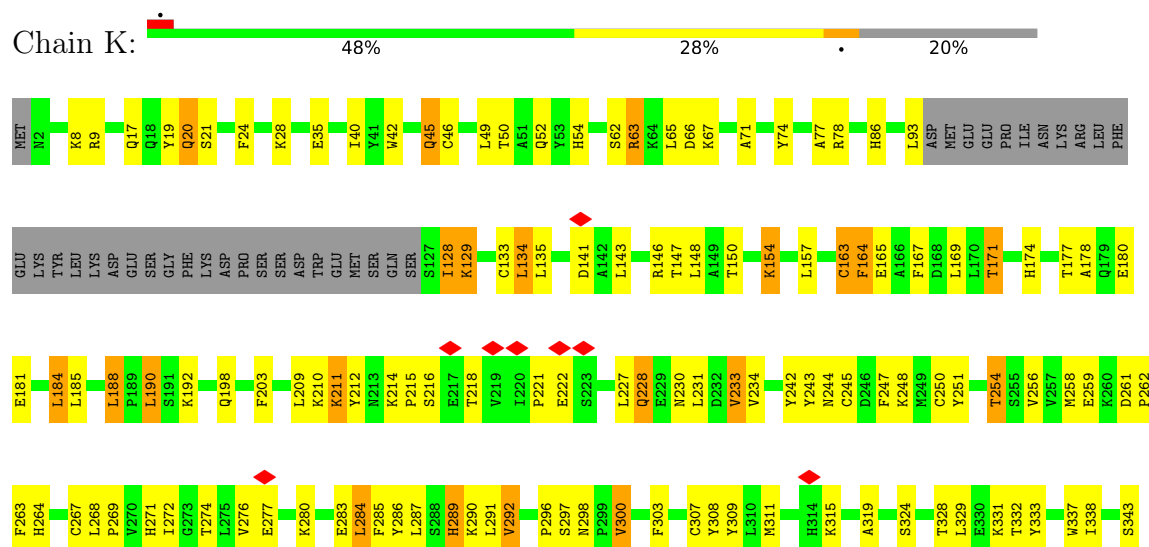
Chain I:  19% 53% 33% 9%

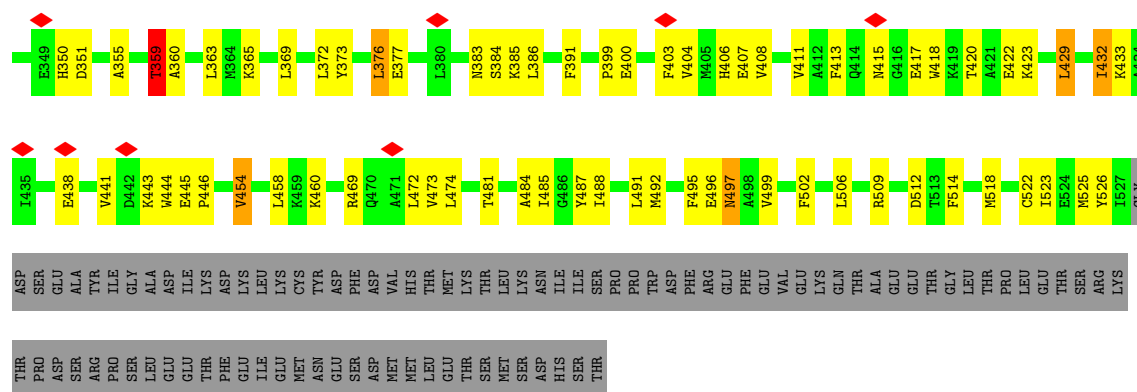


• Molecule 9: Cell division cycle protein 16 homolog

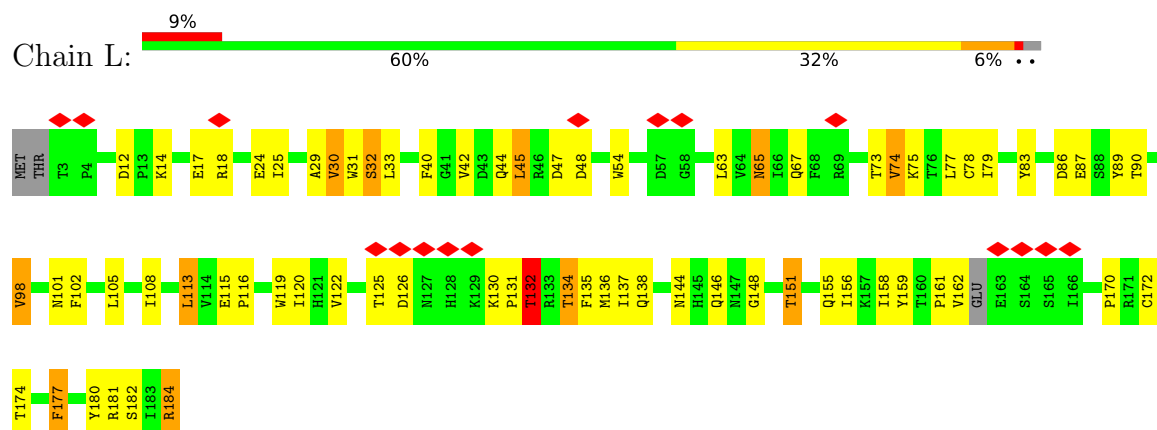


• Molecule 9: Cell division cycle protein 16 homolog

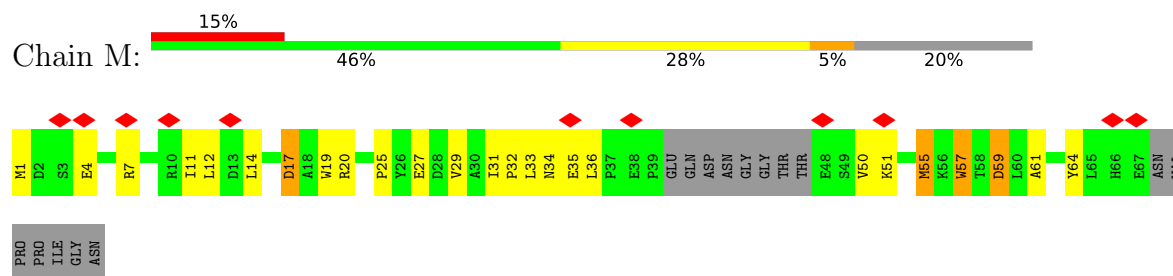




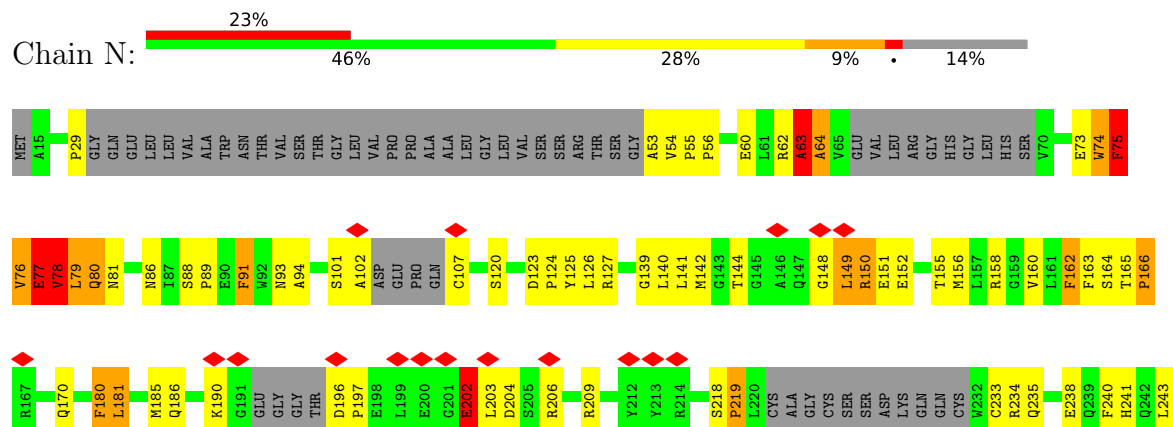
- Molecule 10: Anaphase-promoting complex subunit 10

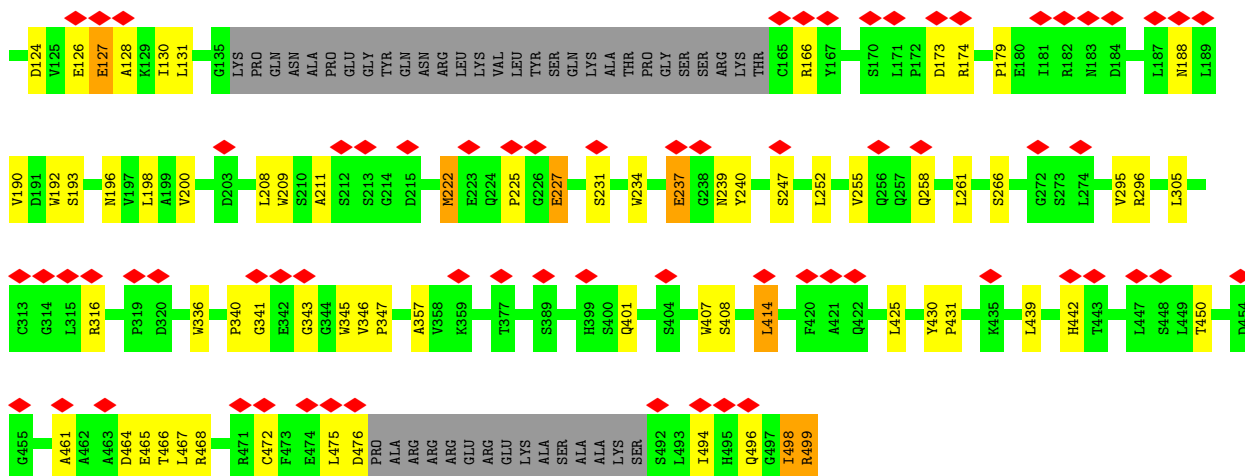


- Molecule 11: Anaphase-promoting complex subunit 13

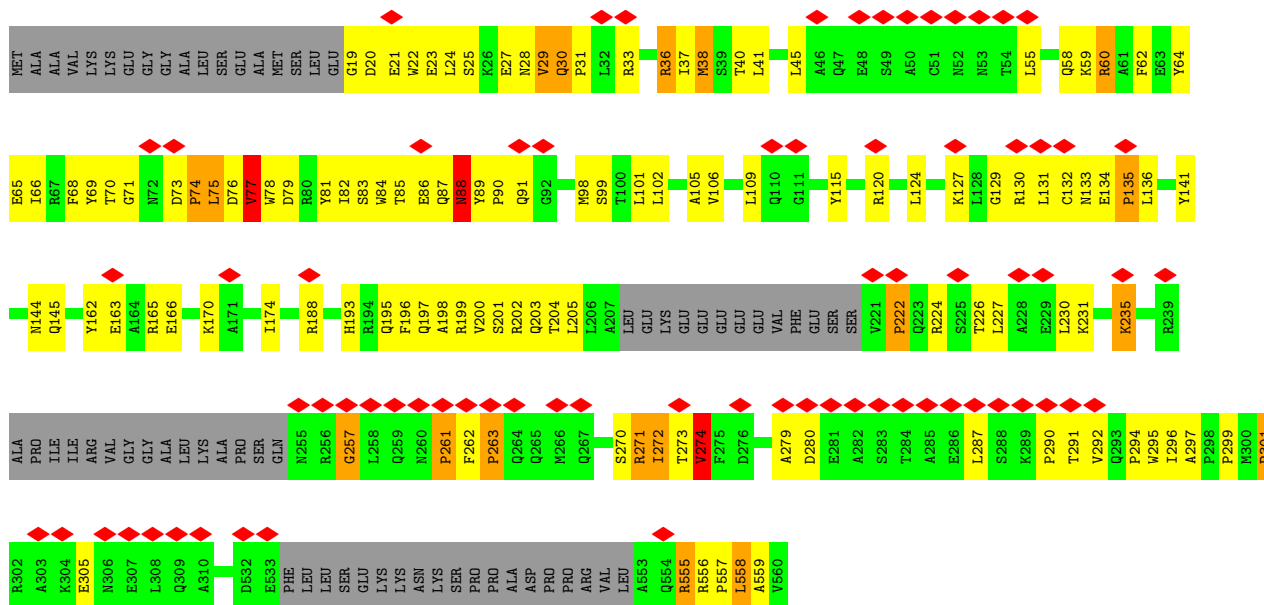
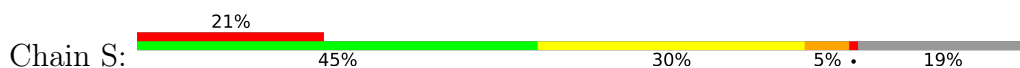


- Molecule 12: Anaphase-promoting complex subunit 2

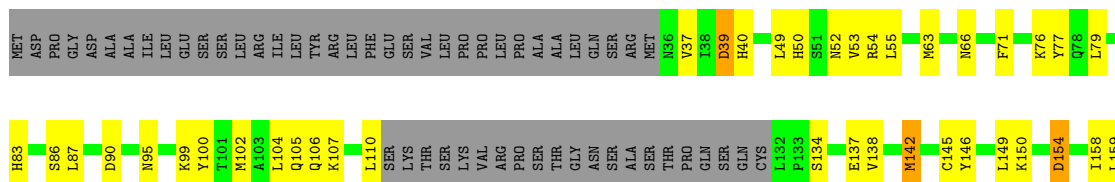


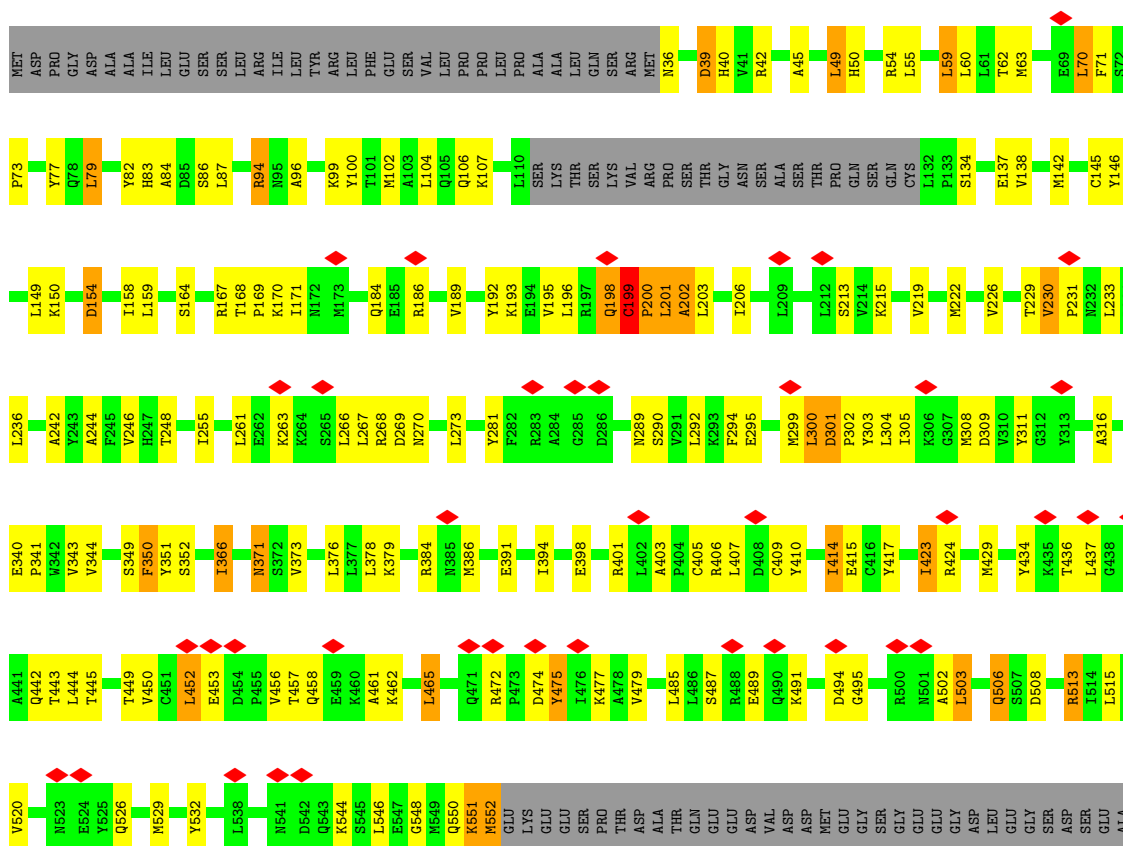


- Molecule 16: Mitotic checkpoint serine/threonine-protein kinase BUB1 beta, Mitotic checkpoint serine/threonine-protein kinase BUB1 beta



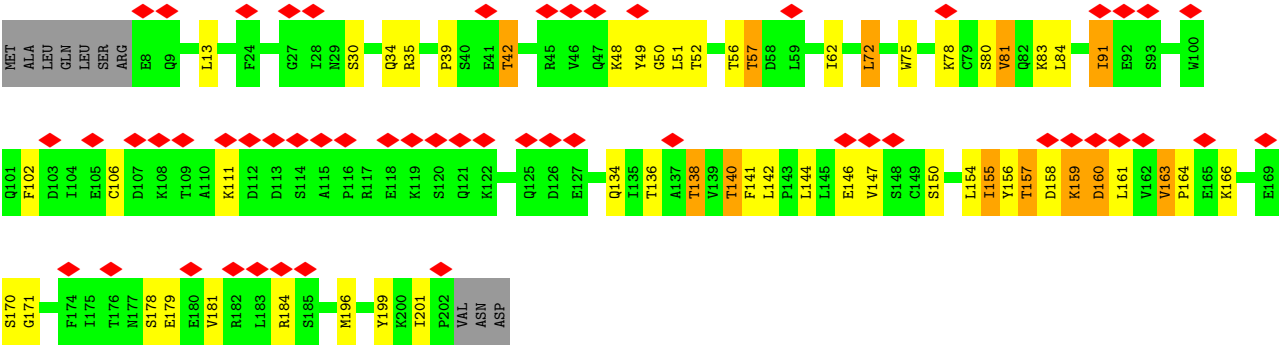
- Molecule 17: Anaphase-promoting complex subunit 7





GLN
TRP
ALA
ASP
GLN
GLU
GLN
TRP
PHE
GLY
MET
GLN

● Molecule 18: Mitotic spindle assembly checkpoint protein MAD2A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155263	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.292	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	359.04, 359.04, 359.04	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.36, 1.36, 1.36	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	0.87	5/11190 (0.0%)	1.29	43/15236 (0.3%)
2	B	0.96	0/665	1.23	1/896 (0.1%)
3	C	0.73	0/4404	1.18	2/5945 (0.0%)
3	P	0.79	0/4138	1.20	1/5587 (0.0%)
4	D	0.93	0/159	1.23	2/218 (0.9%)
5	E	0.76	0/459	1.19	0/619
6	F	0.72	1/3939 (0.0%)	1.26	6/5325 (0.1%)
6	H	0.75	2/3943 (0.1%)	1.27	9/5329 (0.2%)
7	G	0.87	0/214	1.25	0/284
7	W	0.92	0/214	1.26	0/284
8	I	0.89	3/5834 (0.1%)	1.28	22/7909 (0.3%)
9	J	0.97	2/4146 (0.0%)	1.27	16/5616 (0.3%)
9	K	1.00	2/4086 (0.0%)	1.22	9/5534 (0.2%)
10	L	0.77	0/1468	1.18	4/1993 (0.2%)
11	M	0.82	1/502 (0.2%)	1.21	0/680
12	N	0.88	6/5495 (0.1%)	1.39	50/7441 (0.7%)
13	O	0.81	2/5501 (0.0%)	1.26	6/7432 (0.1%)
14	Q	0.98	0/2737	1.10	8/3732 (0.2%)
15	R	1.00	2/3029 (0.1%)	1.10	9/4124 (0.2%)
16	S	0.86	2/2112 (0.1%)	1.24	22/2863 (0.8%)
17	X	0.79	1/3833 (0.0%)	1.24	9/5187 (0.2%)
17	Y	0.80	0/3928	1.25	7/5311 (0.1%)
18	Z	0.87	0/1605	1.14	6/2176 (0.3%)
All	All	0.86	29/73601 (0.0%)	1.25	232/99721 (0.2%)

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	1
8	I	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	J	0	1
12	N	0	16
16	S	0	1
All	All	0	21

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1030	GLU	CD-OE1	12.86	1.49	1.25
12	N	209	ARG	NE-CZ	11.41	1.45	1.33
1	A	1030	GLU	CD-OE2	9.20	1.42	1.25
1	A	1199	LYS	CE-NZ	8.16	1.73	1.49
1	A	795	ARG	NE-CZ	8.06	1.42	1.33
12	N	330	ARG	CZ-NH2	-6.70	1.24	1.33
8	I	97	LYS	CA-C	-6.43	1.47	1.52
12	N	368	THR	CA-C	6.34	1.61	1.52
12	N	330	ARG	CD-NE	6.29	1.55	1.46
9	K	291	LEU	CA-C	-6.19	1.44	1.52
8	I	489	PRO	CA-C	6.10	1.57	1.52
9	J	261	ASP	N-CA	5.89	1.52	1.46
17	X	142	MET	CA-C	-5.75	1.45	1.52
15	R	79	TYR	CA-C	5.68	1.60	1.52
8	I	187	LEU	CA-C	-5.66	1.45	1.52
13	O	752	ILE	CA-CB	5.59	1.60	1.54
6	F	6	GLU	N-CA	5.54	1.50	1.46
11	M	57	TRP	CA-C	-5.37	1.46	1.52
12	N	323	ARG	NE-CZ	5.34	1.39	1.33
6	H	6	GLU	N-CA	5.34	1.50	1.46
15	R	200	VAL	C-O	-5.32	1.18	1.24
9	K	319	ALA	CA-C	-5.28	1.46	1.52
13	O	732	ARG	NE-CZ	5.23	1.38	1.33
12	N	602	PRO	CA-C	5.21	1.57	1.52
1	A	628	ILE	N-CA	5.18	1.52	1.46
6	H	730	LYS	CE-NZ	5.08	1.64	1.49
16	S	231	LYS	CA-C	5.07	1.55	1.52
16	S	60	ARG	NE-CZ	5.06	1.38	1.33
9	J	274	THR	C-O	-5.02	1.18	1.24

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	220	ILE	CA-C-N	13.48	136.70	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	220	ILE	C-N-CA	13.48	136.70	119.84
12	N	496	ARG	N-CA-C	12.00	127.80	111.24
6	H	534	GLU	N-CA-C	9.72	121.47	111.07
6	F	534	GLU	N-CA-C	9.62	121.36	111.07
14	Q	141	PRO	N-CA-CB	9.53	113.25	103.25
8	I	489	PRO	N-CA-C	9.52	122.31	110.70
3	P	96	VAL	N-CA-C	9.49	120.30	110.72
1	A	651	PRO	N-CA-CB	9.37	109.70	101.83
1	A	1589	TYR	CA-C-N	9.27	128.88	119.24
1	A	1589	TYR	C-N-CA	9.27	128.88	119.24
16	S	287	LEU	N-CA-C	9.24	121.43	111.36
16	S	38	MET	CB-CA-C	-9.22	96.26	110.92
3	C	96	VAL	N-CA-C	9.20	120.01	110.72
1	A	1107	LEU	N-CA-C	-8.50	97.90	109.54
8	I	435	PRO	N-CA-CB	8.47	111.22	103.34
12	N	355	ARG	CA-C-N	-8.46	110.90	120.04
12	N	355	ARG	C-N-CA	-8.46	110.90	120.04
18	Z	178	SER	N-CA-C	8.40	122.18	109.41
12	N	395	ASP	N-CA-C	8.38	128.65	110.80
12	N	489	PRO	N-CA-CB	8.32	111.98	103.25
12	N	477	PRO	N-CA-CB	8.26	111.92	103.25
12	N	63	ALA	CA-C-N	8.24	136.54	121.70
12	N	63	ALA	C-N-CA	8.24	136.54	121.70
9	J	211	LYS	N-CA-C	-8.23	97.83	109.69
12	N	63	ALA	N-CA-C	8.17	128.21	110.80
1	A	628	ILE	N-CA-C	8.17	118.26	110.42
12	N	56	PRO	N-CA-CB	8.11	112.25	103.33
1	A	1733	PHE	N-CA-C	7.94	118.46	108.45
16	S	75	LEU	N-CA-C	7.94	119.56	111.07
16	S	557	PRO	N-CA-CB	7.82	110.13	103.25
14	Q	477	PRO	N-CA-CB	7.80	111.44	103.25
8	I	488	SER	CA-C-N	7.80	128.41	120.38
8	I	488	SER	C-N-CA	7.80	128.41	120.38
12	N	125	TYR	CA-C-N	7.68	135.53	121.70
12	N	125	TYR	C-N-CA	7.68	135.53	121.70
13	O	557	MET	N-CA-C	7.66	121.11	111.69
1	A	1653	ALA	N-CA-C	7.62	122.56	112.35
1	A	413	TRP	N-CA-C	7.50	120.86	109.23
16	S	222	PRO	N-CA-CB	7.36	110.98	103.25
17	Y	199	CYS	N-CA-C	7.34	126.03	109.81
12	N	125	TYR	N-CA-C	7.33	118.96	110.97
9	J	247	PHE	N-CA-C	7.31	119.25	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	657	VAL	N-CA-C	7.31	120.07	112.83
12	N	602	PRO	N-CA-C	7.29	119.59	110.70
8	I	223	VAL	CB-CA-C	-7.25	99.82	110.62
6	H	733	VAL	CA-C-N	7.24	127.08	119.05
6	H	733	VAL	C-N-CA	7.24	127.08	119.05
12	N	55	PRO	N-CA-CB	7.24	110.10	103.08
1	A	1933	PRO	N-CA-CB	7.23	111.18	103.52
14	Q	158	PRO	N-CA-CB	7.22	110.95	103.00
9	K	247	PHE	N-CA-C	7.17	119.09	111.28
12	N	388	HIS	CB-CA-C	7.11	119.84	110.81
12	N	509	TYR	N-CA-C	7.09	122.61	113.18
15	R	408	SER	CA-C-N	7.04	126.29	118.97
15	R	408	SER	C-N-CA	7.04	126.29	118.97
12	N	219	PRO	N-CA-CB	7.00	110.60	103.25
8	I	304	PHE	N-CA-C	6.95	118.51	111.07
16	S	290	PRO	N-CA-CB	6.95	110.98	103.33
1	A	759	ILE	N-CA-C	6.95	120.69	112.35
12	N	29	PRO	N-CA-CB	6.84	110.52	103.00
9	K	359	THR	N-CA-CB	6.83	120.15	110.12
6	F	733	VAL	CA-C-N	6.79	126.58	119.05
6	F	733	VAL	C-N-CA	6.79	126.58	119.05
1	A	1760	ASN	N-CA-C	6.71	119.43	111.71
6	H	94	GLY	CA-C-N	6.71	127.38	120.60
6	H	94	GLY	C-N-CA	6.71	127.38	120.60
16	S	29	VAL	N-CA-CB	-6.69	103.08	111.31
14	Q	138	GLN	N-CA-C	6.65	119.11	110.53
1	A	1545	LYS	N-CA-C	6.63	118.16	111.07
14	Q	137	PRO	N-CA-CB	6.62	110.20	103.25
9	J	511	ASP	N-CA-C	6.57	119.28	111.33
12	N	202	GLU	N-CA-C	6.47	119.38	107.73
16	S	261	PRO	N-CA-CB	6.47	110.38	103.52
1	A	758	HIS	CA-C-N	6.47	125.50	120.33
1	A	758	HIS	C-N-CA	6.47	125.50	120.33
18	Z	140	THR	N-CA-C	6.47	117.99	111.07
8	I	659	ARG	N-CA-C	6.46	124.56	110.80
8	I	728	ARG	N-CA-C	-6.46	100.28	109.96
12	N	482	PRO	N-CA-CB	6.43	110.00	103.25
16	S	292	VAL	N-CA-C	6.43	118.05	109.37
16	S	263	PRO	N-CA-CB	6.40	109.97	103.25
8	I	722	VAL	N-CA-C	6.36	117.07	108.17
1	A	1924	PRO	N-CA-CB	6.33	110.65	102.86
9	K	369	LEU	CA-C-N	-6.33	111.95	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	369	LEU	C-N-CA	-6.33	111.95	118.85
16	S	38	MET	CA-CB-CG	6.33	126.75	114.10
12	N	330	ARG	NE-CZ-NH2	-6.32	113.52	119.20
3	C	148	ASN	N-CA-C	6.31	119.45	111.69
10	L	170	PRO	N-CA-CB	6.29	109.25	103.15
1	A	133	ILE	N-CA-C	6.20	116.55	107.37
9	J	369	LEU	CA-C-N	-6.19	112.10	118.85
9	J	369	LEU	C-N-CA	-6.19	112.10	118.85
13	O	461	ASN	N-CA-C	6.18	117.81	111.14
16	S	271	ARG	N-CA-C	6.17	118.44	109.07
8	I	447	PHE	N-CA-CB	-6.14	101.09	110.12
18	Z	57	THR	N-CA-C	-6.14	105.58	114.12
9	J	451	LEU	N-CA-CB	6.08	119.71	110.28
6	F	494	HIS	N-CA-C	-6.06	103.84	111.11
12	N	197	PRO	N-CA-CB	6.05	109.60	103.25
10	L	132	THR	CB-CA-C	-6.05	99.31	109.65
4	D	7	SER	N-CA-C	6.04	118.35	111.11
2	B	14	TRP	CA-CB-CG	6.03	125.06	113.60
13	O	594	SER	N-CA-C	6.03	118.65	111.71
14	Q	408	SER	CA-C-N	6.03	125.24	118.97
14	Q	408	SER	C-N-CA	6.03	125.24	118.97
4	D	16	LEU	N-CA-C	6.00	117.82	111.28
12	N	149	LEU	N-CA-C	5.99	117.74	109.29
9	K	292	VAL	N-CA-CB	5.98	119.55	110.58
15	R	117	ALA	CA-C-N	5.97	128.56	120.38
15	R	117	ALA	C-N-CA	5.97	128.56	120.38
6	H	494	HIS	N-CA-C	-5.96	104.12	111.33
1	A	1601	TYR	N-CA-C	5.93	120.24	112.89
12	N	386	LEU	N-CA-C	5.92	123.41	110.80
9	K	300	VAL	N-CA-CB	5.90	118.57	110.54
1	A	1284	GLU	N-CA-C	5.88	117.25	108.31
1	A	1231	HIS	N-CA-C	5.86	117.67	111.28
9	J	331	LYS	N-CA-C	-5.81	102.45	110.35
13	O	706	CYS	N-CA-C	5.79	117.59	111.28
8	I	337	ILE	CB-CA-C	5.77	119.03	111.81
1	A	841	PRO	N-CA-C	5.76	117.73	110.70
16	S	301	PRO	N-CA-CB	5.76	109.30	103.25
16	S	556	ARG	CA-C-N	5.76	125.78	119.90
16	S	556	ARG	C-N-CA	5.76	125.78	119.90
12	N	78	VAL	N-CA-C	-5.76	97.36	109.34
13	O	409	HIS	CB-CA-C	-5.76	101.84	110.88
12	N	368	THR	CA-C-N	5.75	132.04	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	368	THR	C-N-CA	5.75	132.04	121.70
12	N	497	ARG	N-CA-C	5.73	123.01	110.80
16	S	89	TYR	CA-C-N	-5.70	112.73	119.05
16	S	89	TYR	C-N-CA	-5.70	112.73	119.05
9	K	291	LEU	N-CA-C	5.68	117.55	111.36
17	X	199	CYS	CA-C-N	5.67	125.13	119.24
17	X	199	CYS	C-N-CA	5.67	125.13	119.24
1	A	1255	VAL	CB-CA-C	-5.63	103.14	112.26
12	N	388	HIS	CA-C-N	5.63	125.64	119.90
12	N	388	HIS	C-N-CA	5.63	125.64	119.90
1	A	1879	GLU	N-CA-C	5.62	117.86	111.11
1	A	403	ILE	N-CA-C	5.61	116.32	109.30
9	J	298	ASN	CB-CA-C	5.59	117.47	109.26
16	S	272	ILE	N-CA-C	5.59	116.79	109.58
8	I	287	LEU	N-CA-C	5.56	117.42	111.36
8	I	566	THR	N-CA-C	-5.53	100.66	109.23
12	N	431	ARG	N-CA-C	5.53	117.39	111.36
15	R	227	GLU	CB-CA-C	5.52	118.86	109.53
12	N	476	GLU	CA-C-N	5.51	126.73	119.84
12	N	476	GLU	C-N-CA	5.51	126.73	119.84
1	A	1232	ILE	N-CA-C	5.50	113.89	107.89
18	Z	163	VAL	CA-C-N	5.50	125.81	119.92
18	Z	163	VAL	C-N-CA	5.50	125.81	119.92
12	N	767	SER	N-CA-C	5.50	117.62	108.99
12	N	368	THR	CB-CA-C	5.49	121.35	110.42
1	A	1167	GLU	N-CA-C	-5.48	100.47	109.40
1	A	1030	GLU	CG-CD-OE2	5.47	130.99	118.40
17	Y	230	VAL	CA-C-N	5.47	126.67	119.84
17	Y	230	VAL	C-N-CA	5.47	126.67	119.84
12	N	256	VAL	N-CA-C	5.46	115.66	110.53
12	N	484	PRO	N-CA-CB	5.45	108.60	102.60
1	A	1088	THR	CA-C-N	-5.44	115.49	123.00
1	A	1088	THR	C-N-CA	-5.44	115.49	123.00
12	N	388	HIS	N-CA-CB	-5.44	103.99	111.77
1	A	1761	MET	CB-CA-C	-5.44	109.83	117.23
12	N	637	TRP	N-CA-C	5.44	117.01	111.14
1	A	1894	VAL	N-CA-C	5.43	113.41	107.60
1	A	881	ILE	CB-CA-C	5.43	116.80	110.88
17	X	230	VAL	CA-C-N	5.40	126.59	119.84
17	X	230	VAL	C-N-CA	5.40	126.59	119.84
8	I	139	LEU	N-CA-C	5.39	118.10	110.40
14	Q	227	GLU	CB-CA-C	5.38	118.41	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	218	SER	CA-C-N	5.38	126.56	119.84
12	N	218	SER	C-N-CA	5.38	126.56	119.84
6	F	491	LEU	CA-C-N	5.37	125.08	119.82
6	F	491	LEU	C-N-CA	5.37	125.08	119.82
8	I	628	THR	N-CA-C	5.36	117.21	111.36
12	N	321	LEU	N-CA-C	5.34	117.70	110.06
1	A	474	ILE	CB-CA-C	5.33	115.54	110.16
9	K	164	PHE	N-CA-CB	-5.33	102.09	110.46
8	I	476	GLY	N-CA-C	5.30	120.47	113.37
8	I	150	SER	N-CA-C	-5.29	106.59	113.16
1	A	104	LYS	N-CA-C	5.29	120.22	113.55
1	A	57	LEU	N-CA-C	5.28	117.01	108.08
8	I	446	THR	CA-C-N	5.28	127.36	120.28
8	I	446	THR	C-N-CA	5.28	127.36	120.28
9	J	292	VAL	N-CA-CB	5.26	118.47	110.58
6	H	491	LEU	CA-C-N	5.25	124.96	119.82
6	H	491	LEU	C-N-CA	5.25	124.96	119.82
17	X	350	PHE	CB-CA-C	-5.25	102.42	110.81
17	Y	350	PHE	CB-CA-C	-5.24	102.43	110.81
16	S	37	ILE	CB-CA-C	5.23	117.95	111.15
17	Y	551	LYS	N-CA-C	5.23	117.89	111.82
16	S	291	THR	N-CA-C	5.22	116.97	111.28
1	A	173	LEU	N-CA-C	5.21	116.97	109.04
18	Z	35	ARG	N-CA-C	-5.20	106.78	113.02
17	X	158	ILE	CB-CA-C	-5.20	105.13	112.14
15	R	90	VAL	N-CA-C	-5.19	105.65	110.53
16	S	88	ASN	N-CA-C	5.19	116.94	111.28
10	L	134	THR	N-CA-C	5.19	116.95	108.55
12	N	53	ALA	CA-C-N	5.19	123.51	120.24
12	N	53	ALA	C-N-CA	5.19	123.51	120.24
12	N	54	VAL	CA-C-N	5.18	125.72	120.38
12	N	54	VAL	C-N-CA	5.18	125.72	120.38
16	S	36	ARG	CB-CG-CD	-5.18	99.39	111.30
9	J	485	ILE	CB-CA-C	-5.18	105.15	112.14
13	O	76	SER	N-CA-C	-5.17	105.55	111.14
12	N	54	VAL	O-C-N	5.16	123.73	120.07
15	R	119	ASN	N-CA-C	5.15	119.62	113.23
12	N	784	GLY	CA-C-N	5.13	126.25	119.84
12	N	784	GLY	C-N-CA	5.13	126.25	119.84
1	A	1729	GLU	N-CA-C	5.13	118.20	111.28
6	H	494	HIS	N-CA-CB	5.12	117.74	110.06
9	J	434	ALA	N-CA-C	5.10	117.50	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	296	THR	N-CA-C	5.10	121.66	110.80
9	K	171	THR	N-CA-C	5.10	119.59	113.17
1	A	628	ILE	CB-CA-C	-5.09	105.46	111.97
1	A	1181	LEU	CA-C-N	5.08	127.09	120.28
1	A	1181	LEU	C-N-CA	5.08	127.09	120.28
9	J	220	ILE	C-N-CD	-5.08	104.17	125.00
17	X	37	VAL	CB-CA-C	-5.08	105.28	112.14
9	J	69	TYR	N-CA-C	5.08	119.69	112.93
17	X	366	ILE	N-CA-CB	5.08	117.44	110.54
17	Y	94	ARG	CA-CB-CG	5.05	124.21	114.10
17	Y	158	ILE	CB-CA-C	-5.05	105.32	112.14
1	A	1282	GLY	CA-C-N	5.05	126.15	119.84
1	A	1282	GLY	C-N-CA	5.05	126.15	119.84
1	A	1050	ASN	N-CA-C	5.04	116.74	108.52
15	R	106	THR	CA-C-N	-5.04	113.54	119.84
15	R	106	THR	C-N-CA	-5.04	113.54	119.84
9	J	485	ILE	N-CA-CB	5.04	117.39	110.54
1	A	1391	ASP	N-CA-C	5.03	119.37	113.23
8	I	663	ASP	N-CA-C	5.03	119.57	113.38
10	L	172	CYS	N-CA-C	5.02	117.72	110.28
17	X	349	SER	N-CA-C	5.00	116.81	111.36

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1191	LEU	Peptide
8	I	658	GLY	Peptide
8	I	727	PHE	Peptide
9	J	220	ILE	Peptide
12	N	162	PHE	Peptide
12	N	164	SER	Peptide
12	N	280	GLU	Peptide
12	N	281	TYR	Peptide
12	N	351	PHE	Peptide
12	N	352	PRO	Peptide
12	N	353	ASP	Peptide
12	N	367	ARG	Peptide
12	N	369	ASP	Peptide
12	N	387	LEU	Peptide
12	N	390	GLY	Peptide
12	N	394	CYS	Peptide

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Mol	Chain	Res	Type	Group
12	N	395	ASP	Peptide
12	N	485	VAL	Peptide
12	N	62	ARG	Peptide
12	N	77	GLU	Peptide
16	S	235	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10949	0	10690	435	0
2	B	643	0	617	83	0
3	C	4306	0	4272	166	0
3	P	4043	0	4000	138	0
4	D	153	0	148	8	0
5	E	450	0	435	10	0
6	F	3849	0	3783	114	0
6	H	3853	0	3794	133	0
7	G	213	0	220	13	0
7	W	213	0	220	12	0
8	I	5716	0	5587	359	0
9	J	4047	0	3949	190	0
9	K	3988	0	3908	175	0
10	L	1435	0	1382	58	0
11	M	493	0	469	24	0
12	N	5403	0	5103	293	0
13	O	5402	0	5436	226	0
14	Q	2671	0	2516	107	0
15	R	2953	0	2839	115	0
16	S	2077	0	1827	333	0
17	X	3773	0	3831	167	0
17	Y	3868	0	3925	177	0
18	Z	1577	0	1592	87	0
All	All	72075	0	70543	3012	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 21.

