



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:27 PM EDT

PDB ID : 3BG1 / pdb_00003bg1
Title : Architecture of a Coat for the Nuclear Pore Membrane
Authors : Hoelz, A.
Deposited on : 2007-11-23
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

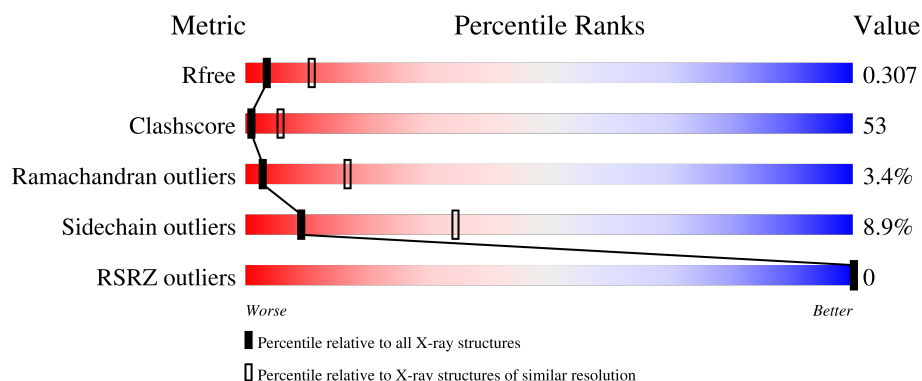
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	316	
1	D	316	
1	E	316	
1	H	316	
2	B	442	

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Mol	Chain	Length	Quality of chain
2	C	442	29%54%11%• 5%
2	F	442	28%54%13%• •
2	G	442	31%52%11%• 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22614 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Protein SEC13 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2233	1407	389	425	12			
1	D	283	Total	C	N	O	S	0	0	0
			2218	1398	386	422	12			
1	E	285	Total	C	N	O	S	0	0	0
			2233	1407	389	425	12			
1	H	283	Total	C	N	O	S	0	0	0
			2218	1398	386	422	12			

- Molecule 2 is a protein called Nucleoporin NUP145.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3438	2201	570	656	11			
2	C	420	Total	C	N	O	S	0	0	0
			3418	2188	566	653	11			
2	F	423	Total	C	N	O	S	0	0	0
			3438	2201	570	656	11			
2	G	420	Total	C	N	O	S	0	0	0
			3418	2188	566	653	11			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	111	MET	-	expression tag	UNP P49687
B	112	GLY	-	expression tag	UNP P49687
B	113	SER	-	expression tag	UNP P49687
B	114	SER	-	expression tag	UNP P49687
B	115	HIS	-	expression tag	UNP P49687
B	116	HIS	-	expression tag	UNP P49687
B	117	HIS	-	expression tag	UNP P49687
B	118	HIS	-	expression tag	UNP P49687

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Chain	Residue	Modelled	Actual	Comment	Reference
B	119	HIS	-	expression tag	UNP P49687
B	120	HIS	-	expression tag	UNP P49687
B	121	SER	-	expression tag	UNP P49687
B	122	GLY	-	expression tag	UNP P49687
B	123	ASP	-	expression tag	UNP P49687
B	124	PRO	-	expression tag	UNP P49687
C	111	MET	-	expression tag	UNP P49687
C	112	GLY	-	expression tag	UNP P49687
C	113	SER	-	expression tag	UNP P49687
C	114	SER	-	expression tag	UNP P49687
C	115	HIS	-	expression tag	UNP P49687
C	116	HIS	-	expression tag	UNP P49687
C	117	HIS	-	expression tag	UNP P49687
C	118	HIS	-	expression tag	UNP P49687
C	119	HIS	-	expression tag	UNP P49687
C	120	HIS	-	expression tag	UNP P49687
C	121	SER	-	expression tag	UNP P49687
C	122	GLY	-	expression tag	UNP P49687
C	123	ASP	-	expression tag	UNP P49687
C	124	PRO	-	expression tag	UNP P49687
F	111	MET	-	expression tag	UNP P49687
F	112	GLY	-	expression tag	UNP P49687
F	113	SER	-	expression tag	UNP P49687
F	114	SER	-	expression tag	UNP P49687
F	115	HIS	-	expression tag	UNP P49687
F	116	HIS	-	expression tag	UNP P49687
F	117	HIS	-	expression tag	UNP P49687
F	118	HIS	-	expression tag	UNP P49687
F	119	HIS	-	expression tag	UNP P49687
F	120	HIS	-	expression tag	UNP P49687
F	121	SER	-	expression tag	UNP P49687
F	122	GLY	-	expression tag	UNP P49687
F	123	ASP	-	expression tag	UNP P49687
F	124	PRO	-	expression tag	UNP P49687
G	111	MET	-	expression tag	UNP P49687
G	112	GLY	-	expression tag	UNP P49687
G	113	SER	-	expression tag	UNP P49687
G	114	SER	-	expression tag	UNP P49687
G	115	HIS	-	expression tag	UNP P49687
G	116	HIS	-	expression tag	UNP P49687
G	117	HIS	-	expression tag	UNP P49687
G	118	HIS	-	expression tag	UNP P49687

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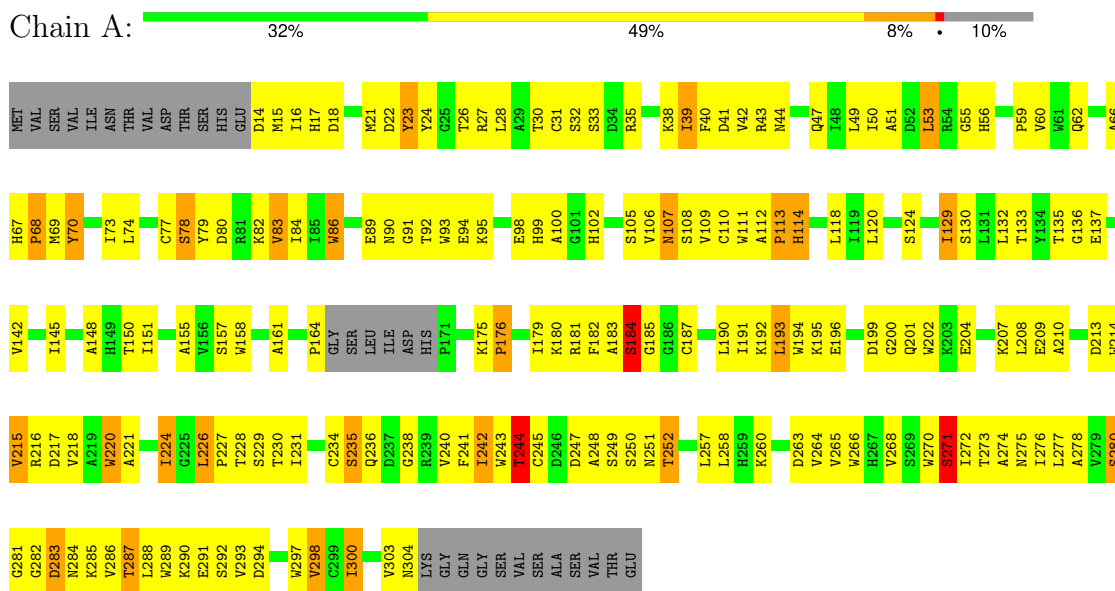
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Chain	Residue	Modelled	Actual	Comment	Reference
G	119	HIS	-	expression tag	UNP P49687
G	120	HIS	-	expression tag	UNP P49687
G	121	SER	-	expression tag	UNP P49687
G	122	GLY	-	expression tag	UNP P49687
G	123	ASP	-	expression tag	UNP P49687
G	124	PRO	-	expression tag	UNP P49687

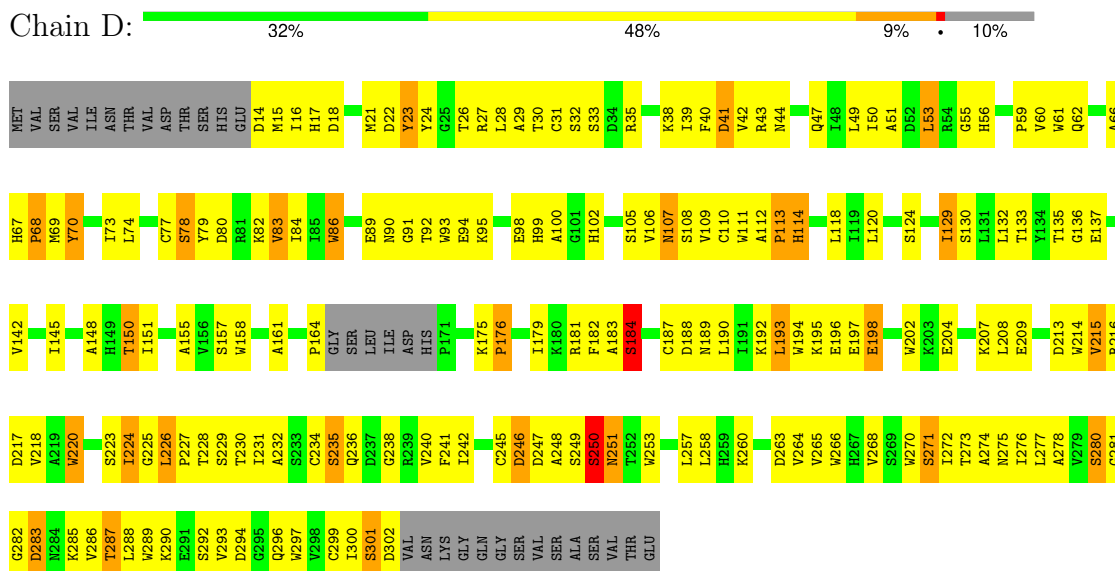
3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Protein SEC13 homolog

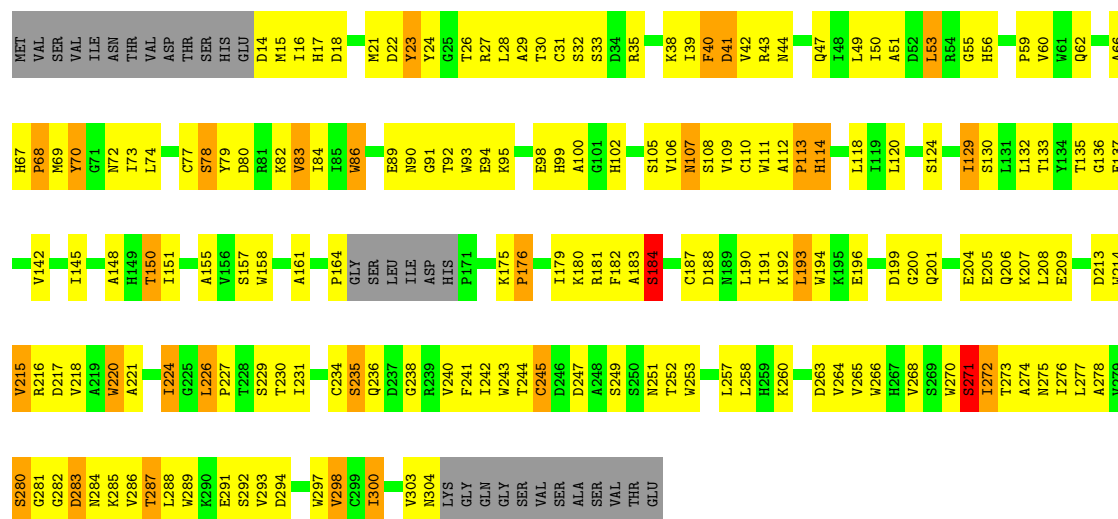


• Molecule 1: Protein SEC13 homolog



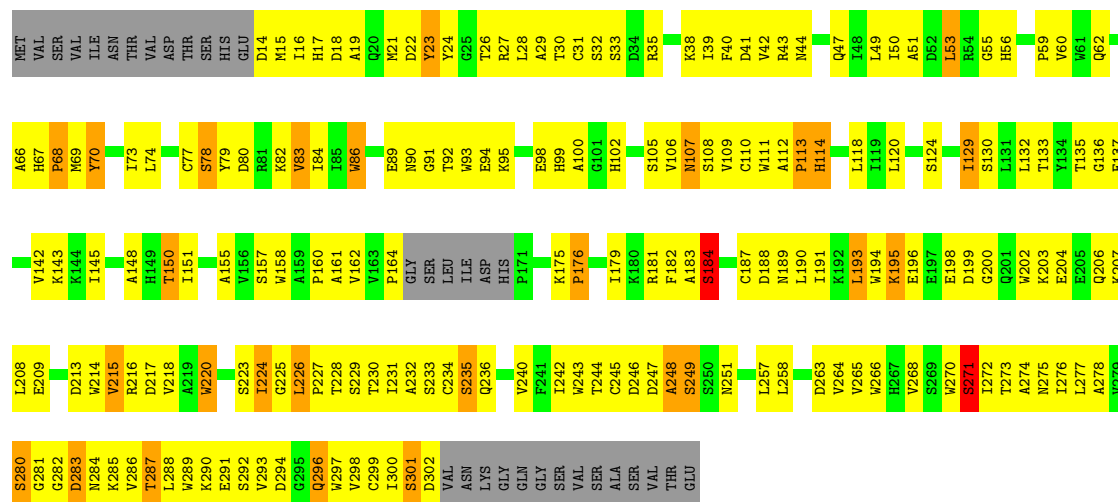
- Molecule 1: Protein SEC13 homolog

Chain E:  33% 48% 9% 10%



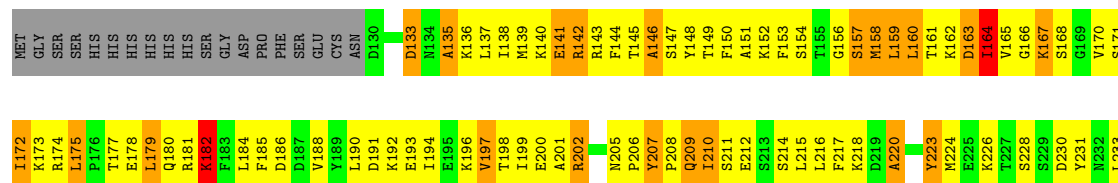
- Molecule 1: Protein SEC13 homolog

Chain H:  29% 51% 9% 10%

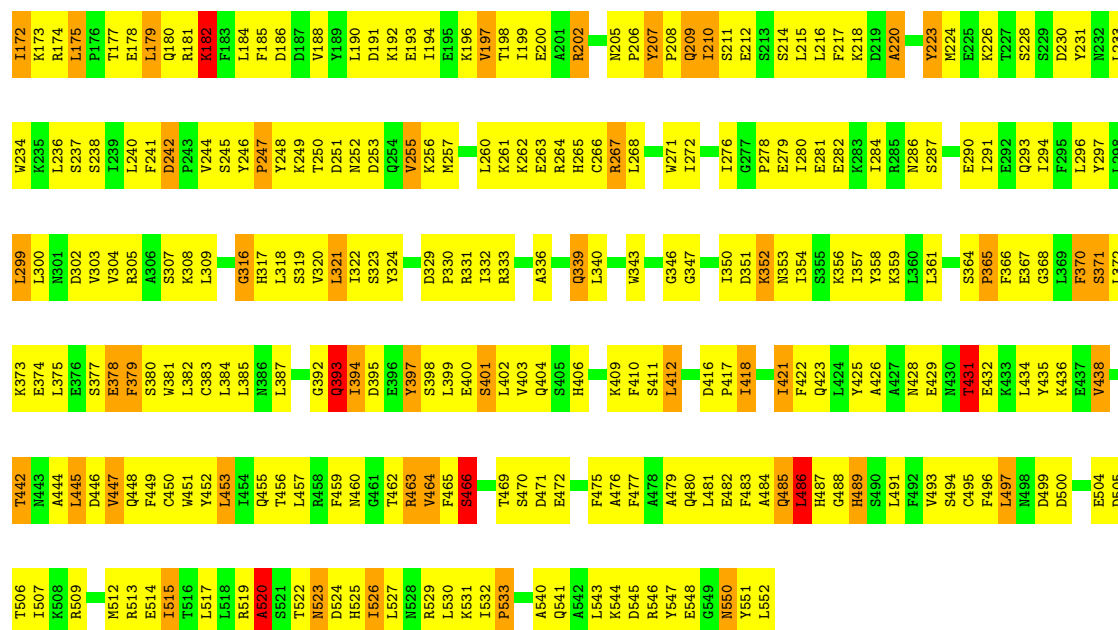


- Molecule 2: Nucleoporin NUP145

Chain B:  28% 54% 13% 5%

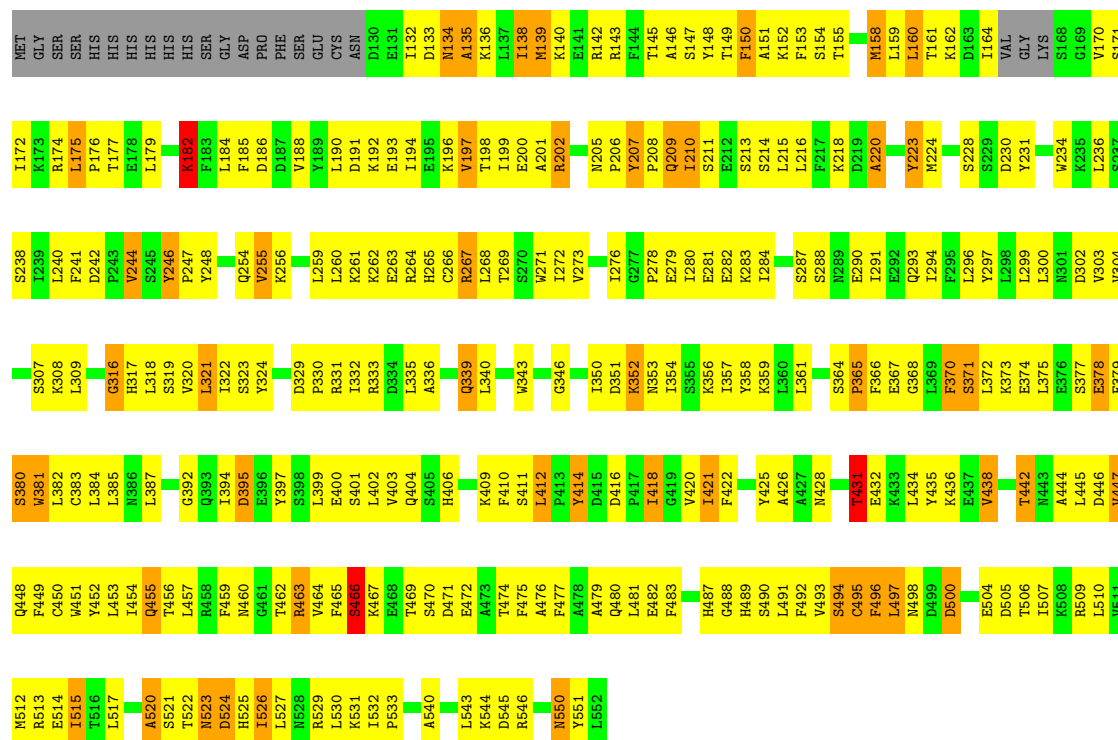






• Molecule 2: Nucleoporin NUP145

Chain G: 31% 52% 11% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	181.37Å 216.79Å 192.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-3.00) 84.3 (20.00-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.98Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.294 0.263 , 0.307	Depositor DCC
R_{free} test set	5815 reflections (8.15%)	wwPDB-VP
Wilson B-factor (Å ²)	87.9	Xtrriage
Anisotropy	0.769	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 78.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22614	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5507e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.61	0/2297	1.16	18/3131 (0.6%)
1	D	0.58	0/2282	1.16	18/3110 (0.6%)
1	E	0.59	0/2297	1.13	16/3131 (0.5%)
1	H	0.55	0/2282	1.13	17/3110 (0.5%)
2	B	0.63	1/3504 (0.0%)	1.20	34/4728 (0.7%)
2	C	0.60	0/3483	1.18	29/4699 (0.6%)
2	F	0.63	0/3504	1.20	36/4728 (0.8%)
2	G	0.59	0/3483	1.17	30/4699 (0.6%)
All	All	0.60	1/23132 (0.0%)	1.17	198/31336 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	487	HIS	CB-CG	5.49	1.57	1.50

