



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:19 PM UTC

PDB ID : 5IZ7 / pdb_00005iz7
EMDB ID : EMD-8139
Title : Cryo-EM structure of thermally stable Zika virus strain H/PF/2013
Authors : Kostyuchenko, V.A.; Zhang, S.; Fibriansah, G.; Lok, S.M.
Deposited on : 2016-03-25
Resolution : 3.70 Å (reported)
Based on initial model : 3J27

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:

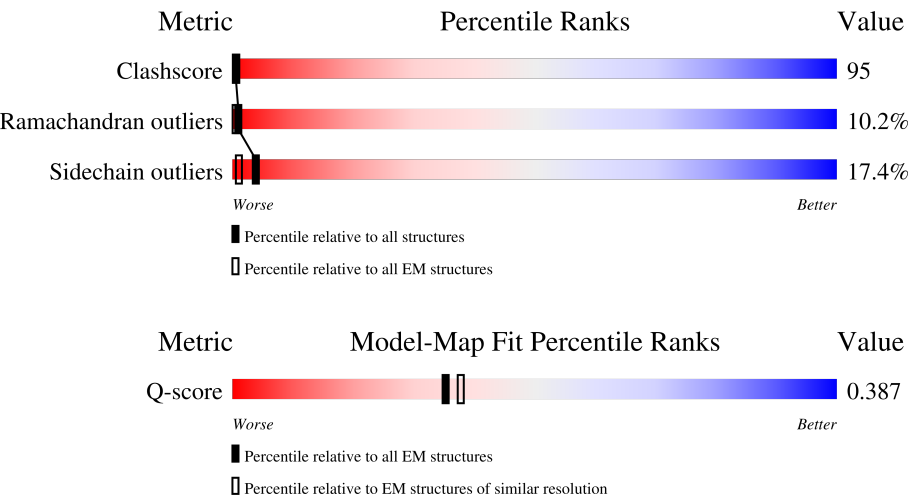
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	504	36% 15%60%23%
1	B	504	32% 16%54%26%
1	C	504	44% 17%57%23%
2	D	75	53% 8%64%24%

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Mol	Chain	Length	Quality of chain
2	E	75	64% 13% 61% 24%
2	F	75	56% 23% 51% 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13268 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 structural protein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	504	Total	C	N	O	S	0	0
			3809	2395	660	723	31		
1	C	504	Total	C	N	O	S	0	0
			3808	2395	660	722	31		
1	B	504	Total	C	N	O	S	0	0
			3809	2395	660	723	31		

- Molecule 2 is a protein called structural protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	75	Total	C	N	O	S	0	0
			600	391	105	103	1		
2	E	75	Total	C	N	O	S	0	0
			600	391	105	103	1		
2	F	75	Total	C	N	O	S	0	0
			600	391	105	103	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

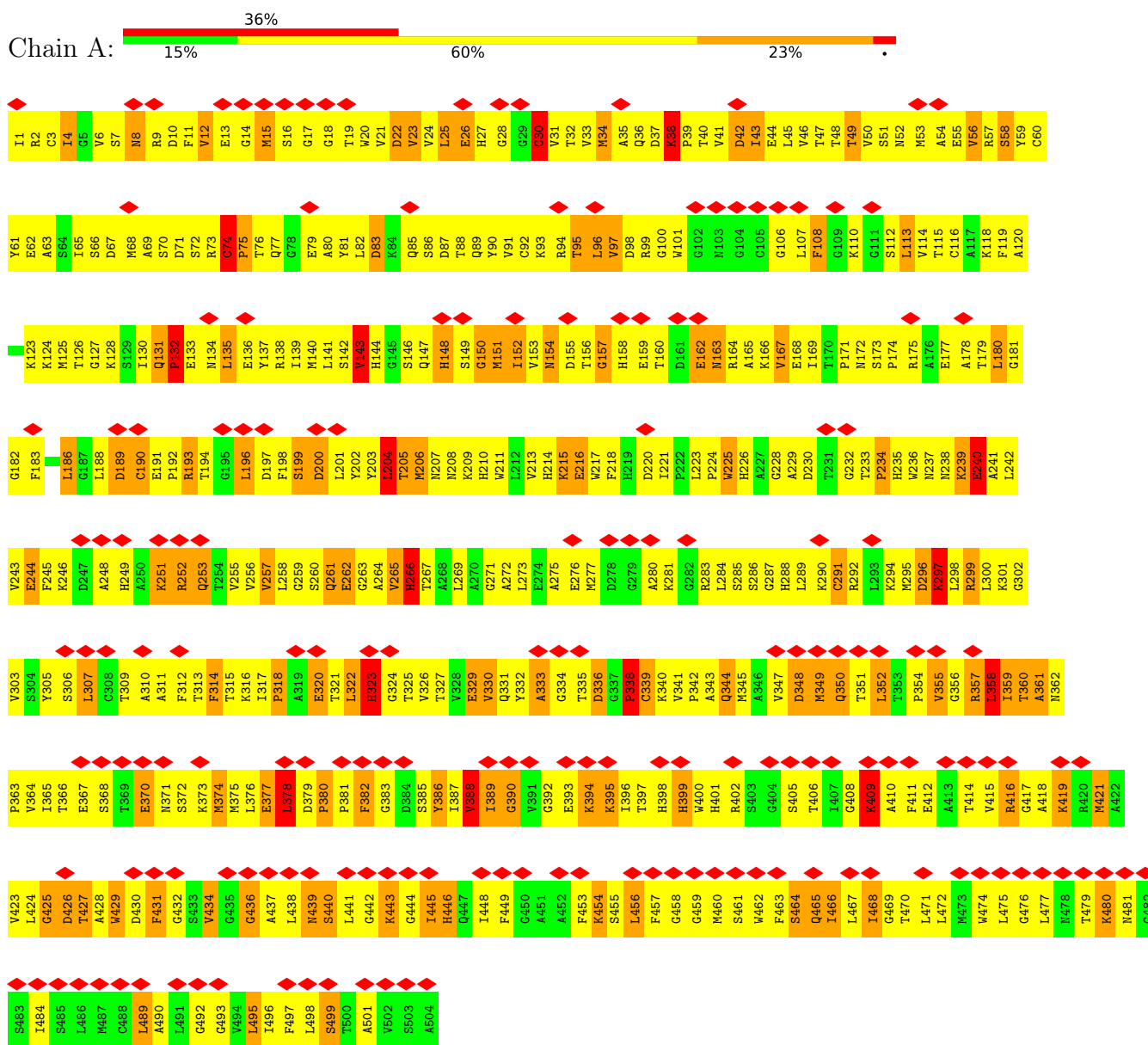


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

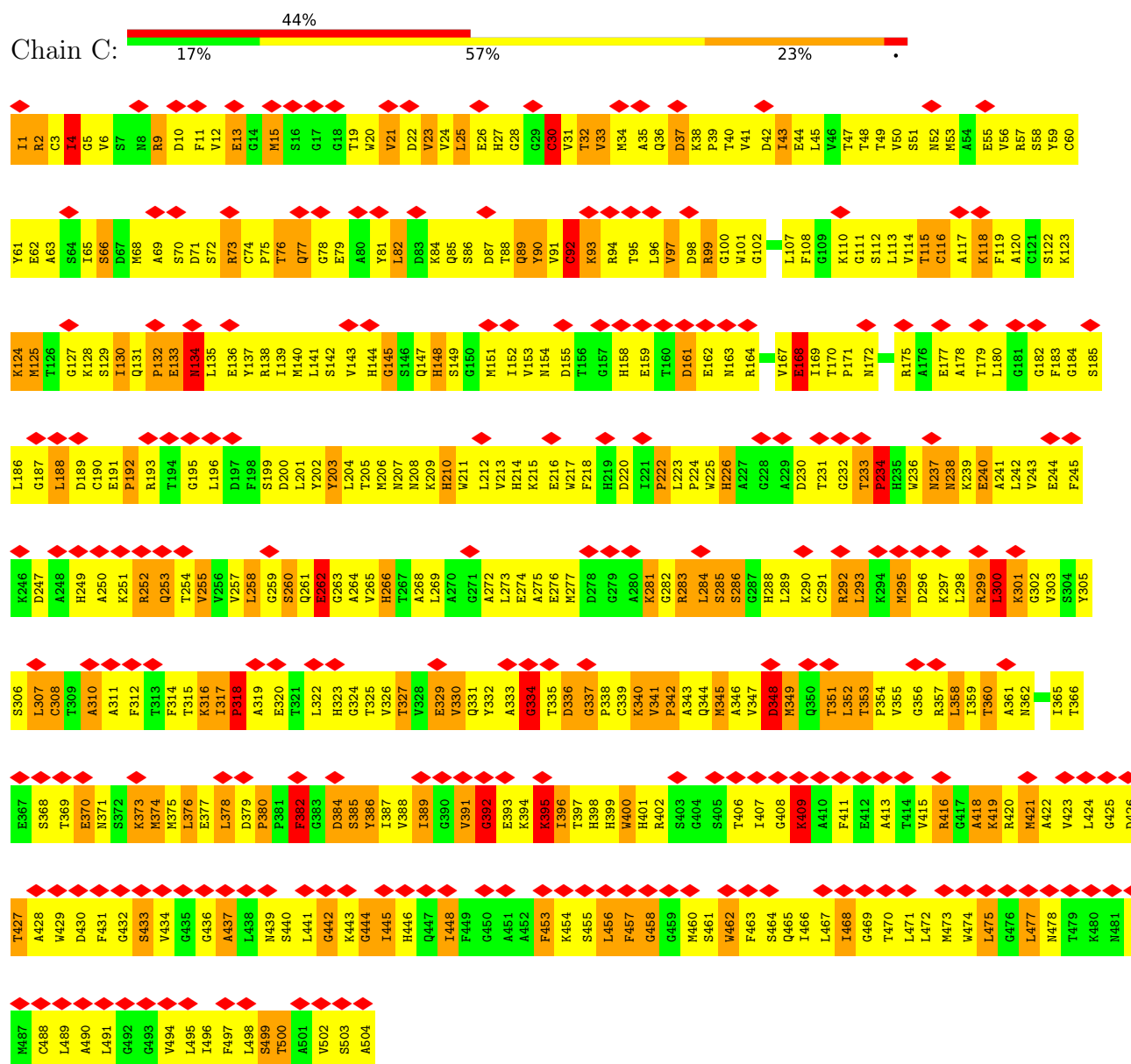
3 Residue-property plots

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.

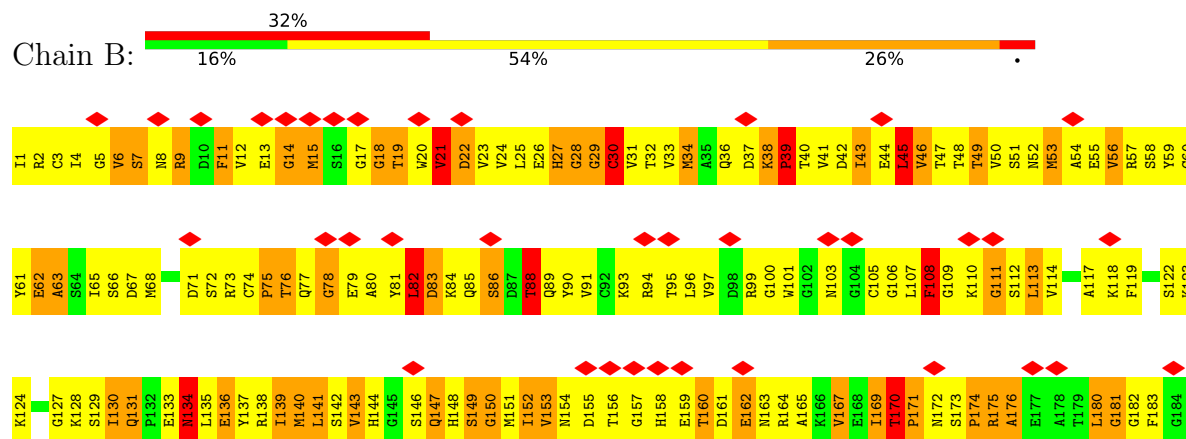
- Molecule 1: structural protein E

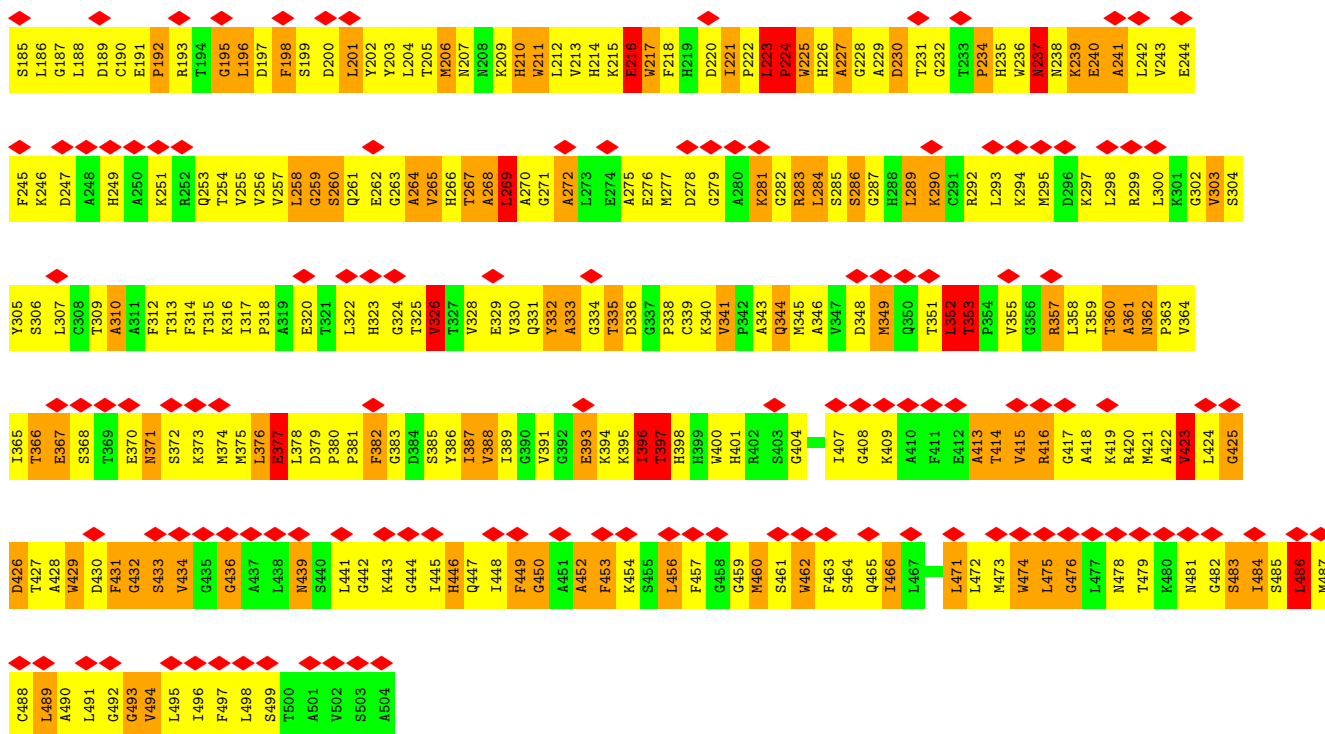


- Molecule 1: structural protein E

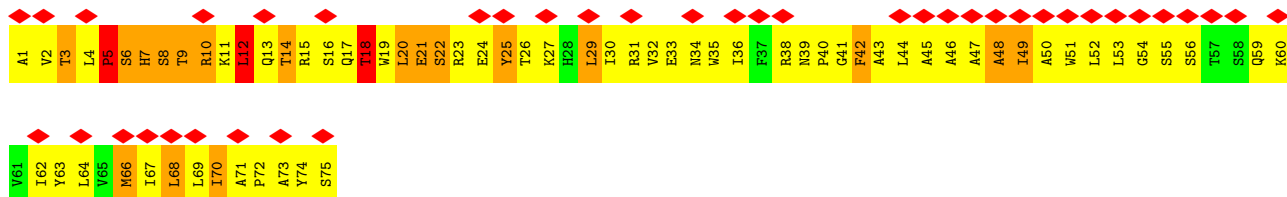
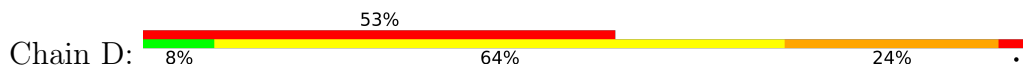


• Molecule 1: structural protein E

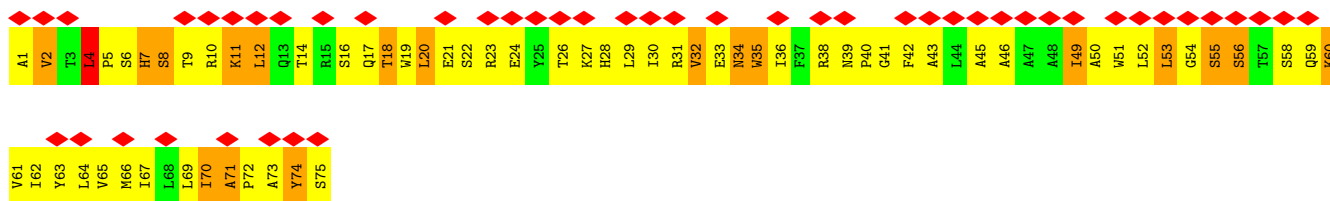
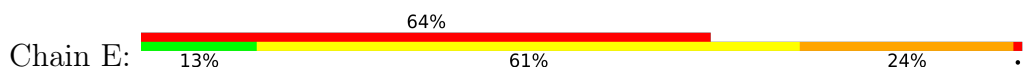




• Molecule 2: structural protein M



• Molecule 2: structural protein M



• Molecule 2: structural protein M



Y61	Y62	Y63	Y64	Y65	Y66	Y67	Y68	Y69	Y70	Y71	Y72	Y73	Y74	Y75

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	7180	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; correction for astigmatism included	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	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	11.108	Depositor
Minimum map value	-6.234	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.75	0/3888	1.31	51/5261 (1.0%)
1	B	0.82	2/3888 (0.1%)	1.40	69/5261 (1.3%)
1	C	0.82	2/3887 (0.1%)	1.35	68/5261 (1.3%)
2	D	0.71	0/615	1.16	6/838 (0.7%)
2	E	0.80	0/615	1.36	12/838 (1.4%)
2	F	0.78	0/615	1.26	10/838 (1.2%)
All	All	0.79	4/13508 (0.0%)	1.34	216/18297 (1.2%)

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
2	F	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	231	THR	CA-CB	5.96	1.61	1.53
1	B	140	MET	SD-CE	5.52	1.93	1.79
1	C	15	MET	SD-CE	5.48	1.93	1.79
1	B	496	ILE	CA-CB	5.27	1.60	1.54

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	LYS	N-CA-C	13.43	125.91	111.28
1	A	393	GLU	N-CA-C	-13.24	97.98	113.21
1	A	427	THR	N-CA-C	-12.45	98.99	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	LEU	N-CA-C	11.54	126.46	112.38
1	A	309	THR	N-CA-C	11.50	125.05	111.02
1	A	360	THR	N-CA-C	-11.24	99.87	112.57
1	B	278	ASP	N-CA-C	-11.18	100.13	113.88
1	A	417	GLY	N-CA-C	-10.77	101.95	115.31
1	C	162	GLU	N-CA-C	-10.43	100.30	113.23
1	A	458	GLY	N-CA-C	-10.38	98.75	112.14
1	B	265	VAL	N-CA-C	-9.98	102.55	113.43
1	C	255	VAL	N-CA-C	9.93	116.84	106.21
1	B	326	VAL	N-CA-C	9.85	122.38	107.99
1	C	30	CYS	N-CA-C	9.49	120.45	107.73
1	C	111	GLY	N-CA-C	-9.45	101.93	112.33
2	E	60	LYS	N-CA-C	-9.25	100.14	111.33
1	A	310	ALA	N-CA-C	9.21	126.10	113.21
1	B	173	SER	CA-C-N	9.12	131.24	119.84
1	B	173	SER	C-N-CA	9.12	131.24	119.84
2	E	7	HIS	N-CA-C	-9.08	102.22	113.20
1	B	466	ILE	N-CA-C	-8.94	102.15	110.82
1	C	77	GLN	N-CA-C	-8.85	102.19	113.16
1	A	280	ALA	N-CA-C	-8.83	103.09	114.04
1	B	224	PRO	N-CA-C	-8.67	94.61	112.47
1	B	230	ASP	N-CA-C	-8.64	96.03	109.25
1	B	475	LEU	N-CA-C	-8.62	102.66	113.01
1	B	223	LEU	CA-C-N	-8.62	109.07	119.84
1	B	223	LEU	C-N-CA	-8.62	109.07	119.84
1	B	82	LEU	N-CA-C	8.53	128.98	110.80
1	C	413	ALA	N-CA-C	-8.47	102.93	113.18
1	B	259	GLY	N-CA-C	8.44	122.85	111.03
1	B	150	GLY	N-CA-C	-8.43	101.91	115.66
1	C	237	ASN	N-CA-C	-8.42	99.18	110.55
1	B	220	ASP	CA-C-N	-8.41	116.54	122.59
1	B	220	ASP	C-N-CA	-8.41	116.54	122.59
1	B	423	VAL	N-CA-C	-8.41	105.72	113.71
1	B	268	ALA	N-CA-C	-8.37	102.11	111.14
2	F	67	ILE	N-CA-C	-8.32	104.41	111.56
1	C	348	ASP	N-CA-C	8.30	128.49	110.80
1	C	370	GLU	CB-CA-C	-8.28	107.02	116.54
1	C	92	CYS	N-CA-C	8.23	121.40	109.14
1	C	285	SER	N-CA-C	-8.23	98.28	110.46
2	F	70	ILE	N-CA-C	-8.13	103.84	111.48
1	C	416	ARG	N-CA-C	-8.00	102.97	112.89
1	C	477	LEU	N-CA-C	-7.91	102.67	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	231	THR	N-CA-C	-7.90	101.83	112.26
1	A	303	VAL	N-CA-C	-7.81	104.28	113.42
1	B	171	PRO	N-CA-C	-7.66	104.77	114.35
1	C	468	ILE	N-CA-C	-7.66	104.46	113.42
1	B	413	ALA	N-CA-C	-7.61	103.06	112.88
1	A	416	ARG	N-CA-C	-7.60	104.62	114.04
2	E	71	ALA	CA-C-N	7.60	127.14	119.24
2	E	71	ALA	C-N-CA	7.60	127.14	119.24
1	B	332	TYR	N-CA-C	7.57	121.84	109.72
1	A	382	PHE	N-CA-C	7.55	120.57	108.41
1	A	336	ASP	N-CA-C	7.54	120.76	108.55
1	A	434	VAL	N-CA-C	-7.46	97.53	108.87
1	A	431	PHE	N-CA-C	-7.45	98.74	109.31
1	B	227	ALA	N-CA-C	7.42	119.41	108.14
1	B	366	THR	N-CA-C	-7.41	99.51	110.48
1	B	220	ASP	N-CA-C	7.35	120.22	111.33
1	C	437	ALA	N-CA-C	-7.32	104.20	113.72
1	A	429	TRP	N-CA-C	-7.26	104.02	114.12
1	C	334	GLY	N-CA-C	7.25	130.37	113.18
1	C	310	ALA	N-CA-C	-7.25	97.25	108.42
1	A	190	CYS	N-CA-C	7.21	120.38	109.63
1	C	252	ARG	N-CA-C	7.21	121.53	107.98
2	D	5	PRO	N-CA-C	7.12	127.13	112.47
1	B	162	GLU	N-CA-C	7.11	121.55	113.01
1	B	88	THR	N-CA-C	-7.11	103.27	112.23
1	B	377	GLU	N-CA-C	7.01	121.23	110.36
1	C	159	GLU	N-CA-C	-6.99	105.38	114.04
2	D	7	HIS	N-CA-C	-6.98	104.77	113.28
1	C	266	HIS	N-CA-C	-6.93	102.56	111.02
1	B	108	PHE	N-CA-C	6.93	120.23	109.07
1	A	495	LEU	N-CA-C	-6.88	103.71	111.07
1	B	449	PHE	N-CA-C	-6.88	103.92	112.72
2	E	39	ASN	CA-C-N	6.80	126.60	119.05
2	E	39	ASN	C-N-CA	6.80	126.60	119.05
1	A	148	HIS	N-CA-C	6.78	120.11	110.14
1	C	360	THR	N-CA-C	-6.78	100.00	110.10
1	A	205	THR	N-CA-C	6.76	118.69	107.20
1	B	170	THR	CA-C-N	-6.75	112.96	120.45
1	B	170	THR	C-N-CA	-6.75	112.96	120.45
1	C	419	LYS	N-CA-C	-6.70	102.51	111.96
2	E	34	ASN	N-CA-C	-6.66	104.19	113.37
1	B	299	ARG	N-CA-C	6.58	120.22	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	450	GLY	N-CA-C	-6.56	104.83	112.83
1	B	393	GLU	N-CA-C	-6.53	103.66	111.69
1	C	406	THR	N-CA-C	-6.52	104.25	111.36
1	C	411	PHE	N-CA-C	-6.50	104.66	112.59
1	B	416	ARG	N-CA-C	-6.42	105.16	112.87
1	C	232	GLY	N-CA-C	-6.40	103.57	111.45
1	C	427	THR	N-CA-C	-6.39	105.86	113.21
1	B	34	MET	N-CA-C	6.34	119.04	108.13
1	A	199	SER	N-CA-C	-6.34	100.45	109.96
1	B	346	ALA	N-CA-C	6.33	118.17	109.18
1	B	130	ILE	N-CA-C	6.31	115.81	106.85
1	B	267	THR	N-CA-C	-6.30	105.42	113.23
1	C	384	ASP	N-CA-C	6.28	119.02	110.35
1	A	206	MET	N-CA-C	-6.28	99.46	109.76
1	C	192	PRO	N-CA-C	-6.28	105.34	113.57
2	E	35	TRP	N-CA-C	-6.26	105.66	113.55
1	C	408	GLY	N-CA-C	-6.26	105.90	115.66
2	F	32	VAL	N-CA-C	-6.23	104.23	113.39
1	A	38	LYS	N-CA-C	6.21	117.53	109.64
1	A	196	LEU	N-CA-C	-6.20	102.78	110.41
1	C	369	THR	N-CA-C	6.17	119.01	109.07
1	A	440	SER	N-CA-C	-6.16	104.83	112.90
1	A	370	GLU	N-CA-C	-6.16	98.93	108.42
1	A	30	CYS	N-CA-C	6.15	117.23	108.74
1	C	226	HIS	N-CA-C	-6.13	96.78	107.20
1	B	439	ASN	N-CA-C	-6.13	104.71	111.82
1	C	392	GLY	N-CA-C	6.10	127.63	113.18
1	C	421	MET	N-CA-C	6.09	118.83	111.40
1	C	486	LEU	N-CA-C	6.08	118.69	111.33
1	C	73	ARG	N-CA-C	-6.07	102.36	110.55
2	F	63	TYR	N-CA-C	-6.04	101.83	111.02
1	C	370	GLU	N-CA-C	6.04	117.49	108.31
1	A	333	ALA	N-CA-C	-6.02	104.64	111.14
1	C	317	ILE	CA-C-N	6.00	127.35	119.84
1	C	317	ILE	C-N-CA	6.00	127.35	119.84
2	D	6	SER	N-CA-C	5.98	123.55	110.80
1	A	108	PHE	N-CA-C	5.97	118.03	110.33
1	C	341	VAL	CA-C-N	5.97	126.47	120.14
1	C	341	VAL	C-N-CA	5.97	126.47	120.14
1	A	394	LYS	N-CA-C	-5.93	104.26	112.03
1	B	482	GLY	N-CA-C	-5.93	105.48	115.80
1	B	429	TRP	N-CA-C	-5.92	104.67	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	LEU	N-CA-C	5.92	118.28	108.99
1	B	119	PHE	N-CA-C	5.90	119.07	107.98
1	C	89	GLN	N-CA-C	5.89	118.18	111.11
2	F	4	LEU	CA-C-N	-5.88	113.91	119.85
2	F	4	LEU	C-N-CA	-5.88	113.91	119.85
1	A	489	LEU	N-CA-C	-5.87	105.78	113.12
1	B	27	HIS	N-CA-C	-5.86	97.18	107.73
1	B	272	ALA	N-CA-C	5.86	120.48	112.68
1	B	353	THR	CA-C-N	-5.86	111.85	120.46
1	B	353	THR	C-N-CA	-5.86	111.85	120.46
1	B	78	GLY	N-CA-C	5.84	119.55	112.49
1	A	74	CYS	CA-C-N	5.83	127.12	119.84
1	A	74	CYS	C-N-CA	5.83	127.12	119.84
1	C	418	ALA	N-CA-C	-5.82	105.79	114.64
1	C	255	VAL	CB-CA-C	-5.82	106.70	113.22
1	B	474	TRP	N-CA-C	-5.76	104.61	111.69
1	C	32	THR	N-CA-C	-5.75	100.51	109.72
1	C	409	LYS	N-CA-C	-5.73	106.12	113.23
1	C	233	THR	CA-C-N	-5.73	112.68	119.84
1	C	233	THR	C-N-CA	-5.73	112.68	119.84
2	F	67	ILE	CB-CA-C	-5.73	106.00	111.44
1	B	431	PHE	N-CA-C	-5.70	105.58	112.54
2	F	54	GLY	N-CA-C	-5.70	99.67	113.18
1	C	386	TYR	CB-CA-C	-5.67	107.31	114.40
1	A	131	GLN	CA-C-N	5.67	126.92	119.84
1	A	131	GLN	C-N-CA	5.67	126.92	119.84
1	A	15	MET	N-CA-C	-5.66	105.20	111.71
2	E	4	LEU	CA-C-N	-5.65	113.39	120.51
2	E	4	LEU	C-N-CA	-5.65	113.39	120.51
1	B	160	THR	N-CA-C	-5.64	106.61	112.93
1	A	419	LYS	N-CA-C	-5.62	104.84	110.97
1	B	228	GLY	N-CA-C	-5.62	99.87	113.18
1	B	489	LEU	N-CA-C	-5.60	106.29	113.01
1	B	486	LEU	N-CA-C	-5.59	104.68	112.45
1	C	97	VAL	CB-CA-C	-5.56	105.90	111.80
1	A	116	CYS	N-CA-C	5.56	117.47	108.41
1	C	15	MET	N-CA-C	-5.56	103.81	111.81
1	B	264	ALA	N-CA-C	-5.55	106.48	113.20
1	A	380	PRO	CA-C-N	5.55	125.54	120.21
1	A	380	PRO	C-N-CA	5.55	125.54	120.21
1	C	281	LYS	N-CA-C	5.54	117.73	109.25
1	B	30	CYS	N-CA-C	5.51	117.17	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	56	SER	N-CA-C	5.49	116.48	108.14
1	A	240	GLU	N-CA-C	5.48	120.84	113.72
1	B	237	ASN	N-CA-C	-5.46	100.76	109.23
1	C	130	ILE	N-CA-C	5.46	116.34	108.48
1	A	204	LEU	N-CA-C	5.45	118.52	110.46
1	A	501	ALA	N-CA-C	-5.42	106.85	112.93
1	C	391	VAL	N-CA-C	5.42	117.45	108.99
2	D	39	ASN	CA-C-N	5.38	124.89	119.19
2	D	39	ASN	C-N-CA	5.38	124.89	119.19
1	B	353	THR	N-CA-C	-5.38	102.66	110.08
1	C	353	THR	N-CA-C	5.37	117.72	110.31
1	A	499	SER	N-CA-C	-5.37	107.39	114.04
1	A	480	LYS	N-CA-C	5.36	116.43	108.60
2	E	74	TYR	N-CA-C	5.34	122.18	110.80
1	C	482	GLY	N-CA-C	5.32	118.48	111.52
1	B	414	THR	N-CA-C	-5.32	105.94	112.90
1	A	414	THR	N-CA-C	-5.31	106.48	113.12
1	A	49	THR	N-CA-C	5.30	116.83	107.61
1	B	28	GLY	N-CA-C	-5.25	100.73	113.18
1	C	349	MET	N-CA-C	5.25	117.22	107.99
1	A	173	SER	CA-C-N	5.21	126.35	119.84
1	A	173	SER	C-N-CA	5.21	126.35	119.84
1	B	39	PRO	CA-C-N	-5.21	115.66	123.00
1	B	39	PRO	C-N-CA	-5.21	115.66	123.00
1	A	201	LEU	N-CA-C	5.19	117.07	108.20
1	C	448	ILE	CB-CA-C	-5.18	105.41	111.94
1	C	483	SER	N-CA-C	-5.17	106.65	113.17
1	B	149	SER	N-CA-C	-5.17	106.06	112.47
2	F	9	THR	N-CA-C	-5.16	105.28	112.45
1	C	199	SER	N-CA-C	-5.15	105.56	111.07
1	C	43	ILE	N-CA-C	-5.14	101.08	108.53
1	C	395	LYS	CA-C-N	-5.13	116.48	123.10
1	C	395	LYS	C-N-CA	-5.13	116.48	123.10
1	B	49	THR	N-CA-C	5.13	117.87	110.28
2	E	56	SER	N-CA-C	-5.13	102.46	110.10
1	C	295	MET	N-CA-C	5.12	117.47	108.56
1	C	453	PHE	N-CA-C	-5.12	105.34	112.45
2	D	8	SER	N-CA-C	-5.12	106.14	112.38
1	B	493	GLY	N-CA-C	-5.12	108.32	114.66
1	C	3	CYS	N-CA-C	5.11	119.08	111.87
1	B	38	LYS	N-CA-C	5.10	116.49	108.23
1	B	362	ASN	CA-C-N	5.08	126.18	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	362	ASN	C-N-CA	5.08	126.18	119.84
1	C	116	CYS	N-CA-C	5.07	118.07	109.76
1	C	358	LEU	N-CA-C	-5.01	100.25	108.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	74	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3809	0	3761	718	0
1	B	3809	0	3760	804	0
1	C	3808	0	3760	723	0
2	D	600	0	624	178	0
2	E	600	0	624	131	0
2	F	600	0	624	131	0
3	A	14	0	13	4	0
3	B	14	0	13	1	0
3	C	14	0	13	6	0
All	All	13268	0	13192	2524	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 95.