All (3012) 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)
16:S:38:MET:CE	18:Z:181:VAL:HG23	1.22	1.65
16:S:22:TRP:CZ3	16:S:41:LEU:HB2	1.31	1.64
16:S:19:GLY:CA	18:Z:134:GLN:HE21	1.16	1.54
8:I:413:ASN:HA	8:I:447:PHE:CZ	1.38	1.53
1:A:1199:LYS:NZ	1:A:1199:LYS:CE	1.73	1.45
16:S:19:GLY:CA	18:Z:134:GLN:NE2	1.74	1.43
16:S:19:GLY:C	18:Z:134:GLN:HE21	1.23	1.42
17:X:442:GLN:CD	17:X:472:ARG:NE	1.78	1.42
16:S:68:PHE:CE2	16:S:81:TYR:CD2	2.10	1.40
16:S:38:MET:CE	18:Z:181:VAL:CG2	2.00	1.38
16:S:30:GLN:N	16:S:36:ARG:HH22	1.20	1.38
16:S:38:MET:HE3	18:Z:181:VAL:CG2	1.50	1.37
16:S:29:VAL:HG13	16:S:36:ARG:NH1	1.40	1.36
16:S:22:TRP:CZ3	16:S:41:LEU:CB	2.10	1.34
16:S:36:ARG:NH1	16:S:90:PRO:HB2	1.42	1.33
16:S:58:GLN:HG3	16:S:62:PHE:CE2	1.61	1.32
16:S:19:GLY:HA3	18:Z:134:GLN:NE2	1.34	1.29
12:N:362:LYS:HB2	12:N:410:LEU:CD2	1.62	1.28
2:B:16:TRP:NE1	2:B:44:CYS:CB	1.96	1.26
8:I:413:ASN:HA	8:I:447:PHE:CE1	1.68	1.25
1:A:1332:GLY:O	1:A:1358:ILE:HD12	1.31	1.25
16:S:68:PHE:CZ	16:S:81:TYR:HD2	1.54	1.25
16:S:21:GLU:O	16:S:45:LEU:HD22	1.35	1.24
17:X:442:GLN:OE1	17:X:472:ARG:CZ	1.85	1.22
1:A:1235:LEU:CD2	1:A:1257:ILE:HG13	1.70	1.21
16:S:29:VAL:HG12	18:Z:140:THR:CG2	1.72	1.20
8:I:430:GLU:HG2	14:Q:429:LYS:CG	1.71	1.20
16:S:71:GLY:C	16:S:74:PRO:HD2	1.68	1.18
17:Y:42:ARG:HA	17:Y:82:TYR:CE2	1.78	1.17
1:A:1332:GLY:O	1:A:1358:ILE:CD1	1.91	1.17
2:B:16:TRP:CD1	2:B:44:CYS:HB3	1.79	1.16
12:N:362:LYS:CB	12:N:410:LEU:HD23	1.76	1.16
16:S:68:PHE:CE2	16:S:81:TYR:HD2	1.51	1.15
16:S:29:VAL:HA	16:S:36:ARG:HH12	1.11	1.15
9:K:129:LYS:O	9:K:133:CYS:SG	2.05	1.14
16:S:132:CYS:HB2	16:S:135:PRO:HG3	1.13	1.13
8:I:279:ILE:HD11	8:I:337:ILE:HA	1.23	1.13
13:O:75:LEU:HD11	13:O:161:TYR:CE2	1.82	1.12
17:X:201:LEU:HD11	17:Y:40:HIS:HB3	1.20	1.12
13:O:75:LEU:CD2	13:O:161:TYR:OH	1.98	1.11
8:I:290:PHE:CA	8:I:320:LEU:HD11	1.81	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:413:ASN:CA	8:I:447:PHE:CZ	2.31	1.11
12:N:765:LEU:HD21	16:S:200:VAL:HG21	1.30	1.11
9:K:250:CYS:SG	9:K:274:THR:HG21	1.91	1.11
16:S:29:VAL:CG1	16:S:36:ARG:NH1	2.14	1.11
16:S:29:VAL:HG12	18:Z:140:THR:HG21	1.29	1.10
16:S:76:ASP:O	16:S:77:VAL:HG23	1.49	1.10
16:S:58:GLN:O	16:S:62:PHE:CD2	2.04	1.10
12:N:362:LYS:HB2	12:N:410:LEU:HD23	1.10	1.10
9:J:441:VAL:HG21	9:J:444:TRP:HD1	1.16	1.09
16:S:21:GLU:O	16:S:45:LEU:CD2	1.99	1.09
2:B:16:TRP:NE1	2:B:44:CYS:HB3	1.58	1.09
6:H:656:MET:HE2	6:H:660:LYS:HE2	1.14	1.09
16:S:22:TRP:CH2	16:S:38:MET:O	2.05	1.09
8:I:313:ALA:HB3	8:I:317:LEU:HB2	1.18	1.08
16:S:132:CYS:HA	16:S:133:ASN:HB2	1.34	1.08
9:J:454:VAL:O	9:J:458:LEU:HD12	1.51	1.08
16:S:20:ASP:OD1	18:Z:184:ARG:HD2	1.53	1.08
8:I:209:CYS:SG	8:I:584:HIS:CE1	2.46	1.07
16:S:30:GLN:H	16:S:91:GLN:HB2	1.18	1.07
16:S:36:ARG:NH1	16:S:90:PRO:CB	2.17	1.07
16:S:38:MET:HE3	18:Z:181:VAL:HG21	1.28	1.07
12:N:180:PHE:CD1	12:N:299:TRP:CZ3	2.43	1.07
13:O:75:LEU:O	13:O:79:TYR:CD2	2.08	1.07
16:S:30:GLN:N	16:S:36:ARG:NH2	2.00	1.07
9:J:332:THR:HA	9:J:363:LEU:HD21	1.37	1.06
16:S:132:CYS:SG	16:S:135:PRO:HA	1.95	1.06
1:A:1235:LEU:HD21	1:A:1257:ILE:CG1	1.85	1.06
8:I:302:ASP:N	8:I:303:GLU:N	2.04	1.06
8:I:209:CYS:SG	8:I:584:HIS:ND1	2.30	1.05
17:X:442:GLN:OE1	17:X:472:ARG:NH2	1.87	1.05
12:N:393:THR:O	12:N:395:ASP:HB3	1.54	1.04
6:F:130:ARG:HG2	17:Y:506:GLN:NE2	1.71	1.04
8:I:300:VAL:HA	8:I:303:GLU:OE1	1.55	1.04
17:Y:452:LEU:HD22	17:Y:461:ALA:N	1.73	1.04
17:X:452:LEU:CD2	17:X:457:THR:O	2.06	1.04
8:I:56:TRP:CE3	8:I:98:PRO:HB3	1.93	1.03
16:S:68:PHE:CZ	16:S:81:TYR:CD2	2.37	1.03
17:X:442:GLN:HG2	17:X:472:ARG:CD	1.86	1.03
12:N:362:LYS:CB	12:N:410:LEU:CD2	2.34	1.03
16:S:30:GLN:N	16:S:91:GLN:HB2	1.74	1.03
17:Y:452:LEU:CD2	17:Y:457:THR:O	2.06	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:98:GLU:CG	15:R:101:PRO:HD3	1.88	1.02
14:Q:185:TYR:CD1	16:S:27:GLU:HB3	1.94	1.02
16:S:79:ASP:OD2	16:S:120:ARG:HG2	1.59	1.02
12:N:425:ARG:HG2	12:N:425:ARG:HH11	1.20	1.02
16:S:19:GLY:C	18:Z:134:GLN:NE2	2.04	1.02
2:B:14:TRP:HA	2:B:15:LEU:HB2	1.41	1.02
16:S:29:VAL:CA	16:S:36:ARG:HH12	1.73	1.02
13:O:581:ILE:HD11	13:O:619:LEU:HB3	1.42	1.01
16:S:38:MET:HE2	18:Z:181:VAL:CG2	1.79	1.01
1:A:1232:ILE:HG13	1:A:1235:LEU:HB2	1.40	1.01
17:X:452:LEU:HD22	17:X:461:ALA:N	1.73	1.01
8:I:295:ASN:O	8:I:316:GLU:HB2	1.61	1.01
14:Q:410:HIS:HB3	14:Q:475:LEU:HD21	1.40	1.01
8:I:289:LYS:HG3	8:I:324:GLN:OE1	1.61	1.00
13:O:75:LEU:CG	13:O:161:TYR:CE2	2.44	1.00
16:S:71:GLY:O	16:S:74:PRO:HD2	1.59	1.00
2:B:16:TRP:HD1	2:B:33:CYS:HA	1.24	1.00
16:S:66:ILE:HA	16:S:69:TYR:HD2	1.24	1.00
8:I:430:GLU:HG2	14:Q:429:LYS:HG3	1.38	1.00
13:O:75:LEU:CD1	13:O:161:TYR:CE2	2.45	0.99
1:A:1162:LYS:HG3	1:A:1163:PRO:HD2	1.44	0.99
17:Y:42:ARG:HG3	17:Y:82:TYR:OH	1.61	0.99
8:I:430:GLU:HG2	14:Q:429:LYS:HG2	1.45	0.99
16:S:22:TRP:HH2	16:S:38:MET:CA	1.76	0.99
17:X:442:GLN:HG2	17:X:472:ARG:HD2	1.40	0.99
13:O:435:SER:HB3	13:O:654:ASP:HB2	1.43	0.98
3:C:344:ARG:HH21	11:M:25:PRO:HG2	1.27	0.98
8:I:313:ALA:HB2	8:I:317:LEU:HD12	1.43	0.98
1:A:1235:LEU:HD21	1:A:1257:ILE:HG13	1.00	0.98
14:Q:128:ALA:HB3	18:Z:156:TYR:CZ	1.99	0.98
16:S:29:VAL:HG13	16:S:36:ARG:HH11	1.26	0.98
15:R:225:PRO:HD2	16:S:166:GLU:O	1.64	0.98
1:A:1786:MET:HE2	1:A:1786:MET:HA	1.43	0.98
9:K:250:CYS:SG	9:K:274:THR:CG2	2.52	0.97
17:X:201:LEU:HD11	17:Y:40:HIS:CB	1.94	0.97
9:J:55:ARG:HH11	9:K:264:HIS:HA	1.24	0.97
16:S:33:ARG:HB2	16:S:130:ARG:HH11	1.30	0.97
6:H:656:MET:HE2	6:H:660:LYS:CE	1.94	0.97
8:I:186:GLU:OE1	8:I:197:ARG:NH1	1.97	0.97
8:I:144:THR:HG21	8:I:159:GLU:HA	1.46	0.97
16:S:132:CYS:HB2	16:S:135:PRO:CG	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:313:ALA:CB	8:I:317:LEU:HD12	1.95	0.96
3:C:134:THR:HG23	3:C:143:LYS:HG3	1.47	0.96
13:O:75:LEU:HD21	13:O:161:TYR:OH	1.62	0.96
16:S:40:THR:HB	16:S:87:GLN:O	1.65	0.96
8:I:313:ALA:HB3	8:I:317:LEU:CB	1.95	0.96
2:B:17:VAL:HG13	2:B:31:ASN:ND2	1.80	0.96
16:S:79:ASP:OD2	16:S:120:ARG:CG	2.13	0.96
16:S:163:GLU:CD	16:S:196:PHE:CE1	2.43	0.95
8:I:209:CYS:HG	8:I:584:HIS:HD1	1.11	0.95
17:X:442:GLN:CD	17:X:472:ARG:HE	1.61	0.95
16:S:79:ASP:OD2	16:S:120:ARG:CB	2.15	0.95
12:N:574:ILE:HD12	12:N:625:LYS:HG2	1.49	0.95
3:P:233:PHE:CZ	3:P:237:ILE:HD11	2.02	0.95
16:S:22:TRP:CH2	16:S:38:MET:HA	2.02	0.95
13:O:75:LEU:CD2	13:O:161:TYR:CZ	2.50	0.94
16:S:22:TRP:HA	16:S:45:LEU:HD11	1.47	0.94
16:S:86:GLU:CG	16:S:98:MET:HE3	1.98	0.94
17:X:442:GLN:NE2	17:X:472:ARG:HE	1.66	0.94
17:Y:305:ILE:HG23	17:Y:340:GLU:OE1	1.68	0.94
1:A:1322:PRO:HG3	1:A:1375:TYR:OH	1.67	0.94
8:I:413:ASN:HA	8:I:447:PHE:HZ	1.24	0.94
9:J:254:THR:HG23	9:J:271:HIS:HD2	1.32	0.94
16:S:86:GLU:HG3	16:S:98:MET:CE	1.98	0.94
8:I:302:ASP:C	8:I:303:GLU:N	2.26	0.94
13:O:75:LEU:HD21	13:O:161:TYR:CE2	2.03	0.94
16:S:22:TRP:CH2	16:S:41:LEU:HB2	2.02	0.94
13:O:75:LEU:O	13:O:79:TYR:HD2	1.47	0.93
9:K:214:LYS:O	9:K:216:SER:N	2.01	0.93
12:N:538:GLU:HG2	12:N:561:LEU:HG	1.47	0.93
6:H:762:TRP:HA	6:H:765:ASP:HB3	1.48	0.93
8:I:290:PHE:HA	8:I:320:LEU:HD11	1.46	0.93
16:S:38:MET:HE1	18:Z:199:TYR:HE2	1.32	0.93
2:B:16:TRP:CZ3	12:N:630:LYS:HE2	2.04	0.93
12:N:78:VAL:O	12:N:81:ASN:N	2.01	0.93
2:B:14:TRP:CA	2:B:15:LEU:HB2	1.99	0.92
9:J:441:VAL:HG21	9:J:444:TRP:CD1	2.03	0.92
12:N:273:MET:HG3	12:N:277:CYS:SG	2.09	0.92
16:S:22:TRP:HZ3	16:S:41:LEU:CB	1.63	0.92
6:H:656:MET:CE	6:H:660:LYS:HE2	1.98	0.92
8:I:290:PHE:C	8:I:320:LEU:HD11	1.93	0.92
17:X:40:HIS:HB3	17:Y:201:LEU:HD11	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:163:GLU:OE1	16:S:196:PHE:CE1	2.22	0.92
9:J:354:MET:HE2	9:J:374:ILE:HG23	1.51	0.92
12:N:180:PHE:CD1	12:N:299:TRP:CH2	2.57	0.92
14:Q:352:THR:HG21	18:Z:50:GLY:O	1.70	0.91
1:A:1332:GLY:O	1:A:1358:ILE:CG1	2.18	0.91
13:O:75:LEU:HD21	13:O:161:TYR:CZ	2.04	0.91
16:S:76:ASP:O	16:S:77:VAL:CG2	2.17	0.91
16:S:30:GLN:NE2	16:S:91:GLN:HG3	1.86	0.91
16:S:71:GLY:O	16:S:74:PRO:O	1.86	0.91
9:K:276:VAL:HA	9:K:311:MET:HE2	1.53	0.91
16:S:19:GLY:HA3	18:Z:134:GLN:CD	1.96	0.91
16:S:36:ARG:HH12	16:S:90:PRO:HB2	1.18	0.90
2:B:46:LEU:HB2	12:N:632:MET:SD	2.09	0.90
8:I:300:VAL:O	8:I:303:GLU:HB2	1.70	0.90
2:B:16:TRP:CD1	2:B:33:CYS:HA	2.05	0.90
13:O:75:LEU:HD23	13:O:161:TYR:OH	1.71	0.90
16:S:163:GLU:OE1	16:S:196:PHE:CD1	2.24	0.90
8:I:26:LEU:HB3	8:I:37:LEU:HB3	1.54	0.90
17:X:267:LEU:HD11	17:Y:59:LEU:CD1	2.01	0.90
16:S:22:TRP:HZ3	16:S:41:LEU:HB2	1.07	0.90
16:S:58:GLN:O	16:S:62:PHE:HD2	1.55	0.90
13:O:75:LEU:HG	13:O:161:TYR:CZ	2.05	0.90
16:S:58:GLN:HG3	16:S:62:PHE:HE2	1.00	0.90
3:C:414:MET:HG2	13:O:330:ILE:CD1	2.02	0.90
14:Q:132:ARG:HG3	18:Z:154:LEU:CD2	2.02	0.90
8:I:301:GLN:C	8:I:303:GLU:N	2.29	0.89
9:J:211:LYS:O	9:J:212:TYR:CD2	2.24	0.89
17:X:442:GLN:OE1	17:X:472:ARG:NE	1.97	0.89
2:B:14:TRP:HA	2:B:15:LEU:CB	1.99	0.89
9:J:354:MET:HE1	9:J:377:GLU:HB2	1.53	0.89
17:Y:452:LEU:HD23	17:Y:457:THR:O	1.72	0.89
16:S:68:PHE:HE2	16:S:81:TYR:CD2	1.82	0.89
16:S:193:HIS:CE1	16:S:197:GLN:OE1	2.25	0.89
16:S:197:GLN:O	16:S:200:VAL:HG22	1.73	0.89
17:X:452:LEU:HD23	17:X:457:THR:O	1.72	0.89
16:S:22:TRP:HH2	16:S:38:MET:C	1.79	0.89
16:S:132:CYS:CB	16:S:135:PRO:HG3	2.03	0.89
6:F:130:ARG:HG2	17:Y:506:GLN:HE21	1.35	0.89
16:S:66:ILE:HA	16:S:69:TYR:CD2	2.07	0.89
11:M:4:GLU:HG2	3:P:50:HIS:CE1	2.08	0.89
8:I:300:VAL:HG21	8:I:456:PHE:CB	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:442:GLN:CG	17:X:472:ARG:CD	2.51	0.88
14:Q:185:TYR:CE1	16:S:27:GLU:HG3	2.09	0.88
13:O:55:MET:SD	13:O:58:ARG:NH1	2.47	0.88
17:X:201:LEU:CD1	17:Y:40:HIS:HB3	2.02	0.88
17:Y:462:LYS:HG2	17:Y:485:LEU:HD13	1.56	0.88
9:J:55:ARG:NH1	9:K:264:HIS:HA	1.89	0.87
13:O:55:MET:SD	13:O:58:ARG:CZ	2.62	0.87
10:L:83:TYR:CD2	10:L:115:GLU:HA	2.09	0.87
12:N:560:MET:HE2	12:N:560:MET:HA	1.54	0.87
16:S:134:GLU:O	16:S:136:LEU:N	2.08	0.87
9:K:222:GLU:OE1	9:K:228:GLN:CD	2.17	0.87
12:N:91:PHE:O	12:N:93:ASN:N	2.07	0.87
16:S:41:LEU:CD1	18:Z:141:PHE:HB3	2.05	0.87
1:A:1175:PHE:CZ	1:A:1179:LEU:HD21	2.10	0.87
14:Q:132:ARG:HB2	18:Z:170:SER:HB2	1.55	0.87
16:S:22:TRP:CH2	16:S:38:MET:CA	2.58	0.87
9:J:445:GLU:OE1	9:J:475:ILE:HG21	1.75	0.87
16:S:38:MET:HE2	18:Z:181:VAL:HG23	0.88	0.87
9:J:167:PHE:O	9:J:170:LEU:HD23	1.75	0.86
12:N:362:LYS:HB2	12:N:410:LEU:HD21	1.55	0.86
14:Q:185:TYR:CD1	16:S:27:GLU:CB	2.59	0.86
16:S:22:TRP:HH2	16:S:38:MET:O	1.56	0.86
16:S:83:SER:O	16:S:87:GLN:HG3	1.74	0.86
16:S:199:ARG:O	16:S:202:ARG:HG2	1.73	0.86
16:S:29:VAL:HA	16:S:90:PRO:HB2	1.57	0.86
17:Y:42:ARG:HA	17:Y:82:TYR:CZ	2.10	0.86
2:B:16:TRP:CD1	2:B:44:CYS:CB	2.52	0.86
3:P:276:ILE:HG22	3:P:277:ARG:H	1.40	0.86
16:S:29:VAL:CG1	18:Z:140:THR:HG21	2.05	0.86
6:H:653:LEU:HD22	9:K:523:ILE:HG21	1.58	0.86
12:N:570:ILE:HD13	12:N:633:ARG:NH1	1.91	0.86
12:N:570:ILE:HD13	12:N:633:ARG:HH12	1.41	0.86
16:S:29:VAL:CG1	18:Z:140:THR:CG2	2.54	0.85
16:S:71:GLY:CA	16:S:74:PRO:HD2	2.05	0.85
16:S:82:ILE:CD1	16:S:124:LEU:CD2	2.54	0.85
1:A:1307:LEU:HD11	1:A:1582:ALA:HB2	1.58	0.85
9:K:472:LEU:HG	9:K:481:THR:HG21	1.58	0.85
13:O:75:LEU:HD11	13:O:161:TYR:HE2	1.40	0.85
16:S:83:SER:HB2	16:S:87:GLN:NE2	1.91	0.85
8:I:286:ARG:HE	8:I:333:LEU:HD13	1.40	0.85
8:I:413:ASN:CA	8:I:447:PHE:CE1	2.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:180:PHE:CD1	12:N:299:TRP:HZ3	1.90	0.85
1:A:1619:LEU:HD21	1:A:1697:LEU:HD22	1.58	0.85
3:C:259:PHE:HB3	3:C:265:ILE:CD1	2.06	0.85
8:I:73:TRP:CZ2	8:I:80:LEU:HD22	2.11	0.85
17:X:442:GLN:HG2	17:X:472:ARG:CG	2.06	0.85
2:B:16:TRP:HE1	2:B:44:CYS:CB	1.47	0.85
8:I:312:LYS:HG3	8:I:428:MET:SD	2.16	0.85
16:S:19:GLY:N	18:Z:134:GLN:NE2	2.25	0.85
8:I:300:VAL:HG21	8:I:456:PHE:HB3	1.59	0.85
10:L:86:ASP:HB3	10:L:89:TYR:HB2	1.58	0.85
17:X:462:LYS:HG2	17:X:485:LEU:HD13	1.57	0.85
13:O:75:LEU:HG	13:O:161:TYR:CE2	2.12	0.84
6:F:571:CYS:SG	6:F:606:LEU:HD12	2.17	0.84
8:I:337:ILE:CG2	8:I:341:TYR:HE2	1.89	0.84
16:S:29:VAL:HG12	18:Z:140:THR:HG22	1.58	0.84
16:S:20:ASP:N	18:Z:134:GLN:NE2	2.25	0.84
17:Y:452:LEU:HD21	17:Y:457:THR:O	1.75	0.84
13:O:114:ASP:O	13:O:117:ASP:OD1	1.93	0.84
16:S:78:TRP:CZ3	16:S:105:ALA:HA	2.13	0.84
17:X:452:LEU:HD21	17:X:457:THR:O	1.75	0.84
9:J:254:THR:HG23	9:J:271:HIS:CD2	2.11	0.84
14:Q:185:TYR:CG	16:S:27:GLU:HB3	2.12	0.84
8:I:262:LEU:HA	8:I:265:ILE:HG22	1.59	0.84
12:N:395:ASP:HB2	12:N:397:ILE:H	1.43	0.83
8:I:310:TRP:HB2	8:I:313:ALA:HA	1.59	0.83
13:O:75:LEU:CD2	13:O:161:TYR:CE2	2.61	0.83
8:I:430:GLU:CG	14:Q:429:LYS:CG	2.55	0.83
8:I:430:GLU:CG	14:Q:429:LYS:HG2	2.08	0.83
16:S:58:GLN:CG	16:S:62:PHE:CE2	2.56	0.83
17:Y:474:ASP:OD1	17:Y:502:ALA:HA	1.78	0.83
9:J:476:PRO:HG2	3:P:182:LEU:HG	1.60	0.83
13:O:75:LEU:HB3	13:O:79:TYR:CE2	2.14	0.83
13:O:539:ASN:HD22	13:O:542:GLU:HB2	1.44	0.83
14:Q:168:ILE:HG23	14:Q:472:CYS:HA	1.61	0.83
13:O:216:LEU:HD22	13:O:256:LEU:HD12	1.59	0.83
17:X:442:GLN:CD	17:X:472:ARG:CD	2.52	0.83
17:X:474:ASP:OD1	17:X:502:ALA:HA	1.78	0.83
8:I:295:ASN:O	8:I:316:GLU:CB	2.27	0.82
16:S:38:MET:CE	18:Z:199:TYR:HE2	1.82	0.82
8:I:276:TRP:CH2	8:I:476:GLY:HA3	2.14	0.82
8:I:290:PHE:HE1	8:I:324:GLN:HB3	1.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:98:GLU:HG3	15:R:101:PRO:HD3	1.58	0.82
3:C:53:LYS:HD3	3:P:96:VAL:HG21	1.61	0.82
8:I:34:LEU:HD12	8:I:46:LEU:HD21	1.61	0.82
8:I:309:LEU:O	13:O:127:HIS:HB2	1.80	0.82
8:I:349:ILE:HD12	13:O:407:LEU:HA	1.62	0.82
16:S:29:VAL:HA	16:S:36:ARG:NH1	1.93	0.82
6:F:537:GLU:OE1	6:F:602:TYR:HB3	1.79	0.82
16:S:30:GLN:H	16:S:36:ARG:HH22	1.23	0.82
3:C:316:LEU:HD21	3:C:340:TYR:HA	1.62	0.81
17:Y:442:GLN:HG2	17:Y:472:ARG:CG	2.07	0.81
3:C:148:ASN:HB3	3:C:151:LEU:HG	1.62	0.81
9:K:192:LYS:HG2	9:K:198:GLN:HG3	1.62	0.81
16:S:132:CYS:HA	16:S:133:ASN:CB	2.10	0.81
17:Y:42:ARG:HA	17:Y:82:TYR:HE2	1.37	0.81
16:S:163:GLU:HB2	16:S:196:PHE:HE1	1.45	0.81
13:O:75:LEU:CG	13:O:161:TYR:CZ	2.63	0.81
16:S:132:CYS:HB3	16:S:135:PRO:CD	2.10	0.81
16:S:29:VAL:C	16:S:36:ARG:HH22	1.88	0.81
1:A:1799:ARG:HD3	1:A:1805:MET:HB3	1.63	0.81
14:Q:128:ALA:CB	18:Z:156:TYR:CZ	2.63	0.81
17:X:267:LEU:HD11	17:Y:59:LEU:HD11	1.60	0.81
12:N:180:PHE:CE1	12:N:299:TRP:CZ3	2.69	0.80
14:Q:163:LYS:HB2	14:Q:167:TYR:CD2	2.16	0.80
17:Y:305:ILE:CG2	17:Y:340:GLU:OE1	2.29	0.80
17:Y:366:ILE:HD11	17:Y:379:LYS:HD2	1.61	0.80
8:I:337:ILE:HG23	8:I:341:TYR:HE2	1.45	0.80
17:X:230:VAL:CG2	17:Y:36:ASN:HB3	2.11	0.80
8:I:32:ARG:HD3	12:N:388:HIS:CE1	2.16	0.80
17:X:230:VAL:HG21	17:Y:36:ASN:HB3	1.62	0.80
14:Q:163:LYS:HB2	14:Q:167:TYR:HD2	1.46	0.80
1:A:1086:MET:HE2	1:A:1564:LEU:HD13	1.62	0.80
2:B:16:TRP:O	2:B:32:GLY:HA2	1.82	0.80
9:J:37:PRO:HB3	9:J:69:TYR:CE2	2.16	0.80
2:B:17:VAL:HG13	2:B:31:ASN:HD22	1.47	0.80
2:B:17:VAL:HG11	12:N:632:MET:HB3	1.64	0.80
16:S:65:GLU:O	16:S:69:TYR:CD2	2.34	0.80
2:B:17:VAL:HG21	12:N:634:THR:H	1.46	0.79
1:A:1232:ILE:HD11	1:A:1235:LEU:HD22	1.63	0.79
17:X:442:GLN:CG	17:X:472:ARG:HD2	2.10	0.79
8:I:56:TRP:HZ3	8:I:58:PHE:HB2	1.46	0.79
8:I:312:LYS:N	8:I:428:MET:SD	2.55	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:293:GLU:CB	8:I:324:GLN:NE2	2.46	0.79
16:S:41:LEU:HD11	18:Z:141:PHE:HB3	1.63	0.79
16:S:145:GLN:HE22	16:S:296:ILE:CB	1.94	0.79
1:A:1209:LEU:HD22	1:A:1228:LEU:HD23	1.64	0.79
13:O:32:PRO:O	13:O:35:ILE:HG22	1.82	0.79
16:S:68:PHE:HZ	16:S:81:TYR:CB	1.95	0.79
16:S:71:GLY:O	16:S:74:PRO:CD	2.29	0.79
17:Y:84:ALA:HB1	17:Y:100:TYR:CE2	2.17	0.79
2:B:43:ASP:HA	12:N:630:LYS:HE3	1.65	0.79
8:I:290:PHE:HD1	8:I:324:GLN:OE1	1.66	0.79
12:N:368:THR:OG1	12:N:369:ASP:HA	1.82	0.78
16:S:30:GLN:O	16:S:36:ARG:NH2	2.16	0.78
6:F:507:ARG:HD3	6:F:538:ILE:HD13	1.65	0.78
16:S:86:GLU:HG3	16:S:98:MET:HE3	1.60	0.78
8:I:306:HIS:ND1	8:I:317:LEU:HG	1.98	0.78
12:N:577:GLU:HB3	12:N:625:LYS:HE3	1.64	0.78
9:J:185:LEU:HD12	9:J:209:LEU:HD21	1.64	0.78
8:I:276:TRP:CH2	8:I:280:LEU:HD22	2.19	0.78
14:Q:128:ALA:CB	18:Z:156:TYR:CE2	2.67	0.78
17:X:442:GLN:CD	17:X:472:ARG:CZ	2.42	0.78
8:I:413:ASN:O	8:I:447:PHE:HE1	1.65	0.78
1:A:873:VAL:HG21	1:A:951:ILE:HG21	1.66	0.78
3:C:493:TYR:CE2	3:C:497:ILE:HD11	2.19	0.78
6:H:527:ARG:HB3	17:Y:302:PRO:HB3	1.66	0.78
13:O:581:ILE:HD13	13:O:611:SER:HB3	1.66	0.78
15:R:110:LYS:HE2	15:R:114:LYS:HB2	1.66	0.78
9:J:445:GLU:HG2	9:J:446:PRO:HD3	1.67	0.77
1:A:1656:LEU:H	1:A:1656:LEU:HD12	1.49	0.77
6:H:128:THR:HG21	6:H:130:ARG:NH1	2.00	0.77
8:I:56:TRP:CE3	8:I:98:PRO:CB	2.67	0.77
6:F:145:ASN:HB2	6:F:146:PRO:C	2.10	0.77
15:R:115:ALA:O	15:R:119:ASN:HB2	1.84	0.77
16:S:163:GLU:CB	16:S:196:PHE:HE1	1.97	0.77
9:K:487:TYR:OH	7:W:15:ASP:O	2.01	0.77
16:S:82:ILE:HD12	16:S:124:LEU:CD2	2.13	0.77
1:A:1097:THR:HG23	13:O:340:LEU:HB3	1.66	0.77
2:B:14:TRP:CZ2	2:B:42:ASP:OD1	2.38	0.77
2:B:16:TRP:CZ2	2:B:45:PRO:N	2.41	0.77
9:J:383:ASN:HB3	9:J:386:LEU:HD13	1.65	0.77
2:B:16:TRP:HZ2	2:B:45:PRO:N	1.65	0.77
8:I:290:PHE:O	8:I:320:LEU:CD1	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:82:ILE:HD12	16:S:124:LEU:HD23	1.66	0.77
8:I:326:THR:O	8:I:330:LEU:N	2.18	0.77
12:N:281:TYR:CE2	12:N:356:PRO:HB2	2.20	0.77
1:A:1791:ILE:HB	13:O:598:THR:HG21	1.66	0.77
3:C:238:TYR:HD1	3:C:243:LEU:HD12	1.49	0.77
16:S:163:GLU:HB2	16:S:196:PHE:CE1	2.20	0.77
3:C:373:HIS:CE1	15:R:79:TYR:HA	2.20	0.76
8:I:304:PHE:CZ	8:I:452:LEU:HG	2.19	0.76
12:N:362:LYS:CA	12:N:410:LEU:CD2	2.62	0.76
14:Q:132:ARG:HB2	18:Z:170:SER:CB	2.13	0.76
16:S:30:GLN:CD	16:S:91:GLN:HG3	2.10	0.76
16:S:201:SER:O	16:S:205:LEU:HG	1.86	0.76
17:X:52:ASN:HD22	17:Y:202:ALA:HB1	1.50	0.76
1:A:1248:ASN:O	1:A:1251:VAL:HG22	1.84	0.76
8:I:297:THR:N	8:I:316:GLU:OE2	2.19	0.76
12:N:289:PHE:O	12:N:291:LYS:N	2.18	0.76
12:N:435:VAL:HA	12:N:438:ILE:HD12	1.67	0.76
16:S:163:GLU:CD	16:S:196:PHE:HE1	1.92	0.76
2:B:14:TRP:CE2	2:B:42:ASP:OD1	2.39	0.76
8:I:679:ASP:OD1	8:I:703:ARG:NH2	2.18	0.76
16:S:22:TRP:CH2	16:S:38:MET:C	2.60	0.76
12:N:666:ILE:HG12	12:N:681:LEU:HD21	1.66	0.76
2:B:16:TRP:CZ2	2:B:44:CYS:N	2.53	0.76
8:I:290:PHE:CD1	8:I:324:GLN:OE1	2.38	0.76
10:L:40:PHE:HA	10:L:44:GLN:OE1	1.86	0.76
12:N:670:PHE:CE1	12:N:715:VAL:HB	2.20	0.76
16:S:86:GLU:HG2	16:S:98:MET:HE3	1.65	0.76
16:S:132:CYS:HB3	16:S:135:PRO:N	2.00	0.76
1:A:1229:SER:HB3	1:A:1236:LEU:HA	1.67	0.76
12:N:425:ARG:HG2	12:N:425:ARG:NH1	1.97	0.76
16:S:82:ILE:CD1	16:S:124:LEU:HD23	2.16	0.76
13:O:411:LYS:HE2	13:O:412:HIS:CE1	2.20	0.76
14:Q:128:ALA:HB3	18:Z:156:TYR:OH	1.85	0.76
15:R:225:PRO:HB2	16:S:166:GLU:HB2	1.68	0.76
1:A:1196:TYR:CB	1:A:1208:LEU:HD11	2.16	0.76
7:G:6:PRO:HB3	9:J:406:HIS:CD2	2.21	0.76
16:S:33:ARG:HB2	16:S:130:ARG:NH1	2.01	0.76
16:S:86:GLU:HG3	16:S:98:MET:HE1	1.68	0.76
8:I:290:PHE:O	8:I:320:LEU:HD13	1.85	0.75
9:K:174:HIS:HA	9:K:211:LYS:NZ	2.00	0.75
12:N:663:GLN:HE21	12:N:695:ARG:HG3	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:225:PRO:CB	16:S:166:GLU:HB2	2.16	0.75
1:A:1254:VAL:HG11	1:A:1298:ALA:HA	1.68	0.75
8:I:48:ARG:HG3	8:I:55:VAL:HG22	1.68	0.75
13:O:356:ASP:HA	13:O:357:SER:HB2	1.69	0.75
16:S:132:CYS:SG	16:S:135:PRO:CA	2.74	0.75
3:C:493:TYR:CZ	3:C:497:ILE:HD11	2.21	0.75
8:I:293:GLU:CB	8:I:324:GLN:HE21	1.99	0.75
13:O:163:GLN:O	13:O:167:LYS:HG3	1.85	0.75
3:P:290:ARG:HH21	3:P:319:LEU:HD12	1.51	0.75
9:J:332:THR:CA	9:J:363:LEU:HD21	2.15	0.75
10:L:126:ASP:OD2	10:L:130:LYS:O	2.05	0.75
12:N:289:PHE:HA	12:N:292:TRP:HB3	1.68	0.75
6:F:730:LYS:HE2	6:F:740:TYR:HE1	1.50	0.75
12:N:180:PHE:HD1	12:N:299:TRP:HZ3	1.34	0.75
1:A:1375:TYR:HB3	1:A:1378:THR:HG21	1.69	0.75
9:J:19:TYR:CD1	9:J:49:LEU:HD13	2.21	0.75
16:S:76:ASP:O	16:S:77:VAL:CB	2.33	0.75
9:J:406:HIS:CE1	9:J:450:ASN:HD22	2.05	0.75
16:S:30:GLN:H	16:S:91:GLN:CB	1.97	0.75
1:A:873:VAL:HG21	1:A:951:ILE:CG2	2.17	0.74
9:K:174:HIS:CE1	9:K:211:LYS:HD3	2.22	0.74
3:C:327:ASP:O	3:C:333:THR:HG21	1.87	0.74
8:I:224:SER:CB	8:I:229:SER:HA	2.17	0.74
8:I:305:MET:HB2	13:O:61:ASN:HD21	1.51	0.74
12:N:120:SER:O	12:N:124:PRO:HD3	1.87	0.74
9:J:451:LEU:HD12	9:J:467:TYR:CE2	2.22	0.74
9:K:184:LEU:O	9:K:188:LEU:HD23	1.87	0.74
13:O:544:VAL:HG23	13:O:567:LEU:HG	1.67	0.74
16:S:22:TRP:CE3	16:S:41:LEU:CB	2.68	0.74
16:S:129:GLY:O	16:S:132:CYS:SG	2.45	0.74
9:J:465:LEU:HA	9:J:488:ILE:HD12	1.67	0.74
1:A:629:LEU:HD11	1:A:634:ALA:HB2	1.69	0.74
12:N:516:ILE:HG13	12:N:554:MET:HE3	1.69	0.74
13:O:312:CYS:SG	13:O:350:LEU:HD21	2.28	0.74
6:F:500:TRP:HB3	6:H:30:ARG:NH2	2.02	0.74
6:F:653:LEU:HA	6:F:656:MET:SD	2.27	0.74
8:I:26:LEU:HB3	8:I:37:LEU:CB	2.17	0.74
8:I:430:GLU:CG	14:Q:429:LYS:HG3	2.17	0.74
16:S:30:GLN:CA	16:S:91:GLN:HB2	2.17	0.74
17:X:52:ASN:ND2	17:Y:202:ALA:HB1	2.01	0.74
8:I:279:ILE:HB	8:I:340:SER:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:452:LEU:HD22	17:Y:461:ALA:H	1.49	0.74
12:N:630:LYS:HD3	12:N:633:ARG:NH1	2.03	0.73
17:X:452:LEU:HD22	17:X:461:ALA:H	1.49	0.73
8:I:417:PHE:HD2	8:I:448:VAL:HG22	1.53	0.73
13:O:75:LEU:HD11	13:O:161:TYR:CD2	2.23	0.73
16:S:41:LEU:O	16:S:45:LEU:HD12	1.88	0.73
3:P:327:ASP:O	3:P:333:THR:HG21	1.89	0.73
16:S:20:ASP:OD1	18:Z:184:ARG:CD	2.35	0.73
12:N:139:GLY:C	12:N:141:LEU:H	1.97	0.73
13:O:405:SER:O	13:O:409:HIS:CD2	2.41	0.73
14:Q:186:TYR:CZ	16:S:27:GLU:HB2	2.23	0.73
9:J:35:GLU:CD	9:J:63:ARG:HE	1.96	0.73
9:K:222:GLU:CD	9:K:228:GLN:HG3	2.14	0.73
12:N:626:TYR:CD2	12:N:633:ARG:HB3	2.22	0.73
3:P:251:TYR:OH	3:P:268:GLN:HG3	1.88	0.73
6:F:550:VAL:HG21	9:K:289:HIS:HB3	1.70	0.73
10:L:44:GLN:HA	10:L:47:ASP:OD2	1.88	0.73
10:L:74:VAL:HG21	10:L:137:ILE:HD11	1.68	0.73
12:N:542:VAL:HG11	12:N:558:GLU:HG2	1.71	0.73
13:O:539:ASN:HD22	13:O:542:GLU:CB	2.01	0.73
1:A:776:ASN:HD22	1:A:779:MET:HG2	1.54	0.72
8:I:81:ALA:HB2	8:I:92:LEU:HB3	1.71	0.72
8:I:177:VAL:HG12	8:I:208:LEU:HD13	1.70	0.72
12:N:542:VAL:HG11	12:N:558:GLU:CG	2.17	0.72
13:O:291:ASN:O	13:O:336:ASP:HB2	1.89	0.72
16:S:40:THR:HG21	16:S:87:GLN:HB3	1.70	0.72
16:S:193:HIS:NE2	16:S:197:GLN:OE1	2.22	0.72
6:H:707:PHE:HB2	6:H:729:LEU:HD11	1.71	0.72
8:I:26:LEU:CB	8:I:37:LEU:HB3	2.19	0.72
17:X:407:LEU:HD13	17:X:443:THR:HG21	1.72	0.72
8:I:302:ASP:CA	8:I:303:GLU:N	2.51	0.72
9:J:24:PHE:CE1	9:J:28:LYS:HE3	2.24	0.72
16:S:30:GLN:CA	16:S:36:ARG:NH2	2.52	0.72
16:S:163:GLU:CG	16:S:196:PHE:HE1	2.02	0.72
1:A:482:VAL:HG12	1:A:487:THR:O	1.90	0.72
1:A:1138:HIS:HE1	1:A:1604:GLN:HE21	1.37	0.72
9:K:185:LEU:HA	9:K:188:LEU:HD21	1.70	0.72
16:S:22:TRP:HZ3	16:S:41:LEU:CG	2.02	0.72
17:Y:442:GLN:HG2	17:Y:472:ARG:HG3	1.71	0.72
3:C:358:LEU:HD21	3:C:368:TRP:CD2	2.24	0.72
9:J:441:VAL:O	9:J:442:ASP:HB3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:63:ARG:HB2	9:K:65:LEU:CD1	2.19	0.72
16:S:132:CYS:CB	16:S:135:PRO:CG	2.64	0.72
1:A:1753:TYR:HD2	13:O:643:LEU:HD12	1.53	0.72
6:H:754:HIS:CE1	6:H:755:LEU:HD13	2.25	0.72
1:A:1284:GLU:HB2	1:A:1350:TYR:CE2	2.24	0.72
8:I:674:VAL:O	8:I:703:ARG:NH1	2.23	0.72
12:N:520:ARG:HD2	12:N:556:PHE:CD1	2.25	0.72
3:C:238:TYR:CD1	3:C:243:LEU:HD12	2.24	0.72
6:F:30:ARG:HD2	6:H:469:MET:HE1	1.71	0.72
8:I:72:ALA:O	8:I:80:LEU:HD12	1.89	0.72
11:M:17:ASP:HA	11:M:20:ARG:HG2	1.71	0.72
16:S:30:GLN:HB2	16:S:91:GLN:HA	1.72	0.72
8:I:48:ARG:HG3	8:I:55:VAL:CG2	2.20	0.72
13:O:620:ALA:O	13:O:624:VAL:HG23	1.90	0.72
8:I:65:GLY:H	8:I:84:LEU:HG	1.54	0.71
3:C:242:GLN:O	3:C:244:ILE:HG13	1.91	0.71
16:S:163:GLU:CG	16:S:196:PHE:CE1	2.73	0.71
2:B:16:TRP:CH2	12:N:630:LYS:HE2	2.24	0.71
3:C:36:LEU:HD21	3:C:58:LEU:HB2	1.73	0.71
1:A:1089:LEU:HD11	1:A:1611:VAL:CG2	2.20	0.71
3:C:414:MET:HG2	13:O:330:ILE:HD11	1.73	0.71
8:I:88:LYS:O	8:I:106:VAL:HG22	1.90	0.71
8:I:294:LYS:CB	8:I:320:LEU:HB2	2.20	0.71
9:K:406:HIS:ND1	7:W:6:PRO:HB3	2.05	0.71
12:N:395:ASP:OD1	12:N:398:THR:N	2.24	0.71
17:Y:45:ALA:HB3	17:Y:82:TYR:CE2	2.25	0.71
1:A:116:ALA:O	13:O:266:ASP:HA	1.90	0.71
6:F:656:MET:HG3	17:Y:526:GLN:HB2	1.72	0.71
12:N:60:GLU:O	12:N:63:ALA:HB2	1.91	0.71
3:P:355:GLN:HA	3:P:358:LEU:HD23	1.70	0.71
16:S:30:GLN:HB2	16:S:91:GLN:HB2	1.73	0.71
8:I:116:MET:SD	8:I:210:LEU:HG	2.31	0.71
12:N:120:SER:O	12:N:124:PRO:CD	2.39	0.71
16:S:83:SER:HB2	16:S:87:GLN:HE21	1.56	0.71
1:A:1469:CYS:HB2	1:A:1488:LEU:CD2	2.19	0.71
9:K:45:GLN:HA	9:K:45:GLN:HE21	1.54	0.71
12:N:343:GLU:O	12:N:347:ILE:N	2.23	0.71
1:A:1624:VAL:HG22	1:A:1698:TYR:HD2	1.56	0.71
7:G:6:PRO:HB3	9:J:406:HIS:HD2	1.55	0.71
8:I:300:VAL:HG21	8:I:456:PHE:HB2	1.73	0.71
8:I:500:PHE:HE2	8:I:507:LEU:HD12	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:362:LYS:CG	12:N:410:LEU:HD23	2.20	0.71
17:Y:42:ARG:CG	17:Y:82:TYR:OH	2.39	0.71
2:B:14:TRP:CB	2:B:15:LEU:HB2	2.21	0.71
17:X:442:GLN:HE21	17:X:472:ARG:HG3	1.55	0.71
9:K:222:GLU:HB3	9:K:228:GLN:OE1	1.90	0.70
12:N:563:ASP:OD2	12:N:597:SER:HB3	1.90	0.70
12:N:425:ARG:CZ	12:N:507:SER:HB2	2.21	0.70
14:Q:410:HIS:CD2	14:Q:475:LEU:HD11	2.26	0.70
15:R:247:SER:HB2	16:S:170:LYS:NZ	2.05	0.70
16:S:64:TYR:O	16:S:68:PHE:CD2	2.44	0.70
16:S:66:ILE:CA	16:S:69:TYR:HD2	2.02	0.70
16:S:68:PHE:CZ	16:S:81:TYR:CB	2.75	0.70
1:A:1645:GLU:HG3	1:A:1646:GLN:H	1.56	0.70
1:A:1786:MET:HA	1:A:1786:MET:CE	2.21	0.70
13:O:706:CYS:HB3	13:O:709:ARG:HB3	1.73	0.70
1:A:801:PRO:HB2	1:A:841:PRO:HG3	1.74	0.70
3:C:39:ILE:HD13	3:C:201:LEU:HB2	1.73	0.70
9:J:254:THR:CG2	9:J:271:HIS:CD2	2.75	0.70
13:O:127:HIS:O	13:O:128:LYS:HB3	1.91	0.70
17:X:442:GLN:NE2	17:X:472:ARG:NE	2.29	0.70
12:N:519:TYR:OH	12:N:541:ASN:HB3	1.90	0.70
16:S:132:CYS:CB	16:S:135:PRO:CD	2.69	0.70
17:X:192:TYR:HA	17:X:195:VAL:HG22	1.73	0.70
8:I:279:ILE:HB	8:I:340:SER:CB	2.22	0.70
9:J:465:LEU:HA	9:J:488:ILE:CD1	2.20	0.70
13:O:479:GLU:O	13:O:656:ALA:O	2.09	0.70
1:A:1390:PRO:HG2	1:A:1396:LEU:HG	1.74	0.70
9:K:417:GLU:HB2	9:K:420:THR:OG1	1.92	0.70
3:P:39:ILE:HD13	3:P:201:LEU:HB2	1.72	0.70
17:X:442:GLN:NE2	17:X:472:ARG:HG3	2.07	0.70
1:A:482:VAL:HG11	1:A:485:ILE:HD12	1.74	0.70
15:R:74:PRO:HB2	15:R:75:GLY:HA2	1.72	0.70
8:I:73:TRP:CG	8:I:80:LEU:HD13	2.26	0.70
8:I:231:VAL:HG21	8:I:557:TYR:CZ	2.27	0.70
8:I:306:HIS:CE1	8:I:313:ALA:O	2.44	0.70
16:S:22:TRP:HH2	16:S:38:MET:HA	1.38	0.70
16:S:25:SER:H	16:S:45:LEU:HD21	1.57	0.70
16:S:78:TRP:CE3	16:S:105:ALA:HB2	2.26	0.70
2:B:16:TRP:C	2:B:31:ASN:O	2.28	0.70
6:H:761:SER:O	6:H:765:ASP:HB2	1.92	0.70
9:J:475:ILE:HD11	9:J:478:ASN:HD22	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:312:LYS:HE2	8:I:428:MET:HA	1.72	0.69
3:P:276:ILE:HG22	3:P:277:ARG:N	2.06	0.69
16:S:79:ASP:OD2	16:S:120:ARG:HB3	1.91	0.69
17:Y:186:ARG:HA	17:Y:189:VAL:HG12	1.75	0.69
2:B:16:TRP:HB3	2:B:33:CYS:N	2.08	0.69
3:C:416:PHE:HB2	3:C:446:LEU:HD11	1.74	0.69
8:I:290:PHE:HE1	8:I:324:GLN:CB	2.05	0.69
3:P:252:GLN:O	3:P:255:ILE:HG22	1.92	0.69
17:Y:192:TYR:HA	17:Y:195:VAL:HG22	1.74	0.69
1:A:980:ARG:NH1	1:A:1674:TRP:CD1	2.61	0.69
8:I:289:LYS:CG	8:I:324:GLN:OE1	2.38	0.69
8:I:290:PHE:HA	8:I:320:LEU:CD1	2.22	0.69
16:S:75:LEU:HD13	16:S:75:LEU:C	2.17	0.69
3:C:358:LEU:HD13	3:C:367:ALA:HB3	1.75	0.69
8:I:46:LEU:HD22	8:I:56:TRP:HE1	1.58	0.69
9:J:185:LEU:HD13	9:J:206:GLU:OE1	1.92	0.69
9:J:439:VAL:HG21	9:J:448:LEU:HD21	1.73	0.69
13:O:657:ILE:HA	13:O:660:LYS:CB	2.22	0.69
16:S:64:TYR:HH	16:S:84:TRP:CD1	2.09	0.69
1:A:1332:GLY:O	1:A:1358:ILE:HG13	1.92	0.69
10:L:105:LEU:HD12	10:L:138:GLN:OE1	1.93	0.69
14:Q:146:ASN:C	14:Q:420:PHE:HE1	2.00	0.69
16:S:195:GLN:O	16:S:199:ARG:HG3	1.91	0.69
17:Y:503:LEU:O	17:Y:506:GLN:NE2	2.25	0.69
14:Q:131:LEU:HD13	18:Z:163:VAL:HG11	1.74	0.69
15:R:112:HIS:NE2	15:R:116:TRP:HZ3	1.91	0.69
6:F:554:VAL:HG21	9:K:286:TYR:HD1	1.56	0.69
8:I:574:PHE:HE2	8:I:576:TRP:HB2	1.57	0.69
12:N:350:ASP:CB	12:N:351:PHE:HA	2.23	0.69
4:D:8:LEU:HD23	13:O:420:ILE:HD11	1.73	0.69
6:H:168:PHE:CB	6:H:467:ARG:HD3	2.23	0.69
6:H:653:LEU:CD2	9:K:523:ILE:HG21	2.22	0.69
13:O:539:ASN:ND2	13:O:542:GLU:HB2	2.08	0.69
16:S:22:TRP:HZ3	16:S:41:LEU:CD1	2.04	0.69
6:H:730:LYS:HD3	6:H:740:TYR:HE1	1.56	0.69
8:I:214:LEU:O	8:I:238:THR:OG1	2.11	0.69
9:J:454:VAL:C	9:J:458:LEU:HD12	2.17	0.69
14:Q:166:ARG:NH2	14:Q:413:GLU:OE1	2.24	0.69
16:S:22:TRP:CZ3	16:S:41:LEU:HB3	2.25	0.69
1:A:763:PHE:CD1	1:A:793:LEU:HD22	2.29	0.68
2:B:17:VAL:O	2:B:30:PHE:O	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:434:ARG:HD2	15:R:80:ILE:HD13	1.74	0.68
6:H:685:SER:O	6:H:689:LEU:HD12	1.92	0.68
12:N:597:SER:OG	12:N:600:PHE:HB2	1.93	0.68
16:S:71:GLY:HA2	16:S:74:PRO:HD2	1.75	0.68
4:D:16:LEU:HD23	4:D:16:LEU:H	1.57	0.68
17:X:445:THR:O	17:X:449:THR:HG23	1.93	0.68
6:F:133:LYS:HA	6:F:136:GLU:OE1	1.94	0.68
12:N:769:SER:OG	12:N:772:ARG:HD3	1.93	0.68
13:O:274:LEU:HD11	13:O:306:ASN:HB3	1.76	0.68
3:P:283:LEU:HD21	3:P:312:MET:CE	2.24	0.68
16:S:29:VAL:CB	16:S:36:ARG:HH12	2.05	0.68
17:Y:270:ASN:HB2	17:Y:273:LEU:HB3	1.74	0.68
1:A:1469:CYS:HB2	1:A:1488:LEU:HD21	1.76	0.68
8:I:269:LEU:CB	8:I:526:LYS:HZ2	2.07	0.68
9:K:285:PHE:HB2	9:K:308:TYR:CE1	2.28	0.68
9:K:384:SER:HB2	9:K:415:ASN:HD21	1.59	0.68
15:R:107:PRO:O	15:R:109:LYS:HE2	1.93	0.68
17:Y:407:LEU:HD13	17:Y:443:THR:HG21	1.74	0.68
1:A:857:MET:CB	1:A:858:PRO:HD3	2.24	0.68
1:A:1089:LEU:HD11	1:A:1611:VAL:HG23	1.74	0.68
17:X:503:LEU:O	17:X:506:GLN:NE2	2.27	0.68
17:Y:371:ASN:H	17:Y:371:ASN:HD22	1.40	0.68
1:A:1329:MET:HE2	1:A:1368:THR:HA	1.76	0.68
2:B:16:TRP:HH2	12:N:630:LYS:HG2	1.59	0.68
8:I:67:GLU:O	8:I:85:ALA:N	2.19	0.68
8:I:414:PHE:CE1	8:I:451:PHE:CE1	2.82	0.68
9:K:185:LEU:HD13	9:K:209:LEU:HD11	1.75	0.68
9:K:495:PHE:CZ	9:K:525:MET:HG2	2.28	0.68
12:N:285:PHE:O	12:N:289:PHE:HD1	1.76	0.68
12:N:350:ASP:HB3	12:N:351:PHE:HA	1.76	0.68
7:G:4:ARG:HH21	9:J:345:ALA:HB1	1.57	0.68
1:A:980:ARG:NH2	1:A:1674:TRP:O	2.27	0.68
3:C:388:TYR:HB2	3:C:405:LEU:HD13	1.76	0.68
6:F:554:VAL:HG21	9:K:286:TYR:CD1	2.29	0.68
8:I:360:LEU:HD21	8:I:390:ILE:HG23	1.76	0.68
8:I:417:PHE:CD2	8:I:448:VAL:HG22	2.28	0.68
9:J:285:PHE:HB2	9:J:308:TYR:CE1	2.28	0.68
16:S:86:GLU:CG	16:S:98:MET:CE	2.64	0.68
1:A:1470:LEU:HA	1:A:1522:SER:OG	1.93	0.68
2:B:27:ARG:CB	12:N:810:TYR:HE2	2.06	0.68
14:Q:166:ARG:CZ	14:Q:436:VAL:HG11	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:417:TYR:CD2	17:X:429:MET:HE1	2.28	0.68
17:Y:294:PHE:CD1	17:Y:294:PHE:C	2.71	0.68
17:Y:407:LEU:CD2	17:Y:437:LEU:HD21	2.24	0.68
1:A:1076:ARG:HE	1:A:1543:HIS:CD2	2.11	0.68
8:I:287:LEU:HG	8:I:456:PHE:CZ	2.29	0.68
3:C:434:ARG:CD	15:R:80:ILE:HG21	2.24	0.67
4:D:13:THR:HG22	13:O:255:TYR:HE2	1.59	0.67
9:J:332:THR:HA	9:J:363:LEU:CD2	2.21	0.67
9:J:397:ILE:HG22	9:J:398:ALA:H	1.59	0.67
8:I:290:PHE:C	8:I:320:LEU:CD1	2.67	0.67
9:K:62:SER:C	9:K:63:ARG:HG3	2.19	0.67
13:O:75:LEU:HB3	13:O:79:TYR:HE2	1.54	0.67
3:P:358:LEU:HD11	3:P:368:TRP:CE2	2.29	0.67
2:B:16:TRP:CD1	2:B:44:CYS:SG	2.88	0.67
2:B:76:CYS:SG	2:B:78:GLN:HG2	2.34	0.67
8:I:317:LEU:HD22	8:I:320:LEU:HD23	1.76	0.67
13:O:114:ASP:C	13:O:117:ASP:OD1	2.37	0.67
8:I:574:PHE:CE2	8:I:576:TRP:HB2	2.28	0.67
16:S:21:GLU:C	16:S:45:LEU:HD13	2.18	0.67
16:S:78:TRP:CE3	16:S:105:ALA:CB	2.77	0.67
16:S:163:GLU:OE1	16:S:196:PHE:HE1	1.75	0.67
8:I:290:PHE:CB	8:I:320:LEU:HD11	2.24	0.67
8:I:306:HIS:ND1	8:I:313:ALA:HB1	2.10	0.67
17:X:442:GLN:HG2	17:X:472:ARG:HG3	1.76	0.67
17:Y:442:GLN:CG	17:Y:472:ARG:HG3	2.24	0.67
17:Y:445:THR:O	17:Y:449:THR:HG23	1.93	0.67
1:A:1153:ILE:HD11	1:A:1184:HIS:HB3	1.76	0.67
8:I:489:PRO:HB2	8:I:490:PRO:C	2.19	0.67
3:P:233:PHE:CE1	3:P:237:ILE:HD11	2.28	0.67
1:A:1186:THR:HG23	1:A:1215:ALA:HB1	1.76	0.67
1:A:1470:LEU:HD12	1:A:1518:VAL:HG13	1.75	0.67
10:L:89:TYR:O	10:L:151:THR:HG22	1.95	0.67
15:R:109:LYS:O	15:R:113:GLN:HG3	1.95	0.67
16:S:197:GLN:O	16:S:200:VAL:CG2	2.41	0.67
17:X:442:GLN:CG	17:X:472:ARG:NE	2.58	0.67
18:Z:158:ASP:O	18:Z:160:ASP:N	2.28	0.67
1:A:939:PHE:HZ	1:A:944:LEU:HD13	1.59	0.67
8:I:15:GLY:O	8:I:743:VAL:N	2.26	0.67
13:O:657:ILE:HA	13:O:660:LYS:HB3	1.77	0.67
16:S:30:GLN:CB	16:S:91:GLN:HB2	2.24	0.67
16:S:83:SER:O	16:S:87:GLN:N	2.21	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:417:TYR:CD2	17:Y:429:MET:HE1	2.29	0.67
3:C:414:MET:CG	13:O:330:ILE:HD11	2.25	0.67
2:B:14:TRP:HB2	2:B:15:LEU:HB2	1.76	0.66
8:I:28:TRP:NE1	8:I:723:ALA:O	2.28	0.66
8:I:312:LYS:HG2	8:I:428:MET:HB3	1.76	0.66
1:A:1287:TYR:CD1	1:A:1287:TYR:O	2.48	0.66
6:F:168:PHE:CB	6:F:467:ARG:HD3	2.24	0.66
6:H:762:TRP:CA	6:H:765:ASP:HB3	2.25	0.66
16:S:22:TRP:CE3	16:S:41:LEU:HB3	2.30	0.66
17:X:66:ASN:ND2	17:Y:268:ARG:HB3	2.10	0.66
6:F:562:MET:HB2	6:H:59:ARG:HH12	1.58	0.66
13:O:544:VAL:CG2	13:O:567:LEU:HG	2.25	0.66
9:K:487:TYR:HE1	9:K:518:MET:HE3	1.59	0.66
12:N:165:THR:N	12:N:166:PRO:HA	2.10	0.66
2:B:16:TRP:NE1	2:B:44:CYS:SG	2.67	0.66
8:I:13:VAL:HG22	8:I:744:PHE:CE2	2.31	0.66
17:Y:104:LEU:HD11	17:Y:142:MET:SD	2.36	0.66
1:A:1399:VAL:HG11	1:A:1404:LEU:HG	1.76	0.66
3:C:411:ILE:HG22	15:R:95:LEU:HD23	1.78	0.66
8:I:73:TRP:CD1	8:I:80:LEU:HD13	2.31	0.66
8:I:269:LEU:HB2	8:I:526:LYS:NZ	2.10	0.66
8:I:290:PHE:CE1	8:I:324:GLN:HB3	2.27	0.66
14:Q:131:LEU:CD1	18:Z:163:VAL:HG11	2.26	0.66
16:S:23:GLU:OE2	18:Z:134:GLN:HA	1.96	0.66
16:S:30:GLN:HB2	16:S:91:GLN:CB	2.25	0.66
1:A:1051:VAL:HG21	1:A:1066:LYS:HB3	1.78	0.66
1:A:1138:HIS:HD2	1:A:1608:HIS:NE2	1.94	0.66
1:A:1750:PHE:HD1	13:O:605:LEU:HD11	1.60	0.66
8:I:349:ILE:CD1	13:O:407:LEU:HA	2.26	0.66
8:I:536:CYS:O	8:I:540:PRO:HD3	1.96	0.66
16:S:58:GLN:HG3	16:S:62:PHE:CZ	2.29	0.66
3:C:416:PHE:CE2	13:O:323:ALA:HB2	2.31	0.66
8:I:295:ASN:O	8:I:316:GLU:CD	2.39	0.66
8:I:313:ALA:HB3	8:I:317:LEU:CG	2.26	0.66
13:O:417:LEU:HA	13:O:420:ILE:HG22	1.78	0.66
14:Q:475:LEU:O	14:Q:476:ASP:HB3	1.94	0.66
3:C:251:TYR:HB3	3:C:269:ILE:HD11	1.78	0.66
12:N:74:TRP:CZ2	12:N:77:GLU:HB2	2.31	0.66
1:A:949:PHE:HA	1:A:952:ALA:HB3	1.77	0.66
3:C:521:PHE:CD1	3:C:553:ILE:HG22	2.31	0.66
6:H:743:ILE:CG2	6:H:759:ASN:HD21	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:24:ILE:O	8:I:569:LEU:HD22	1.96	0.66
6:H:765:ASP:O	17:X:397:ARG:NH2	2.29	0.65
12:N:280:GLU:HA	12:N:281:TYR:HD1	1.61	0.65
1:A:38:GLN:HE21	3:C:396:LYS:H	1.41	0.65
6:F:50:ARG:HE	6:H:19:TYR:HE1	1.44	0.65
9:K:250:CYS:HG	9:K:274:THR:HG21	1.60	0.65
3:P:36:LEU:HD21	3:P:58:LEU:HB2	1.78	0.65
15:R:98:GLU:HG2	15:R:101:PRO:HG3	1.77	0.65
16:S:82:ILE:HD11	16:S:124:LEU:CD2	2.25	0.65
17:X:203:LEU:HD21	17:X:239:TRP:CH2	2.31	0.65
17:X:414:ILE:HD11	17:X:451:CYS:SG	2.36	0.65
1:A:1196:TYR:HB2	1:A:1208:LEU:HD11	1.78	0.65
2:B:39:VAL:N	2:B:40:PRO:HD2	2.12	0.65
3:C:314:SER:HB2	9:J:289:HIS:CE1	2.31	0.65
9:J:37:PRO:HB3	9:J:69:TYR:CZ	2.32	0.65
6:H:121:LEU:HG	6:H:125:TYR:CE1	2.32	0.65
9:J:429:LEU:HA	9:J:432:ILE:HG22	1.79	0.65
12:N:202:GLU:HB2	12:N:282:GLU:OE2	1.96	0.65
3:C:368:TRP:HB3	3:C:391:ALA:HB2	1.78	0.65
6:F:67:THR:HG21	17:Y:263:LYS:HD3	1.78	0.65
6:F:469:MET:HE1	6:H:30:ARG:HD2	1.79	0.65
12:N:538:GLU:HG2	12:N:561:LEU:CG	2.25	0.65
16:S:29:VAL:CA	16:S:36:ARG:NH1	2.55	0.65
1:A:150:CYS:HB3	1:A:163:SER:HA	1.78	0.65
1:A:1797:ILE:HG22	1:A:1852:ILE:HD11	1.78	0.65
8:I:420:TRP:HB2	8:I:440:MET:HE1	1.79	0.65
16:S:163:GLU:OE1	16:S:196:PHE:HD1	1.79	0.65
17:X:40:HIS:HB3	17:Y:201:LEU:CD1	2.24	0.65
1:A:1321:VAL:HG22	1:A:1322:PRO:HD3	1.79	0.65
3:C:477:HIS:HD2	3:C:482:GLU:OE1	1.80	0.65
13:O:75:LEU:C	13:O:79:TYR:CD2	2.75	0.65
13:O:658:LEU:HD13	13:O:704:VAL:HG11	1.78	0.65
1:A:175:PHE:CD1	1:A:191:ARG:HG3	2.31	0.65
1:A:1306:CYS:HB2	1:A:1374:ILE:HG12	1.76	0.65
2:B:17:VAL:CG1	12:N:632:MET:HB3	2.26	0.65
8:I:311:GLY:C	8:I:428:MET:SD	2.79	0.65
8:I:348:VAL:HB	8:I:404:LEU:HD21	1.76	0.65
17:X:371:ASN:HD22	17:X:371:ASN:H	1.43	0.65
1:A:1799:ARG:HD3	1:A:1805:MET:CB	2.26	0.65
3:C:531:THR:O	3:C:535:LYS:HG2	1.97	0.65
8:I:279:ILE:CG1	8:I:340:SER:HB2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:295:ASN:O	8:I:316:GLU:CG	2.45	0.65
9:J:354:MET:HE3	9:J:354:MET:HA	1.79	0.65
9:K:376:LEU:HG	9:K:407:GLU:OE1	1.97	0.65
15:R:98:GLU:CB	15:R:101:PRO:HD3	2.26	0.65
1:A:1333:HIS:HB2	1:A:1357:THR:HA	1.78	0.65
13:O:35:ILE:HG21	13:O:158:LEU:HD13	1.78	0.65
16:S:68:PHE:CZ	16:S:81:TYR:HB2	2.32	0.65
16:S:82:ILE:HD11	16:S:124:LEU:HD22	1.79	0.65
1:A:1405:LEU:HD13	1:A:1467:GLY:HA2	1.78	0.64
8:I:206:LEU:HD22	8:I:570:PHE:CG	2.33	0.64
8:I:337:ILE:HG23	8:I:341:TYR:CE2	2.28	0.64
9:K:254:THR:HG23	9:K:271:HIS:CD2	2.32	0.64
13:O:625:LEU:HD13	13:O:666:LEU:HD22	1.79	0.64
16:S:79:ASP:HB2	16:S:120:ARG:HH11	1.62	0.64
16:S:132:CYS:HB3	16:S:135:PRO:HD3	1.79	0.64
3:P:531:THR:O	3:P:535:LYS:HG2	1.97	0.64
15:R:225:PRO:HB2	16:S:165:ARG:O	1.98	0.64
16:S:144:ASN:HB3	16:S:295:TRP:O	1.97	0.64
17:X:270:ASN:HB2	17:X:273:LEU:CB	2.28	0.64
1:A:611:GLU:O	1:A:645:HIS:NE2	2.30	0.64
8:I:290:PHE:CE1	8:I:324:GLN:CB	2.80	0.64
12:N:74:TRP:CE3	12:N:76:VAL:HG13	2.32	0.64
13:O:460:GLN:HG2	13:O:496:ARG:NH2	2.11	0.64
14:Q:166:ARG:NH1	14:Q:436:VAL:HG11	2.12	0.64
6:F:707:PHE:HB2	6:F:729:LEU:HD11	1.80	0.64
9:K:210:LYS:O	9:K:212:TYR:N	2.28	0.64
17:X:407:LEU:CD2	17:X:437:LEU:HD21	2.26	0.64
1:A:1162:LYS:HG3	1:A:1163:PRO:CD	2.24	0.64
1:A:1475:ARG:HG2	1:A:1476:PHE:CE1	2.32	0.64
8:I:115:TRP:CZ3	8:I:176:LEU:HD22	2.32	0.64
12:N:392:ASN:O	12:N:395:ASP:HA	1.98	0.64
16:S:71:GLY:O	16:S:74:PRO:C	2.40	0.64
3:P:233:PHE:CZ	3:P:237:ILE:CD1	2.79	0.64
16:S:22:TRP:HA	16:S:45:LEU:CD1	2.26	0.64
17:X:270:ASN:HB2	17:X:273:LEU:HB3	1.79	0.64
1:A:1619:LEU:HD11	1:A:1697:LEU:HB2	1.77	0.64
6:H:703:PRO:HB3	6:H:733:VAL:HG21	1.78	0.64
9:J:40:ILE:HD13	9:J:63:ARG:HD3	1.79	0.64
9:J:294:LEU:HD12	9:K:54:HIS:NE2	2.13	0.64
12:N:622:TYR:O	12:N:626:TYR:HB2	1.98	0.64
16:S:134:GLU:O	16:S:134:GLU:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:442:GLN:CG	17:X:472:ARG:HG3	2.27	0.64
6:H:145:ASN:HB2	6:H:146:PRO:O	1.97	0.64
10:L:45:LEU:O	10:L:155:GLN:OE1	2.16	0.64
1:A:1540:ARG:CZ	12:N:486:ASP:O	2.45	0.64
8:I:265:ILE:HD11	8:I:396:PHE:CE2	2.33	0.64
3:P:441:GLU:HG3	3:P:472:LYS:HZ1	1.63	0.64
17:X:159:LEU:HD22	17:X:171:ILE:HG23	1.80	0.64
17:Y:215:LYS:O	17:Y:219:VAL:HG23	1.98	0.64
8:I:321:LEU:HD11	8:I:425:MET:HE2	1.80	0.63
12:N:202:GLU:O	12:N:204:ASP:N	2.31	0.63
3:P:368:TRP:HB3	3:P:391:ALA:HB2	1.80	0.63
17:X:215:LYS:O	17:X:219:VAL:HG23	1.98	0.63
1:A:1100:LEU:HB3	1:A:1101:PRO:HA	1.79	0.63
8:I:73:TRP:CE2	8:I:80:LEU:HD22	2.32	0.63
9:J:445:GLU:HA	9:J:474:LEU:HD23	1.79	0.63
9:K:372:LEU:HD11	9:K:407:GLU:HG3	1.80	0.63
14:Q:166:ARG:NH1	14:Q:413:GLU:OE1	2.31	0.63
16:S:84:TRP:O	16:S:88:ASN:ND2	2.31	0.63
2:B:16:TRP:CH2	12:N:630:LYS:HG2	2.34	0.63
8:I:279:ILE:CB	8:I:340:SER:HB2	2.28	0.63
8:I:305:MET:HB2	13:O:61:ASN:ND2	2.14	0.63
9:K:77:ALA:CB	9:K:93:LEU:HD11	2.27	0.63
12:N:78:VAL:O	12:N:80:GLN:N	2.31	0.63
1:A:174:PRO:HA	1:A:360:VAL:O	1.99	0.63
6:F:696:ILE:HD11	6:F:709:ARG:HD3	1.81	0.63
8:I:24:ILE:HG22	8:I:38:ALA:O	1.98	0.63
1:A:1229:SER:O	1:A:1236:LEU:HB2	1.98	0.63
1:A:1601:TYR:HH	10:L:102:PHE:HD1	1.45	0.63
3:C:61:SER:HB2	3:C:262:SER:HB2	1.79	0.63
6:H:130:ARG:HH12	9:K:473:VAL:HG22	1.64	0.63
8:I:313:ALA:CB	8:I:317:LEU:CD1	2.72	0.63
17:Y:159:LEU:HD22	17:Y:171:ILE:HG23	1.81	0.63
17:Y:373:VAL:HG11	17:Y:403:ALA:HB2	1.79	0.63
1:A:1327:GLN:HA	1:A:1330:VAL:HG12	1.80	0.63
12:N:296:VAL:O	12:N:299:TRP:HB3	1.99	0.63
12:N:765:LEU:HD21	16:S:200:VAL:CG2	2.20	0.63
1:A:1230:ILE:HA	1:A:1236:LEU:HD22	1.81	0.63
1:A:1409:LEU:HG	1:A:1470:LEU:HD22	1.79	0.63
8:I:402:GLU:O	8:I:406:VAL:HG23	1.98	0.63
8:I:427:ARG:HB2	8:I:428:MET:HE2	1.80	0.63
15:R:225:PRO:HG2	16:S:166:GLU:CB	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:452:LEU:HB3	17:X:461:ALA:HB2	1.81	0.63
17:Y:270:ASN:HB2	17:Y:273:LEU:CB	2.28	0.63
1:A:1511:ASN:HD22	1:A:1511:ASN:N	1.96	0.63
8:I:321:LEU:HD21	8:I:425:MET:HG2	1.81	0.63
8:I:330:LEU:HD11	8:I:422:TYR:HB2	1.79	0.63
12:N:501:ILE:H	12:N:501:ILE:HD12	1.62	0.63
12:N:554:MET:HE2	12:N:554:MET:HA	1.80	0.63
15:R:208:LEU:CD1	15:R:255:VAL:CG2	2.77	0.63
6:H:478:SER:HA	6:H:633:ARG:HH22	1.63	0.62
13:O:119:PHE:HE1	13:O:136:LEU:HD21	1.63	0.62
14:Q:208:LEU:CD1	14:Q:255:VAL:CG2	2.77	0.62
17:X:77:TYR:N	17:X:106:GLN:HE21	1.97	0.62
17:X:100:TYR:CD1	17:X:138:VAL:HG13	2.34	0.62
17:X:203:LEU:HD22	17:Y:55:LEU:HB3	1.81	0.62
17:Y:452:LEU:HB3	17:Y:461:ALA:HB2	1.81	0.62
8:I:32:ARG:CD	12:N:388:HIS:CE1	2.82	0.62
9:K:429:LEU:HA	9:K:432:ILE:HG22	1.82	0.62
3:P:475:LYS:O	3:P:479:GLN:NE2	2.32	0.62
15:R:475:LEU:O	15:R:476:ASP:HB2	1.98	0.62
16:S:70:THR:O	16:S:74:PRO:HD3	1.98	0.62
1:A:257:MET:HE3	1:A:266:HIS:HB3	1.80	0.62
1:A:1604:GLN:O	1:A:1607:ARG:HB2	1.99	0.62
8:I:17:LYS:CE	8:I:51:SER:O	2.47	0.62
8:I:430:GLU:CD	14:Q:429:LYS:HG2	2.24	0.62
15:R:95:LEU:HB2	15:R:130:ILE:HD11	1.80	0.62
15:R:192:TRP:CD2	15:R:198:LEU:HD13	2.35	0.62
1:A:1227:LEU:O	1:A:1230:ILE:HG22	1.98	0.62
3:C:341:TYR:OH	11:M:25:PRO:HD3	2.00	0.62
8:I:231:VAL:HG21	8:I:557:TYR:CE1	2.34	0.62
8:I:310:TRP:HB2	8:I:313:ALA:CA	2.29	0.62
9:K:19:TYR:CD1	9:K:49:LEU:HD13	2.35	0.62
9:K:292:VAL:HG21	11:M:57:TRP:HB3	1.81	0.62
10:L:148:GLY:HA2	16:S:270:SER:HB3	1.79	0.62
12:N:180:PHE:HD1	12:N:299:TRP:CZ3	2.08	0.62
3:P:358:LEU:O	3:P:362:PRO:HA	1.98	0.62
1:A:1351:GLN:O	10:L:42:VAL:HG21	2.00	0.62
9:J:219:VAL:C	9:J:221:PRO:HD3	2.24	0.62
9:J:271:HIS:O	9:J:274:THR:HG22	2.00	0.62
9:K:514:PHE:CE2	7:W:11:LEU:HD13	2.34	0.62
10:L:126:ASP:HB2	10:L:132:THR:HG23	1.78	0.62
12:N:619:LEU:HG	12:N:637:TRP:CH2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:704:VAL:HA	12:N:719:GLU:CD	2.25	0.62
17:X:437:LEU:HB2	17:X:444:LEU:HD11	1.82	0.62
1:A:126:ALA:HA	1:A:152:CYS:O	1.99	0.62
1:A:1677:LEU:HD21	1:A:1687:LEU:HG	1.81	0.62
6:F:89:GLU:OE2	6:F:125:TYR:HE1	1.82	0.62
6:F:500:TRP:HB3	6:H:30:ARG:HH22	1.65	0.62
9:J:520:GLY:O	9:J:523:ILE:HG22	1.99	0.62
16:S:22:TRP:HZ3	16:S:41:LEU:HD12	1.64	0.62
17:Y:196:LEU:O	17:Y:200:PRO:HA	1.99	0.62
17:Y:366:ILE:HD11	17:Y:379:LYS:CD	2.29	0.62
1:A:1555:HIS:O	1:A:1559:HIS:HD2	1.82	0.62
8:I:11:PHE:CE1	8:I:746:MET:HE2	2.34	0.62
8:I:27:VAL:C	8:I:35:ILE:HD12	2.25	0.62
16:S:83:SER:O	16:S:87:GLN:CG	2.47	0.62
17:X:304:LEU:O	17:X:308:MET:HG2	1.99	0.62
18:Z:146:GLU:H	18:Z:146:GLU:CD	2.08	0.62
1:A:1196:TYR:HB3	1:A:1208:LEU:HD11	1.80	0.62
2:B:16:TRP:CB	2:B:33:CYS:HB3	2.29	0.62
2:B:16:TRP:CE2	2:B:44:CYS:N	2.67	0.62
3:C:434:ARG:HD3	15:R:80:ILE:HG21	1.81	0.62
8:I:306:HIS:CG	8:I:313:ALA:HB1	2.34	0.62
9:J:476:PRO:HB3	3:P:182:LEU:HB3	1.82	0.62
12:N:386:LEU:C	12:N:388:HIS:HB3	2.25	0.62
1:A:183:THR:HG22	1:A:249:LEU:HG	1.82	0.62
3:C:358:LEU:O	3:C:362:PRO:HA	1.99	0.62
6:H:146:PRO:HG3	6:H:167:THR:HA	1.82	0.62
18:Z:157:THR:OG1	18:Z:158:ASP:N	2.33	0.62
2:B:16:TRP:HD1	2:B:33:CYS:CA	2.04	0.62
3:C:279:ILE:HD11	15:R:76:GLY:O	2.00	0.62
9:J:77:ALA:CB	9:J:93:LEU:HD11	2.29	0.62
9:J:77:ALA:HB1	9:J:93:LEU:HD11	1.81	0.62
1:A:95:VAL:HG22	1:A:100:VAL:HG22	1.81	0.61
6:F:729:LEU:HD13	6:F:739:VAL:HG22	1.81	0.61
8:I:413:ASN:ND2	8:I:450:GLU:OE1	2.33	0.61
16:S:19:GLY:HA2	16:S:22:TRP:HD1	1.65	0.61
1:A:1867:CYS:HB2	1:A:1881:GLN:NE2	2.16	0.61
9:J:445:GLU:HG2	9:J:446:PRO:CD	2.29	0.61
12:N:281:TYR:CZ	12:N:357:ALA:HA	2.35	0.61
12:N:503:SER:O	12:N:507:SER:HB3	1.99	0.61
6:F:146:PRO:HG3	6:F:167:THR:HA	1.82	0.61
8:I:334:GLY:HA2	8:I:418:PHE:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:626:TYR:HD2	12:N:633:ARG:HB3	1.63	0.61
13:O:222:LEU:O	13:O:226:ASP:O	2.19	0.61
3:P:244:ILE:C	3:P:244:ILE:HD12	2.26	0.61
3:P:344:ARG:NH2	3:P:346:GLN:OE1	2.33	0.61
14:Q:410:HIS:CB	14:Q:475:LEU:HD21	2.22	0.61
17:Y:45:ALA:CB	17:Y:82:TYR:CE2	2.83	0.61
18:Z:39:PRO:O	18:Z:42:THR:HB	1.99	0.61
1:A:1791:ILE:HB	13:O:598:THR:CG2	2.30	0.61
2:B:27:ARG:CD	12:N:813:GLY:HA2	2.29	0.61
9:J:173:HIS:CB	9:J:175:MET:HE3	2.30	0.61
16:S:82:ILE:HD13	16:S:102:LEU:CD2	2.29	0.61
17:Y:462:LYS:HG2	17:Y:485:LEU:CD1	2.30	0.61
1:A:844:ILE:O	1:A:848:VAL:HG23	2.00	0.61
1:A:1332:GLY:C	1:A:1358:ILE:HD12	2.21	0.61
1:A:1380:ASN:HD22	1:A:1383:ILE:HD12	1.65	0.61
6:H:515:TYR:HE2	6:H:545:HIS:CD2	2.19	0.61
14:Q:192:TRP:CD2	14:Q:198:LEU:HD13	2.35	0.61
15:R:98:GLU:HG2	15:R:101:PRO:HD3	1.79	0.61
1:A:39:LEU:HD23	1:A:39:LEU:H	1.64	0.61
8:I:56:TRP:CZ3	8:I:58:PHE:HB2	2.34	0.61
8:I:81:ALA:HA	8:I:92:LEU:HA	1.83	0.61
9:K:222:GLU:OE1	9:K:228:GLN:NE2	2.33	0.61
13:O:529:ASP:O	13:O:532:VAL:HG12	1.99	0.61
1:A:1274:LEU:HG	1:A:1302:LEU:HD11	1.81	0.61
12:N:362:LYS:HA	12:N:410:LEU:CD2	2.29	0.61
12:N:456:GLY:HA2	12:N:548:ARG:HH21	1.65	0.61
15:R:225:PRO:CD	16:S:166:GLU:O	2.46	0.61
16:S:36:ARG:HH11	16:S:90:PRO:CB	2.11	0.61
9:J:185:LEU:HD11	9:J:205:PHE:CB	2.31	0.61
12:N:331:PHE:CZ	12:N:335:ILE:HD11	2.36	0.61
13:O:354:ARG:HD2	13:O:573:LYS:O	2.01	0.61
16:S:25:SER:N	16:S:45:LEU:HD21	2.15	0.61
3:C:344:ARG:HH21	11:M:25:PRO:CG	2.10	0.61
12:N:769:SER:OG	12:N:772:ARG:CD	2.49	0.61
3:C:344:ARG:NH2	11:M:25:PRO:HG2	2.07	0.61
3:C:414:MET:CG	13:O:330:ILE:CD1	2.77	0.61
3:P:94:PHE:O	3:P:97:LYS:HB2	2.01	0.61
16:S:19:GLY:HA2	16:S:22:TRP:CD1	2.35	0.61
17:Y:77:TYR:HB2	17:Y:106:GLN:HG3	1.83	0.61
1:A:1137:PHE:O	1:A:1141:VAL:HG23	2.01	0.60
6:F:699:ASP:HB2	6:F:702:ASN:HD21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:37:PRO:HA	9:J:65:LEU:HD11	1.82	0.60
12:N:351:PHE:HE1	12:N:405:LYS:HB2	1.67	0.60
17:X:407:LEU:HD22	17:X:437:LEU:HD21	1.83	0.60
1:A:662:THR:O	1:A:666:ASN:ND2	2.33	0.60
13:O:114:ASP:HA	13:O:117:ASP:OD1	2.00	0.60
14:Q:411:TYR:CE1	14:Q:475:LEU:HD23	2.36	0.60
16:S:58:GLN:CG	16:S:62:PHE:HE2	1.94	0.60
3:P:170:PHE:O	3:P:173:TYR:N	2.33	0.60
14:Q:475:LEU:O	14:Q:476:ASP:CB	2.48	0.60
16:S:22:TRP:CZ3	16:S:41:LEU:HD12	2.36	0.60
14:Q:127:GLU:O	18:Z:159:LYS:HG2	2.01	0.60
14:Q:341:GLY:O	14:Q:343:GLY:N	2.35	0.60
17:Y:304:LEU:O	17:Y:308:MET:HG2	2.01	0.60
1:A:1640:GLY:N	1:A:1645:GLU:O	2.29	0.60
3:C:94:PHE:O	3:C:97:LYS:HB2	2.01	0.60
16:S:41:LEU:CD1	18:Z:141:PHE:CB	2.80	0.60
17:Y:294:PHE:C	17:Y:294:PHE:HD1	2.10	0.60
9:J:167:PHE:HA	9:J:170:LEU:CD2	2.31	0.60
12:N:362:LYS:CA	12:N:410:LEU:HD21	2.31	0.60
15:R:105:GLN:C	15:R:107:PRO:HD3	2.26	0.60
15:R:116:TRP:O	15:R:120:LEU:N	2.32	0.60
15:R:295:VAL:HG23	16:S:274:VAL:HG23	1.84	0.60
1:A:956:ARG:HD2	1:A:1786:MET:HE3	1.83	0.60
6:F:528:ILE:HG22	6:F:529:GLU:HG3	1.82	0.60
14:Q:146:ASN:C	14:Q:420:PHE:CE1	2.79	0.60