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	272	ILE	N-CA-C	15.14	126.06	110.62
1	D	272	ILE	N-CA-C	14.97	125.89	110.62
1	E	272	ILE	N-CA-C	14.88	125.80	110.62
1	A	272	ILE	N-CA-C	14.82	125.74	110.62
2	B	485	GLN	OE1-CD-NE2	-10.19	112.42	122.60
2	G	246	TYR	CA-C-N	9.85	130.11	119.87
2	G	246	TYR	C-N-CA	9.85	130.11	119.87
2	C	246	TYR	CA-C-N	9.54	129.63	119.05
2	C	246	TYR	C-N-CA	9.54	129.63	119.05
2	C	397	TYR	N-CA-C	9.51	126.49	113.37
2	F	485	GLN	OE1-CD-NE2	-9.16	113.44	122.60
2	C	483	PHE	N-CA-C	-9.08	101.46	111.36
2	G	135	ALA	N-CA-C	-9.02	102.29	113.38
2	C	135	ALA	N-CA-C	-8.98	102.34	113.38
2	F	249	LYS	N-CA-C	8.47	122.85	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	180	GLN	N-CA-C	8.41	123.40	107.75
2	B	398	SER	N-CA-C	8.33	122.59	110.42
1	D	23	TYR	N-CA-C	-8.18	100.35	110.41
1	E	23	TYR	N-CA-C	-8.13	100.41	110.41
1	A	23	TYR	N-CA-C	-8.13	100.42	110.41
1	H	23	TYR	N-CA-C	-8.11	100.44	110.41
2	F	316	GLY	N-CA-C	8.07	121.87	112.50
2	C	316	GLY	N-CA-C	8.05	121.84	112.50
2	B	316	GLY	N-CA-C	8.04	121.83	112.50
2	G	316	GLY	N-CA-C	8.01	121.79	112.50
1	A	249	SER	N-CA-C	7.79	122.50	113.38
1	D	250	SER	CA-C-N	-7.71	109.71	122.21
1	D	250	SER	C-N-CA	-7.71	109.71	122.21
1	H	175	LYS	N-CA-C	-7.46	98.87	109.24
1	E	175	LYS	N-CA-C	-7.46	98.87	109.24
1	D	175	LYS	N-CA-C	-7.46	98.87	109.24
2	F	251	ASP	N-CA-C	7.46	122.38	111.87
1	A	175	LYS	N-CA-C	-7.41	98.94	109.24
2	C	207	TYR	CA-C-N	7.31	127.35	119.90
2	C	207	TYR	C-N-CA	7.31	127.35	119.90
2	F	286	ASN	CA-C-N	-7.30	112.70	122.99
2	F	286	ASN	C-N-CA	-7.30	112.70	122.99
2	F	207	TYR	CA-C-N	7.29	127.34	119.90
2	F	207	TYR	C-N-CA	7.29	127.34	119.90
2	B	207	TYR	CA-C-N	7.28	127.32	119.90
2	B	207	TYR	C-N-CA	7.28	127.32	119.90
2	B	465	PHE	N-CA-C	7.20	120.14	108.41
2	G	207	TYR	CA-C-N	7.20	127.24	119.90
2	G	207	TYR	C-N-CA	7.20	127.24	119.90
2	C	465	PHE	N-CA-C	7.10	119.98	108.41
2	F	465	PHE	N-CA-C	7.09	119.97	108.41
2	G	465	PHE	N-CA-C	7.07	119.93	108.41
2	F	287	SER	N-CA-C	6.99	120.29	108.90
2	G	352	LYS	N-CA-C	-6.95	104.06	112.54
2	F	180	GLN	N-CA-C	6.89	120.91	108.17
2	G	134	ASN	N-CA-C	-6.87	104.51	113.17
2	C	134	ASN	N-CA-C	-6.86	104.53	113.17
2	F	352	LYS	N-CA-C	-6.82	104.22	112.54
2	C	352	LYS	N-CA-C	-6.81	104.23	112.54
2	B	463	ARG	N-CA-C	6.80	118.13	108.74
2	G	381	TRP	N-CA-C	-6.79	103.94	111.82
2	B	352	LYS	N-CA-C	-6.78	104.27	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	175	LEU	CA-C-N	6.77	127.14	119.83
2	F	175	LEU	C-N-CA	6.77	127.14	119.83
2	B	286	ASN	CA-C-N	-6.73	112.24	122.81
2	B	286	ASN	C-N-CA	-6.73	112.24	122.81
2	B	350	ILE	N-CA-C	6.73	119.49	108.99
2	C	520	ALA	N-CA-C	6.72	125.12	110.80
2	B	520	ALA	N-CA-C	6.71	125.09	110.80
2	B	175	LEU	CA-C-N	6.69	127.06	119.83
2	B	175	LEU	C-N-CA	6.69	127.06	119.83
2	F	485	GLN	CG-CD-NE2	6.69	126.43	116.40
2	F	520	ALA	N-CA-C	6.68	125.02	110.80
2	G	520	ALA	N-CA-C	6.67	125.02	110.80
1	A	150	THR	N-CA-C	6.66	118.34	111.14
1	H	150	THR	N-CA-C	6.60	118.27	111.14
2	C	438	VAL	N-CA-C	6.58	116.72	110.53
2	B	485	GLN	CG-CD-NE2	6.58	126.26	116.40
2	F	245	SER	N-CA-C	6.56	119.18	108.55
1	D	150	THR	N-CA-C	6.55	118.22	111.14
1	E	150	THR	N-CA-C	6.54	118.21	111.14
2	B	442	THR	N-CA-C	6.51	120.13	109.06
2	B	438	VAL	N-CA-C	6.49	116.63	110.53
2	F	438	VAL	N-CA-C	6.49	116.63	110.53
2	G	442	THR	N-CA-C	6.47	120.05	109.06
2	F	442	THR	N-CA-C	6.45	120.03	109.06
2	F	242	ASP	CA-C-N	6.45	126.47	119.90
2	F	242	ASP	C-N-CA	6.45	126.47	119.90
1	H	248	ALA	N-CA-C	-6.42	105.31	113.02
2	C	442	THR	N-CA-C	6.41	119.96	109.06
2	G	254	GLN	N-CA-C	-6.41	104.39	111.82
1	E	107	ASN	N-CA-C	6.38	119.91	111.75
2	G	438	VAL	N-CA-C	6.37	116.52	110.53
1	A	107	ASN	N-CA-C	6.36	119.89	111.75
1	H	107	ASN	N-CA-C	6.34	119.87	111.75
1	D	107	ASN	N-CA-C	6.29	119.80	111.75
1	D	251	ASN	N-CA-C	6.22	118.63	109.24
2	C	197	VAL	N-CA-C	6.21	117.87	108.80
2	B	197	VAL	N-CA-C	6.21	117.86	108.80
2	B	287	SER	N-CA-C	6.20	119.64	109.72
2	F	197	VAL	N-CA-C	6.19	117.84	108.80
2	B	246	TYR	CA-C-N	6.17	127.55	119.84
2	B	246	TYR	C-N-CA	6.17	127.55	119.84
1	A	133	THR	N-CA-C	-6.14	100.91	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	197	VAL	N-CA-C	6.13	117.76	108.80
2	C	158	MET	N-CA-C	-6.13	101.38	110.46
2	F	463	ARG	N-CA-C	6.13	116.37	108.34
1	E	133	THR	N-CA-C	-6.12	100.94	110.42
1	H	133	THR	N-CA-C	-6.09	100.98	110.42
2	G	158	MET	N-CA-C	-6.06	101.50	110.46
1	H	108	SER	N-CA-C	6.05	118.05	108.79
1	E	108	SER	N-CA-C	6.05	118.05	108.79
1	E	245	CYS	N-CA-C	6.04	118.52	108.13
1	A	108	SER	N-CA-C	6.03	118.02	108.79
1	D	108	SER	N-CA-C	6.03	118.02	108.79
2	F	445	LEU	CA-C-N	6.03	129.94	121.02
2	F	445	LEU	C-N-CA	6.03	129.94	121.02
1	D	250	SER	N-CA-C	-6.02	97.97	110.80
2	G	247	PRO	N-CA-C	6.01	121.42	114.03
2	G	463	ARG	N-CA-C	5.96	118.35	108.99
2	G	288	SER	N-CA-C	-5.91	103.85	113.19
2	F	182	LYS	N-CA-C	5.90	123.36	110.80
2	C	182	LYS	N-CA-C	5.90	123.36	110.80
2	C	247	PRO	N-CA-C	5.89	121.72	113.53
2	F	533	PRO	N-CA-C	5.89	120.49	110.95
2	G	182	LYS	N-CA-C	5.89	123.34	110.80
1	A	215	VAL	N-CA-C	-5.86	101.16	108.89
2	F	146	ALA	N-CA-C	-5.85	106.23	113.19
1	D	215	VAL	N-CA-C	-5.84	101.18	108.89
2	B	182	LYS	N-CA-C	5.84	123.24	110.80
1	E	215	VAL	N-CA-C	-5.83	101.19	108.89
2	B	288	SER	N-CA-C	-5.82	104.74	112.94
2	B	146	ALA	N-CA-C	-5.79	106.30	113.19
1	H	215	VAL	N-CA-C	-5.76	101.29	108.89
1	D	133	THR	N-CA-C	-5.75	100.91	110.17
2	F	466	SER	N-CA-C	5.74	118.56	109.96
1	E	91	GLY	N-CA-C	-5.64	106.74	114.64
2	F	210	ILE	N-CA-C	5.64	116.28	108.84
2	B	464	VAL	N-CA-C	5.64	115.45	106.88
2	C	210	ILE	N-CA-C	5.62	116.25	108.84
2	B	466	SER	N-CA-C	5.60	118.36	109.96
1	A	91	GLY	N-CA-C	-5.59	106.81	114.64
2	G	287	SER	N-CA-C	5.58	118.28	109.96
2	G	466	SER	N-CA-C	5.58	118.34	109.96
2	B	135	ALA	N-CA-C	-5.58	105.20	111.28
2	F	135	ALA	N-CA-C	-5.58	105.20	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	91	GLY	N-CA-C	-5.57	106.84	114.64
2	B	210	ILE	N-CA-C	5.56	116.18	108.84
2	C	466	SER	N-CA-C	5.56	118.30	109.96
1	H	271	SER	N-CA-C	-5.55	101.43	110.20
2	F	464	VAL	N-CA-C	5.54	115.31	106.88
1	H	91	GLY	N-CA-C	-5.54	106.89	114.64
2	G	210	ILE	N-CA-C	5.51	116.12	108.84
1	E	40	PHE	CB-CA-C	-5.48	100.28	109.48
1	D	271	SER	N-CA-C	-5.47	101.55	110.20
1	A	272	ILE	CB-CA-C	-5.45	104.79	112.14
2	C	251	ASP	N-CA-C	5.41	118.00	111.40
2	F	411	SER	N-CA-C	-5.40	102.49	110.48
2	C	464	VAL	N-CA-C	5.39	115.02	107.37
1	E	272	ILE	CB-CA-C	-5.35	104.92	112.14
2	C	377	SER	N-CA-C	5.35	116.80	110.97
1	E	271	SER	N-CA-C	-5.34	101.75	110.20
2	F	377	SER	N-CA-C	5.32	116.77	110.97
2	G	377	SER	N-CA-C	5.32	116.77	110.97
1	H	235	SER	N-CA-C	5.28	117.00	109.14
2	B	377	SER	N-CA-C	5.27	116.72	110.97
1	A	252	THR	CA-C-N	-5.25	115.36	123.14
1	A	252	THR	C-N-CA	-5.25	115.36	123.14
1	D	235	SER	N-CA-C	5.25	116.96	109.14
1	A	235	SER	N-CA-C	5.23	116.94	109.14
1	A	271	SER	N-CA-C	-5.20	101.98	110.20
1	H	272	ILE	CB-CA-C	-5.20	105.12	112.14
2	G	392	GLY	CA-C-N	-5.19	116.09	122.84
2	G	392	GLY	C-N-CA	-5.19	116.09	122.84
2	C	368	GLY	N-CA-C	5.18	120.76	112.58
1	D	137	GLU	N-CA-C	5.17	116.57	109.29
2	G	220	ALA	N-CA-C	5.16	118.36	111.75
2	C	444	ALA	N-CA-C	-5.15	105.74	112.23
2	C	220	ALA	N-CA-C	5.15	118.34	111.75
1	E	235	SER	N-CA-C	5.14	116.79	109.14
2	B	368	GLY	N-CA-C	5.13	120.69	112.58
1	D	272	ILE	CB-CA-C	-5.13	105.21	112.14
2	F	368	GLY	N-CA-C	5.12	120.67	112.58
2	B	220	ALA	N-CA-C	5.12	118.30	111.75
1	H	137	GLU	N-CA-C	5.11	116.50	109.29
1	H	271	SER	CB-CA-C	5.11	118.16	109.53
1	E	137	GLU	N-CA-C	5.11	116.49	109.29
2	C	522	THR	CA-C-N	5.10	131.29	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	522	THR	C-N-CA	5.10	131.29	121.54
2	F	220	ALA	N-CA-C	5.10	118.28	111.75
2	G	368	GLY	N-CA-C	5.10	120.64	112.58
1	A	78	SER	N-CA-C	5.09	115.06	107.88
1	A	137	GLU	N-CA-C	5.09	116.46	109.29
1	H	198	GLU	N-CA-C	5.08	121.61	110.80
1	H	78	SER	N-CA-C	5.07	115.03	107.88
1	E	78	SER	N-CA-C	5.06	115.02	107.88
2	G	160	LEU	N-CA-C	5.06	117.31	108.76
1	D	78	SER	N-CA-C	5.04	114.99	107.88
1	A	244	THR	N-CA-C	5.04	117.46	109.50
2	B	350	ILE	CA-C-N	5.04	128.81	121.31
2	B	350	ILE	C-N-CA	5.04	128.81	121.31
2	G	497	LEU	N-CA-C	5.03	118.32	110.32
2	C	160	LEU	N-CA-C	5.00	117.22	108.76

There are no chirality outliers.

There are no planarity outliers.

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	2233	0	2109	249	0
1	D	2218	0	2094	252	0
1	E	2233	0	2109	265	0
1	H	2218	0	2094	246	0
2	B	3438	0	3452	390	0
2	C	3418	0	3426	363	0
2	F	3438	0	3452	400	0
2	G	3418	0	3426	351	0
All	All	22614	0	22162	2357	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 53.