All (2524) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:MET:SD	1:C:255:VAL:HB	1.79	1.21
1:C:178:ALA:HB3	1:C:186:LEU:H	1.08	1.15
1:A:158:HIS:HB3	1:A:166:LYS:HE3	1.20	1.15
1:B:60:CYS:HB3	1:B:224:PRO:HG2	1.21	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLY:HA3	2:E:7:HIS:CD2	1.83	1.14
1:A:50:VAL:HG11	1:A:130:ILE:HD12	1.15	1.14
1:A:332:TYR:HB3	1:A:335:THR:HG21	1.20	1.14
2:E:55:SER:HA	2:E:60:LYS:HG3	1.29	1.13
1:B:286:SER:HB3	2:E:16:SER:HB3	1.31	1.12
1:A:73:ARG:NH2	1:A:77:GLN:HB3	1.63	1.12
1:C:65:ILE:HD11	1:C:243:VAL:HG22	1.30	1.10
2:E:56:SER:HB3	2:E:59:GLN:HB2	1.35	1.09
1:B:71:ASP:HB2	1:B:82:LEU:HD13	1.30	1.09
1:B:95:THR:HG22	1:B:96:LEU:H	1.01	1.08
1:C:12:VAL:HG13	1:C:33:VAL:HG13	1.31	1.08
1:C:93:LYS:HB2	1:C:245:PHE:HE1	1.12	1.08
1:C:211:TRP:HE1	1:C:269:LEU:HD13	1.04	1.08
1:B:1:ILE:HG21	1:B:147:GLN:HB2	1.36	1.08
2:D:56:SER:HB3	2:D:59:GLN:HG2	1.08	1.06
1:B:41:VAL:HG22	1:B:143:VAL:HG22	1.31	1.06
1:B:364:VAL:N	1:B:374:MET:HE1	1.70	1.06
1:A:152:ILE:HG12	1:A:153:VAL:H	1.17	1.05
1:A:479:THR:HG22	1:A:480:LYS:H	1.19	1.05
1:A:332:TYR:HB3	1:A:335:THR:CG2	1.86	1.05
1:A:263:GLY:O	1:A:267:THR:HG23	1.54	1.05
1:C:25:LEU:HD23	1:C:43:ILE:HD12	1.38	1.04
1:B:21:VAL:HG11	1:B:293:LEU:HB3	1.37	1.04
1:B:100:GLY:HA3	1:B:108:PHE:CE1	1.91	1.04
1:C:34:MET:HE1	1:C:359:ILE:HG23	1.38	1.04
1:C:300:LEU:HD23	1:C:301:LYS:H	1.16	1.04
1:C:337:GLY:HA2	1:C:368:SER:HA	1.04	1.03
2:D:32:VAL:HG23	2:D:72:PRO:HG3	1.38	1.03
2:E:51:TRP:HD1	2:E:60:LYS:HZ2	1.04	1.03
2:D:67:ILE:HA	2:D:70:ILE:HG22	1.41	1.03
1:C:245:PHE:HB3	1:C:255:VAL:HA	1.41	1.02
1:C:460:MET:HE1	1:C:468:ILE:HD12	1.40	1.02
2:D:55:SER:HA	2:D:60:LYS:HE2	1.39	1.01
1:B:21:VAL:HG13	1:B:293:LEU:H	1.23	1.01
1:A:341:VAL:HG21	1:A:374:MET:HE3	1.42	1.01
1:A:46:VAL:HG12	1:A:47:THR:HG23	1.42	1.01
2:D:18:THR:HG23	2:D:21:GLU:HB2	1.39	1.00
1:A:299:ARG:HB2	1:A:299:ARG:NH1	1.77	1.00
1:B:180:LEU:H	1:B:180:LEU:HD12	1.24	1.00
1:B:223:LEU:HB2	1:B:224:PRO:HD3	1.44	1.00
1:B:43:ILE:HG23	1:B:141:LEU:HB3	1.41	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:MET:HE1	1:C:298:LEU:HB3	1.41	0.99
1:A:150:GLY:C	1:A:152:ILE:H	1.69	0.99
1:A:359:ILE:HD11	1:A:377:GLU:HG2	1.42	0.99
1:C:2:ARG:HD2	1:C:44:GLU:OE1	1.61	0.99
1:B:25:LEU:HD13	1:B:139:ILE:HG21	1.40	0.99
1:B:221:ILE:HD12	2:E:4:LEU:HA	1.41	0.98
1:C:59:TYR:O	1:C:124:LYS:HB2	1.64	0.98
1:B:32:THR:HA	1:B:42:ASP:HB3	1.44	0.98
1:B:57:ARG:HA	1:B:227:ALA:CB	1.94	0.98
1:C:20:TRP:HA	1:C:293:LEU:O	1.63	0.97
1:A:152:ILE:HG12	1:A:153:VAL:N	1.70	0.97
1:A:175:ARG:HG2	1:A:189:ASP:HB3	1.46	0.97
1:B:20:TRP:O	1:B:433:SER:HB3	1.63	0.97
1:C:345:MET:HB2	1:C:355:VAL:O	1.63	0.96
2:D:23:ARG:HB3	2:D:27:LYS:HE3	1.47	0.96
2:D:56:SER:CB	2:D:59:GLN:HG2	1.95	0.96
1:C:27:HIS:CE1	1:C:48:THR:HG22	2.01	0.96
1:B:137:TYR:HD2	1:B:289:LEU:HD22	1.29	0.96
1:C:55:GLU:HA	1:C:128:LYS:HA	1.46	0.96
1:B:272:ALA:HB2	2:E:18:THR:HG22	1.45	0.96
1:C:100:GLY:HA3	1:C:108:PHE:CE1	2.00	0.96
1:A:265:VAL:HG23	2:D:4:LEU:HD13	1.47	0.95
1:A:37:ASP:O	1:A:300:LEU:HD11	1.65	0.95
2:E:56:SER:HB3	2:E:59:GLN:CB	1.96	0.95
1:A:204:LEU:HD23	1:A:204:LEU:H	1.29	0.95
1:B:236:TRP:HB2	1:B:239:LYS:HE3	1.44	0.95
1:C:331:GLN:OE1	1:C:371:ASN:HB2	1.65	0.95
1:A:1:ILE:HD13	1:A:144:HIS:HA	1.48	0.95
1:A:302:GLY:HA3	1:A:305:TYR:CD2	2.01	0.95
1:B:1:ILE:HG21	1:B:147:GLN:CB	1.97	0.95
1:A:20:TRP:CE3	1:A:434:VAL:HG12	2.02	0.94
1:A:305:TYR:HB2	1:A:340:LYS:HG3	1.50	0.94
1:A:345:MET:HE2	1:A:378:LEU:HD21	1.50	0.94
1:C:65:ILE:HD13	1:C:257:VAL:HG12	1.49	0.94
1:B:30:CYS:SG	1:B:31:VAL:N	2.39	0.94
1:B:95:THR:HG22	1:B:96:LEU:N	1.80	0.94
1:B:272:ALA:CB	2:E:18:THR:HG22	1.98	0.93
1:A:392:GLY:C	1:A:394:LYS:H	1.75	0.93
1:C:39:PRO:HD2	1:C:298:LEU:HD11	1.49	0.93
1:C:93:LYS:HB2	1:C:245:PHE:CE1	2.04	0.93
1:C:315:THR:HG21	1:C:373:LYS:HE2	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:ILE:HD11	1:C:396:ILE:HG23	1.49	0.92
1:B:375:MET:C	1:B:376:LEU:HG	1.92	0.92
1:B:170:THR:HG22	1:B:171:PRO:HD2	1.52	0.92
1:A:312:PHE:HB3	1:A:396:ILE:HD13	1.51	0.91
1:A:38:LYS:HA	1:A:38:LYS:HE3	1.53	0.91
1:A:331:GLN:HG3	1:A:373:LYS:HG2	1.53	0.91
1:C:211:TRP:NE1	1:C:269:LEU:HD13	1.86	0.91
1:C:154:ASN:HB2	3:C:601:NAG:H82	1.51	0.91
1:B:95:THR:CG2	1:B:96:LEU:H	1.84	0.90
1:B:21:VAL:CG1	1:B:293:LEU:HB3	2.02	0.90
1:A:56:VAL:HG23	1:B:78:GLY:HA3	1.52	0.90
1:A:358:LEU:O	1:A:359:ILE:HG12	1.71	0.90
1:C:217:TRP:NE1	2:F:5:PRO:HB2	1.87	0.90
2:D:23:ARG:CB	2:D:27:LYS:HE3	2.02	0.90
1:C:13:GLU:HG2	1:C:34:MET:HG3	1.52	0.90
1:C:300:LEU:HD23	1:C:301:LYS:N	1.87	0.90
1:B:48:THR:HG23	1:B:284:LEU:HG	1.50	0.90
1:A:47:THR:OG1	1:A:138:ARG:HD3	1.72	0.89
1:C:65:ILE:HD11	1:C:243:VAL:CG2	2.02	0.89
1:C:330:VAL:HG23	1:C:374:MET:HE1	1.53	0.89
1:C:34:MET:HE1	1:C:359:ILE:HD12	1.53	0.89
2:D:1:ALA:CB	2:F:23:ARG:HD2	2.02	0.89
1:A:314:PHE:HD1	1:A:314:PHE:H	1.21	0.89
1:A:305:TYR:CB	1:A:340:LYS:HG3	2.02	0.89
1:C:34:MET:CE	1:C:359:ILE:HG23	2.03	0.89
1:B:486:LEU:HD23	1:B:487:MET:H	1.36	0.89
1:C:439:ASN:C	1:C:441:LEU:H	1.80	0.88
1:B:181:GLY:C	1:B:183:PHE:H	1.79	0.88
1:B:345:MET:HG2	1:B:378:LEU:HD23	1.55	0.88
1:A:171:PRO:HA	1:A:192:PRO:CG	2.03	0.88
1:A:169:ILE:HD11	1:A:289:LEU:HD21	1.54	0.88
1:C:337:GLY:HA2	1:C:368:SER:CA	2.00	0.88
1:C:41:VAL:HG23	1:C:143:VAL:HG22	1.55	0.88
1:B:175:ARG:HA	1:B:188:LEU:O	1.72	0.88
1:C:420:ARG:HD2	1:C:431:PHE:CD2	2.09	0.88
1:A:76:THR:HG21	1:A:107:LEU:HD12	1.55	0.88
1:B:23:VAL:HG21	1:B:31:VAL:HG11	1.56	0.88
1:A:405:SER:HB2	1:A:408:GLY:HA3	1.55	0.87
2:E:71:ALA:N	2:E:72:PRO:HD2	1.88	0.87
1:C:337:GLY:CA	1:C:368:SER:HA	2.00	0.87
1:B:225:TRP:CG	1:B:237:ASN:HD22	1.91	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:HD12	1:A:257:VAL:HG22	1.55	0.87
1:A:171:PRO:HA	1:A:192:PRO:HG2	1.56	0.87
1:C:28:GLY:HA3	2:F:15:ARG:HG3	1.55	0.87
1:B:71:ASP:O	1:B:113:LEU:HB2	1.75	0.86
1:A:352:LEU:H	1:A:352:LEU:HD12	1.40	0.86
1:C:457:PHE:O	1:C:460:MET:HG2	1.75	0.86
1:B:269:LEU:O	2:E:19:TRP:HD1	1.59	0.86
1:A:302:GLY:HA3	1:A:305:TYR:CE2	2.09	0.86
1:C:133:GLU:O	1:C:134:ASN:HB2	1.73	0.86
1:B:40:THR:HG23	1:B:144:HIS:HD2	1.39	0.86
2:D:1:ALA:N	2:F:27:LYS:HD3	1.91	0.86
1:C:154:ASN:CB	3:C:601:NAG:H82	2.06	0.86
1:A:2:ARG:HB2	1:A:142:SER:CB	2.06	0.85
1:A:460:MET:HG3	1:A:464:SER:HB2	1.57	0.85
1:B:320:GLU:HB2	1:B:400:TRP:HZ2	1.41	0.85
1:A:97:VAL:O	1:A:110:LYS:HG3	1.77	0.85
2:F:4:LEU:HD23	2:F:5:PRO:HD3	1.59	0.85
1:B:486:LEU:HD23	1:B:487:MET:N	1.91	0.85
1:C:389:ILE:HD11	1:C:396:ILE:CG2	2.06	0.85
1:A:493:GLY:HA2	1:A:496:ILE:HD12	1.59	0.85
1:A:341:VAL:HG22	1:A:365:ILE:HG13	1.56	0.85
2:D:49:ILE:HA	2:D:52:LEU:HD22	1.57	0.84
1:C:426:ASP:HB3	1:C:446:HIS:CB	2.06	0.84
1:B:137:TYR:CD2	1:B:289:LEU:HD22	2.12	0.84
1:A:115:THR:HG22	1:A:253:GLN:NE2	1.92	0.84
1:A:332:TYR:CB	1:A:335:THR:HG21	2.07	0.84
1:B:60:CYS:H	1:B:224:PRO:HD2	1.42	0.84
1:B:66:SER:OG	1:B:118:LYS:HB3	1.77	0.84
2:F:27:LYS:HG3	2:F:28:HIS:H	1.42	0.84
1:B:364:VAL:H	1:B:374:MET:HE1	1.40	0.84
1:C:273:LEU:N	2:F:12:LEU:HD21	1.93	0.84
1:C:184:GLY:HA3	1:C:297:LYS:O	1.76	0.84
2:E:51:TRP:CD1	2:E:60:LYS:HZ2	1.95	0.84
1:B:262:GLU:O	1:B:265:VAL:HG12	1.77	0.84
1:A:46:VAL:HG21	1:A:140:MET:HG2	1.60	0.83
1:C:178:ALA:O	1:C:185:SER:HB3	1.78	0.83
2:D:73:ALA:HB2	2:F:74:TYR:CE2	2.13	0.83
1:B:97:VAL:HG13	1:B:251:LYS:HA	1.58	0.83
1:B:151:MET:O	1:B:153:VAL:HG22	1.78	0.83
1:A:312:PHE:HD2	1:A:396:ILE:HB	1.40	0.83
1:B:21:VAL:HG13	1:B:293:LEU:N	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLN:CA	1:A:261:GLN:HE21	1.90	0.83
1:C:429:TRP:HB3	1:C:442:GLY:O	1.77	0.83
1:B:21:VAL:HG11	1:B:293:LEU:CB	2.08	0.83
1:B:33:VAL:HG22	1:B:41:VAL:O	1.77	0.83
1:B:57:ARG:HA	1:B:227:ALA:HB2	1.61	0.83
1:C:475:LEU:HD13	2:D:52:LEU:HD23	1.60	0.83
1:A:20:TRP:HE3	1:A:434:VAL:HG12	1.42	0.83
1:C:238:ASN:HA	1:C:240:GLU:OE1	1.77	0.83
1:B:313:THR:HA	1:B:396:ILE:HD12	1.60	0.83
1:B:25:LEU:CD1	1:B:139:ILE:HG21	2.08	0.83
1:C:115:THR:HG21	1:C:253:GLN:HB3	1.59	0.83
1:C:137:TYR:CD2	1:C:289:LEU:HD22	2.12	0.83
1:C:419:LYS:HB3	2:F:15:ARG:HH22	1.41	0.83
2:D:41:GLY:C	2:D:43:ALA:H	1.87	0.83
1:B:1:ILE:HD11	1:B:142:SER:OG	1.79	0.83
1:A:65:ILE:HB	1:A:257:VAL:HG21	1.59	0.82
1:C:210:HIS:CD2	1:C:277:MET:H	1.97	0.82
2:D:66:MET:HE2	2:D:66:MET:HA	1.60	0.82
1:B:99:ARG:HH21	1:B:103:ASN:HB3	1.45	0.82
1:B:396:ILE:O	1:B:396:ILE:HG12	1.77	0.82
1:A:118:LYS:HG2	1:A:119:PHE:H	1.42	0.82
1:B:345:MET:HE1	1:B:380:PRO:HA	1.61	0.82
1:B:223:LEU:CB	1:B:224:PRO:HD3	2.07	0.82
1:A:332:TYR:HD2	1:A:335:THR:HB	1.43	0.82
1:B:107:LEU:HD12	1:B:107:LEU:H	1.43	0.82
1:B:107:LEU:HD12	1:B:107:LEU:N	1.94	0.82
1:B:260:SER:O	1:B:261:GLN:HB2	1.78	0.82
1:B:73:ARG:HB3	1:B:77:GLN:HE21	1.44	0.82
1:A:252:ARG:HB2	1:A:252:ARG:NH1	1.94	0.82
1:B:434:VAL:HG13	1:B:436:GLY:H	1.43	0.82
1:B:382:PHE:HB3	1:B:404:GLY:O	1.80	0.82
1:A:50:VAL:HG11	1:A:130:ILE:CD1	2.04	0.82
1:C:1:ILE:HD12	1:C:1:ILE:H1	1.44	0.82
1:C:97:VAL:O	1:C:99:ARG:HD2	1.79	0.82
1:B:49:THR:HG22	1:B:283:ARG:HG2	1.60	0.82
1:A:43:ILE:HG23	1:A:141:LEU:HD21	1.62	0.81
1:A:305:TYR:HE1	1:A:338:PRO:HG2	1.45	0.81
1:A:314:PHE:CE2	1:A:318:PRO:HD3	2.15	0.81
1:C:68:MET:SD	1:C:255:VAL:CB	2.68	0.81
1:B:12:VAL:CG1	1:B:33:VAL:HG12	2.10	0.81
1:B:40:THR:HG23	1:B:144:HIS:CD2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:TYR:CE2	1:B:289:LEU:HD13	2.14	0.81
1:B:426:ASP:C	1:B:428:ALA:H	1.84	0.81
1:A:225:TRP:NE1	1:A:237:ASN:HD22	1.77	0.81
1:A:240:GLU:HA	1:A:243:VAL:HG22	1.61	0.81
1:B:481:ASN:ND2	1:B:483:SER:HB3	1.95	0.81
1:A:1:ILE:O	1:A:4:ILE:HG13	1.81	0.81
1:C:374:MET:C	1:C:375:MET:HE3	2.04	0.81
1:C:462:TRP:CZ3	1:C:499:SER:HB2	2.15	0.81
2:F:27:LYS:HG3	2:F:28:HIS:N	1.96	0.81
1:B:365:ILE:HG22	1:B:366:THR:O	1.81	0.81
1:C:137:TYR:HE2	1:C:289:LEU:HB2	1.46	0.81
1:C:273:LEU:HD21	1:C:286:SER:HB2	1.60	0.81
1:C:344:GLN:HE21	1:C:354:PRO:HB3	1.44	0.81
2:D:10:ARG:HH21	2:D:10:ARG:HG2	1.45	0.81
2:D:11:LYS:HD2	2:D:18:THR:HG21	1.61	0.81
2:E:62:ILE:O	2:E:65:VAL:HG12	1.81	0.81
1:B:204:LEU:O	1:B:210:HIS:HB3	1.80	0.81
1:A:2:ARG:HB2	1:A:142:SER:HB3	1.63	0.80
1:C:491:LEU:O	1:C:495:LEU:HG	1.81	0.80
1:A:322:LEU:HG	1:A:323:HIS:H	1.46	0.80
2:D:1:ALA:H1	2:F:27:LYS:HD3	1.47	0.80
2:D:31:ARG:HG2	2:F:4:LEU:HB2	1.63	0.80
2:D:50:ALA:HB1	2:D:60:LYS:HB3	1.63	0.80
1:B:27:HIS:CD2	1:B:45:LEU:HD22	2.16	0.80
1:A:2:ARG:HG2	1:A:44:GLU:OE1	1.80	0.80
1:B:198:PHE:HA	1:B:201:LEU:HB2	1.62	0.80
1:B:485:SER:HA	1:B:488:CYS:SG	2.22	0.80
1:C:98:ASP:OD1	1:C:110:LYS:HG3	1.82	0.80
1:C:171:PRO:HB2	1:C:193:ARG:HD2	1.62	0.80
1:A:344:GLN:O	1:A:388:VAL:HG23	1.82	0.80
1:A:373:LYS:O	1:A:374:MET:HB3	1.82	0.80
1:C:423:VAL:HG22	1:C:502:VAL:HG21	1.62	0.80
1:C:178:ALA:HB3	1:C:186:LEU:N	1.92	0.80
1:A:154:ASN:CG	3:A:601:NAG:H82	2.06	0.79
1:B:171:PRO:HA	1:B:192:PRO:HB2	1.62	0.79
1:A:139:ILE:HB	1:A:167:VAL:HG23	1.63	0.79
1:C:89:GLN:HA	1:C:239:LYS:NZ	1.97	0.79
1:B:175:ARG:CZ	1:B:175:ARG:HB2	2.12	0.79
1:C:422:ALA:HB1	1:C:498:LEU:CD1	2.12	0.79
1:B:12:VAL:HG11	1:B:33:VAL:HG12	1.65	0.79
1:B:158:HIS:HB3	1:B:164:ARG:HD3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:VAL:HG11	1:A:432:GLY:HA3	1.65	0.79
1:C:9:ARG:HH11	1:C:32:THR:HG21	1.47	0.79
2:D:67:ILE:HA	2:D:70:ILE:CG2	2.12	0.79
2:E:66:MET:O	2:E:70:ILE:HG22	1.83	0.79
1:B:133:GLU:O	1:B:134:ASN:HB3	1.83	0.79
1:B:357:ARG:HB2	1:B:357:ARG:HH11	1.47	0.79
1:C:423:VAL:CG2	1:C:502:VAL:HG11	2.13	0.79
1:B:223:LEU:HB2	1:B:224:PRO:CD	2.12	0.79
1:B:4:ILE:HA	1:B:9:ARG:HE	1.48	0.79
1:A:360:THR:CG2	1:A:377:GLU:H	1.95	0.78
2:D:67:ILE:HD12	2:D:70:ILE:HG21	1.65	0.78
1:B:27:HIS:CE1	1:B:285:SER:HA	2.18	0.78
1:A:154:ASN:HB2	3:A:601:NAG:H82	1.65	0.78
1:A:336:ASP:HA	1:A:368:SER:O	1.82	0.78
1:A:356:GLY:O	1:A:357:ARG:HB3	1.83	0.78
1:B:261:GLN:HE21	2:E:1:ALA:N	1.82	0.78
1:C:15:MET:SD	1:C:36:GLN:HB2	2.23	0.78
1:C:74:CYS:HB3	1:C:75:PRO:HD2	1.65	0.78
1:B:386:TYR:O	1:B:388:VAL:HG13	1.83	0.78
1:A:95:THR:HG23	1:A:96:LEU:HD12	1.65	0.78
1:A:307:LEU:HD22	1:A:307:LEU:N	1.99	0.78
1:A:409:LYS:NZ	1:A:409:LYS:HB3	1.98	0.78
1:C:300:LEU:HD22	1:C:303:VAL:HG23	1.63	0.78
2:D:35:TRP:HE3	2:D:36:ILE:HD12	1.47	0.78
1:C:273:LEU:H	2:F:12:LEU:HD21	1.48	0.78
1:B:360:THR:OG1	1:B:376:LEU:HB3	1.83	0.78
1:B:32:THR:CA	1:B:42:ASP:HB3	2.14	0.78
1:C:24:VAL:HG11	1:C:424:LEU:HD13	1.65	0.78
1:C:426:ASP:HB3	1:C:446:HIS:HB2	1.63	0.78
1:C:475:LEU:HD11	2:D:52:LEU:HB3	1.66	0.78
1:B:19:THR:HB	1:B:295:MET:HB2	1.66	0.78
1:B:197:ASP:C	1:B:199:SER:H	1.91	0.78
1:A:51:SER:OG	1:A:281:LYS:HE3	1.84	0.78
1:A:65:ILE:HB	1:A:257:VAL:CG2	2.12	0.78
1:C:164:ARG:HG2	1:C:164:ARG:HH11	1.46	0.78
1:C:167:VAL:HG22	1:C:168:GLU:H	1.47	0.77
2:D:9:THR:HG22	2:D:10:ARG:N	1.97	0.77
1:B:138:ARG:NH1	1:B:138:ARG:HB2	1.98	0.77
1:B:269:LEU:O	2:E:19:TRP:CD1	2.37	0.77
2:D:12:LEU:H	2:D:12:LEU:HD12	1.49	0.77
1:B:38:LYS:HG2	1:B:39:PRO:CD	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LYS:HA	1:B:300:LEU:HD11	1.64	0.77
1:B:227:ALA:C	1:B:229:ALA:N	2.36	0.77
1:B:57:ARG:HH11	1:B:225:TRP:CD1	2.03	0.77
1:B:320:GLU:HB2	1:B:400:TRP:CZ2	2.19	0.77
1:B:138:ARG:HB2	1:B:138:ARG:HH11	1.48	0.77
1:B:222:PRO:O	1:B:223:LEU:HG	1.84	0.77
1:A:46:VAL:CG1	1:A:47:THR:HG23	2.15	0.77
1:C:50:VAL:HG11	1:C:130:ILE:HG21	1.65	0.77
1:B:222:PRO:C	1:B:223:LEU:HD12	2.09	0.77
1:C:329:GLU:HG3	1:C:375:MET:HB3	1.66	0.77
2:D:53:LEU:HD13	2:F:62:ILE:HG21	1.67	0.76
1:A:443:LYS:NZ	1:A:443:LYS:HB3	1.99	0.76
1:B:74:CYS:O	1:B:76:THR:N	2.16	0.76
1:B:154:ASN:HB2	1:B:158:HIS:CE1	2.20	0.76
1:B:323:HIS:CD2	1:B:416:ARG:HH12	2.02	0.76
1:B:365:ILE:HA	1:B:374:MET:SD	2.25	0.76
1:C:143:VAL:HB	1:C:163:ASN:ND2	2.00	0.76
1:A:347:VAL:HG23	1:A:355:VAL:HB	1.67	0.76
1:C:2:ARG:NH1	1:C:140:MET:HE2	2.00	0.76
1:A:448:ILE:HG13	1:A:449:PHE:HD1	1.50	0.76
1:C:139:ILE:HB	1:C:167:VAL:CG1	2.16	0.76
1:C:374:MET:O	1:C:374:MET:SD	2.43	0.76
1:C:223:LEU:HD22	1:C:242:LEU:HD21	1.67	0.76
1:A:203:TYR:HE2	1:A:277:MET:CE	1.99	0.76
1:B:330:VAL:O	1:B:373:LYS:HA	1.86	0.76
1:A:476:GLY:HA3	1:A:489:LEU:HG	1.68	0.76
1:B:1:ILE:HD12	1:B:2:ARG:N	2.01	0.76
1:B:74:CYS:SG	1:B:99:ARG:HB3	2.26	0.75
1:B:393:GLU:HG3	1:B:394:LYS:H	1.50	0.75
1:A:154:ASN:CB	3:A:601:NAG:H82	2.16	0.75
1:C:184:GLY:HA3	1:C:297:LYS:C	2.11	0.75
1:B:373:LYS:HG3	1:B:373:LYS:O	1.87	0.75
2:D:44:LEU:O	2:D:48:ALA:HB2	1.84	0.75
1:B:41:VAL:HG22	1:B:143:VAL:CG2	2.15	0.75
1:B:261:GLN:NE2	2:E:1:ALA:H3	1.84	0.75
1:A:131:GLN:O	1:A:133:GLU:N	2.19	0.75
2:D:49:ILE:HD11	2:D:67:ILE:HG21	1.68	0.75
1:B:238:ASN:O	1:B:239:LYS:HB2	1.86	0.75
1:A:174:PRO:O	1:A:189:ASP:HA	1.86	0.75
1:C:307:LEU:HG	1:C:340:LYS:HD2	1.69	0.75
1:B:271:GLY:CA	2:E:7:HIS:CD2	2.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ILE:HB	1:C:167:VAL:HG11	1.66	0.75
1:C:344:GLN:NE2	1:C:354:PRO:HB3	2.02	0.75
2:E:4:LEU:HD23	2:E:4:LEU:C	2.11	0.75
1:B:479:THR:HG21	1:B:485:SER:CB	2.17	0.75
1:A:479:THR:HG22	1:A:480:LYS:N	2.00	0.75
1:C:39:PRO:HG2	1:C:183:PHE:HE2	1.52	0.75
1:C:97:VAL:HG21	1:C:113:LEU:HD23	1.67	0.75
1:B:21:VAL:O	1:B:21:VAL:HG22	1.85	0.75
1:B:60:CYS:CB	1:B:224:PRO:HG2	2.10	0.75
1:A:169:ILE:HD12	1:A:190:CYS:HB2	1.69	0.75
1:C:26:GLU:HB3	1:C:288:HIS:HA	1.69	0.75
1:C:39:PRO:HG2	1:C:183:PHE:CE2	2.22	0.75
1:C:50:VAL:HG11	1:C:130:ILE:CG2	2.17	0.75
1:C:329:GLU:HB3	1:C:373:LYS:HZ1	1.50	0.75
1:B:6:VAL:C	1:B:8:ASN:H	1.95	0.75
1:B:73:ARG:CB	1:B:77:GLN:HE21	2.00	0.75
1:B:141:LEU:CD1	1:B:165:ALA:HB3	2.16	0.75
1:A:73:ARG:HG3	1:A:79:GLU:O	1.87	0.74
1:B:212:LEU:HD12	1:B:275:ALA:HB2	1.69	0.74
1:A:307:LEU:HD22	1:A:307:LEU:H	1.51	0.74
1:A:360:THR:HG21	1:A:377:GLU:H	1.52	0.74
1:C:273:LEU:HD12	1:C:274:GLU:N	2.02	0.74
1:C:276:GLU:OE1	1:C:276:GLU:N	2.20	0.74
2:F:32:VAL:O	2:F:36:ILE:HG12	1.86	0.74
1:A:204:LEU:H	1:A:204:LEU:CD2	2.01	0.74
1:C:137:TYR:CE2	1:C:289:LEU:HB2	2.21	0.74
1:B:57:ARG:NH1	1:B:225:TRP:NE1	2.34	0.74
1:B:261:GLN:NE2	2:E:1:ALA:N	2.34	0.74
1:A:44:GLU:HG3	1:A:46:VAL:HG23	1.70	0.74
1:B:27:HIS:HD2	1:B:45:LEU:HD22	1.50	0.74
1:B:38:LYS:HG2	1:B:39:PRO:HD2	1.69	0.74
1:B:246:LYS:O	1:B:254:THR:HG22	1.87	0.74
1:B:141:LEU:HD11	1:B:165:ALA:HB3	1.69	0.74
1:C:114:VAL:O	1:C:114:VAL:HG13	1.88	0.74
1:C:133:GLU:HB2	1:C:193:ARG:HH12	1.52	0.74
1:B:82:LEU:HG	1:B:82:LEU:O	1.86	0.74
1:A:157:GLY:C	1:A:159:GLU:H	1.92	0.74
1:A:314:PHE:HE2	1:A:318:PRO:HD3	1.51	0.74
1:A:290:LYS:HD2	1:A:427:THR:HG23	1.68	0.74
1:A:329:GLU:HB2	1:C:101:TRP:CZ3	2.23	0.74
1:A:397:THR:HG22	1:A:397:THR:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:TRP:CZ3	1:B:226:HIS:HA	2.22	0.74
1:B:445:ILE:HG23	1:B:446:HIS:H	1.52	0.74
1:A:305:TYR:CE1	1:A:338:PRO:HG2	2.22	0.74
1:A:392:GLY:C	1:A:394:LYS:N	2.46	0.73
1:A:461:SER:OG	2:D:8:SER:HB3	1.88	0.73
1:C:326:VAL:HG21	1:C:380:PRO:HG2	1.69	0.73
2:E:51:TRP:HD1	2:E:60:LYS:NZ	1.85	0.73
1:A:455:SER:O	2:F:41:GLY:HA3	1.88	0.73
1:C:41:VAL:HG23	1:C:143:VAL:CG2	2.17	0.73
1:C:422:ALA:HB1	1:C:498:LEU:HD13	1.68	0.73
1:B:494:VAL:O	1:B:498:LEU:HG	1.88	0.73
1:B:297:LYS:O	1:B:298:LEU:HG	1.86	0.73
1:A:23:VAL:HG13	1:A:25:LEU:HD23	1.70	0.73
1:A:39:PRO:HD3	1:A:300:LEU:HD12	1.71	0.73
1:C:347:VAL:O	1:C:348:ASP:HB2	1.88	0.73
1:A:31:VAL:HB	1:A:43:ILE:HD11	1.70	0.73
1:A:141:LEU:HB2	1:A:165:ALA:HB3	1.71	0.73
1:B:268:ALA:HA	2:E:4:LEU:HD21	1.69	0.73
1:C:332:TYR:O	1:C:371:ASN:HA	1.87	0.73
1:A:1:ILE:HG23	1:A:152:ILE:HG22	1.70	0.73
1:C:312:PHE:O	1:C:396:ILE:HG21	1.88	0.73
1:A:252:ARG:HB2	1:A:252:ARG:CZ	2.19	0.73
1:A:312:PHE:CG	1:A:389:ILE:HB	2.23	0.73
1:B:186:LEU:HD23	1:B:293:LEU:HD11	1.70	0.73
1:A:295:MET:HE2	1:A:295:MET:HA	1.70	0.72
1:B:37:ASP:C	1:B:300:LEU:HD11	2.13	0.72
1:B:40:THR:CG2	1:B:144:HIS:HD2	2.02	0.72
1:B:113:LEU:HD22	1:B:114:VAL:N	2.04	0.72
1:C:196:LEU:HD13	1:C:288:HIS:HB3	1.69	0.72
1:C:34:MET:HE1	1:C:359:ILE:CD1	2.20	0.72
1:C:170:THR:HB	1:C:171:PRO:HD2	1.70	0.72
1:C:300:LEU:HD22	1:C:303:VAL:CG2	2.18	0.72
1:C:445:ILE:HD13	1:C:448:ILE:HD12	1.70	0.72
1:B:345:MET:CE	1:B:380:PRO:HA	2.19	0.72
1:B:442:GLY:HA2	1:B:445:ILE:HG22	1.69	0.72
2:F:56:SER:HB3	2:F:59:GLN:HB2	1.71	0.72
1:A:43:ILE:HG23	1:A:141:LEU:CD2	2.19	0.72
1:A:342:PRO:HG2	1:A:389:ILE:HG13	1.69	0.72
1:C:36:GLN:O	1:C:38:LYS:N	2.23	0.72
1:A:300:LEU:HD12	1:A:300:LEU:N	2.04	0.72
1:C:70:SER:HB2	1:C:115:THR:HA	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:ILE:O	1:C:389:ILE:HD12	1.89	0.72
1:C:319:ALA:O	1:C:326:VAL:HG13	1.90	0.72
1:C:327:THR:HB	1:C:329:GLU:OE2	1.89	0.72
1:B:359:ILE:HB	1:B:377:GLU:HB3	1.70	0.72
1:A:7:SER:O	1:A:8:ASN:HB2	1.89	0.72
1:A:130:ILE:HG21	1:A:198:PHE:HD2	1.54	0.72
1:A:135:LEU:N	1:A:135:LEU:HD23	2.05	0.72
1:B:73:ARG:HG3	1:B:79:GLU:O	1.89	0.72
1:C:100:GLY:HA3	1:C:108:PHE:CD1	2.24	0.72
2:D:55:SER:CA	2:D:60:LYS:HE2	2.15	0.72
1:B:38:LYS:HG3	1:B:298:LEU:CB	2.20	0.71
2:F:9:THR:HG22	2:F:10:ARG:NH2	2.04	0.71
1:A:28:GLY:HA3	2:D:15:ARG:HG3	1.72	0.71
1:C:204:LEU:O	1:C:210:HIS:HB3	1.89	0.71
2:D:71:ALA:HB3	2:D:72:PRO:CD	2.20	0.71
1:C:144:HIS:O	1:C:145:GLY:C	2.34	0.71
1:C:467:LEU:HD13	2:F:69:LEU:HD21	1.72	0.71
1:B:53:MET:HB2	1:B:128:LYS:HD3	1.72	0.71
1:A:85:GLN:HE22	1:A:94:ARG:HH22	1.34	0.71
1:A:144:HIS:ND1	1:A:360:THR:HG22	2.04	0.71
1:A:158:HIS:CB	1:A:166:LYS:HE3	2.12	0.71
1:A:203:TYR:HE2	1:A:277:MET:HE2	1.54	0.71
1:C:92:CYS:HB3	1:C:115:THR:O	1.91	0.71
1:C:284:LEU:HD22	1:C:285:SER:O	1.91	0.71
1:B:23:VAL:CG2	1:B:31:VAL:HG11	2.20	0.71
1:B:181:GLY:C	1:B:183:PHE:N	2.48	0.71
1:A:25:LEU:O	1:A:45:LEU:HB2	1.89	0.71
1:A:426:ASP:C	1:A:428:ALA:H	1.97	0.71
1:C:320:GLU:OE2	1:C:402:ARG:HG3	1.90	0.71
1:A:261:GLN:HE21	1:A:261:GLN:HA	1.55	0.71
1:A:377:GLU:O	1:A:378:LEU:HB2	1.90	0.71
1:C:347:VAL:O	1:C:347:VAL:HG13	1.89	0.71
1:C:384:ASP:O	1:C:385:SER:HB3	1.90	0.71
1:B:12:VAL:HG13	1:B:12:VAL:O	1.89	0.71
1:B:31:VAL:O	1:B:43:ILE:HD12	1.90	0.71
1:B:91:VAL:HG13	1:B:91:VAL:O	1.90	0.71
1:C:426:ASP:HB3	1:C:446:HIS:HB3	1.71	0.71
2:D:1:ALA:HB2	2:F:23:ARG:HD2	1.72	0.71
2:E:6:SER:HB2	2:E:8:SER:HB2	1.73	0.71
2:D:29:LEU:HD23	2:D:29:LEU:O	1.91	0.70
1:B:57:ARG:NH1	1:B:225:TRP:HE1	1.88	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:TYR:HB3	1:B:339:CYS:HA	1.73	0.70
1:B:377:GLU:O	1:B:378:LEU:HD12	1.91	0.70
2:E:28:HIS:O	2:E:32:VAL:HG22	1.91	0.70
1:A:118:LYS:HG2	1:A:119:PHE:N	2.05	0.70
1:A:307:LEU:H	1:A:307:LEU:CD2	2.04	0.70
2:F:71:ALA:HB3	2:F:72:PRO:HD3	1.74	0.70
1:B:357:ARG:HB2	1:B:357:ARG:NH1	2.06	0.70
1:B:316:LYS:HB2	1:B:329:GLU:HB2	1.71	0.70
1:A:150:GLY:HA2	1:A:152:ILE:HG23	1.74	0.70
1:A:299:ARG:HB2	1:A:299:ARG:CZ	2.22	0.70
1:B:38:LYS:HG3	1:B:298:LEU:HB3	1.74	0.70
1:B:432:GLY:HA3	1:B:439:ASN:HD22	1.56	0.70
1:A:27:HIS:CD2	1:A:285:SER:HA	2.27	0.70
1:C:171:PRO:HA	1:C:192:PRO:HB2	1.74	0.70
1:C:460:MET:CE	1:C:468:ILE:HD12	2.19	0.70
1:B:138:ARG:HG2	1:B:138:ARG:O	1.91	0.70
1:A:65:ILE:CG2	1:A:66:SER:N	2.54	0.70
1:A:204:LEU:HD23	1:A:204:LEU:N	2.06	0.70
1:C:39:PRO:HD2	1:C:298:LEU:CD1	2.22	0.70
1:C:300:LEU:HD11	1:C:362:ASN:HB2	1.73	0.70
1:C:329:GLU:HB3	1:C:373:LYS:NZ	2.07	0.70
1:B:187:GLY:O	1:B:293:LEU:HA	1.92	0.70
1:C:475:LEU:CD1	2:D:52:LEU:HD23	2.22	0.69
1:B:4:ILE:H	1:B:151:MET:HE1	1.55	0.69
1:B:197:ASP:O	1:B:199:SER:N	2.24	0.69
1:B:309:THR:HA	1:B:391:VAL:HG22	1.72	0.69
2:E:52:LEU:O	2:E:53:LEU:HD13	1.91	0.69
1:B:357:ARG:HD3	1:B:359:ILE:HD13	1.74	0.69
1:A:360:THR:HG21	1:A:376:LEU:HA	1.75	0.69
1:C:315:THR:CG2	1:C:373:LYS:HE2	2.23	0.69
1:B:473:MET:HE3	1:B:493:GLY:HA2	1.72	0.69
2:F:3:THR:C	2:F:5:PRO:HD2	2.17	0.69
1:A:34:MET:HB3	1:A:40:THR:HG23	1.75	0.69
1:B:286:SER:HB3	2:E:16:SER:CB	2.18	0.69
2:E:46:ALA:O	2:E:49:ILE:HG23	1.92	0.69
1:A:151:MET:O	1:A:151:MET:HG2	1.92	0.69
1:A:169:ILE:HG13	1:A:169:ILE:O	1.90	0.69
1:C:273:LEU:HB2	2:F:12:LEU:CD1	2.23	0.69
2:D:3:THR:OG1	2:F:31:ARG:HD3	1.92	0.69
1:A:299:ARG:HB2	1:A:299:ARG:HH11	1.52	0.69
1:A:341:VAL:HG22	1:A:365:ILE:CG1	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:CYS:O	1:B:9:ARG:NE	2.26	0.69
2:E:70:ILE:C	2:E:72:PRO:HD2	2.16	0.69
2:F:67:ILE:C	2:F:69:LEU:H	2.00	0.69
1:A:175:ARG:HG2	1:A:189:ASP:CB	2.21	0.69
1:B:6:VAL:O	1:B:8:ASN:N	2.26	0.69
1:B:138:ARG:HH11	1:B:138:ARG:CB	2.05	0.69
1:A:6:VAL:HG12	1:A:9:ARG:HB2	1.75	0.69
1:A:56:VAL:HG11	1:A:202:TYR:CE2	2.27	0.69
1:C:454:LYS:O	1:C:458:GLY:HA3	1.92	0.69
2:D:21:GLU:HG3	2:D:22:SER:N	2.08	0.69
1:B:7:SER:H	1:B:322:LEU:HD11	1.57	0.69
1:B:58:SER:HB3	1:B:226:HIS:O	1.92	0.69
1:A:311:ALA:CB	1:A:334:GLY:H	2.05	0.69
1:A:343:ALA:O	1:A:344:GLN:HB3	1.93	0.69
1:A:477:LEU:HD23	1:A:477:LEU:O	1.93	0.69
1:A:191:GLU:HG3	1:A:290:LYS:HB2	1.75	0.69
1:B:38:LYS:HA	1:B:300:LEU:CD1	2.22	0.68
1:B:99:ARG:HH21	1:B:103:ASN:CB	2.06	0.68
1:B:214:HIS:H	2:E:7:HIS:CE1	2.11	0.68
1:C:148:HIS:O	1:C:152:ILE:HG23	1.93	0.68
2:D:67:ILE:CA	2:D:70:ILE:HG22	2.20	0.68
1:B:12:VAL:HG12	1:B:33:VAL:HA	1.76	0.68
1:A:154:ASN:OD1	1:A:156:THR:HG22	1.94	0.68
1:C:135:LEU:O	1:C:171:PRO:HD3	1.93	0.68
1:B:43:ILE:HD12	1:B:43:ILE:H	1.58	0.68
1:B:135:LEU:C	1:B:135:LEU:HD12	2.19	0.68
1:A:360:THR:HG23	1:A:377:GLU:HB2	1.76	0.68
1:C:283:ARG:HB2	1:C:283:ARG:CZ	2.23	0.68
2:D:29:LEU:O	2:D:32:VAL:HG12	1.93	0.68
2:D:55:SER:HA	2:D:60:LYS:CE	2.20	0.68
1:B:343:ALA:CB	1:B:389:ILE:HG22	2.24	0.68
1:B:471:LEU:O	1:B:475:LEU:HG	1.94	0.68
1:C:12:VAL:CG1	1:C:33:VAL:HG13	2.17	0.68
2:D:2:VAL:HG13	2:D:2:VAL:O	1.93	0.68
1:B:57:ARG:NH1	1:B:225:TRP:CD1	2.62	0.68
1:C:12:VAL:HG13	1:C:12:VAL:O	1.93	0.68
1:B:187:GLY:O	1:B:188:LEU:HD23	1.94	0.68
1:A:150:GLY:C	1:A:152:ILE:N	2.42	0.68
1:A:300:LEU:N	1:A:300:LEU:CD1	2.55	0.68
1:A:345:MET:HE3	1:A:381:PRO:HD2	1.76	0.68
1:A:387:ILE:O	1:A:388:VAL:HG13	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:LEU:C	1:C:298:LEU:HD13	2.18	0.68
1:B:221:ILE:CD1	2:E:4:LEU:HA	2.19	0.68
1:B:343:ALA:HB1	1:B:389:ILE:HG22	1.76	0.68
1:A:59:TYR:CE2	1:A:221:ILE:HB	2.27	0.68
2:E:24:GLU:O	2:E:27:LYS:HG2	1.94	0.68
1:C:441:LEU:O	1:C:444:GLY:N	2.25	0.68
1:B:225:TRP:CE3	1:B:225:TRP:C	2.71	0.68
1:B:313:THR:H	1:B:330:VAL:HG13	1.58	0.68
1:C:295:MET:CE	1:C:298:LEU:HB3	2.21	0.67
1:B:32:THR:HA	1:B:42:ASP:CB	2.24	0.67
1:B:100:GLY:CA	1:B:108:PHE:CE1	2.76	0.67
1:B:225:TRP:CE3	1:B:226:HIS:N	2.62	0.67
1:A:138:ARG:HH21	1:A:140:MET:CE	2.07	0.67
1:A:158:HIS:HB3	1:A:166:LYS:CE	2.13	0.67
1:C:141:LEU:O	1:C:164:ARG:HA	1.94	0.67
1:B:93:LYS:HB3	1:B:245:PHE:CD2	2.29	0.67
1:A:157:GLY:C	1:A:159:GLU:N	2.49	0.67
1:A:261:GLN:NE2	1:C:263:GLY:HA3	2.09	0.67
1:C:240:GLU:OE2	1:C:241:ALA:N	2.26	0.67
1:A:423:VAL:C	1:A:425:GLY:H	2.01	0.67
1:C:2:ARG:HH12	1:C:155:ASP:CG	2.02	0.67
1:B:56:VAL:HG11	1:B:202:TYR:CD2	2.30	0.67
1:A:302:GLY:HA3	1:A:305:TYR:HD2	1.58	0.67
1:A:454:LYS:HB2	1:A:454:LYS:NZ	2.10	0.67
1:A:73:ARG:CZ	1:A:77:GLN:HB3	2.23	0.67
1:A:345:MET:O	1:A:354:PRO:HA	1.94	0.67
1:A:497:PHE:C	1:A:499:SER:H	2.03	0.67
1:C:65:ILE:H	1:C:257:VAL:CG1	2.07	0.67
1:C:97:VAL:HG21	1:C:113:LEU:CD2	2.25	0.67
1:B:91:VAL:HG11	1:B:243:VAL:HG21	1.74	0.67
1:C:101:TRP:H	1:C:101:TRP:CD1	2.11	0.67
1:C:161:ASP:HB3	1:C:164:ARG:O	1.95	0.67
1:C:345:MET:CB	1:C:355:VAL:O	2.41	0.67
1:B:58:SER:OG	1:B:124:LYS:HD2	1.95	0.67
1:B:277:MET:HG3	1:B:279:GLY:N	2.09	0.67
1:B:284:LEU:HD12	1:B:285:SER:O	1.95	0.67
1:A:27:HIS:HD2	1:A:285:SER:HA	1.59	0.67
1:C:1:ILE:HD12	1:C:147:GLN:OE1	1.95	0.67
1:C:37:ASP:O	1:C:300:LEU:HB2	1.94	0.67
1:B:75:PRO:HB3	1:B:110:LYS:HB2	1.77	0.67
2:F:9:THR:HG22	2:F:10:ARG:HH22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG12	1:A:144:HIS:H	1.59	0.67
1:C:375:MET:N	1:C:375:MET:SD	2.67	0.67
1:C:426:ASP:CB	1:C:446:HIS:HB2	2.25	0.67
1:B:187:GLY:H	1:B:293:LEU:HD12	1.59	0.67
1:C:245:PHE:HA	1:C:254:THR:O	1.94	0.66
1:B:54:ALA:HB3	1:B:129:SER:HB3	1.77	0.66
1:A:56:VAL:HG23	1:B:78:GLY:CA	2.25	0.66
1:B:180:LEU:HD12	1:B:180:LEU:N	1.99	0.66
1:B:189:ASP:HB2	1:B:292:ARG:HB3	1.77	0.66
1:B:225:TRP:CE3	1:B:226:HIS:HA	2.30	0.66
1:A:73:ARG:HH21	1:A:77:GLN:HB3	1.60	0.66
1:B:186:LEU:HD23	1:B:298:LEU:HD11	1.76	0.66
1:B:227:ALA:C	1:B:229:ALA:H	2.02	0.66
1:A:291:CYS:C	1:A:292:ARG:HD2	2.20	0.66
1:A:459:GLY:HA2	2:D:9:THR:HG23	1.76	0.66
1:C:1:ILE:HD12	1:C:1:ILE:N	2.10	0.66
1:C:138:ARG:HB3	1:C:138:ARG:CZ	2.23	0.66
1:C:179:THR:C	1:C:180:LEU:HD22	2.20	0.66
1:B:56:VAL:HG22	1:B:57:ARG:HG3	1.78	0.66
1:C:392:GLY:O	1:C:395:LYS:HE3	1.95	0.66
1:C:409:LYS:HA	1:C:409:LYS:HZ3	1.61	0.66
1:B:180:LEU:HD11	1:B:186:LEU:HD11	1.76	0.66
1:B:283:ARG:CZ	1:B:283:ARG:HB3	2.24	0.66
1:A:169:ILE:CD1	1:A:190:CYS:HB2	2.25	0.66
1:A:178:ALA:HB1	1:A:180:LEU:HD21	1.76	0.66
1:A:226:HIS:CG	1:A:234:PRO:HB3	2.31	0.66
1:C:70:SER:OG	1:C:253:GLN:NE2	2.28	0.66
1:C:89:GLN:HA	1:C:239:LYS:HZ3	1.61	0.66
1:B:445:ILE:HG23	1:B:446:HIS:N	2.10	0.66
1:A:1:ILE:HG22	1:A:2:ARG:N	2.11	0.66
1:A:493:GLY:O	1:A:496:ILE:HB	1.96	0.66
1:B:20:TRP:CE3	1:B:292:ARG:NH2	2.64	0.66
1:A:359:ILE:CD1	1:A:377:GLU:HG2	2.20	0.66
1:B:38:LYS:CA	1:B:300:LEU:HD11	2.25	0.66
1:B:65:ILE:HD12	1:B:65:ILE:O	1.96	0.66
1:B:190:CYS:C	1:B:192:PRO:HD3	2.20	0.66
2:F:7:HIS:C	2:F:9:THR:H	2.03	0.66
1:A:333:ALA:O	1:A:370:GLU:HA	1.95	0.65
1:A:472:LEU:HD23	1:A:492:GLY:HA2	1.78	0.65
1:C:47:THR:HG23	1:C:283:ARG:HD3	1.77	0.65
1:B:68:MET:HE2	1:B:255:VAL:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:MET:HE3	1:A:17:GLY:O	1.96	0.65
1:A:348:ASP:HB2	1:A:350:GLN:CG	2.26	0.65
1:C:26:GLU:CB	1:C:288:HIS:HA	2.26	0.65
1:B:56:VAL:HG11	1:B:202:TYR:HD2	1.60	0.65
1:B:158:HIS:CB	1:B:164:ARG:HD3	2.26	0.65
1:B:187:GLY:N	1:B:293:LEU:HD12	2.12	0.65
1:B:393:GLU:HG3	1:B:394:LYS:N	2.11	0.65
1:A:266:HIS:O	2:D:20:LEU:HD11	1.96	0.65
1:B:53:MET:HE2	1:B:130:ILE:HG21	1.78	0.65
1:B:281:LYS:NZ	1:B:281:LYS:HB3	2.11	0.65
1:B:74:CYS:HB3	1:B:75:PRO:HD2	1.77	0.65
1:B:137:TYR:CD2	1:B:289:LEU:HD13	2.32	0.65
1:B:479:THR:HG21	1:B:485:SER:OG	1.96	0.65
1:B:159:GLU:HA	1:B:164:ARG:O	1.97	0.65
2:F:4:LEU:HD23	2:F:5:PRO:CD	2.26	0.65
1:A:43:ILE:CG2	1:A:141:LEU:HD21	2.25	0.65
1:A:97:VAL:HG11	1:A:113:LEU:HD13	1.79	0.65
1:B:306:SER:O	1:B:339:CYS:HB2	1.95	0.65
2:F:47:ALA:O	2:F:51:TRP:HB2	1.96	0.65
2:F:56:SER:HB3	2:F:59:GLN:CG	2.27	0.65
1:B:141:LEU:HD12	1:B:165:ALA:O	1.97	0.65
1:B:180:LEU:HD11	1:B:186:LEU:CD1	2.26	0.65
1:C:84:LYS:O	1:C:86:SER:N	2.30	0.65
1:A:58:SER:OG	1:A:126:THR:HG22	1.97	0.65
1:A:265:VAL:CG2	2:D:4:LEU:HD13	2.23	0.65
1:A:305:TYR:HB3	1:A:340:LYS:HG3	1.78	0.65
1:A:365:ILE:HG22	1:A:368:SER:HB2	1.79	0.65
1:C:260:SER:OG	1:C:261:GLN:N	2.27	0.65
1:C:427:THR:HG22	1:C:427:THR:O	1.97	0.65
2:D:29:LEU:HD23	2:D:29:LEU:C	2.22	0.65
1:B:491:LEU:HA	1:B:494:VAL:HG23	1.79	0.65
1:A:156:THR:O	1:A:158:HIS:N	2.29	0.64
1:A:251:LYS:HE2	1:A:252:ARG:HE	1.61	0.64
1:A:470:THR:C	1:A:472:LEU:H	2.05	0.64
2:D:30:ILE:HG13	2:D:31:ARG:N	2.12	0.64
2:E:11:LYS:C	2:E:12:LEU:HD12	2.21	0.64
1:A:27:HIS:NE2	1:A:48:THR:HG22	2.13	0.64
1:A:138:ARG:HH21	1:A:140:MET:HE1	1.61	0.64
1:C:73:ARG:HG2	1:C:79:GLU:N	2.12	0.64
1:C:185:SER:O	1:C:297:LYS:HB2	1.96	0.64
1:B:74:CYS:CB	1:B:75:PRO:HD2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:PRO:HD3	1:B:367:GLU:HG2	1.77	0.64
1:A:63:ALA:HB1	1:A:119:PHE:HE1	1.61	0.64
1:B:474:TRP:HZ2	2:E:58:SER:HB2	1.61	0.64
1:C:334:GLY:CA	1:C:370:GLU:HA	2.28	0.64
1:A:96:LEU:HD12	1:A:96:LEU:H	1.62	0.64
1:C:39:PRO:CG	1:C:300:LEU:HA	2.27	0.64
1:B:56:VAL:O	1:B:227:ALA:HB1	1.96	0.64
1:B:186:LEU:CD2	1:B:293:LEU:HD11	2.28	0.64
1:B:426:ASP:C	1:B:428:ALA:N	2.53	0.64
1:A:225:TRP:NE1	1:A:237:ASN:ND2	2.44	0.64
1:B:345:MET:HG2	1:B:378:LEU:CD2	2.26	0.64
2:F:51:TRP:HA	2:F:60:LYS:HD2	1.80	0.64
1:A:86:SER:OG	1:B:235:HIS:HB2	1.97	0.64
1:C:240:GLU:HA	1:C:243:VAL:HB	1.80	0.64
1:C:357:ARG:HG2	1:C:358:LEU:N	2.12	0.64
1:A:156:THR:O	1:A:157:GLY:C	2.37	0.64
1:B:154:ASN:HB2	1:B:158:HIS:HE1	1.60	0.64
1:B:258:LEU:HD23	1:B:259:GLY:H	1.62	0.64
1:B:472:LEU:HD23	1:B:475:LEU:HD12	1.79	0.64
2:E:65:VAL:HG22	2:E:69:LEU:CD1	2.27	0.64
1:A:18:GLY:O	1:A:19:THR:OG1	2.11	0.64
1:C:27:HIS:HE1	1:C:48:THR:HG22	1.58	0.64
1:A:83:ASP:OD1	1:A:83:ASP:N	2.30	0.64
1:A:131:GLN:C	1:A:133:GLU:H	2.06	0.64
1:A:238:ASN:C	1:A:240:GLU:H	2.04	0.64
1:B:309:THR:HA	1:B:391:VAL:CG2	2.27	0.64
1:A:38:LYS:HE2	1:A:298:LEU:O	1.97	0.63
1:A:312:PHE:CD1	1:A:389:ILE:HB	2.32	0.63
1:C:36:GLN:O	1:C:38:LYS:HG3	1.97	0.63
1:C:63:ALA:HB2	1:C:242:LEU:HD12	1.79	0.63
1:C:70:SER:CB	1:C:115:THR:HA	2.28	0.63
1:C:167:VAL:HG13	1:C:168:GLU:N	2.13	0.63
1:B:429:TRP:HE1	1:B:446:HIS:HD2	1.45	0.63
1:A:45:LEU:HD12	1:A:138:ARG:O	1.97	0.63
2:D:23:ARG:CA	2:D:27:LYS:HE3	2.27	0.63
2:D:71:ALA:HB3	2:D:72:PRO:HD3	1.79	0.63
1:B:349:MET:N	1:B:349:MET:SD	2.72	0.63
1:A:456:LEU:HD13	1:A:457:PHE:CD2	2.33	0.63
1:C:90:TYR:HD1	1:C:90:TYR:H	1.46	0.63
2:D:1:ALA:O	2:D:2:VAL:C	2.42	0.63
1:B:185:SER:C	1:B:186:LEU:HG	2.21	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:HB2	1:A:215:LYS:NZ	2.13	0.63
1:A:248:ALA:HB1	1:A:252:ARG:NH2	2.13	0.63
1:B:360:THR:O	1:B:361:ALA:HB3	1.98	0.63
2:F:27:LYS:O	2:F:29:LEU:N	2.30	0.63
1:A:162:GLU:HG3	1:A:181:GLY:O	1.98	0.63
2:D:60:LYS:HD3	2:D:60:LYS:N	2.12	0.63
1:B:19:THR:CB	1:B:295:MET:H	2.12	0.63
1:B:20:TRP:HE3	1:B:292:ARG:HH21	1.47	0.63
1:B:41:VAL:CG2	1:B:143:VAL:HG22	2.18	0.63
1:C:90:TYR:N	1:C:90:TYR:CD1	2.67	0.63
1:C:445:ILE:HA	1:C:448:ILE:HD12	1.81	0.63
1:B:344:GLN:OE1	1:B:352:LEU:HG	1.98	0.63
2:E:33:GLU:C	2:E:35:TRP:H	2.05	0.63
1:A:115:THR:HG21	1:A:253:GLN:O	1.99	0.63
1:A:330:VAL:HG22	1:A:374:MET:HG3	1.81	0.63
1:B:110:LYS:O	1:B:111:GLY:O	2.17	0.63
1:B:162:GLU:HA	1:B:162:GLU:OE1	1.99	0.63
1:B:489:LEU:O	1:B:489:LEU:HD23	1.98	0.63
2:F:56:SER:O	2:F:60:LYS:HG2	1.98	0.63
1:A:9:ARG:HA	1:A:30:CYS:O	1.99	0.63
1:C:180:LEU:HD23	1:C:184:GLY:O	1.99	0.63
1:B:127:GLY:HA3	1:B:218:PHE:CZ	2.34	0.63
2:F:19:TRP:CG	2:F:20:LEU:N	2.64	0.63
1:A:225:TRP:C	1:A:225:TRP:CD1	2.76	0.62
1:C:40:THR:O	1:C:143:VAL:HG13	1.98	0.62
1:C:305:TYR:HB3	1:C:339:CYS:HA	1.81	0.62
1:C:439:ASN:C	1:C:441:LEU:N	2.47	0.62
2:D:56:SER:HB3	2:D:59:GLN:CG	2.04	0.62
2:D:60:LYS:HD3	2:D:60:LYS:H	1.64	0.62
2:D:69:LEU:O	2:D:69:LEU:HD23	1.99	0.62
2:D:69:LEU:HD22	2:F:70:ILE:HD12	1.81	0.62
1:B:71:ASP:OD2	1:B:80:ALA:HB1	1.99	0.62
1:B:216:GLU:OE1	1:B:216:GLU:HA	1.98	0.62
1:C:63:ALA:HB2	1:C:242:LEU:CD1	2.29	0.62
1:B:32:THR:CB	1:B:42:ASP:HB3	2.29	0.62
1:A:101:TRP:HZ2	1:C:316:LYS:HB2	1.63	0.62
1:B:420:ARG:HB3	1:B:420:ARG:NH1	2.14	0.62
2:F:61:VAL:C	2:F:63:TYR:H	2.06	0.62
1:C:426:ASP:C	1:C:428:ALA:H	2.05	0.62
1:B:169:ILE:HD12	1:B:169:ILE:N	2.15	0.62
1:B:302:GLY:O	1:B:304:SER:N	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:THR:HG21	1:B:485:SER:HB2	1.81	0.62
1:A:225:TRP:CD1	1:A:237:ASN:HD22	2.16	0.62
1:A:321:THR:OG1	1:A:325:THR:OG1	2.17	0.62
1:A:355:VAL:O	1:A:355:VAL:HG12	1.99	0.62
1:C:93:LYS:O	1:C:114:VAL:HA	2.00	0.62
1:C:213:VAL:HG11	1:C:217:TRP:CE3	2.34	0.62
2:D:21:GLU:O	2:D:23:ARG:N	2.33	0.62
1:B:36:GLN:O	1:B:300:LEU:HD21	1.98	0.62
1:B:101:TRP:CD1	1:B:108:PHE:CE2	2.88	0.62
1:B:417:GLY:O	1:B:421:MET:HB2	2.00	0.62
2:E:70:ILE:HG13	2:E:75:SER:C	2.25	0.62
1:A:294:LYS:HB3	1:A:296:ASP:OD1	1.99	0.62
1:A:290:LYS:HE3	1:A:292:ARG:HH12	1.64	0.62
1:A:475:LEU:CD1	2:F:53:LEU:HB2	2.29	0.62
1:C:240:GLU:H	1:C:240:GLU:CD	2.07	0.62
1:B:415:VAL:HG12	1:B:419:LYS:HE3	1.80	0.62
1:B:487:MET:HA	1:B:490:ALA:HB3	1.80	0.62
1:A:150:GLY:O	1:A:152:ILE:N	2.32	0.62
2:E:54:GLY:O	2:E:56:SER:N	2.33	0.62
1:A:72:SER:HB2	1:A:99:ARG:HH11	1.65	0.62
1:C:56:VAL:HG12	1:C:127:GLY:O	1.99	0.62
1:C:70:SER:CB	1:C:253:GLN:HE22	2.12	0.62
2:D:25:TYR:HD1	2:D:25:TYR:C	2.07	0.62
1:B:139:ILE:HD13	1:B:167:VAL:HG23	1.80	0.62
1:C:1:ILE:HG21	1:C:4:ILE:HG23	1.82	0.62
1:C:21:VAL:HA	1:C:433:SER:HB2	1.80	0.62
1:C:211:TRP:HE1	1:C:269:LEU:CD1	1.97	0.62
1:A:2:ARG:HB2	1:A:142:SER:HB2	1.79	0.61
1:B:1:ILE:HD12	1:B:2:ARG:H	1.64	0.61
1:B:55:GLU:CD	1:B:55:GLU:N	2.58	0.61
2:E:42:PHE:O	2:E:46:ALA:CB	2.48	0.61
1:A:3:CYS:O	1:A:9:ARG:HD3	2.00	0.61
1:A:356:GLY:O	1:A:357:ARG:CB	2.48	0.61
2:D:12:LEU:H	2:D:12:LEU:CD1	2.12	0.61
1:B:6:VAL:C	1:B:8:ASN:N	2.57	0.61
1:B:137:TYR:HB2	1:B:169:ILE:CD1	2.31	0.61
1:B:201:LEU:HD12	1:B:212:LEU:HB3	1.82	0.61
2:D:12:LEU:HD12	2:D:12:LEU:N	2.15	0.61
1:B:93:LYS:HB3	1:B:245:PHE:CE2	2.34	0.61
1:B:238:ASN:O	1:B:239:LYS:CB	2.49	0.61
2:F:50:ALA:HB2	2:F:67:ILE:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:THR:HG22	1:A:253:GLN:HE22	1.64	0.61
1:C:273:LEU:HB2	2:F:12:LEU:HD11	1.82	0.61
1:C:345:MET:HE1	1:C:378:LEU:HB3	1.83	0.61
1:B:73:ARG:HD2	1:B:77:GLN:HG3	1.83	0.61
1:B:82:LEU:O	1:B:84:LYS:N	2.32	0.61
1:B:261:GLN:OE1	1:B:261:GLN:HA	1.98	0.61
1:B:409:LYS:NZ	1:B:413:ALA:HB2	2.15	0.61
1:A:49:THR:HG23	1:A:136:GLU:HG3	1.80	0.61
1:A:348:ASP:HB2	1:A:350:GLN:HG2	1.82	0.61
1:C:178:ALA:O	1:C:185:SER:CB	2.48	0.61
1:B:127:GLY:HA2	1:B:204:LEU:HD12	1.82	0.61
1:A:1:ILE:N	1:A:144:HIS:NE2	2.48	0.61
1:A:34:MET:SD	1:A:34:MET:N	2.74	0.61
1:A:199:SER:O	1:A:200:ASP:HB2	2.00	0.61
1:C:308:CYS:HB3	1:C:332:TYR:HE2	1.66	0.61
1:B:45:LEU:HA	1:B:139:ILE:CG2	2.30	0.61
1:B:137:TYR:HB2	1:B:169:ILE:HD11	1.83	0.61
1:B:185:SER:O	1:B:186:LEU:HG	2.01	0.61
1:B:415:VAL:C	1:B:417:GLY:H	2.07	0.61
1:A:321:THR:HG1	1:A:325:THR:HG1	1.49	0.61
1:A:331:GLN:HG2	1:A:372:SER:O	2.01	0.61
1:C:164:ARG:HG2	1:C:164:ARG:NH1	2.15	0.61
1:B:60:CYS:HB3	1:B:224:PRO:CG	2.14	0.61
1:B:130:ILE:HG13	1:B:130:ILE:O	2.00	0.61
1:B:265:VAL:O	1:B:269:LEU:HB2	2.00	0.61
1:C:113:LEU:HD11	1:C:253:GLN:NE2	2.16	0.61
1:C:277:MET:HA	1:C:282:GLY:HA2	1.83	0.61
1:C:330:VAL:HG23	1:C:374:MET:CE	2.28	0.61
1:C:338:PRO:HA	1:C:365:ILE:O	2.00	0.61
1:C:409:LYS:HA	1:C:409:LYS:NZ	2.15	0.61
1:C:421:MET:C	1:C:421:MET:SD	2.84	0.61
1:C:428:ALA:O	1:C:430:ASP:N	2.33	0.61
2:D:9:THR:HG22	2:D:10:ARG:HG2	1.82	0.61
1:B:415:VAL:HA	1:B:418:ALA:CB	2.30	0.61
1:A:324:GLY:CA	1:A:402:ARG:HH22	2.13	0.61
1:A:348:ASP:C	1:A:350:GLN:H	2.08	0.61
1:B:95:THR:O	1:B:112:SER:HA	2.01	0.61
1:C:90:TYR:CZ	1:C:118:LYS:HG3	2.35	0.61
1:B:225:TRP:CE3	1:B:226:HIS:CA	2.83	0.61
1:B:341:VAL:HG23	1:B:363:PRO:HB2	1.83	0.61
1:A:135:LEU:HD23	1:A:135:LEU:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:LEU:HD23	2:F:62:ILE:HD11	1.82	0.60
2:D:25:TYR:C	2:D:25:TYR:CD1	2.78	0.60
2:E:4:LEU:C	2:E:4:LEU:CD2	2.73	0.60
1:A:48:THR:HG23	1:A:284:LEU:HG	1.83	0.60
1:A:235:HIS:HD2	1:B:86:SER:HA	1.65	0.60
1:C:47:THR:HB	1:C:138:ARG:HB2	1.81	0.60
1:A:423:VAL:O	1:A:424:LEU:HB2	2.00	0.60
1:C:131:GLN:O	1:C:133:GLU:O	2.19	0.60
1:C:286:SER:HB3	2:F:16:SER:HB2	1.83	0.60
1:C:295:MET:HE1	1:C:298:LEU:CB	2.26	0.60
1:B:45:LEU:HA	1:B:139:ILE:HG22	1.83	0.60