17:X:279:ASP:OD1	17:X:310:VAL:HG21	2.00	0.60
17:Y:83:HIS:O	17:Y:86:SER:OG	2.16	0.60
1:A:213:MET:HE2	1:A:216:PRO:HA	1.83	0.60
1:A:1153:ILE:HG12	1:A:1184:HIS:CD2	2.37	0.60
2:B:16:TRP:CZ2	2:B:45:PRO:CA	2.85	0.60
6:H:528:ILE:HG22	6:H:529:GLU:HG3	1.82	0.60
12:N:676:TRP:O	12:N:713:PHE:HB2	2.01	0.60
14:Q:140:ALA:O	14:Q:141:PRO:CB	2.49	0.60
1:A:39:LEU:HD12	13:O:248:PRO:HB3	1.84	0.59
6:H:656:MET:HE3	9:K:526:TYR:CD2	2.36	0.59
9:K:74:TYR:CZ	9:K:78:ARG:HD2	2.37	0.59
16:S:71:GLY:C	16:S:74:PRO:CD	2.59	0.59
16:S:78:TRP:CZ3	16:S:105:ALA:CA	2.85	0.59
1:A:1218:GLY:N	1:A:1259:LEU:O	2.35	0.59
7:G:3:ARG:HB2	9:J:443:LYS:NZ	2.17	0.59
6:H:594:ILE:HD11	6:H:604:TYR:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:304:PHE:CE2	8:I:452:LEU:HG	2.37	0.59
9:J:17:GLN:CB	9:K:78:ARG:HH12	2.15	0.59
13:O:619:LEU:O	13:O:623:THR:HG22	2.02	0.59
16:S:19:GLY:N	18:Z:134:GLN:HE22	1.97	0.59
8:I:302:ASP:O	8:I:306:HIS:HB2	2.03	0.59
12:N:77:GLU:O	12:N:78:VAL:HG23	2.03	0.59
3:P:389:ARG:O	3:P:392:ILE:HG23	2.02	0.59
17:X:83:HIS:O	17:X:86:SER:OG	2.15	0.59
1:A:1274:LEU:O	1:A:1277:ILE:HG22	2.01	0.59
3:C:145:GLN:HG3	13:O:246:PHE:CD2	2.38	0.59
6:H:73:TYR:CD1	6:H:117:THR:HG22	2.37	0.59
12:N:180:PHE:CD1	12:N:299:TRP:HH2	2.20	0.59
12:N:619:LEU:HG	12:N:637:TRP:CZ2	2.37	0.59
13:O:417:LEU:HA	13:O:420:ILE:CG2	2.32	0.59
1:A:1255:VAL:HG11	1:A:1606:LEU:HD21	1.84	0.59
3:C:377:GLU:HA	15:R:130:ILE:CG2	2.33	0.59
8:I:290:PHE:CZ	8:I:325:LEU:HB2	2.37	0.59
1:A:485:ILE:CD1	1:A:609:ILE:HB	2.32	0.59
8:I:334:GLY:HA2	8:I:418:PHE:CE2	2.38	0.59
12:N:609:LEU:HD22	12:N:639:HIS:CD2	2.38	0.59
8:I:32:ARG:HB2	8:I:34:LEU:CD2	2.33	0.59
8:I:337:ILE:HG22	8:I:341:TYR:HE2	1.65	0.59
8:I:337:ILE:HD13	8:I:418:PHE:HZ	1.68	0.59
12:N:341:ILE:O	12:N:344:LEU:HB3	2.03	0.59
15:R:341:GLY:O	15:R:343:GLY:N	2.35	0.59
17:X:229:THR:HG21	17:X:233:LEU:HD12	1.84	0.59
1:A:23:PHE:HB2	1:A:111:LEU:HD22	1.83	0.59
3:C:317:SER:CB	11:M:27:GLU:HG3	2.32	0.59
8:I:17:LYS:NZ	8:I:51:SER:O	2.35	0.59
8:I:299:SER:O	8:I:303:GLU:HG3	2.02	0.59
9:K:403:PHE:O	9:K:407:GLU:HG2	2.02	0.59
10:L:125:THR:HA	10:L:126:ASP:HB3	1.84	0.59
12:N:73:GLU:O	12:N:74:TRP:HB3	2.01	0.59
17:X:294:PHE:C	17:X:294:PHE:CD1	2.80	0.59
17:Y:434:TYR:HA	17:Y:444:LEU:HD13	1.84	0.59
3:P:234:LEU:HD22	3:P:238:TYR:CE2	2.38	0.59
3:P:389:ARG:HA	3:P:392:ILE:CG2	2.32	0.59
16:S:84:TRP:CE2	16:S:88:ASN:OD1	2.55	0.59
1:A:1167:GLU:O	1:A:1168:LEU:HB3	2.03	0.59
1:A:1177:MET:HE3	1:A:1181:LEU:HD21	1.84	0.59
2:B:46:LEU:HD23	2:B:47:VAL:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:108:ILE:HB	10:L:125:THR:O	2.03	0.59
17:Y:229:THR:HG21	17:Y:233:LEU:HD12	1.84	0.59
1:A:1134:TRP:CE2	1:A:1203:MET:HE1	2.38	0.58
8:I:65:GLY:HA3	8:I:84:LEU:HB3	1.85	0.58
1:A:1194:HIS:HB2	15:R:121:ASN:HD21	1.69	0.58
2:B:64:LEU:HD22	2:B:71:GLN:HA	1.85	0.58
13:O:75:LEU:C	13:O:79:TYR:HD2	2.09	0.58
1:A:1060:HIS:O	1:A:1063:ILE:HG22	2.03	0.58
1:A:1599:ASN:HB2	1:A:1603:LEU:HA	1.85	0.58
9:J:193:LEU:O	9:J:197:GLU:HB2	2.03	0.58
9:J:211:LYS:O	9:J:212:TYR:CG	2.55	0.58
3:P:358:LEU:HD11	3:P:368:TRP:CZ2	2.38	0.58
14:Q:222:MET:HB3	14:Q:227:GLU:HG3	1.85	0.58
1:A:880:TYR:O	1:A:926:LEU:HD21	2.02	0.58
3:C:389:ARG:HG3	13:O:280:ARG:HD3	1.85	0.58
6:F:152:PHE:HE1	6:F:162:PRO:HG2	1.69	0.58
12:N:148:GLY:HA3	12:N:152:GLU:OE2	2.03	0.58
12:N:520:ARG:HG3	12:N:557:CYS:SG	2.43	0.58
13:O:591:TYR:HA	13:O:594:SER:OG	2.03	0.58
3:P:120:TYR:CZ	3:P:124:LEU:HD11	2.39	0.58
16:S:20:ASP:OD2	18:Z:184:ARG:NH1	2.35	0.58
1:A:436:LEU:H	1:A:501:THR:HG23	1.68	0.58
1:A:1230:ILE:HD12	15:R:116:TRP:CD1	2.39	0.58
9:K:77:ALA:HB1	9:K:93:LEU:HD11	1.85	0.58
13:O:328:ILE:O	13:O:332:GLN:HG3	2.03	0.58
3:P:290:ARG:HH21	3:P:319:LEU:CD1	2.14	0.58
17:Y:45:ALA:HB2	17:Y:82:TYR:CD2	2.38	0.58
17:Y:384:ARG:HH22	17:Y:415:GLU:HB3	1.67	0.58
1:A:1404:LEU:HD22	1:A:1464:ILE:HD11	1.85	0.58
2:B:27:ARG:HB2	12:N:810:TYR:HE2	1.67	0.58
3:C:317:SER:HB3	11:M:27:GLU:HG3	1.84	0.58
8:I:413:ASN:O	8:I:447:PHE:CE1	2.52	0.58
9:K:78:ARG:HG3	9:K:135:LEU:HD22	1.84	0.58
17:X:475:TYR:O	17:X:479:VAL:HG23	2.04	0.58
3:C:389:ARG:CG	13:O:280:ARG:HD3	2.34	0.58
6:H:761:SER:O	6:H:765:ASP:CB	2.52	0.58
8:I:500:PHE:CE2	8:I:507:LEU:HD12	2.37	0.58
12:N:278:ARG:HB3	12:N:343:GLU:OE2	2.04	0.58
12:N:699:TRP:CZ3	12:N:728:VAL:HG21	2.39	0.58
17:Y:407:LEU:HD22	17:Y:437:LEU:HD21	1.86	0.58
1:A:1376:LEU:HD23	1:A:1377:LYS:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:LEU:HD13	1:A:1467:GLY:CA	2.33	0.58
2:B:27:ARG:HD2	12:N:813:GLY:HA2	1.83	0.58
9:K:386:LEU:H	9:K:386:LEU:HD12	1.68	0.58
14:Q:208:LEU:HD11	14:Q:255:VAL:HG23	1.86	0.58
16:S:99:SER:HB2	16:S:131:LEU:HD13	1.85	0.58
17:Y:437:LEU:HB2	17:Y:444:LEU:HD11	1.86	0.58
9:J:185:LEU:HD11	9:J:205:PHE:HB3	1.86	0.58
3:P:400:ARG:HG3	14:Q:498:ILE:HB	1.85	0.58
3:C:414:MET:HB3	13:O:326:GLU:HB3	1.85	0.57
6:F:26:PHE:CD1	6:H:149:TRP:HB2	2.38	0.57
9:J:178:ALA:HB1	9:J:213:ASN:HD22	1.69	0.57
9:K:355:ALA:O	9:K:359:THR:HG22	2.04	0.57
12:N:300:LEU:O	12:N:304:PHE:HD1	1.87	0.57
17:Y:294:PHE:CD1	17:Y:294:PHE:O	2.57	0.57
6:H:42:PHE:HB2	6:H:71:CYS:SG	2.43	0.57
12:N:612:PRO:HG2	12:N:615:ILE:HG12	1.85	0.57
16:S:30:GLN:HB2	16:S:91:GLN:CA	2.33	0.57
17:Y:96:ALA:O	17:Y:100:TYR:HD2	1.86	0.57
9:K:406:HIS:CE1	7:W:6:PRO:HB3	2.39	0.57
10:L:63:LEU:HD13	10:L:138:GLN:NE2	2.18	0.57
13:O:75:LEU:HD21	13:O:161:TYR:HE2	1.62	0.57
3:P:61:SER:HB2	3:P:262:SER:HB2	1.85	0.57
3:P:251:TYR:HB3	3:P:269:ILE:HD11	1.85	0.57
3:P:409:TYR:HA	3:P:412:LEU:HD12	1.85	0.57
15:R:222:MET:HB3	15:R:227:GLU:HG3	1.86	0.57
16:S:30:GLN:C	16:S:36:ARG:NH2	2.62	0.57
1:A:214:LEU:HD21	1:A:407:LEU:HD13	1.87	0.57
1:A:961:HIS:ND1	1:A:964:GLU:OE2	2.37	0.57
3:C:170:PHE:O	3:C:173:TYR:N	2.38	0.57
6:F:544:TRP:CD2	15:R:499:ARG:HD3	2.40	0.57
13:O:414:LEU:CD1	13:O:417:LEU:HB2	2.35	0.57
6:H:621:LEU:HB3	6:H:625:ARG:NH2	2.20	0.57
8:I:36:ALA:CB	8:I:80:LEU:HD21	2.35	0.57
9:J:46:CYS:O	9:J:50:THR:OG1	2.22	0.57
12:N:776:MET:HE2	16:S:198:ALA:HA	1.87	0.57
6:F:533:VAL:HG13	6:F:568:GLU:OE1	2.03	0.57
8:I:730:VAL:HG22	8:I:731:SER:N	2.19	0.57
16:S:68:PHE:CE2	16:S:81:TYR:CG	2.88	0.57
17:X:55:LEU:HB3	17:Y:203:LEU:HD12	1.86	0.57
17:X:462:LYS:HG2	17:X:485:LEU:CD1	2.31	0.57
1:A:629:LEU:HD22	1:A:633:ILE:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:VAL:HG11	2:B:60:ILE:HG21	1.85	0.57
3:C:352:LEU:HD21	3:C:356:ARG:CZ	2.35	0.57
3:C:358:LEU:HD21	3:C:368:TRP:CE2	2.40	0.57
8:I:413:ASN:CA	8:I:447:PHE:HZ	1.93	0.57
12:N:60:GLU:C	12:N:63:ALA:HB2	2.30	0.57
16:S:29:VAL:CG1	16:S:36:ARG:HH12	2.08	0.57
16:S:60:ARG:O	16:S:64:TYR:HD2	1.88	0.57
17:X:170:LYS:HA	17:Y:49:LEU:HD21	1.86	0.57
17:Y:529:MET:HE1	17:Y:552:MET:HB3	1.86	0.57
1:A:215:HIS:CD2	1:A:217:LEU:H	2.23	0.57
3:C:120:TYR:CZ	3:C:124:LEU:HD11	2.40	0.57
8:I:56:TRP:CD2	8:I:98:PRO:HB3	2.38	0.57
12:N:765:LEU:HD11	16:S:200:VAL:HG23	1.87	0.57
16:S:68:PHE:HZ	16:S:81:TYR:HB3	1.69	0.57
6:H:121:LEU:O	6:H:125:TYR:HD1	1.87	0.57
13:O:105:LEU:HD11	13:O:151:VAL:CG1	2.35	0.57
17:Y:475:TYR:O	17:Y:479:VAL:HG23	2.03	0.57
9:J:397:ILE:HG22	9:J:398:ALA:N	2.19	0.57
9:K:296:PRO:HB2	11:M:55:MET:HG3	1.86	0.57
12:N:663:GLN:HB3	12:N:699:TRP:CZ2	2.40	0.57
16:S:79:ASP:OD2	16:S:120:ARG:CA	2.52	0.57
16:S:145:GLN:NE2	16:S:296:ILE:CB	2.68	0.57
1:A:92:GLU:OE2	1:A:111:LEU:HD21	2.05	0.56
1:A:257:MET:CE	1:A:266:HIS:HB3	2.35	0.56
1:A:1033:ARG:NH1	1:A:1531:GLY:O	2.37	0.56
1:A:1290:ASP:OD2	1:A:1600:ARG:HA	2.05	0.56
1:A:1532:ASN:HB3	1:A:1535:VAL:HG23	1.86	0.56
2:B:46:LEU:HD21	2:B:54:CYS:HB3	1.86	0.56
6:F:42:PHE:HB2	6:F:71:CYS:SG	2.44	0.56
8:I:276:TRP:NE1	8:I:475:VAL:HB	2.20	0.56
13:O:75:LEU:CB	13:O:79:TYR:HE2	2.18	0.56
15:R:247:SER:HB2	16:S:170:LYS:HZ1	1.69	0.56
16:S:68:PHE:HE1	16:S:78:TRP:CD2	2.23	0.56
17:X:63:MET:CE	17:Y:266:LEU:HD22	2.35	0.56
6:H:669:SER:HA	6:H:698:ILE:HD11	1.86	0.56
9:J:247:PHE:CD2	9:J:277:GLU:HB3	2.40	0.56
9:J:324:SER:O	9:J:328:THR:HG23	2.05	0.56
12:N:596:LEU:HB3	12:N:601:TRP:NE1	2.19	0.56
13:O:599:ILE:O	13:O:602:PRO:HD2	2.05	0.56
13:O:727:THR:O	13:O:730:ARG:HB2	2.05	0.56
14:Q:208:LEU:HD11	14:Q:255:VAL:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:LEU:HA	1:A:1061:GLU:OE1	2.04	0.56
1:A:1086:MET:HG2	1:A:1610:TYR:CZ	2.40	0.56
1:A:1163:PRO:HG3	1:A:1169:ALA:HA	1.86	0.56
1:A:1235:LEU:HD22	1:A:1257:ILE:HG13	1.79	0.56
1:A:1254:VAL:CG1	1:A:1298:ALA:HA	2.36	0.56
6:F:125:TYR:HD1	6:F:130:ARG:HE	1.49	0.56
8:I:34:LEU:HD13	12:N:389:PRO:O	2.05	0.56
8:I:277:GLU:O	8:I:281:MET:N	2.32	0.56
9:K:284:LEU:HD12	9:K:311:MET:HE3	1.87	0.56
9:K:472:LEU:HG	9:K:481:THR:CG2	2.33	0.56
12:N:386:LEU:HD21	12:N:399:LEU:HD22	1.86	0.56
12:N:501:ILE:HD12	12:N:501:ILE:N	2.20	0.56
13:O:136:LEU:C	13:O:136:LEU:HD12	2.30	0.56
14:Q:410:HIS:CG	14:Q:475:LEU:HD11	2.40	0.56
15:R:208:LEU:HD11	15:R:255:VAL:HG23	1.87	0.56
16:S:88:ASN:HD22	16:S:88:ASN:N	2.02	0.56
17:X:54:ARG:NH2	17:X:90:ASP:OD2	2.39	0.56
12:N:202:GLU:OE2	12:N:283:ARG:HB2	2.05	0.56
12:N:648:VAL:HG13	12:N:650:LEU:HG	1.86	0.56
15:R:225:PRO:HG2	16:S:166:GLU:HB2	1.86	0.56
16:S:38:MET:HE1	18:Z:199:TYR:CE2	2.25	0.56
16:S:79:ASP:CG	16:S:120:ARG:HB3	2.30	0.56
16:S:132:CYS:CB	16:S:135:PRO:N	2.68	0.56
17:X:66:ASN:HD21	17:Y:268:ARG:HB3	1.71	0.56
8:I:218:SER:HA	8:I:235:GLN:HA	1.88	0.56
9:J:451:LEU:HD12	9:J:467:TYR:CD2	2.40	0.56
12:N:344:LEU:HA	12:N:347:ILE:HB	1.87	0.56
15:R:98:GLU:HB3	15:R:101:PRO:HD3	1.85	0.56
15:R:208:LEU:HD11	15:R:255:VAL:CG2	2.35	0.56
16:S:38:MET:HB3	18:Z:181:VAL:HG22	1.87	0.56
16:S:271:ARG:HG2	16:S:272:ILE:N	2.21	0.56
17:X:442:GLN:NE2	17:X:472:ARG:CG	2.68	0.56
3:C:89:LEU:HD12	3:P:60:PHE:CG	2.40	0.56
3:C:97:LYS:HG2	3:C:97:LYS:O	2.06	0.56
8:I:269:LEU:CB	8:I:526:LYS:NZ	2.69	0.56
12:N:556:PHE:HA	12:N:600:PHE:CE1	2.41	0.56
13:O:627:LEU:O	13:O:630:ALA:HB3	2.06	0.56
14:Q:216:ILE:HD13	16:S:558:LEU:HB2	1.87	0.56
16:S:68:PHE:CE1	16:S:78:TRP:CD2	2.93	0.56
17:Y:70:LEU:HD12	17:Y:71:PHE:CE2	2.40	0.56
1:A:105:GLY:O	1:A:111:LEU:HG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ASN:HB3	3:C:151:LEU:CG	2.34	0.56
8:I:669:LEU:CD1	8:I:705:MET:HE1	2.36	0.56
12:N:560:MET:HA	12:N:560:MET:CE	2.31	0.56
12:N:592:TYR:HD1	12:N:593:ALA:N	2.04	0.56
17:X:350:PHE:HB2	17:X:351:TYR:CD1	2.41	0.56
17:Y:350:PHE:HB2	17:Y:351:TYR:CD1	2.40	0.56
1:A:167:LYS:HG2	13:O:319:GLN:HE22	1.70	0.56
1:A:1632:ALA:H	1:A:1653:ALA:HB3	1.70	0.56
6:F:73:TYR:CD1	6:F:117:THR:HG22	2.41	0.56
8:I:231:VAL:HG11	8:I:556:LEU:HD12	1.88	0.56
9:K:222:GLU:CD	9:K:228:GLN:CG	2.79	0.56
12:N:704:VAL:HG23	12:N:705:LEU:HD22	1.86	0.56
13:O:44:MET:HE2	13:O:60:LEU:HD21	1.88	0.56
13:O:104:GLU:N	13:O:107:ASP:OD2	2.39	0.56
15:R:74:PRO:CB	15:R:75:GLY:HA2	2.36	0.56
17:Y:199:CYS:HB3	17:Y:201:LEU:HD12	1.87	0.56
17:Y:475:TYR:CE1	17:Y:477:LYS:HB2	2.41	0.56
2:B:64:LEU:HD11	2:B:80:TRP:CD1	2.41	0.56
3:C:301:ASP:OD2	3:C:335:CYS:HB3	2.06	0.56
4:D:3:THR:O	4:D:5:PHE:CE2	2.58	0.56
8:I:262:LEU:HA	8:I:265:ILE:CG2	2.32	0.56
9:J:212:TYR:HB3	9:J:243:TYR:CD1	2.41	0.56
12:N:502:ILE:HA	12:N:505:LEU:HD12	1.88	0.56
16:S:76:ASP:O	16:S:77:VAL:HB	2.06	0.56
17:X:475:TYR:CE1	17:X:477:LYS:HB2	2.41	0.56
17:Y:100:TYR:HB3	17:Y:142:MET:CG	2.35	0.56
2:B:45:PRO:HB2	12:N:631:ALA:HB3	1.87	0.56
3:C:407:GLN:O	3:C:411:ILE:HG12	2.06	0.56
8:I:290:PHE:HD1	8:I:324:GLN:CD	2.15	0.56
16:S:41:LEU:CD2	16:S:90:PRO:HB3	2.36	0.56
8:I:167:LEU:HD12	8:I:168:LEU:N	2.21	0.55
9:J:465:LEU:CA	9:J:488:ILE:HD12	2.35	0.55
16:S:68:PHE:CZ	16:S:81:TYR:CG	2.93	0.55
17:X:100:TYR:HD1	17:X:138:VAL:HG13	1.70	0.55
17:X:168:THR:HB	17:X:169:PRO:HD2	1.88	0.55
17:Y:50:HIS:ND1	17:Y:86:SER:HA	2.21	0.55
17:Y:168:THR:HB	17:Y:169:PRO:HD2	1.88	0.55
6:H:121:LEU:O	6:H:125:TYR:CD1	2.59	0.55
8:I:291:VAL:HG13	8:I:303:GLU:OE2	2.07	0.55
13:O:394:THR:HG22	13:O:615:ARG:HH12	1.70	0.55
13:O:490:LEU:HD13	13:O:511:ASP:HB2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:303:PHE:CD1	3:P:303:PHE:C	2.83	0.55
1:A:1047:VAL:O	1:A:1109:GLY:HA2	2.06	0.55
1:A:1332:GLY:H	1:A:1358:ILE:HB	1.71	0.55
1:A:1399:VAL:CG1	1:A:1404:LEU:HG	2.36	0.55
1:A:1839:PHE:CE1	1:A:1840:MET:HG3	2.41	0.55
6:F:104:ASP:N	6:F:104:ASP:OD1	2.39	0.55
8:I:64:THR:HG22	8:I:84:LEU:HD11	1.87	0.55
12:N:281:TYR:OH	12:N:357:ALA:HA	2.06	0.55
12:N:560:MET:HE1	12:N:601:TRP:CD1	2.41	0.55
3:P:441:GLU:HG3	3:P:472:LYS:NZ	2.21	0.55
16:S:22:TRP:CZ3	16:S:41:LEU:CD1	2.86	0.55
1:A:1573:SER:HB2	1:A:1617:ARG:NH2	2.22	0.55
6:F:730:LYS:HE2	6:F:740:TYR:CE1	2.38	0.55
8:I:306:HIS:CE1	8:I:316:GLU:HB3	2.41	0.55
9:K:284:LEU:HD13	9:K:308:TYR:HB2	1.88	0.55
14:Q:128:ALA:HB1	18:Z:156:TYR:CE2	2.39	0.55
14:Q:352:THR:HB	18:Z:51:LEU:HA	1.88	0.55
16:S:64:TYR:O	16:S:68:PHE:HD2	1.86	0.55
17:X:76:LYS:CB	17:X:106:GLN:NE2	2.69	0.55
17:Y:203:LEU:HA	17:Y:206:ILE:HD12	1.89	0.55
1:A:1351:GLN:O	10:L:32:SER:HA	2.07	0.55
3:P:407:GLN:O	3:P:411:ILE:HG12	2.06	0.55
16:S:60:ARG:O	16:S:64:TYR:CD2	2.60	0.55
8:I:430:GLU:OE2	14:Q:429:LYS:HB3	2.06	0.55
8:I:497:TRP:CH2	8:I:507:LEU:HD13	2.42	0.55
12:N:102:ALA:HA	12:N:107:CYS:C	2.32	0.55
12:N:676:TRP:HE3	12:N:680:GLU:HB3	1.70	0.55
3:P:180:ARG:HG3	3:P:212:LEU:HD21	1.89	0.55
3:P:441:GLU:HG3	3:P:472:LYS:CE	2.37	0.55
14:Q:185:TYR:CE1	16:S:27:GLU:CG	2.87	0.55
15:R:98:GLU:CG	15:R:101:PRO:CD	2.76	0.55
17:X:52:ASN:HD22	17:Y:202:ALA:CB	2.19	0.55
1:A:1054:TYR:O	1:A:1056:GLU:N	2.40	0.55
1:A:1624:VAL:HG22	1:A:1698:TYR:CD2	2.38	0.55
2:B:38:LYS:C	2:B:40:PRO:HD2	2.31	0.55
2:B:42:ASP:O	2:B:43:ASP:HB2	2.07	0.55
8:I:52:PHE:CD1	8:I:743:VAL:HG21	2.42	0.55
8:I:305:MET:CB	13:O:61:ASN:HD21	2.20	0.55
9:K:174:HIS:HA	9:K:211:LYS:HZ3	1.71	0.55
13:O:163:GLN:HB3	13:O:167:LYS:HE3	1.88	0.55
13:O:219:GLN:HE22	13:O:231:LEU:HD13	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:22:TRP:CZ2	16:S:38:MET:O	2.59	0.55
16:S:79:ASP:OD2	16:S:120:ARG:HA	2.06	0.55
1:A:809:ASP:O	1:A:1807:GLU:O	2.24	0.55
1:A:1531:GLY:HA3	1:A:1566:PHE:CE1	2.42	0.55
6:F:699:ASP:HB3	6:F:702:ASN:OD1	2.06	0.55
9:J:337:TRP:HB3	9:J:360:ALA:HB2	1.88	0.55
13:O:105:LEU:HD11	13:O:151:VAL:HG12	1.89	0.55
13:O:439:LEU:HG	13:O:476:LEU:HD13	1.89	0.55
3:C:259:PHE:HB3	3:C:265:ILE:HD12	1.84	0.55
6:F:594:ILE:HD11	6:F:604:TYR:HA	1.88	0.55
8:I:166:LYS:O	8:I:170:ASP:HB2	2.06	0.55
12:N:165:THR:H	12:N:166:PRO:HA	1.71	0.55
13:O:657:ILE:HA	13:O:660:LYS:HB2	1.89	0.55
17:Y:100:TYR:HD1	17:Y:138:VAL:HG13	1.72	0.55
3:C:363:ARG:HG2	3:C:363:ARG:O	2.05	0.55
8:I:213:ASP:OD1	8:I:215:LYS:N	2.24	0.55
8:I:618:ILE:HD12	8:I:705:MET:HE2	1.87	0.55
9:K:258:MET:HG3	9:K:271:HIS:CD2	2.42	0.55
10:L:75:LYS:HB2	10:L:161:PRO:HG3	1.89	0.55
12:N:520:ARG:HD2	12:N:556:PHE:HD1	1.69	0.55
16:S:68:PHE:CE1	16:S:78:TRP:HA	2.42	0.55
17:X:203:LEU:HA	17:X:206:ILE:HD12	1.89	0.55
1:A:1323:GLU:HG3	1:A:1324:GLN:N	2.22	0.54
1:A:1603:LEU:HD22	1:A:1605:ALA:H	1.72	0.54
3:C:417:TYR:CD2	13:O:307:LEU:HD22	2.42	0.54
9:K:324:SER:O	9:K:328:THR:HG23	2.07	0.54
9:K:373:TYR:CE1	7:W:4:ARG:HG2	2.42	0.54
13:O:119:PHE:CE1	13:O:136:LEU:HD11	2.42	0.54
1:A:1610:TYR:O	1:A:1613:ALA:HB3	2.08	0.54
3:C:429:ARG:HG2	3:C:432:ASP:HB2	1.88	0.54
8:I:46:LEU:HD22	8:I:56:TRP:NE1	2.23	0.54
8:I:497:TRP:CD1	13:O:446:LEU:HB3	2.42	0.54
8:I:607:ILE:HD12	8:I:607:ILE:H	1.72	0.54
9:K:177:THR:HG22	9:K:365:LYS:HB3	1.87	0.54
11:M:59:ASP:C	11:M:61:ALA:H	2.14	0.54
12:N:681:LEU:HD22	12:N:713:PHE:CZ	2.42	0.54
3:P:373:HIS:NE2	14:Q:497:GLY:O	2.39	0.54
15:R:305:LEU:HD23	15:R:336:TRP:CD2	2.43	0.54
1:A:1079:ALA:HB1	1:A:1556:LEU:HA	1.89	0.54
3:C:526:TRP:HE1	3:C:556:LEU:HD23	1.72	0.54
14:Q:305:LEU:HD23	14:Q:336:TRP:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:225:PRO:CG	16:S:166:GLU:HB2	2.38	0.54
16:S:78:TRP:CH2	16:S:105:ALA:HA	2.43	0.54
1:A:1189:ALA:HB3	1:A:1192:ASN:HB2	1.89	0.54
2:B:72:HIS:ND1	2:B:77:ARG:HG3	2.21	0.54
3:C:60:PHE:HB2	3:P:89:LEU:HD12	1.90	0.54
7:G:1:MET:HE1	9:J:364:MET:HE1	1.88	0.54
8:I:23:ILE:HD12	8:I:37:LEU:HD23	1.88	0.54
8:I:79:LEU:HD11	8:I:168:LEU:HD23	1.88	0.54
12:N:670:PHE:CD1	12:N:715:VAL:HB	2.42	0.54
13:O:354:ARG:HD3	13:O:574:LEU:HA	1.89	0.54
15:R:225:PRO:HG2	16:S:166:GLU:HB3	1.89	0.54
17:X:267:LEU:CD1	17:Y:59:LEU:CD1	2.82	0.54
1:A:775:LEU:O	1:A:948:PRO:HD3	2.07	0.54
1:A:1037:VAL:HG22	1:A:1562:LEU:HD21	1.89	0.54
3:C:96:VAL:HG21	3:P:53:LYS:HD3	1.89	0.54
17:X:491:LYS:O	17:X:494:ASP:OD1	2.25	0.54
9:J:55:ARG:HD2	9:K:261:ASP:OD1	2.07	0.54
9:J:322:TYR:HE1	11:M:36:LEU:HD11	1.73	0.54
12:N:77:GLU:HG3	12:N:156:MET:HE2	1.89	0.54
15:R:130:ILE:HG23	15:R:131:LEU:N	2.22	0.54
17:Y:491:LYS:O	17:Y:494:ASP:OD1	2.26	0.54
17:Y:517:ASP:O	17:Y:520:VAL:HG22	2.08	0.54
1:A:612:ILE:O	1:A:641:TRP:CZ3	2.61	0.54
8:I:344:ILE:O	8:I:348:VAL:HG23	2.07	0.54
9:J:277:GLU:OE1	9:J:278:LEU:HD23	2.07	0.54
9:J:406:HIS:HE1	9:J:450:ASN:HD22	1.55	0.54
17:X:394:ILE:HG22	17:X:397:ARG:NH2	2.23	0.54
17:X:517:ASP:O	17:X:520:VAL:HG22	2.08	0.54
6:F:30:ARG:NH2	6:H:500:TRP:HB3	2.22	0.54
8:I:413:ASN:N	8:I:447:PHE:HZ	2.06	0.54
9:J:476:PRO:HB2	3:P:148:ASN:HD21	1.72	0.54
9:K:484:ALA:O	9:K:488:ILE:HG12	2.08	0.54
12:N:395:ASP:HB2	12:N:397:ILE:N	2.18	0.54
3:P:303:PHE:C	3:P:303:PHE:HD1	2.14	0.54
1:A:457:PHE:HB3	1:A:468:PHE:CD1	2.43	0.54
1:A:1378:THR:HG23	1:A:1380:ASN:H	1.72	0.54
2:B:34:CYS:N	2:B:44:CYS:SG	2.79	0.54
2:B:39:VAL:N	2:B:40:PRO:CD	2.71	0.54
8:I:278:GLU:HA	8:I:281:MET:HG2	1.88	0.54
8:I:287:LEU:HG	8:I:456:PHE:CE2	2.43	0.54
8:I:337:ILE:HD13	8:I:418:PHE:CZ	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:204:LEU:HD22	9:K:28:LYS:NZ	2.23	0.54
9:K:242:TYR:O	7:W:3:ARG:NH2	2.40	0.54
12:N:331:PHE:CE2	12:N:335:ILE:HD11	2.42	0.54
1:A:1134:TRP:CD2	1:A:1203:MET:HE1	2.43	0.54
3:C:411:ILE:HD13	15:R:88:MET:HE1	1.90	0.54
9:J:53:TYR:O	9:J:79:CYS:SG	2.66	0.54
9:K:71:ALA:HA	9:K:128:ILE:HD13	1.90	0.54
9:K:154:LYS:HE2	9:K:184:LEU:HD22	1.90	0.54
10:L:78:CYS:SG	10:L:119:TRP:CE3	3.01	0.54
12:N:368:THR:CB	12:N:369:ASP:HA	2.38	0.54
16:S:28:ASN:O	16:S:90:PRO:HG2	2.08	0.54
18:Z:30:SER:O	18:Z:34:GLN:HG3	2.08	0.54
1:A:1921:LEU:HA	12:N:78:VAL:HG21	1.90	0.53
6:F:15:ALA:HA	6:H:116:PHE:CE1	2.43	0.53
6:F:130:ARG:CG	17:Y:506:GLN:HB2	2.38	0.53
8:I:218:SER:OG	8:I:584:HIS:ND1	2.41	0.53
9:J:476:PRO:CG	3:P:182:LEU:HG	2.35	0.53
12:N:123:ASP:O	12:N:127:ARG:N	2.41	0.53
1:A:1636:VAL:HG12	1:A:1666:ILE:HG13	1.91	0.53
6:F:145:ASN:HB2	6:F:146:PRO:O	2.08	0.53
6:H:145:ASN:HB2	6:H:146:PRO:C	2.34	0.53
8:I:186:GLU:OE1	8:I:197:ARG:CZ	2.53	0.53
8:I:262:LEU:CA	8:I:265:ILE:HG22	2.34	0.53
13:O:68:LEU:HD23	13:O:131:VAL:HG12	1.89	0.53
1:A:45:ALA:O	3:C:180:ARG:NH2	2.42	0.53
8:I:412:LYS:C	8:I:447:PHE:HZ	2.15	0.53
17:X:76:LYS:HB2	17:X:106:GLN:NE2	2.23	0.53
1:A:1797:ILE:HG22	1:A:1852:ILE:CD1	2.39	0.53
6:F:537:GLU:CD	6:F:600:TYR:OH	2.52	0.53
8:I:219:VAL:N	8:I:234:PHE:O	2.39	0.53
9:K:174:HIS:CE1	9:K:211:LYS:CD	2.90	0.53
14:Q:132:ARG:HG3	18:Z:154:LEU:HD23	1.90	0.53
17:Y:199:CYS:CB	17:Y:201:LEU:HD12	2.37	0.53
8:I:67:GLU:HB2	8:I:85:ALA:HB3	1.91	0.53
8:I:300:VAL:HA	8:I:303:GLU:CD	2.31	0.53
14:Q:132:ARG:HG3	18:Z:154:LEU:HD21	1.86	0.53
17:X:434:TYR:HA	17:X:444:LEU:HD13	1.91	0.53
6:F:7:PRO:HG2	6:H:459:ALA:HB2	1.91	0.53
6:F:89:GLU:OE1	6:F:130:ARG:NH2	2.41	0.53
13:O:733:CYS:HA	13:O:736:LEU:HD12	1.90	0.53
16:S:20:ASP:CG	18:Z:184:ARG:HD2	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:58:GLN:C	16:S:62:PHE:CD2	2.84	0.53
17:X:104:LEU:HD11	17:X:142:MET:SD	2.49	0.53
17:Y:42:ARG:CA	17:Y:82:TYR:CE2	2.72	0.53
1:A:1568:GLY:O	1:A:1571:ARG:HB3	2.08	0.53
2:B:46:LEU:HD21	2:B:54:CYS:CB	2.39	0.53
3:C:93:TYR:CE1	3:C:98:GLU:OE2	2.61	0.53
8:I:115:TRP:CE3	8:I:176:LEU:HD22	2.44	0.53
8:I:197:ARG:O	8:I:545:GLY:HA3	2.09	0.53
8:I:269:LEU:HB3	8:I:526:LYS:HZ2	1.74	0.53
10:L:78:CYS:SG	10:L:119:TRP:HE3	2.32	0.53
12:N:395:ASP:OD2	12:N:397:ILE:HB	2.09	0.53
12:N:501:ILE:O	12:N:505:LEU:HG	2.09	0.53
12:N:596:LEU:HB3	12:N:601:TRP:HE1	1.73	0.53
13:O:33:TYR:CE1	13:O:37:VAL:HG21	2.43	0.53
13:O:707:LYS:HA	13:O:710:ILE:HG22	1.91	0.53
3:P:488:GLN:HE21	3:P:492:LYS:HD2	1.73	0.53
1:A:1100:LEU:HB3	1:A:1101:PRO:CA	2.39	0.53
6:H:762:TRP:HA	6:H:765:ASP:CB	2.29	0.53
8:I:313:ALA:CB	8:I:317:LEU:CG	2.86	0.53
9:K:62:SER:O	9:K:63:ARG:HG3	2.08	0.53
1:A:799:LEU:C	1:A:801:PRO:HD2	2.33	0.53
3:C:415:PRO:HG3	3:C:445:LYS:CB	2.39	0.53
5:E:86:VAL:HG22	6:H:589:PHE:HE1	1.73	0.53
6:F:540:SER:OG	6:F:575:ASN:ND2	2.34	0.53
9:K:300:VAL:HG12	9:K:333:TYR:OH	2.08	0.53
15:R:247:SER:HB2	16:S:170:LYS:HZ3	1.73	0.53
16:S:141:TYR:CE1	16:S:297:ALA:O	2.62	0.53
16:S:163:GLU:CD	16:S:196:PHE:CD1	2.80	0.53
1:A:214:LEU:CD2	1:A:407:LEU:HD13	2.39	0.52
1:A:1321:VAL:CG2	1:A:1322:PRO:HD3	2.38	0.52
2:B:47:VAL:HG21	2:B:82:PHE:HD2	1.74	0.52
8:I:286:ARG:NE	8:I:333:LEU:HD13	2.18	0.52
9:J:19:TYR:CE1	9:J:49:LEU:HD13	2.44	0.52
9:J:37:PRO:HB3	9:J:69:TYR:OH	2.08	0.52
9:K:46:CYS:O	9:K:50:THR:OG1	2.21	0.52
14:Q:353:GLN:HA	18:Z:52:THR:HB	1.91	0.52
16:S:38:MET:CE	18:Z:199:TYR:CE2	2.69	0.52
3:C:377:GLU:HA	15:R:130:ILE:HG21	1.90	0.52
3:C:449:LEU:HD11	3:C:479:GLN:HE22	1.74	0.52
12:N:241:HIS:CE1	12:N:302:LYS:HE3	2.44	0.52
12:N:267:GLN:O	12:N:271:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:25:SER:HB2	16:S:45:LEU:CD2	2.38	0.52
1:A:1793:MET:HE2	1:A:1848:VAL:HG11	1.90	0.52
6:H:656:MET:CE	9:K:526:TYR:CD2	2.92	0.52
8:I:32:ARG:HG2	12:N:388:HIS:CE1	2.45	0.52
12:N:120:SER:O	12:N:124:PRO:HD2	2.09	0.52
14:Q:128:ALA:HA	18:Z:157:THR:O	2.09	0.52
17:Y:458:GLN:O	17:Y:462:LYS:HG3	2.09	0.52
1:A:159:ILE:HB	1:A:171:ALA:HB3	1.91	0.52
1:A:1307:LEU:CD1	1:A:1582:ALA:HB2	2.36	0.52
9:K:383:ASN:HB3	9:K:386:LEU:HD13	1.90	0.52
16:S:29:VAL:CB	16:S:36:ARG:NH1	2.64	0.52
16:S:197:GLN:C	16:S:200:VAL:HG22	2.34	0.52
1:A:1181:LEU:HB3	1:A:1611:VAL:HG11	1.90	0.52
1:A:1516:LEU:HA	1:A:1519:VAL:HG12	1.91	0.52
8:I:279:ILE:HG12	8:I:340:SER:HB2	1.91	0.52
9:J:481:THR:O	9:J:485:ILE:HG12	2.09	0.52
12:N:596:LEU:HD13	12:N:601:TRP:CE2	2.45	0.52
13:O:378:SER:OG	13:O:417:LEU:HD12	2.09	0.52
3:P:239:THR:O	3:P:275:ASN:ND2	2.43	0.52
15:R:193:SER:HB3	15:R:234:TRP:CE2	2.43	0.52
16:S:141:TYR:CE1	16:S:297:ALA:C	2.88	0.52
17:Y:42:ARG:HA	17:Y:82:TYR:OH	2.09	0.52
1:A:72:GLU:HG3	1:A:94:TYR:OH	2.10	0.52
9:K:509:ARG:HG3	9:K:509:ARG:O	2.09	0.52
12:N:190:LYS:O	12:N:196:ASP:N	2.43	0.52
3:P:283:LEU:HD21	3:P:312:MET:HE3	1.92	0.52
17:Y:100:TYR:CB	17:Y:142:MET:HG2	2.40	0.52
1:A:773:LEU:HD22	1:A:779:MET:HG3	1.92	0.52
3:C:228:TRP:O	3:C:231:GLU:N	2.38	0.52
8:I:116:MET:SD	8:I:210:LEU:HB3	2.50	0.52
12:N:362:LYS:HA	12:N:410:LEU:HD22	1.91	0.52
13:O:479:GLU:OE1	13:O:618:TYR:OH	2.26	0.52
17:X:397:ARG:HD2	17:X:417:TYR:OH	2.10	0.52
17:X:506:GLN:HG3	17:X:508:ASP:OD1	2.10	0.52
17:Y:54:ARG:HG2	17:Y:54:ARG:HH11	1.73	0.52
1:A:1170:ASN:ND2	1:A:1203:MET:HG3	2.25	0.52
1:A:1639:LYS:HG3	1:A:1664:LYS:HB2	1.91	0.52
2:B:11:VAL:HG13	12:N:642:GLY:HA2	1.91	0.52
12:N:362:LYS:CB	12:N:410:LEU:HD21	2.23	0.52
14:Q:184:ASP:HA	16:S:28:ASN:OD1	2.09	0.52
17:Y:42:ARG:HG3	17:Y:82:TYR:HH	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:84:ALA:HB1	17:Y:100:TYR:CZ	2.45	0.52
1:A:436:LEU:HD13	1:A:638:LEU:HD22	1.91	0.52
1:A:1236:LEU:HD12	1:A:1237:PRO:HD2	1.91	0.52
9:J:276:VAL:HA	9:J:311:MET:SD	2.50	0.52
9:J:469:ARG:O	9:J:473:VAL:HG23	2.10	0.52
10:L:33:LEU:HG	10:L:42:VAL:HG22	1.91	0.52
16:S:25:SER:HB2	16:S:45:LEU:HG	1.92	0.52
17:X:423:ILE:HG13	17:X:424:ARG:N	2.25	0.52
17:X:458:GLN:O	17:X:462:LYS:HG3	2.09	0.52
17:Y:506:GLN:HG3	17:Y:508:ASP:OD1	2.09	0.52
1:A:1409:LEU:HD22	1:A:1413:LEU:HG	1.91	0.52
1:A:1502:PRO:O	1:A:1503:ASN:HB3	2.09	0.52
3:C:316:LEU:CD2	3:C:340:TYR:HA	2.35	0.52
6:F:544:TRP:CE3	15:R:499:ARG:HD3	2.45	0.52
6:H:130:ARG:NH1	9:K:473:VAL:HG22	2.24	0.52
6:H:537:GLU:CD	6:H:600:TYR:OH	2.53	0.52
8:I:290:PHE:CE1	8:I:324:GLN:HB2	2.44	0.52
9:J:18:GLN:HE22	9:K:134:LEU:CD1	2.23	0.52
17:X:77:TYR:CE1	17:X:107:LYS:HB2	2.45	0.52
17:X:440:ASN:HA	17:X:471:GLN:HE22	1.75	0.52
6:H:703:PRO:HD2	10:L:180:TYR:CD2	2.45	0.51
9:J:355:ALA:O	9:J:359:THR:HG23	2.11	0.51
13:O:657:ILE:HG13	13:O:704:VAL:HG23	1.92	0.51
3:P:303:PHE:HE1	3:P:307:LEU:HD22	1.75	0.51
16:S:64:TYR:HH	16:S:84:TRP:HD1	1.55	0.51
16:S:71:GLY:O	16:S:74:PRO:N	2.43	0.51
17:Y:495:GLY:HA3	17:Y:518:PHE:HE2	1.75	0.51
1:A:442:LEU:HG	1:A:444:PHE:CE1	2.44	0.51
1:A:482:VAL:CG2	1:A:593:ASN:HA	2.40	0.51
1:A:1237:PRO:CB	1:A:1238:PRO:HD2	2.40	0.51
1:A:1320:ASN:HB3	1:A:1323:GLU:HG2	1.91	0.51
8:I:27:VAL:O	8:I:35:ILE:HD12	2.09	0.51
8:I:70:CYS:C	8:I:71:LEU:HD12	2.35	0.51
8:I:437:LEU:HA	8:I:438:ASN:C	2.35	0.51
8:I:536:CYS:O	8:I:540:PRO:CD	2.58	0.51
9:J:24:PHE:O	9:J:28:LYS:HG2	2.11	0.51
10:L:90:THR:HG21	10:L:116:PRO:HD2	1.91	0.51
15:R:407:TRP:CZ3	15:R:414:LEU:HD11	2.45	0.51
16:S:83:SER:C	16:S:87:GLN:HG3	2.34	0.51
1:A:1385:ASP:O	1:A:1388:ARG:HB2	2.10	0.51
8:I:52:PHE:HD1	8:I:743:VAL:HG21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:74:TRP:CH2	12:N:77:GLU:HB2	2.46	0.51
14:Q:407:TRP:CZ3	14:Q:414:LEU:HD11	2.44	0.51
1:A:1138:HIS:HE1	1:A:1604:GLN:NE2	2.06	0.51
1:A:1230:ILE:HD12	15:R:116:TRP:HD1	1.75	0.51
1:A:1869:HIS:O	1:A:1872:LEU:HG	2.10	0.51
2:B:15:LEU:HD21	12:N:635:LEU:HA	1.91	0.51
6:F:755:LEU:HD13	9:J:393:GLN:HE22	1.76	0.51
8:I:207:ALA:HB1	8:I:575:LEU:HD12	1.91	0.51
8:I:393:VAL:O	8:I:397:ILE:HG13	2.11	0.51
8:I:526:LYS:HA	8:I:529:MET:HE2	1.93	0.51
9:J:180:GLU:O	9:J:184:LEU:N	2.35	0.51
9:J:206:GLU:HA	9:J:209:LEU:HG	1.91	0.51
12:N:60:GLU:O	12:N:63:ALA:CB	2.56	0.51
12:N:281:TYR:CE1	12:N:357:ALA:HA	2.46	0.51
12:N:542:VAL:HG11	12:N:558:GLU:CD	2.35	0.51
12:N:560:MET:SD	12:N:601:TRP:CD1	3.04	0.51
13:O:414:LEU:HD12	13:O:417:LEU:HB2	1.92	0.51
3:P:48:LEU:HD21	3:P:116:PHE:CE2	2.45	0.51
14:Q:193:SER:HB3	14:Q:234:TRP:CE2	2.45	0.51
15:R:110:LYS:O	15:R:114:LYS:N	2.39	0.51
15:R:166:ARG:NH2	15:R:472:CYS:O	2.42	0.51
17:X:281:TYR:CE2	17:X:289:ASN:HB3	2.45	0.51
1:A:42:LEU:HD22	3:C:363:ARG:HB2	1.92	0.51
1:A:766:LEU:HD22	1:A:790:LEU:HD21	1.93	0.51
1:A:1325:LEU:HD21	1:A:1370:ALA:HB1	1.92	0.51
6:F:19:TYR:HE2	6:H:50:ARG:HD3	1.74	0.51
6:F:50:ARG:NE	6:H:19:TYR:HE1	2.09	0.51
9:K:263:PHE:HZ	9:K:290:LYS:HG2	1.76	0.51
12:N:233:CYS:O	12:N:235:GLN:N	2.44	0.51
1:A:957:ASP:CG	1:A:1820:PHE:HZ	2.19	0.51
2:B:15:LEU:HD12	12:N:633:ARG:HG2	1.92	0.51
3:C:117:LEU:HD23	3:C:117:LEU:O	2.11	0.51
3:C:170:PHE:O	3:C:173:TYR:HB3	2.10	0.51
3:C:318:TYR:HD1	9:J:282:ASN:OD1	1.93	0.51
7:G:23:ARG:HG2	9:J:525:MET:HE1	1.92	0.51
8:I:440:MET:HA	8:I:440:MET:HE3	1.93	0.51
12:N:500:ASP:HB2	12:N:501:ILE:HD12	1.92	0.51
13:O:114:ASP:CA	13:O:117:ASP:OD1	2.58	0.51
17:X:76:LYS:HB3	17:X:106:GLN:HE22	1.76	0.51
17:Y:77:TYR:CE1	17:Y:107:LYS:HB2	2.45	0.51
1:A:661:VAL:HG22	1:A:789:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:216:LYS:HG2	3:C:243:LEU:HD11	1.93	0.51
8:I:413:ASN:C	8:I:447:PHE:CE1	2.89	0.51
12:N:362:LYS:N	12:N:410:LEU:HD21	2.25	0.51
12:N:765:LEU:HD13	12:N:768:LEU:HD21	1.93	0.51
17:X:54:ARG:CZ	17:X:90:ASP:OD2	2.59	0.51
17:X:226:VAL:HG22	17:X:236:LEU:HD23	1.93	0.51
17:X:430:ALA:CB	17:X:451:CYS:SG	2.99	0.51
1:A:1375:TYR:HB3	1:A:1378:THR:CG2	2.38	0.51
7:G:11:LEU:HD13	9:J:514:PHE:CE2	2.45	0.51
6:H:540:SER:OG	6:H:575:ASN:ND2	2.35	0.51
8:I:588:PHE:CE1	8:I:599:CYS:HB2	2.46	0.51
9:J:173:HIS:HB2	9:J:175:MET:HE3	1.93	0.51
9:J:245:CYS:HA	9:J:247:PHE:CE1	2.46	0.51
9:K:181:GLU:HB3	9:K:209:LEU:HD13	1.93	0.51
12:N:278:ARG:HA	12:N:343:GLU:OE2	2.10	0.51
3:P:170:PHE:O	3:P:173:TYR:HB3	2.11	0.51
1:A:629:LEU:HB2	1:A:630:PRO:HD2	1.92	0.51
1:A:1235:LEU:CD2	1:A:1257:ILE:CG1	2.61	0.51
2:B:16:TRP:HB2	2:B:33:CYS:HB3	1.92	0.51
12:N:662:VAL:CG2	12:N:695:ARG:HG2	2.41	0.51
13:O:119:PHE:CE1	13:O:136:LEU:HD21	2.45	0.51
14:Q:208:LEU:HD13	14:Q:255:VAL:HG21	1.93	0.51
17:Y:309:ASP:HB2	17:Y:340:GLU:HG2	1.93	0.51
1:A:948:PRO:HB3	1:A:1813:GLN:CD	2.36	0.51
1:A:1388:ARG:HA	1:A:1411:ARG:HD2	1.92	0.51
1:A:1556:LEU:HD12	1:A:1556:LEU:O	2.11	0.51
6:H:703:PRO:HD3	10:L:180:TYR:CE2	2.46	0.51
8:I:304:PHE:HZ	8:I:448:VAL:HG13	1.76	0.51
9:K:222:GLU:OE1	9:K:228:GLN:CG	2.59	0.51
11:M:1:MET:HB2	3:P:50:HIS:HB2	1.92	0.51
12:N:181:LEU:HD22	12:N:299:TRP:CE2	2.46	0.51
15:R:192:TRP:CG	15:R:198:LEU:HD13	2.45	0.51
16:S:36:ARG:CZ	16:S:90:PRO:O	2.59	0.51
1:A:1400:LYS:HA	10:L:135:PHE:CZ	2.46	0.50
1:A:1674:TRP:CD1	1:A:1674:TRP:N	2.79	0.50
8:I:269:LEU:HB2	8:I:526:LYS:HZ1	1.74	0.50
10:L:87:GLU:CD	10:L:146:GLN:HE22	2.19	0.50
12:N:570:ILE:HA	12:N:573:ASN:ND2	2.26	0.50
13:O:460:GLN:HG2	13:O:496:ARG:HH22	1.74	0.50
3:P:228:TRP:O	3:P:231:GLU:N	2.38	0.50
3:P:494:ILE:HG21	3:P:516:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:235:TRP:CE3	17:X:236:LEU:HA	2.47	0.50
17:Y:294:PHE:CE2	17:Y:311:TYR:HB2	2.46	0.50
18:Z:158:ASP:C	18:Z:160:ASP:H	2.19	0.50
1:A:1294:TYR:CD1	1:A:1294:TYR:C	2.89	0.50
3:C:225:PRO:O	3:C:230:LYS:HD2	2.11	0.50
12:N:555:HIS:O	12:N:559:VAL:HG12	2.11	0.50
13:O:648:ILE:CD1	13:O:663:ALA:HB1	2.41	0.50
15:R:111:GLU:O	15:R:115:ALA:N	2.42	0.50
17:X:495:GLY:HA3	17:X:518:PHE:CE2	2.46	0.50
17:Y:281:TYR:CE2	17:Y:289:ASN:HB3	2.46	0.50
3:C:277:ARG:HB3	15:R:75:GLY:O	2.11	0.50
8:I:138:LEU:HD13	8:I:253:ARG:HG2	1.92	0.50
8:I:413:ASN:N	8:I:447:PHE:CZ	2.78	0.50
9:J:37:PRO:HB3	9:J:69:TYR:HE2	1.75	0.50
9:K:42:TRP:HA	9:K:42:TRP:CE3	2.46	0.50
12:N:751:LEU:HA	12:N:754:PHE:HD2	1.75	0.50
13:O:75:LEU:CD1	13:O:161:TYR:CD2	2.89	0.50
14:Q:340:PRO:HD3	14:Q:345:TRP:CZ2	2.47	0.50
15:R:98:GLU:HG2	15:R:101:PRO:CD	2.41	0.50
17:Y:73:PRO:O	17:Y:106:GLN:OE1	2.29	0.50
17:Y:196:LEU:O	17:Y:200:PRO:CA	2.59	0.50
17:Y:423:ILE:HG13	17:Y:424:ARG:N	2.25	0.50
17:Y:452:LEU:CD2	17:Y:461:ALA:H	2.23	0.50
6:H:537:GLU:OE2	6:H:568:GLU:OE1	2.28	0.50
12:N:75:PHE:O	12:N:78:VAL:N	2.44	0.50
12:N:676:TRP:CE3	12:N:680:GLU:HB3	2.46	0.50
3:P:225:PRO:O	3:P:230:LYS:HD2	2.11	0.50
16:S:21:GLU:O	16:S:45:LEU:HD13	2.10	0.50
17:X:495:GLY:HA3	17:X:518:PHE:HE2	1.75	0.50
1:A:442:LEU:HG	1:A:444:PHE:HE1	1.77	0.50
1:A:873:VAL:CG2	1:A:951:ILE:CG2	2.89	0.50
6:F:26:PHE:CD1	6:H:149:TRP:CB	2.94	0.50
8:I:72:ALA:C	8:I:80:LEU:HD12	2.37	0.50
8:I:174:ASN:OD1	8:I:190:TYR:HA	2.12	0.50
8:I:304:PHE:CZ	8:I:448:VAL:CG1	2.95	0.50
12:N:370:GLN:HG2	12:N:373:GLN:HB2	1.93	0.50
3:P:234:LEU:HD22	3:P:238:TYR:CZ	2.46	0.50
14:Q:192:TRP:CG	14:Q:198:LEU:HD13	2.46	0.50
17:X:269:ASP:HB3	17:X:300:LEU:HD21	1.92	0.50
1:A:1234:ALA:HB1	1:A:1272:VAL:HB	1.93	0.50
1:A:1300:LEU:HD13	1:A:1369:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1601:TYR:OH	10:L:102:PHE:HD1	1.95	0.50
3:C:361:ASN:HB3	3:C:363:ARG:N	2.27	0.50
8:I:245:LEU:HB3	8:I:246:PRO:HD3	1.93	0.50
10:L:65:ASN:HB3	10:L:136:MET:HE3	1.94	0.50
14:Q:425:LEU:HD12	14:Q:425:LEU:N	2.27	0.50
17:Y:146:TYR:CD1	17:Y:154:ASP:HB2	2.47	0.50
17:Y:495:GLY:HA3	17:Y:518:PHE:CE2	2.46	0.50
18:Z:138:THR:HG23	18:Z:142:LEU:HD12	1.93	0.50
1:A:1523:LEU:O	1:A:1526:VAL:HG22	2.11	0.50
8:I:306:HIS:CE1	8:I:313:ALA:HB1	2.46	0.50
8:I:317:LEU:CD2	8:I:320:LEU:HD23	2.40	0.50
8:I:441:THR:O	8:I:445:ILE:HG12	2.12	0.50
12:N:659:VAL:HG22	12:N:660:THR:N	2.27	0.50
15:R:81:PRO:HG3	15:R:131:LEU:HD21	1.94	0.50
18:Z:72:LEU:HD11	18:Z:155:ILE:HD11	1.92	0.50
1:A:39:LEU:HD21	3:C:393:GLU:HG2	1.93	0.50
1:A:489:LEU:HD22	1:A:497:LEU:HD22	1.94	0.50
1:A:852:LEU:HD11	1:A:1819:GLU:HB3	1.93	0.50
3:C:415:PRO:HG3	3:C:445:LYS:HB3	1.92	0.50
6:H:164:PRO:HG3	6:H:471:LYS:HG3	1.93	0.50
6:H:704:LEU:HD22	10:L:181:ARG:HA	1.93	0.50
8:I:47:HIS:CE1	8:I:54:ARG:NH1	2.79	0.50
9:K:185:LEU:HA	9:K:188:LEU:CD2	2.40	0.50
12:N:180:PHE:CE2	12:N:240:PHE:HB3	2.47	0.50
15:R:77:ASP:OD1	15:R:77:ASP:N	2.45	0.50
1:A:95:VAL:HG21	1:A:126:ALA:HB3	1.93	0.50
1:A:436:LEU:HB3	1:A:638:LEU:HD13	1.93	0.50
8:I:282:GLN:O	8:I:285:SER:HB3	2.12	0.50
8:I:300:VAL:C	8:I:303:GLU:HB2	2.36	0.50
15:R:340:PRO:HD3	15:R:345:TRP:CZ2	2.47	0.50
17:X:294:PHE:CE2	17:X:311:TYR:HB2	2.46	0.50
17:Y:235:TRP:CE3	17:Y:236:LEU:HA	2.47	0.50
1:A:1325:LEU:HD21	1:A:1370:ALA:CB	2.42	0.49
3:C:273:TYR:HB3	3:C:282:ALA:HB2	1.94	0.49
8:I:266:ASN:HA	8:I:526:LYS:NZ	2.26	0.49
9:J:17:GLN:HB3	9:K:78:ARG:HH12	1.77	0.49
9:J:204:LEU:HD22	9:K:28:LYS:HZ2	1.77	0.49
15:R:209:TRP:HB2	16:S:227:LEU:HD13	1.94	0.49
1:A:485:ILE:HD11	1:A:609:ILE:HB	1.94	0.49
1:A:1230:ILE:HA	1:A:1236:LEU:HD13	1.94	0.49
3:C:414:MET:HE1	13:O:300:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:311:HIS:HB2	13:O:320:ALA:HB2	1.92	0.49
13:O:657:ILE:HG22	13:O:660:LYS:HE2	1.94	0.49
16:S:23:GLU:OE2	18:Z:134:GLN:CA	2.60	0.49
16:S:199:ARG:O	16:S:203:GLN:HG2	2.11	0.49
1:A:480:ALA:HB1	1:A:590:PRO:HG3	1.94	0.49
3:C:126:GLY:C	3:C:148:ASN:OD1	2.55	0.49
3:C:251:TYR:HB3	3:C:269:ILE:CD1	2.42	0.49
6:H:465:LEU:HD22	6:H:495:HIS:CE1	2.47	0.49
9:J:213:ASN:OD1	9:J:214:LYS:N	2.45	0.49
9:J:247:PHE:CE2	9:J:277:GLU:CB	2.96	0.49
9:K:227:LEU:O	9:K:230:ASN:HB3	2.13	0.49
9:K:406:HIS:CE1	7:W:6:PRO:CB	2.95	0.49
12:N:393:THR:HG23	12:N:434:THR:HG22	1.94	0.49
12:N:409:VAL:O	12:N:410:LEU:HB2	2.11	0.49
12:N:577:GLU:HB3	12:N:625:LYS:CE	2.40	0.49
15:R:112:HIS:CD2	15:R:116:TRP:HZ3	2.29	0.49
17:Y:226:VAL:HG22	17:Y:236:LEU:HD23	1.94	0.49
1:A:1229:SER:HA	1:A:1235:LEU:HB3	1.94	0.49
1:A:1401:PRO:HD3	10:L:135:PHE:CE2	2.47	0.49
1:A:1555:HIS:O	1:A:1559:HIS:CD2	2.64	0.49
5:E:94:TRP:CZ2	6:F:592:ARG:HG2	2.46	0.49
6:F:739:VAL:O	6:F:743:ILE:HG13	2.13	0.49
6:H:656:MET:O	6:H:660:LYS:HG3	2.12	0.49
8:I:203:GLY:HA3	8:I:223:VAL:HG22	1.94	0.49
9:J:441:VAL:O	9:J:442:ASP:CB	2.59	0.49
9:K:372:LEU:HD22	9:K:404:VAL:HG22	1.94	0.49
15:R:208:LEU:HD13	15:R:255:VAL:HG21	1.93	0.49
16:S:134:GLU:C	16:S:136:LEU:N	2.68	0.49
17:Y:269:ASP:HB3	17:Y:300:LEU:HD21	1.94	0.49
1:A:1551:ASN:OD1	1:A:1554:PHE:CD2	2.65	0.49
6:H:743:ILE:HG22	6:H:759:ASN:HD21	1.77	0.49
8:I:116:MET:HE1	8:I:211:SER:O	2.12	0.49
10:L:63:LEU:HD22	10:L:138:GLN:HE21	1.77	0.49
12:N:249:ARG:HB3	12:N:250:LEU:HD23	1.94	0.49
3:P:117:LEU:HD23	3:P:117:LEU:O	2.11	0.49
14:Q:430:TYR:CD1	14:Q:431:PRO:HA	2.48	0.49
15:R:430:TYR:CD1	15:R:431:PRO:HA	2.48	0.49
3:C:313:LYS:HG2	3:C:343:LEU:HD22	1.95	0.49
8:I:639:LEU:HB2	8:I:652:VAL:HG12	1.93	0.49
13:O:233:PRO:HA	13:O:263:ARG:HH21	1.77	0.49
15:R:239:ASN:ND2	15:R:240:TYR:CE2	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:55:LEU:O	16:S:59:LYS:HD3	2.12	0.49
9:J:397:ILE:CG2	9:J:398:ALA:H	2.25	0.49
13:O:707:LYS:CA	13:O:710:ILE:HG22	2.42	0.49
15:R:425:LEU:N	15:R:425:LEU:HD12	2.28	0.49
1:A:78:LYS:HD3	1:A:592:HIS:HB2	1.94	0.49
1:A:248:PHE:CZ	1:A:250:ASN:HB2	2.48	0.49
1:A:945:GLU:O	13:O:599:ILE:HD13	2.13	0.49
3:C:48:LEU:HD21	3:C:116:PHE:CZ	2.47	0.49
6:H:739:VAL:O	6:H:743:ILE:HG13	2.13	0.49
8:I:207:ALA:CB	8:I:575:LEU:HD12	2.43	0.49
8:I:337:ILE:O	8:I:341:TYR:CD2	2.66	0.49
9:J:376:LEU:HD23	9:J:407:GLU:HG2	1.93	0.49
9:K:256:VAL:O	9:K:259:GLU:HG2	2.12	0.49
9:K:441:VAL:HG13	9:K:474:LEU:HD22	1.95	0.49
12:N:63:ALA:HB3	12:N:64:ALA:CB	2.42	0.49
13:O:402:LEU:HD13	13:O:425:LYS:CG	2.42	0.49
13:O:509:LEU:HG	13:O:513:LYS:HE3	1.95	0.49
17:X:170:LYS:HA	17:Y:49:LEU:CD2	2.42	0.49
17:X:376:LEU:HD11	17:X:398:GLU:OE2	2.13	0.49
17:X:393:ILE:HG22	17:X:397:ARG:HD3	1.94	0.49
1:A:1160:TYR:HB2	13:O:332:GLN:HB3	1.93	0.49
1:A:1770:LEU:HD13	1:A:1798:ARG:HH22	1.78	0.49
7:G:3:ARG:HB2	9:J:443:LYS:HZ1	1.77	0.49
9:J:165:GLU:HB2	9:K:21:SER:HB2	1.94	0.49
10:L:24:GLU:HG3	10:L:159:TYR:CE1	2.48	0.49
12:N:156:MET:O	12:N:160:VAL:HG23	2.12	0.49
12:N:180:PHE:CG	12:N:299:TRP:HH2	2.30	0.49
16:S:273:THR:O	16:S:274:VAL:HB	2.12	0.49
1:A:455:VAL:HB	1:A:471:VAL:HG12	1.94	0.49
1:A:1157:TRP:HA	13:O:332:GLN:OE1	2.12	0.49
3:C:296:ARG:HD3	3:P:101:ARG:HH22	1.78	0.49
8:I:36:ALA:HB2	8:I:80:LEU:HD21	1.94	0.49
9:K:178:ALA:HA	9:K:181:GLU:CD	2.38	0.49
10:L:45:LEU:HD11	10:L:156:ILE:HD12	1.95	0.49
12:N:545:LEU:O	12:N:549:PHE:N	2.46	0.49
13:O:36:ALA:CB	13:O:75:LEU:HD21	2.43	0.49
13:O:78:LEU:HD12	13:O:78:LEU:O	2.13	0.49
3:P:119:MET:HG2	3:P:158:LEU:HD21	1.95	0.49
16:S:21:GLU:O	16:S:45:LEU:HD21	2.06	0.49
1:A:436:LEU:H	1:A:501:THR:CG2	2.26	0.48
6:F:89:GLU:CD	6:F:130:ARG:NH2	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:44:VAL:C	8:I:45:LEU:HD12	2.37	0.48
8:I:424:ALA:O	8:I:428:MET:HG2	2.13	0.48
12:N:659:VAL:HG22	12:N:660:THR:H	1.77	0.48
3:P:334:CYS:HB3	3:P:357:ALA:HB2	1.94	0.48
6:F:500:TRP:CB	6:H:30:ARG:NH2	2.74	0.48
12:N:286:LEU:O	12:N:288:GLU:N	2.46	0.48
13:O:99:LEU:C	13:O:99:LEU:HD12	2.37	0.48
16:S:68:PHE:HE1	16:S:78:TRP:CG	2.31	0.48
17:X:168:THR:OG1	17:X:171:ILE:CD1	2.61	0.48
17:Y:376:LEU:HD11	17:Y:398:GLU:OE2	2.12	0.48
1:A:1644:TYR:O	1:A:1645:GLU:HG2	2.13	0.48
3:C:466:GLU:HG3	15:R:82:HIS:CD2	2.49	0.48
6:F:130:ARG:HG2	17:Y:506:GLN:HB2	1.96	0.48
8:I:446:THR:O	8:I:449:ALA:HB3	2.12	0.48
9:J:20:GLN:OE1	9:J:20:GLN:HA	2.14	0.48
9:J:215:PRO:HB2	9:J:435:ILE:HD11	1.95	0.48
9:J:297:SER:O	9:J:329:LEU:HD11	2.13	0.48
12:N:281:TYR:CZ	12:N:284:SER:HB3	2.48	0.48
12:N:700:LEU:HD13	12:N:707:GLU:HG3	1.95	0.48
13:O:422:ILE:O	13:O:426:THR:HG22	2.14	0.48
14:Q:239:ASN:ND2	14:Q:240:TYR:CE2	2.81	0.48
18:Z:91:ILE:HG12	18:Z:150:SER:HB3	1.95	0.48
1:A:612:ILE:O	1:A:641:TRP:HZ3	1.95	0.48
1:A:1082:VAL:HG22	1:A:1138:HIS:CG	2.48	0.48
1:A:1136:SER:O	1:A:1139:ASN:HB3	2.13	0.48
3:C:33:LYS:NZ	3:C:64:ALA:HA	2.29	0.48
6:F:459:ALA:HB2	6:H:7:PRO:HG2	1.95	0.48
6:H:102:SER:OG	6:H:104:ASP:OD1	2.17	0.48
6:H:736:GLU:OE1	10:L:177:PHE:HB2	2.13	0.48
6:H:743:ILE:HG22	6:H:759:ASN:ND2	2.29	0.48
12:N:523:LEU:HD22	12:N:538:GLU:OE1	2.12	0.48
14:Q:208:LEU:CD1	14:Q:255:VAL:HG21	2.43	0.48
17:X:63:MET:HE3	17:Y:266:LEU:HD22	1.95	0.48
3:C:334:CYS:HB3	3:C:357:ALA:HB2	1.95	0.48
3:C:413:LYS:O	3:C:415:PRO:HD3	2.14	0.48
6:F:164:PRO:CG	6:F:471:LYS:HG3	2.43	0.48
8:I:290:PHE:CE2	8:I:325:LEU:HD12	2.47	0.48
12:N:268:VAL:HA	12:N:271:GLU:CD	2.38	0.48
16:S:82:ILE:CD1	16:S:102:LEU:HD23	2.43	0.48
16:S:84:TRP:O	16:S:88:ASN:CG	2.57	0.48
1:A:1405:LEU:CD1	1:A:1467:GLY:HA2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:265:ILE:O	3:C:269:ILE:HG12	2.14	0.48
6:F:541:THR:HG23	15:R:499:ARG:HG2	1.96	0.48
6:H:564:LYS:O	6:H:565:ASN:HB2	2.14	0.48
8:I:290:PHE:HB3	8:I:320:LEU:HD11	1.95	0.48
9:K:228:GLN:HA	9:K:233:VAL:HG21	1.95	0.48
9:K:458:LEU:HB3	9:K:460:LYS:HG3	1.95	0.48
12:N:88:SER:O	12:N:91:PHE:HB3	2.13	0.48
12:N:91:PHE:CZ	12:N:94:ALA:HB2	2.49	0.48
15:R:208:LEU:CD1	15:R:255:VAL:HG21	2.43	0.48
17:X:393:ILE:HG22	17:X:397:ARG:HH11	1.78	0.48
1:A:772:GLU:HG3	1:A:867:CYS:HA	1.95	0.48
1:A:1080:LEU:N	1:A:1081:PRO:HD2	2.29	0.48
1:A:1602:HIS:O	1:A:1603:LEU:HB3	2.13	0.48
8:I:49:LEU:HD13	8:I:730:VAL:HG21	1.95	0.48
8:I:202:ALA:C	8:I:223:VAL:HG22	2.38	0.48
12:N:91:PHE:CE1	12:N:94:ALA:HB2	2.48	0.48
12:N:139:GLY:C	12:N:141:LEU:N	2.70	0.48
13:O:281:LEU:HD21	13:O:283:LEU:HD12	1.95	0.48
13:O:356:ASP:HA	13:O:357:SER:CB	2.42	0.48
15:R:105:GLN:O	15:R:107:PRO:HD3	2.14	0.48
16:S:19:GLY:HA3	18:Z:134:GLN:CG	2.44	0.48
17:X:99:LYS:HD3	17:X:102:MET:CE	2.43	0.48
17:X:339:ALA:O	17:X:343:VAL:HG23	2.14	0.48
17:Y:168:THR:OG1	17:Y:171:ILE:CD1	2.61	0.48
17:Y:338:HIS:O	17:Y:341:PRO:HD2	2.14	0.48
1:A:437:CYS:HA	1:A:626:LYS:HD2	1.96	0.48
6:F:152:PHE:CE1	6:F:162:PRO:HG2	2.49	0.48
6:H:486:ASN:O	6:H:490:HIS:CD2	2.67	0.48
8:I:410:SER:O	8:I:414:PHE:HD2	1.95	0.48
8:I:430:GLU:CD	14:Q:429:LYS:CG	2.86	0.48
12:N:519:TYR:CE1	12:N:523:LEU:HD21	2.49	0.48
13:O:635:GLY:O	13:O:637:PRO:HD3	2.14	0.48
17:X:436:THR:HG23	17:X:437:LEU:HD12	1.96	0.48
18:Z:138:THR:HG23	18:Z:142:LEU:CD1	2.44	0.48
1:A:1201:HIS:CE1	1:A:1203:MET:HB2	2.49	0.48
1:A:1573:SER:HB2	1:A:1617:ARG:HH21	1.78	0.48
1:A:1610:TYR:CD1	1:A:1610:TYR:C	2.92	0.48
3:C:521:PHE:HD1	3:C:553:ILE:HG22	1.74	0.48
8:I:188:TYR:HA	8:I:193:PHE:O	2.14	0.48
9:J:413:PHE:CD1	9:J:454:VAL:HG12	2.49	0.48
10:L:144:ASN:ND2	10:L:151:THR:HG23	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:706:ARG:HB2	12:N:716:ILE:HD13	1.94	0.48
13:O:423:ALA:O	13:O:426:THR:HG23	2.13	0.48
13:O:681:PRO:O	13:O:682:LYS:HB2	2.14	0.48
3:P:437:VAL:HG22	3:P:469:ALA:HB2	1.96	0.48
15:R:98:GLU:HG2	15:R:101:PRO:CG	2.41	0.48
1:A:174:PRO:HG2	1:A:175:PHE:CD2	2.49	0.48
3:C:209:LEU:O	3:C:213:ILE:HG12	2.14	0.48
6:F:130:ARG:HH11	17:Y:506:GLN:CB	2.27	0.48
6:F:564:LYS:O	6:F:565:ASN:HB2	2.13	0.48
6:H:537:GLU:CD	6:H:568:GLU:OE1	2.57	0.48
8:I:294:LYS:CB	8:I:320:LEU:HD13	2.43	0.48
9:J:230:ASN:OD1	9:J:231:LEU:N	2.47	0.48
12:N:560:MET:HE3	12:N:600:PHE:HB2	1.96	0.48
17:Y:339:ALA:O	17:Y:343:VAL:HG23	2.13	0.48
18:Z:81:VAL:HG21	18:Z:155:ILE:HD12	1.96	0.48
1:A:1621:PRO:HG3	1:A:1653:ALA:CB	2.44	0.47
3:C:48:LEU:HD21	3:C:116:PHE:CE2	2.49	0.47
3:C:145:GLN:CG	13:O:246:PHE:HA	2.43	0.47
6:F:59:ARG:HH12	6:H:562:MET:HB2	1.79	0.47
6:F:673:CYS:O	6:F:677:VAL:HG23	2.14	0.47
10:L:75:LYS:HA	10:L:131:PRO:HB3	1.95	0.47
3:P:48:LEU:HD21	3:P:116:PHE:CZ	2.48	0.47
16:S:79:ASP:CB	16:S:120:ARG:HH11	2.27	0.47
17:X:452:LEU:CD2	17:X:461:ALA:H	2.23	0.47
3:C:317:SER:OG	11:M:27:GLU:HG3	2.14	0.47
6:F:130:ARG:HG2	17:Y:506:GLN:CD	2.38	0.47
6:H:121:LEU:HG	6:H:125:TYR:HE1	1.79	0.47
9:J:393:GLN:O	9:J:396:SER:HB3	2.13	0.47
12:N:765:LEU:HD23	12:N:765:LEU:HA	1.70	0.47
3:P:265:ILE:O	3:P:269:ILE:HG12	2.14	0.47
1:A:1235:LEU:HD21	1:A:1257:ILE:CD1	2.40	0.47
8:I:427:ARG:HB2	8:I:428:MET:CE	2.42	0.47
8:I:673:LEU:HA	8:I:676:ASN:HB2	1.95	0.47
12:N:556:PHE:CZ	12:N:600:PHE:HA	2.49	0.47
13:O:39:VAL:HG11	13:O:97:ILE:HG13	1.94	0.47
13:O:411:LYS:HE2	13:O:412:HIS:HE1	1.74	0.47
3:P:308:TYR:CD2	14:Q:499:ARG:HD2	2.49	0.47
16:S:188:ARG:HH12	18:Z:147:VAL:CG1	2.26	0.47
8:I:206:LEU:HD22	8:I:570:PHE:CD2	2.50	0.47
9:K:227:LEU:O	9:K:230:ASN:N	2.48	0.47
9:K:263:PHE:CZ	9:K:290:LYS:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:282:GLU:O	12:N:284:SER:N	2.44	0.47
3:P:316:LEU:CD1	3:P:340:TYR:HB2	2.44	0.47
14:Q:166:ARG:CZ	14:Q:413:GLU:OE1	2.62	0.47
15:R:112:HIS:CE1	15:R:116:TRP:HZ3	2.31	0.47
16:S:134:GLU:O	16:S:135:PRO:C	2.57	0.47
1:A:1172:TYR:CZ	1:A:1176:LEU:HD23	2.49	0.47
3:C:101:ARG:CZ	3:P:296:ARG:HA	2.44	0.47
6:F:537:GLU:OE1	6:F:600:TYR:CE2	2.67	0.47
8:I:325:LEU:HD13	8:I:425:MET:HE1	1.95	0.47
9:J:272:ILE:HD11	9:J:304:ALA:HB2	1.97	0.47
9:K:350:HIS:ND1	9:K:377:GLU:OE1	2.47	0.47
10:L:29:ALA:O	10:L:31:TRP:CD1	2.67	0.47
13:O:91:ASN:O	13:O:95:ILE:HG12	2.14	0.47
3:P:209:LEU:O	3:P:213:ILE:HG12	2.15	0.47
1:A:1078:MET:HB2	1:A:1552:TYR:CE1	2.50	0.47
1:A:1511:ASN:HD22	1:A:1511:ASN:H	1.60	0.47
3:C:180:ARG:HG3	3:C:212:LEU:HD21	1.97	0.47
8:I:276:TRP:HA	8:I:279:ILE:HG22	1.96	0.47
9:J:69:TYR:O	9:J:70:GLU:CB	2.62	0.47
9:J:456:ARG:CG	9:J:488:ILE:HG22	2.44	0.47
18:Z:80:SER:O	18:Z:157:THR:HB	2.14	0.47
1:A:93:LEU:HD11	1:A:151:ILE:HD12	1.97	0.47
1:A:280:ASN:C	1:A:346:ASN:N	2.71	0.47
1:A:665:MET:O	1:A:669:GLY:N	2.44	0.47
1:A:1064:GLU:HA	1:A:1125:ILE:HD11	1.97	0.47
1:A:1413:LEU:HD22	1:A:1416:TRP:HZ3	1.80	0.47
3:C:550:LEU:HD22	3:C:553:ILE:HD11	1.97	0.47
8:I:291:VAL:HG12	8:I:298:THR:HA	1.96	0.47
8:I:442:GLN:HE21	13:O:69:GLN:HG2	1.80	0.47
9:J:58:HIS:CD2	9:K:262:PRO:HD3	2.50	0.47
9:J:191:SER:O	9:J:193:LEU:HG	2.14	0.47
13:O:129:THR:O	13:O:130:SER:CB	2.61	0.47
13:O:628:ALA:HB2	13:O:643:LEU:HD22	1.97	0.47
13:O:710:ILE:O	13:O:713:VAL:HG12	2.14	0.47
16:S:21:GLU:O	16:S:45:LEU:CD1	2.62	0.47
16:S:25:SER:HB2	16:S:45:LEU:HD21	1.96	0.47
17:X:349:SER:HA	17:X:352:SER:OG	2.15	0.47
3:C:333:THR:O	3:C:337:ILE:HG12	2.15	0.47
6:F:96:VAL:HG12	6:F:97:PHE:CD1	2.50	0.47
9:J:220:ILE:HG12	9:J:240:ARG:NH1	2.30	0.47
9:J:475:ILE:HD11	9:J:478:ASN:ND2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:499:VAL:HG11	9:K:523:ILE:CD1	2.45	0.47
12:N:202:GLU:O	12:N:202:GLU:OE1	2.33	0.47
12:N:567:SER:HB2	12:N:594:VAL:O	2.14	0.47
14:Q:196:ASN:ND2	14:Q:211:ALA:HB3	2.30	0.47
17:Y:42:ARG:CB	17:Y:82:TYR:OH	2.63	0.47
2:B:16:TRP:CH2	12:N:630:LYS:CE	2.98	0.47
3:C:119:MET:HG2	3:C:158:LEU:HD21	1.97	0.47
6:H:146:PRO:CG	6:H:167:THR:HA	2.45	0.47
9:J:78:ARG:NH1	9:K:17:GLN:HB3	2.29	0.47
12:N:73:GLU:O	12:N:74:TRP:CB	2.63	0.47
12:N:273:MET:CG	12:N:277:CYS:SG	2.95	0.47
12:N:577:GLU:HG2	12:N:583:ALA:HB2	1.97	0.47
3:P:274:HIS:O	3:P:276:ILE:O	2.33	0.47
3:P:358:LEU:CD1	3:P:368:TRP:CE2	2.98	0.47
3:P:365:LEU:HB3	3:P:395:ASN:HD21	1.80	0.47
1:A:162:HIS:HD2	1:A:168:ASP:HB3	1.79	0.47
1:A:804:ASP:OD1	1:A:804:ASP:N	2.48	0.47
1:A:845:TYR:HB3	1:A:1812:TRP:CZ3	2.50	0.47
2:B:27:ARG:HD3	12:N:813:GLY:HA2	1.97	0.47
6:H:97:PHE:HA	9:K:433:LYS:HD3	1.97	0.47
8:I:301:GLN:O	8:I:304:PHE:N	2.48	0.47
8:I:578:ASN:ND2	8:I:646:ASP:HB3	2.30	0.47
9:J:496:GLU:HB2	9:J:526:TYR:CE1	2.50	0.47
9:K:248:LYS:N	9:K:438:GLU:OE2	2.48	0.47
13:O:36:ALA:O	13:O:39:VAL:HG12	2.15	0.47
13:O:123:GLU:N	13:O:124:PRO:HA	2.30	0.47
13:O:425:LYS:HB2	13:O:441:GLN:HG2	1.96	0.47
14:Q:186:TYR:CE2	16:S:27:GLU:HB2	2.49	0.47
16:S:141:TYR:CE2	16:S:299:PRO:HD3	2.50	0.47
3:C:259:PHE:HB3	3:C:265:ILE:HD13	1.94	0.46
6:F:146:PRO:CG	6:F:167:THR:HA	2.46	0.46
6:F:481:CYS:HB2	6:F:512:LEU:HD13	1.96	0.46
8:I:195:ILE:HD11	8:I:251:MET:HE3	1.98	0.46
8:I:287:LEU:O	8:I:291:VAL:HG23	2.15	0.46
8:I:399:LYS:HG2	8:I:525:VAL:HG21	1.98	0.46
8:I:669:LEU:HD11	8:I:705:MET:HE1	1.97	0.46
9:J:322:TYR:CZ	11:M:31:ILE:HD13	2.50	0.46
9:K:443:LYS:O	9:K:446:PRO:HD2	2.15	0.46
11:M:32:PRO:C	11:M:34:ASN:H	2.22	0.46
12:N:258:ALA:HA	12:N:261:VAL:HG22	1.97	0.46
3:P:361:ASN:HB3	3:P:363:ARG:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:388:TYR:HB3	3:P:405:LEU:HG	1.98	0.46
14:Q:442:HIS:CE1	14:Q:468:ARG:HD2	2.51	0.46
15:R:461:ALA:HB2	15:R:467:LEU:CD1	2.45	0.46
17:Y:349:SER:HA	17:Y:352:SER:OG	2.15	0.46
1:A:442:LEU:HB3	1:A:455:VAL:HG13	1.96	0.46
2:B:16:TRP:CZ2	2:B:45:PRO:HA	2.50	0.46
5:E:99:ILE:HD11	5:E:103:LEU:HD13	1.98	0.46
6:F:98:ASN:OD1	6:F:98:ASN:N	2.47	0.46
7:G:4:ARG:HB2	9:J:373:TYR:HE1	1.81	0.46
6:H:541:THR:CG2	10:L:184:ARG:HB3	2.45	0.46
6:H:592:ARG:HD3	6:H:592:ARG:HA	1.66	0.46
8:I:25:PHE:CD1	8:I:71:LEU:HD13	2.50	0.46