All (2357) 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:E:278:ALA:HB2	2:F:153:PHE:CE1	1.79	1.18
2:G:481:LEU:HD13	2:G:489:HIS:HB3	1.23	1.17
2:C:479:ALA:CB	1:D:273:THR:HG21	1.76	1.14
1:E:107:ASN:HD21	2:F:142:ARG:NH2	1.47	1.12
1:E:278:ALA:HB2	2:F:153:PHE:HE1	0.98	1.10
2:C:479:ALA:HB1	1:D:273:THR:HG21	1.34	1.09
1:A:278:ALA:HB2	2:B:153:PHE:HE1	1.07	1.08
1:A:278:ALA:HB2	2:B:153:PHE:CE1	1.89	1.07
1:D:135:THR:HG22	1:D:136:GLY:H	1.17	1.05
1:A:135:THR:HG22	1:A:136:GLY:H	1.17	1.05
2:B:432:GLU:OE2	2:B:466:SER:HB3	1.56	1.05
1:A:41:ASP:HB2	1:A:50:ILE:HD11	1.38	1.04
2:B:350:ILE:HG23	2:B:354:ILE:HD12	1.39	1.04
2:G:479:ALA:CB	1:H:273:THR:HG21	1.87	1.04
2:C:481:LEU:HD13	2:C:489:HIS:HB3	1.39	1.04
2:G:432:GLU:OE2	2:G:466:SER:HB3	1.56	1.03
1:E:135:THR:HG22	1:E:136:GLY:H	1.17	1.03
2:B:404:GLN:HG2	2:B:426:ALA:HB1	1.39	1.03
1:H:135:THR:HG22	1:H:136:GLY:H	1.17	1.02
2:G:155:THR:HG22	2:G:513:ARG:HD2	1.42	1.01
2:G:479:ALA:HB1	1:H:273:THR:CG2	1.90	1.01
2:F:484:ALA:HB3	2:F:486:LEU:CD1	1.90	1.01
2:C:479:ALA:HB1	1:D:273:THR:CG2	1.90	1.00
1:A:107:ASN:HD21	2:B:142:ARG:NH2	1.57	1.00
1:A:69:MET:HE3	1:A:70:TYR:HE1	1.27	0.99
2:F:202:ARG:HG3	2:F:500:ASP:OD1	1.61	0.98
1:E:70:TYR:CE2	1:E:118:LEU:HB2	1.98	0.98
2:F:432:GLU:OE2	2:F:466:SER:HB3	1.63	0.98
1:D:69:MET:HE3	1:D:70:TYR:HE1	1.28	0.98
2:C:442:THR:HG22	2:C:444:ALA:H	1.28	0.98
1:E:69:MET:HE3	1:E:70:TYR:HE1	1.28	0.98
1:A:70:TYR:CE2	1:A:118:LEU:HB2	1.98	0.98
1:D:70:TYR:CE2	1:D:118:LEU:HB2	1.99	0.98
1:E:102:HIS:ND1	1:E:124:SER:HB3	1.79	0.98
1:H:102:HIS:ND1	1:H:124:SER:HB3	1.79	0.98
1:E:206:GLN:OE1	1:E:251:ASN:HB3	1.62	0.98
1:A:102:HIS:ND1	1:A:124:SER:HB3	1.79	0.97
2:B:276:ILE:HD13	2:B:383:CYS:HA	1.44	0.97
2:C:479:ALA:CB	1:D:273:THR:CG2	2.41	0.97
1:H:70:TYR:CE2	1:H:118:LEU:HB2	1.99	0.97
2:F:442:THR:HG22	2:F:444:ALA:H	1.29	0.97
1:H:69:MET:HE3	1:H:70:TYR:HE1	1.28	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:479:ALA:CB	1:H:273:THR:CG2	2.41	0.96
1:D:102:HIS:ND1	1:D:124:SER:HB3	1.79	0.96
2:B:522:THR:O	2:B:523:ASN:CG	2.09	0.95
2:B:487:HIS:HD2	2:B:517:LEU:HD23	1.31	0.95
2:C:162:LYS:NZ	1:D:15:MET:HE2	1.80	0.95
2:G:479:ALA:HB1	1:H:273:THR:HG21	1.46	0.95
2:G:291:ILE:HG22	2:G:353:ASN:HB2	1.47	0.94
2:G:177:THR:HG22	2:G:179:LEU:H	1.29	0.94
2:G:276:ILE:HD13	2:G:383:CYS:HA	1.47	0.94
2:G:442:THR:HG22	2:G:444:ALA:H	1.30	0.94
2:C:291:ILE:HG22	2:C:353:ASN:HB2	1.49	0.93
2:B:149:THR:HG22	2:B:150:PHE:H	1.32	0.93
2:F:522:THR:O	2:F:523:ASN:CG	2.12	0.93
2:C:177:THR:HG22	2:C:179:LEU:H	1.29	0.93
2:F:149:THR:HG22	2:F:150:PHE:H	1.33	0.93
2:B:201:ALA:H	2:B:531:LYS:HZ2	1.12	0.92
1:E:242:ILE:HD13	1:E:297:TRP:NE1	1.84	0.92
2:G:159:LEU:HD12	2:G:160:LEU:H	1.35	0.91
2:G:462:THR:O	2:G:463:ARG:HD3	1.71	0.91
2:C:159:LEU:HD12	2:C:160:LEU:H	1.35	0.91
1:E:107:ASN:ND2	2:F:142:ARG:HH22	1.67	0.91
1:A:28:LEU:HD21	2:B:170:VAL:HG11	1.54	0.90
2:B:184:LEU:HD21	2:B:448:GLN:HE22	1.34	0.90
2:F:207:TYR:CD2	2:F:504:GLU:HA	2.05	0.90
2:G:267:ARG:HH11	2:G:267:ARG:HG3	1.37	0.90
1:H:288:LEU:H	1:H:301:SER:HB3	1.37	0.89
1:E:41:ASP:HB2	1:E:50:ILE:HD11	1.51	0.89
1:A:40:PHE:CZ	2:B:168:SER:HB2	2.07	0.89
1:E:107:ASN:HD21	2:F:142:ARG:HH22	1.10	0.89
2:G:294:ILE:HG12	2:G:309:LEU:HD23	1.54	0.89
2:F:238:SER:HA	2:F:242:ASP:OD2	1.73	0.89
1:A:214:TRP:O	1:A:235:SER:HB2	1.74	0.88
1:D:195:LYS:HG2	1:D:196:GLU:H	1.36	0.88
1:E:214:TRP:O	1:E:235:SER:HB2	1.73	0.88
1:A:107:ASN:HD21	2:B:142:ARG:HH22	1.14	0.88
2:F:484:ALA:HB3	2:F:486:LEU:HD12	1.52	0.88
2:F:267:ARG:HH11	2:F:267:ARG:HG3	1.38	0.88
1:H:82:LYS:HG2	1:H:100:ALA:HB2	1.56	0.88
2:B:163:ASP:HB2	2:B:171:SER:OG	1.73	0.88
1:D:82:LYS:HG2	1:D:100:ALA:HB2	1.56	0.88
2:F:404:GLN:HG2	2:F:426:ALA:HB1	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:THR:HG22	1:E:136:GLY:N	1.90	0.87
2:F:163:ASP:HB2	2:F:171:SER:OG	1.73	0.87
1:A:82:LYS:HG2	1:A:100:ALA:HB2	1.56	0.87
2:B:442:THR:HG22	2:B:444:ALA:H	1.39	0.87
1:D:214:TRP:O	1:D:235:SER:HB2	1.74	0.87
2:G:551:TYR:HD1	1:H:27:ARG:HE	1.23	0.87
2:B:267:ARG:HH11	2:B:267:ARG:HG3	1.38	0.87
1:H:135:THR:HG22	1:H:136:GLY:N	1.90	0.87
2:B:202:ARG:HG3	2:B:500:ASP:OD1	1.75	0.87
1:D:249:SER:O	1:D:250:SER:HB2	1.73	0.86
1:E:107:ASN:ND2	2:F:142:ARG:NH2	2.20	0.86
1:A:49:LEU:HD12	1:A:50:ILE:H	1.40	0.86
1:H:151:ILE:HB	1:H:187:CYS:HB2	1.55	0.86
1:A:135:THR:HG22	1:A:136:GLY:N	1.90	0.86
2:B:515:ILE:HD11	2:B:540:ALA:HB3	1.54	0.86
2:C:267:ARG:HH11	2:C:267:ARG:HG3	1.37	0.86
2:B:487:HIS:CD2	2:B:517:LEU:HD23	2.08	0.86
1:E:82:LYS:HG2	1:E:100:ALA:HB2	1.56	0.86
1:A:107:ASN:ND2	2:B:142:ARG:HH22	1.73	0.86
2:G:291:ILE:HG22	2:G:353:ASN:CB	2.04	0.86
1:E:49:LEU:HD12	1:E:50:ILE:H	1.40	0.86
1:H:41:ASP:HB2	1:H:50:ILE:HD11	1.58	0.86
1:H:49:LEU:HD12	1:H:50:ILE:H	1.40	0.85
2:B:365:PRO:HB2	2:B:372:LEU:HD12	1.58	0.85
2:F:276:ILE:HD13	2:F:383:CYS:HA	1.56	0.85
1:H:214:TRP:O	1:H:235:SER:HB2	1.74	0.85
1:E:40:PHE:CZ	2:F:168:SER:HB2	2.12	0.85
2:F:365:PRO:HB2	2:F:372:LEU:HD12	1.59	0.85
2:G:218:LYS:HG2	2:G:238:SER:OG	1.76	0.85
2:F:218:LYS:HG2	2:F:238:SER:OG	1.76	0.85
2:C:365:PRO:HB2	2:C:372:LEU:HD12	1.59	0.85
2:C:218:LYS:HG2	2:C:238:SER:OG	1.76	0.84
2:C:280:ILE:HG13	2:C:300:LEU:HD21	1.58	0.84
2:F:481:LEU:HD13	2:F:489:HIS:HB3	1.58	0.84
2:B:184:LEU:HD21	2:B:448:GLN:NE2	1.93	0.84
1:D:155:ALA:HB2	1:D:217:ASP:HA	1.60	0.84
2:B:218:LYS:HG2	2:B:238:SER:OG	1.76	0.84
1:D:49:LEU:HD12	1:D:50:ILE:H	1.41	0.84
2:F:149:THR:HG22	2:F:150:PHE:N	1.92	0.84
2:G:343:TRP:CZ3	2:G:350:ILE:HG13	2.12	0.84
1:A:28:LEU:HD11	2:B:160:LEU:HD13	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:416:ASP:OD1	2:C:418:ILE:HG13	1.78	0.83
2:B:151:ALA:HB1	2:B:159:LEU:HD11	1.60	0.83
2:B:416:ASP:OD1	2:B:418:ILE:HG13	1.78	0.83
2:C:276:ILE:HD13	2:C:383:CYS:HA	1.59	0.83
2:F:151:ALA:HB1	2:F:159:LEU:HD11	1.60	0.83
2:G:365:PRO:HB2	2:G:372:LEU:HD12	1.58	0.83
2:G:416:ASP:OD1	2:G:418:ILE:HG13	1.78	0.83
2:G:175:LEU:HD13	2:G:176:PRO:HD2	1.60	0.82
2:G:494:SER:O	2:G:497:LEU:HG	1.79	0.82
2:F:416:ASP:OD1	2:F:418:ILE:HG13	1.78	0.82
2:C:175:LEU:HD13	2:C:176:PRO:HD2	1.60	0.82
1:D:135:THR:HG22	1:D:136:GLY:N	1.90	0.82
2:F:484:ALA:HB3	2:F:486:LEU:HD11	1.60	0.82
1:H:69:MET:HE3	1:H:70:TYR:CE1	2.15	0.82
2:B:350:ILE:CG2	2:B:354:ILE:HD12	2.09	0.82
2:F:216:LEU:HB3	2:F:242:ASP:OD1	1.78	0.82
2:B:218:LYS:HG3	2:B:242:ASP:OD2	1.80	0.82
1:H:155:ALA:HB2	1:H:217:ASP:HA	1.59	0.82
2:F:515:ILE:HD11	2:F:540:ALA:HB3	1.62	0.81
2:G:162:LYS:NZ	1:H:15:MET:HE2	1.95	0.81
2:C:142:ARG:O	2:C:143:ARG:HB2	1.79	0.81
2:B:497:LEU:HD12	2:B:503:ALA:HA	1.62	0.81
1:D:69:MET:HE3	1:D:70:TYR:CE1	2.15	0.81
2:C:162:LYS:HZ3	1:D:15:MET:HE2	1.43	0.81
2:C:276:ILE:CD1	2:C:383:CYS:HA	2.10	0.81
2:C:522:THR:O	2:C:523:ASN:CG	2.23	0.81
2:F:320:VAL:O	2:F:323:SER:HB3	1.81	0.81
2:C:291:ILE:HG22	2:C:353:ASN:CB	2.10	0.80
2:C:145:THR:HG22	2:C:147:SER:H	1.46	0.80
2:C:515:ILE:HD11	2:C:540:ALA:HB3	1.62	0.80
2:F:159:LEU:C	2:F:160:LEU:HD23	2.06	0.80
2:G:145:THR:HG22	2:G:147:SER:H	1.46	0.80
2:G:471:ASP:OD1	2:G:497:LEU:HD22	1.82	0.80
2:C:155:THR:HG22	2:C:513:ARG:HD2	1.63	0.80
1:E:245:CYS:HB2	1:E:253:TRP:CE3	2.17	0.80
2:B:320:VAL:O	2:B:323:SER:HB3	1.82	0.80
2:B:159:LEU:HD12	2:B:160:LEU:N	1.97	0.80
2:F:159:LEU:HD12	2:F:160:LEU:N	1.96	0.80
2:G:320:VAL:O	2:G:323:SER:HB3	1.82	0.80
1:H:220:TRP:CE2	1:H:231:ILE:HD11	2.17	0.80
2:B:149:THR:HG22	2:B:150:PHE:N	1.92	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:431:THR:HG22	2:F:432:GLU:N	1.97	0.79
2:B:190:LEU:HD13	2:B:489:HIS:ND1	1.97	0.79
2:B:431:THR:HG22	2:B:432:GLU:N	1.96	0.79
1:E:69:MET:HE3	1:E:70:TYR:CE1	2.14	0.79
1:E:208:LEU:HB3	1:E:243:TRP:CZ3	2.18	0.79
1:A:220:TRP:CE2	1:A:231:ILE:HD11	2.18	0.79
2:C:149:THR:HG23	2:C:162:LYS:HG2	1.64	0.79
2:G:479:ALA:CA	1:H:273:THR:HG21	2.11	0.79
2:B:207:TYR:CD2	2:B:504:GLU:HA	2.18	0.79
2:C:320:VAL:O	2:C:323:SER:HB3	1.82	0.79
2:G:149:THR:HG23	2:G:162:LYS:HG2	1.64	0.79
2:B:159:LEU:C	2:B:160:LEU:HD23	2.07	0.79
2:F:238:SER:O	2:F:242:ASP:HB2	1.81	0.79
1:E:28:LEU:HD21	2:F:170:VAL:HG11	1.65	0.79
2:G:431:THR:HG22	2:G:432:GLU:N	1.97	0.79
1:A:107:ASN:ND2	2:B:142:ARG:NH2	2.30	0.79
2:C:494:SER:O	2:C:497:LEU:HG	1.82	0.79
1:E:220:TRP:CE2	1:E:231:ILE:HD11	2.17	0.79
1:A:69:MET:HE3	1:A:70:TYR:CE1	2.14	0.78
2:F:445:LEU:HD22	2:F:449:PHE:CD2	2.18	0.78
2:G:142:ARG:O	2:G:143:ARG:HB2	1.79	0.78
2:B:276:ILE:CD1	2:B:383:CYS:HA	2.13	0.78
1:D:220:TRP:CE2	1:D:231:ILE:HD11	2.18	0.78
2:B:172:ILE:O	2:B:172:ILE:HG22	1.83	0.78
1:E:180:LYS:HD2	1:E:196:GLU:OE1	1.82	0.78
2:G:479:ALA:HB1	1:H:273:THR:HG22	1.65	0.78
1:H:244:THR:HG22	1:H:245:CYS:H	1.48	0.78
1:A:41:ASP:HB2	1:A:50:ILE:CD1	2.13	0.78
2:C:431:THR:HG22	2:C:432:GLU:N	1.97	0.78
2:B:398:SER:OG	2:B:401:SER:HB3	1.83	0.78
1:E:273:THR:HG21	2:F:479:ALA:CB	2.14	0.77
2:G:512:MET:SD	2:G:540:ALA:HB2	2.24	0.77
2:F:177:THR:HG21	2:F:179:LEU:HD23	1.67	0.77
2:B:177:THR:HG21	2:B:179:LEU:HD23	1.67	0.77
2:C:442:THR:CG2	2:C:444:ALA:H	1.96	0.77
2:C:432:GLU:OE2	2:C:466:SER:HB3	1.85	0.77
1:E:135:THR:CG2	1:E:136:GLY:H	1.98	0.77
2:C:158:MET:HE1	2:C:174:ARG:HG3	1.66	0.77
2:F:442:THR:CG2	2:F:444:ALA:H	1.97	0.77
2:C:134:ASN:O	2:C:138:ILE:HB	1.85	0.76
2:C:487:HIS:HD2	2:C:517:LEU:HD23	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:172:ILE:HG22	2:F:172:ILE:O	1.84	0.76
2:F:250:THR:HG21	2:G:335:LEU:HD13	1.67	0.76
2:G:134:ASN:O	2:G:138:ILE:HB	1.85	0.76
2:G:158:MET:HE1	2:G:174:ARG:HG3	1.66	0.76
2:G:352:LYS:CE	2:G:374:GLU:OE2	2.33	0.76
2:G:291:ILE:CG2	2:G:353:ASN:HB2	2.16	0.76
1:H:226:LEU:HD13	1:H:227:PRO:HD2	1.67	0.76
1:A:220:TRP:CZ3	1:A:229:SER:HB2	2.21	0.76
2:B:210:ILE:HD11	2:B:495:CYS:HB2	1.65	0.76
2:F:343:TRP:CZ3	2:F:350:ILE:HG21	2.21	0.76
2:G:359:LYS:HD2	2:G:365:PRO:HA	1.68	0.76
1:D:220:TRP:CZ3	1:D:229:SER:HB2	2.21	0.76
1:E:220:TRP:CZ3	1:E:229:SER:HB2	2.21	0.76
1:H:220:TRP:CZ3	1:H:229:SER:HB2	2.21	0.76
2:B:177:THR:CG2	2:B:179:LEU:HD23	2.16	0.75
2:G:162:LYS:HZ3	1:H:15:MET:HE2	1.49	0.75
2:C:284:ILE:HD13	2:C:297:TYR:CE1	2.22	0.75
1:D:226:LEU:HD13	1:D:227:PRO:HD2	1.68	0.75
1:A:102:HIS:HE2	1:A:130:SER:HB3	1.52	0.75
2:F:364:SER:HB3	2:F:394:ILE:HG12	1.69	0.75
1:H:79:TYR:HA	1:H:105:SER:HB2	1.68	0.75
2:B:321:LEU:HB3	2:B:361:LEU:HD11	1.67	0.75
2:B:359:LYS:HD2	2:B:365:PRO:HA	1.68	0.75
2:G:276:ILE:CD1	2:G:383:CYS:HA	2.15	0.75
2:G:216:LEU:HB3	2:G:242:ASP:OD1	1.86	0.75
1:H:102:HIS:HE2	1:H:130:SER:HB3	1.52	0.75
1:A:226:LEU:HD13	1:A:227:PRO:HD2	1.67	0.74
1:D:102:HIS:HE2	1:D:130:SER:HB3	1.52	0.74
2:F:359:LYS:HD2	2:F:365:PRO:HA	1.68	0.74
2:F:484:ALA:CB	2:F:486:LEU:HD11	2.17	0.74
2:C:359:LYS:HD2	2:C:365:PRO:HA	1.68	0.74
1:D:195:LYS:HG2	1:D:196:GLU:N	2.01	0.74
1:E:79:TYR:HA	1:E:105:SER:HB2	1.69	0.74
1:A:242:ILE:HD11	1:A:258:LEU:HD22	1.69	0.74
1:E:226:LEU:HD13	1:E:227:PRO:HD2	1.68	0.74
1:A:135:THR:CG2	1:A:136:GLY:H	1.98	0.74
2:C:151:ALA:HA	2:C:160:LEU:O	1.87	0.74
2:G:151:ALA:HA	2:G:160:LEU:O	1.87	0.74
2:C:294:ILE:HG12	2:C:309:LEU:HD23	1.67	0.74
1:A:41:ASP:CB	1:A:50:ILE:HD11	2.17	0.74
1:A:79:TYR:HA	1:A:105:SER:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ILE:HB	1:D:187:CYS:HB2	1.70	0.74
2:F:177:THR:CG2	2:F:179:LEU:HD23	2.16	0.74
2:G:284:ILE:HD13	2:G:297:TYR:CE1	2.23	0.74
1:D:29:ALA:HB2	1:D:39:ILE:CD1	2.18	0.74
1:D:79:TYR:HA	1:D:105:SER:HB2	1.68	0.74
1:D:135:THR:CG2	1:D:136:GLY:H	1.98	0.74
2:F:179:LEU:O	2:F:179:LEU:HG	1.88	0.74
1:E:107:ASN:OD1	2:F:142:ARG:NH1	2.21	0.74
2:G:280:ILE:HB	2:G:300:LEU:HD21	1.68	0.74
2:B:177:THR:HG22	2:B:179:LEU:HB3	1.70	0.73
1:E:17:HIS:CE1	2:F:148:TYR:CE2	2.76	0.73
1:D:290:LYS:HB3	1:D:300:ILE:HD11	1.70	0.73
2:G:240:LEU:HD21	2:G:268:LEU:CD1	2.17	0.73
1:D:249:SER:O	1:D:250:SER:CB	2.34	0.73
1:E:102:HIS:HE2	1:E:130:SER:HB3	1.52	0.73
2:B:244:VAL:HG23	2:B:264:ARG:HH21	1.54	0.73
2:C:483:PHE:O	2:C:485:GLN:HG2	1.88	0.73
2:B:197:VAL:HG12	2:B:198:THR:N	2.03	0.73
2:B:216:LEU:HB3	2:B:242:ASP:OD2	1.88	0.73
2:C:421:ILE:HD11	2:C:449:PHE:HZ	1.54	0.73
2:F:432:GLU:CD	2:F:466:SER:HB3	2.13	0.73
2:G:197:VAL:HG12	2:G:198:THR:N	2.03	0.73
2:G:412:LEU:N	2:G:412:LEU:HD12	2.04	0.73
1:H:95:LYS:HE3	1:H:98:GLU:HB2	1.71	0.73
1:D:95:LYS:HE3	1:D:98:GLU:HB2	1.71	0.73
2:F:336:ALA:O	2:F:340:LEU:HD23	1.89	0.73
2:C:162:LYS:NZ	1:D:15:MET:CE	2.52	0.73
2:C:199:ILE:CD1	2:C:530:LEU:HA	2.19	0.72
2:F:179:LEU:HD11	2:F:184:LEU:CD1	2.19	0.72
2:G:442:THR:CG2	2:G:444:ALA:H	2.01	0.72
1:H:195:LYS:HE2	1:H:203:LYS:HB2	1.71	0.72
1:E:41:ASP:CB	1:E:50:ILE:HD11	2.18	0.72
2:C:428:ASN:HA	2:C:463:ARG:NH1	2.04	0.72
2:C:471:ASP:OD1	2:C:497:LEU:HA	1.89	0.72
1:D:41:ASP:CB	1:D:50:ILE:HD11	2.19	0.72
1:A:95:LYS:HE3	1:A:98:GLU:HB2	1.71	0.72
2:B:336:ALA:O	2:B:340:LEU:HD23	1.89	0.72
1:E:230:THR:HG22	1:E:231:ILE:H	1.55	0.72
2:F:197:VAL:HG12	2:F:198:THR:N	2.04	0.72
2:C:336:ALA:O	2:C:340:LEU:HD23	1.90	0.72
2:C:421:ILE:HD11	2:C:449:PHE:CZ	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:177:THR:HG22	2:F:179:LEU:HB3	1.70	0.72
2:G:336:ALA:O	2:G:340:LEU:HD23	1.89	0.72
1:H:69:MET:CE	1:H:114:HIS:HB2	2.20	0.72
2:F:184:LEU:HD21	2:F:448:GLN:HE22	1.52	0.72
2:B:179:LEU:HG	2:B:179:LEU:O	1.87	0.72
2:G:175:LEU:CD1	2:G:176:PRO:HD2	2.18	0.72
2:C:175:LEU:CD1	2:C:176:PRO:HD2	2.18	0.71
2:G:149:THR:HG22	2:G:150:PHE:H	1.55	0.71
1:D:69:MET:CE	1:D:114:HIS:HB2	2.20	0.71
2:C:223:TYR:CD1	2:C:223:TYR:N	2.58	0.71
2:B:223:TYR:N	2:B:223:TYR:CD1	2.58	0.71
1:D:234:CYS:SG	1:D:268:VAL:HG23	2.30	0.71
2:F:343:TRP:CE3	2:F:350:ILE:HD13	2.25	0.71
1:A:69:MET:CE	1:A:114:HIS:HB2	2.20	0.71
1:A:230:THR:HG22	1:A:231:ILE:H	1.55	0.71
2:C:197:VAL:HG12	2:C:198:THR:N	2.04	0.71
1:E:69:MET:CE	1:E:114:HIS:HB2	2.20	0.71
2:G:148:TYR:HB2	1:H:266:TRP:CG	2.24	0.71
2:G:280:ILE:CB	2:G:300:LEU:HD21	2.19	0.71
2:C:512:MET:SD	2:C:540:ALA:HB2	2.30	0.71
2:C:149:THR:HG22	2:C:150:PHE:H	1.55	0.71
2:C:194:ILE:HG12	2:C:492:PHE:CE2	2.26	0.71
2:F:276:ILE:CD1	2:F:383:CYS:HA	2.21	0.71
1:D:29:ALA:CB	1:D:39:ILE:CD1	2.69	0.71
1:E:95:LYS:HE3	1:E:98:GLU:HB2	1.72	0.71
2:F:247:PRO:HG2	2:F:248:TYR:CE1	2.26	0.71
2:F:385:LEU:HA	2:F:406:HIS:CE1	2.26	0.71
2:C:162:LYS:HZ2	1:D:15:MET:HE2	1.54	0.70
2:F:343:TRP:HZ3	2:F:350:ILE:CG2	2.04	0.70
2:C:216:LEU:HB3	2:C:242:ASP:OD1	1.92	0.70
1:H:230:THR:HG22	1:H:231:ILE:H	1.56	0.70
2:C:149:THR:HG22	2:C:150:PHE:N	2.06	0.70
2:F:223:TYR:CD1	2:F:223:TYR:N	2.58	0.70
1:A:22:ASP:OD1	1:A:23:TYR:N	2.24	0.70
2:F:445:LEU:HD22	2:F:449:PHE:HD2	1.56	0.70
1:H:22:ASP:OD1	1:H:23:TYR:N	2.25	0.70
1:D:230:THR:HG22	1:D:231:ILE:H	1.56	0.70
2:F:480:GLN:OE1	2:F:480:GLN:HA	1.91	0.70
2:F:524:ASP:OD1	2:F:524:ASP:O	2.10	0.70
2:C:480:GLN:OE1	2:C:480:GLN:HA	1.92	0.70
1:E:145:ILE:HD13	1:E:194:TRP:CZ3	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASN:OD1	2:B:142:ARG:NH1	2.24	0.70
1:E:22:ASP:OD1	1:E:23:TYR:N	2.24	0.70
1:A:242:ILE:HD12	1:A:297:TRP:CE2	2.27	0.70
2:C:291:ILE:CG2	2:C:353:ASN:HB2	2.21	0.70
2:F:294:ILE:HG12	2:F:309:LEU:HD23	1.72	0.70
2:G:149:THR:HG22	2:G:150:PHE:N	2.06	0.70
2:C:487:HIS:O	2:C:488:GLY:C	2.35	0.70
2:G:223:TYR:N	2:G:223:TYR:CD1	2.58	0.70
1:D:22:ASP:OD1	1:D:23:TYR:N	2.25	0.70
1:D:190:LEU:CD2	1:D:209:GLU:HB3	2.22	0.69
1:E:179:ILE:HG21	1:E:181:ARG:HE	1.57	0.69
2:F:244:VAL:HG23	2:F:264:ARG:HH21	1.56	0.69
2:F:395:ASP:HB2	2:F:397:TYR:CE2	2.27	0.69
2:F:431:THR:HG22	2:F:432:GLU:H	1.56	0.69
2:G:215:LEU:O	2:G:456:THR:HG23	1.92	0.69
1:D:179:ILE:HG21	1:D:181:ARG:HE	1.57	0.69
1:E:26:THR:HB	2:F:547:TYR:OH	1.92	0.69
1:H:135:THR:CG2	1:H:136:GLY:H	1.98	0.69
2:F:343:TRP:HZ3	2:F:350:ILE:HG21	1.56	0.69