1:B:137:TYR:HE2	1:B:289:LEU:HD13	1.66	0.60
1:B:366:THR:O	1:B:368:SER:N	2.34	0.60
1:A:143:VAL:HG11	1:A:183:PHE:CD2	2.36	0.60
1:A:228:GLY:HA3	1:B:73:ARG:HH12	1.66	0.60
1:A:338:PRO:HA	1:A:365:ILE:O	2.01	0.60
1:A:376:LEU:HD12	1:A:376:LEU:O	2.02	0.60
1:B:341:VAL:CG2	1:B:363:PRO:HB2	2.32	0.60
1:B:382:PHE:N	1:B:382:PHE:CD1	2.69	0.60
1:A:382:PHE:CD2	1:A:406:THR:HA	2.37	0.60
1:C:329:GLU:CG	1:C:375:MET:HB3	2.31	0.60
1:C:461:SER:O	1:C:464:SER:OG	2.15	0.60
2:D:47:ALA:HA	2:D:64:LEU:HD23	1.84	0.60
1:B:75:PRO:HB3	1:B:110:LYS:CB	2.32	0.60
1:B:181:GLY:O	1:B:183:PHE:N	2.32	0.60
1:B:216:GLU:O	1:B:218:PHE:N	2.33	0.60
2:E:56:SER:C	2:E:58:SER:H	2.09	0.60
1:A:1:ILE:HG12	1:A:147:GLN:CB	2.32	0.60
1:A:2:ARG:NH1	1:A:140:MET:HG3	2.16	0.60
1:A:238:ASN:O	1:A:240:GLU:N	2.35	0.60
1:A:244:GLU:O	1:A:255:VAL:HA	2.01	0.60
1:C:20:TRP:CD1	1:C:20:TRP:O	2.54	0.60
1:C:175:ARG:HG2	1:C:189:ASP:OD1	2.01	0.60
2:D:3:THR:O	2:D:4:LEU:C	2.45	0.60
2:D:72:PRO:O	2:D:73:ALA:HB3	2.01	0.60
1:B:4:ILE:HD11	1:B:144:HIS:HE1	1.67	0.60
1:B:22:ASP:HB2	1:B:433:SER:HA	1.82	0.60
1:B:196:LEU:HD21	1:B:287:GLY:HA2	1.84	0.60
1:B:277:MET:HG3	1:B:279:GLY:H	1.66	0.60
2:F:54:GLY:O	2:F:59:GLN:NE2	2.35	0.60
1:A:150:GLY:CA	1:A:152:ILE:HD13	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ASN:HB2	3:C:601:NAG:C8	2.30	0.60
1:C:210:HIS:HD2	1:C:277:MET:H	1.47	0.60
1:C:336:ASP:C	1:C:336:ASP:OD1	2.45	0.60
1:B:2:ARG:HH12	1:B:140:MET:HB3	1.66	0.60
1:B:107:LEU:H	1:B:107:LEU:CD1	2.13	0.60
1:B:348:ASP:HB2	1:B:349:MET:HE2	1.84	0.60
2:F:29:LEU:O	2:F:31:ARG:N	2.35	0.60
1:A:1:ILE:HD13	1:A:144:HIS:CA	2.29	0.60
1:A:21:VAL:O	1:A:21:VAL:HG13	2.01	0.60
1:A:409:LYS:HB3	1:A:409:LYS:HZ2	1.65	0.60
1:C:375:MET:HE3	1:C:375:MET:N	2.16	0.60
1:B:149:SER:C	1:B:151:MET:H	2.08	0.60
1:B:272:ALA:HB2	2:E:18:THR:CG2	2.27	0.60
1:A:411:PHE:O	1:A:415:VAL:HG22	2.02	0.60
1:C:15:MET:SD	1:C:36:GLN:CB	2.90	0.60
1:C:255:VAL:O	1:C:255:VAL:HG12	2.02	0.60
1:C:302:GLY:CA	1:C:305:TYR:CD2	2.85	0.60
1:C:396:ILE:HD12	1:C:397:THR:H	1.65	0.60
1:B:446:HIS:CG	1:B:446:HIS:O	2.55	0.60
1:B:491:LEU:HD12	1:B:494:VAL:HG21	1.84	0.60
1:A:65:ILE:HG23	1:A:66:SER:H	1.66	0.59
1:A:457:PHE:O	1:A:460:MET:HB2	2.02	0.59
1:C:462:TRP:CD1	1:C:463:PHE:N	2.70	0.59
1:B:191:GLU:O	1:B:193:ARG:N	2.28	0.59
2:E:53:LEU:C	2:E:55:SER:H	2.10	0.59
1:A:349:MET:O	1:A:349:MET:SD	2.60	0.59
1:C:1:ILE:O	1:C:2:ARG:HB3	2.03	0.59
1:C:61:TYR:HE1	1:C:123:LYS:HE2	1.66	0.59
1:C:70:SER:HA	1:C:82:LEU:HD11	1.84	0.59
1:B:23:VAL:HG21	1:B:31:VAL:HG21	1.82	0.59
1:B:385:SER:C	1:B:386:TYR:CD2	2.80	0.59
1:A:261:GLN:OE1	2:D:2:VAL:HG21	2.02	0.59
1:C:1:ILE:N	1:C:1:ILE:CD1	2.65	0.59
1:C:373:LYS:NZ	1:C:373:LYS:HB3	2.16	0.59
2:D:66:MET:HA	2:D:66:MET:CE	2.32	0.59
1:B:23:VAL:CG2	1:B:31:VAL:HG21	2.33	0.59
1:A:418:ALA:HA	1:A:421:MET:HB2	1.84	0.59
1:B:160:THR:O	1:B:160:THR:HG22	2.03	0.59
1:B:171:PRO:CA	1:B:192:PRO:HB2	2.30	0.59
1:A:43:ILE:HD12	1:A:43:ILE:O	2.02	0.59
1:A:90:TYR:N	1:A:239:LYS:NZ	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:PRO:O	1:A:390:GLY:N	2.33	0.59
1:B:286:SER:HB2	2:E:14:THR:HG21	1.85	0.59
1:B:345:MET:CG	1:B:378:LEU:HD23	2.31	0.59
1:B:374:MET:HE2	1:B:376:LEU:HD11	1.84	0.59
1:B:415:VAL:C	1:B:417:GLY:N	2.60	0.59
1:A:261:GLN:HE21	1:A:261:GLN:N	2.01	0.59
1:A:419:LYS:O	1:A:423:VAL:HG12	2.02	0.59
1:C:72:SER:HB3	1:C:113:LEU:HD13	1.85	0.59
1:B:49:THR:HG22	1:B:283:ARG:CG	2.32	0.59
1:B:66:SER:HG	1:B:118:LYS:HB3	1.68	0.59
2:F:4:LEU:N	2:F:5:PRO:HD2	2.17	0.59
1:C:307:LEU:N	1:C:307:LEU:HD12	2.17	0.59
1:B:1:ILE:CD1	1:B:142:SER:OG	2.49	0.59
1:B:109:GLY:O	1:B:110:LYS:HB2	2.02	0.59
2:E:12:LEU:HD12	2:E:12:LEU:N	2.18	0.59
1:A:307:LEU:N	1:A:307:LEU:CD2	2.64	0.59
1:A:464:SER:O	1:A:465:GLN:C	2.45	0.59
1:C:125:MET:HB3	1:C:206:MET:HB3	1.85	0.59
1:B:258:LEU:HD23	1:B:259:GLY:N	2.17	0.59
2:F:50:ALA:HB1	2:F:63:TYR:HB3	1.84	0.59
1:A:416:ARG:C	1:A:418:ALA:H	2.11	0.59
2:D:19:TRP:C	2:D:21:GLU:H	2.11	0.59
1:B:46:VAL:HG13	1:B:47:THR:H	1.68	0.59
1:A:265:VAL:C	1:A:267:THR:H	2.11	0.59
1:B:415:VAL:HA	1:B:418:ALA:HB3	1.85	0.59
1:A:233:THR:O	1:A:234:PRO:C	2.45	0.58
1:A:382:PHE:CE2	1:A:406:THR:HA	2.38	0.58
1:C:268:ALA:HB1	2:F:5:PRO:O	2.03	0.58
1:C:407:ILE:HG22	1:C:407:ILE:O	2.02	0.58
1:C:443:LYS:O	1:C:443:LYS:HG2	2.02	0.58
2:D:27:LYS:HA	2:D:30:ILE:HG12	1.85	0.58
1:B:190:CYS:O	1:B:192:PRO:HD3	2.03	0.58
1:C:22:ASP:HA	1:C:292:ARG:HG2	1.85	0.58
1:C:496:ILE:O	1:C:500:THR:OG1	2.19	0.58
1:B:447:GLN:C	1:B:449:PHE:H	2.11	0.58
2:F:56:SER:HB3	2:F:59:GLN:CB	2.33	0.58
1:A:220:ASP:OD2	2:F:38:ARG:HD2	2.03	0.58
1:C:65:ILE:H	1:C:257:VAL:HG11	1.67	0.58
1:C:127:GLY:O	1:C:128:LYS:C	2.45	0.58
1:C:180:LEU:CB	1:C:183:PHE:HB2	2.33	0.58
1:C:374:MET:HE2	1:C:376:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:ARG:O	1:C:420:ARG:HG3	2.03	0.58
1:B:5:GLY:C	1:B:7:SER:H	2.11	0.58
1:B:12:VAL:CG1	1:B:12:VAL:O	2.52	0.58
1:A:39:PRO:HG3	1:A:300:LEU:HA	1.85	0.58
1:C:334:GLY:HA2	1:C:370:GLU:HA	1.85	0.58
1:B:137:TYR:HD2	1:B:289:LEU:CD2	2.12	0.58
1:B:151:MET:HG2	1:B:152:ILE:HG12	1.85	0.58
1:B:303:VAL:O	1:B:303:VAL:HG12	2.02	0.58
2:E:21:GLU:O	2:E:24:GLU:CB	2.52	0.58
2:F:7:HIS:C	2:F:9:THR:N	2.59	0.58
1:A:96:LEU:HD12	1:A:96:LEU:N	2.17	0.58
1:C:65:ILE:CD1	1:C:257:VAL:HG12	2.31	0.58
1:B:170:THR:O	1:B:192:PRO:HG2	2.03	0.58
1:B:322:LEU:O	1:B:323:HIS:CD2	2.56	0.58
1:C:214:HIS:NE2	1:C:216:GLU:HG3	2.19	0.58
1:C:262:GLU:O	1:C:263:GLY:C	2.47	0.58
1:C:262:GLU:OE1	1:C:262:GLU:N	2.36	0.58
2:D:26:THR:O	2:D:29:LEU:HB3	2.02	0.58
2:D:27:LYS:HB3	2:F:2:VAL:HG21	1.84	0.58
1:A:63:ALA:HB1	1:A:119:PHE:CE1	2.38	0.58
1:A:305:TYR:HE1	1:A:338:PRO:CG	2.16	0.58
1:A:313:THR:HG23	1:A:313:THR:O	2.04	0.58
1:C:355:VAL:HG12	1:C:356:GLY:N	2.18	0.58
1:B:38:LYS:N	1:B:300:LEU:HD11	2.19	0.58
1:B:73:ARG:HH11	1:B:77:GLN:HG3	1.67	0.58
1:B:272:ALA:CA	2:E:18:THR:HG22	2.34	0.58
1:B:314:PHE:HA	1:B:330:VAL:HG22	1.86	0.58
1:B:358:LEU:O	1:B:359:ILE:C	2.44	0.58
1:B:360:THR:HG21	1:B:363:PRO:HB3	1.86	0.58
2:E:26:THR:O	2:E:30:ILE:HG13	2.04	0.58
1:A:107:LEU:N	1:A:107:LEU:HD23	2.17	0.58
1:C:389:ILE:HD11	1:C:396:ILE:O	2.04	0.58
1:C:423:VAL:HG23	1:C:502:VAL:HG11	1.86	0.58
1:B:1:ILE:CG2	1:B:147:GLN:HB2	2.23	0.58
1:B:31:VAL:HG13	1:B:43:ILE:CD1	2.34	0.58
1:B:38:LYS:CG	1:B:39:PRO:HD2	2.32	0.58
1:B:268:ALA:HB2	2:E:4:LEU:HD11	1.85	0.58
1:A:383:GLY:O	1:A:401:HIS:ND1	2.36	0.58
1:C:39:PRO:CG	1:C:183:PHE:HE2	2.15	0.58
1:C:154:ASN:CA	3:C:601:NAG:H82	2.34	0.58
1:C:257:VAL:O	1:C:258:LEU:CB	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:LEU:HD12	1:C:307:LEU:H	1.68	0.58
2:D:10:ARG:HH21	2:D:10:ARG:CG	2.17	0.58
1:B:202:TYR:CE1	1:B:215:LYS:HB2	2.38	0.58
1:C:211:TRP:HB3	1:C:274:GLU:HA	1.85	0.58
1:C:301:LYS:NZ	1:C:301:LYS:HB3	2.18	0.58
1:B:4:ILE:N	1:B:151:MET:HE1	2.19	0.58
1:B:38:LYS:HG2	1:B:39:PRO:N	2.18	0.58
1:B:74:CYS:C	1:B:76:THR:H	2.11	0.58
1:A:156:THR:C	1:A:158:HIS:N	2.61	0.57
1:B:375:MET:O	1:B:376:LEU:HG	2.04	0.57
1:C:395:LYS:O	1:C:395:LYS:HD3	2.04	0.57
1:C:445:ILE:HA	1:C:448:ILE:CD1	2.34	0.57
2:D:46:ALA:O	2:D:49:ILE:HG12	2.03	0.57
2:E:14:THR:HG23	2:E:16:SER:O	2.04	0.57
1:A:331:GLN:HA	1:A:373:LYS:HA	1.86	0.57
1:C:151:MET:HE2	3:C:601:NAG:H4	1.85	0.57
1:C:213:VAL:HG12	1:C:214:HIS:N	2.18	0.57
1:B:100:GLY:O	1:B:105:CYS:HB2	2.04	0.57
1:B:261:GLN:HE21	2:E:1:ALA:H1	1.52	0.57
1:B:332:TYR:O	1:B:333:ALA:C	2.48	0.57
2:F:27:LYS:CG	2:F:28:HIS:H	2.16	0.57
1:A:246:LYS:O	1:A:253:GLN:HA	2.03	0.57
1:C:101:TRP:CD1	1:C:101:TRP:N	2.70	0.57
1:C:164:ARG:O	1:C:164:ARG:HG3	2.04	0.57
1:C:171:PRO:HB2	1:C:193:ARG:HH11	1.69	0.57
1:C:340:LYS:HG2	1:C:341:VAL:N	2.18	0.57
1:B:61:TYR:CZ	1:B:206:MET:HE3	2.39	0.57
1:B:113:LEU:HD13	1:B:113:LEU:C	2.29	0.57
2:E:51:TRP:HA	2:E:60:LYS:HE3	1.86	0.57
2:E:65:VAL:HG22	2:E:69:LEU:HG	1.86	0.57
1:A:10:ASP:O	1:A:31:VAL:HG13	2.05	0.57
1:A:125:MET:SD	1:A:206:MET:HE3	2.44	0.57
1:C:65:ILE:CD1	1:C:243:VAL:HG22	2.20	0.57
1:C:469:GLY:O	1:C:472:LEU:HB2	2.04	0.57
1:B:137:TYR:CE2	1:B:289:LEU:HB2	2.38	0.57
1:B:351:THR:O	1:B:353:THR:N	2.35	0.57
1:A:24:VAL:HG11	1:A:424:LEU:HD21	1.85	0.57
1:A:327:THR:HG21	1:C:108:PHE:HE2	1.70	0.57
1:A:479:THR:CG2	1:A:480:LYS:H	2.03	0.57
1:B:73:ARG:HB3	1:B:77:GLN:NE2	2.19	0.57
1:B:101:TRP:CD1	1:B:108:PHE:CD2	2.92	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:THR:O	1:B:310:ALA:HB2	2.04	0.57
1:A:314:PHE:CD1	1:A:314:PHE:N	2.72	0.57
1:C:95:THR:O	1:C:96:LEU:HD23	2.04	0.57
1:C:462:TRP:CE3	1:C:499:SER:HB2	2.39	0.57
1:B:23:VAL:HG21	1:B:31:VAL:CG1	2.32	0.57
1:B:205:THR:HG23	1:B:210:HIS:HD2	1.70	0.57
1:B:332:TYR:CD1	1:B:333:ALA:N	2.73	0.57
1:A:216:GLU:HB3	2:F:38:ARG:HD3	1.86	0.57
1:C:26:GLU:HG2	1:C:28:GLY:H	1.68	0.57
1:B:241:ALA:O	1:B:242:LEU:HG	2.05	0.57
2:E:28:HIS:H	2:E:28:HIS:CD2	2.21	0.57
1:B:225:TRP:CB	1:B:237:ASN:HD22	2.18	0.57
1:B:457:PHE:CD2	1:B:495:LEU:HD21	2.40	0.57
1:A:74:CYS:C	1:A:76:THR:H	2.13	0.57
1:A:6:VAL:CG1	1:A:9:ARG:HB2	2.35	0.56
2:D:1:ALA:HB1	2:F:23:ARG:HD2	1.84	0.56
2:D:67:ILE:HD12	2:D:70:ILE:CG2	2.34	0.56
1:B:39:PRO:HG3	1:B:183:PHE:HD1	1.68	0.56
1:B:52:ASN:C	1:B:53:MET:HG2	2.30	0.56
1:B:95:THR:HG22	1:B:96:LEU:HD23	1.87	0.56
1:B:99:ARG:NH2	1:B:105:CYS:SG	2.78	0.56
2:E:62:ILE:O	2:E:65:VAL:N	2.37	0.56
1:A:85:GLN:NE2	1:A:94:ARG:HH22	2.01	0.56
1:A:101:TRP:CZ2	1:C:316:LYS:HB2	2.39	0.56
1:C:19:THR:HG22	1:C:19:THR:O	2.04	0.56
1:B:11:PHE:HA	1:B:32:THR:HG22	1.86	0.56
1:B:246:LYS:O	1:B:254:THR:CG2	2.53	0.56
1:B:442:GLY:C	1:B:444:GLY:N	2.62	0.56
1:A:44:GLU:CG	1:A:46:VAL:HG23	2.34	0.56
1:A:55:GLU:HA	1:A:128:LYS:HA	1.86	0.56
1:C:33:VAL:O	1:C:40:THR:HA	2.05	0.56
1:C:251:LYS:HG3	1:C:251:LYS:O	2.04	0.56
1:C:276:GLU:HG2	1:C:276:GLU:O	2.05	0.56
1:C:315:THR:HG21	1:C:373:LYS:CE	2.31	0.56
1:C:467:LEU:HD13	2:F:69:LEU:CD2	2.35	0.56
1:B:39:PRO:HG3	1:B:183:PHE:CD1	2.40	0.56
1:B:62:GLU:HA	1:B:260:SER:HA	1.86	0.56
1:B:133:GLU:O	1:B:134:ASN:CB	2.53	0.56
1:B:135:LEU:HD12	1:B:136:GLU:N	2.19	0.56
1:B:335:THR:O	1:B:335:THR:HG22	2.05	0.56
1:B:345:MET:HE1	1:B:381:PRO:CD	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ILE:CA	1:B:374:MET:SD	2.94	0.56
1:A:2:ARG:HB3	1:A:42:ASP:HB3	1.87	0.56
1:A:364:VAL:HG12	1:A:365:ILE:N	2.20	0.56
1:A:467:LEU:C	1:A:469:GLY:H	2.12	0.56
1:B:418:ALA:HA	1:B:421:MET:HE3	1.86	0.56
1:A:182:GLY:O	1:A:301:LYS:HA	2.05	0.56
1:C:212:LEU:HD13	1:C:284:LEU:HD23	1.85	0.56
1:B:63:ALA:HB2	1:B:242:LEU:HD22	1.88	0.56
1:B:100:GLY:HA3	1:B:108:PHE:CZ	2.39	0.56
1:A:193:ARG:NH1	1:A:193:ARG:HB2	2.20	0.56
1:A:366:THR:O	1:A:367:GLU:HG3	2.05	0.56
1:A:387:ILE:C	1:A:388:VAL:HG22	2.31	0.56
1:C:148:HIS:CB	1:C:151:MET:HB3	2.36	0.56
2:D:41:GLY:O	2:D:43:ALA:N	2.39	0.56
1:B:21:VAL:CG1	1:B:293:LEU:CB	2.75	0.56
1:B:53:MET:HB3	1:B:130:ILE:HG22	1.88	0.56
1:B:214:HIS:CE1	1:B:216:GLU:HB2	2.40	0.56
1:B:364:VAL:C	1:B:374:MET:SD	2.88	0.56
1:A:329:GLU:HB2	1:C:101:TRP:HZ3	1.69	0.56
1:A:366:THR:C	1:A:367:GLU:HG3	2.30	0.56
1:C:11:PHE:CD1	1:C:32:THR:OG1	2.58	0.56
1:C:315:THR:OG1	1:C:373:LYS:HE3	2.06	0.56
1:A:56:VAL:HG22	1:A:57:ARG:HG3	1.88	0.56
1:A:51:SER:HB2	1:A:134:ASN:HB3	1.88	0.56
1:A:209:LYS:HB2	1:A:211:TRP:CH2	2.41	0.56
1:C:469:GLY:HA2	1:C:472:LEU:HD12	1.88	0.56
2:D:72:PRO:C	2:D:74:TYR:H	2.14	0.56
1:B:24:VAL:HG11	1:B:424:LEU:HD21	1.86	0.56
1:B:27:HIS:HB3	1:B:287:GLY:H	1.70	0.56
1:B:247:ASP:HA	1:B:253:GLN:HA	1.87	0.56
1:A:65:ILE:HG23	1:A:66:SER:N	2.20	0.56
1:A:466:ILE:O	1:A:470:THR:N	2.39	0.56
1:C:9:ARG:HA	1:C:30:CYS:O	2.06	0.56
1:C:222:PRO:O	1:C:223:LEU:HD23	2.05	0.56
1:C:302:GLY:HA2	1:C:305:TYR:CE2	2.41	0.56
1:C:358:LEU:HG	1:C:360:THR:O	2.06	0.56
2:D:19:TRP:O	2:D:21:GLU:N	2.40	0.56
1:A:150:GLY:O	1:A:152:ILE:HD13	2.06	0.55
1:A:470:THR:C	1:A:472:LEU:N	2.64	0.55
1:C:315:THR:CG2	1:C:331:GLN:HG2	2.36	0.55
1:B:44:GLU:O	1:B:46:VAL:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:LYS:CG	2:F:28:HIS:N	2.69	0.55
1:A:82:LEU:O	1:A:85:GLN:HG3	2.05	0.55
1:C:9:ARG:NH1	1:C:32:THR:HG21	2.16	0.55
1:C:58:SER:HB2	1:C:226:HIS:HB3	1.88	0.55
1:C:207:ASN:O	1:C:208:ASN:HB2	2.06	0.55
1:B:72:SER:OG	1:B:99:ARG:NH1	2.40	0.55
1:B:222:PRO:C	1:B:223:LEU:CD1	2.80	0.55
1:B:244:GLU:HB3	1:B:256:VAL:HG23	1.88	0.55
1:B:429:TRP:NE1	1:B:446:HIS:HD2	2.04	0.55
1:A:261:GLN:HA	1:A:261:GLN:NE2	2.19	0.55
1:C:41:VAL:CG2	1:C:143:VAL:HG22	2.33	0.55
1:B:152:ILE:HG22	1:B:153:VAL:N	2.21	0.55
1:A:65:ILE:CD1	1:A:257:VAL:HG22	2.34	0.55
1:C:32:THR:HG22	1:C:42:ASP:OD2	2.06	0.55
1:B:99:ARG:NH2	1:B:103:ASN:HD22	2.03	0.55
1:B:345:MET:HE1	1:B:381:PRO:HD2	1.89	0.55
1:B:345:MET:HB3	1:B:387:ILE:HA	1.88	0.55
1:B:459:GLY:H	1:B:460:MET:HE3	1.71	0.55
1:A:91:VAL:HG22	1:A:239:LYS:HE3	1.89	0.55
1:A:163:ASN:O	1:A:164:ARG:HD2	2.06	0.55
1:A:360:THR:HG23	1:A:377:GLU:H	1.70	0.55
1:A:370:GLU:O	1:A:371:ASN:HB2	2.06	0.55
1:C:217:TRP:CE2	2:F:5:PRO:HB2	2.42	0.55
2:D:1:ALA:H2	2:F:27:LYS:HD3	1.68	0.55
1:B:483:SER:C	1:B:485:SER:H	2.15	0.55
2:E:19:TRP:CD1	2:E:20:LEU:HG	2.41	0.55
1:A:225:TRP:CD1	1:A:226:HIS:N	2.75	0.55
1:A:232:GLY:O	1:A:233:THR:C	2.50	0.55
1:A:246:LYS:HE2	2:F:17:GLN:HB3	1.88	0.55
1:C:34:MET:CE	1:C:359:ILE:HD12	2.30	0.55
2:D:32:VAL:O	2:D:32:VAL:HG22	2.06	0.55
1:B:38:LYS:HE3	1:B:39:PRO:O	2.07	0.55
1:B:484:ILE:O	1:B:484:ILE:HG22	2.07	0.55
1:A:49:THR:CG2	1:A:136:GLU:HG3	2.37	0.55
1:A:366:THR:C	1:A:368:SER:N	2.63	0.55
1:C:114:VAL:O	1:C:114:VAL:CG1	2.55	0.55
1:C:179:THR:O	1:C:180:LEU:HD13	2.07	0.55
1:C:261:GLN:O	1:C:265:VAL:HG22	2.07	0.55
1:C:456:LEU:HB3	1:C:457:PHE:CD1	2.42	0.55
1:B:11:PHE:N	1:B:11:PHE:CD1	2.75	0.55
1:B:38:LYS:C	1:B:39:PRO:O	2.48	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:LEU:HD12	1:B:492:GLY:HA2	1.88	0.55
1:A:237:ASN:O	1:A:238:ASN:HB2	2.06	0.55
1:C:265:VAL:O	1:C:266:HIS:C	2.49	0.55
1:B:148:HIS:C	1:B:150:GLY:N	2.60	0.55
1:B:338:PRO:HG3	1:B:367:GLU:HG2	1.89	0.55
1:B:389:ILE:HG13	1:B:389:ILE:O	2.07	0.55
1:B:472:LEU:HA	1:B:475:LEU:HG	1.89	0.55
1:A:19:THR:O	1:A:294:LYS:HA	2.06	0.55
1:A:31:VAL:O	1:A:43:ILE:HD12	2.07	0.55
1:A:132:PRO:O	1:A:135:LEU:HD21	2.07	0.55
1:C:40:THR:HG21	1:C:360:THR:HA	1.87	0.55
1:B:12:VAL:HG12	1:B:33:VAL:HG12	1.86	0.55
1:B:37:ASP:O	1:B:300:LEU:HD11	2.07	0.55
1:B:38:LYS:HG3	1:B:298:LEU:HB2	1.87	0.55
1:B:186:LEU:HD21	1:B:298:LEU:HD21	1.88	0.55
1:B:382:PHE:HD1	1:B:382:PHE:H	1.53	0.55
1:B:420:ARG:HB3	1:B:420:ARG:HH11	1.72	0.55
1:A:89:GLN:O	1:A:89:GLN:HG2	2.06	0.55
1:A:197:ASP:O	1:A:199:SER:O	2.24	0.55
1:A:263:GLY:O	1:A:267:THR:CG2	2.42	0.55
1:A:324:GLY:HA3	1:A:402:ARG:HH22	1.71	0.55
1:C:20:TRP:O	1:C:20:TRP:HD1	1.90	0.55
1:C:315:THR:HG23	1:C:331:GLN:HG2	1.89	0.55
1:B:71:ASP:HB2	1:B:82:LEU:CD1	2.21	0.55
2:E:22:SER:O	2:E:23:ARG:HB2	2.06	0.55
1:A:224:PRO:HA	1:A:237:ASN:O	2.06	0.54
1:A:290:LYS:HB3	1:A:290:LYS:NZ	2.21	0.54
1:C:329:GLU:HG3	1:C:375:MET:CB	2.34	0.54
1:C:382:PHE:CD1	1:C:382:PHE:C	2.86	0.54
1:C:445:ILE:HD13	1:C:448:ILE:CD1	2.37	0.54
1:B:2:ARG:HA	1:B:151:MET:HE3	1.88	0.54
1:B:4:ILE:HD11	1:B:144:HIS:CE1	2.42	0.54
1:B:107:LEU:N	1:B:107:LEU:CD1	2.67	0.54
1:B:135:LEU:CD1	1:B:136:GLU:N	2.70	0.54
1:B:322:LEU:O	1:B:323:HIS:CG	2.60	0.54
2:F:71:ALA:O	2:F:75:SER:HB3	2.07	0.54
1:A:241:ALA:O	1:A:242:LEU:HD12	2.06	0.54
1:C:1:ILE:HD13	1:C:152:ILE:HG22	1.88	0.54
1:C:47:THR:HG22	1:C:49:THR:HG23	1.89	0.54
2:D:47:ALA:O	2:D:50:ALA:HB3	2.06	0.54
1:B:276:GLU:O	1:B:283:ARG:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:LEU:CD2	1:C:212:LEU:HD23	2.37	0.54
1:B:21:VAL:O	1:B:21:VAL:CG2	2.56	0.54
1:B:365:ILE:N	1:B:374:MET:SD	2.80	0.54
1:A:172:ASN:C	1:A:172:ASN:OD1	2.51	0.54
1:A:238:ASN:C	1:A:240:GLU:N	2.59	0.54
1:A:311:ALA:O	1:A:332:TYR:HA	2.08	0.54
1:C:113:LEU:HD21	1:C:253:GLN:HE21	1.71	0.54
1:C:131:GLN:O	1:C:132:PRO:C	2.50	0.54
1:C:302:GLY:CA	1:C:305:TYR:CE2	2.90	0.54
1:B:81:TYR:O	1:B:82:LEU:CB	2.54	0.54
1:B:360:THR:HG1	1:B:376:LEU:HB3	1.69	0.54
1:A:49:THR:HB	1:A:283:ARG:NH2	2.22	0.54
1:A:72:SER:CB	1:A:99:ARG:HH11	2.21	0.54
1:A:113:LEU:HD21	1:A:253:GLN:HE21	1.72	0.54
1:C:74:CYS:CB	1:C:75:PRO:HD2	2.37	0.54
1:C:322:LEU:HD12	1:C:322:LEU:N	2.23	0.54
2:D:19:TRP:C	2:D:21:GLU:N	2.64	0.54
2:D:70:ILE:O	2:D:70:ILE:HD13	2.07	0.54
1:B:7:SER:HA	1:B:322:LEU:HD13	1.89	0.54
1:B:74:CYS:C	1:B:76:THR:N	2.66	0.54
1:B:371:ASN:O	1:B:371:ASN:OD1	2.26	0.54
1:A:332:TYR:CD2	1:A:335:THR:HB	2.34	0.54
1:A:443:LYS:HB3	1:A:443:LYS:HZ3	1.69	0.54
2:D:21:GLU:O	2:D:22:SER:C	2.51	0.54
2:D:51:TRP:HA	2:D:60:LYS:NZ	2.23	0.54
1:B:7:SER:HA	1:B:322:LEU:CD1	2.38	0.54
1:B:236:TRP:HB2	1:B:239:LYS:CE	2.28	0.54
1:B:330:VAL:CG1	1:B:331:GLN:N	2.71	0.54
1:B:338:PRO:HG3	1:B:367:GLU:CG	2.37	0.54
1:A:37:ASP:N	1:A:37:ASP:OD1	2.40	0.54
1:A:74:CYS:SG	1:A:75:PRO:HD2	2.47	0.54
1:A:204:LEU:CD2	1:A:204:LEU:N	2.66	0.54
1:A:259:GLY:O	1:A:261:GLN:NE2	2.41	0.54
1:A:332:TYR:O	1:A:372:SER:OG	2.24	0.54
1:C:28:GLY:HA3	2:F:15:ARG:CG	2.33	0.54
1:C:36:GLN:C	1:C:38:LYS:H	2.15	0.54
1:B:169:ILE:CD1	1:B:169:ILE:H	2.20	0.54
1:B:260:SER:O	1:B:261:GLN:CB	2.54	0.54
1:B:364:VAL:CA	1:B:374:MET:HE1	2.38	0.54
1:A:38:LYS:HE3	1:A:38:LYS:CA	2.33	0.54
1:A:203:TYR:CE2	1:A:277:MET:HE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PRO:HD2	1:A:242:LEU:HD22	1.89	0.54
1:A:315:THR:O	1:A:316:LYS:HG2	2.08	0.54
1:C:2:ARG:HH11	1:C:140:MET:HE2	1.71	0.54
1:B:151:MET:CG	1:B:152:ILE:HG12	2.37	0.54
1:B:204:LEU:HG	1:B:205:THR:H	1.73	0.54
1:B:310:ALA:HB1	1:B:333:ALA:HB2	1.90	0.54
1:B:357:ARG:CG	1:B:358:LEU:N	2.71	0.54
1:B:472:LEU:HD23	1:B:475:LEU:CD1	2.37	0.54
2:E:38:ARG:C	2:E:40:PRO:HD3	2.33	0.54
1:A:125:MET:HG2	1:A:125:MET:O	2.08	0.54
1:C:131:GLN:O	1:C:133:GLU:N	2.41	0.54
1:C:170:THR:O	1:C:192:PRO:HG2	2.08	0.54
1:C:357:ARG:CG	1:C:358:LEU:N	2.69	0.54
1:C:423:VAL:O	1:C:423:VAL:HG12	2.08	0.54
1:B:223:LEU:HD12	1:B:223:LEU:N	2.23	0.54
1:C:314:PHE:H	1:C:314:PHE:HD1	1.56	0.54
1:C:399:HIS:CE1	1:B:191:GLU:OE1	2.61	0.54
2:F:19:TRP:CD1	2:F:20:LEU:H	2.25	0.54
1:C:460:MET:C	2:D:75:SER:O	2.51	0.53
1:B:396:ILE:O	1:B:396:ILE:CG1	2.55	0.53
1:A:72:SER:C	1:A:73:ARG:HG2	2.34	0.53
1:A:466:ILE:HG13	1:A:467:LEU:H	1.73	0.53
1:C:127:GLY:HA3	1:C:218:PHE:CE2	2.43	0.53
1:B:57:ARG:CZ	1:B:225:TRP:HE1	2.19	0.53
1:B:73:ARG:CA	1:B:77:GLN:HE21	2.21	0.53
1:B:313:THR:CA	1:B:396:ILE:HD12	2.36	0.53
1:A:396:ILE:HD12	1:A:396:ILE:N	2.22	0.53
1:A:472:LEU:HA	1:A:475:LEU:HD23	1.90	0.53
1:C:1:ILE:HG21	1:C:4:ILE:HG13	1.89	0.53
1:C:1:ILE:O	1:C:2:ARG:CB	2.56	0.53
1:C:72:SER:HA	1:C:112:SER:O	2.08	0.53
1:A:273:LEU:HG	2:D:12:LEU:HB2	1.90	0.53
1:A:398:HIS:ND1	1:A:399:HIS:O	2.42	0.53
1:C:32:THR:HA	1:C:41:VAL:O	2.07	0.53
1:B:351:THR:O	1:B:351:THR:HG22	2.09	0.53
2:D:9:THR:CG2	2:D:10:ARG:N	2.67	0.53
1:B:223:LEU:HB3	1:B:242:LEU:HD11	1.91	0.53
2:E:40:PRO:HG2	2:E:41:GLY:N	2.23	0.53
1:A:108:PHE:HB2	1:C:320:GLU:O	2.08	0.53
1:A:273:LEU:CG	2:D:12:LEU:HD22	2.39	0.53
1:A:12:VAL:C	1:A:14:GLY:N	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ASP:OD1	1:A:446:HIS:HB3	2.09	0.53
1:C:320:GLU:OE2	1:C:324:GLY:HA2	2.09	0.53
1:B:56:VAL:HG13	1:B:57:ARG:H	1.73	0.53
1:B:217:TRP:CD1	2:E:7:HIS:HB2	2.44	0.53
1:B:268:ALA:CA	2:E:4:LEU:HD21	2.37	0.53
1:B:268:ALA:CB	2:E:4:LEU:HD21	2.39	0.53
1:B:283:ARG:HG2	1:B:283:ARG:HH11	1.72	0.53
1:B:302:GLY:C	1:B:304:SER:H	2.15	0.53
1:B:330:VAL:HG12	1:B:331:GLN:N	2.23	0.53
1:A:2:ARG:CB	1:A:142:SER:HB3	2.36	0.53
1:A:215:LYS:O	1:A:216:GLU:C	2.51	0.53
1:A:359:ILE:HG12	1:A:377:GLU:HB3	1.91	0.53
1:C:113:LEU:HD11	1:C:253:GLN:HE22	1.73	0.53
2:D:33:GLU:C	2:D:35:TRP:N	2.65	0.53
1:B:20:TRP:O	1:B:22:ASP:N	2.41	0.53
1:B:326:VAL:HG12	1:B:380:PRO:HD3	1.91	0.53
2:E:63:TYR:O	2:E:67:ILE:HG22	2.08	0.53
1:A:74:CYS:O	1:A:76:THR:N	2.42	0.53
1:A:101:TRP:HB3	1:C:152:ILE:HD11	1.91	0.53
1:B:148:HIS:C	1:B:150:GLY:H	2.16	0.53
2:E:71:ALA:N	2:E:72:PRO:CD	2.66	0.53
2:F:48:ALA:HA	2:F:51:TRP:HB3	1.90	0.53
1:A:130:ILE:HG21	1:A:198:PHE:CD2	2.41	0.53
1:A:347:VAL:CG2	1:A:355:VAL:HB	2.37	0.53
1:C:355:VAL:CG1	1:C:356:GLY:N	2.72	0.53
1:B:99:ARG:NH2	1:B:103:ASN:HB3	2.21	0.53
1:B:191:GLU:C	1:B:193:ARG:H	2.14	0.53
1:B:240:GLU:C	1:B:242:LEU:H	2.17	0.53
2:F:62:ILE:HG23	2:F:62:ILE:O	2.08	0.53
1:A:70:SER:HA	1:A:115:THR:HA	1.91	0.52
1:A:113:LEU:HD23	1:A:113:LEU:C	2.34	0.52
1:A:265:VAL:C	1:A:267:THR:N	2.64	0.52
1:A:378:LEU:HD23	1:A:379:ASP:N	2.24	0.52
2:D:64:LEU:O	2:D:68:LEU:HB2	2.08	0.52
1:B:2:ARG:HG2	1:B:3:CYS:H	1.74	0.52
1:B:75:PRO:HG2	1:B:107:LEU:HB2	1.90	0.52
1:B:169:ILE:HD12	1:B:169:ILE:H	1.71	0.52
1:B:180:LEU:H	1:B:180:LEU:CD1	1.98	0.52
1:B:338:PRO:CD	1:B:367:GLU:HG2	2.39	0.52
1:A:23:VAL:HG22	1:A:24:VAL:N	2.24	0.52
1:A:87:ASP:C	1:A:89:GLN:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:MET:SD	1:A:158:HIS:CE1	3.03	0.52
1:A:352:LEU:H	1:A:352:LEU:CD1	2.16	0.52
1:C:115:THR:CG2	1:C:253:GLN:HB3	2.37	0.52
2:D:9:THR:HG21	2:D:10:ARG:NH2	2.24	0.52
2:D:41:GLY:C	2:D:43:ALA:N	2.55	0.52
1:B:4:ILE:HG13	1:B:9:ARG:HH21	1.73	0.52
2:F:32:VAL:HG13	2:F:72:PRO:HG2	1.90	0.52
1:C:113:LEU:HD12	1:C:114:VAL:N	2.24	0.52
1:C:300:LEU:CD2	1:C:301:LYS:O	2.57	0.52
1:C:399:HIS:CE1	1:C:400:TRP:O	2.62	0.52
2:D:53:LEU:CD1	2:F:62:ILE:HG21	2.37	0.52
1:B:40:THR:CG2	1:B:144:HIS:CD2	2.86	0.52
1:B:62:GLU:HB3	1:B:122:SER:HB2	1.91	0.52
2:F:67:ILE:C	2:F:69:LEU:N	2.67	0.52
1:A:17:GLY:C	1:A:19:THR:H	2.17	0.52
1:C:56:VAL:HG13	1:C:57:ARG:N	2.24	0.52
1:C:155:ASP:OD1	1:C:158:HIS:CE1	2.63	0.52
1:C:225:TRP:HB2	1:C:237:ASN:HD22	1.73	0.52
1:C:226:HIS:CD2	1:C:234:PRO:HB2	2.44	0.52
2:D:30:ILE:HG13	2:D:31:ARG:H	1.72	0.52
1:A:34:MET:HB3	1:A:40:THR:CG2	2.39	0.52
1:C:69:ALA:O	1:C:116:CYS:N	2.39	0.52
1:C:188:LEU:N	1:C:188:LEU:HD23	2.24	0.52
1:C:494:VAL:HG13	1:C:495:LEU:HD23	1.92	0.52
1:B:22:ASP:H	1:B:433:SER:HB3	1.75	0.52
1:B:65:ILE:HD12	1:B:65:ILE:C	2.34	0.52
1:B:374:MET:HB3	1:B:376:LEU:HD11	1.90	0.52
1:B:388:VAL:CG2	1:B:388:VAL:O	2.57	0.52
1:A:215:LYS:HB2	1:A:215:LYS:HZ2	1.74	0.52
1:A:366:THR:O	1:A:367:GLU:CG	2.58	0.52
1:A:423:VAL:C	1:A:425:GLY:N	2.66	0.52
1:C:201:LEU:HD21	1:C:212:LEU:HD23	1.90	0.52
1:C:420:ARG:HD2	1:C:431:PHE:CE2	2.44	0.52
1:B:377:GLU:C	1:B:378:LEU:HD12	2.35	0.52
1:B:419:LYS:C	1:B:421:MET:H	2.18	0.52
1:A:22:ASP:O	1:A:23:VAL:HB	2.10	0.52
1:C:247:ASP:CG	1:C:252:ARG:O	2.53	0.52
1:C:387:ILE:HG22	1:C:387:ILE:O	2.10	0.52
1:C:389:ILE:CD1	1:C:396:ILE:O	2.58	0.52
1:C:420:ARG:O	1:C:428:ALA:HB1	2.09	0.52
2:E:4:LEU:HD23	2:E:5:PRO:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:LEU:HD21	2:F:1:ALA:HA	1.92	0.52
1:C:273:LEU:HB2	2:F:12:LEU:HD13	1.92	0.52
1:C:466:ILE:HD13	1:C:496:ILE:HG22	1.92	0.52
1:B:223:LEU:CB	1:B:224:PRO:CD	2.78	0.52
2:E:49:ILE:O	2:E:53:LEU:CD2	2.57	0.52
2:F:20:LEU:C	2:F:20:LEU:HD12	2.35	0.52
1:A:416:ARG:C	1:A:418:ALA:N	2.64	0.52
1:C:107:LEU:HD12	1:C:108:PHE:H	1.74	0.52
1:C:119:PHE:C	1:C:119:PHE:CD1	2.88	0.52
1:C:203:TYR:CE2	1:C:277:MET:HB2	2.44	0.52
1:C:391:VAL:O	1:C:395:LYS:HB3	2.09	0.52
2:D:9:THR:CG2	2:D:10:ARG:HH21	2.23	0.52
1:B:38:LYS:HD3	1:B:298:LEU:HD13	1.91	0.52
1:B:142:SER:HA	1:B:163:ASN:O	2.10	0.52
1:B:172:ASN:C	1:B:174:PRO:HD3	2.34	0.52
2:F:27:LYS:O	2:F:28:HIS:C	2.53	0.52
1:A:171:PRO:HB3	1:A:192:PRO:HB2	1.92	0.52
1:A:342:PRO:HG2	1:A:389:ILE:CG1	2.40	0.52
1:C:148:HIS:C	1:C:375:MET:HE2	2.35	0.52
1:C:244:GLU:HG2	2:D:20:LEU:HD23	1.91	0.52
1:C:346:ALA:HB2	1:C:388:VAL:HG23	1.91	0.52
2:D:49:ILE:O	2:D:52:LEU:HB2	2.10	0.52
1:B:41:VAL:HG23	1:B:143:VAL:HG13	1.92	0.52
1:B:60:CYS:H	1:B:224:PRO:CD	2.18	0.52
2:F:21:GLU:O	2:F:22:SER:C	2.52	0.52
1:A:97:VAL:CG1	1:A:113:LEU:HD22	2.40	0.51
1:A:141:LEU:O	1:A:164:ARG:HA	2.09	0.51
1:A:320:GLU:O	1:C:108:PHE:HB2	2.09	0.51
1:C:93:LYS:HD2	1:C:245:PHE:CE1	2.45	0.51
1:C:308:CYS:HB3	1:C:332:TYR:CE2	2.45	0.51
1:B:191:GLU:HG3	1:B:290:LYS:HE3	1.91	0.51
2:F:61:VAL:C	2:F:63:TYR:N	2.67	0.51
1:A:114:VAL:HG22	1:A:115:THR:N	2.24	0.51
1:A:399:HIS:ND1	1:A:399:HIS:C	2.68	0.51
1:C:45:LEU:HD22	1:C:289:LEU:HB3	1.92	0.51
1:C:65:ILE:H	1:C:257:VAL:HG12	1.75	0.51
2:D:54:GLY:HA2	2:F:59:GLN:OE1	2.10	0.51
1:B:43:ILE:HD12	1:B:43:ILE:N	2.26	0.51
1:B:421:MET:O	1:B:425:GLY:N	2.43	0.51
2:E:56:SER:HB3	2:E:59:GLN:HB3	1.88	0.51
1:A:348:ASP:HB2	1:A:350:GLN:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:THR:C	1:A:368:SER:H	2.18	0.51
2:D:38:ARG:O	2:D:40:PRO:HD3	2.09	0.51
1:B:283:ARG:CG	1:B:283:ARG:HH11	2.24	0.51
1:A:412:GLU:C	1:A:412:GLU:CD	2.79	0.51
1:C:133:GLU:O	1:C:134:ASN:CB	2.52	0.51
1:C:138:ARG:HB3	1:C:138:ARG:NH2	2.25	0.51
1:C:477:LEU:HD23	1:C:489:LEU:HD23	1.91	0.51
1:B:28:GLY:O	1:B:29:GLY:O	2.29	0.51
1:B:175:ARG:CZ	1:B:175:ARG:CB	2.85	0.51
1:B:175:ARG:O	1:B:176:ALA:O	2.29	0.51
1:B:202:TYR:N	1:B:202:TYR:CD1	2.79	0.51
1:B:330:VAL:HG21	1:B:389:ILE:HD11	1.91	0.51
1:A:317:ILE:HG23	1:A:317:ILE:O	2.10	0.51
1:C:340:LYS:NZ	1:C:340:LYS:CB	2.73	0.51
1:C:453:PHE:CZ	1:C:495:LEU:HD22	2.46	0.51
2:D:33:GLU:C	2:D:35:TRP:H	2.18	0.51
1:B:313:THR:O	1:B:330:VAL:HG13	2.11	0.51
1:B:314:PHE:CE2	1:B:398:HIS:HB2	2.45	0.51
1:B:320:GLU:OE2	1:B:324:GLY:HA2	2.11	0.51
1:B:474:TRP:C	1:B:476:GLY:H	2.18	0.51
2:E:33:GLU:C	2:E:35:TRP:N	2.69	0.51
1:A:4:ILE:HG22	1:A:4:ILE:O	2.10	0.51
1:A:412:GLU:OE2	1:A:416:ARG:HB2	2.11	0.51
1:C:225:TRP:O	1:C:236:TRP:HA	2.11	0.51
1:B:283:ARG:HB3	1:B:283:ARG:NH1	2.26	0.51
1:A:273:LEU:HB2	2:D:12:LEU:HD22	1.93	0.51
1:C:201:LEU:HD12	1:C:213:VAL:O	2.09	0.51
1:B:202:TYR:CE1	1:B:215:LYS:HG3	2.45	0.51
1:B:357:ARG:HB3	1:B:379:ASP:HB3	1.91	0.51
2:E:19:TRP:CG	2:E:20:LEU:HG	2.46	0.51
1:C:66:SER:HB3	1:C:118:LYS:HB3	1.93	0.51
1:C:400:TRP:CZ3	1:C:401:HIS:O	2.64	0.51
1:C:423:VAL:HG13	2:F:13:GLN:HB3	1.93	0.51
2:D:18:THR:OG1	2:D:19:TRP:N	2.44	0.51
1:B:41:VAL:CG2	1:B:143:VAL:HG13	2.41	0.51
2:F:38:ARG:HB3	2:F:38:ARG:HH11	1.76	0.51
1:A:256:VAL:HG13	1:C:209:LYS:NZ	2.26	0.51
1:A:359:ILE:C	1:A:361:ALA:H	2.16	0.51
1:C:373:LYS:HB3	1:C:373:LYS:HZ3	1.75	0.51
1:C:467:LEU:CD1	2:F:69:LEU:HD21	2.39	0.51
1:C:471:LEU:HD23	2:F:62:ILE:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:LEU:CD2	2:F:70:ILE:HD12	2.39	0.51
1:B:34:MET:HE1	1:B:359:ILE:HD12	1.93	0.51
1:A:290:LYS:HB3	1:A:290:LYS:HZ2	1.76	0.51
1:C:60:CYS:O	1:C:223:LEU:HD13	2.11	0.51
1:C:93:LYS:O	1:C:114:VAL:HG23	2.10	0.51
1:C:125:MET:SD	1:C:206:MET:HE2	2.51	0.51
1:C:374:MET:C	1:C:374:MET:SD	2.93	0.51
1:C:468:ILE:O	1:C:472:LEU:HG	2.11	0.51
1:B:13:GLU:O	1:B:14:GLY:O	2.28	0.51
1:B:445:ILE:CG2	1:B:446:HIS:H	2.21	0.51
2:E:59:GLN:C	2:E:61:VAL:N	2.64	0.51
1:A:65:ILE:HB	1:A:257:VAL:HG22	1.92	0.50
1:A:306:SER:O	1:A:339:CYS:HB2	2.11	0.50
1:C:27:HIS:NE2	1:C:48:THR:HG22	2.26	0.50
1:C:439:ASN:O	1:C:441:LEU:N	2.44	0.50
2:D:9:THR:HG22	2:D:10:ARG:CG	2.41	0.50
2:E:42:PHE:O	2:E:46:ALA:HB2	2.11	0.50
1:A:131:GLN:O	1:A:133:GLU:O	2.30	0.50
1:C:22:ASP:OD1	1:C:433:SER:HA	2.11	0.50
1:C:203:TYR:HE2	1:C:277:MET:HB2	1.77	0.50
1:C:320:GLU:HA	1:C:325:THR:O	2.11	0.50
2:D:40:PRO:C	2:D:42:PHE:N	2.69	0.50
1:B:149:SER:C	1:B:151:MET:N	2.67	0.50
1:B:156:THR:O	1:B:159:GLU:HG2	2.11	0.50
1:B:272:ALA:HA	2:E:18:THR:HA	1.94	0.50
2:E:50:ALA:O	2:E:60:LYS:HG2	2.11	0.50
2:E:65:VAL:HG22	2:E:69:LEU:HD11	1.92	0.50
1:A:135:LEU:N	1:A:135:LEU:CD2	2.74	0.50
1:A:199:SER:O	1:A:200:ASP:CB	2.59	0.50
1:A:453:PHE:HA	1:A:456:LEU:HD11	1.91	0.50
1:C:91:VAL:HG13	1:C:91:VAL:O	2.11	0.50
1:C:133:GLU:HB2	1:C:193:ARG:NH1	2.23	0.50
1:C:312:PHE:CZ	1:C:341:VAL:HG11	2.46	0.50
1:C:396:ILE:HD12	1:C:397:THR:N	2.26	0.50
1:C:457:PHE:CD1	1:C:457:PHE:N	2.79	0.50
1:B:11:PHE:HD1	1:B:11:PHE:H	1.59	0.50
1:B:169:ILE:HG21	1:B:190:CYS:HB2	1.94	0.50
1:B:234:PRO:O	1:B:236:TRP:CD1	2.64	0.50
1:B:444:GLY:O	1:B:447:GLN:CB	2.58	0.50
1:A:300:LEU:CD1	1:A:300:LEU:H	2.23	0.50
1:A:322:LEU:HG	1:A:323:HIS:N	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LYS:O	1:C:87:ASP:N	2.44	0.50
1:C:236:TRP:O	1:C:239:LYS:HG3	2.12	0.50
1:A:62:GLU:OE2	1:A:260:SER:HB2	2.12	0.50
1:C:273:LEU:CD2	1:C:286:SER:HB2	2.36	0.50
1:B:21:VAL:HG13	1:B:293:LEU:CA	2.41	0.50
1:B:61:TYR:O	1:B:61:TYR:CD1	2.65	0.50
1:B:146:SER:HA	1:B:374:MET:HE3	1.94	0.50
2:E:49:ILE:O	2:E:53:LEU:HD22	2.11	0.50
2:F:61:VAL:O	2:F:63:TYR:N	2.44	0.50
1:A:52:ASN:C	1:A:53:MET:HG3	2.35	0.50
1:A:423:VAL:HG22	1:A:424:LEU:H	1.77	0.50
1:A:425:GLY:O	1:A:426:ASP:HB3	2.11	0.50
1:C:90:TYR:HA	1:C:117:ALA:O	2.11	0.50
1:B:31:VAL:O	1:B:31:VAL:HG13	2.11	0.50
1:B:323:HIS:HD2	1:B:416:ARG:HH12	1.58	0.50
1:A:47:THR:OG1	1:A:138:ARG:HB2	2.11	0.50
1:A:191:GLU:HG3	1:A:290:LYS:CB	2.41	0.50
1:A:271:GLY:O	2:D:11:LYS:HA	2.12	0.50
1:C:375:MET:N	1:C:375:MET:CE	2.74	0.50
1:B:175:ARG:O	1:B:176:ALA:C	2.55	0.50
1:B:487:MET:HA	1:B:490:ALA:CB	2.42	0.50
2:E:59:GLN:O	2:E:60:LYS:C	2.53	0.50
1:A:179:THR:C	1:A:180:LEU:HD23	2.36	0.50
1:A:423:VAL:O	1:A:425:GLY:N	2.42	0.50
1:C:213:VAL:HG11	1:C:217:TRP:CZ3	2.46	0.50
1:C:434:VAL:HG13	1:C:434:VAL:O	2.11	0.50
1:B:57:ARG:HA	1:B:227:ALA:HB1	1.88	0.50
1:B:415:VAL:CG1	1:B:419:LYS:HE3	2.42	0.50
1:A:65:ILE:HG22	1:A:66:SER:N	2.27	0.50
1:A:101:TRP:HZ2	1:C:316:LYS:CB	2.24	0.50
1:A:163:ASN:C	1:A:164:ARG:HD2	2.37	0.50
1:A:418:ALA:O	1:A:421:MET:HB2	2.12	0.50
1:C:201:LEU:HD12	1:C:214:HIS:HA	1.93	0.50
2:D:18:THR:HG23	2:D:21:GLU:CB	2.28	0.50
1:B:7:SER:CA	1:B:322:LEU:HD13	2.42	0.50
1:B:91:VAL:O	1:B:91:VAL:CG1	2.59	0.50
1:B:113:LEU:HD13	1:B:113:LEU:O	2.12	0.50
2:E:50:ALA:CB	2:E:64:LEU:HA	2.42	0.50
2:F:19:TRP:CD1	2:F:20:LEU:N	2.80	0.50
2:F:54:GLY:HA2	2:F:63:TYR:CD2	2.47	0.50
1:A:74:CYS:HA	1:A:99:ARG:HD3	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:SER:O	1:A:150:GLY:C	2.55	0.49
1:A:214:HIS:ND1	2:D:10:ARG:HG3	2.26	0.49
1:A:263:GLY:HA3	1:C:260:SER:O	2.12	0.49
1:A:321:THR:C	1:A:322:LEU:O	2.51	0.49
1:C:36:GLN:C	1:C:38:LYS:N	2.70	0.49
1:C:379:ASP:O	1:C:380:PRO:C	2.55	0.49
1:C:424:LEU:HB2	1:C:428:ALA:HB2	1.94	0.49
1:B:312:PHE:CZ	1:B:341:VAL:HG12	2.46	0.49
2:F:73:ALA:O	2:F:75:SER:N	2.43	0.49
1:A:99:ARG:HB2	1:A:99:ARG:NH2	2.27	0.49
1:A:221:ILE:HG22	1:A:223:LEU:HB2	1.94	0.49
1:A:463:PHE:HD1	1:A:466:ILE:HD11	1.77	0.49
1:C:133:GLU:HG2	1:C:134:ASN:N	2.26	0.49
1:C:437:ALA:C	1:C:439:ASN:N	2.69	0.49
1:B:139:ILE:CD1	1:B:167:VAL:HG23	2.41	0.49
1:B:429:TRP:CE3	1:B:442:GLY:HA3	2.47	0.49
1:A:1:ILE:HG23	1:A:152:ILE:CG2	2.41	0.49
1:A:119:PHE:O	1:A:120:ALA:HB2	2.11	0.49
1:A:496:ILE:O	1:A:499:SER:HB2	2.12	0.49
1:C:247:ASP:OD2	1:C:250:ALA:O	2.29	0.49
2:D:64:LEU:C	2:D:64:LEU:HD13	2.37	0.49
1:B:20:TRP:HE3	1:B:292:ARG:NH2	2.08	0.49
1:B:81:TYR:O	1:B:82:LEU:HB3	2.13	0.49
2:F:58:SER:O	2:F:61:VAL:HG23	2.12	0.49
1:A:99:ARG:HB2	1:A:99:ARG:HH21	1.76	0.49
1:A:236:TRP:HB2	1:A:239:LYS:HG2	1.94	0.49
1:A:276:GLU:OE1	1:A:283:ARG:HG2	2.13	0.49
1:A:296:ASP:O	1:A:298:LEU:N	2.45	0.49
1:A:497:PHE:C	1:A:499:SER:N	2.70	0.49
1:C:34:MET:HB3	1:C:40:THR:HB	1.93	0.49
1:C:191:GLU:HG3	1:C:191:GLU:O	2.13	0.49
1:C:315:THR:C	1:C:316:LYS:HD3	2.37	0.49
2:D:3:THR:HB	2:F:31:ARG:NH1	2.27	0.49
1:B:7:SER:N	1:B:322:LEU:HD11	2.26	0.49
1:B:20:TRP:HE3	1:B:292:ARG:HE	1.58	0.49
1:B:157:GLY:HA3	3:B:601:NAG:O6	2.12	0.49
1:B:225:TRP:O	1:B:236:TRP:CE3	2.65	0.49
1:B:272:ALA:CB	2:E:18:THR:CG2	2.82	0.49
1:A:67:ASP:O	1:A:68:MET:C	2.56	0.49
1:A:262:GLU:HG2	1:C:259:GLY:HA3	1.94	0.49
1:A:392:GLY:O	1:A:395:LYS:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LYS:HB3	1:A:443:LYS:HZ2	1.73	0.49
1:A:456:LEU:HD13	1:A:457:PHE:HD2	1.77	0.49
1:C:214:HIS:HB2	2:F:7:HIS:NE2	2.26	0.49
1:C:430:ASP:OD1	1:C:443:LYS:HD2	2.13	0.49
1:B:4:ILE:H	1:B:151:MET:CE	2.22	0.49
1:B:148:HIS:HB2	1:B:373:LYS:HG3	1.94	0.49
1:B:444:GLY:O	1:B:447:GLN:HB3	2.11	0.49
1:A:43:ILE:CG2	1:A:141:LEU:CD2	2.89	0.49
1:A:332:TYR:OH	1:A:389:ILE:CD1	2.60	0.49
1:C:61:TYR:CE1	1:C:123:LYS:HE2	2.45	0.49
1:C:84:LYS:C	1:C:86:SER:H	2.20	0.49
1:C:138:ARG:HH21	1:C:138:ARG:HG3	1.78	0.49
1:C:298:LEU:HD13	1:C:298:LEU:O	2.13	0.49
2:D:21:GLU:C	2:D:23:ARG:N	2.71	0.49
2:D:63:TYR:O	2:D:66:MET:HB2	2.13	0.49
1:B:203:TYR:OH	1:B:275:ALA:HB1	2.13	0.49
1:C:182:GLY:O	1:C:299:ARG:NH1	2.45	0.49
1:C:434:VAL:HG23	1:C:439:ASN:CG	2.38	0.49
1:B:65:ILE:HG13	1:B:257:VAL:HB	1.93	0.49
1:B:215:LYS:O	1:B:216:GLU:C	2.55	0.49
2:F:48:ALA:HA	2:F:51:TRP:CB	2.42	0.49
1:A:246:LYS:CE	2:F:17:GLN:HB3	2.42	0.49
1:A:358:LEU:O	1:A:377:GLU:HB3	2.13	0.49
1:C:39:PRO:HG3	1:C:300:LEU:HA	1.94	0.49
1:C:42:ASP:O	1:C:141:LEU:HA	2.13	0.49
1:C:325:THR:HB	1:C:377:GLU:HG3	1.94	0.49
1:B:1:ILE:HG12	1:B:147:GLN:HG3	1.94	0.49
1:B:175:ARG:HB2	1:B:175:ARG:NH1	2.27	0.49
1:A:49:THR:HB	1:A:283:ARG:HH22	1.78	0.49
1:A:225:TRP:HD1	1:A:226:HIS:N	2.10	0.49
1:A:385:SER:O	1:A:400:TRP:N	2.43	0.49
1:C:52:ASN:O	1:C:134:ASN:CG	2.56	0.49
1:C:97:VAL:CG2	1:C:113:LEU:HD23	2.42	0.49
1:C:263:GLY:O	1:C:265:VAL:N	2.46	0.49
1:C:288:HIS:CE1	1:C:424:LEU:HD22	2.48	0.49
1:B:143:VAL:HG23	1:B:163:ASN:O	2.13	0.49
1:B:474:TRP:C	1:B:476:GLY:N	2.65	0.49
1:A:133:GLU:O	1:A:134:ASN:HB2	2.13	0.49
1:A:150:GLY:C	1:A:152:ILE:HD13	2.38	0.49
1:A:272:ALA:HB2	2:D:7:HIS:ND1	2.26	0.49
1:C:70:SER:HA	1:C:82:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ASN:O	1:C:208:ASN:CB	2.60	0.49
1:C:306:SER:O	1:C:308:CYS:N	2.46	0.49
1:C:461:SER:O	1:C:462:TRP:C	2.55	0.49
1:C:475:LEU:HB3	1:C:488:CYS:SG	2.53	0.49
1:B:135:LEU:C	1:B:135:LEU:CD1	2.86	0.49
1:B:152:ILE:HG22	1:B:153:VAL:H	1.76	0.49
1:B:225:TRP:H	1:B:236:TRP:HE3	1.60	0.49
1:B:261:GLN:OE1	1:B:264:ALA:HB3	2.13	0.49
1:B:263:GLY:O	1:B:266:HIS:HB2	2.13	0.49
1:B:300:LEU:HB3	1:B:362:ASN:ND2	2.28	0.49
1:B:457:PHE:O	1:B:460:MET:HE3	2.12	0.49
2:E:58:SER:HA	2:E:61:VAL:HG21	1.94	0.49
2:F:4:LEU:N	2:F:5:PRO:CD	2.75	0.49
2:F:29:LEU:C	2:F:31:ARG:H	2.21	0.49
1:A:15:MET:SD	1:A:295:MET:HG3	2.53	0.48
1:A:233:THR:O	1:A:235:HIS:N	2.46	0.48
1:A:244:GLU:OE2	1:A:244:GLU:HA	2.12	0.48
1:A:314:PHE:HE2	1:A:318:PRO:CD	2.21	0.48
1:A:454:LYS:HB2	1:A:454:LYS:HZ2	1.77	0.48
1:C:474:TRP:CD1	1:C:474:TRP:C	2.90	0.48
2:D:54:GLY:O	2:D:55:SER:HB2	2.11	0.48
1:B:25:LEU:HD13	1:B:139:ILE:CG2	2.27	0.48
1:B:97:VAL:HG13	1:B:251:LYS:CA	2.38	0.48
1:B:457:PHE:CE2	1:B:495:LEU:HD11	2.48	0.48
1:A:7:SER:O	1:A:8:ASN:CB	2.61	0.48
1:A:89:GLN:C	1:A:239:LYS:NZ	2.71	0.48
1:A:154:ASN:CG	3:A:601:NAG:C8	2.81	0.48
1:A:399:HIS:ND1	1:A:400:TRP:N	2.61	0.48
1:C:384:ASP:O	1:C:385:SER:CB	2.56	0.48
1:B:5:GLY:HA2	1:B:322:LEU:CD1	2.43	0.48
1:B:30:CYS:SG	1:B:43:ILE:O	2.71	0.48
1:B:261:GLN:NE2	2:E:1:ALA:H1	2.10	0.48
1:B:357:ARG:HD3	1:B:359:ILE:CD1	2.43	0.48
2:E:65:VAL:HG22	2:E:69:LEU:CG	2.43	0.48
2:F:19:TRP:CG	2:F:20:LEU:H	2.30	0.48
2:F:54:GLY:HA2	2:F:63:TYR:CE2	2.47	0.48
1:A:61:TYR:HE2	1:A:262:GLU:HB2	1.77	0.48
1:A:216:GLU:O	1:A:217:TRP:C	2.56	0.48
1:A:255:VAL:HG12	1:A:256:VAL:N	2.29	0.48
1:A:261:GLN:O	1:A:264:ALA:HB3	2.13	0.48
1:A:409:LYS:HB3	1:A:409:LYS:HZ3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:VAL:HG12	1:C:32:THR:N	2.26	0.48
1:C:312:PHE:HB3	1:C:330:VAL:CG1	2.43	0.48
1:C:418:ALA:O	1:C:422:ALA:HB3	2.13	0.48
1:C:420:ARG:HG2	1:C:431:PHE:CE2	2.48	0.48
1:B:59:TYR:CE2	1:B:221:ILE:O	2.66	0.48
1:B:97:VAL:O	1:B:99:ARG:N	2.46	0.48
1:B:338:PRO:CG	1:B:367:GLU:HG2	2.43	0.48
1:B:428:ALA:C	1:B:430:ASP:H	2.21	0.48
2:E:31:ARG:CZ	2:E:31:ARG:HB2	2.43	0.48
1:A:47:THR:OG1	1:A:138:ARG:CD	2.54	0.48
1:A:228:GLY:CA	1:B:73:ARG:HH12	2.26	0.48
1:A:410:ALA:C	1:A:412:GLU:N	2.72	0.48
1:C:24:VAL:HG22	1:C:290:LYS:HG3	1.96	0.48
1:C:25:LEU:HD12	1:C:25:LEU:H	1.78	0.48
1:B:32:THR:OG1	1:B:42:ASP:HB3	2.14	0.48
1:B:97:VAL:CG1	1:B:251:LYS:HA	2.37	0.48
1:A:54:ALA:HB3	1:B:76:THR:O	2.14	0.48
1:A:232:GLY:O	1:A:234:PRO:N	2.45	0.48
1:A:265:VAL:O	1:A:267:THR:N	2.47	0.48
1:A:429:TRP:HB2	1:A:443:LYS:HE2	1.95	0.48
1:C:21:VAL:O	1:C:22:ASP:C	2.56	0.48
1:C:55:GLU:CA	1:C:128:LYS:HA	2.31	0.48
1:C:214:HIS:HD2	1:C:216:GLU:HB2	1.78	0.48
1:C:345:MET:CE	1:C:378:LEU:HB3	2.42	0.48
1:C:399:HIS:ND1	1:C:400:TRP:N	2.61	0.48
1:C:471:LEU:HD13	1:C:471:LEU:O	2.14	0.48
1:B:61:TYR:CE1	1:B:262:GLU:HG2	2.48	0.48
1:A:35:ALA:O	1:A:37:ASP:N	2.46	0.48
1:A:38:LYS:HG3	1:A:298:LEU:HB2	1.94	0.48
1:A:73:ARG:NH2	1:A:77:GLN:CB	2.56	0.48
1:A:101:TRP:N	1:A:106:GLY:HA2	2.27	0.48
1:A:386:TYR:C	1:A:387:ILE:O	2.54	0.48
1:C:39:PRO:CD	1:C:298:LEU:HD11	2.33	0.48
1:C:61:TYR:CE1	1:C:123:LYS:HB2	2.49	0.48
1:C:343:ALA:HA	1:C:388:VAL:O	2.13	0.48
1:C:357:ARG:CG	1:C:358:LEU:H	2.26	0.48
1:C:382:PHE:C	1:C:382:PHE:HD1	2.21	0.48
1:B:90:TYR:CD1	1:B:90:TYR:N	2.82	0.48
1:B:196:LEU:HB2	1:B:198:PHE:CZ	2.48	0.48
1:B:244:GLU:O	1:B:255:VAL:HA	2.13	0.48