8:I:330:LEU:HD13	8:I:330:LEU:C	2.41	0.46
8:I:440:MET:HB3	8:I:445:ILE:HD11	1.97	0.46
8:I:561:ARG:NH2	8:I:589:THR:O	2.44	0.46
9:K:280:LYS:HB3	9:K:283:GLU:HG2	1.97	0.46
12:N:753:LEU:HG	12:N:757:TYR:HE1	1.81	0.46
3:P:405:LEU:HA	3:P:408:THR:HG22	1.97	0.46
17:X:339:ALA:HB2	17:X:369:ASN:HB2	1.97	0.46
17:Y:494:ASP:OD1	17:Y:494:ASP:N	2.48	0.46
1:A:256:VAL:HB	1:A:269:TRP:HB2	1.98	0.46
3:C:477:HIS:CD2	3:C:482:GLU:OE1	2.64	0.46
4:D:5:PHE:CE1	13:O:427:ALA:HB1	2.51	0.46
6:F:533:VAL:HG23	6:F:559:LEU:HD22	1.97	0.46
8:I:145:LEU:HD13	8:I:267:LEU:HD22	1.98	0.46
8:I:669:LEU:HD13	8:I:705:MET:HE1	1.97	0.46
12:N:286:LEU:O	12:N:287:ARG:C	2.57	0.46
15:R:130:ILE:HG23	15:R:131:LEU:H	1.78	0.46
17:X:40:HIS:CB	17:Y:201:LEU:HD11	2.36	0.46
1:A:252:ASP:HB2	1:A:253:PRO:HD3	1.98	0.46
1:A:1477:ALA:HA	1:A:1525:MET:O	2.14	0.46
1:A:1621:PRO:HG3	1:A:1653:ALA:HB1	1.97	0.46
5:E:89:LEU:HD11	6:H:592:ARG:HB2	1.97	0.46
6:F:164:PRO:HG3	6:F:471:LYS:HG3	1.98	0.46
6:H:98:ASN:OD1	6:H:98:ASN:N	2.49	0.46
8:I:414:PHE:CE1	8:I:451:PHE:HE1	2.31	0.46
9:J:219:VAL:O	9:J:221:PRO:HD3	2.14	0.46
9:K:8:LYS:HA	9:K:8:LYS:HD2	1.82	0.46
9:K:93:LEU:HD12	9:K:93:LEU:N	2.31	0.46
9:K:167:PHE:O	9:K:171:THR:HG22	2.15	0.46
9:K:298:ASN:OD1	9:K:300:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:496:GLU:HB2	9:K:526:TYR:CE1	2.50	0.46
13:O:629:PHE:CE1	13:O:755:LEU:C	2.94	0.46
15:R:124:ASP:O	15:R:127:GLU:O	2.33	0.46
16:S:36:ARG:NH2	16:S:90:PRO:O	2.48	0.46
17:X:63:MET:SD	17:Y:235:TRP:NE1	2.89	0.46
17:X:146:TYR:CD1	17:X:154:ASP:HB2	2.50	0.46
17:X:373:VAL:O	17:X:376:LEU:N	2.46	0.46
17:X:406:ARG:HB2	17:X:409:CYS:SG	2.56	0.46
1:A:1753:TYR:CD2	13:O:643:LEU:HD12	2.42	0.46
3:C:170:PHE:O	3:C:171:GLY:C	2.57	0.46
3:C:358:LEU:O	3:C:362:PRO:HB3	2.15	0.46
8:I:28:TRP:CD1	8:I:723:ALA:HB1	2.51	0.46
8:I:139:LEU:HD21	8:I:192:MET:CE	2.45	0.46
8:I:238:THR:HG22	8:I:548:MET:SD	2.55	0.46
9:J:36:GLU:HG2	9:J:37:PRO:HD2	1.98	0.46
9:J:185:LEU:HD11	9:J:205:PHE:HB2	1.96	0.46
9:K:230:ASN:OD1	9:K:231:LEU:N	2.48	0.46
3:P:120:TYR:CE2	3:P:124:LEU:HD11	2.51	0.46
14:Q:163:LYS:HD3	15:R:466:THR:HG22	1.97	0.46
15:R:190:VAL:HG12	15:R:450:THR:HG21	1.98	0.46
17:Y:350:PHE:CZ	17:Y:378:LEU:HD12	2.50	0.46
3:C:101:ARG:NH2	3:P:296:ARG:HA	2.31	0.46
3:C:120:TYR:CE2	3:C:124:LEU:HD11	2.50	0.46
3:C:359:LYS:HG2	11:M:14:LEU:HD22	1.97	0.46
6:H:58:TYR:OH	6:H:62:LYS:HD2	2.16	0.46
8:I:11:PHE:HD1	8:I:746:MET:HA	1.80	0.46
8:I:45:LEU:CD2	8:I:54:ARG:NH1	2.79	0.46
8:I:73:TRP:CD2	8:I:80:LEU:HD13	2.50	0.46
8:I:142:LEU:HD13	8:I:264:TYR:CE2	2.51	0.46
8:I:189:ALA:N	8:I:193:PHE:O	2.48	0.46
8:I:202:ALA:O	8:I:221:THR:OG1	2.30	0.46
8:I:513:LEU:HD23	13:O:473:LEU:HD11	1.98	0.46
8:I:685:PHE:HA	8:I:701:PRO:HD3	1.98	0.46
9:J:42:TRP:CE3	9:J:42:TRP:HA	2.50	0.46
13:O:126:VAL:HG13	13:O:132:VAL:HG12	1.98	0.46
13:O:292:GLY:HA3	13:O:336:ASP:CB	2.45	0.46
13:O:621:SER:HB3	13:O:651:ILE:HG12	1.96	0.46
15:R:196:ASN:ND2	15:R:211:ALA:HB3	2.31	0.46
15:R:296:ARG:CD	16:S:272:ILE:HG12	2.46	0.46
17:X:87:LEU:HD22	17:X:95:ASN:HD22	1.80	0.46
1:A:40:ARG:HG2	13:O:248:PRO:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:ARG:NH1	1:A:1785:GLU:OE1	2.48	0.46
1:A:1037:VAL:HA	1:A:1040:LEU:HB2	1.98	0.46
9:J:334:GLY:N	9:J:335:PRO:CD	2.79	0.46
9:J:397:ILE:O	9:J:398:ALA:C	2.59	0.46
17:Y:436:THR:HG23	17:Y:437:LEU:HD12	1.98	0.46
1:A:40:ARG:CZ	13:O:248:PRO:HB2	2.46	0.46
1:A:657:TRP:CD1	1:A:785:SER:HG	2.33	0.46
1:A:1079:ALA:HB1	1:A:1556:LEU:CA	2.45	0.46
1:A:1326:TYR:HB2	1:A:1386:TRP:CZ2	2.50	0.46
1:A:1790:TYR:OH	1:A:1840:MET:HE3	2.16	0.46
6:F:58:TYR:OH	6:F:62:LYS:HD2	2.16	0.46
6:F:612:VAL:HG11	6:F:643:MET:HE3	1.98	0.46
6:H:142:LEU:HA	6:H:146:PRO:HB3	1.97	0.46
6:H:702:ASN:ND2	10:L:180:TYR:CD1	2.84	0.46
9:J:93:LEU:HD12	9:J:93:LEU:N	2.31	0.46
9:J:147:THR:O	9:J:150:THR:HG22	2.16	0.46
9:K:222:GLU:OE1	9:K:228:GLN:HG3	2.16	0.46
13:O:354:ARG:CD	13:O:573:LYS:O	2.63	0.46
3:P:290:ARG:NH2	3:P:319:LEU:HD12	2.26	0.46
15:R:85:ALA:O	15:R:88:MET:HB2	2.15	0.46
18:Z:159:LYS:HE2	18:Z:159:LYS:HB3	1.78	0.46
1:A:1745:PRO:HB3	13:O:609:ALA:HB1	1.97	0.46
3:C:66:PRO:O	3:C:67:LEU:HB3	2.16	0.46
3:C:516:LEU:HD22	3:C:520:TYR:CE2	2.50	0.46
6:H:473:TYR:HD2	6:H:500:TRP:CZ2	2.34	0.46
8:I:45:LEU:HG	8:I:57:SER:HA	1.98	0.46
8:I:286:ARG:O	8:I:290:PHE:CG	2.69	0.46
9:J:445:GLU:CA	9:J:474:LEU:HD23	2.43	0.46
9:J:514:PHE:O	9:J:518:MET:HB2	2.16	0.46
9:K:502:PHE:CZ	9:K:518:MET:HG3	2.51	0.46
13:O:143:TYR:CD1	13:O:143:TYR:C	2.94	0.46
13:O:571:CYS:SG	13:O:579:MET:HB3	2.56	0.46
3:P:358:LEU:O	3:P:362:PRO:HB3	2.15	0.46
3:P:365:LEU:HD23	3:P:395:ASN:ND2	2.31	0.46
15:R:127:GLU:HA	15:R:128:ALA:HA	1.70	0.46
16:S:29:VAL:HG11	18:Z:140:THR:HB	1.98	0.46
17:X:494:ASP:OD1	17:X:494:ASP:N	2.48	0.46
1:A:776:ASN:HA	1:A:869:ARG:NE	2.31	0.46
1:A:1230:ILE:HG21	15:R:120:LEU:HD23	1.98	0.46
1:A:1246:PRO:HB2	1:A:1249:VAL:HG23	1.98	0.46
3:C:145:GLN:HG3	13:O:246:PHE:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:335:CYS:HG	3:C:354:PHE:HE1	1.64	0.46
6:F:563:ASP:OD1	6:F:564:LYS:O	2.34	0.46
6:H:656:MET:SD	9:K:523:ILE:HG23	2.56	0.46
6:H:729:LEU:HD13	6:H:739:VAL:HG22	1.98	0.46
9:K:180:GLU:O	9:K:184:LEU:N	2.35	0.46
12:N:235:GLN:HA	12:N:238:GLU:CD	2.41	0.46
12:N:531:PHE:O	12:N:533:PHE:HA	2.15	0.46
13:O:159:GLN:O	13:O:163:GLN:HG2	2.15	0.46
13:O:274:LEU:HD23	13:O:275:LEU:HD12	1.98	0.46
3:P:170:PHE:O	3:P:171:GLY:C	2.56	0.46
3:P:373:HIS:O	3:P:377:GLU:HG2	2.15	0.46
17:Y:145:CYS:O	17:Y:149:LEU:HG	2.15	0.46
18:Z:146:GLU:CD	18:Z:146:GLU:N	2.72	0.46
1:A:617:LEU:HD11	1:A:782:GLY:CA	2.46	0.45
3:C:390:HIS:CD2	13:O:280:ARG:NH2	2.84	0.45
8:I:202:ALA:O	8:I:223:VAL:CG2	2.64	0.45
9:K:481:THR:O	9:K:485:ILE:HG13	2.16	0.45
10:L:73:THR:HG22	10:L:131:PRO:HB2	1.97	0.45
12:N:155:THR:HA	12:N:158:ARG:HD2	1.99	0.45
3:P:33:LYS:NZ	3:P:64:ALA:HA	2.30	0.45
17:X:145:CYS:O	17:X:149:LEU:HG	2.15	0.45
1:A:94:TYR:HE1	1:A:96:ALA:HB2	1.81	0.45
1:A:94:TYR:O	1:A:100:VAL:HA	2.16	0.45
1:A:780:GLY:C	1:A:782:GLY:H	2.23	0.45
1:A:1176:LEU:HD22	1:A:1176:LEU:HA	1.67	0.45
1:A:1522:SER:O	1:A:1526:VAL:HG13	2.17	0.45
1:A:1543:HIS:CD2	1:A:1559:HIS:HE1	2.34	0.45
3:C:92:ALA:O	3:C:96:VAL:HG23	2.16	0.45
3:C:93:TYR:CD1	3:C:98:GLU:OE2	2.69	0.45
8:I:278:GLU:HA	8:I:281:MET:SD	2.55	0.45
9:J:69:TYR:O	9:J:70:GLU:HB3	2.16	0.45
15:R:261:LEU:CD1	15:R:261:LEU:N	2.79	0.45
17:X:283:ARG:O	17:X:407:LEU:HD12	2.16	0.45
1:A:629:LEU:C	1:A:629:LEU:HD12	2.42	0.45
1:A:872:LEU:HD11	1:A:939:PHE:CD2	2.52	0.45
1:A:957:ASP:OD2	1:A:1820:PHE:HZ	1.99	0.45
2:B:17:VAL:CG2	12:N:634:THR:H	2.21	0.45
5:E:55:CYS:O	5:E:58:VAL:HG12	2.17	0.45
6:F:19:TYR:HE2	6:H:50:ARG:CD	2.28	0.45
8:I:74:ARG:HD2	8:I:174:ASN:HD22	1.81	0.45
8:I:166:LYS:O	8:I:170:ASP:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:224:SER:OG	8:I:228:ALA:O	2.29	0.45
9:J:332:THR:H	9:J:363:LEU:HD11	1.82	0.45
9:J:334:GLY:HA3	9:J:364:MET:SD	2.57	0.45
12:N:519:TYR:HE1	12:N:523:LEU:HD21	1.82	0.45
13:O:62:GLN:O	13:O:66:PRO:CD	2.64	0.45
13:O:226:ASP:OD1	13:O:227:GLU:N	2.48	0.45
13:O:738:ARG:CZ	13:O:738:ARG:HB3	2.45	0.45
3:P:515:TYR:HA	3:P:518:GLN:HG2	1.99	0.45
14:Q:188:ASN:O	14:Q:231:SER:HA	2.16	0.45
15:R:442:HIS:CE1	15:R:468:ARG:HD2	2.51	0.45
17:X:338:HIS:O	17:X:341:PRO:HD2	2.16	0.45
1:A:613:ALA:HB1	1:A:619:GLN:HB2	1.98	0.45
1:A:628:ILE:HG12	1:A:765:VAL:HG11	1.98	0.45
1:A:860:TYR:CG	1:A:861:PRO:HD2	2.51	0.45
1:A:1019:MET:HB2	1:A:1021:HIS:CE1	2.52	0.45
1:A:1086:MET:HG2	1:A:1610:TYR:CE1	2.52	0.45
1:A:1702:ARG:HD3	1:A:1782:GLU:CD	2.41	0.45
8:I:737:ASN:OD1	8:I:738:LEU:N	2.49	0.45
9:K:248:LYS:HB2	9:K:438:GLU:OE2	2.17	0.45
12:N:202:GLU:HB2	12:N:282:GLU:CD	2.40	0.45
13:O:402:LEU:HD13	13:O:425:LYS:HE2	1.98	0.45
16:S:58:GLN:O	16:S:62:PHE:CE2	2.65	0.45
16:S:200:VAL:HG23	16:S:201:SER:N	2.32	0.45
16:S:261:PRO:O	16:S:263:PRO:N	2.49	0.45
17:X:87:LEU:HD22	17:X:95:ASN:ND2	2.30	0.45
17:X:168:THR:OG1	17:X:171:ILE:HD12	2.17	0.45
17:X:442:GLN:CD	17:X:472:ARG:HG3	2.41	0.45
17:Y:316:ALA:HB1	17:Y:351:TYR:CZ	2.52	0.45
18:Z:75:TRP:NE1	18:Z:161:LEU:HD21	2.31	0.45
1:A:1089:LEU:CD1	1:A:1611:VAL:HG23	2.45	0.45
2:B:42:ASP:O	2:B:43:ASP:CB	2.64	0.45
6:F:639:TYR:CD1	15:R:498:ILE:HG21	2.52	0.45
6:H:515:TYR:CE2	6:H:545:HIS:CD2	3.03	0.45
9:J:289:HIS:C	9:J:289:HIS:CD2	2.94	0.45
9:K:384:SER:HB3	9:K:415:ASN:OD1	2.16	0.45
10:L:98:VAL:HB	10:L:134:THR:HG21	1.99	0.45
13:O:83:GLU:HG3	13:O:90:ALA:CB	2.47	0.45
3:P:92:ALA:O	3:P:96:VAL:HG23	2.16	0.45
14:Q:179:PRO:HB3	16:S:555:ARG:CZ	2.47	0.45
14:Q:261:LEU:N	14:Q:261:LEU:CD1	2.79	0.45
14:Q:498:ILE:O	14:Q:499:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:88:MET:O	15:R:91:ALA:HB3	2.16	0.45
16:S:29:VAL:CG1	16:S:36:ARG:CZ	2.91	0.45
16:S:41:LEU:HD12	18:Z:141:PHE:CB	2.47	0.45
17:X:63:MET:HE2	17:Y:266:LEU:HD22	1.97	0.45
18:Z:83:LYS:HA	18:Z:102:PHE:O	2.17	0.45
1:A:617:LEU:HD11	1:A:782:GLY:HA3	1.97	0.45
1:A:1540:ARG:NH1	12:N:486:ASP:O	2.50	0.45
5:E:96:PHE:HB2	6:H:595:GLN:HE21	1.82	0.45
9:J:376:LEU:CD2	9:J:407:GLU:HG2	2.47	0.45
12:N:76:VAL:O	12:N:80:GLN:HB3	2.16	0.45
3:P:379:LYS:HA	3:P:379:LYS:HD2	1.75	0.45
14:Q:190:VAL:HG12	14:Q:450:THR:HG21	1.99	0.45
17:X:442:GLN:CD	17:X:472:ARG:CG	2.89	0.45
1:A:42:LEU:HD21	3:C:394:VAL:HG13	1.99	0.45
1:A:1138:HIS:O	1:A:1141:VAL:N	2.50	0.45
8:I:118:VAL:HG12	8:I:173:LEU:O	2.16	0.45
9:K:231:LEU:HA	9:K:234:VAL:HG22	1.98	0.45
12:N:281:TYR:HE2	12:N:356:PRO:HB2	1.71	0.45
13:O:119:PHE:CZ	13:O:136:LEU:HD11	2.52	0.45
16:S:85:THR:HB	16:S:98:MET:CE	2.47	0.45
17:X:442:GLN:CG	17:X:472:ARG:CG	2.79	0.45
17:Y:341:PRO:O	17:Y:344:VAL:HG12	2.16	0.45
17:Y:485:LEU:O	17:Y:489:GLU:HG2	2.17	0.45
18:Z:56:THR:HG23	18:Z:62:ILE:HG13	1.99	0.45
1:A:239:VAL:HG21	1:A:409:ILE:HD12	1.97	0.45
1:A:616:GLU:CD	1:A:779:MET:HE1	2.41	0.45
1:A:1145:LEU:HD22	1:A:1611:VAL:HG21	1.99	0.45
5:E:89:LEU:HD21	6:H:588:LYS:HB3	1.98	0.45
6:H:639:TYR:CD1	6:H:658:PHE:HE1	2.35	0.45
8:I:116:MET:SD	8:I:210:LEU:CG	3.02	0.45
8:I:304:PHE:CZ	8:I:448:VAL:HG13	2.51	0.45
9:J:418:TRP:CZ3	9:J:457:LYS:HG3	2.52	0.45
12:N:570:ILE:CD1	12:N:633:ARG:NH1	2.73	0.45
13:O:604:LEU:HB3	13:O:627:LEU:CD2	2.46	0.45
3:P:115:TYR:C	3:P:115:TYR:CD1	2.95	0.45
3:P:312:MET:H	3:P:312:MET:HG2	1.62	0.45
3:P:402:TRP:CH2	3:P:424:ARG:HG2	2.52	0.45
3:P:487:ALA:HB1	3:P:519:TYR:HE1	1.82	0.45
16:S:65:GLU:C	16:S:69:TYR:CD2	2.94	0.45
17:X:134:SER:O	17:X:138:VAL:HG23	2.17	0.45
1:A:93:LEU:HD21	1:A:151:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:ARG:HG2	1:A:1280:PRO:HD2	1.98	0.45
2:B:16:TRP:CD1	2:B:33:CYS:CA	2.86	0.45
3:C:494:ILE:HA	3:C:497:ILE:HD12	1.99	0.45
6:H:556:SER:OG	6:H:573:ALA:HA	2.17	0.45
8:I:12:ARG:O	8:I:744:PHE:HA	2.17	0.45
8:I:17:LYS:HE3	8:I:51:SER:O	2.15	0.45
8:I:224:SER:HB2	8:I:230:GLU:H	1.81	0.45
8:I:276:TRP:CZ2	8:I:280:LEU:HD22	2.51	0.45
9:K:277:GLU:OE1	9:K:277:GLU:HA	2.16	0.45
13:O:394:THR:HA	13:O:615:ARG:NH1	2.32	0.45
3:P:273:TYR:HB3	3:P:282:ALA:HB2	1.99	0.45
14:Q:355:GLN:O	18:Z:136:THR:HG21	2.17	0.45
17:Y:532:TYR:CE1	17:Y:548:GLY:HA3	2.52	0.45
1:A:87:VAL:HG12	1:A:88:ASP:N	2.32	0.45
1:A:1189:ALA:HB3	1:A:1192:ASN:HD22	1.81	0.45
1:A:1391:ASP:C	1:A:1433:ILE:HG13	2.42	0.45
3:C:550:LEU:O	3:C:553:ILE:HG12	2.17	0.45
6:F:465:LEU:HD22	6:F:495:HIS:CE1	2.52	0.45
6:H:762:TRP:C	6:H:765:ASP:HB3	2.42	0.45
9:J:50:THR:O	9:J:50:THR:HG22	2.16	0.45
9:K:50:THR:HG22	9:K:50:THR:O	2.17	0.45
10:L:24:GLU:HA	10:L:158:ILE:O	2.16	0.45
12:N:434:THR:O	12:N:437:GLN:N	2.50	0.45
3:P:66:PRO:HD2	3:P:68:ALA:O	2.17	0.45
15:R:84:SER:HB2	15:R:87:GLN:HB3	1.99	0.45
16:S:58:GLN:C	16:S:62:PHE:HD2	2.22	0.45
17:Y:406:ARG:HB2	17:Y:409:CYS:SG	2.57	0.45
1:A:1781:GLN:HB2	1:A:1783:THR:HG22	1.98	0.44
6:F:130:ARG:HD2	6:F:133:LYS:HD3	1.99	0.44
8:I:347:LEU:O	8:I:351:HIS:HB2	2.17	0.44
9:J:354:MET:HE1	9:J:377:GLU:CB	2.35	0.44
9:J:468:HIS:HB3	9:J:485:ILE:HG23	1.99	0.44
12:N:185:MET:HE1	12:N:295:ARG:HD3	1.99	0.44
12:N:400:TYR:CZ	12:N:404:ILE:HD11	2.52	0.44
12:N:574:ILE:HG13	12:N:625:LYS:HE2	1.99	0.44
12:N:655:LEU:HA	12:N:724:ARG:O	2.17	0.44
14:Q:461:ALA:HB2	14:Q:467:LEU:CD1	2.47	0.44
17:X:87:LEU:HD13	17:X:95:ASN:ND2	2.31	0.44
17:X:134:SER:N	17:X:137:GLU:OE1	2.50	0.44
17:X:235:TRP:NE1	17:Y:63:MET:SD	2.90	0.44
1:A:1386:TRP:C	1:A:1386:TRP:CD1	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:LEU:HD12	3:P:60:PHE:HB2	1.99	0.44
3:C:96:VAL:N	3:C:97:LYS:HA	2.32	0.44
6:H:689:LEU:HD11	6:H:716:ASN:HD21	1.81	0.44
12:N:74:TRP:CG	12:N:75:PHE:N	2.85	0.44
3:P:242:GLN:O	3:P:243:LEU:HB2	2.17	0.44
16:S:162:TYR:HD2	16:S:174:ILE:CD1	2.30	0.44
17:Y:168:THR:OG1	17:Y:171:ILE:HD12	2.18	0.44
1:A:173:LEU:HA	1:A:174:PRO:HD2	1.88	0.44
1:A:268:VAL:O	1:A:412:LEU:HD23	2.17	0.44
7:G:15:ASP:O	9:J:487:TYR:OH	2.34	0.44
6:H:473:TYR:CD2	6:H:500:TRP:HZ2	2.35	0.44
6:H:703:PRO:CD	10:L:180:TYR:CD2	3.00	0.44
8:I:269:LEU:HD11	8:I:522:LEU:HD13	1.99	0.44
8:I:276:TRP:CZ3	8:I:476:GLY:HA3	2.52	0.44
8:I:410:SER:O	8:I:413:ASN:HB2	2.17	0.44
9:J:163:CYS:O	9:J:163:CYS:SG	2.75	0.44
9:J:227:LEU:HD22	9:J:233:VAL:HG11	2.00	0.44
9:J:405:MET:HE1	9:J:431:LYS:CG	2.47	0.44
9:J:476:PRO:HB2	3:P:148:ASN:ND2	2.32	0.44
12:N:550:GLY:HA2	12:N:551:GLU:HB2	1.99	0.44
12:N:609:LEU:HD22	12:N:639:HIS:HD2	1.83	0.44
16:S:25:SER:HB2	16:S:45:LEU:CG	2.47	0.44
16:S:30:GLN:CB	16:S:91:GLN:CB	2.92	0.44
17:X:485:LEU:O	17:X:489:GLU:HG2	2.17	0.44
17:Y:87:LEU:HD11	17:Y:99:LYS:HG3	1.99	0.44
17:Y:261:LEU:HD22	17:Y:267:LEU:HD23	1.99	0.44
1:A:482:VAL:HG22	1:A:593:ASN:HA	2.00	0.44
1:A:1790:TYR:O	1:A:1793:MET:HB2	2.17	0.44
7:G:13:LEU:HA	7:G:16:ILE:HD12	1.98	0.44
6:H:545:HIS:HE1	10:L:182:SER:O	2.00	0.44
8:I:65:GLY:O	8:I:84:LEU:HD12	2.18	0.44
8:I:397:ILE:HG22	13:O:444:MET:HE3	1.99	0.44
9:K:509:ARG:HG3	9:K:512:ASP:HB2	2.00	0.44
12:N:478:GLU:H	12:N:479:ASP:HA	1.82	0.44
12:N:699:TRP:HB3	12:N:705:LEU:HD23	2.00	0.44
3:P:286:PHE:HB3	3:P:303:PHE:CE2	2.53	0.44
17:X:410:TYR:O	17:X:414:ILE:HG22	2.17	0.44
17:Y:546:LEU:O	17:Y:550:GLN:HG2	2.17	0.44
1:A:1216:LYS:HD2	1:A:1216:LYS:N	2.32	0.44
1:A:1279:ARG:NH1	1:A:1287:TYR:OH	2.51	0.44
6:F:639:TYR:CD1	6:F:639:TYR:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:734:PRO:HB2	9:J:144:ASP:HB3	1.99	0.44
8:I:224:SER:HB3	8:I:229:SER:HA	1.96	0.44
8:I:430:GLU:HA	14:Q:429:LYS:HE2	1.99	0.44
8:I:578:ASN:OD1	8:I:578:ASN:C	2.60	0.44
12:N:186:GLN:O	12:N:190:LYS:HG3	2.18	0.44
13:O:416:GLU:O	13:O:420:ILE:HG22	2.18	0.44
3:P:283:LEU:HD13	3:P:306:LEU:HD11	2.00	0.44
17:Y:99:LYS:HD3	17:Y:102:MET:CE	2.48	0.44
17:Y:200:PRO:C	17:Y:202:ALA:H	2.24	0.44
17:Y:281:TYR:HB3	17:Y:290:SER:OG	2.17	0.44
1:A:872:LEU:HD11	1:A:939:PHE:HB2	1.99	0.44
1:A:1194:HIS:CG	15:R:121:ASN:HD21	2.36	0.44
1:A:1845:LEU:N	1:A:1846:PRO:HD2	2.32	0.44
4:D:14:GLU:HB2	4:D:17:TRP:CZ3	2.53	0.44
6:F:26:PHE:CD1	6:H:149:TRP:CG	3.06	0.44
6:H:483:GLU:O	6:H:487:ILE:HG12	2.17	0.44
6:H:703:PRO:HB3	6:H:733:VAL:CG2	2.47	0.44
8:I:360:LEU:HD12	8:I:397:ILE:CD1	2.47	0.44
9:K:147:THR:O	9:K:150:THR:HG22	2.18	0.44
9:K:163:CYS:O	9:K:163:CYS:SG	2.76	0.44
9:K:404:VAL:O	9:K:408:VAL:HG23	2.18	0.44
14:Q:185:TYR:CD1	16:S:27:GLU:CG	3.01	0.44
14:Q:425:LEU:HB2	14:Q:439:LEU:HB2	1.99	0.44
17:X:149:LEU:O	17:X:150:LYS:HB2	2.17	0.44
17:X:199:CYS:HA	17:X:200:PRO:HD2	1.81	0.44
17:X:371:ASN:HD22	17:X:371:ASN:N	2.09	0.44
17:Y:305:ILE:HG22	17:Y:340:GLU:OE1	2.17	0.44
1:A:454:CYS:O	1:A:471:VAL:HA	2.18	0.44
1:A:1136:SER:OG	1:A:1171:GLU:HB3	2.17	0.44
1:A:1599:ASN:HB2	1:A:1603:LEU:H	1.83	0.44
6:H:522:PHE:O	6:H:525:VAL:HB	2.18	0.44
9:J:306:GLY:HA3	9:J:323:LEU:HD13	1.99	0.44
9:K:24:PHE:CD1	9:K:24:PHE:C	2.95	0.44
9:K:222:GLU:OE2	9:K:228:GLN:HG3	2.18	0.44
9:K:337:TRP:HB3	9:K:360:ALA:HB2	1.98	0.44
12:N:648:VAL:CG1	12:N:650:LEU:HG	2.47	0.44
13:O:44:MET:HE2	13:O:60:LEU:CD2	2.47	0.44
16:S:30:GLN:CB	16:S:36:ARG:HH21	2.30	0.44
16:S:41:LEU:HD21	16:S:90:PRO:HB3	1.98	0.44
16:S:59:LYS:HA	16:S:62:PHE:HD2	1.82	0.44
16:S:83:SER:O	16:S:87:GLN:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:270:ASN:HA	17:Y:62:THR:HG21	1.99	0.44
17:X:281:TYR:HB3	17:X:290:SER:OG	2.17	0.44
1:A:42:LEU:HD13	3:C:363:ARG:HG3	2.00	0.44
1:A:174:PRO:HG3	1:A:356:PHE:CE2	2.53	0.44
1:A:1671:PRO:HB2	1:A:1705:GLN:HE22	1.82	0.44
3:C:60:PHE:CG	3:P:89:LEU:HD12	2.52	0.44
3:C:61:SER:CB	3:C:262:SER:HB2	2.46	0.44
3:C:66:PRO:HD2	3:C:68:ALA:O	2.17	0.44
3:C:296:ARG:HA	3:P:101:ARG:NH2	2.33	0.44
6:F:483:GLU:O	6:F:487:ILE:HG12	2.17	0.44
6:H:621:LEU:HG	6:H:644:ILE:HG21	1.99	0.44
8:I:96:GLU:OE1	12:N:427:TYR:HE1	2.01	0.44
9:J:477:GLN:O	9:J:508:LEU:HD13	2.17	0.44
9:J:509:ARG:HD2	9:J:512:ASP:HB2	1.99	0.44
10:L:113:LEU:HD13	10:L:120:ILE:HD13	1.99	0.44
12:N:761:MET:HE2	16:S:205:LEU:HD21	2.00	0.44
3:P:48:LEU:N	3:P:48:LEU:HD23	2.33	0.44
3:P:96:VAL:N	3:P:97:LYS:HA	2.33	0.44
3:P:402:TRP:HZ3	3:P:421:TYR:HD1	1.66	0.44
14:Q:411:TYR:CE1	14:Q:475:LEU:CD2	3.01	0.44
16:S:75:LEU:O	16:S:75:LEU:HD22	2.18	0.44
17:Y:100:TYR:HB2	17:Y:142:MET:HG2	2.00	0.44
1:A:1194:HIS:CD2	15:R:121:ASN:HD21	2.36	0.44
1:A:1552:TYR:OH	1:A:1604:GLN:NE2	2.51	0.44
1:A:1571:ARG:NH1	1:A:1694:ASP:O	2.51	0.44
2:B:15:LEU:O	2:B:16:TRP:C	2.61	0.44
6:F:522:PHE:O	6:F:525:VAL:HB	2.18	0.44
9:K:391:PHE:CE2	9:K:411:VAL:HG21	2.53	0.44
12:N:165:THR:N	12:N:166:PRO:CA	2.79	0.44
17:X:316:ALA:HB1	17:X:351:TYR:CZ	2.53	0.44
17:Y:39:ASP:OD1	17:Y:39:ASP:N	2.50	0.44
1:A:1621:PRO:HA	1:A:1697:LEU:O	2.18	0.43
2:B:36:ASP:O	2:B:38:LYS:N	2.51	0.43
3:C:148:ASN:HB3	3:C:151:LEU:CD1	2.48	0.43
3:C:358:LEU:O	3:C:362:PRO:CA	2.65	0.43
5:E:78:ARG:NH2	6:H:554:VAL:HG22	2.33	0.43
6:F:556:SER:OG	6:F:573:ALA:HA	2.18	0.43
6:H:489:SER:O	17:X:105:GLN:NE2	2.51	0.43
6:H:552:LEU:HG	6:H:576:CYS:SG	2.57	0.43
9:K:74:TYR:OH	9:K:78:ARG:HD2	2.17	0.43
9:K:272:ILE:HG21	9:K:303:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:289:HIS:CD2	11:M:57:TRP:CE3	3.06	0.43
9:K:372:LEU:HD11	9:K:407:GLU:CG	2.47	0.43
12:N:574:ILE:HA	12:N:625:LYS:HE2	2.00	0.43
13:O:386:GLN:HB2	13:O:424:GLN:NE2	2.32	0.43
15:R:96:SER:O	15:R:99:ASN:HB2	2.18	0.43
16:S:58:GLN:NE2	16:S:62:PHE:CZ	2.75	0.43
16:S:134:GLU:N	16:S:135:PRO:HD3	2.33	0.43
1:A:119:VAL:HG11	1:A:153:ILE:HG21	2.00	0.43
1:A:1041:LEU:HD13	1:A:1084:ARG:HA	2.00	0.43
1:A:1254:VAL:HG11	1:A:1298:ALA:CA	2.44	0.43
1:A:1634:LEU:O	1:A:1650:GLU:HA	2.18	0.43
1:A:1637:THR:OG1	1:A:1665:GLN:HG3	2.18	0.43
3:C:36:LEU:O	3:C:39:ILE:HG22	2.19	0.43
8:I:294:LYS:CB	8:I:320:LEU:HD22	2.49	0.43
9:J:432:ILE:HD11	9:J:444:TRP:CD1	2.53	0.43
9:K:146:ARG:CZ	9:K:332:THR:HG22	2.48	0.43
9:K:167:PHE:CE1	9:K:171:THR:HG21	2.53	0.43
12:N:404:ILE:HA	12:N:417:LEU:HD11	2.00	0.43
3:P:158:LEU:HD11	3:P:174:LEU:CD1	2.48	0.43
15:R:188:ASN:O	15:R:231:SER:HA	2.17	0.43
15:R:425:LEU:HB2	15:R:439:LEU:HB2	1.99	0.43
16:S:85:THR:HB	16:S:98:MET:HE1	2.00	0.43
16:S:134:GLU:C	16:S:136:LEU:H	2.25	0.43
17:Y:134:SER:N	17:Y:137:GLU:OE1	2.51	0.43
1:A:161:MET:HG3	1:A:216:PRO:HB3	2.00	0.43
1:A:790:LEU:HD13	1:A:806:TYR:OH	2.18	0.43
2:B:16:TRP:HB3	2:B:33:CYS:HB3	1.99	0.43
2:B:17:VAL:HA	2:B:31:ASN:CG	2.43	0.43
3:C:89:LEU:HD12	3:P:60:PHE:CB	2.49	0.43
3:C:145:GLN:HG2	13:O:246:PHE:HA	1.99	0.43
6:H:657:HIS:HA	6:H:660:LYS:HE3	2.00	0.43
6:H:747:TYR:CD2	6:H:755:LEU:HB3	2.53	0.43
8:I:11:PHE:CD1	8:I:746:MET:HE2	2.52	0.43
9:J:441:VAL:HG23	9:J:442:ASP:N	2.33	0.43
12:N:602:PRO:N	12:N:603:PRO:HD2	2.32	0.43
3:P:242:GLN:NE2	3:P:428:LEU:O	2.51	0.43
14:Q:185:TYR:CD1	16:S:27:GLU:HG3	2.53	0.43
15:R:84:SER:O	15:R:88:MET:N	2.51	0.43
16:S:38:MET:HB3	18:Z:181:VAL:CG2	2.46	0.43
17:X:39:ASP:OD1	17:X:39:ASP:N	2.51	0.43
17:Y:100:TYR:CB	17:Y:142:MET:CG	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:170:SER:OG	18:Z:171:GLY:N	2.51	0.43
1:A:409:ILE:HG22	1:A:410:ASP:N	2.33	0.43
1:A:1731:ARG:HE	1:A:1731:ARG:C	2.26	0.43
2:B:38:LYS:HG2	2:B:40:PRO:HG2	1.99	0.43
2:B:62:LYS:O	2:B:69:VAL:HG21	2.17	0.43
8:I:101:LEU:HD23	8:I:101:LEU:C	2.43	0.43
9:J:167:PHE:HA	9:J:170:LEU:HD21	1.99	0.43
9:J:242:TYR:HB2	9:J:250:CYS:SG	2.59	0.43
10:L:33:LEU:HD13	10:L:54:TRP:CD2	2.53	0.43
12:N:527:LEU:HD11	12:N:561:LEU:HD22	2.00	0.43
13:O:402:LEU:HD13	13:O:425:LYS:HG2	1.99	0.43
3:P:209:LEU:HB3	3:P:233:PHE:HE1	1.82	0.43
16:S:162:TYR:CD2	16:S:174:ILE:CD1	3.01	0.43
17:X:341:PRO:O	17:X:344:VAL:HG12	2.18	0.43
17:Y:149:LEU:O	17:Y:150:LYS:HB2	2.18	0.43
17:Y:437:LEU:CB	17:Y:444:LEU:HD11	2.48	0.43
1:A:777:THR:HB	1:A:946:THR:O	2.18	0.43
1:A:1138:HIS:CE1	1:A:1604:GLN:HE21	2.26	0.43
1:A:1194:HIS:CB	15:R:121:ASN:HD21	2.31	0.43
1:A:1230:ILE:CA	1:A:1236:LEU:HD13	2.49	0.43
1:A:1404:LEU:CD2	1:A:1464:ILE:HD11	2.46	0.43
1:A:1839:PHE:CD1	1:A:1840:MET:HG3	2.53	0.43
3:C:356:ARG:NH2	11:M:19:TRP:HA	2.33	0.43
4:D:6:PRO:HB2	13:O:420:ILE:HG13	2.01	0.43
4:D:18:PHE:O	4:D:18:PHE:CG	2.71	0.43
8:I:266:ASN:HA	8:I:526:LYS:HZ3	1.82	0.43
8:I:312:LYS:CG	8:I:428:MET:HB3	2.45	0.43
9:J:247:PHE:CE2	9:J:277:GLU:HG3	2.54	0.43
13:O:663:ALA:O	13:O:667:VAL:HG23	2.18	0.43
3:P:116:PHE:CD2	3:P:116:PHE:C	2.96	0.43
1:A:845:TYR:CE1	1:A:951:ILE:HD11	2.52	0.43
1:A:1512:LEU:HA	1:A:1515:CYS:SG	2.58	0.43
1:A:1618:LEU:HA	1:A:1656:LEU:HA	2.01	0.43
1:A:1666:ILE:HG21	1:A:1687:LEU:HD11	2.01	0.43
1:A:1803:ARG:CB	1:A:1884:MET:HE1	2.49	0.43
2:B:16:TRP:HB3	2:B:33:CYS:CA	2.48	0.43
6:F:75:LEU:HG	6:F:91:ILE:HD13	2.00	0.43
8:I:95:VAL:HG12	12:N:389:PRO:HG2	2.01	0.43
8:I:231:VAL:CG1	8:I:556:LEU:HD12	2.48	0.43
8:I:578:ASN:CG	8:I:646:ASP:CG	2.87	0.43
10:L:125:THR:CA	10:L:126:ASP:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:601:LEU:HB2	13:O:602:PRO:HD3	2.00	0.43
15:R:179:PRO:HG2	16:S:226:THR:HG22	2.00	0.43
16:S:88:ASN:ND2	16:S:88:ASN:N	2.67	0.43
17:X:50:HIS:HA	17:X:53:VAL:HG22	1.99	0.43
1:A:501:THR:HB	1:A:504:VAL:HG22	2.01	0.43
1:A:871:ARG:HG3	1:A:872:LEU:N	2.34	0.43
1:A:1024:MET:HG2	1:A:1034:VAL:HG11	2.00	0.43
1:A:1110:ARG:HG2	1:A:1117:THR:HG22	2.00	0.43
1:A:1166:ALA:HA	1:A:1169:ALA:HB2	1.99	0.43
1:A:1170:ASN:HD21	1:A:1203:MET:HG3	1.83	0.43
1:A:1304:MET:O	1:A:1307:LEU:HB2	2.18	0.43
2:B:27:ARG:CB	12:N:810:TYR:CE2	2.96	0.43
6:F:130:ARG:HD3	17:Y:506:GLN:HB2	2.00	0.43
6:H:513:SER:HA	6:H:515:TYR:CE1	2.54	0.43
9:J:404:VAL:O	9:J:408:VAL:HG23	2.19	0.43
9:J:465:LEU:HD22	9:J:469:ARG:HH11	1.83	0.43
9:K:268:LEU:N	9:K:269:PRO:HD2	2.34	0.43
9:K:432:ILE:HD11	9:K:444:TRP:CD1	2.54	0.43
10:L:14:LYS:HA	10:L:17:GLU:OE1	2.19	0.43
13:O:324:LEU:HD22	13:O:350:LEU:HD12	2.00	0.43
13:O:385:VAL:HG11	13:O:402:LEU:HG	2.01	0.43
3:P:283:LEU:HD21	3:P:312:MET:HE1	1.99	0.43
14:Q:163:LYS:NZ	16:S:224:ARG:HH22	2.16	0.43
1:A:457:PHE:HB3	1:A:468:PHE:CE1	2.53	0.43
3:C:67:LEU:HD22	3:P:78:GLU:HA	2.01	0.43
6:H:761:SER:O	6:H:765:ASP:N	2.51	0.43
8:I:207:ALA:HB3	8:I:220:VAL:HB	2.00	0.43
8:I:320:LEU:HA	8:I:320:LEU:HD12	1.75	0.43
8:I:497:TRP:HH2	8:I:507:LEU:HD13	1.81	0.43
9:J:405:MET:HE3	9:J:427:ASP:CG	2.44	0.43
9:K:230:ASN:O	9:K:233:VAL:HG22	2.18	0.43
9:K:272:ILE:HG23	9:K:307:CYS:SG	2.59	0.43
9:K:309:TYR:HD2	9:K:315:LYS:HB3	1.83	0.43
12:N:75:PHE:O	12:N:76:VAL:C	2.62	0.43
3:P:209:LEU:HB3	3:P:233:PHE:CE1	2.53	0.43
15:R:357:ALA:CB	16:S:305:GLU:HG3	2.48	0.43
15:R:498:ILE:O	15:R:499:ARG:HB2	2.19	0.43
16:S:78:TRP:CD1	16:S:109:LEU:HD11	2.54	0.43
17:X:267:LEU:CD1	17:Y:59:LEU:HD11	2.39	0.43
2:B:47:VAL:HG21	2:B:82:PHE:CD2	2.53	0.43
3:C:46:ARG:HB3	3:C:116:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:414:MET:HG2	13:O:330:ILE:HD13	1.95	0.43
6:F:96:VAL:O	6:F:97:PHE:HB2	2.18	0.43
6:H:515:TYR:HD1	6:H:515:TYR:H	1.66	0.43
6:H:673:CYS:O	6:H:677:VAL:HG23	2.19	0.43
8:I:290:PHE:HE2	8:I:325:LEU:HD12	1.84	0.43
8:I:306:HIS:HE1	8:I:316:GLU:HB3	1.83	0.43
9:J:268:LEU:N	9:J:269:PRO:HD2	2.33	0.43
12:N:501:ILE:HD13	12:N:548:ARG:NH2	2.34	0.43
12:N:560:MET:HE3	12:N:600:PHE:CB	2.49	0.43
13:O:648:ILE:O	13:O:652:LEU:HG	2.19	0.43
16:S:66:ILE:O	16:S:69:TYR:HB2	2.19	0.43
16:S:68:PHE:HE1	16:S:78:TRP:HA	1.82	0.43
16:S:261:PRO:C	16:S:263:PRO:N	2.76	0.43
17:X:222:MET:O	17:X:226:VAL:HG23	2.19	0.43
1:A:1165:HIS:HD2	1:A:1167:GLU:H	1.67	0.43
1:A:1550:MET:SD	1:A:1558:HIS:HE1	2.42	0.43
1:A:1595:HIS:NE2	1:A:1598:ASP:HB2	2.34	0.43
2:B:8:TRP:NE1	12:N:644:VAL:HG12	2.34	0.43
2:B:26:CYS:HB3	2:B:59:CYS:SG	2.59	0.43
3:C:54:TRP:CE3	3:C:203:TRP:HB2	2.54	0.43
6:F:142:LEU:HA	6:F:146:PRO:HB3	2.00	0.43
6:H:702:ASN:HA	6:H:703:PRO:HD3	1.91	0.43
8:I:74:ARG:HD2	8:I:174:ASN:ND2	2.34	0.43
8:I:313:ALA:HB3	8:I:317:LEU:CD1	2.47	0.43
12:N:556:PHE:CE1	12:N:600:PHE:HA	2.54	0.43
13:O:56:GLU:HB3	13:O:86:CYS:SG	2.59	0.43
15:R:258:GLN:O	15:R:258:GLN:HG2	2.19	0.43
16:S:70:THR:O	16:S:74:PRO:CD	2.65	0.43
16:S:75:LEU:C	16:S:75:LEU:CD1	2.90	0.43
16:S:200:VAL:O	16:S:204:THR:HG23	2.19	0.43
7:W:5:LYS:HB3	7:W:5:LYS:HE3	1.76	0.43
17:Y:134:SER:O	17:Y:138:VAL:HG23	2.18	0.43
1:A:1036:ASP:O	1:A:1040:LEU:HD13	2.19	0.42
1:A:1250:GLN:O	1:A:1254:VAL:HG23	2.19	0.42
8:I:19:LEU:HD13	8:I:23:ILE:HG13	2.00	0.42
12:N:151:GLU:O	12:N:155:THR:HG23	2.19	0.42
15:R:112:HIS:NE2	15:R:116:TRP:CZ3	2.80	0.42
16:S:33:ARG:HA	18:Z:144:LEU:HG	2.01	0.42
7:W:13:LEU:HA	7:W:16:ILE:HD12	2.01	0.42
17:X:430:ALA:HB2	17:X:451:CYS:SG	2.59	0.42
17:Y:170:LYS:HG2	17:Y:171:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:222:MET:O	17:Y:226:VAL:HG23	2.18	0.42
17:Y:410:TYR:O	17:Y:414:ILE:HG22	2.19	0.42
1:A:131:PHE:HE1	1:A:187:LEU:HB2	1.84	0.42
1:A:487:THR:HG22	1:A:501:THR:HA	2.00	0.42
1:A:1190:THR:O	1:A:1193:ILE:HB	2.19	0.42
1:A:1813:GLN:O	1:A:1817:VAL:HG23	2.19	0.42
3:C:414:MET:HG3	13:O:330:ILE:HD11	1.99	0.42
8:I:280:LEU:O	8:I:280:LEU:HG	2.19	0.42
9:J:42:TRP:HA	9:J:42:TRP:HE3	1.83	0.42
9:J:482:TYR:CD1	9:J:485:ILE:HD11	2.54	0.42
9:K:386:LEU:HD12	9:K:386:LEU:N	2.34	0.42
12:N:395:ASP:OD1	12:N:398:THR:HG23	2.18	0.42
12:N:455:THR:CB	12:N:501:ILE:HD11	2.49	0.42
13:O:40:LEU:HD22	13:O:82:ILE:HD12	2.00	0.42
16:S:75:LEU:CB	16:S:115:TYR:OH	2.62	0.42
17:X:417:TYR:CE2	17:X:429:MET:HE1	2.53	0.42
17:Y:199:CYS:HB2	17:Y:200:PRO:C	2.44	0.42
18:Z:163:VAL:HA	18:Z:164:PRO:HD3	1.85	0.42
1:A:250:ASN:HD22	1:A:251:THR:N	2.17	0.42
1:A:1360:VAL:HB	1:A:1364:CYS:HB2	2.00	0.42
6:F:61:LEU:HD23	6:F:61:LEU:HA	1.94	0.42
6:F:135:SER:OG	6:F:160:GLU:HG3	2.18	0.42
9:J:210:LYS:HE3	9:J:212:TYR:CZ	2.54	0.42
9:K:289:HIS:ND1	11:M:57:TRP:CZ3	2.87	0.42
12:N:570:ILE:CD1	12:N:633:ARG:HH12	2.22	0.42
12:N:662:VAL:HB	12:N:687:MET:SD	2.58	0.42
3:P:399:TYR:CE2	14:Q:498:ILE:CG2	3.02	0.42
14:Q:258:GLN:HG2	14:Q:258:GLN:O	2.19	0.42
16:S:82:ILE:HG21	16:S:127:LYS:HD3	2.02	0.42
17:X:76:LYS:C	17:X:106:GLN:NE2	2.77	0.42
17:Y:465:LEU:HD23	17:Y:485:LEU:HD11	2.01	0.42
1:A:877:ILE:HG23	1:A:881:ILE:HD12	2.00	0.42
3:C:60:PHE:CB	3:P:89:LEU:HD12	2.49	0.42
3:C:402:TRP:HZ3	3:C:421:TYR:HD1	1.66	0.42
6:F:621:LEU:HG	6:F:644:ILE:HG21	2.00	0.42
6:H:703:PRO:CD	10:L:180:TYR:CE2	3.02	0.42
8:I:285:SER:O	8:I:289:LYS:HG2	2.19	0.42
8:I:474:ARG:O	8:I:477:GLN:HG3	2.19	0.42
10:L:83:TYR:N	10:L:116:PRO:O	2.53	0.42
12:N:86:ASN:C	12:N:89:PRO:HD2	2.45	0.42
12:N:574:ILE:CD1	12:N:625:LYS:HG2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:669:TYR:CZ	12:N:684:ALA:HB1	2.53	0.42
13:O:418:ILE:HG21	13:O:448:MET:HE1	2.01	0.42
3:P:151:LEU:HB3	3:P:182:LEU:HD11	2.02	0.42
17:X:270:ASN:HB2	17:X:273:LEU:HB2	2.01	0.42
1:A:802:TYR:CZ	1:A:841:PRO:HA	2.54	0.42
1:A:1194:HIS:NE2	15:R:117:ALA:HA	2.35	0.42
1:A:1220:MET:HE1	3:C:544:GLU:HB2	2.01	0.42
1:A:1316:MET:O	1:A:1319:LEU:O	2.38	0.42
1:A:1322:PRO:CG	1:A:1375:TYR:OH	2.54	0.42
6:F:134:GLY:O	6:F:137:CYS:HB3	2.19	0.42
6:H:473:TYR:CD2	6:H:500:TRP:CZ2	3.08	0.42
9:J:18:GLN:NE2	9:K:134:LEU:CD1	2.83	0.42
9:K:251:TYR:HA	9:K:254:THR:HG22	2.01	0.42
12:N:506:VAL:O	12:N:510:GLY:HA3	2.19	0.42
13:O:594:SER:O	13:O:595:SER:HB3	2.19	0.42
3:P:417:TYR:O	3:P:421:TYR:CD2	2.72	0.42
14:Q:420:PHE:HB3	16:S:31:PRO:HD2	2.02	0.42
17:X:465:LEU:HD23	17:X:485:LEU:HD11	2.02	0.42
1:A:93:LEU:HB2	1:A:128:TRP:CH2	2.54	0.42
1:A:1249:VAL:O	1:A:1252:ALA:HB3	2.20	0.42
1:A:1307:LEU:HD21	1:A:1579:SER:HA	2.01	0.42
3:C:158:LEU:HD11	3:C:174:LEU:CD1	2.49	0.42
6:H:480:ASN:HD22	6:H:480:ASN:C	2.28	0.42
8:I:310:TRP:CG	8:I:314:SER:H	2.38	0.42
9:J:61:ARG:HG2	9:J:61:ARG:NH1	2.34	0.42
9:J:497:ASN:N	9:J:497:ASN:OD1	2.53	0.42
11:M:31:ILE:HG22	11:M:33:LEU:HD22	2.02	0.42
12:N:523:LEU:O	12:N:527:LEU:HG	2.20	0.42
13:O:434:ARG:HA	13:O:434:ARG:HD2	1.75	0.42
13:O:493:LEU:HD13	13:O:507:TRP:HB2	2.01	0.42
3:P:203:TRP:HE3	3:P:229:MET:HE1	1.84	0.42
3:P:244:ILE:HD11	3:P:276:ILE:HD11	2.02	0.42
3:P:297:ILE:HD11	3:P:333:THR:HB	2.01	0.42
15:R:193:SER:HB3	15:R:234:TRP:CD2	2.55	0.42
15:R:237:GLU:CD	15:R:237:GLU:H	2.28	0.42
16:S:30:GLN:CB	16:S:36:ARG:NH2	2.83	0.42
17:Y:391:GLU:O	17:Y:394:ILE:HG12	2.19	0.42
17:Y:417:TYR:CE2	17:Y:429:MET:HE1	2.54	0.42
1:A:971:PRO:HG2	1:A:974:VAL:HG23	2.01	0.42
3:C:515:TYR:HA	3:C:518:GLN:HG2	2.00	0.42
3:C:554:LEU:HD12	9:K:386:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:762:TRP:NE1	9:J:362:GLN:HB2	2.35	0.42
8:I:398:LEU:HD23	13:O:444:MET:HG3	2.01	0.42
9:J:482:TYR:HD1	9:J:485:ILE:HD11	1.85	0.42
12:N:180:PHE:CG	12:N:299:TRP:CH2	3.05	0.42
12:N:411:ASP:O	12:N:412:PRO:C	2.61	0.42
13:O:256:LEU:HD23	13:O:256:LEU:HA	1.85	0.42
13:O:508:MET:HA	13:O:511:ASP:OD2	2.19	0.42
13:O:547:LYS:HG3	13:O:563:LEU:HD21	2.02	0.42
3:P:151:LEU:HD22	3:P:178:VAL:HG13	2.01	0.42
3:P:424:ARG:NH1	3:P:424:ARG:HG3	2.33	0.42
14:Q:193:SER:HB3	14:Q:234:TRP:CD2	2.55	0.42
17:X:452:LEU:HD22	17:X:461:ALA:CA	2.47	0.42
18:Z:13:LEU:HD22	18:Z:111:LYS:HB3	2.00	0.42
1:A:857:MET:CB	1:A:858:PRO:CD	2.95	0.42
1:A:1261:TYR:O	1:A:1264:THR:OG1	2.37	0.42
3:C:262:SER:O	3:C:266:VAL:HG23	2.20	0.42
6:H:481:CYS:O	6:H:485:ILE:HG12	2.19	0.42
8:I:248:VAL:HA	8:I:251:MET:HE2	2.01	0.42
8:I:370:ALA:HB2	8:I:386:ILE:HD12	2.01	0.42
8:I:586:LEU:HD12	8:I:587:LEU:N	2.34	0.42
12:N:411:ASP:CG	12:N:416:ILE:HB	2.44	0.42
12:N:556:PHE:HA	12:N:600:PHE:CD1	2.55	0.42
13:O:350:LEU:HA	13:O:350:LEU:HD23	1.86	0.42
13:O:568:LEU:HD13	13:O:583:VAL:HG13	2.02	0.42
13:O:711:ARG:HH12	13:O:745:PRO:HB3	1.84	0.42
3:P:127:GLU:HA	3:P:127:GLU:OE2	2.20	0.42
17:Y:230:VAL:HA	17:Y:231:PRO:HD2	1.88	0.42
18:Z:48:LYS:HG3	18:Z:49:TYR:CD2	2.55	0.42
18:Z:81:VAL:CG2	18:Z:155:ILE:HD12	2.49	0.42
1:A:1638:TYR:N	1:A:1638:TYR:CD1	2.88	0.42
1:A:1739:SER:N	1:A:1740:ALA:HB3	2.35	0.42
2:B:17:VAL:O	2:B:30:PHE:C	2.63	0.42
3:C:434:ARG:HH11	15:R:80:ILE:HD13	1.85	0.42
5:E:102:LEU:HD13	6:H:594:ILE:HG22	2.01	0.42
6:F:699:ASP:CB	6:F:702:ASN:HD21	2.31	0.42
6:H:515:TYR:CD1	6:H:515:TYR:N	2.88	0.42
8:I:403:LEU:HG	8:I:407:ILE:HD11	2.02	0.42
9:J:19:TYR:CD1	9:J:49:LEU:CD1	2.97	0.42
9:J:230:ASN:O	9:J:233:VAL:HG22	2.20	0.42
9:K:289:HIS:CG	11:M:57:TRP:CZ3	3.08	0.42
9:K:499:VAL:HG11	9:K:523:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:180:PHE:HD1	12:N:180:PHE:C	2.28	0.42
12:N:414:MET:SD	12:N:498:SER:N	2.93	0.42
13:O:648:ILE:HA	13:O:651:ILE:HD12	2.02	0.42
16:S:272:ILE:HG13	16:S:273:THR:N	2.35	0.42
17:X:242:ALA:O	17:X:246:VAL:HG23	2.20	0.42
1:A:1867:CYS:CB	1:A:1881:GLN:CD	2.93	0.42
3:C:89:LEU:HD21	3:C:93:TYR:CE2	2.55	0.42
3:C:116:PHE:CD2	3:C:116:PHE:C	2.98	0.42
6:H:130:ARG:NH1	9:K:473:VAL:CG2	2.82	0.42
8:I:556:LEU:HD11	8:I:586:LEU:HD21	2.02	0.42
9:J:17:GLN:HB3	9:K:78:ARG:NH1	2.34	0.42
9:K:284:LEU:HD11	9:K:307:CYS:SG	2.60	0.42
9:K:422:GLU:OE1	9:K:458:LEU:HD22	2.20	0.42
9:K:491:LEU:HA	7:W:22:ILE:HG21	2.02	0.42
10:L:14:LYS:HB3	10:L:18:ARG:CZ	2.50	0.42
12:N:152:GLU:O	12:N:156:MET:HG2	2.19	0.42
13:O:707:LYS:HA	13:O:710:ILE:CG2	2.49	0.42
3:P:123:TYR:CE1	3:P:151:LEU:HD21	2.55	0.42
3:P:303:PHE:CE1	3:P:307:LEU:HD22	2.54	0.42
14:Q:169:PRO:C	14:Q:171:LEU:H	2.27	0.42
17:X:261:LEU:HD22	17:X:267:LEU:HD23	2.02	0.42
17:Y:513:ARG:NH1	17:Y:544:LYS:HB3	2.34	0.42
1:A:1191:LEU:HD23	1:A:1191:LEU:H	1.84	0.41
1:A:1424:LYS:HA	1:A:1427:ASP:OD2	2.20	0.41
3:C:202:HIS:CD2	3:C:202:HIS:C	2.98	0.41
6:F:130:ARG:NH1	17:Y:506:GLN:HB3	2.35	0.41
6:F:550:VAL:HG21	9:K:289:HIS:CB	2.43	0.41
6:F:726:LEU:HD21	6:F:742:LEU:HD22	2.02	0.41
8:I:86:ASP:OD1	8:I:87:THR:N	2.53	0.41
9:K:20:GLN:CA	9:K:20:GLN:HE21	2.32	0.41
9:K:258:MET:HA	9:K:261:ASP:O	2.20	0.41
9:K:444:TRP:CZ3	7:W:6:PRO:HG2	2.54	0.41
10:L:144:ASN:CG	10:L:151:THR:HG23	2.45	0.41
11:M:32:PRO:O	11:M:33:LEU:HB2	2.20	0.41
12:N:180:PHE:CD1	12:N:180:PHE:C	2.98	0.41
14:Q:163:LYS:NZ	15:R:465:GLU:O	2.48	0.41
1:A:269:TRP:CZ3	1:A:411:HIS:HB2	2.55	0.41
1:A:1588:LEU:O	1:A:1589:TYR:C	2.63	0.41
3:C:48:LEU:N	3:C:48:LEU:HD23	2.35	0.41
8:I:427:ARG:CB	8:I:428:MET:HE2	2.48	0.41
9:J:24:PHE:CE1	9:J:28:LYS:CE	3.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:40:PHE:CA	10:L:44:GLN:OE1	2.64	0.41
12:N:432:GLU:C	12:N:434:THR:H	2.26	0.41
12:N:456:GLY:C	12:N:544:LEU:HG	2.45	0.41
12:N:528:LEU:HD11	12:N:641:LEU:HD13	2.01	0.41
12:N:681:LEU:HD23	12:N:692:LEU:HD21	2.01	0.41
17:X:391:GLU:O	17:X:394:ILE:HG12	2.20	0.41
1:A:129:CYS:SG	1:A:187:LEU:HD13	2.60	0.41
1:A:860:TYR:CD1	1:A:861:PRO:HD2	2.55	0.41
1:A:1371:LEU:HD23	1:A:1371:LEU:HA	1.86	0.41
1:A:1574:LEU:H	1:A:1574:LEU:HG	1.61	0.41
1:A:1814:ILE:O	1:A:1818:LEU:HD12	2.19	0.41
6:H:32:TYR:CE1	6:H:41:LEU:HB2	2.55	0.41
6:H:624:PHE:O	6:H:628:ILE:HG12	2.21	0.41
8:I:28:TRP:HZ3	8:I:33:ASP:O	2.04	0.41
9:J:21:SER:HB2	9:K:165:GLU:HG3	2.02	0.41
9:J:290:LYS:O	9:J:294:LEU:HD23	2.19	0.41
9:J:323:LEU:HD12	9:J:323:LEU:HA	1.88	0.41
9:J:340:TYR:HE1	9:J:344:PHE:CE2	2.38	0.41
10:L:105:LEU:HD11	10:L:136:MET:HE2	2.01	0.41
12:N:149:LEU:HB3	12:N:150:ARG:H	1.60	0.41
14:Q:163:LYS:HE2	15:R:464:ASP:O	2.21	0.41
15:R:107:PRO:C	15:R:109:LYS:H	2.28	0.41
17:Y:244:ALA:O	17:Y:248:THR:HG23	2.20	0.41
1:A:616:GLU:HB2	13:O:556:GLN:HA	2.03	0.41
1:A:1236:LEU:HA	1:A:1237:PRO:HD3	1.89	0.41
3:C:415:PRO:HG3	3:C:445:LYS:HB2	2.03	0.41
6:F:457:ALA:HA	6:F:460:GLU:OE1	2.21	0.41
6:F:502:LEU:HA	6:F:505:ILE:HD12	2.02	0.41
6:H:502:LEU:HA	6:H:505:ILE:HD12	2.03	0.41
6:H:689:LEU:O	6:H:693:ASN:HB2	2.20	0.41
8:I:73:TRP:CH2	8:I:80:LEU:HD22	2.55	0.41
9:J:28:LYS:HD3	9:K:230:ASN:ND2	2.35	0.41
9:J:231:LEU:HA	9:J:234:VAL:HG22	2.01	0.41
9:J:322:TYR:CE1	11:M:36:LEU:HD11	2.54	0.41
9:J:386:LEU:HD12	9:J:386:LEU:H	1.85	0.41
9:K:203:PHE:HE1	9:K:218:THR:HB	1.85	0.41
9:K:203:PHE:CD1	9:K:221:PRO:CG	3.04	0.41
12:N:632:MET:HB2	12:N:632:MET:HE3	1.57	0.41
3:P:97:LYS:HG3	3:P:99:TYR:CZ	2.55	0.41
14:Q:498:ILE:O	14:Q:498:ILE:HG22	2.21	0.41
16:S:20:ASP:O	16:S:24:LEU:HG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:S:36:ARG:CZ	16:S:90:PRO:C	2.93	0.41
17:X:170:LYS:HG2	17:X:171:ILE:HD12	2.01	0.41
17:X:437:LEU:CB	17:X:444:LEU:HD11	2.48	0.41
1:A:811:PRO:HG3	1:A:1806:SER:HB3	2.01	0.41
1:A:1364:CYS:N	1:A:1365:PRO:HD2	2.36	0.41
3:C:389:ARG:HA	3:C:389:ARG:HD3	1.65	0.41
6:F:45:ALA:CB	6:F:61:LEU:HD11	2.51	0.41
7:G:3:ARG:HB2	9:J:443:LYS:HZ3	1.86	0.41
8:I:231:VAL:HG12	8:I:232:SER:N	2.35	0.41
8:I:290:PHE:HB3	8:I:320:LEU:HD21	2.01	0.41
8:I:333:LEU:HG	8:I:337:ILE:HD12	2.02	0.41
9:K:20:GLN:HE21	9:K:20:GLN:HA	1.86	0.41
13:O:541:ILE:O	13:O:544:VAL:HG22	2.20	0.41
3:P:248:LEU:O	3:P:252:GLN:HG2	2.20	0.41
17:X:434:TYR:HA	17:X:444:LEU:HD22	2.03	0.41
17:Y:70:LEU:O	17:Y:70:LEU:HD13	2.20	0.41
1:A:957:ASP:HA	1:A:1839:PHE:HE2	1.85	0.41
1:A:1251:VAL:HG12	1:A:1294:TYR:HA	2.03	0.41
1:A:1325:LEU:HD23	1:A:1371:LEU:CD2	2.50	0.41
1:A:1387:LEU:HD12	1:A:1407:ARG:HG3	2.03	0.41
2:B:16:TRP:HZ3	12:N:633:ARG:HG3	1.85	0.41
2:B:28:MET:HG2	2:B:33:CYS:O	2.20	0.41
3:C:307:LEU:HD21	3:C:316:LEU:HB2	2.02	0.41
6:F:666:PRO:O	6:F:667:GLN:HG3	2.21	0.41
8:I:34:LEU:HD13	12:N:390:GLY:HA3	2.03	0.41
8:I:306:HIS:NE2	8:I:313:ALA:O	2.53	0.41
9:J:447:LEU:O	9:J:451:LEU:HD23	2.20	0.41
9:K:497:ASN:OD1	9:K:497:ASN:N	2.52	0.41
12:N:386:LEU:HD12	12:N:387:LEU:HG	2.02	0.41
12:N:389:PRO:HA	12:N:431:ARG:HH22	1.85	0.41
12:N:501:ILE:H	12:N:501:ILE:CD1	2.29	0.41
13:O:604:LEU:HB3	13:O:627:LEU:HD21	2.02	0.41
3:P:389:ARG:HA	3:P:392:ILE:HG22	2.02	0.41
3:P:396:LYS:HA	3:P:396:LYS:HD3	1.88	0.41
1:A:107:LYS:HB2	1:A:110:ALA:HB3	2.03	0.41
1:A:773:LEU:HB2	1:A:783:ILE:HD12	2.01	0.41
1:A:1329:MET:HE1	1:A:1371:LEU:HD12	2.02	0.41
1:A:1750:PHE:HD2	1:A:1775:LEU:HD12	1.86	0.41
3:C:206:TRP:O	3:C:209:LEU:HB2	2.21	0.41
6:F:705:CYS:SG	6:F:706:LYS:N	2.93	0.41
8:I:237:GLU:CG	8:I:607:ILE:HD13	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:35:GLU:HB3	9:K:40:ILE:HD11	2.03	0.41
9:K:66:ASP:OD1	9:K:67:LYS:N	2.54	0.41
9:K:297:SER:O	9:K:329:LEU:HD21	2.20	0.41
12:N:321:LEU:HD22	12:N:324:TRP:CD2	2.56	0.41
13:O:266:ASP:CB	13:O:269:SER:HB3	2.51	0.41
13:O:592:TRP:CH2	13:O:630:ALA:HA	2.55	0.41
3:P:358:LEU:O	3:P:362:PRO:CA	2.65	0.41
15:R:430:TYR:CG	15:R:431:PRO:HA	2.56	0.41
1:A:1645:GLU:CG	1:A:1646:GLN:H	2.27	0.41
3:C:276:ILE:O	3:C:276:ILE:HG22	2.21	0.41
6:F:559:LEU:O	6:F:562:MET:HG3	2.21	0.41
8:I:32:ARG:HD2	8:I:34:LEU:HD21	2.03	0.41
8:I:101:LEU:HD23	8:I:102:HIS:N	2.36	0.41
8:I:184:PHE:HB2	8:I:198:VAL:O	2.20	0.41
8:I:231:VAL:HG21	8:I:557:TYR:CE2	2.56	0.41
8:I:719:ALA:HA	8:I:735:SER:HA	2.02	0.41
9:J:485:ILE:O	9:J:488:ILE:HG12	2.21	0.41
12:N:427:TYR:O	12:N:430:THR:HB	2.21	0.41
13:O:208:SER:HB3	13:O:211:GLN:NE2	2.36	0.41
3:P:434:ARG:NH1	14:Q:498:ILE:HD13	2.35	0.41
14:Q:139:ASN:O	14:Q:140:ALA:CB	2.68	0.41
15:R:461:ALA:CA	15:R:467:LEU:HD12	2.51	0.41
16:S:73:ASP:HB3	16:S:74:PRO:HD3	2.02	0.41
1:A:154:LEU:HD13	1:A:159:ILE:HG12	2.02	0.41
1:A:439:GLN:NE2	1:A:456:LYS:HG3	2.35	0.41
1:A:628:ILE:HD11	1:A:762:ILE:HD13	2.03	0.41
1:A:767:HIS:O	1:A:770:TYR:HB3	2.20	0.41
1:A:1016:MET:HE2	1:A:1084:ARG:HG3	2.03	0.41
1:A:1036:ASP:O	1:A:1039:ARG:HB3	2.20	0.41
1:A:1039:ARG:O	1:A:1042:GLN:HG3	2.21	0.41
1:A:1525:MET:HA	1:A:1528:ALA:HB2	2.03	0.41
1:A:1658:PRO:HG2	1:A:1663:LEU:HD13	2.03	0.41
2:B:13:THR:O	2:B:15:LEU:HD23	2.20	0.41
3:C:150:ALA:O	3:C:154:LEU:HD13	2.21	0.41
6:F:462:LEU:HD13	6:F:465:LEU:HD23	2.02	0.41
6:F:703:PRO:HB3	6:F:733:VAL:CG2	2.50	0.41
6:H:762:TRP:HD1	6:H:765:ASP:CG	2.28	0.41
9:J:180:GLU:CA	9:J:180:GLU:OE1	2.69	0.41
9:J:441:VAL:CG2	9:J:444:TRP:CD1	2.91	0.41
9:K:243:TYR:HA	7:W:3:ARG:HH22	1.85	0.41
9:K:418:TRP:HB3	9:K:458:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:445:GLU:HA	9:K:474:LEU:HD12	2.03	0.41
12:N:63:ALA:HB3	12:N:64:ALA:HB3	2.02	0.41
12:N:330:ARG:HB2	12:N:334:ARG:NH2	2.36	0.41
12:N:457:GLN:HA	12:N:544:LEU:HD11	2.02	0.41
12:N:550:GLY:HA2	12:N:551:GLU:CB	2.51	0.41
13:O:62:GLN:O	13:O:66:PRO:HD2	2.21	0.41
13:O:678:TYR:O	13:O:683:LYS:HB2	2.20	0.41
13:O:682:LYS:O	13:O:685:GLU:HB3	2.20	0.41
3:P:46:ARG:HG3	3:P:116:PHE:CD2	2.55	0.41
3:P:91:LYS:O	3:P:94:PHE:HB3	2.21	0.41
14:Q:237:GLU:CD	14:Q:237:GLU:H	2.28	0.41
14:Q:496:GLN:HA	14:Q:497:GLY:HA2	1.78	0.41
15:R:174:ARG:HH11	16:S:257:GLY:N	2.19	0.41
16:S:279:ALA:N	16:S:280:ASP:HA	2.36	0.41
17:X:244:ALA:O	17:X:248:THR:HG23	2.21	0.41
17:X:335:SER:HB2	17:X:338:HIS:CD2	2.56	0.41
17:Y:45:ALA:HB3	17:Y:82:TYR:HE2	1.79	0.41
17:Y:100:TYR:CD1	17:Y:138:VAL:HG13	2.55	0.41
17:Y:242:ALA:O	17:Y:246:VAL:HG23	2.20	0.41
17:Y:434:TYR:HA	17:Y:444:LEU:HD22	2.03	0.41
1:A:845:TYR:HB3	1:A:1812:TRP:CE3	2.56	0.41
1:A:1787:LEU:O	1:A:1791:ILE:HG12	2.21	0.41
3:C:185:VAL:HG13	3:C:212:LEU:HD22	2.02	0.41
6:F:507:ARG:HD3	6:F:538:ILE:CD1	2.42	0.41
9:J:165:GLU:OE2	9:K:20:GLN:HB2	2.21	0.41
9:J:168:ASP:HA	9:J:171:THR:HG22	2.03	0.41
12:N:76:VAL:C	12:N:78:VAL:H	2.29	0.41
12:N:580:LYS:HB3	12:N:582:PRO:HD2	2.03	0.41
12:N:595:ILE:CD1	12:N:626:TYR:OH	2.69	0.41
13:O:321:GLU:HA	13:O:350:LEU:HD13	2.02	0.41
13:O:592:TRP:HH2	13:O:630:ALA:HA	1.86	0.41
13:O:688:GLU:O	13:O:691:ILE:HG22	2.21	0.41
3:P:251:TYR:CZ	3:P:268:GLN:HG3	2.55	0.41
14:Q:352:THR:CB	18:Z:51:LEU:HA	2.51	0.41
14:Q:461:ALA:CA	14:Q:467:LEU:HD12	2.51	0.41
17:X:316:ALA:HB1	17:X:351:TYR:CE1	2.56	0.41
1:A:1031:ASP:OD1	12:N:489:PRO:N	2.54	0.40
1:A:1131:MET:O	1:A:1132:THR:HB	2.21	0.40
1:A:1619:LEU:HD23	1:A:1634:LEU:HD11	2.02	0.40
3:C:217:GLU:O	3:C:221:PHE:HD1	2.03	0.40
3:C:416:PHE:CB	3:C:446:LEU:HD11	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:702:ASN:HB2	6:F:705:CYS:SG	2.61	0.40
6:H:163:ASP:HA	6:H:164:PRO:HD2	1.98	0.40
6:H:639:TYR:CZ	6:H:643:MET:HG3	2.57	0.40
8:I:209:CYS:HG	8:I:584:HIS:CG	2.22	0.40
8:I:413:ASN:C	8:I:447:PHE:HE1	2.21	0.40
8:I:585:TYR:CE1	8:I:602:ARG:HD3	2.56	0.40
10:L:79:ILE:HG13	10:L:156:ILE:HG12	2.03	0.40
10:L:119:TRP:HH2	10:L:155:GLN:HG2	1.86	0.40
12:N:595:ILE:HD12	12:N:626:TYR:OH	2.21	0.40
13:O:127:HIS:O	13:O:128:LYS:CB	2.61	0.40
13:O:375:TYR:CE1	13:O:417:LEU:HD23	2.56	0.40
3:P:58:LEU:HD13	3:P:259:PHE:HE2	1.86	0.40
3:P:276:ILE:CG2	3:P:277:ARG:H	2.22	0.40
16:S:75:LEU:HA	16:S:115:TYR:OH	2.21	0.40
16:S:82:ILE:HD13	16:S:102:LEU:HD21	2.02	0.40
18:Z:78:LYS:HB2	18:Z:78:LYS:HE3	1.96	0.40
1:A:799:LEU:O	1:A:801:PRO:HD2	2.21	0.40
1:A:1071:LEU:O	1:A:1074:CYS:HB2	2.22	0.40
1:A:1208:LEU:O	1:A:1212:VAL:HG23	2.21	0.40
1:A:1227:LEU:O	1:A:1231:HIS:ND1	2.55	0.40
1:A:1359:ASN:HB3	10:L:30:VAL:HG11	2.04	0.40
1:A:1694:ASP:OD1	1:A:1696:VAL:HB	2.21	0.40
1:A:1867:CYS:CB	1:A:1881:GLN:NE2	2.83	0.40
3:C:412:LEU:O	3:C:413:LYS:HB2	2.20	0.40
6:F:32:TYR:CE1	6:F:41:LEU:HB2	2.56	0.40
6:H:158:ILE:HG22	6:H:159:GLY:N	2.36	0.40
6:H:162:PRO:HD2	6:H:474:LEU:HD13	2.03	0.40
6:H:557:LYS:HE2	6:H:557:LYS:HB3	1.93	0.40
9:J:337:TRP:O	9:J:340:TYR:HB3	2.21	0.40
9:J:397:ILE:CG2	9:J:398:ALA:N	2.84	0.40
9:K:244:ASN:O	9:K:245:CYS:HB2	2.21	0.40
12:N:563:ASP:C	12:N:564:MET:N	2.78	0.40
12:N:596:LEU:HD13	12:N:601:TRP:CZ2	2.56	0.40
12:N:611:VAL:HG11	12:N:637:TRP:CH2	2.56	0.40
13:O:65:LEU:HB3	13:O:66:PRO:HD3	2.03	0.40
13:O:351:GLY:O	13:O:352:GLN:HG3	2.21	0.40
13:O:516:PHE:CD1	13:O:516:PHE:C	2.99	0.40
13:O:516:PHE:HB2	13:O:535:ILE:HD11	2.02	0.40
16:S:19:GLY:O	16:S:23:GLU:HG3	2.20	0.40
17:X:164:SER:HA	17:X:167:ARG:NE	2.37	0.40
17:Y:301:ASP:HA	17:Y:302:PRO:HD2	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:350:PHE:CE2	17:Y:378:LEU:HD12	2.56	0.40
3:C:116:PHE:HE1	3:C:174:LEU:HB2	1.86	0.40
3:C:312:MET:H	3:C:312:MET:HG2	1.60	0.40
6:F:146:PRO:C	6:F:148:LEU:H	2.29	0.40
6:F:624:PHE:O	6:F:628:ILE:HG12	2.21	0.40
6:H:146:PRO:C	6:H:148:LEU:H	2.29	0.40
6:H:698:ILE:HG13	6:H:699:ASP:N	2.36	0.40
6:H:765:ASP:O	17:X:397:ARG:CZ	2.68	0.40
8:I:279:ILE:HD12	8:I:279:ILE:HA	1.92	0.40
9:K:19:TYR:CE1	9:K:49:LEU:HD13	2.56	0.40
9:K:413:PHE:HD1	9:K:454:VAL:HG23	1.86	0.40
12:N:803:VAL:HG21	12:N:810:TYR:HB2	2.03	0.40
13:O:340:LEU:HD23	13:O:340:LEU:HA	1.93	0.40
3:P:66:PRO:O	3:P:67:LEU:HB3	2.20	0.40
3:P:464:ASP:OD2	3:P:469:ALA:HB3	2.20	0.40
14:Q:128:ALA:HB1	18:Z:156:TYR:CZ	2.50	0.40
14:Q:163:LYS:HD3	15:R:466:THR:CG2	2.51	0.40
14:Q:430:TYR:CG	14:Q:431:PRO:HA	2.56	0.40
15:R:346:VAL:HA	15:R:347:PRO:HD3	1.98	0.40
16:S:41:LEU:HD11	18:Z:141:PHE:CB	2.44	0.40
17:Y:60:LEU:HB3	17:Y:79:LEU:HD11	2.04	0.40
17:Y:169:PRO:HG3	17:Y:198:GLN:CD	2.46	0.40
17:Y:452:LEU:HD22	17:Y:461:ALA:CA	2.47	0.40
1:A:181:TRP:HA	1:A:182:PRO:HD3	2.01	0.40
1:A:941:LEU:HB2	1:A:977:LEU:HA	2.03	0.40
1:A:957:ASP:CG	1:A:1820:PHE:CZ	3.00	0.40
3:C:62:LEU:HB3	3:C:63:PRO:HD2	2.03	0.40
5:E:60:SER:O	5:E:63:VAL:HG12	2.21	0.40
6:F:550:VAL:HG13	6:F:551:ALA:N	2.37	0.40
7:G:23:ARG:CG	9:J:525:MET:HE1	2.51	0.40
9:J:342:HIS:CD2	9:J:357:TYR:OH	2.74	0.40
9:K:63:ARG:HB2	9:K:65:LEU:HD13	2.01	0.40
9:K:190:LEU:O	9:K:198:GLN:NE2	2.54	0.40
12:N:354:SER:O	12:N:357:ALA:HB3	2.22	0.40
12:N:556:PHE:CG	12:N:600:PHE:HD1	2.39	0.40
12:N:596:LEU:HD22	12:N:601:TRP:CZ2	2.56	0.40
3:P:54:TRP:CE3	3:P:203:TRP:HB2	2.56	0.40
14:Q:128:ALA:HB3	18:Z:156:TYR:CE2	2.39	0.40
17:X:71:PHE:O	17:X:76:LYS:HE3	2.22	0.40
17:X:154:ASP:OD1	17:X:154:ASP:N	2.54	0.40
17:Y:164:SER:HA	17:Y:167:ARG:NE	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.98	0.40
1:A:474:ILE:HD11	1:A:490:VAL:HG21	2.03	0.40
1:A:657:TRP:NE1	1:A:785:SER:OG	2.55	0.40
1:A:808:ARG:NH2	1:A:1894:VAL:O	2.54	0.40
1:A:1800:LEU:HD11	1:A:1811:LEU:HD21	2.03	0.40
2:B:16:TRP:O	2:B:31:ASN:O	2.39	0.40
3:C:91:LYS:O	3:C:94:PHE:HB3	2.22	0.40
6:F:689:LEU:O	6:F:693:ASN:HB2	2.22	0.40
6:H:726:LEU:HD21	6:H:742:LEU:HD22	2.03	0.40
6:H:765:ASP:O	17:X:397:ARG:NE	2.54	0.40
8:I:14:VAL:N	8:I:743:VAL:O	2.54	0.40
9:K:250:CYS:SG	9:K:274:THR:HG23	2.55	0.40
10:L:86:ASP:HB3	10:L:89:TYR:CB	2.40	0.40
12:N:370:GLN:HE21	12:N:373:GLN:HB3	1.87	0.40
13:O:267:VAL:O	13:O:271:THR:HG22	2.21	0.40
13:O:544:VAL:HG23	13:O:567:LEU:CG	2.45	0.40
14:Q:342:GLU:C	14:Q:344:GLY:H	2.29	0.40
16:S:20:ASP:H	18:Z:134:GLN:NE2	2.12	0.40
18:Z:179:GLU:HG2	18:Z:201:ILE:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1397/1944 (72%)	1267 (91%)	106 (8%)	24 (2%)	7	35
2	B	75/84 (89%)	62 (83%)	8 (11%)	5 (7%)	1	12
3	C	520/597 (87%)	498 (96%)	20 (4%)	2 (0%)	30	66
3	P	485/597 (81%)	465 (96%)	20 (4%)	0	100	100
4	D	16/121 (13%)	14 (88%)	2 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	54/110 (49%)	53 (98%)	1 (2%)	0	100	100
6	F	479/824 (58%)	458 (96%)	13 (3%)	8 (2%)	7	35
6	H	479/824 (58%)	459 (96%)	14 (3%)	6 (1%)	9	41
7	G	23/85 (27%)	23 (100%)	0	0	100	100
7	W	23/85 (27%)	23 (100%)	0	0	100	100
8	I	725/808 (90%)	683 (94%)	35 (5%)	7 (1%)	12	47
9	J	500/620 (81%)	467 (93%)	29 (6%)	4 (1%)	16	52
9	K	489/620 (79%)	456 (93%)	27 (6%)	6 (1%)	10	42
10	L	180/185 (97%)	165 (92%)	14 (8%)	1 (1%)	21	58
11	M	55/74 (74%)	46 (84%)	9 (16%)	0	100	100
12	N	679/822 (83%)	557 (82%)	68 (10%)	54 (8%)	1	10
13	O	677/755 (90%)	640 (94%)	29 (4%)	8 (1%)	10	42
14	Q	348/374 (93%)	317 (91%)	21 (6%)	10 (3%)	3	24
15	R	377/499 (76%)	344 (91%)	26 (7%)	7 (2%)	6	32
16	S	267/342 (78%)	237 (89%)	18 (7%)	12 (4%)	2	18
17	X	480/599 (80%)	464 (97%)	13 (3%)	3 (1%)	21	58
17	Y	492/599 (82%)	474 (96%)	13 (3%)	5 (1%)	12	47
18	Z	193/205 (94%)	186 (96%)	6 (3%)	1 (0%)	24	62
All	All	9013/11773 (77%)	8358 (93%)	492 (6%)	163 (2%)	9	33