2:C:170:VAL:HG12	2:C:171:SER:N	2.07	0.69
2:C:479:ALA:HB2	1:D:273:THR:CG2	2.21	0.69
2:F:475:PHE:HE2	2:F:497:LEU:HD21	1.56	0.69
2:B:480:GLN:OE1	2:B:480:GLN:HA	1.92	0.69
2:C:431:THR:HG22	2:C:432:GLU:H	1.57	0.69
1:D:41:ASP:HB3	1:D:50:ILE:HD11	1.75	0.69
2:G:353:ASN:O	2:G:357:ILE:HG13	1.92	0.69
2:B:385:LEU:HA	2:B:406:HIS:CE1	2.28	0.69
2:G:480:GLN:OE1	2:G:480:GLN:HA	1.92	0.69
2:B:524:ASP:O	2:B:524:ASP:OD1	2.10	0.69
2:C:479:ALA:CA	1:D:273:THR:HG21	2.23	0.69
2:F:353:ASN:O	2:F:357:ILE:HG13	1.93	0.69
1:H:29:ALA:HB2	1:H:39:ILE:CD1	2.23	0.69
1:A:179:ILE:CG2	1:A:181:ARG:HE	2.06	0.69
2:B:404:GLN:CG	2:B:426:ALA:HB1	2.21	0.69
1:H:179:ILE:HG21	1:H:181:ARG:HE	1.57	0.69
2:B:304:VAL:HG21	2:C:302:ASP:HA	1.75	0.68
1:E:29:ALA:HB2	1:E:39:ILE:CD1	2.23	0.68
2:F:224:MET:CE	2:F:230:ASP:HB3	2.24	0.68
2:C:224:MET:CE	2:C:230:ASP:HB3	2.23	0.68
2:G:479:ALA:HA	1:H:273:THR:HG21	1.74	0.68
2:G:291:ILE:HD12	2:G:351:ASP:OD2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:53:LEU:N	1:H:53:LEU:HD23	2.09	0.68
1:A:28:LEU:HD11	2:B:160:LEU:CD1	2.23	0.68
2:C:353:ASN:O	2:C:357:ILE:HG13	1.93	0.68
1:E:39:ILE:HD11	1:E:74:LEU:HD22	1.75	0.68
1:H:288:LEU:N	1:H:301:SER:HB3	2.06	0.68
1:A:193:LEU:C	1:A:194:TRP:CD1	2.72	0.68
2:B:353:ASN:O	2:B:357:ILE:HG13	1.92	0.68
2:B:491:LEU:O	2:B:494:SER:HB2	1.93	0.68
1:D:193:LEU:C	1:D:194:TRP:CD1	2.72	0.68
2:G:202:ARG:HG2	2:G:209:GLN:OE1	1.94	0.68
2:G:284:ILE:HG12	2:G:296:LEU:HD12	1.76	0.68
1:H:220:TRP:HZ3	1:H:229:SER:HB2	1.58	0.68
2:B:202:ARG:HG2	2:B:209:GLN:OE1	1.94	0.68
2:B:223:TYR:HD1	2:B:223:TYR:H	1.42	0.68
2:C:215:LEU:O	2:C:456:THR:HG23	1.93	0.68
2:G:352:LYS:HG2	2:G:356:LYS:HE3	1.73	0.68
2:G:400:GLU:HG3	2:G:425:TYR:CZ	2.28	0.68
2:G:404:GLN:HG2	2:G:426:ALA:HB1	1.74	0.68
1:E:193:LEU:C	1:E:194:TRP:CD1	2.72	0.68
2:G:431:THR:HG22	2:G:432:GLU:H	1.56	0.68
1:E:107:ASN:OD1	2:F:142:ARG:CZ	2.42	0.68
2:F:202:ARG:HG2	2:F:209:GLN:OE1	1.94	0.68
2:C:238:SER:O	2:C:242:ASP:HB2	1.93	0.68
2:C:378:GLU:OE1	2:C:378:GLU:N	2.27	0.68
2:F:280:ILE:HG13	2:F:300:LEU:HD21	1.75	0.68
1:A:53:LEU:N	1:A:53:LEU:HD23	2.09	0.68
2:C:159:LEU:HD12	2:C:160:LEU:N	2.09	0.68
2:F:184:LEU:HD21	2:F:448:GLN:NE2	2.08	0.68
2:B:431:THR:HG22	2:B:432:GLU:H	1.56	0.67
1:H:179:ILE:CG2	1:H:181:ARG:HE	2.06	0.67
1:A:42:VAL:HG12	1:A:42:VAL:O	1.94	0.67
1:A:224:ILE:C	1:A:226:LEU:H	2.03	0.67
1:E:53:LEU:N	1:E:53:LEU:HD23	2.08	0.67
2:F:378:GLU:OE1	2:F:378:GLU:N	2.27	0.67
2:G:210:ILE:CD1	2:G:495:CYS:HB3	2.24	0.67
2:G:224:MET:CE	2:G:230:ASP:HB3	2.23	0.67
1:A:268:VAL:CG1	1:A:277:LEU:HD11	2.25	0.67
2:C:202:ARG:HG2	2:C:209:GLN:OE1	1.94	0.67
1:D:224:ILE:C	1:D:226:LEU:H	2.03	0.67
1:H:193:LEU:C	1:H:194:TRP:CD1	2.72	0.67
1:E:271:SER:HB2	2:F:153:PHE:CD2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:MET:CE	2:B:230:ASP:HB3	2.23	0.67
2:C:280:ILE:CG1	2:C:300:LEU:HD21	2.24	0.67
2:C:364:SER:HB2	2:C:367:GLU:HG2	1.76	0.67
1:D:179:ILE:CG2	1:D:181:ARG:HE	2.06	0.67
1:D:288:LEU:H	1:D:301:SER:HB3	1.59	0.67
2:G:170:VAL:HG12	2:G:171:SER:N	2.08	0.67
2:G:352:LYS:HE2	2:G:374:GLU:OE2	1.94	0.67
1:A:179:ILE:HG21	1:A:181:ARG:HE	1.57	0.67
2:B:378:GLU:OE1	2:B:378:GLU:N	2.27	0.67
2:B:487:HIS:CE1	2:B:514:GLU:HG3	2.30	0.67
1:D:53:LEU:N	1:D:53:LEU:HD23	2.08	0.67
1:H:268:VAL:CG1	1:H:277:LEU:HD11	2.25	0.67
1:D:232:ALA:HB2	1:D:270:TRP:CZ2	2.29	0.67
2:G:202:ARG:CZ	2:G:209:GLN:HB3	2.25	0.67
1:H:23:TYR:HD2	1:H:24:TYR:CD1	2.12	0.67
2:B:156:GLY:O	2:B:157:SER:HB2	1.94	0.67
1:E:28:LEU:HD11	2:F:160:LEU:HD13	1.76	0.67
2:F:177:THR:C	2:F:179:LEU:H	2.03	0.67
2:F:202:ARG:CZ	2:F:209:GLN:HB3	2.25	0.67
2:B:177:THR:C	2:B:179:LEU:H	2.02	0.67
1:E:179:ILE:CG2	1:E:181:ARG:HE	2.06	0.67
2:F:421:ILE:HD11	2:F:449:PHE:HZ	1.59	0.67
2:G:138:ILE:HG22	2:G:139:MET:HG2	1.77	0.67
2:G:432:GLU:CD	2:G:466:SER:HB3	2.18	0.67
1:H:230:THR:CG2	1:H:242:ILE:HG23	2.25	0.67
1:A:273:THR:HG21	2:B:479:ALA:CB	2.25	0.66
1:E:23:TYR:HD2	1:E:24:TYR:CD1	2.13	0.66
2:B:167:LYS:O	2:B:167:LYS:HD3	1.95	0.66
2:B:284:ILE:HG12	2:B:296:LEU:HD12	1.76	0.66
2:C:202:ARG:CZ	2:C:209:GLN:HB3	2.25	0.66
2:F:167:LYS:O	2:F:167:LYS:HD3	1.95	0.66
1:A:17:HIS:CE1	2:B:148:TYR:CE2	2.83	0.66
2:C:223:TYR:H	2:C:223:TYR:HD1	1.42	0.66
1:D:268:VAL:CG1	1:D:277:LEU:HD11	2.24	0.66
1:E:208:LEU:HD13	1:E:243:TRP:CE3	2.30	0.66
2:F:156:GLY:O	2:F:157:SER:HB2	1.94	0.66
2:G:240:LEU:HD21	2:G:268:LEU:HD12	1.75	0.66
1:H:224:ILE:C	1:H:226:LEU:H	2.03	0.66
2:B:364:SER:HB2	2:B:367:GLU:HG2	1.77	0.66
2:B:491:LEU:HD21	2:B:532:ILE:HD11	1.78	0.66
2:B:522:THR:CG2	2:B:526:ILE:HD11	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:ALA:HB1	1:D:290:LYS:HE3	1.78	0.66
1:E:220:TRP:HZ3	1:E:229:SER:HB2	1.58	0.66
1:E:242:ILE:HD13	1:E:297:TRP:CE2	2.30	0.66
2:G:223:TYR:HD1	2:G:223:TYR:H	1.42	0.66
1:H:39:ILE:HD11	1:H:74:LEU:HD22	1.75	0.66
1:A:23:TYR:HD2	1:A:24:TYR:CD1	2.13	0.66
2:C:487:HIS:CD2	2:C:517:LEU:HD23	2.31	0.66
1:D:23:TYR:HD2	1:D:24:TYR:CD1	2.12	0.66
2:F:223:TYR:H	2:F:223:TYR:HD1	1.42	0.66
2:G:479:ALA:CB	1:H:273:THR:HG22	2.24	0.66
1:A:26:THR:HB	2:B:547:TYR:OH	1.96	0.66
2:C:240:LEU:HD21	2:C:268:LEU:CD1	2.26	0.66
1:E:224:ILE:C	1:E:226:LEU:H	2.02	0.66
2:B:202:ARG:CZ	2:B:209:GLN:HB3	2.25	0.66
2:C:177:THR:HG22	2:C:179:LEU:N	2.08	0.66
2:C:321:LEU:HB3	2:C:361:LEU:HD11	1.76	0.66
1:E:26:THR:HG22	1:E:27:ARG:HD2	1.78	0.66
2:G:364:SER:HB2	2:G:367:GLU:HG2	1.77	0.66
1:A:220:TRP:HZ3	1:A:229:SER:HB2	1.58	0.66
2:B:246:TYR:CD1	2:B:247:PRO:HD2	2.31	0.66
1:D:39:ILE:HD11	1:D:74:LEU:HD22	1.77	0.65
1:E:268:VAL:CG1	1:E:277:LEU:HD11	2.25	0.65
1:E:288:LEU:HB2	1:E:300:ILE:HG13	1.78	0.65
2:F:364:SER:HB2	2:F:367:GLU:HG2	1.77	0.65
2:G:202:ARG:HG3	2:G:500:ASP:OD1	1.97	0.65
2:G:378:GLU:OE1	2:G:378:GLU:N	2.27	0.65
1:A:26:THR:HG22	1:A:27:ARG:HD2	1.78	0.65
2:C:138:ILE:HG22	2:C:139:MET:HG2	1.77	0.65
1:D:220:TRP:HZ3	1:D:229:SER:HB2	1.58	0.65
2:C:223:TYR:N	2:C:223:TYR:HD1	1.94	0.65
1:E:21:MET:HE1	2:F:172:ILE:HD13	1.78	0.65
1:A:15:MET:HG3	2:B:162:LYS:NZ	2.12	0.65
1:A:107:ASN:OD1	2:B:142:ARG:CZ	2.45	0.65
2:G:421:ILE:HD11	2:G:449:PHE:HZ	1.62	0.65
1:H:26:THR:HG22	1:H:27:ARG:HD2	1.78	0.65
1:H:29:ALA:CB	1:H:39:ILE:CD1	2.75	0.65
1:H:244:THR:HG22	1:H:245:CYS:N	2.11	0.65
2:C:291:ILE:HD12	2:C:351:ASP:OD2	1.96	0.65
2:C:491:LEU:O	2:C:494:SER:HB3	1.97	0.65
2:F:484:ALA:CB	2:F:486:LEU:CD1	2.70	0.65
2:B:280:ILE:CB	2:B:300:LEU:HD21	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:THR:HG22	1:D:27:ARG:HD2	1.78	0.65
2:F:149:THR:CG2	2:F:150:PHE:H	2.06	0.65
2:F:223:TYR:N	2:F:223:TYR:HD1	1.94	0.65
2:G:280:ILE:HG13	2:G:300:LEU:HD21	1.78	0.65
2:G:421:ILE:HD11	2:G:449:PHE:CZ	2.31	0.65
1:E:29:ALA:CB	1:E:39:ILE:CD1	2.75	0.65
2:B:431:THR:CG2	2:B:432:GLU:N	2.60	0.65
2:B:522:THR:O	2:B:523:ASN:ND2	2.29	0.65
2:C:435:TYR:CE2	2:C:454:ILE:HD11	2.32	0.65
1:E:288:LEU:CB	1:E:300:ILE:HG13	2.27	0.65
2:G:159:LEU:HD12	2:G:160:LEU:N	2.09	0.65
2:G:431:THR:CG2	2:G:432:GLU:N	2.60	0.65
1:A:190:LEU:CD2	1:A:209:GLU:HB3	2.27	0.64
2:B:149:THR:CG2	2:B:150:PHE:H	2.06	0.64
2:C:210:ILE:HG22	2:C:459:PHE:HE2	1.61	0.64
1:H:16:ILE:HD12	1:H:30:THR:HG21	1.79	0.64
1:A:151:ILE:HB	1:A:187:CYS:HB2	1.80	0.64
1:E:16:ILE:HD12	1:E:30:THR:HG21	1.79	0.64
2:F:252:ASN:HB3	2:F:255:VAL:HB	1.79	0.64
1:A:113:PRO:CB	1:A:161:ALA:HB2	2.27	0.64
1:H:209:GLU:O	1:H:209:GLU:HG3	1.97	0.64
2:B:280:ILE:HB	2:B:300:LEU:HD21	1.79	0.64
2:C:479:ALA:HB1	1:D:273:THR:HG22	1.79	0.64
2:G:210:ILE:HD12	2:G:495:CYS:HB3	1.77	0.64
1:A:16:ILE:HD12	1:A:30:THR:HG21	1.79	0.64
1:A:182:PHE:CD1	1:A:182:PHE:O	2.51	0.64
2:B:197:VAL:CG1	2:B:198:THR:N	2.61	0.64
2:C:524:ASP:OD1	2:C:524:ASP:O	2.15	0.64
1:D:29:ALA:HB2	1:D:39:ILE:HD12	1.80	0.64
1:E:182:PHE:O	1:E:182:PHE:CD1	2.50	0.64
1:E:278:ALA:CB	2:F:153:PHE:HE1	1.93	0.64
1:A:155:ALA:HB2	1:A:217:ASP:HA	1.79	0.64
2:G:223:TYR:N	2:G:223:TYR:HD1	1.94	0.64
2:G:246:TYR:HE2	2:G:248:TYR:HB2	1.63	0.64
1:E:15:MET:HG3	2:F:162:LYS:NZ	2.12	0.64
2:F:431:THR:CG2	2:F:432:GLU:N	2.60	0.64
2:B:179:LEU:HD11	2:B:184:LEU:CD1	2.28	0.64
2:B:384:LEU:O	2:B:387:LEU:HB2	1.98	0.64
2:F:197:VAL:CG1	2:F:198:THR:N	2.61	0.64
2:F:284:ILE:HG12	2:F:296:LEU:HD12	1.80	0.64
1:A:274:ALA:HB3	1:A:276:ILE:HG13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:170:VAL:HG12	2:C:171:SER:H	1.63	0.64
2:C:384:LEU:O	2:C:387:LEU:HB2	1.98	0.64
2:C:420:VAL:HG11	2:C:445:LEU:HD11	1.80	0.64
2:G:481:LEU:CD1	2:G:489:HIS:HB3	2.15	0.64
2:B:404:GLN:HG2	2:B:426:ALA:CB	2.23	0.63
2:C:152:LYS:NZ	1:D:62:GLN:HE21	1.96	0.63
1:D:182:PHE:CD1	1:D:182:PHE:O	2.51	0.63
1:H:151:ILE:HB	1:H:187:CYS:CB	2.28	0.63
2:C:280:ILE:CB	2:C:300:LEU:HD21	2.29	0.63
2:C:381:TRP:CZ3	2:C:382:LEU:HD13	2.33	0.63
1:A:209:GLU:HG3	1:A:209:GLU:O	1.97	0.63
2:B:485:GLN:HE21	2:B:517:LEU:HD22	1.63	0.63
1:E:274:ALA:O	1:E:275:ASN:HB2	1.98	0.63
2:F:321:LEU:HB3	2:F:361:LEU:HD11	1.78	0.63
2:C:431:THR:CG2	2:C:432:GLU:N	2.61	0.63
2:G:384:LEU:O	2:G:387:LEU:HB2	1.98	0.63
2:B:223:TYR:N	2:B:223:TYR:HD1	1.94	0.63
2:G:512:MET:HA	2:G:540:ALA:HB1	1.81	0.63
2:C:197:VAL:CG1	2:C:198:THR:N	2.61	0.63
1:D:79:TYR:CD1	1:D:105:SER:HB3	2.34	0.63
1:D:274:ALA:O	1:D:275:ASN:HB2	1.97	0.63
1:E:209:GLU:O	1:E:209:GLU:HG3	1.98	0.63
2:G:197:VAL:CG1	2:G:198:THR:N	2.61	0.63
2:G:201:ALA:HB2	2:G:531:LYS:NZ	2.14	0.63
1:H:274:ALA:HB3	1:H:276:ILE:HG13	1.80	0.63
1:A:274:ALA:O	1:A:275:ASN:HB2	1.98	0.63
2:B:164:ILE:HG23	2:B:164:ILE:O	1.98	0.63
2:B:494:SER:O	2:B:497:LEU:HG	1.99	0.63
1:D:16:ILE:HD12	1:D:30:THR:HG21	1.79	0.63
2:G:155:THR:HG22	2:G:513:ARG:CD	2.25	0.63
1:H:226:LEU:HD13	1:H:227:PRO:CD	2.29	0.63
1:A:79:TYR:CD1	1:A:105:SER:HB3	2.34	0.63
2:C:381:TRP:CE3	2:C:412:LEU:CD2	2.82	0.63
1:H:190:LEU:CD2	1:H:209:GLU:HB3	2.29	0.63
1:H:274:ALA:O	1:H:275:ASN:HB2	1.98	0.63
2:C:240:LEU:HD21	2:C:268:LEU:HD12	1.81	0.62
1:E:17:HIS:ND1	2:F:148:TYR:HE2	1.96	0.62
2:B:238:SER:O	2:B:242:ASP:HB3	1.99	0.62
2:C:151:ALA:HB2	1:D:286:VAL:HG21	1.81	0.62
2:G:138:ILE:HG22	2:G:139:MET:H	1.64	0.62
1:A:226:LEU:HD13	1:A:227:PRO:CD	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:ARG:HH11	2:C:267:ARG:CG	2.10	0.62
1:E:230:THR:HG22	1:E:231:ILE:N	2.14	0.62
1:E:274:ALA:HB3	1:E:276:ILE:HG13	1.80	0.62
1:H:182:PHE:O	1:H:182:PHE:CD1	2.51	0.62
2:C:136:LYS:O	2:C:140:LYS:HB2	1.99	0.62
2:C:492:PHE:CD1	2:C:492:PHE:C	2.77	0.62
1:D:209:GLU:HG3	1:D:209:GLU:O	1.97	0.62
1:A:15:MET:HE2	2:B:162:LYS:NZ	2.15	0.62
1:D:274:ALA:HB3	1:D:276:ILE:HG13	1.80	0.62
2:F:149:THR:CG2	2:F:150:PHE:N	2.63	0.62
2:F:164:ILE:HG23	2:F:164:ILE:O	1.99	0.62
2:F:240:LEU:HD21	2:F:268:LEU:HD12	1.80	0.62
1:H:42:VAL:O	1:H:42:VAL:HG12	1.98	0.62
1:H:79:TYR:CD1	1:H:105:SER:HB3	2.34	0.62
1:D:226:LEU:HD13	1:D:227:PRO:CD	2.29	0.62
1:E:226:LEU:HD13	1:E:227:PRO:CD	2.29	0.62
2:F:237:SER:OG	2:F:421:ILE:CD1	2.48	0.62
2:G:515:ILE:HD11	2:G:540:ALA:HB3	1.82	0.62
2:C:148:TYR:HB2	1:D:266:TRP:CG	2.35	0.62
1:E:79:TYR:CD1	1:E:105:SER:HB3	2.35	0.62
2:F:155:THR:HG22	2:F:513:ARG:CD	2.30	0.62
2:F:384:LEU:O	2:F:387:LEU:HB2	1.98	0.62
1:H:39:ILE:HD11	1:H:74:LEU:CD2	2.29	0.62
2:B:276:ILE:HD13	2:B:383:CYS:CA	2.27	0.62
2:C:162:LYS:HZ3	1:D:15:MET:CE	2.12	0.62
2:F:522:THR:O	2:F:523:ASN:ND2	2.32	0.62
2:G:136:LYS:O	2:G:140:LYS:HB2	1.99	0.62
2:G:194:ILE:HG12	2:G:492:PHE:CE2	2.35	0.62
1:A:238:GLY:O	1:A:260:LYS:HA	2.00	0.62
2:C:224:MET:HE1	2:C:230:ASP:HB3	1.82	0.62
1:E:15:MET:HE2	2:F:162:LYS:NZ	2.15	0.62
1:E:221:ALA:HB2	1:E:270:TRP:CE2	2.34	0.62
2:F:155:THR:HG22	2:F:513:ARG:HD2	1.82	0.62
1:H:208:LEU:HB3	1:H:243:TRP:CZ3	2.35	0.62
2:B:240:LEU:HD21	2:B:268:LEU:CD1	2.30	0.61
2:B:267:ARG:HH11	2:B:267:ARG:CG	2.11	0.61
2:B:421:ILE:HD11	2:B:449:PHE:HZ	1.63	0.61
2:C:138:ILE:HG22	2:C:139:MET:H	1.64	0.61
2:F:210:ILE:HD11	2:F:495:CYS:HB2	1.81	0.61
2:G:524:ASP:O	2:G:524:ASP:OD1	2.18	0.61
1:A:30:THR:HG22	1:A:31:CYS:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:ARG:HE	2:F:551:TYR:HD1	1.46	0.61
1:E:41:ASP:C	1:E:41:ASP:OD1	2.43	0.61
1:E:190:LEU:HD13	1:E:207:LYS:HD3	1.80	0.61
2:G:343:TRP:HZ3	2:G:350:ILE:HG21	1.65	0.61
1:H:292:SER:C	1:H:294:ASP:H	2.08	0.61
1:D:30:THR:HG22	1:D:31:CYS:N	2.15	0.61
2:F:280:ILE:CB	2:F:300:LEU:HD21	2.30	0.61
1:H:30:THR:HG22	1:H:31:CYS:N	2.15	0.61
1:A:180:LYS:HD2	1:A:196:GLU:OE1	2.00	0.61
1:D:263:ASP:OD1	1:D:264:VAL:N	2.34	0.61
1:E:70:TYR:CD2	1:E:118:LEU:HB2	2.35	0.61
2:G:224:MET:HE1	2:G:230:ASP:HB3	1.82	0.61
1:A:271:SER:HB2	2:B:153:PHE:CD2	2.35	0.61
2:C:160:LEU:HA	2:C:171:SER:O	2.00	0.61
2:C:512:MET:HA	2:C:540:ALA:HB1	1.81	0.61
1:D:230:THR:HG22	1:D:231:ILE:N	2.16	0.61
2:G:175:LEU:HG	2:G:483:PHE:CD2	2.35	0.61
1:A:70:TYR:CD2	1:A:118:LEU:HB2	2.35	0.61
1:A:263:ASP:OD1	1:A:264:VAL:N	2.33	0.61
1:D:145:ILE:HD11	1:D:202:TRP:CB	2.30	0.61
1:E:263:ASP:OD1	1:E:264:VAL:N	2.33	0.61
2:F:263:GLU:HA	2:G:320:VAL:HG22	1.83	0.61
2:F:512:MET:SD	2:F:540:ALA:HB2	2.41	0.61
2:G:160:LEU:HA	2:G:171:SER:O	2.00	0.61
2:G:479:ALA:HB2	1:H:273:THR:CG2	2.29	0.61
2:B:138:ILE:O	2:B:142:ARG:HB2	2.00	0.61
1:D:39:ILE:HD11	1:D:74:LEU:CD2	2.30	0.61
1:D:70:TYR:CD2	1:D:118:LEU:HB2	2.35	0.61
1:E:30:THR:HG22	1:E:31:CYS:N	2.14	0.61
1:E:39:ILE:HD11	1:E:74:LEU:CD2	2.30	0.61
2:F:145:THR:HG22	2:F:147:SER:H	1.66	0.61
2:F:392:GLY:C	2:F:394:ILE:H	2.08	0.61
2:F:491:LEU:HD21	2:F:532:ILE:CD1	2.30	0.61
1:H:70:TYR:CD2	1:H:118:LEU:HB2	2.36	0.61
1:H:263:ASP:OD1	1:H:264:VAL:N	2.33	0.61
2:B:284:ILE:HG12	2:B:296:LEU:CD1	2.30	0.61
1:D:248:ALA:O	1:D:249:SER:OG	2.16	0.61
2:G:238:SER:HA	2:G:242:ASP:OD2	2.01	0.61
2:C:138:ILE:CG2	2:C:139:MET:N	2.64	0.61
2:G:236:LEU:HD22	2:G:418:ILE:HG22	1.83	0.61
1:H:208:LEU:HB3	1:H:243:TRP:CH2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:HG22	1:A:231:ILE:N	2.15	0.61
1:D:70:TYR:HE2	1:D:118:LEU:HB2	1.64	0.61
1:D:238:GLY:O	1:D:260:LYS:HA	2.01	0.61
2:F:138:ILE:O	2:F:142:ARG:HB2	2.01	0.60
2:F:399:LEU:HD23	2:F:425:TYR:OH	2.01	0.60
2:F:487:HIS:CD2	2:F:517:LEU:HD23	2.36	0.60
2:G:177:THR:HG22	2:G:179:LEU:N	2.08	0.60
2:G:205:ASN:HB2	2:G:206:PRO:HD2	1.83	0.60
1:H:208:LEU:HD13	1:H:243:TRP:CE3	2.36	0.60
2:B:375:LEU:HB2	2:B:384:LEU:HD21	1.82	0.60
2:F:142:ARG:HB3	2:F:144:PHE:CD1	2.36	0.60
2:B:240:LEU:HD21	2:B:268:LEU:HD12	1.82	0.60
1:H:230:THR:HG22	1:H:231:ILE:N	2.15	0.60
2:B:205:ASN:HB2	2:B:206:PRO:HD2	1.84	0.60
2:G:142:ARG:NH2	1:H:107:ASN:OD1	2.35	0.60
2:B:442:THR:HG22	2:B:444:ALA:N	2.15	0.60
2:F:412:LEU:CD1	2:F:412:LEU:H	2.10	0.60
2:G:210:ILE:HG22	2:G:459:PHE:HE2	1.66	0.60
2:B:237:SER:OG	2:B:421:ILE:CD1	2.49	0.60
1:E:183:ALA:O	1:E:184:SER:HB3	2.00	0.60
1:H:287:THR:CG2	1:H:299:CYS:SG	2.89	0.60
1:A:70:TYR:HE2	1:A:118:LEU:HB2	1.64	0.60
2:F:224:MET:HE1	2:F:230:ASP:HB3	1.82	0.60
2:F:240:LEU:HD21	2:F:268:LEU:CD1	2.32	0.60
2:G:170:VAL:HG12	2:G:171:SER:H	1.64	0.60
2:G:283:LYS:NZ	2:G:378:GLU:HB2	2.16	0.60
2:G:138:ILE:CG2	2:G:139:MET:N	2.64	0.60
2:B:149:THR:CG2	2:B:150:PHE:N	2.63	0.60
2:F:446:ASP:O	2:F:449:PHE:N	2.35	0.60
2:B:294:ILE:HG12	2:B:309:LEU:HD23	1.83	0.60
2:B:446:ASP:O	2:B:449:PHE:N	2.35	0.60
1:E:151:ILE:HB	1:E:187:CYS:HB2	1.83	0.60
2:F:485:GLN:O	2:F:487:HIS:N	2.35	0.60
2:G:451:TRP:CZ2	2:G:493:VAL:HG13	2.36	0.60
1:H:113:PRO:HB2	1:H:161:ALA:HB2	1.84	0.60
2:B:142:ARG:HB3	2:B:144:PHE:CD1	2.37	0.59
2:B:522:THR:HG22	2:B:526:ILE:HD11	1.83	0.59
2:C:205:ASN:HB2	2:C:206:PRO:HD2	1.83	0.59
1:D:195:LYS:CG	1:D:196:GLU:H	2.11	0.59
1:E:190:LEU:CD2	1:E:209:GLU:HB3	2.32	0.59
2:F:205:ASN:HB2	2:F:206:PRO:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:532:ILE:HG23	2:F:533:PRO:HD2	1.84	0.59