1:B:255:VAL:O	1:B:255:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ALA:HB3	2:E:12:LEU:HD13	1.94	0.48
1:A:12:VAL:HG23	1:A:33:VAL:HG22	1.96	0.48
1:A:58:SER:HA	1:A:126:THR:HA	1.95	0.48
1:A:235:HIS:CD2	1:B:86:SER:HA	2.47	0.48
1:C:49:THR:OG1	1:C:136:GLU:OE1	2.29	0.48
1:C:55:GLU:HA	1:C:128:LYS:CA	2.31	0.48
1:C:180:LEU:HD22	1:C:180:LEU:N	2.28	0.48
2:D:60:LYS:H	2:D:60:LYS:CD	2.24	0.48
1:B:382:PHE:CB	1:B:404:GLY:O	2.57	0.48
2:E:50:ALA:HB2	2:E:64:LEU:HA	1.96	0.48
1:A:60:CYS:O	1:A:223:LEU:HG	2.13	0.48
1:A:97:VAL:HG23	1:A:98:ASP:N	2.28	0.48
1:A:312:PHE:CZ	1:A:388:VAL:O	2.67	0.48
1:C:61:TYR:HB2	1:C:261:GLN:HB2	1.96	0.48
1:C:139:ILE:HB	1:C:167:VAL:HG12	1.93	0.48
1:C:149:SER:HG	1:C:373:LYS:HZ2	1.61	0.48
1:C:154:ASN:HA	3:C:601:NAG:H82	1.94	0.48
1:C:223:LEU:HB3	1:C:224:PRO:CD	2.43	0.48
1:C:302:GLY:HA2	1:C:305:TYR:CD2	2.49	0.48
1:C:305:TYR:CZ	1:C:338:PRO:HB2	2.49	0.48
1:B:247:ASP:HB3	1:B:253:GLN:HG3	1.94	0.48
1:B:336:ASP:O	1:B:368:SER:O	2.31	0.48
1:B:465:GLN:HG3	1:B:499:SER:HB3	1.95	0.48
1:A:423:VAL:HG22	1:A:424:LEU:N	2.29	0.48
1:A:425:GLY:O	1:A:426:ASP:CB	2.62	0.48
1:A:437:ALA:C	1:A:439:ASN:H	2.21	0.48
1:A:462:TRP:NE1	1:A:499:SER:HB3	2.29	0.48
1:C:434:VAL:HG23	1:C:439:ASN:OD1	2.14	0.48
2:F:46:ALA:HA	2:F:49:ILE:HB	1.96	0.48
1:A:96:LEU:HA	1:A:112:SER:HA	1.96	0.48
1:A:240:GLU:HA	1:A:243:VAL:CG2	2.38	0.48
1:C:20:TRP:CD1	1:C:20:TRP:C	2.91	0.48
1:C:273:LEU:H	2:F:12:LEU:CD2	2.22	0.48
1:C:340:LYS:HB3	1:C:340:LYS:HZ3	1.79	0.48
2:D:11:LYS:O	2:D:13:GLN:N	2.46	0.48
1:B:302:GLY:HA2	1:B:364:VAL:HG11	1.94	0.48
2:F:24:GLU:O	2:F:27:LYS:HG2	2.14	0.48
1:A:99:ARG:NH2	1:A:99:ARG:CB	2.76	0.47
1:C:40:THR:HG23	1:C:144:HIS:HB2	1.96	0.47
1:C:84:LYS:C	1:C:86:SER:N	2.70	0.47
1:C:215:LYS:O	1:C:216:GLU:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:LEU:O	1:C:443:LYS:N	2.47	0.47
1:C:465:GLN:OE1	1:C:499:SER:HB3	2.14	0.47
1:B:114:VAL:O	1:B:114:VAL:HG13	2.14	0.47
1:B:226:HIS:O	1:B:227:ALA:HB2	2.14	0.47
1:B:231:THR:O	1:B:232:GLY:C	2.56	0.47
1:B:300:LEU:HD12	1:B:300:LEU:N	2.29	0.47
1:B:313:THR:H	1:B:330:VAL:CG1	2.25	0.47
1:B:364:VAL:H	1:B:374:MET:CE	2.20	0.47
1:B:452:ALA:O	1:B:453:PHE:C	2.57	0.47
2:E:21:GLU:O	2:E:24:GLU:HB3	2.13	0.47
2:E:72:PRO:HG2	2:E:73:ALA:H	1.79	0.47
1:A:10:ASP:HB2	1:A:431:PHE:HZ	1.78	0.47
1:C:31:VAL:HG12	1:C:32:THR:O	2.14	0.47
2:D:9:THR:CG2	2:D:10:ARG:NH2	2.77	0.47
1:B:462:TRP:O	1:B:463:PHE:C	2.56	0.47
1:B:479:THR:HG23	1:B:481:ASN:O	2.14	0.47
2:F:44:LEU:O	2:F:47:ALA:HB3	2.14	0.47
2:F:56:SER:OG	2:F:57:THR:N	2.44	0.47
1:A:43:ILE:HA	1:A:140:MET:O	2.14	0.47
1:A:50:VAL:CG1	1:A:130:ILE:HD12	2.10	0.47
1:A:171:PRO:HB2	1:A:193:ARG:HH12	1.79	0.47
1:A:311:ALA:CB	1:A:334:GLY:N	2.77	0.47
1:A:434:VAL:O	1:A:434:VAL:HG23	2.14	0.47
1:C:213:VAL:CG1	1:C:214:HIS:N	2.76	0.47
1:C:277:MET:HG3	1:C:282:GLY:HA2	1.96	0.47
1:C:471:LEU:CD2	2:F:62:ILE:HG12	2.43	0.47
1:C:497:PHE:HA	1:C:500:THR:OG1	2.14	0.47
1:B:73:ARG:HB3	1:B:77:GLN:CG	2.44	0.47
1:B:338:PRO:HG3	1:B:367:GLU:CB	2.44	0.47
1:B:345:MET:HA	1:B:386:TYR:O	2.15	0.47
1:B:449:PHE:O	1:B:450:GLY:C	2.58	0.47
1:B:456:LEU:HD12	1:B:457:PHE:HE1	1.78	0.47
2:F:3:THR:HG22	2:F:5:PRO:HG2	1.95	0.47
1:A:196:LEU:HG	1:A:287:GLY:HA2	1.96	0.47
1:A:476:GLY:CA	1:A:489:LEU:HG	2.41	0.47
1:C:202:TYR:CZ	1:C:215:LYS:HG3	2.48	0.47
2:D:10:ARG:HG2	2:D:10:ARG:NH2	2.22	0.47
1:B:61:TYR:O	1:B:62:GLU:HB2	2.13	0.47
1:B:461:SER:O	1:B:462:TRP:C	2.57	0.47
1:A:65:ILE:HD13	1:A:255:VAL:HG11	1.96	0.47
1:C:97:VAL:HG23	1:C:113:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:THR:HG23	1:C:210:HIS:ND1	2.30	0.47
1:C:349:MET:CE	1:C:352:LEU:HD22	2.45	0.47
2:D:62:ILE:O	2:D:66:MET:HG2	2.14	0.47
1:B:34:MET:HE2	1:B:34:MET:HB3	1.79	0.47
1:B:37:ASP:C	1:B:37:ASP:OD1	2.57	0.47
1:B:73:ARG:HB3	1:B:77:GLN:HG2	1.95	0.47
1:B:137:TYR:HE2	1:B:289:LEU:HB2	1.79	0.47
1:A:34:MET:HB3	1:A:40:THR:OG1	2.14	0.47
1:A:37:ASP:O	1:A:300:LEU:HD21	2.15	0.47
1:C:125:MET:SD	1:C:206:MET:CE	3.02	0.47
1:C:209:LYS:O	1:C:211:TRP:CZ3	2.68	0.47
1:C:209:LYS:HB2	1:C:211:TRP:HZ3	1.79	0.47
1:B:61:TYR:CZ	1:B:123:LYS:CB	2.97	0.47
2:E:65:VAL:HG13	2:E:66:MET:N	2.29	0.47
1:A:38:LYS:C	1:A:39:PRO:O	2.58	0.47
1:A:151:MET:O	1:A:151:MET:CG	2.61	0.47
1:A:152:ILE:CG1	1:A:153:VAL:N	2.58	0.47
1:A:204:LEU:HD21	1:A:213:VAL:HG13	1.97	0.47
1:A:312:PHE:CD2	1:A:396:ILE:HB	2.32	0.47
1:C:13:GLU:CG	1:C:34:MET:HG3	2.33	0.47
1:C:171:PRO:CA	1:C:192:PRO:HB2	2.43	0.47
1:C:277:MET:HG3	1:C:282:GLY:CA	2.44	0.47
1:C:300:LEU:CD2	1:C:301:LYS:N	2.69	0.47
1:C:399:HIS:CD2	1:B:191:GLU:HA	2.50	0.47
2:D:13:GLN:O	2:D:14:THR:HG23	2.15	0.47
2:D:18:THR:O	2:D:21:GLU:HB3	2.13	0.47
1:B:20:TRP:CZ3	1:B:292:ARG:NH2	2.83	0.47
1:B:36:GLN:OE1	1:B:36:GLN:CA	2.62	0.47
1:B:175:ARG:CA	1:B:188:LEU:O	2.52	0.47
1:B:222:PRO:C	1:B:223:LEU:CG	2.88	0.47
1:B:370:GLU:HG3	1:B:371:ASN:N	2.30	0.47
1:A:31:VAL:O	1:A:43:ILE:CD1	2.63	0.47
1:A:81:TYR:C	1:A:81:TYR:CD1	2.93	0.47
1:C:75:PRO:O	1:C:77:GLN:N	2.48	0.47
1:C:187:GLY:C	1:C:188:LEU:HD23	2.40	0.47
1:C:429:TRP:CD1	1:C:442:GLY:HA3	2.49	0.47
1:C:468:ILE:HD13	2:D:42:PHE:CZ	2.50	0.47
1:B:21:VAL:O	1:B:292:ARG:HA	2.14	0.47
1:B:99:ARG:NH2	1:B:103:ASN:ND2	2.63	0.47
1:B:105:CYS:O	1:B:106:GLY:C	2.55	0.47
2:E:20:LEU:O	2:E:21:GLU:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:O	1:A:154:ASN:C	2.57	0.47
1:C:209:LYS:CB	1:C:211:TRP:HZ3	2.28	0.47
1:C:326:VAL:CG2	1:C:380:PRO:HG2	2.41	0.47
1:C:389:ILE:CD1	1:C:396:ILE:HG23	2.33	0.47
1:C:420:ARG:HG2	1:C:431:PHE:HE2	1.80	0.47
1:C:436:GLY:O	1:C:439:ASN:OD1	2.32	0.47
1:C:473:MET:O	1:C:477:LEU:HG	2.15	0.47
1:B:38:LYS:O	1:B:39:PRO:O	2.33	0.47
1:B:281:LYS:HB3	1:B:281:LYS:HZ3	1.77	0.47
1:B:491:LEU:HD12	1:B:494:VAL:CG2	2.44	0.47
2:F:48:ALA:C	2:F:50:ALA:N	2.68	0.47
1:A:93:LYS:HB3	1:A:245:PHE:CD2	2.50	0.47
1:A:264:ALA:HB1	2:D:4:LEU:HD12	1.97	0.47
1:A:305:TYR:HB2	1:A:340:LYS:CG	2.33	0.47
1:A:313:THR:CG2	1:A:331:GLN:O	2.63	0.47
1:C:331:GLN:OE1	1:C:371:ASN:CB	2.50	0.47
1:C:374:MET:C	1:C:375:MET:CE	2.85	0.47
1:B:222:PRO:O	1:B:223:LEU:CG	2.60	0.47
1:B:309:THR:O	1:B:310:ALA:CB	2.62	0.47
1:B:310:ALA:HB3	1:B:332:TYR:CE1	2.50	0.47
1:A:454:LYS:HG2	1:A:455:SER:N	2.30	0.46
1:A:460:MET:C	1:A:461:SER:O	2.57	0.46
1:A:472:LEU:C	1:A:474:TRP:N	2.71	0.46
1:C:1:ILE:HG21	1:C:4:ILE:CG2	2.44	0.46
1:C:307:LEU:HD23	1:C:342:PRO:HG3	1.96	0.46
1:C:347:VAL:O	1:C:348:ASP:CB	2.61	0.46
1:B:41:VAL:HG13	1:B:142:SER:O	2.15	0.46
1:B:147:GLN:O	1:B:375:MET:HB3	2.16	0.46
1:B:170:THR:C	1:B:172:ASN:N	2.73	0.46
1:B:357:ARG:HH11	1:B:357:ARG:CB	2.22	0.46
1:B:479:THR:CG2	1:B:485:SER:OG	2.64	0.46
1:A:225:TRP:HD1	1:A:226:HIS:C	2.23	0.46
1:A:234:PRO:O	1:A:236:TRP:N	2.48	0.46
1:C:34:MET:HE1	1:C:359:ILE:CG2	2.27	0.46
1:C:240:GLU:CD	1:C:240:GLU:N	2.73	0.46
1:C:312:PHE:CD2	1:C:331:GLN:O	2.68	0.46
1:C:347:VAL:O	1:C:347:VAL:HG22	2.15	0.46
1:A:138:ARG:NH2	1:A:140:MET:HE1	2.29	0.46
1:A:427:THR:HG22	1:A:427:THR:O	2.15	0.46
1:A:477:LEU:HD23	1:A:477:LEU:C	2.39	0.46
1:C:20:TRP:HB2	1:C:292:ARG:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:ARG:HG3	1:C:292:ARG:NH1	2.30	0.46
1:C:300:LEU:HD23	1:C:301:LYS:O	2.16	0.46
1:C:311:ALA:HB2	1:C:394:LYS:HE2	1.98	0.46
1:B:61:TYR:CZ	1:B:123:LYS:HB2	2.50	0.46
1:B:93:LYS:C	1:B:114:VAL:HG23	2.41	0.46
1:B:148:HIS:CG	1:B:148:HIS:O	2.68	0.46
1:B:225:TRP:CD2	1:B:226:HIS:N	2.84	0.46
1:B:360:THR:HG23	1:B:376:LEU:HD22	1.96	0.46
1:B:426:ASP:O	1:B:428:ALA:N	2.48	0.46
1:C:307:LEU:H	1:C:307:LEU:CD1	2.28	0.46
1:C:397:THR:OG1	1:B:175:ARG:HD3	2.15	0.46
1:C:463:PHE:CE1	1:C:467:LEU:HD11	2.50	0.46
1:C:490:ALA:O	1:C:494:VAL:HG12	2.15	0.46
2:E:67:ILE:O	2:E:70:ILE:HG23	2.15	0.46
2:F:48:ALA:O	2:F:49:ILE:C	2.59	0.46
1:A:157:GLY:O	1:A:159:GLU:N	2.48	0.46
1:A:159:GLU:CD	1:A:160:THR:N	2.74	0.46
1:A:203:TYR:HE2	1:A:277:MET:HE1	1.79	0.46
1:A:312:PHE:CD2	1:A:389:ILE:HB	2.50	0.46
1:A:355:VAL:O	1:A:355:VAL:CG1	2.64	0.46
1:C:200:ASP:HA	1:C:215:LYS:HB2	1.96	0.46
1:C:273:LEU:HD12	1:C:273:LEU:C	2.40	0.46
1:B:223:LEU:HA	1:B:241:ALA:HB3	1.96	0.46
1:B:386:TYR:O	1:B:388:VAL:N	2.49	0.46
1:B:442:GLY:O	1:B:444:GLY:N	2.49	0.46
1:A:24:VAL:HG23	1:A:430:ASP:O	2.15	0.46
1:A:202:TYR:HE1	1:A:215:LYS:HB2	1.81	0.46
1:A:362:ASN:N	1:A:363:PRO:CD	2.78	0.46
1:C:22:ASP:CA	1:C:292:ARG:HG2	2.46	0.46
1:C:292:ARG:HG3	1:C:292:ARG:HH11	1.79	0.46
1:C:386:TYR:O	1:C:387:ILE:HG13	2.15	0.46
1:C:393:GLU:C	1:C:393:GLU:CD	2.83	0.46
1:C:423:VAL:HG21	1:C:502:VAL:HG11	1.94	0.46
1:B:128:LYS:O	1:B:202:TYR:HB3	2.15	0.46
1:B:360:THR:O	1:B:361:ALA:CB	2.64	0.46
2:F:29:LEU:C	2:F:31:ARG:N	2.74	0.46
1:A:12:VAL:CG2	1:A:33:VAL:HG22	2.45	0.46
1:A:69:ALA:O	1:A:70:SER:HB2	2.15	0.46
1:A:96:LEU:H	1:A:96:LEU:CD1	2.18	0.46
1:C:35:ALA:HB3	1:C:38:LYS:HD2	1.97	0.46
1:C:39:PRO:HG3	1:C:300:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:ALA:C	1:C:439:ASN:H	2.24	0.46
2:D:29:LEU:C	2:D:29:LEU:CD2	2.88	0.46
1:B:9:ARG:HG3	1:B:11:PHE:CE1	2.51	0.46
1:B:34:MET:HE1	1:B:359:ILE:HG23	1.98	0.46
1:B:442:GLY:C	1:B:444:GLY:H	2.23	0.46
1:B:494:VAL:HG12	1:B:498:LEU:HD11	1.96	0.46
1:A:101:TRP:CZ2	1:C:316:LYS:HG3	2.51	0.46
1:C:19:THR:HG23	1:C:295:MET:O	2.16	0.46
1:C:25:LEU:HD12	1:C:289:LEU:O	2.16	0.46
1:B:26:GLU:OE2	1:B:420:ARG:HG2	2.16	0.46
1:A:61:TYR:CE2	1:A:262:GLU:HB2	2.50	0.46
1:A:149:SER:O	1:A:151:MET:N	2.49	0.46
1:A:150:GLY:CA	1:A:152:ILE:HG23	2.44	0.46
1:A:193:ARG:HB2	1:A:193:ARG:HH11	1.80	0.46
1:A:378:LEU:HD11	1:A:387:ILE:HG22	1.98	0.46
1:C:40:THR:CG2	1:C:360:THR:HA	2.46	0.46
1:C:139:ILE:O	1:C:167:VAL:HG12	2.15	0.46
1:C:148:HIS:HB3	1:C:151:MET:HB3	1.96	0.46
1:B:7:SER:N	1:B:322:LEU:CD1	2.79	0.46
1:B:36:GLN:OE1	1:B:36:GLN:HA	2.16	0.46
1:B:159:GLU:C	1:B:161:ASP:H	2.23	0.46
1:B:241:ALA:C	1:B:242:LEU:HD12	2.40	0.46
2:E:31:ARG:HG3	2:E:32:VAL:H	1.81	0.46
1:A:223:LEU:HD13	2:D:4:LEU:HD21	1.98	0.46
1:A:261:GLN:CA	1:A:261:GLN:NE2	2.63	0.46
1:A:264:ALA:CB	2:D:4:LEU:HD12	2.46	0.46
1:A:321:THR:O	1:A:322:LEU:O	2.33	0.46
1:A:396:ILE:HD12	1:A:396:ILE:H	1.81	0.46
1:C:68:MET:HA	1:C:116:CYS:O	2.16	0.46
1:C:97:VAL:HG13	1:C:250:ALA:C	2.41	0.46
1:C:133:GLU:CB	1:C:193:ARG:HH12	2.26	0.46
1:C:147:GLN:NE2	1:C:163:ASN:HB2	2.31	0.46
1:C:148:HIS:C	1:C:375:MET:CE	2.89	0.46
1:C:366:THR:O	1:C:366:THR:HG22	2.16	0.46
1:B:99:ARG:NH2	1:B:103:ASN:CB	2.75	0.46
1:A:302:GLY:HA3	1:A:305:TYR:HE2	1.75	0.45
1:A:362:ASN:O	1:A:364:VAL:HG23	2.15	0.45
1:C:4:ILE:HG12	1:C:152:ILE:HD12	1.98	0.45
1:C:89:GLN:HA	1:C:239:LYS:HZ2	1.80	0.45
1:C:180:LEU:HB3	1:C:183:PHE:HB2	1.97	0.45
1:B:1:ILE:HG21	1:B:147:GLN:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:TYR:N	1:B:202:TYR:HD1	2.14	0.45
1:B:221:ILE:HA	1:B:222:PRO:HD3	1.75	0.45
1:A:202:TYR:OH	1:A:215:LYS:HD3	2.15	0.45
1:A:364:VAL:CG1	1:A:365:ILE:N	2.77	0.45
1:B:93:LYS:HD2	1:B:94:ARG:N	2.30	0.45
1:B:364:VAL:HG23	1:B:364:VAL:O	2.16	0.45
1:A:12:VAL:C	1:A:14:GLY:H	2.24	0.45
1:A:396:ILE:H	1:A:396:ILE:CD1	2.30	0.45
1:A:464:SER:HB3	2:F:75:SER:HB2	1.99	0.45
1:C:220:ASP:HB3	2:D:34:ASN:OD1	2.17	0.45
2:E:23:ARG:HB2	2:E:23:ARG:HH11	1.81	0.45
1:A:62:GLU:HG2	1:A:260:SER:HA	1.99	0.45
1:A:204:LEU:HD11	1:A:269:LEU:HD21	1.97	0.45
1:A:223:LEU:HD12	1:A:242:LEU:CD1	2.47	0.45
1:A:358:LEU:O	1:A:359:ILE:CG1	2.56	0.45
1:A:378:LEU:CD1	1:A:387:ILE:HG22	2.46	0.45
1:C:1:ILE:CG2	1:C:4:ILE:HG13	2.47	0.45
1:C:138:ARG:HH21	1:C:138:ARG:CG	2.29	0.45
1:C:295:MET:HE1	1:C:298:LEU:HD12	1.98	0.45
1:B:264:ALA:HA	1:B:267:THR:HG22	1.98	0.45
1:B:395:LYS:C	1:B:397:THR:H	2.24	0.45
2:F:27:LYS:C	2:F:29:LEU:N	2.73	0.45
1:A:49:THR:OG1	1:A:281:LYS:HB3	2.16	0.45
1:A:477:LEU:N	1:A:489:LEU:HD21	2.31	0.45
1:C:186:LEU:HD23	1:C:186:LEU:HA	1.57	0.45
1:B:151:MET:O	1:B:152:ILE:C	2.60	0.45
1:B:202:TYR:CE1	1:B:215:LYS:CB	3.00	0.45
1:A:265:VAL:HG23	2:D:4:LEU:CD1	2.32	0.45
1:A:475:LEU:HD13	2:F:53:LEU:HB2	1.97	0.45
1:A:480:LYS:O	1:A:484:ILE:HD11	2.17	0.45
1:C:51:SER:HA	1:C:281:LYS:HB3	1.99	0.45
1:C:143:VAL:H	1:C:163:ASN:HB3	1.82	0.45
1:C:333:ALA:O	1:C:335:THR:HG23	2.16	0.45
1:C:349:MET:HE3	1:C:352:LEU:HD22	1.97	0.45
1:B:41:VAL:CG1	1:B:42:ASP:N	2.80	0.45
1:B:409:LYS:HZ3	1:B:413:ALA:HB2	1.82	0.45
1:B:452:ALA:O	1:B:454:LYS:N	2.50	0.45
2:E:20:LEU:N	2:E:20:LEU:HD12	2.32	0.45
1:A:93:LYS:HD3	1:A:245:PHE:CB	2.47	0.45
1:A:263:GLY:HA2	1:A:266:HIS:HB2	1.97	0.45
1:A:273:LEU:HG	2:D:12:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:PRO:O	1:A:355:VAL:HG23	2.17	0.45
1:C:149:SER:OG	1:C:373:LYS:NZ	2.39	0.45
2:D:14:THR:HB	2:D:15:ARG:H	1.49	0.45
1:B:190:CYS:HB3	1:B:289:LEU:HD11	1.99	0.45
1:B:312:PHE:O	1:B:313:THR:HG23	2.17	0.45
2:E:23:ARG:HA	2:E:26:THR:HG22	1.99	0.45
2:E:28:HIS:CD2	2:E:28:HIS:N	2.84	0.45
2:E:38:ARG:HA	2:E:38:ARG:HE	1.81	0.45
1:A:139:ILE:O	1:A:167:VAL:CG2	2.65	0.45
1:A:148:HIS:ND1	1:A:373:LYS:HB2	2.31	0.45
1:C:59:TYR:O	1:C:124:LYS:CB	2.50	0.45
1:C:153:VAL:O	1:C:154:ASN:C	2.60	0.45
1:C:302:GLY:HA3	1:C:305:TYR:CE2	2.52	0.45
1:C:324:GLY:HA3	1:C:402:ARG:HE	1.81	0.45
1:C:400:TRP:HZ3	1:C:402:ARG:HB2	1.81	0.45
1:C:497:PHE:C	1:C:497:PHE:CD2	2.95	0.45
2:D:23:ARG:HB3	2:D:27:LYS:CE	2.32	0.45
1:A:20:TRP:HZ3	1:A:434:VAL:HA	1.82	0.45
1:A:89:GLN:CA	1:A:239:LYS:HZ3	2.30	0.45
1:A:357:ARG:O	1:A:357:ARG:HG2	2.17	0.45
1:C:113:LEU:CD2	1:C:251:LYS:HD2	2.47	0.45
1:C:392:GLY:O	1:C:395:LYS:CE	2.65	0.45
1:C:444:GLY:O	1:C:446:HIS:N	2.50	0.45
1:B:211:TRP:CD1	1:B:211:TRP:N	2.85	0.45
1:B:340:LYS:HA	1:B:364:VAL:HG12	1.99	0.45
1:B:400:TRP:CG	1:B:401:HIS:N	2.85	0.45
1:A:31:VAL:HB	1:A:43:ILE:CD1	2.43	0.45
1:A:223:LEU:HA	1:A:224:PRO:HD3	1.88	0.45
1:A:283:ARG:CZ	1:A:283:ARG:HB2	2.42	0.45
1:A:329:GLU:HG2	1:A:375:MET:HG2	1.98	0.45
1:A:468:ILE:HG22	1:A:468:ILE:O	2.17	0.45
1:A:484:ILE:C	1:A:484:ILE:HD12	2.41	0.45
1:C:6:VAL:HG23	1:C:6:VAL:O	2.17	0.45
1:C:400:TRP:CE3	1:C:401:HIS:N	2.85	0.45
1:C:420:ARG:CG	1:C:431:PHE:CE2	3.00	0.45
2:D:67:ILE:O	2:D:70:ILE:HG22	2.17	0.45
1:B:99:ARG:HG3	1:B:99:ARG:HH11	1.82	0.45
1:B:151:MET:HG3	1:B:152:ILE:N	2.32	0.45
1:B:180:LEU:O	1:B:181:GLY:O	2.35	0.45
2:E:51:TRP:CD1	2:E:60:LYS:NZ	2.72	0.45
1:A:101:TRP:C	1:C:152:ILE:HD11	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LEU:C	1:A:378:LEU:CD2	2.90	0.44
1:C:10:ASP:O	1:C:31:VAL:HA	2.17	0.44
1:C:60:CYS:HB3	1:C:224:PRO:HD2	1.98	0.44
1:C:101:TRP:N	1:C:101:TRP:HD1	2.14	0.44
1:C:164:ARG:NH1	1:C:164:ARG:CG	2.74	0.44
1:C:240:GLU:O	1:C:243:VAL:O	2.35	0.44
2:D:69:LEU:HD21	2:F:74:TYR:CD2	2.53	0.44
1:B:21:VAL:CG1	1:B:293:LEU:CA	2.95	0.44
1:B:65:ILE:HG22	1:B:117:ALA:HB1	1.99	0.44
1:B:151:MET:CG	1:B:152:ILE:N	2.79	0.44
1:B:158:HIS:O	1:B:164:ARG:HB2	2.17	0.44
2:E:40:PRO:HG2	2:E:41:GLY:H	1.82	0.44
1:A:398:HIS:ND1	1:A:398:HIS:C	2.74	0.44
1:C:100:GLY:HA2	1:C:107:LEU:O	2.18	0.44
2:D:2:VAL:O	2:D:2:VAL:CG1	2.65	0.44
1:B:193:ARG:C	1:B:195:GLY:H	2.24	0.44
1:B:474:TRP:CZ2	2:E:58:SER:HB2	2.48	0.44
1:A:73:ARG:N	1:A:112:SER:O	2.51	0.44
1:A:100:GLY:O	1:A:101:TRP:C	2.60	0.44
1:C:53:MET:HB2	1:C:129:SER:O	2.17	0.44
1:C:74:CYS:O	1:C:75:PRO:C	2.59	0.44
1:C:295:MET:CE	1:C:298:LEU:HD12	2.48	0.44
2:E:65:VAL:CG1	2:E:66:MET:N	2.80	0.44
1:A:17:GLY:C	1:A:19:THR:N	2.75	0.44
1:A:397:THR:O	1:A:397:THR:CG2	2.58	0.44
1:C:217:TRP:HE1	2:F:5:PRO:HB2	1.79	0.44
1:C:322:LEU:N	1:C:322:LEU:CD1	2.80	0.44
1:C:338:PRO:HB3	1:C:366:THR:HA	1.98	0.44
1:C:392:GLY:O	1:C:395:LYS:HD2	2.17	0.44
1:C:419:LYS:O	1:C:420:ARG:C	2.60	0.44
2:D:19:TRP:CD2	2:D:20:LEU:HG	2.52	0.44
1:B:459:GLY:O	1:B:460:MET:HE2	2.17	0.44
1:A:178:ALA:HB3	1:A:186:LEU:HB3	2.00	0.44
1:A:240:GLU:CA	1:A:243:VAL:HG22	2.40	0.44
1:A:290:LYS:HE3	1:A:292:ARG:NH1	2.32	0.44
1:A:351:THR:O	1:A:352:LEU:C	2.59	0.44
1:A:374:MET:SD	1:A:376:LEU:HD23	2.58	0.44
1:A:386:TYR:CB	1:A:397:THR:HG23	2.47	0.44
1:A:445:ILE:O	1:A:445:ILE:CG2	2.64	0.44
1:C:161:ASP:CB	1:C:164:ARG:O	2.65	0.44
1:C:169:ILE:HG22	1:C:192:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:PRO:HG2	1:C:172:ASN:N	2.33	0.44
1:C:251:LYS:O	1:C:251:LYS:CG	2.65	0.44
1:C:441:LEU:C	1:C:443:LYS:H	2.26	0.44
1:C:474:TRP:NE1	1:C:478:ASN:HD22	2.16	0.44
1:B:1:ILE:CG1	1:B:147:GLN:HG3	2.48	0.44
1:B:27:HIS:NE2	1:B:46:VAL:O	2.51	0.44
1:B:53:MET:HE2	1:B:130:ILE:CG2	2.45	0.44
1:B:85:GLN:OE1	1:B:94:ARG:NH1	2.47	0.44
1:B:93:LYS:HE2	1:B:95:THR:OG1	2.17	0.44
1:B:196:LEU:HD21	1:B:287:GLY:CA	2.48	0.44
1:B:344:GLN:OE1	1:B:352:LEU:CG	2.64	0.44
1:B:445:ILE:CG2	1:B:446:HIS:N	2.78	0.44
1:A:312:PHE:HB2	1:A:389:ILE:HD12	2.00	0.44
1:A:389:ILE:CG2	1:A:395:LYS:HA	2.47	0.44
1:C:332:TYR:CD1	1:C:332:TYR:C	2.95	0.44
2:D:51:TRP:HA	2:D:60:LYS:HZ2	1.81	0.44
2:D:67:ILE:CG2	2:D:68:LEU:N	2.80	0.44
1:B:71:ASP:O	1:B:113:LEU:CB	2.58	0.44
1:B:249:HIS:HE1	1:B:251:LYS:HB2	1.83	0.44
1:B:343:ALA:HB2	1:B:389:ILE:HG22	2.00	0.44
2:E:30:ILE:O	2:E:34:ASN:HB3	2.18	0.44
1:A:26:GLU:HA	1:A:288:HIS:HA	2.00	0.44
1:A:296:ASP:C	1:A:298:LEU:H	2.25	0.44
1:C:60:CYS:HB2	1:C:236:TRP:CZ3	2.52	0.44
1:C:94:ARG:HH21	1:C:94:ARG:HG2	1.82	0.44
1:C:97:VAL:HG13	1:C:250:ALA:O	2.18	0.44
1:C:225:TRP:HE3	1:C:237:ASN:HD22	1.65	0.44
1:C:276:GLU:H	1:C:276:GLU:CD	2.21	0.44
1:C:421:MET:HA	1:C:428:ALA:CB	2.48	0.44
1:C:475:LEU:HD21	2:D:52:LEU:HG	2.00	0.44
2:D:43:ALA:C	2:D:45:ALA:N	2.75	0.44
2:D:48:ALA:O	2:D:50:ALA:N	2.51	0.44
1:B:136:GLU:HG3	1:B:137:TYR:N	2.32	0.44
1:B:204:LEU:HG	1:B:205:THR:N	2.32	0.44
1:A:86:SER:HB3	1:B:88:THR:HG21	1.98	0.44
1:A:169:ILE:O	1:A:169:ILE:CG1	2.62	0.44
1:A:296:ASP:C	1:A:298:LEU:N	2.73	0.44
1:A:300:LEU:O	1:A:301:LYS:C	2.60	0.44
1:A:442:GLY:O	1:A:446:HIS:HB2	2.18	0.44
1:C:323:HIS:CD2	1:C:416:ARG:HH22	2.35	0.44
1:C:420:ARG:CD	1:C:431:PHE:CE2	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:VAL:O	1:C:424:LEU:HD23	2.18	0.44
1:C:437:ALA:O	1:C:440:SER:N	2.44	0.44
1:C:484:ILE:O	1:C:485:SER:C	2.61	0.44
2:D:26:THR:O	2:D:29:LEU:N	2.42	0.44
2:D:40:PRO:O	2:D:42:PHE:N	2.50	0.44
1:B:40:THR:HG21	1:B:359:ILE:O	2.18	0.44
1:B:282:GLY:O	1:B:284:LEU:HD23	2.18	0.44
1:B:420:ARG:O	1:B:424:LEU:HB2	2.17	0.44
1:B:459:GLY:HA2	2:E:9:THR:CG2	2.47	0.44
1:B:491:LEU:HA	1:B:494:VAL:CG2	2.47	0.44
2:E:30:ILE:O	2:E:34:ASN:CB	2.66	0.44
2:E:35:TRP:HE3	2:E:36:ILE:HG12	1.82	0.44
2:E:65:VAL:HG13	2:E:66:MET:HE2	1.99	0.44
2:F:58:SER:O	2:F:59:GLN:C	2.61	0.44
1:A:56:VAL:HG11	1:A:202:TYR:HE2	1.79	0.44
1:A:210:HIS:HB2	1:A:275:ALA:O	2.18	0.44
1:A:363:PRO:CB	1:A:374:MET:HE1	2.47	0.44
1:C:84:LYS:HD2	1:C:90:TYR:CZ	2.53	0.44
1:C:161:ASP:N	1:C:161:ASP:OD1	2.51	0.44
1:C:247:ASP:HB2	1:C:253:GLN:HA	1.99	0.44
1:C:283:ARG:CZ	1:C:283:ARG:CB	2.93	0.44
2:D:72:PRO:C	2:D:74:TYR:N	2.76	0.44
1:B:48:THR:HG23	1:B:48:THR:O	2.17	0.44
1:B:54:ALA:O	1:B:128:LYS:HA	2.18	0.44
2:E:56:SER:C	2:E:58:SER:N	2.73	0.44
2:F:59:GLN:O	2:F:60:LYS:C	2.61	0.44
1:A:137:TYR:CE2	1:A:289:LEU:HD13	2.53	0.43
1:C:70:SER:HB3	1:C:253:GLN:OE1	2.18	0.43
1:C:210:HIS:O	1:C:275:ALA:O	2.35	0.43
1:C:382:PHE:O	1:C:402:ARG:O	2.35	0.43
1:C:423:VAL:C	1:C:424:LEU:HG	2.42	0.43
1:C:466:ILE:O	1:C:470:THR:N	2.32	0.43
1:B:45:LEU:HA	1:B:139:ILE:HG23	1.99	0.43
1:B:331:GLN:OE1	1:B:371:ASN:ND2	2.51	0.43
1:A:324:GLY:HA3	1:A:402:ARG:NH2	2.32	0.43
1:C:300:LEU:CD1	1:C:362:ASN:HD22	2.32	0.43
1:C:357:ARG:HG2	1:C:358:LEU:H	1.83	0.43
1:C:434:VAL:HG23	1:C:439:ASN:ND2	2.33	0.43
1:C:503:SER:O	1:C:504:ALA:HB2	2.18	0.43
1:B:17:GLY:O	1:B:18:GLY:O	2.36	0.43
1:B:268:ALA:O	1:B:270:ALA:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:THR:HG23	1:B:355:VAL:HG23	2.00	0.43
1:B:364:VAL:C	1:B:374:MET:HE1	2.44	0.43
1:B:409:LYS:HZ2	1:B:413:ALA:HB2	1.82	0.43
2:E:56:SER:CB	2:E:59:GLN:HB2	2.25	0.43
2:F:50:ALA:O	2:F:51:TRP:C	2.59	0.43
1:A:24:VAL:HG11	1:A:424:LEU:CD2	2.49	0.43
1:A:39:PRO:CD	1:A:300:LEU:HD12	2.45	0.43
1:A:101:TRP:HH2	1:C:317:ILE:O	2.00	0.43
1:A:136:GLU:HB2	1:A:168:GLU:OE1	2.17	0.43
1:A:223:LEU:HD12	1:A:242:LEU:HD11	2.01	0.43
1:C:148:HIS:HB2	1:C:151:MET:HB3	1.99	0.43
1:C:310:ALA:CB	1:C:332:TYR:CE1	3.02	0.43
1:C:462:TRP:CG	1:C:463:PHE:N	2.84	0.43
1:A:292:ARG:HD2	1:A:292:ARG:N	2.31	0.43
1:C:50:VAL:HG22	1:C:135:LEU:CD1	2.48	0.43
1:C:324:GLY:HA3	1:C:402:ARG:HH21	1.83	0.43
1:C:462:TRP:O	1:C:463:PHE:C	2.61	0.43
1:B:331:GLN:HA	1:B:372:SER:O	2.18	0.43
1:B:459:GLY:CA	2:E:9:THR:HG23	2.49	0.43
1:A:13:GLU:HG2	1:A:34:MET:HE2	2.00	0.43
1:A:32:THR:HA	1:A:41:VAL:O	2.17	0.43
1:C:320:GLU:CD	1:C:324:GLY:HA2	2.43	0.43
2:D:4:LEU:N	2:D:5:PRO:HD3	2.33	0.43
1:B:204:LEU:HD12	1:B:204:LEU:HA	1.74	0.43
1:A:1:ILE:N	1:A:144:HIS:CD2	2.85	0.43
1:A:314:PHE:HB3	1:A:330:VAL:HA	2.00	0.43
1:A:365:ILE:HG21	1:A:368:SER:OG	2.19	0.43
1:C:26:GLU:C	1:C:28:GLY:H	2.26	0.43
1:C:27:HIS:CD2	1:C:27:HIS:N	2.87	0.43
1:C:75:PRO:O	1:C:76:THR:C	2.62	0.43
1:C:316:LYS:HE2	1:C:373:LYS:HE3	2.01	0.43
1:C:395:LYS:HD2	1:C:395:LYS:H	1.84	0.43
1:B:191:GLU:C	1:B:193:ARG:N	2.73	0.43
1:B:216:GLU:O	1:B:217:TRP:C	2.62	0.43
2:E:36:ILE:O	2:E:40:PRO:HB3	2.18	0.43
1:A:300:LEU:H	1:A:300:LEU:HD13	1.83	0.43
1:A:472:LEU:C	1:A:474:TRP:H	2.25	0.43
1:C:13:GLU:HG2	1:C:34:MET:CG	2.38	0.43
1:C:20:TRP:CZ2	1:C:434:VAL:CG1	3.01	0.43
1:C:202:TYR:CE2	1:C:215:LYS:HG3	2.54	0.43
1:C:466:ILE:HA	1:C:496:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LEU:CD2	1:B:298:LEU:HD11	2.47	0.43
1:B:383:GLY:O	1:B:401:HIS:HA	2.19	0.43
1:B:407:ILE:HG23	1:B:408:GLY:N	2.33	0.43
2:F:69:LEU:HD12	2:F:69:LEU:HA	1.70	0.43
1:A:259:GLY:HA3	1:C:262:GLU:HB3	2.00	0.43
1:C:20:TRP:CE3	1:C:292:ARG:NE	2.87	0.43
1:C:169:ILE:HD11	1:C:188:LEU:HD12	2.00	0.43
1:C:389:ILE:HD12	1:C:389:ILE:C	2.43	0.43
1:C:428:ALA:C	1:C:430:ASP:N	2.77	0.43
1:B:170:THR:C	1:B:172:ASN:H	2.24	0.43
1:B:227:ALA:O	1:B:229:ALA:N	2.51	0.43
1:A:67:ASP:HB2	1:A:118:LYS:HB2	2.00	0.43
1:A:127:GLY:HA3	1:A:218:PHE:CZ	2.53	0.43
1:A:242:LEU:HD11	2:D:2:VAL:HG23	1.99	0.43
1:A:398:HIS:C	1:A:398:HIS:HD1	2.27	0.43
1:A:441:LEU:O	1:A:442:GLY:C	2.62	0.43
1:C:71:ASP:OD2	1:C:82:LEU:HG	2.18	0.43
1:C:177:GLU:HA	1:C:186:LEU:O	2.19	0.43
1:C:401:HIS:ND1	1:C:402:ARG:N	2.67	0.43
2:D:27:LYS:HD2	2:F:2:VAL:CG2	2.48	0.43
2:D:63:TYR:HE1	2:F:62:ILE:CG2	2.32	0.43
1:B:357:ARG:HG3	1:B:358:LEU:N	2.34	0.43
2:E:21:GLU:O	2:E:22:SER:C	2.59	0.43
1:A:34:MET:HE3	1:A:359:ILE:HB	2.01	0.43
1:A:139:ILE:O	1:A:167:VAL:HG23	2.19	0.43
1:A:148:HIS:O	1:A:149:SER:C	2.61	0.43
1:A:229:ALA:H	1:B:73:ARG:HH22	1.67	0.43
1:A:248:ALA:O	1:A:249:HIS:C	2.62	0.43
1:A:253:GLN:HE21	1:A:253:GLN:HB3	1.47	0.43
1:A:376:LEU:HD12	1:A:376:LEU:C	2.44	0.43
1:C:1:ILE:HG21	1:C:4:ILE:CG1	2.49	0.43
1:C:19:THR:HG23	1:C:295:MET:C	2.44	0.43
1:C:119:PHE:CD1	1:C:120:ALA:N	2.87	0.43
2:D:69:LEU:CD2	2:F:74:TYR:CD2	3.02	0.43
1:B:2:ARG:NH1	1:B:140:MET:HB3	2.34	0.43
1:B:40:THR:HG23	1:B:40:THR:O	2.18	0.43
1:B:97:VAL:HG23	1:B:113:LEU:HD12	2.01	0.43
1:B:375:MET:C	1:B:376:LEU:CG	2.78	0.43
1:A:50:VAL:HA	1:A:134:ASN:O	2.19	0.42
1:A:350:GLN:HE21	1:A:350:GLN:HB2	1.65	0.42
1:A:424:LEU:HA	1:A:424:LEU:HD23	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:MET:HE2	1:C:376:LEU:CD1	2.49	0.42
2:D:75:SER:HB2	2:F:9:THR:OG1	2.19	0.42
1:B:65:ILE:CG2	1:B:117:ALA:HB1	2.49	0.42
1:B:216:GLU:C	1:B:218:PHE:N	2.77	0.42
1:B:314:PHE:CZ	1:B:398:HIS:HB2	2.53	0.42
2:F:42:PHE:CZ	2:F:46:ALA:HB2	2.54	0.42
1:A:386:TYR:HB3	1:A:397:THR:HG23	2.00	0.42
1:A:410:ALA:C	1:A:412:GLU:H	2.26	0.42
1:C:185:SER:O	1:C:297:LYS:CB	2.63	0.42
1:C:444:GLY:C	1:C:446:HIS:N	2.74	0.42
1:C:455:SER:O	1:C:456:LEU:C	2.60	0.42
1:C:462:TRP:CD1	1:C:463:PHE:H	2.37	0.42
1:B:28:GLY:C	1:B:29:GLY:O	2.62	0.42
1:B:128:LYS:O	1:B:202:TYR:CB	2.67	0.42
1:B:472:LEU:CD2	1:B:475:LEU:HD12	2.48	0.42
1:B:474:TRP:O	1:B:478:ASN:HB3	2.19	0.42
2:E:22:SER:O	2:E:23:ARG:CB	2.67	0.42
2:E:62:ILE:O	2:E:63:TYR:C	2.60	0.42
1:A:23:VAL:HG13	1:A:25:LEU:CD2	2.45	0.42
1:A:271:GLY:HA2	2:D:11:LYS:HG3	2.01	0.42
1:C:258:LEU:CD1	2:D:20:LEU:HD21	2.49	0.42
1:C:373:LYS:HZ3	1:C:373:LYS:CB	2.31	0.42
2:D:9:THR:HG21	2:D:10:ARG:HH21	1.83	0.42
2:D:64:LEU:O	2:D:64:LEU:HD22	2.18	0.42
1:B:56:VAL:O	1:B:227:ALA:CB	2.66	0.42
1:B:202:TYR:HE1	1:B:215:LYS:HB2	1.81	0.42
1:B:312:PHE:CZ	1:B:332:TYR:HE2	2.37	0.42
1:B:364:VAL:C	1:B:374:MET:CE	2.92	0.42
1:B:388:VAL:O	1:B:388:VAL:HG23	2.18	0.42
2:E:6:SER:C	2:E:8:SER:H	2.25	0.42
2:E:19:TRP:CD1	2:E:20:LEU:HD11	2.54	0.42
1:A:297:LYS:N	1:A:297:LYS:HD2	2.35	0.42
1:C:169:ILE:HD13	1:C:190:CYS:SG	2.59	0.42
1:C:204:LEU:N	1:C:204:LEU:HD12	2.33	0.42
1:C:272:ALA:O	2:F:19:TRP:HB2	2.20	0.42
1:C:376:LEU:CD1	1:C:376:LEU:N	2.82	0.42
1:C:475:LEU:HD11	2:D:52:LEU:CB	2.45	0.42
1:B:45:LEU:C	1:B:45:LEU:CD2	2.93	0.42
1:B:82:LEU:O	1:B:82:LEU:CG	2.57	0.42
1:B:230:ASP:O	1:B:231:THR:C	2.63	0.42
1:B:419:LYS:C	1:B:421:MET:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:GLY:O	1:B:454:LYS:HB3	2.19	0.42
2:E:21:GLU:O	2:E:24:GLU:N	2.52	0.42
1:A:2:ARG:NH2	1:A:44:GLU:OE2	2.53	0.42
1:A:286:SER:HB2	2:D:16:SER:HB2	2.01	0.42
1:C:341:VAL:HG23	1:C:365:ILE:HG12	2.01	0.42
1:C:392:GLY:O	1:C:395:LYS:CD	2.67	0.42
1:C:444:GLY:C	1:C:446:HIS:H	2.27	0.42
1:C:460:MET:HE3	1:C:464:SER:OG	2.20	0.42
2:D:63:TYR:HE1	2:F:62:ILE:HG23	1.83	0.42
1:B:38:LYS:CG	1:B:298:LEU:HB3	2.47	0.42
2:E:19:TRP:CD1	2:E:20:LEU:CD1	3.02	0.42
1:A:1:ILE:O	1:A:2:ARG:C	2.61	0.42
1:A:20:TRP:CZ3	1:A:434:VAL:HG12	2.51	0.42
1:A:252:ARG:HB2	1:A:252:ARG:HH11	1.80	0.42
1:A:290:LYS:HE2	1:A:430:ASP:OD2	2.19	0.42
1:A:463:PHE:CD1	1:A:463:PHE:O	2.72	0.42
1:C:47:THR:O	1:C:138:ARG:HB2	2.19	0.42
1:C:74:CYS:HB3	1:C:75:PRO:CD	2.44	0.42
1:C:276:GLU:OE2	1:C:283:ARG:HG2	2.20	0.42
2:D:70:ILE:O	2:D:71:ALA:C	2.62	0.42
2:D:74:TYR:O	2:D:75:SER:C	2.62	0.42
1:B:73:ARG:HD2	1:B:77:GLN:CG	2.48	0.42
1:B:76:THR:HB	1:B:77:GLN:OE1	2.20	0.42
1:B:133:GLU:OE2	1:B:193:ARG:NH1	2.52	0.42
1:B:142:SER:OG	1:B:164:ARG:HG2	2.20	0.42
1:B:202:TYR:HD1	1:B:202:TYR:H	1.66	0.42
1:B:217:TRP:C	1:B:217:TRP:CE3	2.98	0.42
1:B:360:THR:OG1	1:B:377:GLU:N	2.53	0.42
1:B:395:LYS:O	1:B:397:THR:HG23	2.19	0.42
2:E:24:GLU:C	2:E:24:GLU:CD	2.88	0.42
1:A:101:TRP:HB2	1:A:108:PHE:CZ	2.54	0.42
1:A:204:LEU:HD21	1:A:211:TRP:HB2	2.00	0.42
1:A:441:LEU:O	1:A:444:GLY:N	2.53	0.42
1:A:470:THR:O	1:A:472:LEU:N	2.52	0.42
1:C:281:LYS:HB2	1:C:281:LYS:HE3	1.79	0.42
1:C:398:HIS:CD2	1:B:172:ASN:HA	2.55	0.42
1:B:67:ASP:OD1	1:B:67:ASP:C	2.62	0.42
1:B:225:TRP:HB3	1:B:237:ASN:HD22	1.83	0.42
1:B:257:VAL:O	1:B:257:VAL:HG13	2.19	0.42
1:B:257:VAL:O	1:B:258:LEU:C	2.62	0.42
2:E:4:LEU:HD23	2:E:5:PRO:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLY:HA3	1:C:261:GLN:NE2	2.35	0.42
1:A:396:ILE:N	1:A:396:ILE:CD1	2.83	0.42
1:C:353:THR:HG23	1:C:354:PRO:HD2	2.02	0.42
2:D:74:TYR:HE2	2:F:69:LEU:O	2.02	0.42
1:B:442:GLY:O	1:B:443:LYS:C	2.63	0.42
2:E:29:LEU:O	2:E:30:ILE:C	2.62	0.42
1:A:12:VAL:CG1	1:A:432:GLY:HA3	2.42	0.42
1:A:20:TRP:HE3	1:A:434:VAL:CG1	2.23	0.42
1:A:87:ASP:C	1:A:89:GLN:N	2.78	0.42
1:A:211:TRP:HE1	2:D:19:TRP:CD1	2.38	0.42
1:A:234:PRO:O	1:A:235:HIS:C	2.61	0.42
1:A:496:ILE:O	1:A:499:SER:CB	2.68	0.42
1:C:23:VAL:HG21	1:C:43:ILE:HD11	2.02	0.42
2:D:73:ALA:HB1	2:F:73:ALA:CB	2.50	0.42
1:B:9:ARG:HG3	1:B:9:ARG:HH11	1.84	0.42
1:B:314:PHE:O	1:B:315:THR:C	2.59	0.42
1:B:317:ILE:O	1:B:317:ILE:HG23	2.19	0.42
1:A:74:CYS:HA	1:A:99:ARG:CD	2.50	0.42
1:A:223:LEU:CD1	1:A:242:LEU:HD11	2.50	0.42
1:A:248:ALA:HB2	1:A:252:ARG:NH1	2.35	0.42
1:A:272:ALA:HB2	2:D:7:HIS:CE1	2.54	0.42
1:C:230:ASP:OD1	1:C:230:ASP:C	2.63	0.42
1:B:41:VAL:HG12	1:B:42:ASP:N	2.35	0.42
1:B:158:HIS:CG	1:B:164:ARG:HD3	2.55	0.42
1:B:186:LEU:HB3	1:B:293:LEU:CD1	2.50	0.42
1:B:221:ILE:HG12	1:B:223:LEU:HD11	2.00	0.42
2:E:41:GLY:C	2:E:43:ALA:N	2.76	0.42
2:F:56:SER:HB3	2:F:59:GLN:HG3	1.99	0.42
2:F:70:ILE:O	2:F:71:ALA:C	2.63	0.42
1:A:65:ILE:HD12	1:A:257:VAL:CG2	2.39	0.41
1:A:155:ASP:C	1:A:155:ASP:OD1	2.62	0.41
1:A:162:GLU:C	1:A:162:GLU:CD	2.87	0.41
1:A:313:THR:HG22	1:A:331:GLN:O	2.20	0.41
1:C:107:LEU:HD12	1:C:107:LEU:HA	1.80	0.41
1:C:171:PRO:HG2	1:C:172:ASN:H	1.85	0.41
1:C:210:HIS:C	1:C:211:TRP:CE3	2.98	0.41
1:C:351:THR:HG22	1:C:388:VAL:HG21	2.02	0.41
2:D:17:GLN:H	2:D:17:GLN:HG3	1.45	0.41
1:B:20:TRP:HE3	1:B:292:ARG:NE	2.18	0.41
1:B:82:LEU:HD22	1:B:114:VAL:O	2.19	0.41
1:B:163:ASN:OD1	1:B:163:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ASP:O	1:B:201:LEU:HD22	2.19	0.41
2:F:26:THR:HG23	2:F:27:LYS:N	2.35	0.41
1:A:1:ILE:HG12	1:A:147:GLN:HB2	2.00	0.41
1:A:215:LYS:NZ	1:A:215:LYS:CB	2.82	0.41
1:A:359:ILE:HD11	1:A:377:GLU:CG	2.31	0.41
1:C:317:ILE:HA	1:C:318:PRO:HD3	1.85	0.41
1:C:389:ILE:HD11	1:C:396:ILE:H	1.84	0.41
1:C:389:ILE:CD1	1:C:396:ILE:H	2.32	0.41
1:B:2:ARG:CA	1:B:151:MET:HE3	2.50	0.41
1:B:88:THR:HG23	1:B:89:GLN:N	2.35	0.41
1:B:371:ASN:O	1:B:371:ASN:CG	2.63	0.41
1:B:423:VAL:HG12	1:B:424:LEU:HD12	2.01	0.41
1:B:460:MET:HB2	1:B:464:SER:OG	2.20	0.41
1:A:40:THR:OG1	1:A:359:ILE:O	2.36	0.41
1:A:74:CYS:C	1:A:76:THR:N	2.78	0.41
1:A:191:GLU:HB3	1:A:194:THR:OG1	2.20	0.41
1:A:207:ASN:C	1:A:208:ASN:OD1	2.64	0.41
1:A:332:TYR:O	1:A:335:THR:HG22	2.20	0.41
1:C:34:MET:HE2	1:C:359:ILE:HG23	1.98	0.41
1:C:97:VAL:HG23	1:C:113:LEU:CB	2.50	0.41
2:D:19:TRP:CE2	2:D:20:LEU:HG	2.55	0.41
1:B:45:LEU:CA	1:B:139:ILE:HG22	2.50	0.41
1:B:206:MET:O	1:B:207:ASN:HB3	2.19	0.41
1:B:215:LYS:O	1:B:218:PHE:HB3	2.21	0.41
1:B:454:LYS:HB3	1:B:454:LYS:HE3	1.91	0.41
2:E:31:ARG:HG3	2:E:32:VAL:N	2.36	0.41
1:A:72:SER:O	1:A:73:ARG:HG2	2.19	0.41
1:A:196:LEU:CG	1:A:287:GLY:HA2	2.50	0.41
1:A:236:TRP:CB	1:A:239:LYS:HG2	2.50	0.41
1:A:290:LYS:NZ	1:A:430:ASP:HB3	2.36	0.41
1:C:47:THR:CG2	1:C:49:THR:HG23	2.49	0.41
1:C:73:ARG:HG2	1:C:78:GLY:C	2.45	0.41
1:C:180:LEU:HD23	1:C:185:SER:HA	2.01	0.41
1:C:240:GLU:O	1:C:241:ALA:C	2.62	0.41
1:C:306:SER:O	1:C:339:CYS:HB2	2.19	0.41
1:C:441:LEU:C	1:C:443:LYS:N	2.79	0.41
1:C:488:CYS:C	1:C:490:ALA:H	2.28	0.41
2:D:1:ALA:C	2:D:3:THR:N	2.77	0.41
2:D:48:ALA:C	2:D:50:ALA:N	2.77	0.41
2:D:70:ILE:HD13	2:D:70:ILE:C	2.46	0.41
1:B:7:SER:CA	1:B:322:LEU:CD1	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LEU:HD12	1:B:294:LYS:H	1.84	0.41
1:B:456:LEU:HD12	1:B:457:PHE:CE1	2.56	0.41
1:B:481:ASN:HD22	1:B:483:SER:HB3	1.82	0.41
2:E:31:ARG:NH2	2:E:31:ARG:CB	2.83	0.41
1:A:38:LYS:O	1:A:39:PRO:C	2.64	0.41
1:A:139:ILE:HB	1:A:167:VAL:CG2	2.43	0.41
1:A:366:THR:HG22	1:A:367:GLU:N	2.35	0.41
1:C:40:THR:HG22	1:C:361:ALA:H	1.85	0.41
2:D:69:LEU:HD23	2:F:74:TYR:HD2	1.85	0.41
1:B:19:THR:HB	1:B:295:MET:CB	2.43	0.41
1:B:456:LEU:C	1:B:457:PHE:CD1	2.99	0.41
1:A:1:ILE:H1	1:A:144:HIS:CD2	2.39	0.41
1:A:101:TRP:HE3	1:C:327:THR:HG1	1.62	0.41
1:A:147:GLN:HE22	1:A:151:MET:HE3	1.86	0.41
1:A:190:CYS:HB3	1:A:290:LYS:O	2.21	0.41
1:A:204:LEU:CD2	1:A:211:TRP:HB2	2.50	0.41
1:A:392:GLY:O	1:A:395:LYS:CB	2.68	0.41
1:C:42:ASP:N	1:C:142:SER:O	2.49	0.41
1:C:312:PHE:CZ	1:C:341:VAL:HG21	2.55	0.41
1:C:420:ARG:CG	1:C:431:PHE:HE2	2.34	0.41
1:B:245:PHE:HA	1:B:255:VAL:HG12	2.02	0.41
1:B:290:LYS:O	1:B:290:LYS:HG2	2.20	0.41
1:A:99:ARG:HB3	1:A:99:ARG:CZ	2.51	0.41
1:C:21:VAL:O	1:C:23:VAL:HG12	2.21	0.41
1:C:41:VAL:HG22	1:C:42:ASP:N	2.35	0.41
1:C:52:ASN:O	1:C:134:ASN:OD1	2.39	0.41
1:C:399:HIS:NE2	1:B:193:ARG:HB3	2.35	0.41
1:B:6:VAL:HG22	1:B:9:ARG:HB3	2.02	0.41
1:B:224:PRO:HG3	1:B:242:LEU:HD13	2.03	0.41
1:A:72:SER:HB2	1:A:99:ARG:NH1	2.33	0.41
1:A:445:ILE:O	1:A:445:ILE:HG22	2.20	0.41
1:A:454:LYS:CG	1:A:455:SER:N	2.81	0.41
1:C:471:LEU:HD21	2:F:62:ILE:HG12	2.01	0.41
1:B:1:ILE:CG2	1:B:147:GLN:CG	2.99	0.41
1:B:213:VAL:HG11	1:B:269:LEU:HD21	2.02	0.41
1:B:329:GLU:OE2	1:B:375:MET:HB2	2.21	0.41
1:B:395:LYS:C	1:B:397:THR:N	2.78	0.41
1:B:494:VAL:O	1:B:497:PHE:HB3	2.21	0.41
2:E:45:ALA:O	2:E:46:ALA:C	2.63	0.41
2:F:3:THR:HG22	2:F:5:PRO:CG	2.51	0.41
2:F:68:LEU:HD23	2:F:68:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG21	1:A:140:MET:CG	2.39	0.41
1:A:68:MET:SD	1:A:255:VAL:HB	2.61	0.41
1:A:71:ASP:OD1	1:A:72:SER:N	2.54	0.41
1:A:226:HIS:CE1	1:A:230:ASP:HB3	2.56	0.41
1:A:348:ASP:C	1:A:350:GLN:N	2.75	0.41
1:A:365:ILE:CG2	1:A:368:SER:HB2	2.48	0.41
1:A:490:ALA:C	1:A:492:GLY:H	2.29	0.41
1:C:73:ARG:HB2	1:C:79:GLU:C	2.46	0.41
1:C:118:LYS:HB3	1:C:118:LYS:NZ	2.36	0.41
1:C:206:MET:C	1:C:208:ASN:H	2.28	0.41
1:C:291:CYS:HB3	1:C:292:ARG:H	1.47	0.41
1:C:322:LEU:CD1	1:C:322:LEU:H	2.34	0.41
1:C:471:LEU:HD13	1:C:471:LEU:C	2.46	0.41
2:D:30:ILE:O	2:D:31:ARG:C	2.62	0.41
2:D:40:PRO:C	2:D:42:PHE:H	2.29	0.41
2:D:67:ILE:C	2:D:70:ILE:HG22	2.46	0.41
1:B:19:THR:OG1	1:B:295:MET:HG2	2.21	0.41
1:B:23:VAL:O	1:B:23:VAL:HG13	2.21	0.41
1:B:61:TYR:CZ	1:B:123:LYS:HB3	2.56	0.41
1:B:131:GLN:HE21	1:B:131:GLN:HB3	1.67	0.41
1:B:225:TRP:C	1:B:225:TRP:CD2	2.98	0.41
1:B:432:GLY:O	1:B:434:VAL:N	2.54	0.41
2:E:31:ARG:NH2	2:E:31:ARG:HB3	2.36	0.41
2:E:54:GLY:C	2:E:56:SER:N	2.79	0.41
2:E:64:LEU:O	2:E:67:ILE:HG23	2.20	0.41
2:F:65:VAL:C	2:F:67:ILE:H	2.29	0.41
1:A:38:LYS:HG3	1:A:298:LEU:CB	2.51	0.41
1:A:61:TYR:CE2	1:A:123:LYS:NZ	2.89	0.41
1:A:147:GLN:O	1:A:375:MET:N	2.52	0.41
1:A:314:PHE:CD2	1:A:318:PRO:HD3	2.54	0.41
1:A:335:THR:O	1:A:336:ASP:CG	2.64	0.41
1:A:466:ILE:HG13	1:A:467:LEU:N	2.36	0.41
1:C:62:GLU:CG	1:C:122:SER:HB3	2.50	0.41
1:C:81:TYR:CD1	1:C:81:TYR:C	2.99	0.41
1:C:98:ASP:OD1	1:C:110:LYS:CG	2.60	0.41
1:C:213:VAL:HG12	1:C:214:HIS:O	2.21	0.41
1:C:355:VAL:CG1	1:C:356:GLY:H	2.34	0.41
1:C:420:ARG:HD2	1:C:431:PHE:HD2	1.75	0.41
1:C:488:CYS:C	1:C:490:ALA:N	2.79	0.41
2:D:19:TRP:HA	2:D:19:TRP:CE3	2.56	0.41
2:D:23:ARG:O	2:D:27:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:PHE:O	2:D:46:ALA:CB	2.69	0.41
1:B:217:TRP:CD1	2:E:7:HIS:N	2.89	0.41
1:B:476:GLY:HA3	1:B:489:LEU:HD12	2.02	0.41
2:F:42:PHE:CE2	2:F:46:ALA:HB2	2.56	0.41
1:C:94:ARG:HG2	1:C:94:ARG:NH2	2.37	0.40
1:C:257:VAL:O	1:C:258:LEU:HB3	2.21	0.40
1:C:429:TRP:O	1:C:430:ASP:OD1	2.39	0.40
1:B:50:VAL:HB	1:B:53:MET:CE	2.51	0.40
1:B:447:GLN:C	1:B:449:PHE:N	2.78	0.40
2:E:35:TRP:CE3	2:E:36:ILE:HG12	2.56	0.40
1:A:59:TYR:HD1	1:A:59:TYR:HA	1.74	0.40
1:A:89:GLN:HA	1:A:239:LYS:HZ3	1.87	0.40
1:A:326:VAL:HG23	1:A:380:PRO:HG3	2.02	0.40
1:A:349:MET:HB2	1:A:386:TYR:CD2	2.56	0.40
1:A:405:SER:HB2	1:A:408:GLY:CA	2.39	0.40
1:C:143:VAL:O	1:C:163:ASN:OD1	2.38	0.40
1:C:432:GLY:O	1:C:433:SER:C	2.64	0.40
2:D:73:ALA:HB1	2:F:73:ALA:HB1	2.03	0.40
1:B:108:PHE:HD1	1:B:109:GLY:N	2.20	0.40
1:B:153:VAL:HG23	1:B:154:ASN:N	2.36	0.40
1:B:226:HIS:NE2	1:B:231:THR:HA	2.36	0.40
2:F:53:LEU:HD13	2:F:53:LEU:HA	1.98	0.40
1:A:152:ILE:HD11	1:C:102:GLY:HA3	2.03	0.40
1:A:398:HIS:O	1:A:399:HIS:C	2.65	0.40
1:C:171:PRO:HB2	1:C:193:ARG:CD	2.43	0.40
1:C:312:PHE:CE2	1:C:341:VAL:HG11	2.57	0.40
2:D:67:ILE:O	2:D:68:LEU:C	2.63	0.40
1:B:1:ILE:CG2	1:B:147:GLN:HG3	2.51	0.40
1:B:24:VAL:HG11	1:B:424:LEU:CD2	2.52	0.40
1:B:101:TRP:HD1	1:B:108:PHE:CE2	2.38	0.40
1:B:211:TRP:CG	1:B:269:LEU:HD11	2.57	0.40
1:B:283:ARG:CG	1:B:283:ARG:NH1	2.82	0.40
2:E:42:PHE:O	2:E:46:ALA:HB3	2.19	0.40
2:E:53:LEU:C	2:E:55:SER:N	2.76	0.40
1:A:20:TRP:HE1	1:A:292:ARG:HG2	1.86	0.40
1:A:60:CYS:HB2	1:A:236:TRP:CH2	2.57	0.40
1:A:61:TYR:CD1	1:A:61:TYR:N	2.90	0.40
1:A:65:ILE:HG13	1:A:257:VAL:HG13	2.04	0.40
1:A:73:ARG:CG	1:A:80:ALA:HB2	2.51	0.40
1:A:242:LEU:HD11	2:D:2:VAL:CG2	2.52	0.40
1:A:360:THR:HG21	1:A:377:GLU:N	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:VAL:HG12	1:C:32:THR:O	2.21	0.40
1:B:3:CYS:O	1:B:9:ARG:CZ	2.70	0.40
1:B:131:GLN:HG2	1:B:133:GLU:O	2.21	0.40
1:B:209:LYS:O	1:B:211:TRP:CE2	2.73	0.40
1:B:237:ASN:O	1:B:238:ASN:HB2	2.21	0.40
1:B:264:ALA:O	2:E:4:LEU:CD1	2.70	0.40
1:B:373:LYS:O	1:B:373:LYS:CG	2.58	0.40
1:B:444:GLY:O	1:B:447:GLN:HB2	2.21	0.40
1:A:9:ARG:NH1	1:A:11:PHE:HZ	2.18	0.40
1:A:34:MET:HG2	1:A:34:MET:O	2.21	0.40
1:A:436:GLY:O	1:A:440:SER:HB3	2.21	0.40
1:C:33:VAL:N	1:C:41:VAL:O	2.52	0.40
1:B:101:TRP:CD1	1:B:101:TRP:N	2.89	0.40
1:B:263:GLY:C	1:B:266:HIS:H	2.29	0.40
1:B:312:PHE:CE1	1:B:332:TYR:CD2	3.09	0.40
1:B:386:TYR:CD2	1:B:386:TYR:N	2.89	0.40
2:E:40:PRO:CG	2:E:41:GLY:N	2.84	0.40
2:E:60:LYS:HE2	2:E:60:LYS:HB3	1.70	0.40
2:F:63:TYR:O	2:F:67:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/504 (100%)	332 (66%)	123 (24%)	47 (9%)	0	7
1	B	502/504 (100%)	331 (66%)	104 (21%)	67 (13%)	0	3
1	C	502/504 (100%)	365 (73%)	96 (19%)	41 (8%)	0	9
2	D	73/75 (97%)	37 (51%)	26 (36%)	10 (14%)	0	3
2	E	73/75 (97%)	48 (66%)	20 (27%)	5 (7%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	73/75 (97%)	43 (59%)	24 (33%)	6 (8%)	0	9
All	All	1725/1737 (99%)	1156 (67%)	393 (23%)	176 (10%)	1	6