All (163) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	VAL
1	A	630	PRO
1	A	857	MET
1	A	1125	ILE
1	A	1358	ILE
2	B	15	LEU
2	B	37	CYS
2	B	43	ASP
2	B	67	GLN
8	I	431	ASP
8	I	489	PRO
8	I	503	ASN
9	J	221	PRO

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Mol	Chain	Res	Type
9	K	211	LYS
9	K	215	PRO
12	N	74	TRP
12	N	75	PHE
12	N	78	VAL
12	N	79	LEU
12	N	91	PHE
12	N	126	LEU
12	N	140	LEU
12	N	203	LEU
12	N	234	ARG
12	N	252	LEU
12	N	286	LEU
12	N	287	ARG
12	N	290	HIS
12	N	350	ASP
12	N	368	THR
12	N	395	ASP
12	N	412	PRO
12	N	477	PRO
12	N	488	ASP
12	N	489	PRO
12	N	492	SER
12	N	497	ARG
12	N	530	GLN
12	N	606	ASP
12	N	632	MET
12	N	674	ALA
12	N	716	ILE
14	Q	140	ALA
14	Q	141	PRO
14	Q	476	ASP
14	Q	477	PRO
14	Q	478	ALA
14	Q	479	ARG
15	R	106	THR
16	S	77	VAL
16	S	135	PRO
16	S	222	PRO
16	S	230	LEU
16	S	262	PHE
16	S	274	VAL