1:A:221:ALA:HB2	1:A:270:TRP:CE2	2.38	0.59
2:B:224:MET:HE1	2:B:230:ASP:HB3	1.82	0.59
1:D:145:ILE:HD11	1:D:202:TRP:HB2	1.83	0.59
1:D:183:ALA:O	1:D:184:SER:HB3	2.01	0.59
1:D:213:ASP:HB3	1:D:236:GLN:HB2	1.84	0.59
1:E:238:GLY:O	1:E:260:LYS:HA	2.01	0.59
1:H:287:THR:HA	1:H:301:SER:CB	2.32	0.59
1:A:89:GLU:O	1:A:90:ASN:HB2	2.02	0.59
2:B:162:LYS:HG3	2:B:162:LYS:O	2.02	0.59
2:B:332:ILE:HD12	2:B:332:ILE:H	1.67	0.59
1:D:77:CYS:HB3	1:D:109:VAL:CG2	2.32	0.59
1:E:192:LYS:HD3	1:E:204:GLU:OE1	2.02	0.59
2:F:162:LYS:HG3	2:F:162:LYS:O	2.02	0.59
2:F:198:THR:HG22	2:F:211:SER:HB3	1.84	0.59
2:F:332:ILE:H	2:F:332:ILE:HD12	1.67	0.59
2:B:497:LEU:CD1	2:B:503:ALA:HA	2.31	0.59
2:C:202:ARG:HG3	2:C:500:ASP:OD1	2.02	0.59
1:E:155:ALA:HB2	1:E:217:ASP:HA	1.84	0.59
1:E:258:LEU:HD13	1:E:297:TRP:CB	2.32	0.59
2:B:145:THR:HG22	2:B:147:SER:H	1.66	0.59
2:C:451:TRP:CD1	2:C:474:THR:HA	2.37	0.59
1:H:183:ALA:O	1:H:184:SER:HB3	2.01	0.59
1:E:49:LEU:HD12	1:E:50:ILE:N	2.16	0.59
2:F:423:GLN:HB3	2:F:434:LEU:HD21	1.84	0.59
1:H:190:LEU:HD22	1:H:209:GLU:HB3	1.85	0.59
2:B:464:VAL:HG23	2:B:464:VAL:O	2.03	0.59
1:D:29:ALA:HA	1:D:39:ILE:HD13	1.85	0.59
1:E:213:ASP:HB3	1:E:236:GLN:HB2	1.84	0.59
1:A:183:ALA:O	1:A:184:SER:HB3	2.01	0.59
1:A:213:ASP:HB3	1:A:236:GLN:HB2	1.84	0.59
2:C:446:ASP:O	2:C:449:PHE:N	2.36	0.59
2:G:321:LEU:HB3	2:G:361:LEU:HD11	1.84	0.59
1:A:77:CYS:HB3	1:A:109:VAL:CG2	2.33	0.59
2:B:198:THR:HG22	2:B:211:SER:HB3	1.84	0.59
2:C:160:LEU:CD2	2:C:172:ILE:HG12	2.33	0.59
2:C:482:GLU:CD	2:C:509:ARG:HH22	2.11	0.59
1:D:41:ASP:C	1:D:41:ASP:OD1	2.46	0.59
1:D:41:ASP:HB2	1:D:50:ILE:HD11	1.85	0.58
2:F:384:LEU:HD13	2:F:410:PHE:CE1	2.38	0.58
1:H:89:GLU:O	1:H:90:ASN:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:332:ILE:H	2:C:332:ILE:HD12	1.67	0.58
1:D:242:ILE:HG12	1:D:297:TRP:CE2	2.38	0.58
2:B:491:LEU:HD21	2:B:532:ILE:CD1	2.33	0.58
2:G:199:ILE:CD1	2:G:530:LEU:HA	2.32	0.58
2:G:464:VAL:HG23	2:G:464:VAL:O	2.04	0.58
2:G:491:LEU:HD13	2:G:510:LEU:HD23	1.85	0.58
1:H:77:CYS:HB3	1:H:109:VAL:CG2	2.33	0.58
2:C:152:LYS:HZ1	1:D:62:GLN:NE2	2.00	0.58
2:C:218:LYS:HG3	2:C:242:ASP:OD2	2.03	0.58
2:F:233:LEU:HD13	2:F:417:PRO:HB2	1.85	0.58
2:G:332:ILE:H	2:G:332:ILE:HD12	1.67	0.58
1:E:89:GLU:O	1:E:90:ASN:HB2	2.02	0.58
2:F:267:ARG:HH11	2:F:267:ARG:CG	2.11	0.58
2:G:160:LEU:CD2	2:G:172:ILE:HG12	2.33	0.58
1:H:213:ASP:HB3	1:H:236:GLN:HB2	1.84	0.58
2:C:351:ASP:HB2	2:C:354:ILE:HG13	1.86	0.58
1:D:89:GLU:O	1:D:90:ASN:HB2	2.02	0.58
1:E:70:TYR:N	1:E:70:TYR:CD1	2.72	0.58
2:F:247:PRO:HG2	2:F:248:TYR:CD1	2.38	0.58
2:G:198:THR:HG22	2:G:211:SER:HB3	1.84	0.58
2:G:238:SER:O	2:G:242:ASP:HB2	2.04	0.58
1:A:208:LEU:HB3	1:A:243:TRP:CZ3	2.39	0.58
2:C:152:LYS:NZ	1:D:62:GLN:NE2	2.51	0.58
2:G:495:CYS:C	2:G:497:LEU:H	2.11	0.58
1:H:70:TYR:CD1	1:H:70:TYR:N	2.72	0.58
1:A:193:LEU:N	1:A:193:LEU:CD2	2.67	0.58
2:B:210:ILE:CD1	2:B:495:CYS:HB2	2.33	0.58
2:C:262:LYS:O	2:C:265:HIS:N	2.36	0.58
1:E:23:TYR:CD2	1:E:68:PRO:HG3	2.39	0.58
1:E:29:ALA:HB2	1:E:39:ILE:HD12	1.85	0.58
2:F:340:LEU:HD21	2:F:358:TYR:HB3	1.85	0.58
1:H:191:ILE:HG23	1:H:218:VAL:HG21	1.86	0.58
1:A:190:LEU:HD22	1:A:209:GLU:HB3	1.86	0.58
2:B:160:LEU:N	2:B:160:LEU:HD23	2.18	0.58
2:B:210:ILE:CD1	2:B:495:CYS:CB	2.82	0.58
1:E:77:CYS:HB3	1:E:109:VAL:CG2	2.33	0.58
2:F:381:TRP:CG	2:F:382:LEU:N	2.71	0.58
2:F:421:ILE:HD11	2:F:449:PHE:CZ	2.39	0.58
2:G:487:HIS:HD2	2:G:517:LEU:HD23	1.69	0.58
1:H:132:LEU:HD23	1:H:142:VAL:HG13	1.86	0.58
2:C:400:GLU:HG3	2:C:425:TYR:CZ	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:LEU:HD23	1:D:142:VAL:HG13	1.86	0.58
1:E:109:VAL:HG12	1:E:120:LEU:HD11	1.86	0.58
2:G:175:LEU:HG	2:G:483:PHE:HD2	1.69	0.58
1:H:287:THR:HA	1:H:301:SER:HB3	1.86	0.58
1:H:291:GLU:HG3	1:H:291:GLU:O	2.01	0.58
1:A:16:ILE:HG22	1:A:17:HIS:N	2.19	0.57
1:D:16:ILE:HG22	1:D:17:HIS:N	2.19	0.57
1:E:208:LEU:HB3	1:E:243:TRP:CH2	2.38	0.57
2:F:262:LYS:O	2:F:265:HIS:N	2.36	0.57
2:G:351:ASP:HB2	2:G:354:ILE:HG13	1.86	0.57
1:D:193:LEU:CD2	1:D:193:LEU:N	2.68	0.57
2:G:207:TYR:CD2	2:G:504:GLU:HA	2.39	0.57
2:G:291:ILE:HG22	2:G:353:ASN:HB3	1.86	0.57
2:G:551:TYR:HD1	1:H:27:ARG:NE	1.99	0.57
1:H:23:TYR:CD2	1:H:68:PRO:HG3	2.39	0.57
2:B:532:ILE:HG23	2:B:533:PRO:HD2	1.84	0.57
1:E:286:VAL:O	1:E:303:VAL:HG23	2.05	0.57
1:A:17:HIS:ND1	2:B:148:TYR:HE2	2.03	0.57
1:A:208:LEU:HB3	1:A:243:TRP:CH2	2.39	0.57
1:D:42:VAL:O	1:D:42:VAL:HG12	2.05	0.57
2:F:215:LEU:O	2:F:456:THR:HG23	2.04	0.57
2:G:202:ARG:NH2	2:G:209:GLN:HB3	2.20	0.57
2:G:294:ILE:CG1	2:G:309:LEU:HD23	2.31	0.57
1:H:16:ILE:HG22	1:H:17:HIS:N	2.19	0.57
2:B:280:ILE:HG13	2:B:300:LEU:HD21	1.87	0.57
2:C:289:ASN:O	2:C:292:GLU:N	2.37	0.57
1:D:23:TYR:CD2	1:D:68:PRO:HG3	2.39	0.57
1:E:109:VAL:CG1	1:E:120:LEU:HD11	2.35	0.57
2:F:177:THR:OG1	2:F:483:PHE:HB2	2.05	0.57
2:F:339:GLN:O	2:F:343:TRP:HD1	1.87	0.57
2:G:210:ILE:HD13	2:G:496:PHE:CD1	2.39	0.57
2:C:149:THR:CG2	2:C:162:LYS:HG2	2.35	0.57
2:F:351:ASP:HB2	2:F:354:ILE:HG13	1.86	0.57
2:G:446:ASP:O	2:G:449:PHE:N	2.36	0.57
1:A:70:TYR:N	1:A:70:TYR:CD1	2.72	0.57
2:B:246:TYR:CG	2:B:247:PRO:HD2	2.40	0.57
2:B:262:LYS:O	2:B:265:HIS:N	2.36	0.57
1:E:132:LEU:HD23	1:E:142:VAL:HG13	1.86	0.57
1:E:193:LEU:CD2	1:E:193:LEU:N	2.67	0.57
2:F:267:ARG:HG3	2:F:267:ARG:NH1	2.15	0.57
1:H:292:SER:C	1:H:294:ASP:N	2.62	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HD23	1:A:142:VAL:HG13	1.86	0.57
2:C:198:THR:HG22	2:C:211:SER:HB3	1.84	0.57
2:C:371:SER:OG	2:C:373:LYS:HG3	2.05	0.57
1:A:258:LEU:HD13	1:A:297:TRP:CB	2.35	0.57
1:E:16:ILE:HG22	1:E:17:HIS:N	2.18	0.57
1:H:29:ALA:HB2	1:H:39:ILE:HD12	1.85	0.57
1:A:113:PRO:HB2	1:A:161:ALA:HB2	1.86	0.57
2:C:201:ALA:HB2	2:C:531:LYS:HE2	1.87	0.57
2:C:464:VAL:O	2:C:464:VAL:HG23	2.04	0.57
1:D:109:VAL:CG1	1:D:120:LEU:HD11	2.35	0.57
2:G:149:THR:CG2	2:G:150:PHE:H	2.18	0.57
1:A:23:TYR:CD2	1:A:68:PRO:HG3	2.39	0.56
2:B:190:LEU:O	2:B:194:ILE:HG13	2.05	0.56
2:C:149:THR:CG2	2:C:150:PHE:H	2.18	0.56
2:C:190:LEU:O	2:C:194:ILE:HG13	2.05	0.56
2:C:451:TRP:CZ2	2:C:493:VAL:HG13	2.39	0.56
2:F:371:SER:OG	2:F:373:LYS:HG3	2.05	0.56
2:G:371:SER:OG	2:G:373:LYS:HG3	2.05	0.56
1:H:193:LEU:N	1:H:193:LEU:CD2	2.68	0.56
2:B:351:ASP:HB2	2:B:354:ILE:HG13	1.86	0.56
2:C:194:ILE:HG12	2:C:492:PHE:HE2	1.69	0.56
2:F:284:ILE:HD13	2:F:297:TYR:CE1	2.40	0.56
2:G:280:ILE:CG1	2:G:300:LEU:HD21	2.35	0.56
2:G:332:ILE:HD12	2:G:332:ILE:N	2.21	0.56
2:G:532:ILE:HG23	2:G:533:PRO:HD2	1.87	0.56
1:H:109:VAL:HG12	1:H:120:LEU:HD11	1.88	0.56
1:H:150:THR:HB	1:H:188:ASP:HB3	1.86	0.56
1:A:35:ARG:HD3	1:A:56:HIS:O	2.05	0.56
2:B:233:LEU:HD13	2:B:417:PRO:HB2	1.87	0.56
2:C:339:GLN:O	2:C:343:TRP:HD1	1.87	0.56
2:C:381:TRP:CE3	2:C:412:LEU:HD21	2.40	0.56
1:D:70:TYR:N	1:D:70:TYR:CD1	2.72	0.56
1:D:80:ASP:OD2	1:D:82:LYS:HB2	2.05	0.56
1:E:35:ARG:HD3	1:E:56:HIS:O	2.05	0.56
1:E:151:ILE:O	1:E:151:ILE:HG22	2.06	0.56
2:F:151:ALA:HB1	2:F:159:LEU:CD1	2.33	0.56
2:F:352:LYS:O	2:F:356:LYS:HG3	2.05	0.56
2:G:339:GLN:O	2:G:343:TRP:HD1	1.87	0.56
1:H:234:CYS:SG	1:H:268:VAL:HG23	2.45	0.56
1:A:80:ASP:OD2	1:A:82:LYS:HB2	2.05	0.56
2:C:284:ILE:HD13	2:C:297:TYR:HE1	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ARG:HD3	1:D:56:HIS:O	2.05	0.56
2:F:280:ILE:HB	2:F:300:LEU:HD21	1.85	0.56
2:F:332:ILE:HD12	2:F:332:ILE:N	2.21	0.56
2:G:262:LYS:O	2:G:265:HIS:N	2.37	0.56
1:H:35:ARG:HD3	1:H:56:HIS:O	2.05	0.56
1:H:80:ASP:OD2	1:H:82:LYS:HB2	2.06	0.56
1:D:292:SER:C	1:D:294:ASP:H	2.13	0.56
2:F:482:GLU:CD	2:F:509:ARG:HH22	2.14	0.56
2:B:177:THR:OG1	2:B:483:PHE:HB3	2.06	0.56
2:B:321:LEU:N	2:B:321:LEU:HD23	2.20	0.56
2:B:431:THR:OG1	2:B:463:ARG:HG2	2.06	0.56
2:C:267:ARG:HG3	2:C:267:ARG:NH1	2.14	0.56
1:D:112:ALA:HB2	1:D:158:TRP:CZ2	2.41	0.56
2:G:487:HIS:O	2:G:488:GLY:C	2.47	0.56
1:H:232:ALA:HB2	1:H:270:TRP:CZ2	2.41	0.56
2:B:339:GLN:O	2:B:343:TRP:HD1	1.87	0.56
2:C:202:ARG:NH2	2:C:209:GLN:HB3	2.20	0.56
2:F:160:LEU:HD23	2:F:160:LEU:N	2.18	0.56
2:F:181:ARG:HD2	2:F:448:GLN:OE1	2.05	0.56
2:G:352:LYS:O	2:G:356:LYS:HG3	2.06	0.56
1:H:109:VAL:CG1	1:H:120:LEU:HD11	2.36	0.56
2:C:162:LYS:HZ2	1:D:15:MET:CE	2.16	0.56
1:E:80:ASP:OD2	1:E:82:LYS:HB2	2.05	0.56
2:G:495:CYS:O	2:G:497:LEU:N	2.38	0.56
1:A:304:ASN:OD1	2:B:161:THR:HG21	2.06	0.56
2:B:448:GLN:HB2	2:B:477:PHE:CE1	2.41	0.56
2:C:352:LYS:O	2:C:356:LYS:HG3	2.05	0.56
2:C:449:PHE:O	2:C:450:CYS:C	2.49	0.56
1:E:112:ALA:HB2	1:E:158:TRP:CZ2	2.41	0.56
2:G:321:LEU:N	2:G:321:LEU:HD23	2.20	0.56
1:H:70:TYR:HE2	1:H:118:LEU:HB2	1.64	0.56
1:A:190:LEU:HD13	1:A:207:LYS:HD3	1.88	0.56
2:B:179:LEU:HD11	2:B:184:LEU:HD13	1.87	0.56
2:B:197:VAL:CG1	2:B:198:THR:H	2.19	0.56
2:B:371:SER:OG	2:B:373:LYS:HG3	2.05	0.56
1:E:31:CYS:HB2	1:E:60:VAL:HB	1.88	0.56
1:E:292:SER:C	1:E:294:ASP:H	2.13	0.56
2:F:156:GLY:O	2:F:157:SER:CB	2.54	0.56
2:F:202:ARG:NH2	2:F:209:GLN:HB3	2.20	0.56
2:F:464:VAL:HG23	2:F:464:VAL:O	2.04	0.56
2:G:190:LEU:O	2:G:194:ILE:HG13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:290:LYS:HB3	1:H:300:ILE:HD11	1.87	0.56
2:C:321:LEU:N	2:C:321:LEU:HD23	2.20	0.55
2:F:190:LEU:O	2:F:194:ILE:HG13	2.05	0.55
2:G:162:LYS:NZ	1:H:15:MET:CE	2.68	0.55
2:G:451:TRP:CD1	2:G:474:THR:HA	2.41	0.55
1:A:112:ALA:HB2	1:A:158:TRP:CZ2	2.41	0.55
1:A:292:SER:C	1:A:294:ASP:H	2.13	0.55
2:B:202:ARG:NH2	2:B:209:GLN:HB3	2.20	0.55
2:B:210:ILE:HD12	2:B:495:CYS:HB3	1.89	0.55
2:B:332:ILE:HD12	2:B:332:ILE:N	2.20	0.55
2:F:321:LEU:HD23	2:F:321:LEU:N	2.21	0.55
2:F:343:TRP:HE3	2:F:350:ILE:HD13	1.69	0.55
1:H:151:ILE:O	1:H:151:ILE:HG22	2.06	0.55
1:A:31:CYS:HB2	1:A:60:VAL:HB	1.89	0.55
1:A:109:VAL:CG1	1:A:120:LEU:HD11	2.35	0.55
1:A:151:ILE:HG22	1:A:151:ILE:O	2.06	0.55
1:A:273:THR:HG21	2:B:479:ALA:HB2	1.87	0.55
2:B:352:LYS:O	2:B:356:LYS:HG3	2.05	0.55
1:D:49:LEU:HD12	1:D:50:ILE:N	2.17	0.55
1:H:112:ALA:HB2	1:H:158:TRP:CZ2	2.41	0.55
1:D:31:CYS:HB2	1:D:60:VAL:HB	1.88	0.55
1:A:304:ASN:HA	2:B:173:LYS:NZ	2.22	0.55
2:C:512:MET:HA	2:C:540:ALA:CB	2.37	0.55
1:D:29:ALA:CB	1:D:39:ILE:HD13	2.36	0.55
1:E:289:TRP:HA	1:E:298:VAL:O	2.06	0.55
2:G:149:THR:CG2	2:G:162:LYS:HG2	2.34	0.55
2:G:190:LEU:HB2	2:G:489:HIS:CE1	2.42	0.55
1:E:15:MET:HE2	2:F:162:LYS:HZ3	1.71	0.55
2:F:158:MET:HE2	2:F:174:ARG:HG3	1.89	0.55
2:F:197:VAL:CG1	2:F:198:THR:H	2.19	0.55
2:F:268:LEU:HD21	2:F:272:ILE:HD11	1.88	0.55
2:B:241:PHE:O	2:B:242:ASP:C	2.49	0.55
1:D:109:VAL:HG12	1:D:120:LEU:HD11	1.87	0.55
1:E:113:PRO:CB	1:E:161:ALA:HB2	2.36	0.55
1:E:207:LYS:O	1:E:208:LEU:HD23	2.07	0.55
2:F:491:LEU:HD21	2:F:532:ILE:HD11	1.88	0.55
1:A:109:VAL:HG12	1:A:120:LEU:HD11	1.87	0.55
2:C:154:SER:HB2	1:D:21:MET:HB3	1.88	0.55
2:F:462:THR:O	2:F:463:ARG:HD3	2.07	0.55
2:G:512:MET:SD	2:G:540:ALA:CB	2.95	0.55
2:C:210:ILE:HG22	2:C:459:PHE:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:332:ILE:HD12	2:C:332:ILE:N	2.21	0.55
2:G:197:VAL:CG1	2:G:198:THR:H	2.19	0.55
2:G:409:LYS:C	2:G:410:PHE:CD2	2.85	0.55
1:H:242:ILE:HD11	1:H:258:LEU:HD22	1.89	0.55
1:A:250:SER:O	1:A:252:THR:N	2.35	0.55
2:B:151:ALA:HB1	2:B:159:LEU:CD1	2.33	0.55
2:B:158:MET:HE2	2:B:174:ARG:HG3	1.88	0.55
2:B:268:LEU:HD21	2:B:272:ILE:HD11	1.89	0.55
2:C:268:LEU:HD21	2:C:272:ILE:HD11	1.89	0.55
2:C:375:LEU:HB3	2:C:379:PHE:HD2	1.71	0.55
2:C:375:LEU:HB2	2:C:384:LEU:HD21	1.88	0.55
1:D:207:LYS:O	1:D:208:LEU:HD23	2.07	0.55
1:E:42:VAL:O	1:E:42:VAL:HG12	2.05	0.55
2:F:381:TRP:CZ2	2:F:382:LEU:HD13	2.42	0.55
2:B:449:PHE:O	2:B:450:CYS:C	2.49	0.54
2:B:512:MET:SD	2:B:540:ALA:HB2	2.46	0.54
2:C:207:TYR:CD2	2:C:504:GLU:HA	2.43	0.54
1:D:190:LEU:HD13	1:D:207:LYS:HD3	1.89	0.54
1:E:145:ILE:HD13	1:E:194:TRP:CE3	2.43	0.54
2:G:267:ARG:HH11	2:G:267:ARG:CG	2.10	0.54
2:G:268:LEU:HD21	2:G:272:ILE:HD11	1.89	0.54
2:C:409:LYS:C	2:C:410:PHE:CD2	2.85	0.54
1:D:79:TYR:HD1	1:D:105:SER:HB3	1.72	0.54
2:G:343:TRP:CZ3	2:G:350:ILE:HG21	2.42	0.54
1:A:265:VAL:HA	1:A:281:GLY:HA3	1.89	0.54
2:B:156:GLY:O	2:B:157:SER:CB	2.55	0.54
1:D:151:ILE:O	1:D:151:ILE:HG22	2.06	0.54
1:D:190:LEU:HD22	1:D:209:GLU:HB3	1.90	0.54
1:E:242:ILE:HD13	1:E:297:TRP:CD1	2.43	0.54
2:F:449:PHE:O	2:F:450:CYS:C	2.49	0.54
1:A:207:LYS:O	1:A:208:LEU:HD23	2.07	0.54
2:B:484:ALA:O	2:B:485:GLN:HB3	2.07	0.54
2:F:280:ILE:CG1	2:F:300:LEU:HD21	2.37	0.54
2:F:491:LEU:O	2:F:494:SER:HB2	2.08	0.54
2:G:242:ASP:O	2:G:264:ARG:NH2	2.40	0.54
2:B:145:THR:C	2:B:147:SER:H	2.15	0.54
2:B:409:LYS:C	2:B:410:PHE:CD2	2.86	0.54
2:B:477:PHE:CE2	2:B:493:VAL:HG21	2.43	0.54
2:C:194:ILE:HG12	2:C:492:PHE:CD2	2.42	0.54
2:C:451:TRP:HE1	2:C:474:THR:HG23	1.73	0.54
1:D:60:VAL:HG13	1:D:77:CYS:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:409:LYS:C	2:F:410:PHE:CD2	2.86	0.54
2:G:210:ILE:HD13	2:G:496:PHE:CG	2.42	0.54
2:G:449:PHE:O	2:G:450:CYS:C	2.49	0.54
1:H:31:CYS:HB2	1:H:60:VAL:HB	1.88	0.54
1:H:265:VAL:HA	1:H:281:GLY:HA3	1.89	0.54
1:A:15:MET:HE2	2:B:162:LYS:HZ3	1.72	0.54
2:C:138:ILE:HG22	2:C:139:MET:N	2.23	0.54
1:E:60:VAL:HG13	1:E:77:CYS:O	2.08	0.54
1:E:304:ASN:OD1	2:F:161:THR:HG21	2.08	0.54
2:G:382:LEU:HD12	2:G:385:LEU:HD23	1.90	0.54
1:H:291:GLU:HB3	1:H:297:TRP:CD2	2.42	0.54
2:C:267:ARG:CG	2:C:267:ARG:NH1	2.71	0.54
2:F:512:MET:HA	2:F:540:ALA:HB1	1.90	0.54
2:G:170:VAL:H	1:H:47:GLN:HE22	1.55	0.54
2:G:284:ILE:HG12	2:G:296:LEU:CD1	2.37	0.54
2:G:367:GLU:HG3	2:G:367:GLU:O	2.08	0.54
1:A:56:HIS:NE2	1:A:84:ILE:HD12	2.22	0.54
2:B:145:THR:HG22	2:B:146:ALA:N	2.23	0.54
1:D:67:HIS:ND1	1:D:69:MET:HB3	2.23	0.54
1:D:82:LYS:HG2	1:D:100:ALA:CB	2.35	0.54
1:D:265:VAL:HA	1:D:281:GLY:HA3	1.89	0.54
1:E:67:HIS:ND1	1:E:69:MET:HB3	2.23	0.54
1:E:70:TYR:HE2	1:E:118:LEU:HB2	1.64	0.54
2:F:145:THR:HG22	2:F:146:ALA:N	2.23	0.54
2:F:375:LEU:HB2	2:F:384:LEU:HD21	1.90	0.54
2:F:379:PHE:N	2:F:379:PHE:CD1	2.75	0.54
2:G:409:LYS:C	2:G:410:PHE:HD2	2.16	0.54
1:H:60:VAL:HG13	1:H:77:CYS:O	2.07	0.54
1:A:67:HIS:ND1	1:A:69:MET:HB3	2.23	0.54
2:B:382:LEU:HD12	2:B:385:LEU:HD23	1.90	0.54
2:F:236:LEU:HD21	2:F:422:PHE:CE1	2.43	0.54
1:H:79:TYR:HD1	1:H:105:SER:HB3	1.72	0.54
1:A:102:HIS:HE2	1:A:130:SER:CB	2.21	0.54
2:B:177:THR:OG1	2:B:483:PHE:CB	2.56	0.54
2:B:201:ALA:H	2:B:531:LYS:NZ	1.96	0.54
2:C:197:VAL:CG1	2:C:198:THR:H	2.19	0.54
2:C:236:LEU:HD21	2:C:422:PHE:CE1	2.42	0.54
2:C:366:PHE:CZ	2:C:384:LEU:HD22	2.42	0.54
2:C:428:ASN:HA	2:C:463:ARG:HH12	1.73	0.54
2:G:244:VAL:HG12	2:G:263:GLU:OE2	2.08	0.54
1:A:82:LYS:HG2	1:A:100:ALA:CB	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ILE:HG21	1:A:181:ARG:NE	2.23	0.53
2:F:145:THR:C	2:F:147:SER:H	2.15	0.53
1:A:60:VAL:HG13	1:A:77:CYS:O	2.07	0.53
2:G:241:PHE:CD2	2:G:457:LEU:HD21	2.43	0.53
1:H:113:PRO:CB	1:H:161:ALA:HB2	2.38	0.53
1:A:49:LEU:HD12	1:A:50:ILE:N	2.16	0.53
2:B:159:LEU:HD12	2:B:160:LEU:H	1.74	0.53
2:C:142:ARG:HG3	1:D:61:TRP:CZ2	2.44	0.53
1:E:205:GLU:HG2	1:E:251:ASN:ND2	2.22	0.53
2:G:487:HIS:HA	2:G:490:SER:HB2	1.91	0.53
1:H:56:HIS:NE2	1:H:84:ILE:HD12	2.23	0.53
1:H:207:LYS:O	1:H:208:LEU:HD23	2.07	0.53
1:A:145:ILE:HD13	1:A:194:TRP:CZ3	2.43	0.53
2:B:409:LYS:C	2:B:410:PHE:HD2	2.16	0.53
2:F:174:ARG:HG2	2:F:175:LEU:H	1.74	0.53
1:A:291:GLU:N	1:A:297:TRP:CE3	2.77	0.53
2:B:291:ILE:HG22	2:B:353:ASN:HB2	1.90	0.53
1:D:245:CYS:SG	1:D:251:ASN:HB2	2.48	0.53
1:E:273:THR:HG21	2:F:479:ALA:HB2	1.89	0.53
2:F:272:ILE:HG23	2:F:382:LEU:HG	1.90	0.53
1:A:145:ILE:O	1:A:145:ILE:HG22	2.08	0.53
2:B:236:LEU:HD21	2:B:422:PHE:CE1	2.44	0.53
2:C:515:ILE:HD12	2:C:541:GLN:N	2.24	0.53
1:D:38:LYS:HB2	1:D:40:PHE:HE1	1.73	0.53
1:D:242:ILE:HD11	1:D:258:LEU:HB2	1.89	0.53
2:G:138:ILE:HG22	2:G:139:MET:N	2.22	0.53