All (176) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	132	PRO
1	A	322	LEU
1	A	323	HIS
1	A	357	ARG
1	A	359	ILE
1	A	465	GLN
1	C	37	ASP
1	C	66	SER
1	C	85	GLN
1	C	249	HIS
1	C	300	LEU
1	C	334	GLY
1	C	385	SER
1	C	433	SER
1	C	462	TRP
2	D	18	THR
1	B	7	SER
1	B	14	GLY
1	B	62	GLU
1	B	75	PRO
1	B	82	LEU
1	B	134	ASN
1	B	176	ALA
1	B	198	PHE
1	B	216	GLU
1	B	217	TRP
1	B	223	LEU
1	B	260	SER
1	B	303	VAL
1	B	310	ALA
2	E	55	SER
2	E	74	TYR
2	F	28	HIS
2	F	30	ILE
1	A	16	SER

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Mol	Chain	Res	Type
1	A	23	VAL
1	A	75	PRO
1	A	151	MET
1	A	239	LYS
1	A	297	LYS
1	A	339	CYS
1	A	374	MET
1	A	378	LEU
1	A	425	GLY
1	C	76	THR
1	C	88	THR
1	C	134	ASN
1	C	161	ASP
1	C	195	GLY
1	C	234	PRO
1	C	258	LEU
1	C	264	ALA
1	C	307	LEU
1	C	348	ASP
1	C	392	GLY
1	C	442	GLY
1	C	444	GLY
1	C	456	LEU
2	D	6	SER
2	D	20	LEU
2	D	22	SER
2	D	24	GLU
1	B	18	GLY
1	B	29	GLY
1	B	45	LEU
1	B	46	VAL
1	B	63	ALA
1	B	111	GLY
1	B	147	GLN
1	B	181	GLY
1	B	195	GLY
1	B	234	PRO
1	B	333	ALA
1	B	335	THR
1	B	352	LEU
1	B	367	GLU
1	B	397	THR