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Mol	Chain	Res	Type
17	X	213	SER
17	Y	201	LEU
17	Y	213	SER
18	Z	159	LYS
1	A	87	VAL
1	A	860	TYR
1	A	1099	PRO
1	A	1164	LYS
1	A	1307	LEU
1	A	1925	VAL
3	C	27	SER
6	F	129	ASP
6	F	147	PHE
6	F	165	ASP
6	F	493	SER
6	H	129	ASP
6	H	147	PHE
6	H	493	SER
8	I	296	THR
8	I	433	VAL
9	J	70	GLU
12	N	63	ALA
12	N	64	ALA
12	N	101	SER
12	N	278	ARG
12	N	289	PHE
12	N	531	PHE
12	N	550	GLY
13	O	505	GLN
14	Q	137	PRO
14	Q	266	SER
15	R	101	PRO
15	R	266	SER
15	R	494	ILE
16	S	74	PRO
16	S	235	LYS
17	X	202	ALA
17	Y	202	ALA
1	A	1100	LEU
1	A	1283	PRO
1	A	1314	ILE
6	F	103	HIS

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Mol	Chain	Res	Type
8	I	487	VAL
9	J	397	ILE
9	K	129	LYS
9	K	228	GLN
10	L	174	THR
12	N	77	GLU
12	N	144	THR
12	N	280	GLU
12	N	480	TRP
12	N	500	ASP
12	N	629	LEU
12	N	672	ASP
13	O	707	LYS
15	R	108	THR
16	S	559	ALA
17	Y	456	VAL
1	A	253	PRO
1	A	1055	PRO
1	A	1822	SER
2	B	65	HIS
6	F	145	ASN
6	H	145	ASN
9	J	382	ASN
9	K	86	HIS
12	N	219	PRO
12	N	283	ARG
12	N	352	PRO
12	N	353	ASP
12	N	482	PRO
12	N	484	PRO
12	N	595	ILE
13	O	462	ASN
13	O	540	SER
13	O	657	ILE
13	O	745	PRO
17	X	456	VAL
1	A	1356	ASP
1	A	1603	LEU
6	F	96	VAL
6	H	97	PHE
12	N	282	GLU
12	N	499	SER