1:H:78:SER:HB3	1:H:80:ASP:OD1	2.09	0.53
2:B:175:LEU:HD23	2:B:483:PHE:CE2	2.44	0.53
2:C:492:PHE:C	2:C:492:PHE:HD1	2.16	0.53
2:G:332:ILE:O	2:G:333:ARG:C	2.52	0.53
2:C:208:PRO:HG3	2:C:530:LEU:O	2.08	0.53
2:C:409:LYS:C	2:C:410:PHE:HD2	2.16	0.53
2:F:382:LEU:HD12	2:F:385:LEU:HD23	1.90	0.53
2:F:409:LYS:C	2:F:410:PHE:HD2	2.16	0.53
1:H:82:LYS:HG2	1:H:100:ALA:CB	2.34	0.53
2:C:524:ASP:O	2:C:524:ASP:CG	2.51	0.53
1:D:263:ASP:HB3	1:D:282:GLY:HA2	1.91	0.53
2:B:291:ILE:HG22	2:B:353:ASN:CB	2.39	0.53
2:C:404:GLN:HG2	2:C:426:ALA:HB1	1.90	0.53
1:E:29:ALA:CB	1:E:39:ILE:HD13	2.39	0.53
1:E:56:HIS:NE2	1:E:84:ILE:HD12	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:HIS:ND1	1:H:69:MET:HB3	2.23	0.53
1:H:145:ILE:O	1:H:145:ILE:HG22	2.08	0.53
2:B:210:ILE:HD12	2:B:495:CYS:CB	2.39	0.52
2:B:331:ARG:HB2	2:B:332:ILE:HD12	1.91	0.52
2:C:149:THR:CG2	2:C:150:PHE:N	2.72	0.52
2:C:236:LEU:HD22	2:C:418:ILE:HG22	1.89	0.52
2:C:280:ILE:HB	2:C:300:LEU:HD21	1.91	0.52
2:C:382:LEU:HD12	2:C:385:LEU:HD23	1.90	0.52
1:D:56:HIS:NE2	1:D:84:ILE:HD12	2.24	0.52
1:E:38:LYS:HB2	1:E:40:PHE:HE1	1.73	0.52
1:E:67:HIS:O	1:E:69:MET:N	2.42	0.52
1:E:145:ILE:O	1:E:145:ILE:HG22	2.08	0.52
1:E:243:TRP:N	1:E:243:TRP:CD1	2.76	0.52
1:E:276:ILE:CG2	1:E:300:ILE:HD11	2.38	0.52
2:F:155:THR:O	2:F:513:ARG:NH1	2.39	0.52
1:H:49:LEU:HD12	1:H:50:ILE:N	2.16	0.52
1:A:78:SER:HB3	1:A:80:ASP:OD1	2.09	0.52
2:B:332:ILE:O	2:B:333:ARG:C	2.52	0.52
2:F:272:ILE:CG2	2:F:382:LEU:HG	2.39	0.52
2:F:284:ILE:HG12	2:F:296:LEU:CD1	2.38	0.52
1:H:102:HIS:HE2	1:H:130:SER:CB	2.21	0.52
2:C:495:CYS:C	2:C:497:LEU:H	2.17	0.52
1:D:197:GLU:O	1:D:198:GLU:HB2	2.08	0.52
1:E:79:TYR:HD1	1:E:105:SER:HB3	1.73	0.52
1:E:263:ASP:HB3	1:E:282:GLY:HA2	1.91	0.52
2:F:302:ASP:HA	2:G:304:VAL:HG21	1.92	0.52
2:C:367:GLU:O	2:C:367:GLU:HG3	2.08	0.52
1:D:290:LYS:CB	1:D:300:ILE:HD11	2.36	0.52
1:E:265:VAL:HA	1:E:281:GLY:HA3	1.90	0.52
1:A:39:ILE:HD11	1:A:74:LEU:HD22	1.90	0.52
1:A:79:TYR:HD1	1:A:105:SER:HB3	1.72	0.52
2:C:170:VAL:H	1:D:47:GLN:HE22	1.58	0.52
1:D:67:HIS:O	1:D:69:MET:N	2.43	0.52
1:E:264:VAL:HG12	1:E:265:VAL:N	2.25	0.52
2:F:302:ASP:OD1	2:F:305:ARG:HB2	2.10	0.52
1:H:29:ALA:HA	1:H:39:ILE:HD13	1.91	0.52
1:H:38:LYS:HB2	1:H:40:PHE:HE1	1.73	0.52
1:A:234:CYS:HB2	1:A:265:VAL:HB	1.91	0.52
2:B:174:ARG:HG2	2:B:175:LEU:H	1.74	0.52
2:F:367:GLU:HG3	2:F:367:GLU:O	2.08	0.52
1:H:263:ASP:HB3	1:H:282:GLY:HA2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:TRP:CH2	1:A:229:SER:HB2	2.45	0.52
2:B:181:ARG:HD2	2:B:448:GLN:OE1	2.09	0.52
2:C:332:ILE:O	2:C:333:ARG:C	2.52	0.52
1:D:145:ILE:HG22	1:D:145:ILE:O	2.09	0.52
2:F:175:LEU:HD23	2:F:483:PHE:CE2	2.44	0.52
2:F:332:ILE:O	2:F:333:ARG:C	2.52	0.52
1:H:29:ALA:CB	1:H:39:ILE:HD13	2.39	0.52
1:H:189:ASN:OD1	1:H:213:ASP:C	2.52	0.52
1:H:258:LEU:CD1	1:H:297:TRP:HB2	2.40	0.52
1:A:28:LEU:HD13	2:B:172:ILE:HD11	1.92	0.52
2:B:471:ASP:OD1	2:B:497:LEU:HA	2.10	0.52
2:C:375:LEU:HB3	2:C:379:PHE:CD2	2.44	0.52
1:E:78:SER:HB3	1:E:80:ASP:OD1	2.09	0.52
1:E:220:TRP:CH2	1:E:229:SER:HB2	2.45	0.52
2:F:304:VAL:HG21	2:G:302:ASP:HA	1.92	0.52
1:H:109:VAL:HG12	1:H:110:CYS:N	2.25	0.52
2:B:140:LYS:C	2:B:142:ARG:H	2.16	0.52
2:B:367:GLU:HG3	2:B:367:GLU:O	2.08	0.52
2:B:432:GLU:CD	2:B:466:SER:HB3	2.34	0.52
1:E:273:THR:CG2	2:F:479:ALA:CB	2.85	0.52
1:E:273:THR:CG2	2:F:479:ALA:HB2	2.40	0.52
2:G:372:LEU:O	2:G:375:LEU:HG	2.10	0.52
1:A:67:HIS:O	1:A:69:MET:N	2.43	0.52
2:B:372:LEU:O	2:B:375:LEU:HG	2.10	0.52
2:B:421:ILE:HD11	2:B:449:PHE:CZ	2.44	0.52
1:D:220:TRP:CH2	1:D:229:SER:HB2	2.45	0.52
1:E:29:ALA:HA	1:E:39:ILE:HD13	1.91	0.52
2:F:140:LYS:C	2:F:142:ARG:H	2.16	0.52
2:F:236:LEU:HD23	2:F:421:ILE:HG21	1.92	0.52
2:F:372:LEU:O	2:F:375:LEU:HG	2.10	0.52
2:F:412:LEU:H	2:F:412:LEU:HD12	1.75	0.52
2:G:148:TYR:HB2	1:H:266:TRP:CD2	2.44	0.52
2:G:175:LEU:HD12	2:G:176:PRO:N	2.24	0.52
2:G:412:LEU:N	2:G:412:LEU:CD1	2.71	0.52
2:G:420:VAL:HG11	2:G:445:LEU:HD11	1.92	0.52
1:H:67:HIS:O	1:H:69:MET:N	2.43	0.52
2:C:175:LEU:HD12	2:C:176:PRO:N	2.24	0.51
2:C:242:ASP:O	2:C:264:ARG:NH2	2.42	0.51
1:D:78:SER:HB3	1:D:80:ASP:OD1	2.09	0.51
1:D:151:ILE:HB	1:D:187:CYS:CB	2.38	0.51
1:E:28:LEU:HD13	2:F:172:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:138:ILE:HD11	1:H:79:TYR:CD2	2.45	0.51
2:C:340:LEU:HD21	2:C:358:TYR:HB3	1.92	0.51
1:H:23:TYR:CD2	1:H:24:TYR:CD1	2.97	0.51
1:A:263:ASP:HB3	1:A:282:GLY:HA2	1.91	0.51
1:A:264:VAL:HG12	1:A:265:VAL:N	2.25	0.51
2:C:522:THR:HG21	2:C:526:ILE:CD1	2.41	0.51
1:D:110:CYS:O	1:D:120:LEU:HD12	2.11	0.51
2:G:210:ILE:HG22	2:G:459:PHE:CE2	2.45	0.51
1:H:268:VAL:HG13	1:H:277:LEU:HD11	1.93	0.51
1:D:290:LYS:HB2	1:D:300:ILE:HD12	1.93	0.51
1:E:110:CYS:O	1:E:120:LEU:HD12	2.10	0.51
1:H:264:VAL:HG12	1:H:265:VAL:N	2.25	0.51
1:A:258:LEU:CD1	1:A:297:TRP:CB	2.89	0.51
2:C:551:TYR:HD1	1:D:27:ARG:HE	1.57	0.51
1:D:102:HIS:HE2	1:D:130:SER:CB	2.22	0.51
1:D:109:VAL:HG12	1:D:110:CYS:N	2.25	0.51
1:E:234:CYS:HB2	1:E:265:VAL:HB	1.93	0.51
2:F:548:GLU:O	2:F:552:LEU:HG	2.10	0.51
2:G:385:LEU:HD21	2:G:422:PHE:CE2	2.45	0.51
1:H:157:SER:HB2	1:H:218:VAL:O	2.11	0.51
2:B:400:GLU:HG3	2:B:425:TYR:CZ	2.46	0.51
2:F:210:ILE:CD1	2:F:495:CYS:HB2	2.40	0.51
2:F:320:VAL:HG22	2:G:263:GLU:HA	1.92	0.51
2:G:175:LEU:CD1	2:G:176:PRO:CD	2.88	0.51
2:G:236:LEU:HD21	2:G:422:PHE:CE1	2.46	0.51
2:G:366:PHE:CZ	2:G:387:LEU:HD12	2.46	0.51
2:B:359:LYS:HZ1	2:B:368:GLY:HA3	1.76	0.51
2:B:475:PHE:CE2	2:B:497:LEU:HD21	2.46	0.51
2:C:170:VAL:CG1	2:C:171:SER:N	2.74	0.51
2:C:475:PHE:HE2	2:C:497:LEU:HD11	1.74	0.51
1:E:41:ASP:HB2	1:E:50:ILE:CD1	2.33	0.51
2:G:381:TRP:CD1	2:G:381:TRP:H	2.27	0.51
2:C:175:LEU:CD1	2:C:176:PRO:CD	2.88	0.51
1:D:23:TYR:CD2	1:D:24:TYR:CD1	2.98	0.51
1:D:179:ILE:HG21	1:D:181:ARG:NE	2.23	0.51
1:E:17:HIS:ND1	2:F:148:TYR:CE2	2.76	0.51
1:E:109:VAL:HG12	1:E:110:CYS:N	2.26	0.51
1:E:289:TRP:CE3	1:E:298:VAL:C	2.89	0.51
2:F:331:ARG:HB2	2:F:332:ILE:HD12	1.91	0.51
2:F:381:TRP:CD1	2:F:382:LEU:H	2.28	0.51
1:H:220:TRP:CH2	1:H:229:SER:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:216:LEU:HD13	2:C:243:PRO:HD2	1.93	0.51
2:C:385:LEU:HA	2:C:406:HIS:CE1	2.46	0.51
2:F:179:LEU:HD11	2:F:184:LEU:HD13	1.91	0.51
2:F:196:LYS:HD2	2:F:214:SER:O	2.11	0.51
2:G:331:ARG:HB2	2:G:332:ILE:HD12	1.92	0.51
2:G:462:THR:O	2:G:463:ARG:CD	2.53	0.51
1:H:179:ILE:HG21	1:H:181:ARG:NE	2.23	0.51
1:A:38:LYS:HB2	1:A:40:PHE:HE1	1.74	0.51
1:A:98:GLU:HG2	1:A:99:HIS:N	2.26	0.51
1:A:109:VAL:HG12	1:A:110:CYS:N	2.25	0.51
2:C:199:ILE:HD12	2:C:530:LEU:HA	1.92	0.51
2:C:210:ILE:HD13	2:C:496:PHE:CG	2.46	0.51
2:C:366:PHE:CE2	2:C:384:LEU:HD22	2.46	0.51
2:C:479:ALA:CB	1:D:273:THR:HG22	2.35	0.51
1:D:111:TRP:CD2	1:D:120:LEU:HD13	2.47	0.51
2:F:398:SER:OG	2:F:401:SER:HB3	2.11	0.51
2:G:267:ARG:CG	2:G:267:ARG:NH1	2.71	0.51
1:A:28:LEU:CD2	2:B:170:VAL:HG11	2.35	0.50
1:A:110:CYS:O	1:A:120:LEU:HD12	2.10	0.50
1:A:185:GLY:HA3	1:A:215:VAL:HG11	1.91	0.50
1:A:268:VAL:HG13	1:A:277:LEU:HD11	1.93	0.50
2:B:196:LYS:HD2	2:B:214:SER:O	2.11	0.50
2:C:457:LEU:HD13	2:C:463:ARG:HG3	1.93	0.50
1:D:264:VAL:HG12	1:D:265:VAL:N	2.25	0.50
2:F:434:LEU:O	2:F:438:VAL:HG23	2.11	0.50
2:G:170:VAL:CG1	2:G:171:SER:N	2.74	0.50
2:G:191:ASP:OD1	2:G:529:ARG:NH1	2.44	0.50
1:A:230:THR:CG2	1:A:242:ILE:HG22	2.42	0.50
2:B:208:PRO:HB3	2:B:531:LYS:HB3	1.93	0.50
2:C:153:PHE:CE2	1:D:278:ALA:HB2	2.46	0.50
2:C:431:THR:HG21	2:C:463:ARG:HB3	1.93	0.50
2:C:471:ASP:OD2	2:C:498:ASN:ND2	2.44	0.50
1:E:92:THR:HG22	1:E:94:GLU:HG3	1.93	0.50
1:E:111:TRP:CD2	1:E:120:LEU:HD13	2.46	0.50
2:F:347:GLY:O	2:F:350:ILE:HD12	2.12	0.50
1:H:16:ILE:HD12	1:H:30:THR:CG2	2.41	0.50
1:A:111:TRP:CD2	1:A:120:LEU:HD13	2.46	0.50
2:C:276:ILE:HD13	2:C:383:CYS:CA	2.38	0.50
2:C:372:LEU:O	2:C:375:LEU:HG	2.10	0.50
1:E:98:GLU:HG2	1:E:99:HIS:N	2.26	0.50
2:F:486:LEU:HD12	2:F:486:LEU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:184:LEU:HD21	2:G:448:GLN:HE22	1.76	0.50
1:A:40:PHE:CZ	2:B:168:SER:CB	2.89	0.50
2:B:174:ARG:HG2	2:B:175:LEU:N	2.27	0.50
2:B:215:LEU:O	2:B:456:THR:HG23	2.11	0.50
2:B:236:LEU:HD23	2:B:421:ILE:HG21	1.93	0.50
2:B:477:PHE:HD2	2:B:493:VAL:HG11	1.75	0.50
2:C:142:ARG:NH2	1:D:107:ASN:OD1	2.44	0.50
2:G:162:LYS:HZ2	1:H:15:MET:HE2	1.74	0.50
2:G:196:LYS:HD2	2:G:214:SER:O	2.12	0.50
2:G:359:LYS:HZ1	2:G:370:PHE:H	1.58	0.50
2:B:255:VAL:HG12	2:B:256:LYS:N	2.27	0.50
2:C:331:ARG:HB2	2:C:332:ILE:HD12	1.91	0.50
1:E:102:HIS:HE2	1:E:130:SER:CB	2.21	0.50
2:F:159:LEU:HD12	2:F:160:LEU:H	1.74	0.50
2:G:474:THR:CG2	2:G:493:VAL:HG12	2.42	0.50
2:G:474:THR:HG23	2:G:493:VAL:HG12	1.93	0.50
1:H:111:TRP:CD2	1:H:120:LEU:HD13	2.46	0.50
1:A:16:ILE:HD12	1:A:30:THR:CG2	2.41	0.50
1:A:43:ARG:O	1:A:44:ASN:HB2	2.11	0.50
2:C:448:GLN:HB2	2:C:477:PHE:CE1	2.46	0.50
1:D:245:CYS:HB2	1:D:253:TRP:CE3	2.46	0.50
1:E:179:ILE:HG21	1:E:181:ARG:NE	2.23	0.50
2:F:451:TRP:HZ2	2:F:496:PHE:CD1	2.30	0.50
1:H:43:ARG:O	1:H:44:ASN:HB2	2.11	0.50
1:H:92:THR:HG22	1:H:94:GLU:HG3	1.93	0.50
1:H:110:CYS:O	1:H:120:LEU:HD12	2.11	0.50
1:A:49:LEU:CD1	1:A:50:ILE:H	2.20	0.50
2:B:215:LEU:HD22	2:B:452:TYR:OH	2.11	0.50
2:B:482:GLU:CD	2:B:509:ARG:HH22	2.20	0.50
2:C:434:LEU:O	2:C:438:VAL:HG23	2.12	0.50
1:E:43:ARG:O	1:E:44:ASN:HB2	2.11	0.50
1:E:258:LEU:HD13	1:E:297:TRP:HB2	1.92	0.50
1:E:205:GLU:HG2	1:E:251:ASN:HD21	1.77	0.50
2:F:332:ILE:H	2:F:332:ILE:CD1	2.25	0.50
2:F:359:LYS:HZ1	2:F:370:PHE:H	1.59	0.50
1:H:230:THR:HG21	1:H:242:ILE:HG23	1.92	0.50
2:B:434:LEU:O	2:B:438:VAL:HG23	2.11	0.50
2:C:184:LEU:O	2:C:486:LEU:HD13	2.12	0.50
1:D:98:GLU:HG2	1:D:99:HIS:N	2.26	0.50
1:D:292:SER:C	1:D:294:ASP:N	2.69	0.50
1:E:23:TYR:CD2	1:E:24:TYR:CD1	2.98	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:255:VAL:HG12	2:F:256:LYS:N	2.27	0.50
2:G:175:LEU:HD12	2:G:176:PRO:CD	2.42	0.50
2:G:255:VAL:HG12	2:G:256:LYS:N	2.27	0.50
2:G:380:SER:OG	2:G:382:LEU:N	2.45	0.50
2:G:436:LYS:HE3	2:G:469:THR:OG1	2.12	0.50
2:B:267:ARG:CG	2:B:267:ARG:NH1	2.71	0.49
2:C:196:LYS:HD2	2:C:214:SER:O	2.12	0.49
2:C:477:PHE:CD2	2:C:493:VAL:HG21	2.47	0.49
2:C:479:ALA:HA	1:D:273:THR:HG21	1.94	0.49
2:F:224:MET:HE2	2:F:230:ASP:HB3	1.94	0.49
2:F:372:LEU:HD22	2:F:375:LEU:HD11	1.94	0.49
2:G:266:CYS:O	2:G:267:ARG:C	2.55	0.49
1:A:27:ARG:HE	2:B:551:TYR:HD1	1.60	0.49
1:A:30:THR:CG2	1:A:31:CYS:N	2.75	0.49
1:D:92:THR:HG22	1:D:94:GLU:HG3	1.93	0.49
1:E:16:ILE:HD12	1:E:30:THR:CG2	2.41	0.49
1:E:268:VAL:HG13	1:E:277:LEU:HD11	1.93	0.49
2:F:174:ARG:HG2	2:F:175:LEU:N	2.27	0.49
2:F:385:LEU:CA	2:F:406:HIS:CE1	2.95	0.49
2:G:224:MET:HE2	2:G:230:ASP:HB3	1.94	0.49
2:B:244:VAL:HG23	2:B:264:ARG:NH2	2.24	0.49
2:C:255:VAL:HG12	2:C:256:LYS:N	2.27	0.49
2:C:332:ILE:H	2:C:332:ILE:CD1	2.25	0.49
1:D:241:PHE:CD2	1:D:257:LEU:HA	2.48	0.49
1:E:292:SER:C	1:E:294:ASP:N	2.69	0.49
2:G:290:GLU:O	2:G:293:GLN:HB2	2.12	0.49
1:A:111:TRP:CE2	1:A:120:LEU:HD13	2.48	0.49
2:B:525:HIS:O	2:B:527:LEU:N	2.45	0.49
2:C:175:LEU:HD12	2:C:176:PRO:CD	2.42	0.49
1:E:242:ILE:HD11	1:E:258:LEU:HD22	1.94	0.49
2:F:404:GLN:CG	2:F:426:ALA:HB1	2.34	0.49
1:H:287:THR:HG22	1:H:299:CYS:SG	2.52	0.49
2:B:332:ILE:H	2:B:332:ILE:CD1	2.25	0.49
2:B:340:LEU:HD21	2:B:358:TYR:HB3	1.94	0.49
2:C:372:LEU:HD22	2:C:375:LEU:HD11	1.94	0.49
1:D:240:VAL:O	1:D:258:LEU:HB3	2.11	0.49
1:E:82:LYS:HG2	1:E:100:ALA:CB	2.34	0.49
1:E:190:LEU:HD22	1:E:209:GLU:HB3	1.94	0.49
2:F:217:PHE:HE2	2:F:449:PHE:CE1	2.31	0.49
2:F:475:PHE:CE2	2:F:497:LEU:HD21	2.44	0.49
2:G:170:VAL:CG1	2:G:171:SER:H	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:356:LYS:O	2:G:359:LYS:HB3	2.12	0.49
1:A:92:THR:HG22	1:A:94:GLU:HG3	1.93	0.49
1:A:192:LYS:HD3	1:A:204:GLU:OE1	2.13	0.49
2:B:290:GLU:O	2:B:293:GLN:HB2	2.13	0.49
2:B:548:GLU:O	2:B:552:LEU:HG	2.13	0.49
2:C:170:VAL:CG1	2:C:171:SER:H	2.25	0.49
2:C:252:ASN:OD1	2:C:253:ASP:N	2.46	0.49
1:D:157:SER:HB2	1:D:218:VAL:O	2.13	0.49
2:F:191:ASP:OD1	2:F:529:ARG:NH1	2.45	0.49
2:F:210:ILE:HG22	2:F:459:PHE:HE2	1.78	0.49
1:H:106:VAL:HA	1:H:124:SER:HA	1.94	0.49
2:B:515:ILE:HD12	2:B:541:GLN:N	2.26	0.49
2:C:280:ILE:HG13	2:C:300:LEU:CD2	2.37	0.49
2:C:356:LYS:O	2:C:359:LYS:HB3	2.13	0.49
1:D:16:ILE:HD12	1:D:30:THR:CG2	2.41	0.49
1:D:242:ILE:HG12	1:D:297:TRP:NE1	2.28	0.49
2:F:290:GLU:O	2:F:293:GLN:HB2	2.13	0.49
2:F:525:HIS:O	2:F:527:LEU:N	2.46	0.49
2:G:152:LYS:NZ	1:H:62:GLN:HE21	2.11	0.49
1:H:112:ALA:HA	1:H:158:TRP:CD2	2.48	0.49
1:A:56:HIS:CE1	1:A:84:ILE:HD12	2.48	0.49
1:A:157:SER:HB2	1:A:218:VAL:O	2.12	0.49
2:B:170:VAL:O	2:B:170:VAL:HG12	2.12	0.49
2:B:280:ILE:HD11	2:B:383:CYS:SG	2.53	0.49
1:D:49:LEU:CD1	1:D:50:ILE:H	2.21	0.49
1:D:70:TYR:N	1:D:70:TYR:HD1	2.11	0.49
2:F:182:LYS:O	2:F:185:PHE:HD1	1.96	0.49
2:F:356:LYS:O	2:F:359:LYS:HB3	2.13	0.49
1:H:111:TRP:CE2	1:H:120:LEU:HD13	2.48	0.49
1:A:70:TYR:N	1:A:70:TYR:HD1	2.10	0.49
1:D:268:VAL:HG13	1:D:277:LEU:HD11	1.92	0.49
1:E:291:GLU:N	1:E:297:TRP:CE3	2.80	0.49
2:F:135:ALA:O	2:F:139:MET:HB3	2.12	0.49
2:G:267:ARG:HG3	2:G:267:ARG:NH1	2.14	0.49
1:H:98:GLU:HG2	1:H:99:HIS:N	2.27	0.49
2:B:236:LEU:HD22	2:B:418:ILE:HG22	1.95	0.49
2:C:139:MET:HA	2:C:139:MET:HE2	1.95	0.49
2:C:145:THR:HG22	2:C:146:ALA:N	2.28	0.49
2:C:246:TYR:CD1	2:C:247:PRO:HD2	2.48	0.49
2:C:290:GLU:O	2:C:293:GLN:HB2	2.13	0.49
2:C:385:LEU:HD21	2:C:422:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:491:LEU:HD13	2:C:510:LEU:HD23	1.94	0.49
1:D:43:ARG:O	1:D:44:ASN:HB2	2.11	0.49
1:D:164:PRO:CD	1:D:176:PRO:HB2	2.43	0.49
2:G:208:PRO:HG3	2:G:530:LEU:O	2.12	0.49
2:G:372:LEU:HD22	2:G:375:LEU:HD11	1.95	0.49
2:B:266:CYS:O	2:B:267:ARG:C	2.56	0.48
2:C:199:ILE:HG22	2:C:200:GLU:N	2.27	0.48
2:C:216:LEU:HB3	2:C:242:ASP:CG	2.37	0.48
1:E:28:LEU:HD11	2:F:160:LEU:CD1	2.40	0.48
1:E:208:LEU:HD22	1:E:243:TRP:CZ3	2.48	0.48
2:G:145:THR:HG22	2:G:146:ALA:N	2.28	0.48
2:G:434:LEU:O	2:G:438:VAL:HG23	2.12	0.48
1:H:49:LEU:CD1	1:H:50:ILE:H	2.20	0.48
1:H:70:TYR:N	1:H:70:TYR:HD1	2.11	0.48
1:H:244:THR:CG2	1:H:245:CYS:H	2.23	0.48
1:A:292:SER:C	1:A:294:ASP:N	2.69	0.48
2:B:135:ALA:O	2:B:139:MET:HB3	2.13	0.48
2:B:238:SER:O	2:B:242:ASP:CB	2.60	0.48
2:B:436:LYS:HE3	2:B:469:THR:OG1	2.13	0.48
2:C:182:LYS:O	2:C:185:PHE:HD1	1.96	0.48
1:E:113:PRO:HB2	1:E:161:ALA:HB2	1.95	0.48
2:F:207:TYR:CZ	2:F:504:GLU:HG3	2.49	0.48
2:F:266:CYS:O	2:F:267:ARG:C	2.55	0.48
2:G:446:ASP:O	2:G:447:VAL:C	2.56	0.48
1:H:30:THR:CG2	1:H:31:CYS:N	2.75	0.48
2:C:398:SER:HB3	2:C:401:SER:HB3	1.96	0.48
2:C:432:GLU:CD	2:C:466:SER:HB3	2.38	0.48
1:D:30:THR:CG2	1:D:31:CYS:N	2.75	0.48
1:D:74:LEU:O	1:D:86:TRP:HD1	1.96	0.48
1:D:112:ALA:HA	1:D:158:TRP:CD2	2.48	0.48
1:D:182:PHE:HE2	1:D:202:TRP:CD1	2.31	0.48
1:E:30:THR:CG2	1:E:31:CYS:N	2.75	0.48
1:E:240:VAL:HB	1:E:258:LEU:HB3	1.96	0.48
2:F:487:HIS:HD2	2:F:517:LEU:HD23	1.77	0.48
1:A:164:PRO:CD	1:A:176:PRO:HB2	2.44	0.48
1:A:288:LEU:HB2	1:A:300:ILE:HG13	1.95	0.48
2:B:210:ILE:HD12	2:B:495:CYS:C	2.38	0.48
2:B:372:LEU:HD22	2:B:375:LEU:HD11	1.95	0.48
2:C:423:GLN:HB3	2:C:434:LEU:HD21	1.94	0.48
2:C:525:HIS:O	2:C:527:LEU:N	2.46	0.48
1:E:112:ALA:HA	1:E:158:TRP:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:ARG:HG3	2:F:142:ARG:HH11	1.79	0.48
2:F:215:LEU:HD13	2:F:452:TYR:HE1	1.78	0.48
2:F:515:ILE:HD12	2:F:541:GLN:N	2.28	0.48
2:G:283:LYS:HZ3	2:G:378:GLU:HB2	1.77	0.48
2:G:332:ILE:H	2:G:332:ILE:CD1	2.25	0.48
1:H:220:TRP:NE1	1:H:231:ILE:HD11	2.28	0.48
1:A:21:MET:HE1	2:B:172:ILE:HD13	1.94	0.48
1:A:220:TRP:NE1	1:A:231:ILE:HD11	2.28	0.48
2:B:294:ILE:HD11	2:B:310:ALA:HA	1.95	0.48
2:B:330:PRO:O	2:B:331:ARG:C	2.57	0.48