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Mol	Chain	Res	Type
1	B	425	GLY
1	B	433	SER
1	B	434	VAL
1	B	462	TRP
1	B	476	GLY
1	A	8	ASN
1	A	154	ASN
1	A	157	GLY
1	A	216	GLU
1	A	266	HIS
1	A	344	GLN
1	A	352	LEU
1	A	377	GLU
1	A	481	ASN
1	C	2	ARG
1	C	9	ARG
1	C	262	GLU
1	C	337	GLY
1	C	380	PRO
2	D	5	PRO
2	D	12	LEU
2	D	48	ALA
2	D	49	ILE
1	B	15	MET
1	B	51	SER
1	B	83	ASP
1	B	136	GLU
1	B	152	ILE
1	B	153	VAL
1	B	182	GLY
1	B	224	PRO
1	B	239	LYS
1	B	269	LEU
1	B	286	SER
1	B	360	THR
1	B	361	ALA
1	B	371	ASN
1	B	387	ILE
1	B	427	THR
1	B	436	GLY
1	B	453	PHE
1	A	88	THR

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Mol	Chain	Res	Type
1	A	150	GLY
1	A	262	GLU
1	A	318	PRO
1	A	338	PRO
1	A	355	VAL
1	A	361	ALA
1	A	426	ASP
1	A	436	GLY
1	C	382	PHE
1	C	485	SER
1	B	241	ALA
1	B	422	ALA
1	B	460	MET
1	B	483	SER
1	B	484	ILE
2	E	32	VAL
2	F	19	TRP
2	F	62	ILE
2	F	68	LEU
1	A	146	SER
1	A	200	ASP
1	A	390	GLY
1	A	471	LEU
1	A	498	LEU
1	C	4	ILE
1	C	132	PRO
1	C	168	GLU
1	C	222	PRO
1	C	352	LEU
1	C	425	GLY
1	C	458	GLY
2	D	42	PHE
1	B	39	PRO
1	B	396	ILE
1	B	452	ALA
2	E	2	VAL
2	E	11	LYS
2	F	22	SER
1	A	143	VAL
1	A	409	LYS
1	A	97	VAL
1	A	234	PRO