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Mol	Chain	Res	Type
13	O	126	VAL
15	R	498	ILE
16	S	301	PRO
1	A	502	GLY
1	A	590	PRO
1	A	781	GLU
1	A	1239	THR
3	C	229	MET
6	F	97	PHE
6	H	96	VAL
12	N	142	MET
12	N	551	GLU
14	Q	161	SER
15	R	76	GLY
9	K	399	PRO
16	S	257	GLY
8	I	291	VAL
16	S	294	PRO
1	A	858	PRO
12	N	490	GLY
14	Q	498	ILE
17	Y	200	PRO
12	N	166	PRO
13	O	124	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	1151/1720 (67%)	989 (86%)	162 (14%)	3	16
2	B	71/75 (95%)	60 (84%)	11 (16%)	2	14
3	C	452/520 (87%)	390 (86%)	62 (14%)	3	16
3	P	422/520 (81%)	368 (87%)	54 (13%)	4	18
4	D	18/115 (16%)	15 (83%)	3 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	47/89 (53%)	35 (74%)	12 (26%)	0	4
6	F	407/727 (56%)	360 (88%)	47 (12%)	5	20
6	H	408/727 (56%)	366 (90%)	42 (10%)	7	23
7	G	23/77 (30%)	21 (91%)	2 (9%)	9	30
7	W	23/77 (30%)	22 (96%)	1 (4%)	26	48
8	I	617/730 (84%)	572 (93%)	45 (7%)	13	35
9	J	424/548 (77%)	370 (87%)	54 (13%)	4	18
9	K	423/548 (77%)	381 (90%)	42 (10%)	7	25
10	L	155/170 (91%)	136 (88%)	19 (12%)	4	19
11	M	55/67 (82%)	44 (80%)	11 (20%)	1	9
12	N	518/724 (72%)	445 (86%)	73 (14%)	3	16
13	O	577/650 (89%)	497 (86%)	80 (14%)	3	16
14	Q	271/310 (87%)	262 (97%)	9 (3%)	33	55
15	R	311/411 (76%)	290 (93%)	21 (7%)	14	37
16	S	186/293 (64%)	178 (96%)	8 (4%)	26	48
17	X	407/513 (79%)	375 (92%)	32 (8%)	11	33
17	Y	418/513 (82%)	381 (91%)	37 (9%)	9	29
18	Z	181/190 (95%)	168 (93%)	13 (7%)	13	35
All	All	7565/10314 (73%)	6725 (89%)	840 (11%)	8	21

All (840) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	36	ASN
1	A	37	LEU
1	A	39	LEU
1	A	47	GLU
1	A	88	ASP
1	A	90	ASP
1	A	92	GLU
1	A	98	ASN
1	A	113	VAL
1	A	118	THR
1	A	120	ASP
1	A	127	LEU

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Mol	Chain	Res	Type
1	A	133	ILE
1	A	151	ILE
1	A	153	ILE
1	A	159	ILE
1	A	172	SER
1	A	176	GLN
1	A	180	VAL
1	A	183	THR
1	A	210	MET
1	A	212	SER
1	A	223	LEU
1	A	249	LEU
1	A	271	LEU
1	A	403	ILE
1	A	429	LYS
1	A	430	VAL
1	A	437	CYS
1	A	439	GLN
1	A	444	PHE
1	A	449	GLN
1	A	450	LEU
1	A	459	GLU
1	A	474	ILE
1	A	491	LEU
1	A	497	LEU
1	A	508	LYS
1	A	584	ILE
1	A	609	ILE
1	A	614	THR
1	A	628	ILE
1	A	638	LEU
1	A	640	LYS
1	A	664	LEU
1	A	766	LEU
1	A	781	GLU
1	A	798	LYS
1	A	808	ARG
1	A	871	ARG
1	A	934	MET
1	A	945	GLU
1	A	947	LEU
1	A	953	LEU

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Mol	Chain	Res	Type
1	A	962	CYS
1	A	964	GLU
1	A	1016	MET
1	A	1026	LEU
1	A	1037	VAL
1	A	1049	VAL
1	A	1057	LEU
1	A	1075	GLN
1	A	1081	PRO
1	A	1089	LEU
1	A	1100	LEU
1	A	1107	LEU
1	A	1118	VAL
1	A	1120	LEU
1	A	1146	LYS
1	A	1168	LEU
1	A	1170	ASN
1	A	1176	LEU
1	A	1177	MET
1	A	1179	LEU
1	A	1181	LEU
1	A	1202	GLU
1	A	1216	LYS
1	A	1217	LEU
1	A	1220	MET
1	A	1224	ILE
1	A	1227	LEU
1	A	1230	ILE
1	A	1232	ILE
1	A	1235	LEU
1	A	1243	LEU
1	A	1255	VAL
1	A	1273	LEU
1	A	1279	ARG
1	A	1292	GLU
1	A	1304	MET
1	A	1312	ASN
1	A	1313	LEU
1	A	1314	ILE
1	A	1319	LEU
1	A	1321	VAL
1	A	1323	GLU

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Mol	Chain	Res	Type
1	A	1325	LEU
1	A	1327	GLN
1	A	1359	ASN
1	A	1369	LEU
1	A	1378	THR
1	A	1386	TRP
1	A	1400	LYS
1	A	1404	LEU
1	A	1405	LEU
1	A	1409	LEU
1	A	1455	GLU
1	A	1457	LEU
1	A	1482	LEU
1	A	1487	CYS
1	A	1488	LEU
1	A	1511	ASN
1	A	1516	LEU
1	A	1523	LEU
1	A	1536	LEU
1	A	1538	LEU
1	A	1539	CYS
1	A	1540	ARG
1	A	1556	LEU
1	A	1562	LEU
1	A	1564	LEU
1	A	1573	SER
1	A	1574	LEU
1	A	1586	CYS
1	A	1588	LEU
1	A	1597	THR
1	A	1603	LEU
1	A	1607	ARG
1	A	1611	VAL
1	A	1638	TYR
1	A	1646	GLN
1	A	1650	GLU
1	A	1656	LEU
1	A	1662	LEU
1	A	1663	LEU
1	A	1665	GLN
1	A	1666	ILE
1	A	1672	ARG

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Mol	Chain	Res	Type
1	A	1674	TRP
1	A	1687	LEU
1	A	1688	LYS
1	A	1693	LYS
1	A	1694	ASP
1	A	1706	LEU
1	A	1731	ARG
1	A	1742	THR
1	A	1748	LEU
1	A	1749	SER
1	A	1756	LYS
1	A	1767	ILE
1	A	1770	LEU
1	A	1798	ARG
1	A	1805	MET
1	A	1811	LEU
1	A	1824	ARG
1	A	1851	THR
1	A	1854	ASN
1	A	1858	GLN
1	A	1869	HIS
1	A	1882	LEU
1	A	1893	SER
2	B	11	VAL
2	B	14	TRP
2	B	15	LEU
2	B	16	TRP
2	B	17	VAL
2	B	23	CYS
2	B	34	CYS
2	B	40	PRO
2	B	62	LYS
2	B	71	GLN
2	B	79	GLU
3	C	26	PHE
3	C	37	LEU
3	C	38	LEU
3	C	42	LEU
3	C	44	ARG
3	C	48	LEU
3	C	49	LEU
3	C	57	GLU

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Mol	Chain	Res	Type
3	C	70	LEU
3	C	76	ILE
3	C	77	THR
3	C	78	GLU
3	C	85	ASP
3	C	89	LEU
3	C	122	ARG
3	C	127	GLU
3	C	128	LYS
3	C	138	LEU
3	C	146	VAL
3	C	147	LYS
3	C	157	GLU
3	C	172	LEU
3	C	182	LEU
3	C	183	ASP
3	C	197	HIS
3	C	201	LEU
3	C	234	LEU
3	C	237	ILE
3	C	239	THR
3	C	244	ILE
3	C	268	GLN
3	C	280	ASP
3	C	289	LEU
3	C	300	MET
3	C	302	THR
3	C	306	LEU
3	C	307	LEU
3	C	310	ARG
3	C	312	MET
3	C	313	LYS
3	C	324	CYS
3	C	325	GLU
3	C	328	LYS
3	C	334	CYS
3	C	343	LEU
3	C	359	LYS
3	C	361	ASN
3	C	376	MET
3	C	379	LYS
3	C	381	THR

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Mol	Chain	Res	Type
3	C	386	GLN
3	C	389	ARG
3	C	397	ARG
3	C	414	MET
3	C	424	ARG
3	C	428	LEU
3	C	441	GLU
3	C	446	LEU
3	C	451	GLU
3	C	516	LEU
3	C	518	GLN
3	C	542	THR
4	D	11	ARG
4	D	12	VAL
4	D	16	LEU
5	E	56	GLU
5	E	57	SER
5	E	58	VAL
5	E	60	SER
5	E	61	TYR
5	E	66	THR
5	E	69	GLN
5	E	70	VAL
5	E	81	LYS
5	E	85	LEU
5	E	87	GLU
5	E	99	ILE
6	F	22	ARG
6	F	27	LEU
6	F	43	LEU
6	F	70	GLN
6	F	78	CYS
6	F	90	GLN
6	F	98	ASN
6	F	104	ASP
6	F	118	LEU
6	F	121	LEU
6	F	131	LEU
6	F	141	SER
6	F	143	SER
6	F	145	ASN
6	F	165	ASP

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Mol	Chain	Res	Type
6	F	462	LEU
6	F	476	LEU
6	F	477	CYS
6	F	480	ASN
6	F	494	HIS
6	F	507	ARG
6	F	520	ARG
6	F	521	ILE
6	F	527	ARG
6	F	530	ASN
6	F	536	MET
6	F	538	ILE
6	F	549	ASP
6	F	562	MET
6	F	564	LYS
6	F	576	CYS
6	F	578	SER
6	F	588	LYS
6	F	614	THR
6	F	616	GLU
6	F	623	CYS
6	F	625	ARG
6	F	655	GLU
6	F	656	MET
6	F	667	GLN
6	F	705	CYS
6	F	720	LYS
6	F	721	SER
6	F	729	LEU
6	F	733	VAL
6	F	748	LYS
6	F	757	LEU
7	G	15	ASP
7	G	23	ARG
6	H	27	LEU
6	H	43	LEU
6	H	61	LEU
6	H	78	CYS
6	H	90	GLN
6	H	98	ASN
6	H	141	SER
6	H	143	SER

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Mol	Chain	Res	Type
6	H	154	SER
6	H	462	LEU
6	H	476	LEU
6	H	477	CYS
6	H	480	ASN
6	H	494	HIS
6	H	503	CYS
6	H	507	ARG
6	H	515	TYR
6	H	520	ARG
6	H	521	ILE
6	H	530	ASN
6	H	536	MET
6	H	546	LEU
6	H	562	MET
6	H	564	LYS
6	H	571	CYS
6	H	588	LYS
6	H	592	ARG
6	H	599	ASN
6	H	613	LEU
6	H	623	CYS
6	H	643	MET
6	H	655	GLU
6	H	667	GLN
6	H	702	ASN
6	H	720	LYS
6	H	729	LEU
6	H	733	VAL
6	H	755	LEU
6	H	757	LEU
6	H	758	MET
6	H	761	SER
6	H	762	TRP
8	I	26	LEU
8	I	34	LEU
8	I	35	ILE
8	I	37	LEU
8	I	71	LEU
8	I	75	PRO
8	I	89	LYS
8	I	92	LEU

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Mol	Chain	Res	Type
8	I	101	LEU
8	I	110	VAL
8	I	210	LEU
8	I	218	SER
8	I	224	SER
8	I	232	SER
8	I	259	SER
8	I	266	ASN
8	I	267	LEU
8	I	269	LEU
8	I	273	CYS
8	I	304	PHE
8	I	316	GLU
8	I	322	MET
8	I	325	LEU
8	I	348	VAL
8	I	349	ILE
8	I	352	LEU
8	I	353	GLN
8	I	359	LEU
8	I	360	LEU
8	I	371	SER
8	I	372	TRP
8	I	397	ILE
8	I	445	ILE
8	I	448	VAL
8	I	452	LEU
8	I	477	GLN
8	I	505	SER
8	I	522	LEU
8	I	564	ASP
8	I	571	LYS
8	I	609	GLN
8	I	652	VAL
8	I	688	THR
8	I	718	LYS
8	I	736	SER
9	J	23	LEU
9	J	36	GLU
9	J	61	ARG
9	J	134	LEU
9	J	141	ASP

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Mol	Chain	Res	Type
9	J	148	LEU
9	J	157	LEU
9	J	163	CYS
9	J	164	PHE
9	J	169	LEU
9	J	180	GLU
9	J	185	LEU
9	J	188	LEU
9	J	202	ARG
9	J	206	GLU
9	J	214	LYS
9	J	233	VAL
9	J	248	LYS
9	J	254	THR
9	J	256	VAL
9	J	258	MET
9	J	259	GLU
9	J	267	CYS
9	J	287	LEU
9	J	290	LYS
9	J	298	ASN
9	J	307	CYS
9	J	323	LEU
9	J	329	LEU
9	J	331	LYS
9	J	338	ILE
9	J	343	SER
9	J	351	ASP
9	J	354	MET
9	J	372	LEU
9	J	385	LYS
9	J	386	LEU
9	J	395	LEU
9	J	400	GLU
9	J	423	LYS
9	J	429	LEU
9	J	439	VAL
9	J	445	GLU
9	J	448	LEU
9	J	451	LEU
9	J	465	LEU
9	J	472	LEU

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Mol	Chain	Res	Type
9	J	485	ILE
9	J	488	ILE
9	J	497	ASN
9	J	506	LEU
9	J	523	ILE
9	J	525	MET
9	J	527	ILE
9	K	9	ARG
9	K	20	GLN
9	K	45	GLN
9	K	52	GLN
9	K	63	ARG
9	K	128	ILE
9	K	134	LEU
9	K	141	ASP
9	K	143	LEU
9	K	148	LEU
9	K	154	LYS
9	K	157	LEU
9	K	163	CYS
9	K	164	PHE
9	K	169	LEU
9	K	184	LEU
9	K	188	LEU
9	K	190	LEU
9	K	233	VAL
9	K	254	THR
9	K	267	CYS
9	K	284	LEU
9	K	287	LEU
9	K	289	HIS
9	K	331	LYS
9	K	338	ILE
9	K	343	SER
9	K	351	ASP
9	K	359	THR
9	K	363	LEU
9	K	376	LEU
9	K	385	LYS
9	K	400	GLU
9	K	423	LYS
9	K	429	LEU