2:B:356:LYS:O	2:B:359:LYS:HB3	2.13	0.48
2:B:495:CYS:C	2:B:497:LEU:H	2.20	0.48
2:C:544:LYS:O	2:C:545:ASP:C	2.56	0.48
1:E:47:GLN:OE1	2:F:167:LYS:N	2.46	0.48
2:F:237:SER:OG	2:F:421:ILE:HD13	2.13	0.48
2:G:404:GLN:HG2	2:G:426:ALA:C	2.39	0.48
1:A:73:ILE:HG22	1:A:74:LEU:N	2.28	0.48
1:A:74:LEU:O	1:A:86:TRP:HD1	1.97	0.48
2:C:409:LYS:O	2:C:410:PHE:HD2	1.97	0.48
1:D:106:VAL:HA	1:D:124:SER:HA	1.94	0.48
1:D:111:TRP:CE2	1:D:120:LEU:HD13	2.48	0.48
1:D:242:ILE:HG12	1:D:297:TRP:CZ2	2.48	0.48
1:E:40:PHE:CZ	2:F:168:SER:CB	2.93	0.48
2:F:207:TYR:CE2	2:F:504:GLU:HA	2.45	0.48
2:F:241:PHE:CD2	2:F:457:LEU:HD21	2.48	0.48
2:F:267:ARG:CG	2:F:267:ARG:NH1	2.71	0.48
2:G:139:MET:HE2	2:G:139:MET:HA	1.95	0.48
2:G:330:PRO:O	2:G:331:ARG:C	2.57	0.48
2:G:394:ILE:O	2:G:397:TYR:CE1	2.66	0.48
1:A:23:TYR:CD2	1:A:24:TYR:CD1	2.98	0.48
1:A:112:ALA:HA	1:A:158:TRP:CD2	2.48	0.48
2:B:485:GLN:HE21	2:B:517:LEU:CD2	2.26	0.48
2:C:266:CYS:O	2:C:267:ARG:C	2.56	0.48
1:D:274:ALA:O	1:D:275:ASN:CB	2.61	0.48
2:F:170:VAL:O	2:F:170:VAL:HG12	2.13	0.48
2:F:525:HIS:CD2	2:F:529:ARG:HG3	2.49	0.48
2:G:210:ILE:HD11	2:G:495:CYS:HB3	1.93	0.48
2:G:262:LYS:O	2:G:263:GLU:C	2.56	0.48
1:A:112:ALA:HB2	1:A:158:TRP:CH2	2.49	0.48
2:B:182:LYS:O	2:B:185:PHE:HD1	1.96	0.48
2:B:262:LYS:O	2:B:263:GLU:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:525:HIS:CD2	2:C:529:ARG:HG3	2.49	0.48
1:E:70:TYR:N	1:E:70:TYR:HD1	2.10	0.48
2:F:544:LYS:O	2:F:545:ASP:C	2.56	0.48
2:G:492:PHE:O	2:G:495:CYS:HB2	2.14	0.48
1:H:16:ILE:HA	1:H:32:SER:HB3	1.96	0.48
1:H:112:ALA:HB2	1:H:158:TRP:CH2	2.49	0.48
1:A:284:ASN:HA	2:B:149:THR:OG1	2.12	0.48
2:B:199:ILE:HG22	2:B:200:GLU:N	2.27	0.48
2:B:446:ASP:O	2:B:447:VAL:C	2.56	0.48
2:B:471:ASP:OD2	2:B:498:ASN:ND2	2.37	0.48
2:B:544:LYS:O	2:B:545:ASP:C	2.56	0.48
2:C:135:ALA:O	2:C:139:MET:HG3	2.14	0.48
2:C:297:TYR:CE2	2:C:305:ARG:HB3	2.48	0.48
1:D:112:ALA:HB2	1:D:158:TRP:CH2	2.49	0.48
1:D:213:ASP:OD1	1:D:214:TRP:N	2.38	0.48
1:E:106:VAL:HA	1:E:124:SER:HA	1.94	0.48
1:E:111:TRP:CE2	1:E:120:LEU:HD13	2.48	0.48
1:E:215:VAL:HA	1:E:235:SER:HB3	1.96	0.48
2:F:364:SER:CB	2:F:394:ILE:HG12	2.42	0.48
2:F:448:GLN:HB2	2:F:477:PHE:CE1	2.48	0.48
2:F:485:GLN:O	2:F:487:HIS:CG	2.67	0.48
2:G:199:ILE:HG22	2:G:200:GLU:N	2.27	0.48
1:A:106:VAL:HA	1:A:124:SER:HA	1.95	0.48
2:B:299:LEU:HD13	2:B:379:PHE:HE2	1.79	0.48
2:B:409:LYS:O	2:B:410:PHE:HD2	1.97	0.48
2:C:289:ASN:O	2:C:290:GLU:C	2.56	0.48
2:C:291:ILE:HG22	2:C:353:ASN:HB3	1.95	0.48
2:C:451:TRP:CE2	2:C:493:VAL:HG13	2.49	0.48
1:D:16:ILE:HA	1:D:32:SER:HB3	1.96	0.48
1:E:164:PRO:CD	1:E:176:PRO:HB2	2.44	0.48
2:F:262:LYS:O	2:F:263:GLU:C	2.56	0.48
2:G:210:ILE:CD1	2:G:496:PHE:CD1	2.97	0.48
2:G:284:ILE:HD13	2:G:297:TYR:HE1	1.78	0.48
1:A:17:HIS:ND1	2:B:148:TYR:CE2	2.82	0.47
1:A:18:ASP:OD2	2:B:152:LYS:NZ	2.43	0.47
1:A:234:CYS:SG	1:A:268:VAL:HG23	2.54	0.47
1:A:258:LEU:CD1	1:A:297:TRP:HB2	2.43	0.47
2:B:142:ARG:HH11	2:B:142:ARG:HG3	1.79	0.47
2:B:217:PHE:HZ	2:B:453:LEU:HD23	1.77	0.47
2:B:487:HIS:CD2	2:B:517:LEU:CD2	2.91	0.47
2:B:532:ILE:CG2	2:B:533:PRO:HD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:446:ASP:O	2:C:447:VAL:C	2.57	0.47
2:F:199:ILE:HG22	2:F:200:GLU:N	2.27	0.47
2:F:215:LEU:HD22	2:F:452:TYR:OH	2.14	0.47
2:F:446:ASP:O	2:F:447:VAL:C	2.56	0.47
2:G:409:LYS:O	2:G:410:PHE:HD2	1.97	0.47
1:E:112:ALA:HB2	1:E:158:TRP:CH2	2.49	0.47
1:E:276:ILE:HG21	1:E:300:ILE:HD11	1.96	0.47
2:F:190:LEU:HD13	2:F:489:HIS:ND1	2.29	0.47
2:F:409:LYS:O	2:F:410:PHE:HD2	1.97	0.47
2:B:174:ARG:NH2	2:B:485:GLN:OE1	2.47	0.47
2:B:485:GLN:HG3	2:B:485:GLN:O	2.13	0.47
2:C:190:LEU:HB2	2:C:489:HIS:CE1	2.48	0.47
2:C:299:LEU:HD22	2:C:383:CYS:SG	2.54	0.47
2:C:330:PRO:O	2:C:331:ARG:C	2.57	0.47
2:C:471:ASP:OD1	2:C:497:LEU:CA	2.59	0.47
1:D:56:HIS:CE1	1:D:84:ILE:HD12	2.49	0.47
2:F:471:ASP:OD1	2:F:497:LEU:HA	2.14	0.47
2:F:543:LEU:O	2:F:546:ARG:HB3	2.14	0.47
2:G:215:LEU:HD22	2:G:452:TYR:OH	2.15	0.47
2:G:284:ILE:HD13	2:G:297:TYR:CD1	2.48	0.47
2:G:525:HIS:O	2:G:527:LEU:N	2.47	0.47
1:H:274:ALA:O	1:H:275:ASN:CB	2.62	0.47
1:A:224:ILE:C	1:A:226:LEU:N	2.72	0.47
2:C:370:PHE:O	2:C:371:SER:O	2.33	0.47
1:D:220:TRP:NE1	1:D:231:ILE:HD11	2.29	0.47
1:D:251:ASN:ND2	1:D:253:TRP:HE1	2.13	0.47
1:E:74:LEU:O	1:E:86:TRP:HD1	1.96	0.47
2:F:370:PHE:O	2:F:371:SER:O	2.32	0.47
2:G:525:HIS:CD2	2:G:529:ARG:HG3	2.49	0.47
1:H:56:HIS:CE1	1:H:84:ILE:HD12	2.49	0.47
1:H:215:VAL:HA	1:H:235:SER:HB3	1.96	0.47
2:B:149:THR:O	2:B:150:PHE:HB3	2.15	0.47
2:B:215:LEU:HD13	2:B:452:TYR:HE1	1.78	0.47
2:B:525:HIS:CD2	2:B:529:ARG:HG3	2.49	0.47
2:C:217:PHE:HE2	2:C:449:PHE:CE1	2.32	0.47
2:C:276:ILE:O	2:C:276:ILE:HG22	2.14	0.47
2:C:522:THR:O	2:C:523:ASN:OD1	2.31	0.47
1:D:21:MET:HE2	1:D:21:MET:HB2	1.68	0.47
1:E:182:PHE:O	1:E:182:PHE:CG	2.68	0.47
2:G:135:ALA:O	2:G:139:MET:HG3	2.14	0.47
2:G:370:PHE:O	2:G:371:SER:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:524:ASP:O	2:G:524:ASP:CG	2.55	0.47
1:H:74:LEU:O	1:H:86:TRP:HD1	1.97	0.47
1:H:129:ILE:O	1:H:129:ILE:HG22	2.15	0.47
2:B:145:THR:HG22	2:B:147:SER:N	2.29	0.47
2:B:237:SER:OG	2:B:421:ILE:HD13	2.15	0.47
2:B:425:TYR:O	2:B:463:ARG:NH2	2.47	0.47
2:B:432:GLU:CD	2:B:466:SER:H	2.23	0.47
2:C:152:LYS:HZ2	1:D:62:GLN:HE21	1.62	0.47
2:C:224:MET:HE2	2:C:230:ASP:HB3	1.94	0.47
2:C:497:LEU:HD12	2:C:503:ALA:HA	1.97	0.47
1:H:73:ILE:HG22	1:H:74:LEU:N	2.30	0.47
1:H:79:TYR:HD1	1:H:105:SER:CB	2.28	0.47
1:A:16:ILE:HA	1:A:32:SER:HB3	1.96	0.47
1:A:27:ARG:HH12	1:A:93:TRP:HZ2	1.62	0.47
1:A:240:VAL:HB	1:A:258:LEU:HB3	1.97	0.47
2:B:280:ILE:CG1	2:B:300:LEU:HD21	2.45	0.47
2:B:323:SER:OG	2:C:262:LYS:HE2	2.14	0.47
2:B:515:ILE:HD11	2:B:540:ALA:CB	2.35	0.47
2:B:524:ASP:O	2:B:524:ASP:CG	2.58	0.47
2:C:276:ILE:HG21	2:C:383:CYS:SG	2.55	0.47
1:D:79:TYR:HD1	1:D:105:SER:CB	2.28	0.47
1:E:27:ARG:HH12	1:E:93:TRP:HZ2	1.62	0.47
1:E:56:HIS:CE1	1:E:84:ILE:HD12	2.49	0.47
1:E:220:TRP:NE1	1:E:231:ILE:HD11	2.28	0.47
1:E:291:GLU:HA	1:E:297:TRP:HA	1.96	0.47
2:F:217:PHE:HA	2:F:452:TYR:HE2	1.78	0.47
2:G:172:ILE:CD1	1:H:42:VAL:HG21	2.44	0.47
2:G:182:LYS:O	2:G:185:PHE:HD1	1.96	0.47
2:G:271:TRP:HE3	2:G:272:ILE:HG12	1.80	0.47
2:G:474:THR:HG23	2:G:493:VAL:CG1	2.45	0.47
1:H:280:SER:HA	1:H:286:VAL:HG22	1.96	0.47
1:A:241:PHE:HD2	1:A:257:LEU:HA	1.80	0.47
2:B:145:THR:C	2:B:147:SER:N	2.71	0.47
2:C:199:ILE:HD13	2:C:530:LEU:HA	1.95	0.47
1:E:16:ILE:HA	1:E:32:SER:HB3	1.96	0.47
2:F:177:THR:CG2	2:F:179:LEU:HB3	2.43	0.47
2:F:495:CYS:C	2:F:497:LEU:H	2.22	0.47
1:H:145:ILE:HD11	1:H:202:TRP:HB2	1.97	0.47
1:D:224:ILE:C	1:D:226:LEU:N	2.72	0.47
2:F:177:THR:C	2:F:179:LEU:N	2.72	0.47
1:H:27:ARG:HH12	1:H:93:TRP:HZ2	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:THR:HG22	1:A:245:CYS:N	2.30	0.47
2:C:209:GLN:HG2	2:C:497:LEU:O	2.15	0.47
1:D:73:ILE:HG22	1:D:74:LEU:N	2.30	0.47
2:F:207:TYR:CE1	2:F:504:GLU:HG3	2.50	0.47
2:F:291:ILE:HG22	2:F:353:ASN:HB2	1.97	0.47
2:G:543:LEU:O	2:G:546:ARG:HB3	2.15	0.47
1:H:53:LEU:HD23	1:H:53:LEU:H	1.80	0.47
1:A:79:TYR:HD1	1:A:105:SER:CB	2.28	0.46
2:B:370:PHE:O	2:B:371:SER:O	2.33	0.46
1:E:43:ARG:NH2	2:F:551:TYR:CE2	2.83	0.46
2:F:299:LEU:HD22	2:F:383:CYS:SG	2.55	0.46
2:F:515:ILE:HD11	2:F:540:ALA:CB	2.40	0.46
2:G:394:ILE:O	2:G:395:ASP:HB2	2.15	0.46
1:H:164:PRO:CD	1:H:176:PRO:HB2	2.43	0.46
1:A:283:ASP:C	1:A:285:LYS:H	2.23	0.46
2:B:276:ILE:O	2:B:276:ILE:HG22	2.15	0.46
2:B:423:GLN:HB3	2:B:434:LEU:HD21	1.97	0.46
2:C:262:LYS:O	2:C:263:GLU:C	2.56	0.46
1:D:290:LYS:CB	1:D:300:ILE:CD1	2.93	0.46
1:E:242:ILE:CD1	1:E:297:TRP:CD1	2.99	0.46
1:E:273:THR:HG21	2:F:479:ALA:HB1	1.94	0.46
1:E:276:ILE:HG23	1:E:289:TRP:O	2.15	0.46
2:F:343:TRP:CE3	2:F:350:ILE:HG21	2.51	0.46
2:G:194:ILE:HG12	2:G:492:PHE:CD2	2.50	0.46
2:G:445:LEU:HD23	2:G:445:LEU:HA	1.74	0.46
2:G:525:HIS:O	2:G:526:ILE:C	2.57	0.46
2:B:142:ARG:HA	2:B:142:ARG:HD3	1.52	0.46
2:B:543:LEU:O	2:B:546:ARG:HB3	2.15	0.46
2:C:543:LEU:O	2:C:546:ARG:HB3	2.15	0.46
1:E:49:LEU:CD1	1:E:50:ILE:H	2.20	0.46
2:F:149:THR:O	2:F:150:PHE:HB3	2.14	0.46
2:G:544:LYS:O	2:G:545:ASP:C	2.56	0.46
1:H:21:MET:HB2	1:H:21:MET:HE2	1.68	0.46
1:H:214:TRP:O	1:H:235:SER:CB	2.56	0.46
1:H:224:ILE:C	1:H:226:LEU:N	2.72	0.46
1:A:215:VAL:HA	1:A:235:SER:HB3	1.96	0.46
2:B:140:LYS:C	2:B:142:ARG:N	2.73	0.46
2:B:224:MET:HE2	2:B:230:ASP:HB3	1.94	0.46
2:B:241:PHE:CD2	2:B:457:LEU:HD21	2.51	0.46
1:E:14:ASP:CG	1:E:15:MET:H	2.24	0.46
2:F:153:PHE:HE2	2:F:175:LEU:HD22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:255:VAL:HG11	2:G:335:LEU:HD22	1.97	0.46
2:G:153:PHE:CE2	1:H:278:ALA:HB2	2.51	0.46
2:G:482:GLU:CD	2:G:509:ARG:HH22	2.24	0.46
1:A:50:ILE:O	1:A:50:ILE:HG22	2.16	0.46
2:B:177:THR:CG2	2:B:179:LEU:HB3	2.43	0.46
1:D:27:ARG:HH12	1:D:93:TRP:HZ2	1.62	0.46
1:E:234:CYS:SG	1:E:268:VAL:HG23	2.56	0.46
1:E:247:ASP:C	1:E:249:SER:H	2.23	0.46
2:F:202:ARG:HD3	2:F:202:ARG:HA	1.55	0.46
2:G:161:THR:O	2:G:170:VAL:HG13	2.15	0.46
1:H:16:ILE:HG22	1:H:17:HIS:H	1.80	0.46
1:H:224:ILE:HG13	1:H:226:LEU:HB2	1.98	0.46
2:B:136:LYS:O	2:B:140:LYS:HB2	2.15	0.46
2:C:161:THR:O	2:C:170:VAL:HG13	2.15	0.46
1:D:16:ILE:HG22	1:D:17:HIS:H	1.81	0.46
1:D:190:LEU:HD21	1:D:209:GLU:HB3	1.97	0.46
1:D:215:VAL:HA	1:D:235:SER:HB3	1.96	0.46
1:D:280:SER:HA	1:D:286:VAL:HG22	1.96	0.46
1:E:53:LEU:N	1:E:53:LEU:CD2	2.77	0.46
1:E:280:SER:HA	1:E:286:VAL:HG22	1.96	0.46
2:F:165:VAL:O	2:F:165:VAL:HG12	2.14	0.46
2:F:276:ILE:HG22	2:F:276:ILE:O	2.15	0.46
2:G:151:ALA:HB2	1:H:286:VAL:HG21	1.97	0.46
2:G:303:VAL:HG13	2:G:322:ILE:CG2	2.46	0.46
1:H:283:ASP:C	1:H:285:LYS:H	2.23	0.46
1:H:296:GLN:O	1:H:296:GLN:NE2	2.48	0.46
1:A:16:ILE:HG22	1:A:17:HIS:H	1.80	0.46
1:A:280:SER:HA	1:A:286:VAL:HG22	1.96	0.46
2:B:271:TRP:HE3	2:B:272:ILE:HG12	1.80	0.46
2:B:272:ILE:HG23	2:B:382:LEU:HG	1.98	0.46
1:E:241:PHE:C	1:E:242:ILE:HG13	2.40	0.46
1:E:272:ILE:HD11	2:F:155:THR:HA	1.97	0.46
2:F:343:TRP:CZ3	2:F:350:ILE:CG2	2.88	0.46
2:F:429:GLU:O	2:F:464:VAL:HG21	2.16	0.46
1:H:143:LYS:HD2	1:H:200:GLY:O	2.15	0.46
1:H:296:GLN:HE21	1:H:298:VAL:HG23	1.80	0.46
2:B:284:ILE:HD13	2:B:297:TYR:CE1	2.51	0.46
2:C:525:HIS:O	2:C:526:ILE:C	2.58	0.46
1:D:145:ILE:HG22	1:D:148:ALA:HB2	1.98	0.46
1:E:304:ASN:HA	2:F:173:LYS:NZ	2.30	0.46
2:F:136:LYS:O	2:F:140:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:177:THR:HG22	2:F:179:LEU:HD23	1.97	0.46
2:G:471:ASP:OD1	2:G:497:LEU:CD2	2.58	0.46
1:H:216:ARG:HA	1:H:216:ARG:HD3	1.67	0.46
2:B:230:ASP:O	2:B:231:TYR:C	2.59	0.46
1:D:14:ASP:CG	1:D:15:MET:H	2.24	0.46
1:E:50:ILE:HG22	1:E:50:ILE:O	2.16	0.46
2:F:137:LEU:O	2:F:141:GLU:HB3	2.16	0.46
2:F:271:TRP:HE3	2:F:272:ILE:HG12	1.81	0.46
1:H:14:ASP:CG	1:H:15:MET:H	2.24	0.46
1:H:145:ILE:HG22	1:H:148:ALA:HB2	1.98	0.46
1:A:53:LEU:N	1:A:53:LEU:CD2	2.78	0.46
2:B:256:LYS:O	2:B:260:LEU:HG	2.16	0.46
1:D:50:ILE:O	1:D:50:ILE:HG22	2.16	0.46
1:D:53:LEU:N	1:D:53:LEU:CD2	2.77	0.46
1:D:77:CYS:HB3	1:D:109:VAL:HG23	1.98	0.46
1:D:129:ILE:O	1:D:129:ILE:HG22	2.15	0.46
1:E:73:ILE:HG22	1:E:74:LEU:N	2.30	0.46
1:E:107:ASN:CG	2:F:142:ARG:NH2	2.73	0.46
1:E:192:LYS:HE2	1:E:207:LYS:HE2	1.98	0.46
2:F:217:PHE:HZ	2:F:453:LEU:HD23	1.80	0.46
2:F:532:ILE:HG23	2:F:533:PRO:CD	2.45	0.46
1:A:15:MET:HG3	2:B:162:LYS:HZ2	1.81	0.45
1:A:77:CYS:HB3	1:A:109:VAL:HG23	1.98	0.45
1:A:182:PHE:O	1:A:182:PHE:CG	2.68	0.45
1:A:224:ILE:HG13	1:A:226:LEU:HB2	1.98	0.45
2:B:137:LEU:O	2:B:141:GLU:N	2.32	0.45
2:B:295:PHE:CE1	2:B:360:LEU:HD11	2.52	0.45
2:C:213:SER:HB3	2:C:459:PHE:CD2	2.52	0.45
2:F:230:ASP:O	2:F:231:TYR:C	2.59	0.45
2:F:244:VAL:HG11	2:F:263:GLU:HB3	1.98	0.45
2:F:330:PRO:O	2:F:331:ARG:C	2.57	0.45
2:F:550:ASN:OD1	2:F:550:ASN:N	2.50	0.45
2:G:411:SER:C	2:G:412:LEU:HD12	2.41	0.45
1:H:50:ILE:O	1:H:50:ILE:HG22	2.16	0.45
1:A:14:ASP:CG	1:A:15:MET:H	2.24	0.45
2:B:165:VAL:HG12	2:B:165:VAL:O	2.15	0.45
2:C:271:TRP:HE3	2:C:272:ILE:HG12	1.80	0.45
2:C:303:VAL:HG13	2:C:322:ILE:CG2	2.46	0.45
1:D:182:PHE:O	1:D:182:PHE:CG	2.69	0.45
1:E:53:LEU:HD12	1:E:86:TRP:CD2	2.52	0.45
1:E:191:ILE:HB	1:E:208:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:186:ASP:OD1	2:F:186:ASP:C	2.59	0.45
2:F:303:VAL:HG13	2:F:322:ILE:CG2	2.47	0.45
2:F:475:PHE:CE2	2:F:497:LEU:HD11	2.50	0.45
2:G:276:ILE:O	2:G:276:ILE:HG22	2.14	0.45
2:G:350:ILE:HG22	2:G:351:ASP:N	2.30	0.45
2:G:394:ILE:O	2:G:397:TYR:CD1	2.70	0.45
2:G:550:ASN:N	2:G:550:ASN:OD1	2.49	0.45
1:A:28:LEU:HD13	2:B:172:ILE:CD1	2.46	0.45
1:A:129:ILE:O	1:A:129:ILE:HG22	2.14	0.45
2:B:487:HIS:HE1	2:B:513:ARG:HH21	1.65	0.45
2:C:359:LYS:HZ1	2:C:370:PHE:H	1.65	0.45
1:E:79:TYR:HD1	1:E:105:SER:CB	2.29	0.45
1:E:145:ILE:HG22	1:E:148:ALA:HB2	1.98	0.45
1:E:150:THR:HB	1:E:188:ASP:HB3	1.99	0.45
1:E:294:ASP:OD1	1:E:294:ASP:O	2.34	0.45
2:F:524:ASP:O	2:F:524:ASP:CG	2.58	0.45
2:G:162:LYS:HZ3	1:H:15:MET:CE	2.22	0.45
2:G:375:LEU:HB2	2:G:384:LEU:HD21	1.98	0.45
2:G:495:CYS:C	2:G:497:LEU:N	2.74	0.45
2:B:137:LEU:O	2:B:141:GLU:HB3	2.15	0.45
2:B:186:ASP:C	2:B:186:ASP:OD1	2.59	0.45
2:B:202:ARG:HG2	2:B:209:GLN:CD	2.42	0.45
2:C:489:HIS:O	2:C:490:SER:C	2.60	0.45
1:D:242:ILE:CD1	1:D:258:LEU:HB2	2.46	0.45
2:G:414:TYR:C	2:G:414:TYR:CD2	2.94	0.45
1:H:248:ALA:O	1:H:249:SER:HB3	2.16	0.45
1:H:276:ILE:HG23	1:H:289:TRP:O	2.16	0.45
1:A:53:LEU:HD12	1:A:86:TRP:CD2	2.52	0.45
1:A:276:ILE:HG23	1:A:289:TRP:O	2.16	0.45
2:B:153:PHE:HE2	2:B:175:LEU:HD22	1.81	0.45
2:B:409:LYS:H	2:B:409:LYS:HG2	1.56	0.45
2:B:484:ALA:O	2:B:485:GLN:CB	2.65	0.45
2:B:512:MET:HA	2:B:540:ALA:HB1	1.98	0.45
1:D:189:ASN:HA	1:D:215:VAL:HG23	1.98	0.45
1:D:232:ALA:HB2	1:D:270:TRP:HZ2	1.77	0.45
1:D:283:ASP:C	1:D:285:LYS:H	2.23	0.45
1:E:266:TRP:HD1	1:E:281:GLY:HA2	1.81	0.45
2:F:164:ILE:O	2:F:164:ILE:CG2	2.63	0.45
2:G:155:THR:CG2	2:G:513:ARG:HD2	2.30	0.45
1:H:145:ILE:HD11	1:H:202:TRP:CB	2.47	0.45
1:H:266:TRP:HD1	1:H:281:GLY:HA2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:N	1:A:193:LEU:HD23	2.32	0.45
2:B:199:ILE:HG21	2:B:208:PRO:HB2	1.99	0.45
2:C:519:ARG:HB3	2:C:520:ALA:H	1.48	0.45
1:D:214:TRP:O	1:D:235:SER:CB	2.56	0.45
1:E:70:TYR:CD2	1:E:118:LEU:HD13	2.52	0.45
1:E:77:CYS:SG	1:E:106:VAL:O	2.67	0.45
1:E:129:ILE:O	1:E:129:ILE:HG22	2.14	0.45
1:E:224:ILE:HG13	1:E:226:LEU:HB2	1.98	0.45
1:E:258:LEU:CD1	1:E:297:TRP:CB	2.94	0.45
2:G:209:GLN:HG3	2:G:495:CYS:O	2.17	0.45
2:G:256:LYS:O	2:G:260:LEU:HG	2.16	0.45
2:G:522:THR:O	2:G:523:ASN:CG	2.59	0.45
1:A:213:ASP:OD1	1:A:214:TRP:N	2.38	0.45
1:A:216:ARG:HD3	1:A:216:ARG:HA	1.66	0.45
2:B:299:LEU:HD13	2:B:379:PHE:CE2	2.52	0.45
2:C:522:THR:CG2	2:C:526:ILE:HG13	2.47	0.45
1:D:150:THR:HB	1:D:188:ASP:HB3	1.98	0.45
1:D:294:ASP:OD1	1:D:294:ASP:O	2.34	0.45
2:F:163:ASP:O	2:F:164:ILE:HB	2.16	0.45
2:F:513:ARG:HE	2:F:514:GLU:HG2	1.82	0.45
2:G:177:THR:C	2:G:179:LEU:H	2.25	0.45
2:G:201:ALA:HB2	2:G:531:LYS:HZ2	1.80	0.45
2:G:385:LEU:HA	2:G:406:HIS:CE1	2.52	0.45
2:B:177:THR:O	2:B:179:LEU:N	2.49	0.45
2:B:272:ILE:CG2	2:B:382:LEU:HG	2.47	0.45
2:B:469:THR:O	2:B:472:GLU:HB3	2.17	0.45
2:B:513:ARG:HE	2:B:514:GLU:HG2	1.81	0.45
2:C:215:LEU:HD22	2:C:452:TYR:OH	2.17	0.45
2:C:256:LYS:O	2:C:260:LEU:HG	2.17	0.45
2:C:469:THR:O	2:C:472:GLU:HB3	2.17	0.45
2:C:486:LEU:HD23	2:C:486:LEU:HA	1.83	0.45
2:C:522:THR:C	2:C:523:ASN:CG	2.85	0.45
1:D:290:LYS:HB2	1:D:300:ILE:CD1	2.46	0.45
1:E:213:ASP:OD1	1:E:214:TRP:N	2.38	0.45
1:E:284:ASN:HA	2:F:149:THR:OG1	2.16	0.45
2:F:469:THR:O	2:F:472:GLU:HB3	2.17	0.45
2:G:373:LYS:HE2	2:G:410:PHE:HE2	1.81	0.45
2:B:525:HIS:O	2:B:526:ILE:C	2.60	0.45
2:C:184:LEU:HD21	2:C:448:GLN:HE22	1.81	0.45