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Mol	Chain	Res	Type
1	A	388	VAL
1	C	445	ILE
1	B	6	VAL
1	B	56	VAL
1	A	4	ILE
1	A	468	ILE
1	C	5	GLY
1	C	145	GLY
1	B	192	PRO
1	C	318	PRO
1	B	21	VAL
1	B	334	GLY
1	B	432	GLY
1	B	448	ILE

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	410/410 (100%)	333 (81%)	77 (19%)	1	10
1	B	410/410 (100%)	337 (82%)	73 (18%)	2	12
1	C	410/410 (100%)	344 (84%)	66 (16%)	2	14
2	D	64/64 (100%)	52 (81%)	12 (19%)	1	10
2	E	64/64 (100%)	53 (83%)	11 (17%)	2	13
2	F	64/64 (100%)	55 (86%)	9 (14%)	3	18
All	All	1422/1422 (100%)	1174 (83%)	248 (17%)	4	12

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	22	ASP
1	A	25	LEU
1	A	26	GLU

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Mol	Chain	Res	Type
1	A	30	CYS
1	A	34	MET
1	A	38	LYS
1	A	42	ASP
1	A	43	ILE
1	A	56	VAL
1	A	58	SER
1	A	74	CYS
1	A	83	ASP
1	A	92	CYS
1	A	95	THR
1	A	96	LEU
1	A	113	LEU
1	A	124	LYS
1	A	132	PRO
1	A	135	LEU
1	A	143	VAL
1	A	152	ILE
1	A	162	GLU
1	A	163	ASN
1	A	167	VAL
1	A	177	GLU
1	A	180	LEU
1	A	186	LEU
1	A	188	LEU
1	A	189	ASP
1	A	193	ARG
1	A	204	LEU
1	A	205	THR
1	A	215	LYS
1	A	225	TRP
1	A	240	GLU
1	A	244	GLU
1	A	252	ARG
1	A	253	GLN
1	A	257	VAL
1	A	258	LEU
1	A	261	GLN
1	A	265	VAL
1	A	266	HIS
1	A	291	CYS
1	A	296	ASP

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Mol	Chain	Res	Type
1	A	297	LYS
1	A	299	ARG
1	A	307	LEU
1	A	314	PHE
1	A	320	GLU
1	A	323	HIS
1	A	329	GLU
1	A	330	VAL
1	A	338	PRO
1	A	348	ASP
1	A	349	MET
1	A	350	GLN
1	A	358	LEU
1	A	378	LEU
1	A	386	TYR
1	A	388	VAL
1	A	389	ILE
1	A	395	LYS
1	A	399	HIS
1	A	409	LYS
1	A	421	MET
1	A	438	LEU
1	A	439	ASN
1	A	443	LYS
1	A	445	ILE
1	A	446	HIS
1	A	454	LYS
1	A	456	LEU
1	A	464	SER
1	A	466	ILE
1	A	495	LEU
1	C	1	ILE
1	C	4	ILE
1	C	13	GLU
1	C	21	VAL
1	C	23	VAL
1	C	25	LEU
1	C	30	CYS
1	C	33	VAL
1	C	82	LEU
1	C	90	TYR
1	C	92	CYS