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Mol	Chain	Res	Type
9	K	432	ILE
9	K	454	VAL
9	K	469	ARG
9	K	492	MET
9	K	497	ASN
9	K	506	LEU
9	K	522	CYS
10	L	12	ASP
10	L	25	ILE
10	L	30	VAL
10	L	32	SER
10	L	45	LEU
10	L	48	ASP
10	L	65	ASN
10	L	67	GLN
10	L	74	VAL
10	L	77	LEU
10	L	98	VAL
10	L	101	ASN
10	L	113	LEU
10	L	122	VAL
10	L	132	THR
10	L	151	THR
10	L	162	VAL
10	L	177	PHE
10	L	184	ARG
11	M	7	ARG
11	M	11	ILE
11	M	12	LEU
11	M	17	ASP
11	M	29	VAL
11	M	35	GLU
11	M	50	VAL
11	M	51	LYS
11	M	55	MET
11	M	59	ASP
11	M	64	TYR
12	N	75	PHE
12	N	76	VAL
12	N	77	GLU
12	N	79	LEU
12	N	80	GLN

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Mol	Chain	Res	Type
12	N	150	ARG
12	N	162	PHE
12	N	163	PHE
12	N	170	GLN
12	N	180	PHE
12	N	181	LEU
12	N	202	GLU
12	N	206	ARG
12	N	243	LEU
12	N	250	LEU
12	N	251	SER
12	N	256	VAL
12	N	271	GLU
12	N	274	GLU
12	N	277	CYS
12	N	278	ARG
12	N	281	TYR
12	N	285	PHE
12	N	287	ARG
12	N	322	ARG
12	N	330	ARG
12	N	334	ARG
12	N	340	ARG
12	N	344	LEU
12	N	351	PHE
12	N	364	CYS
12	N	365	LEU
12	N	366	GLU
12	N	370	GLN
12	N	372	GLN
12	N	373	GLN
12	N	379	LYS
12	N	386	LEU
12	N	388	HIS
12	N	392	ASN
12	N	394	CYS
12	N	397	ILE
12	N	398	THR
12	N	424	ILE
12	N	425	ARG
12	N	435	VAL
12	N	501	ILE

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Mol	Chain	Res	Type
12	N	503	SER
12	N	504	LEU
12	N	505	LEU
12	N	513	ASP
12	N	516	ILE
12	N	517	ASN
12	N	522	LEU
12	N	544	LEU
12	N	557	CYS
12	N	560	MET
12	N	561	LEU
12	N	564	MET
12	N	570	ILE
12	N	594	VAL
12	N	609	LEU
12	N	613	GLU
12	N	622	TYR
12	N	625	LYS
12	N	626	TYR
12	N	632	MET
12	N	638	LYS
12	N	640	THR
12	N	670	PHE
12	N	699	TRP
12	N	728	VAL
12	N	787	LEU
13	O	38	LEU
13	O	40	LEU
13	O	43	GLU
13	O	44	MET
13	O	62	GLN
13	O	64	LEU
13	O	73	ILE
13	O	78	LEU
13	O	98	LYS
13	O	99	LEU
13	O	104	GLU
13	O	108	MET
13	O	129	THR
13	O	132	VAL
13	O	136	LEU
13	O	166	GLU

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Mol	Chain	Res	Type
13	O	207	LEU
13	O	216	LEU
13	O	223	LEU
13	O	256	LEU
13	O	275	LEU
13	O	280	ARG
13	O	319	GLN
13	O	328	ILE
13	O	330	ILE
13	O	344	LEU
13	O	347	LEU
13	O	367	LYS
13	O	369	VAL
13	O	381	ILE
13	O	387	GLN
13	O	396	ASN
13	O	398	LEU
13	O	404	ASP
13	O	408	LEU
13	O	411	LYS
13	O	414	LEU
13	O	417	LEU
13	O	420	ILE
13	O	426	THR
13	O	435	SER
13	O	441	GLN
13	O	448	MET
13	O	462	ASN
13	O	496	ARG
13	O	506	LEU
13	O	510	CYS
13	O	511	ASP
13	O	533	THR
13	O	535	ILE
13	O	563	LEU
13	O	567	LEU
13	O	574	LEU
13	O	575	LYS
13	O	579	MET
13	O	581	ILE
13	O	586	SER
13	O	608	LEU

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Mol	Chain	Res	Type
13	O	610	LEU
13	O	616	LEU
13	O	619	LEU
13	O	623	THR
13	O	625	LEU
13	O	626	ASN
13	O	632	LEU
13	O	633	ILE
13	O	636	ILE
13	O	641	LEU
13	O	643	LEU
13	O	649	GLU
13	O	657	ILE
13	O	685	GLU
13	O	691	ILE
13	O	694	LEU
13	O	706	CYS
13	O	713	VAL
13	O	719	ARG
13	O	723	THR
13	O	735	MET
13	O	752	ILE
3	P	37	LEU
3	P	38	LEU
3	P	42	LEU
3	P	48	LEU
3	P	70	LEU
3	P	77	THR
3	P	78	GLU
3	P	89	LEU
3	P	97	LYS
3	P	98	GLU
3	P	122	ARG
3	P	128	LYS
3	P	172	LEU
3	P	182	LEU
3	P	183	ASP
3	P	201	LEU
3	P	234	LEU
3	P	239	THR
3	P	244	ILE
3	P	248	LEU

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Mol	Chain	Res	Type
3	P	268	GLN
3	P	289	LEU
3	P	299	ASN
3	P	300	MET
3	P	302	THR
3	P	303	PHE
3	P	306	LEU
3	P	310	ARG
3	P	312	MET
3	P	313	LYS
3	P	316	LEU
3	P	319	LEU
3	P	321	HIS
3	P	324	CYS
3	P	325	GLU
3	P	334	CYS
3	P	335	CYS
3	P	343	LEU
3	P	346	GLN
3	P	358	LEU
3	P	359	LYS
3	P	365	LEU
3	P	379	LYS
3	P	381	THR
3	P	392	ILE
3	P	395	ASN
3	P	412	LEU
3	P	423	ARG
3	P	424	ARG
3	P	428	LEU
3	P	441	GLU
3	P	451	GLU
3	P	472	LYS
3	P	524	LYS
14	Q	133	LEU
14	Q	173	ASP
14	Q	222	MET
14	Q	237	GLU
14	Q	252	LEU
14	Q	316	ARG
14	Q	401	GLN
14	Q	414	LEU

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Mol	Chain	Res	Type
14	Q	494	ILE
15	R	77	ASP
15	R	78	ARG
15	R	79	TYR
15	R	83	ARG
15	R	89	GLU
15	R	94	LEU
15	R	97	LYS
15	R	109	LYS
15	R	110	LYS
15	R	121	ASN
15	R	126	GLU
15	R	127	GLU
15	R	173	ASP
15	R	222	MET
15	R	237	GLU
15	R	252	LEU
15	R	316	ARG
15	R	401	GLN
15	R	414	LEU
15	R	496	GLN
15	R	499	ARG
16	S	30	GLN
16	S	77	VAL
16	S	88	ASN
16	S	101	LEU
16	S	106	VAL
16	S	274	VAL
16	S	555	ARG
16	S	558	LEU
7	W	5	LYS
17	X	39	ASP
17	X	49	LEU
17	X	79	LEU
17	X	110	LEU
17	X	154	ASP
17	X	184	GLN
17	X	189	VAL
17	X	193	LYS
17	X	201	LEU
17	X	214	VAL
17	X	255	ILE

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Mol	Chain	Res	Type
17	X	292	LEU
17	X	295	GLU
17	X	299	MET
17	X	300	LEU
17	X	303	TYR
17	X	366	ILE
17	X	371	ASN
17	X	386	MET
17	X	401	ARG
17	X	414	ILE
17	X	423	ILE
17	X	450	VAL
17	X	452	LEU
17	X	453	GLU
17	X	460	LYS
17	X	465	LEU
17	X	487	SER
17	X	503	LEU
17	X	506	GLN
17	X	513	ARG
17	X	515	LEU
17	Y	39	ASP
17	Y	49	LEU
17	Y	59	LEU
17	Y	70	LEU
17	Y	79	LEU
17	Y	94	ARG
17	Y	154	ASP
17	Y	184	GLN
17	Y	193	LYS
17	Y	198	GLN
17	Y	199	CYS
17	Y	255	ILE
17	Y	292	LEU
17	Y	295	GLU
17	Y	299	MET
17	Y	300	LEU
17	Y	301	ASP
17	Y	303	TYR
17	Y	366	ILE
17	Y	371	ASN
17	Y	386	MET

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Mol	Chain	Res	Type
17	Y	401	ARG
17	Y	405	CYS
17	Y	414	ILE
17	Y	423	ILE
17	Y	450	VAL
17	Y	452	LEU
17	Y	453	GLU
17	Y	465	LEU
17	Y	475	TYR
17	Y	487	SER
17	Y	503	LEU
17	Y	506	GLN
17	Y	513	ARG
17	Y	515	LEU
17	Y	551	LYS
17	Y	552	MET
18	Z	42	THR
18	Z	57	THR
18	Z	72	LEU
18	Z	81	VAL
18	Z	84	LEU
18	Z	91	ILE
18	Z	106	CYS
18	Z	138	THR
18	Z	155	ILE
18	Z	157	THR
18	Z	160	ASP
18	Z	166	LYS
18	Z	196	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (210) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	43	GLN
1	A	124	GLN
1	A	125	GLN
1	A	162	HIS
1	A	176	GLN
1	A	250	ASN
1	A	266	HIS
1	A	439	GLN

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Mol	Chain	Res	Type
1	A	592	HIS
1	A	776	ASN
1	A	792	GLN
1	A	1021	HIS
1	A	1045	HIS
1	A	1060	HIS
1	A	1138	HIS
1	A	1161	ASN
1	A	1165	HIS
1	A	1170	ASN
1	A	1182	ASN
1	A	1184	HIS
1	A	1192	ASN
1	A	1266	HIS
1	A	1351	GLN
1	A	1359	ASN
1	A	1380	ASN
1	A	1453	ASN
1	A	1511	ASN
1	A	1543	HIS
1	A	1558	HIS
1	A	1559	HIS
1	A	1604	GLN
2	B	9	ASN
2	B	31	ASN
2	B	65	HIS
2	B	71	GLN
3	C	71	GLN
3	C	107	HIS
3	C	163	GLN
3	C	287	ASN
3	C	299	ASN
3	C	305	ASN
3	C	322	ASN
3	C	347	HIS
3	C	355	GLN
3	C	361	ASN
3	C	373	HIS
3	C	386	GLN
3	C	390	HIS
3	C	477	HIS
3	C	479	GLN

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Mol	Chain	Res	Type
3	C	518	GLN
6	F	495	HIS
6	F	634	HIS
6	F	636	ASN
6	F	659	GLN
6	F	667	GLN
6	H	166	GLN
6	H	480	ASN
6	H	494	HIS
6	H	495	HIS
6	H	545	HIS
6	H	580	GLN
6	H	583	HIS
6	H	595	GLN
6	H	634	HIS
6	H	648	GLN
6	H	657	HIS
6	H	659	GLN
6	H	716	ASN
6	H	754	HIS
6	H	759	ASN
8	I	18	GLN
8	I	53	HIS
8	I	323	ASN
8	I	345	GLN
8	I	374	GLN
8	I	442	GLN
8	I	496	GLN
8	I	523	HIS
8	I	535	GLN
8	I	538	GLN
8	I	604	HIS
8	I	613	ASN
8	I	684	GLN
9	J	16	GLN
9	J	17	GLN
9	J	18	GLN
9	J	52	GLN
9	J	58	HIS
9	J	87	GLN
9	J	173	HIS
9	J	271	HIS

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Mol	Chain	Res	Type
9	J	289	HIS
9	J	316	ASN
9	J	342	HIS
9	J	352	GLN
9	J	362	GLN
9	J	382	ASN
9	J	393	GLN
9	J	406	HIS
9	K	20	GLN
9	K	86	HIS
9	K	87	GLN
9	K	264	HIS
9	K	271	HIS
9	K	314	HIS
9	K	316	ASN
9	K	352	GLN
9	K	449	ASN
9	K	477	GLN
10	L	49	ASN
10	L	67	GLN
10	L	101	ASN
10	L	103	HIS
10	L	104	ASN
10	L	128	HIS
10	L	146	GLN
10	L	152	HIS
12	N	81	ASN
12	N	248	HIS
12	N	290	HIS
12	N	370	GLN
12	N	388	HIS
12	N	571	ASN
12	N	639	HIS
12	N	663	GLN
12	N	671	GLN
12	N	726	ASN
12	N	759	GLN
12	N	775	ASN
13	O	61	ASN
13	O	69	GLN
13	O	91	ASN
13	O	211	GLN

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Mol	Chain	Res	Type
13	O	219	GLN
13	O	242	ASN
13	O	247	ASN
13	O	319	GLN
13	O	363	HIS
13	O	387	GLN
13	O	412	HIS
13	O	441	GLN
13	O	449	ASN
13	O	460	GLN
13	O	462	ASN
13	O	539	ASN
13	O	626	ASN
13	O	639	GLN
13	O	671	GLN
13	O	693	ASN
13	O	728	GLN
13	O	741	HIS
3	P	50	HIS
3	P	71	GLN
3	P	148	ASN
3	P	287	ASN
3	P	305	ASN
3	P	321	HIS
3	P	322	ASN
3	P	347	HIS
3	P	395	ASN
3	P	448	GLN
3	P	488	GLN
3	P	495	GLN
14	Q	221	GLN
14	Q	367	GLN
15	R	99	ASN
15	R	119	ASN
15	R	121	ASN
15	R	221	GLN
16	S	52	ASN
16	S	87	GLN
16	S	88	ASN
16	S	97	ASN
16	S	133	ASN
16	S	145	GLN

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Mol	Chain	Res	Type
16	S	153	GLN
16	S	197	GLN
16	S	278	ASN
16	S	306	ASN
17	X	36	ASN
17	X	50	HIS
17	X	67	ASN
17	X	89	HIS
17	X	95	ASN
17	X	106	GLN
17	X	151	GLN
17	X	251	ASN
17	X	298	GLN
17	X	326	ASN
17	X	337	GLN
17	X	371	ASN
17	X	471	GLN
17	X	501	ASN
17	X	506	GLN
17	Y	184	GLN
17	Y	251	ASN
17	Y	326	ASN
17	Y	337	GLN
17	Y	338	HIS
17	Y	367	GLN
17	Y	371	ASN
17	Y	471	GLN
17	Y	506	GLN
17	Y	541	ASN
18	Z	66	ASN
18	Z	125	GLN
18	Z	134	GLN
18	Z	173	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	N	2
16	S	1
8	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	310:ALA	C	529:SER	N	39.42
1	N	92:TRP	C	93:ASN	N	3.29
1	N	563:ASP	C	564:MET	N	2.78
1	I	302:ASP	C	303:GLU	N	2.26

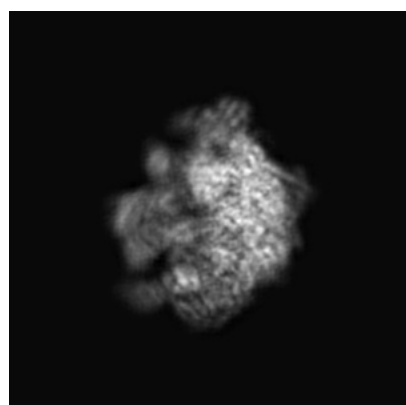
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4037. These allow visual inspection of the internal detail of the map and identification of artifacts.

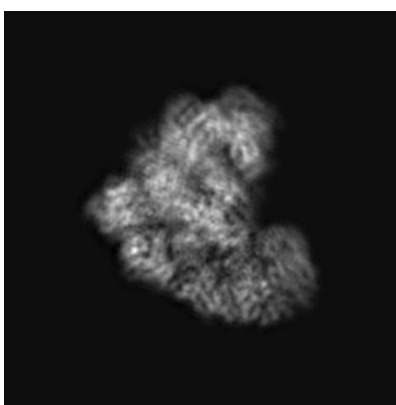
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

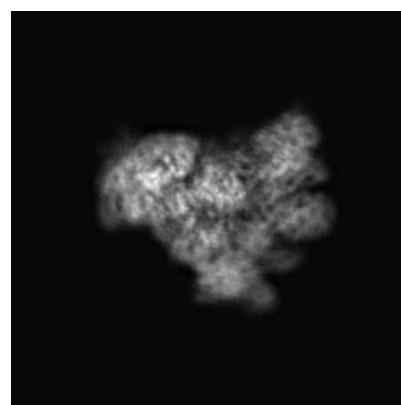
6.1.1 Primary map



X



Y

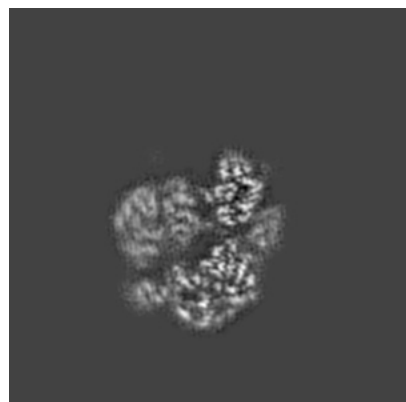


Z

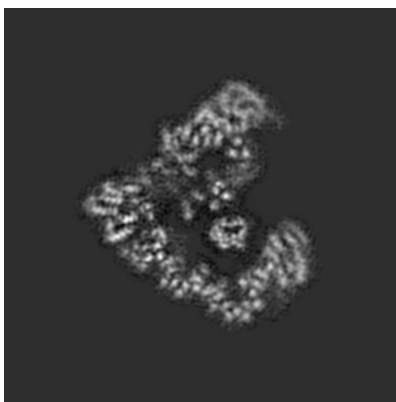
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

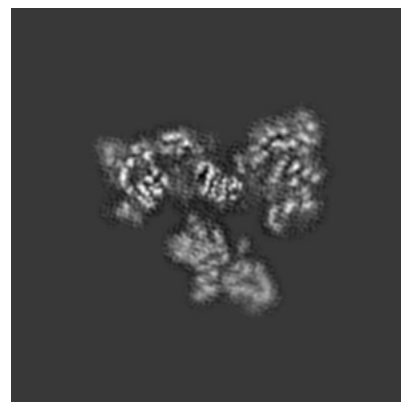
6.2.1 Primary map



X Index: 132



Y Index: 132

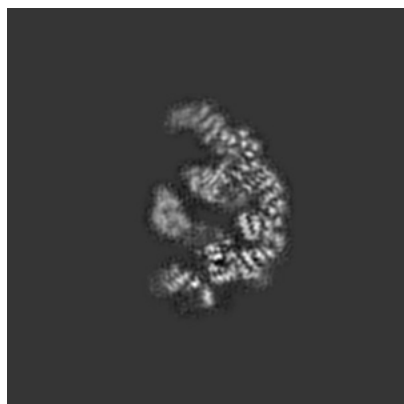


Z Index: 132

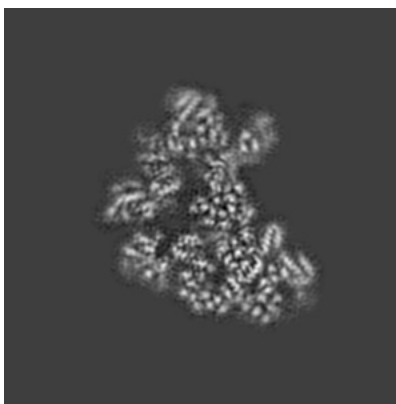
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

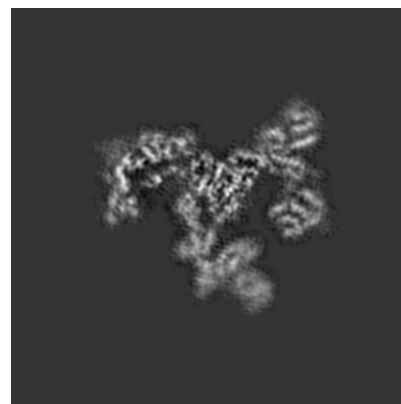
6.3.1 Primary map



X Index: 112



Y Index: 155

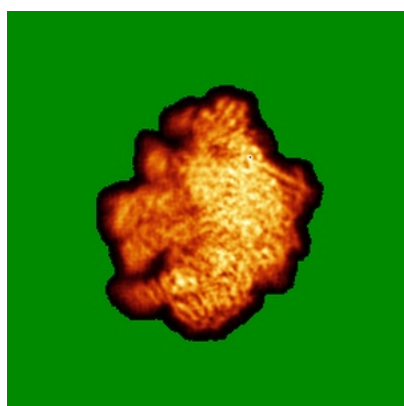


Z Index: 140

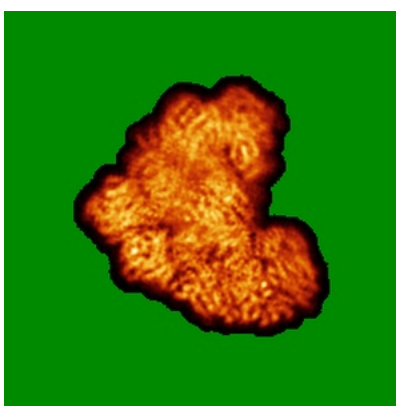
The images above show the largest variance slices of the map in three orthogonal directions.

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

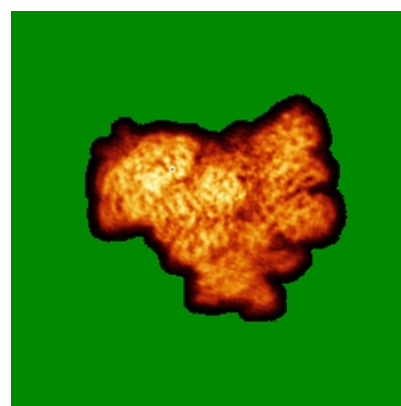
6.4.1 Primary map



X



Y

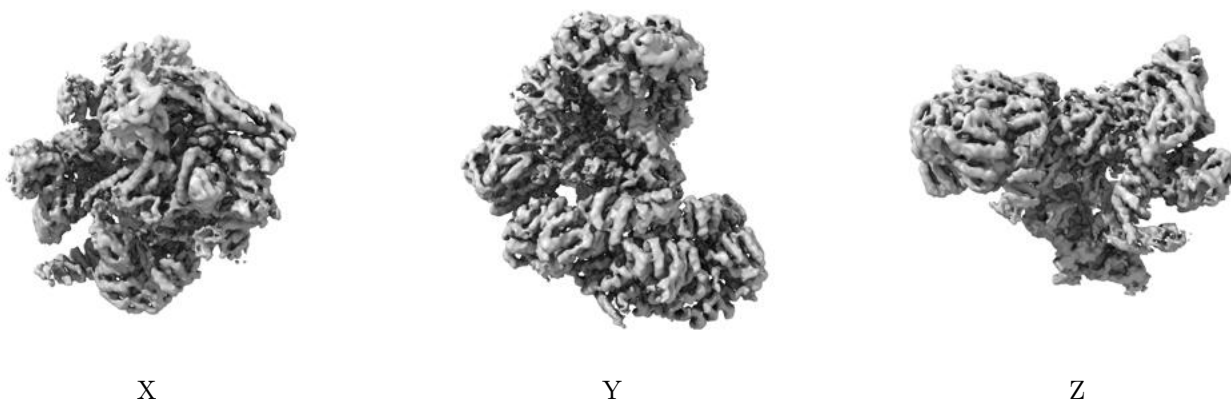


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

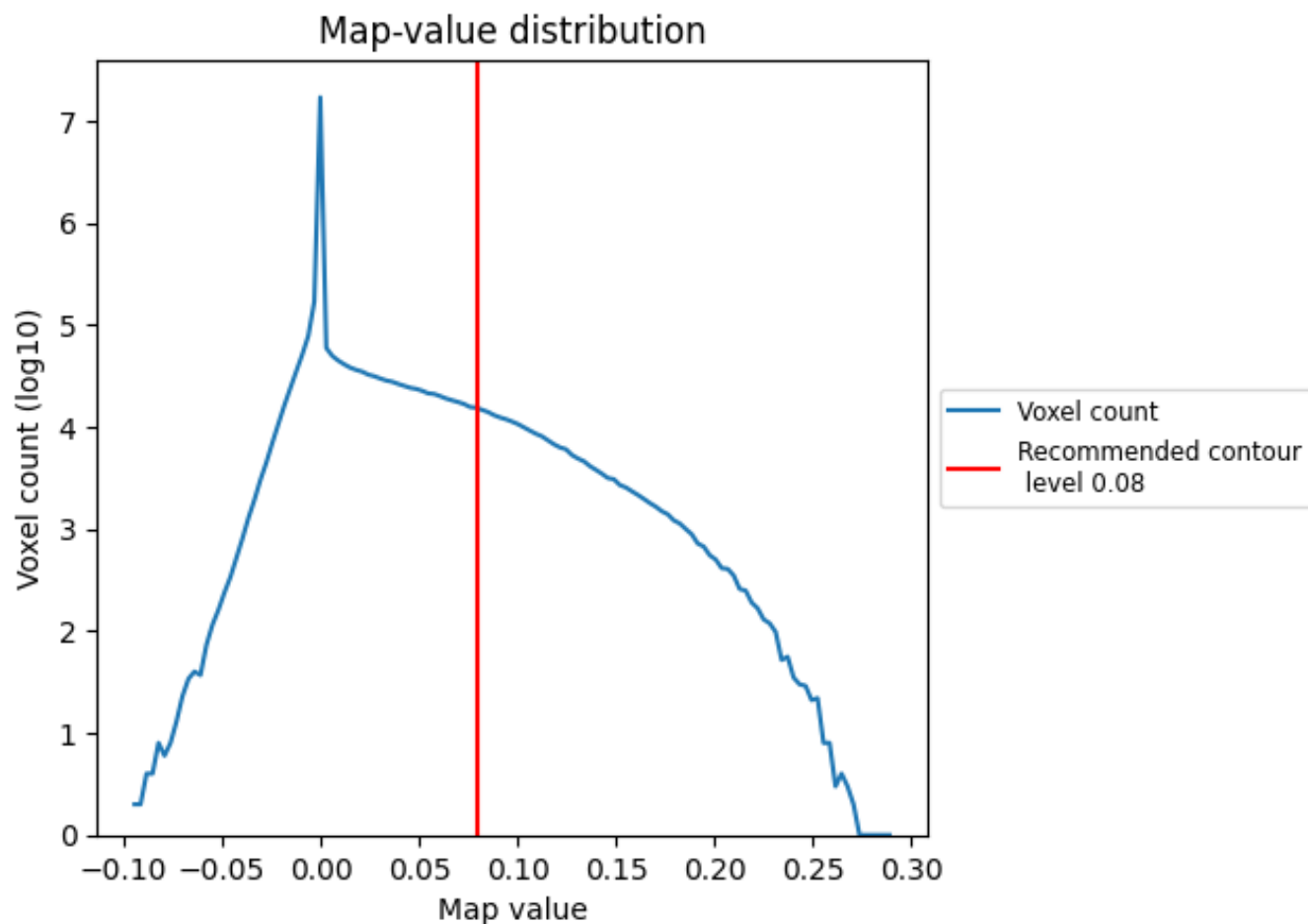
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

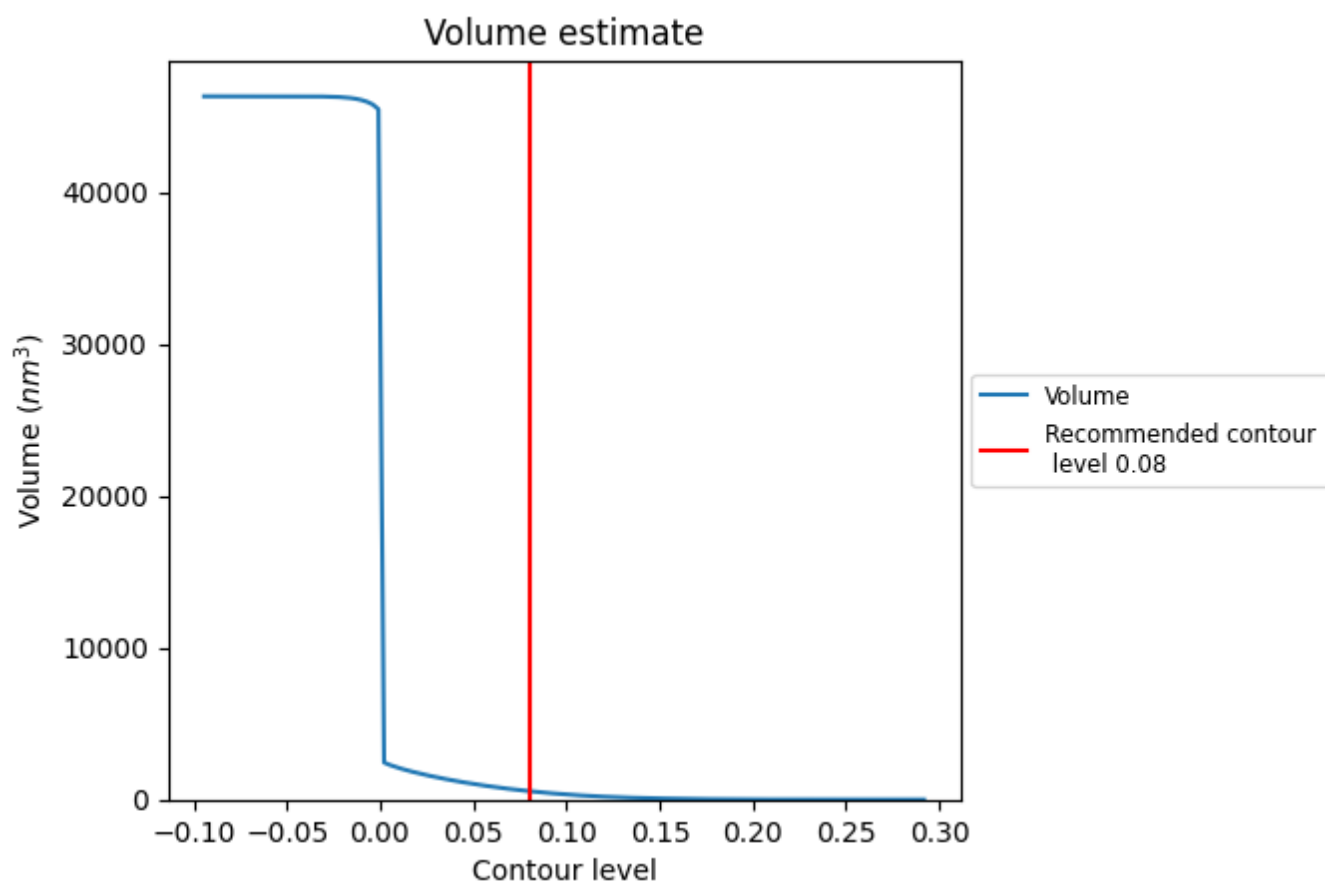
This section contains the results of statistical analysis of the map.

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.

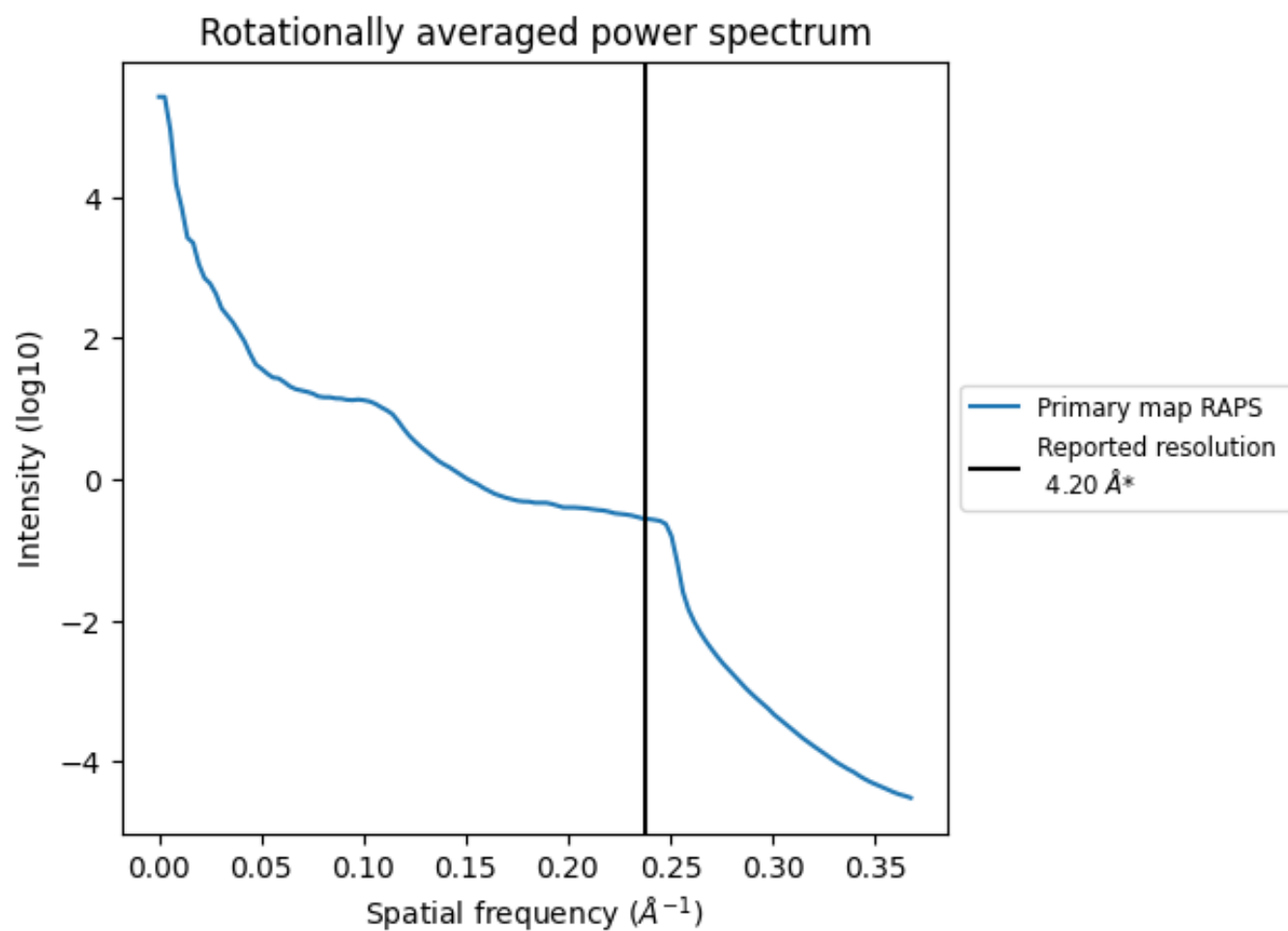
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 554 nm³; this corresponds to an approximate mass of 501 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 0.238 Å⁻¹

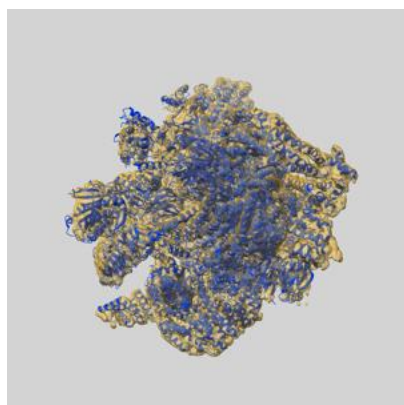
8 Fourier-Shell correlation

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

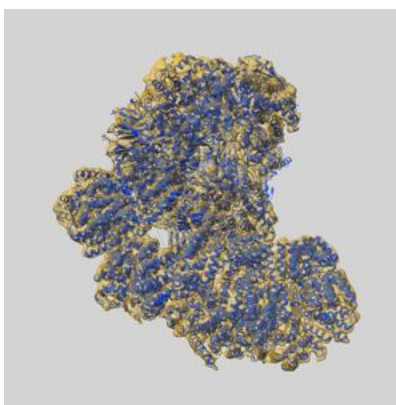
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4037 and PDB model 5LCW. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

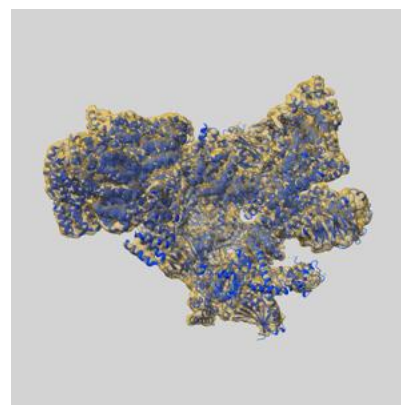
9.1 Map-model overlay [i](#)



X



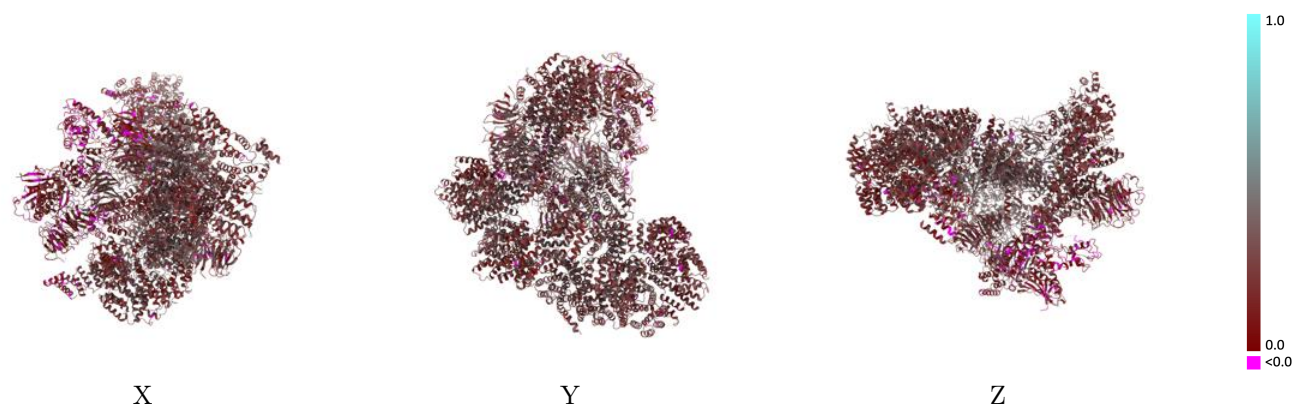
Y



Z

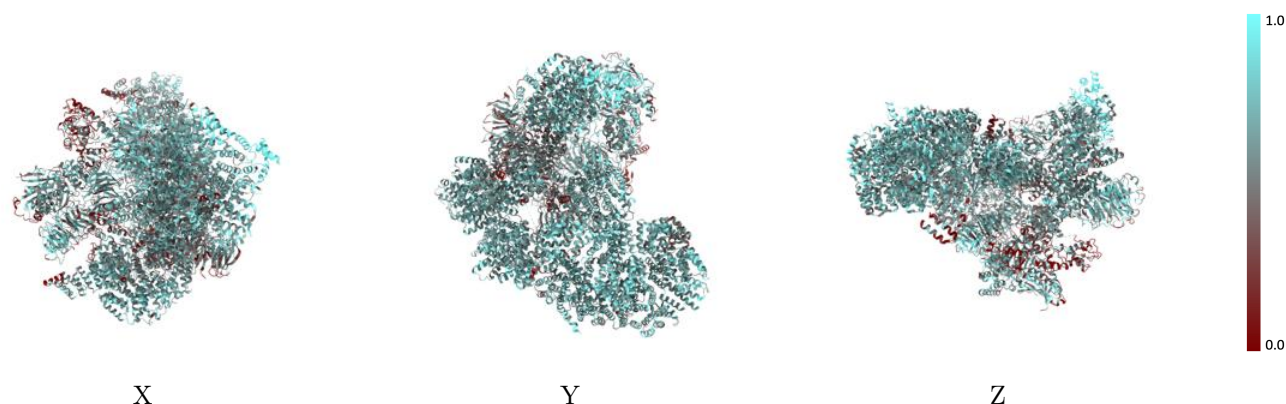
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



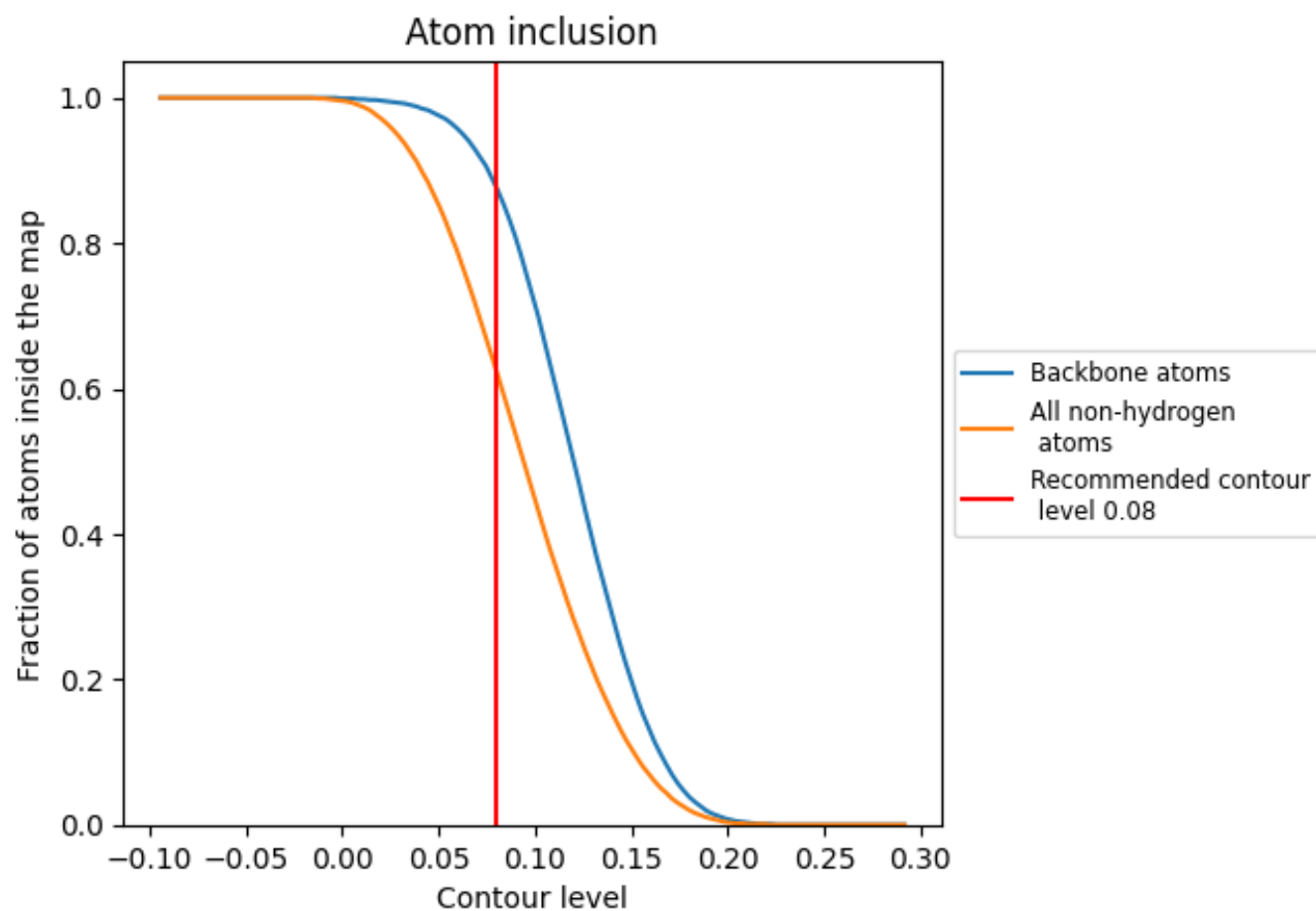
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6250	 0.2520
A	 0.6230	 0.3020
B	 0.1260	 0.0340
C	 0.6190	 0.2630
D	 0.4400	 0.3690
E	 0.6760	 0.3320
F	 0.6860	 0.2920
G	 0.6240	 0.3050
H	 0.7130	 0.3030
I	 0.6010	 0.2160
J	 0.7110	 0.2910
K	 0.6910	 0.2680
L	 0.6840	 0.3260
M	 0.5570	 0.3280
N	 0.5600	 0.1860
O	 0.5680	 0.2670
P	 0.6460	 0.2500
Q	 0.6250	 0.2000
R	 0.6390	 0.2310
S	 0.5830	 0.1970
W	 0.5900	 0.2950
X	 0.6020	 0.2040
Y	 0.6430	 0.2340
Z	 0.5440	 0.1520