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Mol	Chain	Res	Type
1	C	93	LYS
1	C	99	ARG
1	C	115	THR
1	C	118	LYS
1	C	124	LYS
1	C	125	MET
1	C	133	GLU
1	C	134	ASN
1	C	148	HIS
1	C	168	GLU
1	C	188	LEU
1	C	203	TYR
1	C	210	HIS
1	C	233	THR
1	C	234	PRO
1	C	238	ASN
1	C	240	GLU
1	C	253	GLN
1	C	260	SER
1	C	262	GLU
1	C	283	ARG
1	C	284	LEU
1	C	286	SER
1	C	292	ARG
1	C	293	LEU
1	C	296	ASP
1	C	299	ARG
1	C	300	LEU
1	C	301	LYS
1	C	308	CYS
1	C	316	LYS
1	C	318	PRO
1	C	327	THR
1	C	329	GLU
1	C	330	VAL
1	C	336	ASP
1	C	340	LYS
1	C	342	PRO
1	C	345	MET
1	C	351	THR
1	C	373	LYS
1	C	374	MET

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Mol	Chain	Res	Type
1	C	376	LEU
1	C	378	LEU
1	C	382	PHE
1	C	389	ILE
1	C	395	LYS
1	C	396	ILE
1	C	400	TRP
1	C	409	LYS
1	C	415	VAL
1	C	457	PHE
1	C	475	LEU
1	C	499	SER
1	C	500	THR
2	D	3	THR
2	D	9	THR
2	D	10	ARG
2	D	12	LEU
2	D	14	THR
2	D	18	THR
2	D	21	GLU
2	D	25	TYR
2	D	29	LEU
2	D	66	MET
2	D	68	LEU
2	D	70	ILE
1	B	9	ARG
1	B	11	PHE
1	B	15	MET
1	B	19	THR
1	B	21	VAL
1	B	22	ASP
1	B	30	CYS
1	B	43	ILE
1	B	45	LEU
1	B	53	MET
1	B	76	THR
1	B	83	ASP
1	B	86	SER
1	B	88	THR
1	B	108	PHE
1	B	113	LEU
1	B	131	GLN

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Mol	Chain	Res	Type
1	B	134	ASN
1	B	139	ILE
1	B	141	LEU
1	B	143	VAL
1	B	155	ASP
1	B	167	VAL
1	B	169	ILE
1	B	170	THR
1	B	174	PRO
1	B	175	ARG
1	B	180	LEU
1	B	196	LEU
1	B	201	LEU
1	B	206	MET
1	B	210	HIS
1	B	211	TRP
1	B	216	GLU
1	B	221	ILE
1	B	225	TRP
1	B	237	ASN
1	B	240	GLU
1	B	258	LEU
1	B	269	LEU
1	B	281	LYS
1	B	283	ARG
1	B	284	LEU
1	B	289	LEU
1	B	290	LYS
1	B	307	LEU
1	B	318	PRO
1	B	325	THR
1	B	326	VAL
1	B	328	VAL
1	B	341	VAL
1	B	344	GLN
1	B	349	MET
1	B	352	LEU
1	B	353	THR
1	B	357	ARG
1	B	377	GLU
1	B	382	PHE
1	B	388	VAL

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Mol	Chain	Res	Type
1	B	396	ILE
1	B	397	THR
1	B	414	THR
1	B	415	VAL
1	B	423	VAL
1	B	426	ASP
1	B	431	PHE
1	B	441	LEU
1	B	446	HIS
1	B	456	LEU
1	B	466	ILE
1	B	471	LEU
1	B	486	LEU
1	B	494	VAL
2	E	2	VAL
2	E	4	LEU
2	E	8	SER
2	E	10	ARG
2	E	12	LEU
2	E	17	GLN
2	E	18	THR
2	E	20	LEU
2	E	49	ILE
2	E	53	LEU
2	E	70	ILE
2	F	2	VAL
2	F	12	LEU
2	F	20	LEU
2	F	38	ARG
2	F	61	VAL
2	F	62	ILE
2	F	63	TYR
2	F	66	MET
2	F	69	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	85	GLN
1	A	89	GLN
1	A	131	GLN

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Mol	Chain	Res	Type
1	A	134	ASN
1	A	207	ASN
1	A	226	HIS
1	A	235	HIS
1	A	237	ASN
1	A	253	GLN
1	A	261	GLN
1	A	331	GLN
1	A	465	GLN
1	C	8	ASN
1	C	85	GLN
1	C	89	GLN
1	C	134	ASN
1	C	144	HIS
1	C	207	ASN
1	C	210	HIS
1	C	237	ASN
1	C	253	GLN
1	C	261	GLN
1	C	344	GLN
1	C	399	HIS
1	C	478	ASN
1	C	481	ASN
2	D	59	GLN
1	B	27	HIS
1	B	77	GLN
1	B	103	ASN
1	B	134	ASN
1	B	144	HIS
1	B	147	GLN
1	B	158	HIS
1	B	219	HIS
1	B	253	GLN
1	B	261	GLN
1	B	323	HIS
1	B	362	ASN
1	B	439	ASN
2	E	7	HIS
2	E	28	HIS
2	F	34	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	B	601	1	14,14,15	0.69	0	17,19,21	0.67	0
3	NAG	C	601	1	14,14,15	1.18	2 (14%)	17,19,21	0.90	0
3	NAG	A	601	1	14,14,15	1.06	1 (7%)	17,19,21	0.96	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	601	1	-	3/6/23/26	0/1/1/1
3	NAG	C	601	1	-	4/6/23/26	0/1/1/1
3	NAG	A	601	1	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	NAG	C1-C2	3.23	1.56	1.52
3	C	601	NAG	C3-C2	2.34	1.57	1.52
3	A	601	NAG	C1-C2	2.06	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	NAG	C8-C7-N2-C2
3	A	601	NAG	O7-C7-N2-C2
3	C	601	NAG	C8-C7-N2-C2
3	C	601	NAG	O7-C7-N2-C2
3	B	601	NAG	C8-C7-N2-C2
3	B	601	NAG	O7-C7-N2-C2
3	C	601	NAG	O5-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	A	601	NAG	C4-C5-C6-O6
3	C	601	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	NAG	1	0
3	C	601	NAG	6	0
3	A	601	NAG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

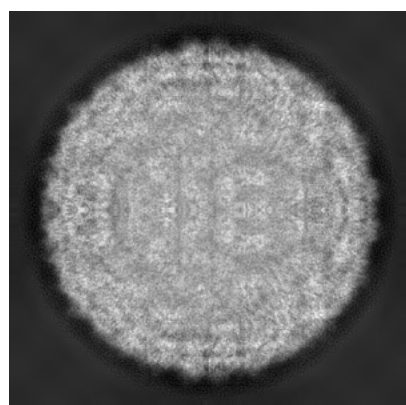
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8139. These allow visual inspection of the internal detail of the map and identification of artifacts.

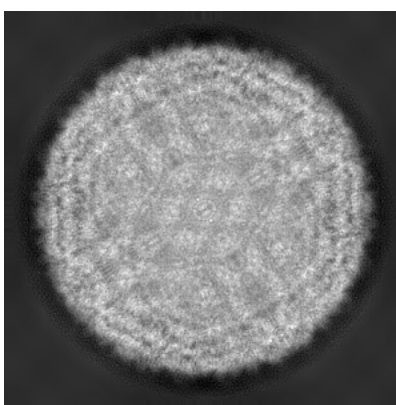
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

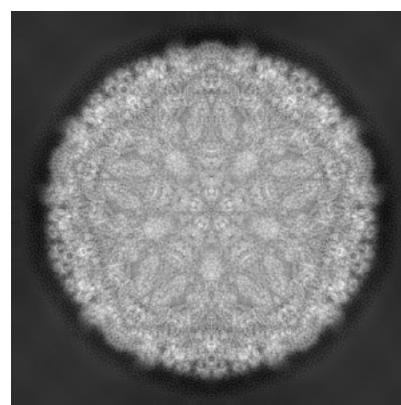
6.1.1 Primary map



X



Y

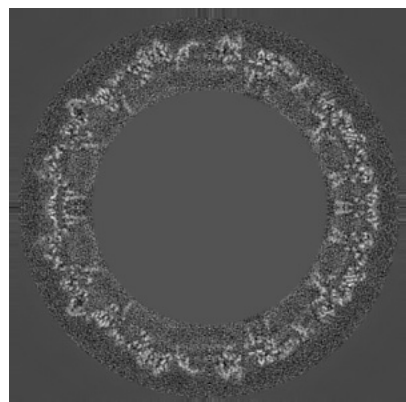


Z

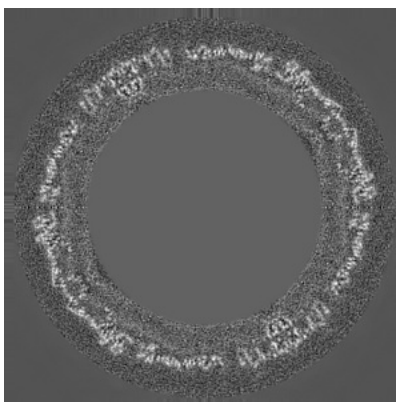
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

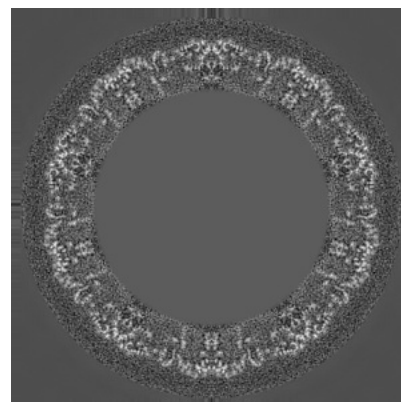
6.2.1 Primary map



X Index: 200



Y Index: 200

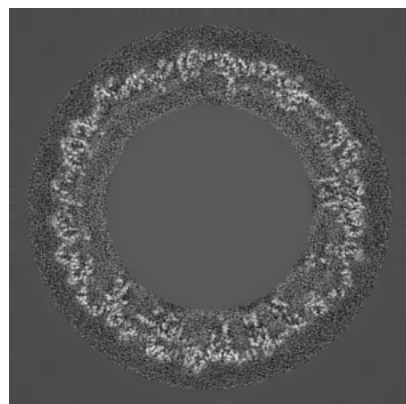


Z Index: 200

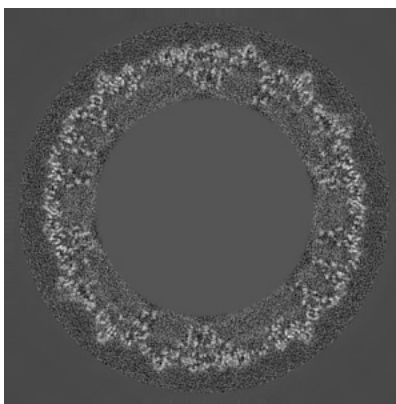
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

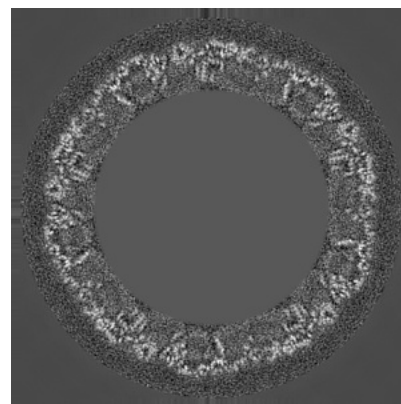
6.3.1 Primary map



X Index: 256



Y Index: 156

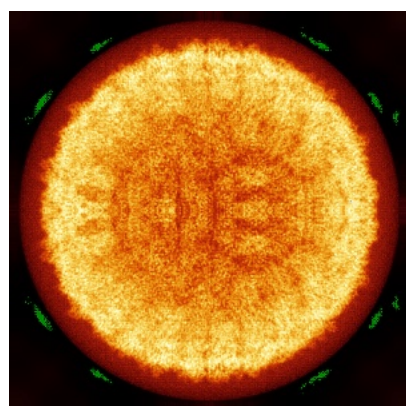


Z Index: 194

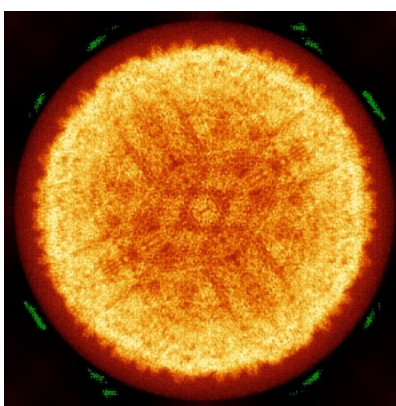
The images above show the largest variance slices of the map in three orthogonal directions.

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

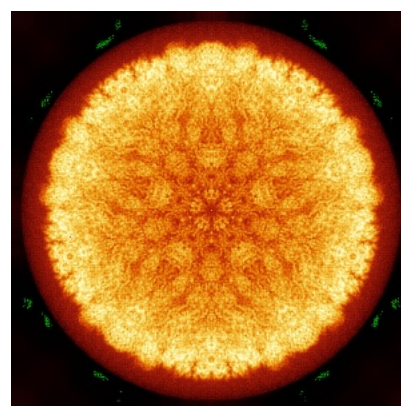
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

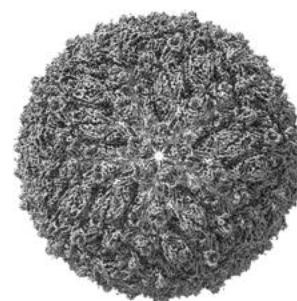
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

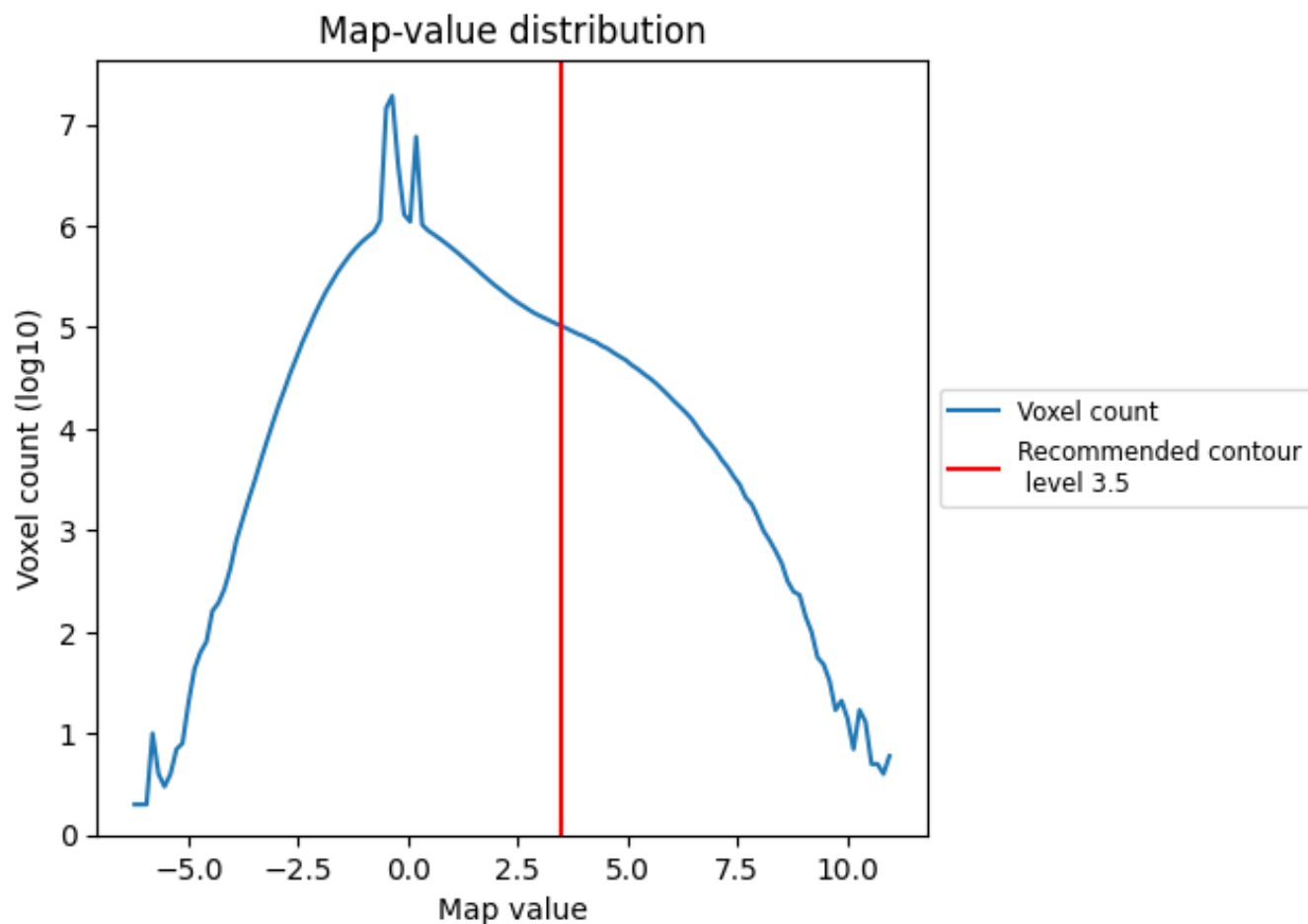
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

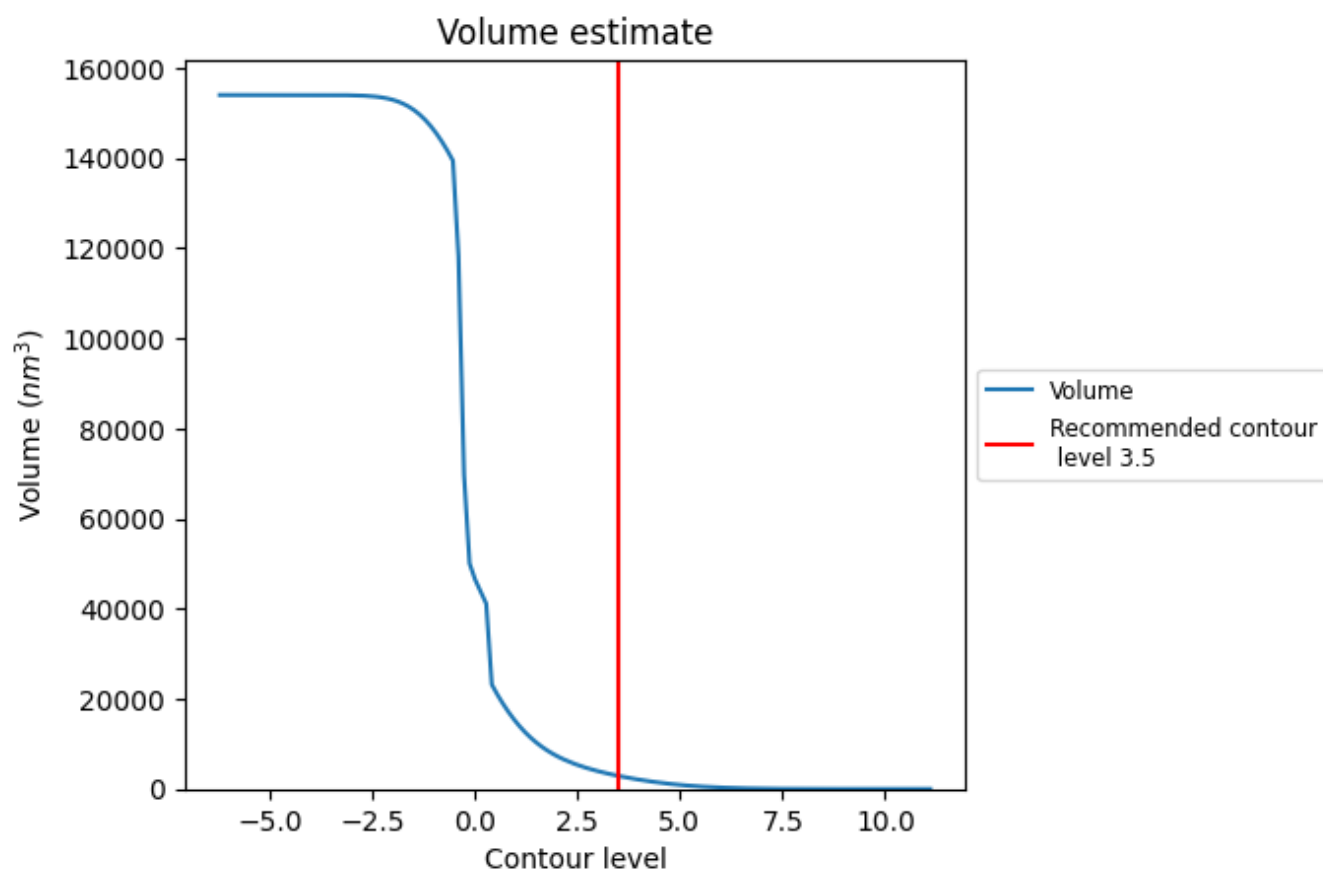
This section contains the results of statistical analysis of the map.

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.

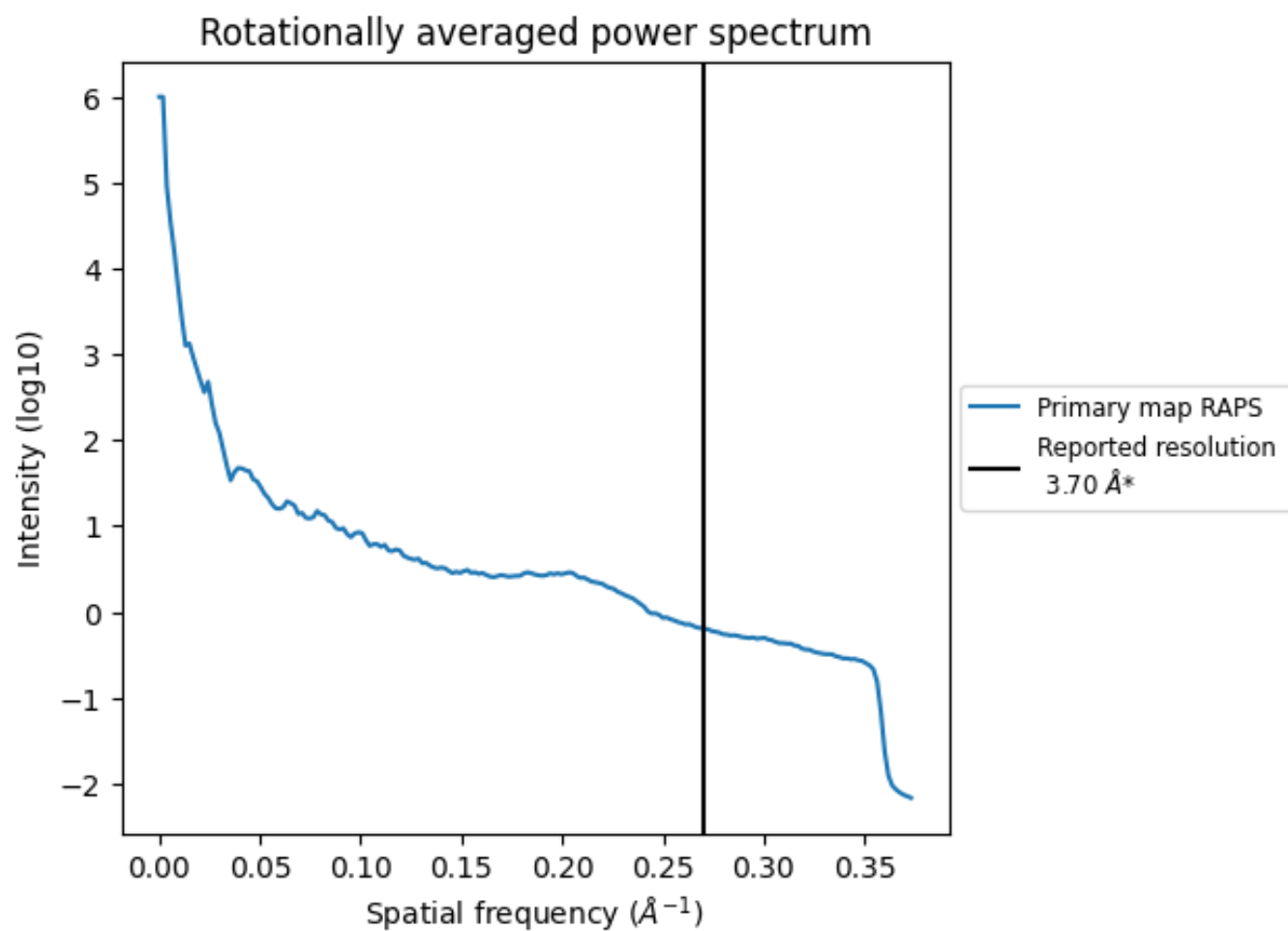
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2891 nm³; this corresponds to an approximate mass of 2612 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 0.270 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

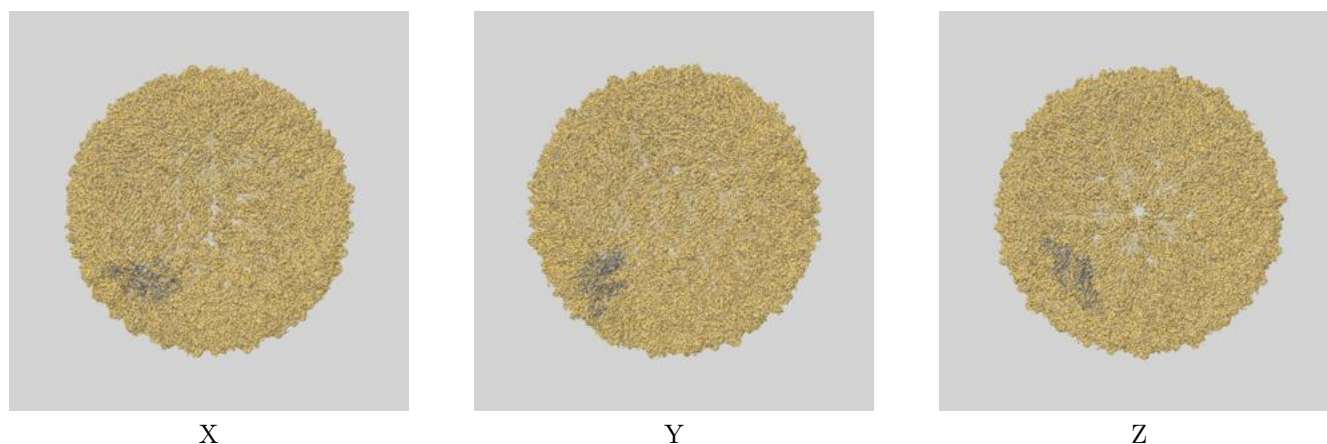
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

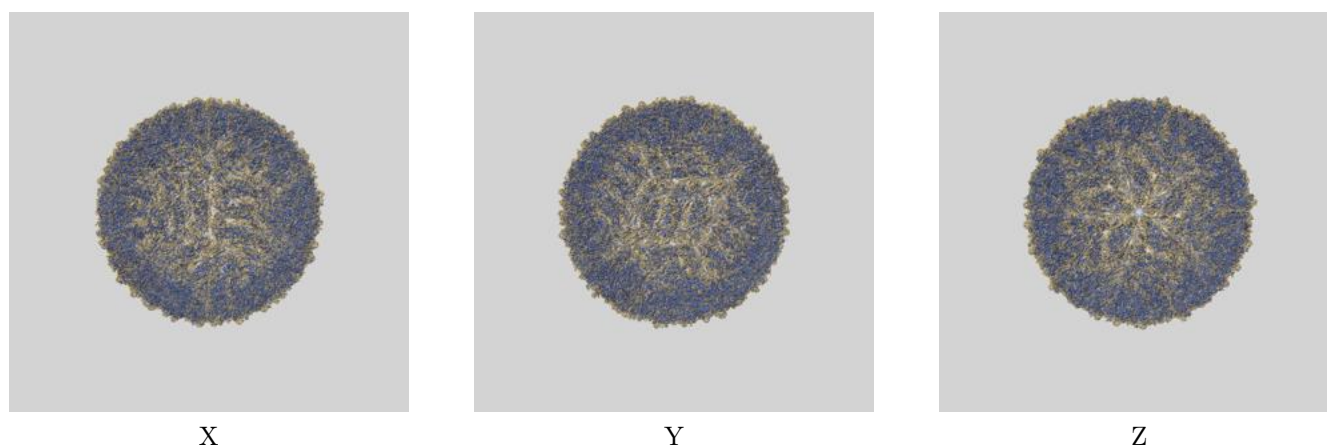
This section contains information regarding the fit between EMDB map EMD-8139 and PDB model 5IZ7. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

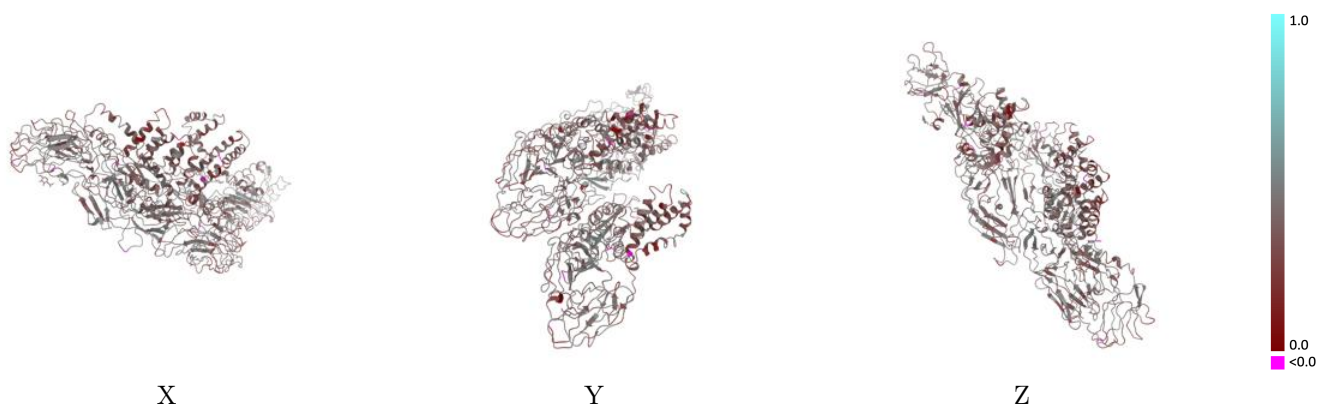


9.1.2 Map-model assembly overlay [i](#)



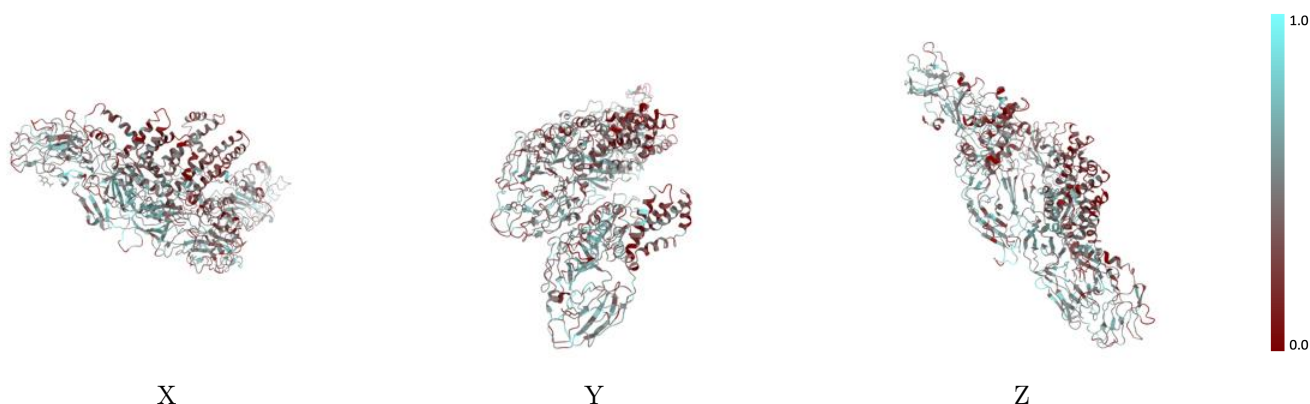
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



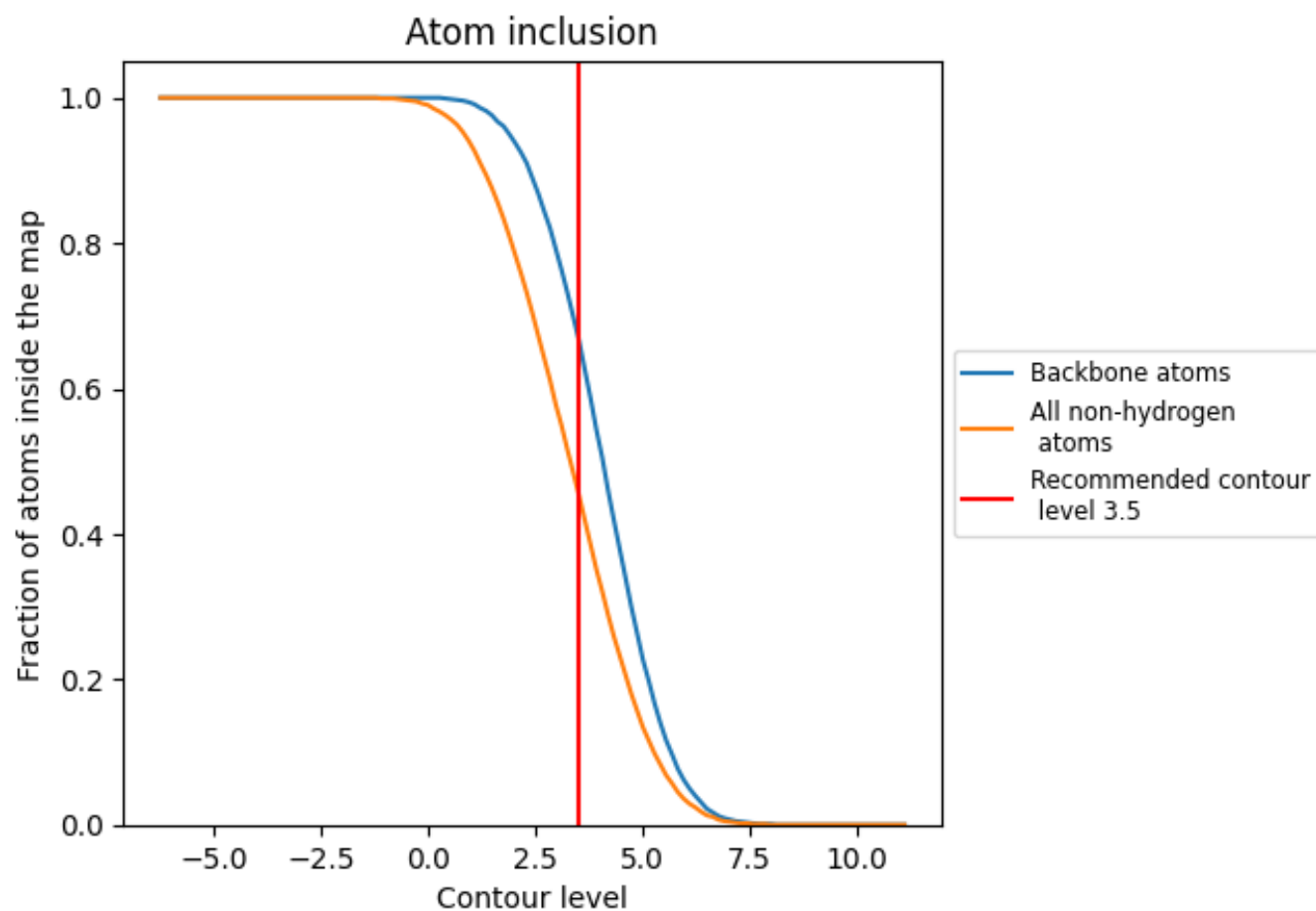
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 46% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4580	0.3870
A	0.4700	0.3950
B	0.4880	0.3910
C	0.4510	0.3860
D	0.3920	0.3770
E	0.3750	0.3420
F	0.3960	0.3710

1.0

0.0

<0.0