2:C:475:PHE:HE2	2:C:497:LEU:CD1	2.30	0.45
1:E:41:ASP:OD1	1:E:42:VAL:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:LEU:N	1:E:193:LEU:HD23	2.32	0.45
1:E:199:ASP:OD1	1:E:200:GLY:N	2.50	0.45
1:E:258:LEU:CD1	1:E:297:TRP:HB2	2.47	0.45
2:F:140:LYS:C	2:F:142:ARG:N	2.73	0.45
2:G:202:ARG:HD3	2:G:202:ARG:HA	1.55	0.45
2:G:230:ASP:O	2:G:231:TYR:C	2.59	0.45
1:A:199:ASP:OD1	1:A:200:GLY:N	2.50	0.45
1:A:208:LEU:HD13	1:A:243:TRP:CE3	2.52	0.45
2:B:163:ASP:O	2:B:164:ILE:HB	2.16	0.45
2:B:350:ILE:CG2	2:B:351:ASP:N	2.80	0.45
2:B:402:LEU:O	2:B:403:VAL:C	2.60	0.45
2:C:155:THR:HG22	2:C:513:ARG:CD	2.42	0.45
2:F:145:THR:HG22	2:F:147:SER:N	2.30	0.45
2:F:256:LYS:O	2:F:260:LEU:HG	2.16	0.45
2:F:393:GLN:O	2:F:394:ILE:C	2.59	0.45
2:G:469:THR:O	2:G:472:GLU:HB3	2.18	0.45
2:G:513:ARG:HE	2:G:514:GLU:HG2	1.81	0.45
1:H:182:PHE:O	1:H:182:PHE:CG	2.69	0.45
1:H:232:ALA:HB2	1:H:270:TRP:HZ2	1.79	0.45
1:A:145:ILE:HD13	1:A:194:TRP:CE3	2.53	0.44
2:B:487:HIS:CE1	2:B:513:ARG:HH21	2.35	0.44
2:C:177:THR:C	2:C:179:LEU:H	2.25	0.44
2:C:402:LEU:O	2:C:403:VAL:C	2.60	0.44
1:D:38:LYS:HB2	1:D:40:PHE:CE1	2.52	0.44
1:E:157:SER:HB2	1:E:218:VAL:O	2.17	0.44
1:E:283:ASP:C	1:E:285:LYS:H	2.23	0.44
2:F:250:THR:O	2:F:256:LYS:HE3	2.17	0.44
2:G:149:THR:CG2	2:G:150:PHE:N	2.72	0.44
2:G:276:ILE:HD13	2:G:383:CYS:CA	2.34	0.44
2:G:366:PHE:HZ	2:G:387:LEU:HD12	1.82	0.44
1:A:21:MET:HB3	2:B:154:SER:OG	2.17	0.44
1:A:191:ILE:HB	1:A:208:LEU:HB2	1.99	0.44
1:A:210:ALA:HB3	1:A:243:TRP:CZ2	2.52	0.44
1:A:258:LEU:HD13	1:A:297:TRP:HB2	1.99	0.44
1:A:294:ASP:OD1	1:A:294:ASP:O	2.34	0.44
2:B:133:ASP:OD1	2:B:133:ASP:N	2.50	0.44
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.83	0.44
2:B:321:LEU:HB3	2:B:361:LEU:CD1	2.42	0.44
2:B:491:LEU:HD23	2:B:530:LEU:HD12	1.99	0.44
2:C:193:GLU:O	2:C:196:LYS:HB2	2.18	0.44
2:C:202:ARG:HG2	2:C:209:GLN:CD	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:295:PHE:CE2	2:C:356:LYS:HD3	2.53	0.44
2:C:474:THR:CG2	2:C:493:VAL:HG12	2.47	0.44
2:C:481:LEU:O	2:C:484:ALA:HB3	2.18	0.44
2:C:513:ARG:HE	2:C:514:GLU:HG2	1.82	0.44
1:D:53:LEU:HD12	1:D:86:TRP:CD2	2.51	0.44
1:D:266:TRP:HD1	1:D:281:GLY:HA2	1.82	0.44
2:F:210:ILE:HG22	2:F:459:PHE:CE2	2.53	0.44
1:A:43:ARG:O	1:A:44:ASN:CB	2.66	0.44
1:A:70:TYR:CD2	1:A:118:LEU:HD13	2.53	0.44
1:A:145:ILE:HG22	1:A:148:ALA:HB2	1.98	0.44
1:A:280:SER:HB2	2:B:150:PHE:HA	1.99	0.44
1:A:300:ILE:H	1:A:300:ILE:HG12	1.59	0.44
2:B:210:ILE:CD1	2:B:495:CYS:C	2.91	0.44
2:B:210:ILE:HD12	2:B:210:ILE:H	1.82	0.44
2:C:208:PRO:HD3	2:C:533:PRO:HD3	1.98	0.44
1:D:77:CYS:HB3	1:D:109:VAL:HG21	1.99	0.44
1:E:16:ILE:HG22	1:E:17:HIS:H	1.80	0.44
1:E:43:ARG:O	1:E:44:ASN:CB	2.66	0.44
1:E:95:LYS:O	1:E:95:LYS:HG2	2.17	0.44
2:F:133:ASP:OD1	2:F:133:ASP:N	2.50	0.44
2:F:193:GLU:O	2:F:196:LYS:HB2	2.17	0.44
2:F:246:TYR:CD1	2:F:246:TYR:C	2.95	0.44
2:G:202:ARG:HG2	2:G:209:GLN:CD	2.42	0.44
1:H:77:CYS:HB3	1:H:109:VAL:HG23	1.98	0.44
1:H:95:LYS:HG2	1:H:95:LYS:O	2.17	0.44
2:B:316:GLY:O	2:B:317:HIS:C	2.60	0.44
2:B:492:PHE:CD1	2:B:492:PHE:C	2.95	0.44
1:D:224:ILE:HG13	1:D:226:LEU:HB2	1.98	0.44
2:G:316:GLY:O	2:G:317:HIS:C	2.60	0.44
2:G:551:TYR:CE2	1:H:43:ARG:NH2	2.85	0.44
1:H:53:LEU:HD12	1:H:86:TRP:CD2	2.52	0.44
1:H:199:ASP:OD1	1:H:199:ASP:O	2.36	0.44
1:A:266:TRP:HD1	1:A:281:GLY:HA2	1.82	0.44
2:B:135:ALA:O	2:B:139:MET:CB	2.65	0.44
2:C:230:ASP:O	2:C:231:TYR:C	2.59	0.44
2:C:284:ILE:O	2:C:287:SER:HB3	2.17	0.44
2:C:396:GLU:OE1	2:C:396:GLU:HA	2.16	0.44
2:C:435:TYR:CD2	2:C:454:ILE:HD11	2.53	0.44
2:C:550:ASN:OD1	2:C:550:ASN:N	2.49	0.44
1:D:53:LEU:HD23	1:D:53:LEU:H	1.80	0.44
1:D:78:SER:OG	1:D:79:TYR:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:LEU:N	1:D:193:LEU:HD23	2.33	0.44
1:E:264:VAL:CG1	1:E:265:VAL:N	2.81	0.44
1:E:287:THR:O	1:E:288:LEU:HD23	2.17	0.44
2:F:210:ILE:H	2:F:210:ILE:HD12	1.82	0.44
1:A:40:PHE:N	1:A:40:PHE:CD1	2.84	0.44
1:A:95:LYS:O	1:A:95:LYS:HG2	2.17	0.44
2:B:193:GLU:O	2:B:196:LYS:HB2	2.17	0.44
2:C:178:GLU:HG2	2:C:480:GLN:NE2	2.32	0.44
1:D:29:ALA:CA	1:D:39:ILE:HD13	2.46	0.44
1:E:21:MET:HB2	1:E:21:MET:HE2	1.68	0.44
1:E:245:CYS:HB2	1:E:253:TRP:CZ3	2.51	0.44
2:F:199:ILE:HG21	2:F:208:PRO:HB2	1.99	0.44
2:B:475:PHE:O	2:B:476:ALA:C	2.61	0.44
2:C:185:PHE:HA	2:C:486:LEU:HD11	2.00	0.44
2:C:246:TYR:CE2	2:C:250:THR:OG1	2.67	0.44
1:D:276:ILE:HG23	1:D:289:TRP:O	2.17	0.44
1:E:78:SER:OG	1:E:79:TYR:N	2.51	0.44
2:F:137:LEU:O	2:F:141:GLU:N	2.33	0.44
2:F:238:SER:CA	2:F:242:ASP:OD2	2.54	0.44
2:F:323:SER:OG	2:G:262:LYS:HE2	2.18	0.44
2:F:530:LEU:O	2:F:531:LYS:C	2.61	0.44
2:G:186:ASP:OD1	2:G:186:ASP:C	2.59	0.44
1:H:77:CYS:HB3	1:H:109:VAL:HG21	2.00	0.44
1:A:38:LYS:HB2	1:A:40:PHE:CE1	2.52	0.44
2:B:185:PHE:CD1	2:B:185:PHE:N	2.86	0.44
2:B:276:ILE:HG21	2:B:383:CYS:SG	2.58	0.44
2:B:412:LEU:HB3	2:B:413:PRO:HD2	1.99	0.44
2:C:249:LYS:O	2:C:250:THR:C	2.61	0.44
2:C:272:ILE:HG23	2:C:382:LEU:HG	2.00	0.44
2:C:448:GLN:HB2	2:C:477:PHE:HE1	1.81	0.44
1:E:280:SER:HB2	2:F:150:PHE:HA	1.98	0.44
2:F:177:THR:CG2	2:F:179:LEU:CD2	2.93	0.44
2:F:519:ARG:HB3	2:F:520:ALA:H	1.48	0.44
2:G:199:ILE:HG21	2:G:208:PRO:HB2	1.99	0.44
2:G:278:PRO:HG2	2:G:279:GLU:H	1.83	0.44
1:A:77:CYS:HB3	1:A:109:VAL:HG21	2.00	0.44
1:A:107:ASN:CG	2:B:142:ARG:NH2	2.76	0.44
2:B:303:VAL:HG13	2:B:322:ILE:CG2	2.46	0.44
2:B:380:SER:O	2:B:381:TRP:C	2.60	0.44
2:B:451:TRP:CD1	2:B:474:THR:HA	2.53	0.44
2:B:485:GLN:NE2	2:B:517:LEU:HD22	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:172:ILE:CD1	1:D:42:VAL:HG21	2.47	0.44
2:C:210:ILE:HD13	2:C:496:PHE:HA	2.00	0.44
2:C:297:TYR:HB3	2:C:306:ALA:HB2	2.00	0.44
1:D:70:TYR:CD2	1:D:118:LEU:HD13	2.53	0.44
1:D:216:ARG:HD3	1:D:216:ARG:HA	1.67	0.44
1:E:183:ALA:O	1:E:184:SER:CB	2.66	0.44
1:E:303:VAL:O	1:E:304:ASN:HB2	2.17	0.44
2:F:142:ARG:HD3	2:F:142:ARG:HA	1.51	0.44
2:F:525:HIS:O	2:F:526:ILE:C	2.60	0.44
2:G:152:LYS:HZ1	1:H:62:GLN:NE2	2.16	0.44
2:G:475:PHE:O	2:G:476:ALA:C	2.61	0.44
1:A:89:GLU:O	1:A:90:ASN:CB	2.66	0.43
2:B:297:TYR:CE2	2:B:305:ARG:HB3	2.53	0.43
2:C:188:VAL:O	2:C:192:LYS:HB2	2.18	0.43
2:C:199:ILE:HG21	2:C:208:PRO:HB2	1.99	0.43
2:C:317:HIS:O	2:C:320:VAL:HB	2.18	0.43
1:D:66:ALA:HB3	1:D:73:ILE:HB	2.00	0.43
1:E:245:CYS:HB2	1:E:253:TRP:CD2	2.53	0.43
2:F:177:THR:O	2:F:179:LEU:N	2.50	0.43
2:F:218:LYS:CG	2:F:238:SER:OG	2.59	0.43
2:G:152:LYS:NZ	1:H:62:GLN:NE2	2.66	0.43
2:G:153:PHE:HE1	2:G:175:LEU:HD22	1.82	0.43
2:G:404:GLN:CG	2:G:426:ALA:HB1	2.46	0.43
1:H:247:ASP:C	1:H:249:SER:H	2.25	0.43
1:A:303:VAL:O	1:A:304:ASN:HB2	2.17	0.43
2:B:199:ILE:CD1	2:B:530:LEU:HA	2.48	0.43
2:B:299:LEU:HD22	2:B:383:CYS:SG	2.58	0.43
2:B:481:LEU:HB2	2:B:490:SER:HB2	1.99	0.43
2:B:522:THR:HG21	2:B:526:ILE:HD11	1.98	0.43
2:B:550:ASN:OD1	2:B:550:ASN:N	2.50	0.43
2:C:153:PHE:HE1	2:C:175:LEU:HD22	1.82	0.43
2:C:316:GLY:O	2:C:317:HIS:C	2.60	0.43
2:C:475:PHE:O	2:C:476:ALA:C	2.61	0.43
1:D:204:GLU:O	1:D:204:GLU:HG3	2.18	0.43
1:E:77:CYS:HB3	1:E:109:VAL:HG23	1.98	0.43
1:E:79:TYR:CE2	2:F:138:ILE:CD1	3.01	0.43
1:E:288:LEU:HB3	1:E:300:ILE:HG13	2.00	0.43
2:F:188:VAL:O	2:F:192:LYS:HB2	2.19	0.43
2:F:380:SER:O	2:F:383:CYS:N	2.45	0.43
2:F:522:THR:CG2	2:F:526:ILE:CD1	2.96	0.43
2:G:188:VAL:O	2:G:192:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:317:HIS:O	2:G:320:VAL:HB	2.19	0.43
1:H:160:PRO:O	1:H:162:VAL:HG23	2.18	0.43
1:A:78:SER:OG	1:A:79:TYR:N	2.51	0.43
1:A:204:GLU:HG3	1:A:204:GLU:O	2.18	0.43
2:B:487:HIS:HD2	2:B:517:LEU:CD2	2.15	0.43
2:C:194:ILE:CG1	2:C:492:PHE:CE2	2.99	0.43
2:C:359:LYS:NZ	2:C:370:PHE:H	2.16	0.43
1:E:33:SER:HA	1:E:59:PRO:HB3	2.00	0.43
1:E:182:PHE:CD1	1:E:182:PHE:C	2.97	0.43
2:F:135:ALA:O	2:F:139:MET:CB	2.65	0.43
2:F:253:ASP:O	2:F:257:MET:HB2	2.18	0.43
2:F:317:HIS:O	2:F:320:VAL:HB	2.19	0.43
2:G:402:LEU:O	2:G:403:VAL:C	2.60	0.43
1:H:70:TYR:CD2	1:H:118:LEU:HD13	2.53	0.43
1:H:193:LEU:HD21	1:H:208:LEU:CD1	2.48	0.43
1:A:21:MET:HE2	1:A:21:MET:HB2	1.68	0.43
2:B:188:VAL:O	2:B:192:LYS:HB2	2.18	0.43
2:B:217:PHE:HA	2:B:452:TYR:HE2	1.82	0.43
2:C:410:PHE:CD2	2:C:410:PHE:N	2.84	0.43
1:D:234:CYS:HB2	1:D:265:VAL:CG1	2.47	0.43
2:F:402:LEU:O	2:F:403:VAL:C	2.61	0.43
2:F:410:PHE:CD2	2:F:410:PHE:N	2.84	0.43
2:G:193:GLU:O	2:G:196:LYS:HB2	2.18	0.43
1:H:78:SER:OG	1:H:79:TYR:N	2.51	0.43
1:H:89:GLU:O	1:H:90:ASN:CB	2.66	0.43
1:H:193:LEU:N	1:H:193:LEU:HD23	2.33	0.43
1:H:213:ASP:OD1	1:H:214:TRP:N	2.38	0.43
1:A:33:SER:HA	1:A:59:PRO:HB3	2.01	0.43
1:A:287:THR:O	1:A:288:LEU:HD23	2.19	0.43
2:C:246:TYR:HA	2:C:247:PRO:HD2	1.80	0.43
2:C:348:CYS:O	2:C:349:SER:C	2.62	0.43
2:C:359:LYS:HZ1	2:C:368:GLY:HA3	1.83	0.43
1:D:77:CYS:SG	1:D:106:VAL:O	2.66	0.43
1:E:79:TYR:CD2	2:F:138:ILE:HD13	2.53	0.43
2:F:145:THR:C	2:F:147:SER:N	2.70	0.43
2:F:244:VAL:HG23	2:F:264:ARG:NH2	2.27	0.43
2:F:475:PHE:O	2:F:476:ALA:C	2.61	0.43
1:H:40:PHE:N	1:H:40:PHE:CD1	2.85	0.43
1:A:53:LEU:HD23	1:A:53:LEU:H	1.81	0.43
2:B:278:PRO:HG2	2:B:279:GLU:H	1.84	0.43
2:B:359:LYS:NZ	2:B:370:PHE:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:PHE:CD2	2:B:410:PHE:N	2.84	0.43
2:B:522:THR:O	2:B:522:THR:HG22	2.18	0.43
2:C:185:PHE:N	2:C:185:PHE:CD1	2.87	0.43
2:C:220:ALA:HB3	2:C:234:TRP:CE3	2.54	0.43
2:C:484:ALA:O	2:C:485:GLN:HB2	2.19	0.43
1:D:69:MET:HE1	1:D:114:HIS:CD2	2.53	0.43
1:D:95:LYS:O	1:D:95:LYS:HG2	2.18	0.43
1:E:69:MET:HE1	1:E:114:HIS:CD2	2.54	0.43
2:F:202:ARG:HG2	2:F:209:GLN:CD	2.42	0.43
2:F:379:PHE:N	2:F:379:PHE:HD1	2.17	0.43
2:B:294:ILE:HD13	2:B:310:ALA:HB2	1.99	0.43
2:C:339:GLN:O	2:C:343:TRP:CD1	2.71	0.43
2:C:399:LEU:O	2:C:402:LEU:HB3	2.19	0.43
1:D:43:ARG:O	1:D:44:ASN:CB	2.66	0.43
1:D:264:VAL:CG1	1:D:265:VAL:N	2.82	0.43
1:D:287:THR:O	1:D:288:LEU:HD23	2.19	0.43
1:E:66:ALA:HB3	1:E:73:ILE:HB	2.01	0.43
1:E:77:CYS:HB3	1:E:109:VAL:HG21	2.00	0.43
1:E:216:ARG:HD3	1:E:216:ARG:HA	1.67	0.43
2:F:262:LYS:HE2	2:G:323:SER:OG	2.19	0.43
2:F:359:LYS:NZ	2:F:370:PHE:H	2.16	0.43
2:G:220:ALA:HB3	2:G:234:TRP:CE3	2.54	0.43
2:G:272:ILE:HG23	2:G:382:LEU:HG	1.99	0.43
1:H:43:ARG:O	1:H:44:ASN:CB	2.66	0.43
1:H:69:MET:HE1	1:H:114:HIS:CD2	2.54	0.43
2:B:267:ARG:HG3	2:B:267:ARG:NH1	2.15	0.43
2:B:280:ILE:O	2:B:281:GLU:C	2.62	0.43
2:C:186:ASP:C	2:C:186:ASP:OD1	2.60	0.43
2:C:194:ILE:CG1	2:C:492:PHE:HE2	2.29	0.43
1:E:69:MET:HE1	1:E:114:HIS:HB2	1.98	0.43
1:E:89:GLU:O	1:E:90:ASN:CB	2.66	0.43
2:F:381:TRP:CD1	2:F:382:LEU:N	2.86	0.43
2:G:201:ALA:HB2	2:G:531:LYS:HZ3	1.80	0.43
2:G:410:PHE:CD2	2:G:410:PHE:N	2.84	0.43
1:H:287:THR:HG21	1:H:299:CYS:SG	2.58	0.43
1:A:264:VAL:CG1	1:A:265:VAL:N	2.81	0.43
1:A:266:TRP:CZ3	2:B:144:PHE:HD2	2.37	0.43
2:B:339:GLN:O	2:B:343:TRP:CD1	2.71	0.43
2:C:435:TYR:O	2:C:436:LYS:C	2.62	0.43
2:F:215:LEU:HD23	2:F:215:LEU:HA	1.84	0.43
2:F:278:PRO:HG2	2:F:279:GLU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:399:LEU:O	2:G:402:LEU:HB3	2.19	0.43
2:G:431:THR:HG21	2:G:463:ARG:HB3	2.00	0.43
1:H:33:SER:HA	1:H:59:PRO:HB3	2.01	0.43
1:H:164:PRO:HD2	1:H:176:PRO:HB2	2.01	0.43
1:H:292:SER:OG	1:H:294:ASP:HB2	2.19	0.43
1:A:69:MET:HE1	1:A:114:HIS:CD2	2.54	0.43
2:B:317:HIS:O	2:B:320:VAL:HB	2.19	0.43
2:B:487:HIS:HB3	2:B:518:LEU:HD21	2.01	0.43
1:D:183:ALA:O	1:D:184:SER:CB	2.67	0.43
1:E:164:PRO:HD2	1:E:176:PRO:HB2	2.01	0.43
2:F:494:SER:O	2:F:497:LEU:HB2	2.18	0.43
2:B:399:LEU:O	2:B:402:LEU:HB3	2.19	0.42
2:B:493:VAL:O	2:B:493:VAL:HG12	2.19	0.42
2:C:210:ILE:H	2:C:210:ILE:HD12	1.83	0.42
2:C:399:LEU:O	2:C:400:GLU:C	2.62	0.42
1:E:38:LYS:HB2	1:E:40:PHE:CE1	2.53	0.42
1:E:224:ILE:C	1:E:226:LEU:N	2.72	0.42
2:F:400:GLU:HG3	2:F:425:TYR:CZ	2.54	0.42
2:F:487:HIS:O	2:F:488:GLY:C	2.61	0.42
2:G:244:VAL:CG1	2:G:263:GLU:OE2	2.66	0.42
1:H:49:LEU:HD11	1:H:51:ALA:O	2.19	0.42
1:H:66:ALA:HB3	1:H:73:ILE:HB	2.01	0.42
1:H:204:GLU:HG3	1:H:204:GLU:O	2.18	0.42
1:A:21:MET:HA	1:A:28:LEU:HD12	2.01	0.42
1:A:47:GLN:OE1	2:B:166:GLY:CA	2.67	0.42
2:B:399:LEU:O	2:B:400:GLU:C	2.62	0.42
2:C:384:LEU:O	2:C:385:LEU:C	2.62	0.42
2:C:393:GLN:HA	2:C:393:GLN:OE1	2.19	0.42
1:D:89:GLU:O	1:D:90:ASN:CB	2.66	0.42
1:E:274:ALA:O	1:E:275:ASN:CB	2.62	0.42
2:F:199:ILE:CG2	2:F:200:GLU:N	2.83	0.42
2:F:202:ARG:HG2	2:F:209:GLN:HB2	2.02	0.42
2:F:280:ILE:O	2:F:281:GLU:C	2.62	0.42
2:F:316:GLY:O	2:F:317:HIS:C	2.60	0.42
2:F:384:LEU:O	2:F:387:LEU:N	2.51	0.42
2:G:218:LYS:CG	2:G:238:SER:OG	2.59	0.42
2:G:409:LYS:H	2:G:409:LYS:HG2	1.56	0.42
2:G:506:THR:HG22	2:G:507:ILE:N	2.35	0.42
1:H:38:LYS:HB2	1:H:40:PHE:CE1	2.53	0.42
1:A:274:ALA:HB1	1:A:290:LYS:HE3	2.01	0.42
2:B:431:THR:HG21	2:B:463:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:THR:HG21	2:C:147:SER:OG	2.19	0.42
2:C:208:PRO:HD3	2:C:531:LYS:O	2.19	0.42
2:C:218:LYS:CG	2:C:238:SER:OG	2.59	0.42
2:C:278:PRO:HG2	2:C:279:GLU:H	1.83	0.42
1:D:240:VAL:HB	1:D:258:LEU:HB3	2.00	0.42
1:E:257:LEU:HD12	1:E:258:LEU:N	2.34	0.42
2:G:210:ILE:HD12	2:G:210:ILE:H	1.83	0.42
2:G:384:LEU:O	2:G:387:LEU:N	2.52	0.42
1:A:274:ALA:O	1:A:275:ASN:CB	2.62	0.42
2:B:506:THR:HG22	2:B:507:ILE:N	2.34	0.42
2:C:199:ILE:CG2	2:C:200:GLU:N	2.82	0.42
2:C:271:TRP:CE3	2:C:272:ILE:HG12	2.54	0.42
2:C:321:LEU:O	2:C:324:TYR:N	2.53	0.42
2:F:162:LYS:O	2:F:162:LYS:CG	2.67	0.42
2:F:207:TYR:HA	2:F:208:PRO:HD2	1.81	0.42
2:F:271:TRP:CE3	2:F:272:ILE:HG12	2.55	0.42
2:G:448:GLN:HB2	2:G:477:PHE:CE1	2.55	0.42
2:G:455:GLN:CG	2:G:496:PHE:CD2	3.03	0.42
1:A:77:CYS:HA	1:A:83:VAL:HG22	2.01	0.42
1:A:182:PHE:CD1	1:A:182:PHE:C	2.97	0.42
1:A:288:LEU:CB	1:A:300:ILE:HG13	2.50	0.42
2:B:414:TYR:CD1	2:F:143:ARG:HD3	2.54	0.42
2:B:460:ASN:C	2:B:462:THR:H	2.28	0.42
1:D:164:PRO:HD2	1:D:176:PRO:HB2	2.01	0.42
1:D:257:LEU:HD12	1:D:258:LEU:N	2.35	0.42
1:D:301:SER:O	1:D:302:ASP:C	2.62	0.42
2:F:143:ARG:HG3	2:F:143:ARG:HH11	1.84	0.42
2:F:399:LEU:O	2:F:402:LEU:HB3	2.19	0.42
2:G:236:LEU:HD23	2:G:421:ILE:HG21	2.01	0.42
2:G:359:LYS:NZ	2:G:370:PHE:H	2.16	0.42
1:H:77:CYS:HA	1:H:83:VAL:HG22	2.00	0.42
1:A:102:HIS:NE2	1:A:130:SER:HB3	2.29	0.42
1:A:257:LEU:HD12	1:A:258:LEU:N	2.35	0.42
1:A:289:TRP:HA	1:A:298:VAL:O	2.19	0.42
1:A:291:GLU:N	1:A:297:TRP:CZ3	2.87	0.42
2:B:320:VAL:HG22	2:C:263:GLU:HA	2.01	0.42
2:B:525:HIS:N	2:B:525:HIS:ND1	2.67	0.42
2:C:343:TRP:CZ3	2:C:349:SER:CB	3.03	0.42
2:C:455:GLN:HE21	2:C:496:PHE:HD2	1.66	0.42
1:D:33:SER:HA	1:D:59:PRO:HB3	2.01	0.42
1:D:241:PHE:HD2	1:D:257:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:185:PHE:CD1	2:F:185:PHE:N	2.86	0.42
2:G:185:PHE:CD1	2:G:185:PHE:N	2.87	0.42
2:G:321:LEU:O	2:G:324:TYR:N	2.52	0.42
2:G:487:HIS:CD2	2:G:517:LEU:HD23	2.52	0.42
1:H:182:PHE:CD1	1:H:182:PHE:C	2.97	0.42
1:A:195:LYS:O	1:A:202:TRP:HA	2.20	0.42
1:A:289:TRP:CE3	1:A:298:VAL:C	2.97	0.42
2:B:162:LYS:O	2:B:162:LYS:CG	2.67	0.42
2:B:263:GLU:HA	2:C:320:VAL:HG22	2.01	0.42
2:B:384:LEU:O	2:B:387:LEU:N	2.51	0.42
1:D:40:PHE:N	1:D:40:PHE:CD1	2.88	0.42
1:D:69:MET:HE1	1:D:114:HIS:HB2	1.98	0.42
1:D:293:VAL:O	1:D:293:VAL:HG12	2.19	0.42
1:E:204:GLU:HG3	1:E:204:GLU:O	2.18	0.42
1:E:293:VAL:O	1:E:293:VAL:HG12	2.20	0.42
2:F:148:TYR:CD1	2:F:148:TYR:C	2.98	0.42
2:F:385:LEU:N	2:F:406:HIS:CE1	2.87	0.42
2:G:145:THR:HG21	2:G:147:SER:OG	2.19	0.42
2:G:154:SER:OG	2:G:158:MET:HB2	2.20	0.42
2:G:246:TYR:CE1	2:G:259:LEU:HD13	2.55	0.42
2:G:460:ASN:C	2:G:462:THR:H	2.28	0.42
2:G:481:LEU:HD13	2:G:489:HIS:CB	2.17	0.42
1:A:66:ALA:HB3	1:A:73:ILE:HB	2.01	0.42
1:A:164:PRO:HD2	1:A:176:PRO:HB2	2.01	0.42
1:A:214:TRP:O	1:A:235:SER:CB	2.56	0.42
1:A:258:LEU:HD13	1:A:297:TRP:CG	2.53	0.42
2:B:199:ILE:CG2	2:B:200:GLU:N	2.82	0.42
1:E:271:SER:HB2	2:F:153:PHE:CE2	2.55	0.42
2:F:148:TYR:CE1	2:F:149:THR:O	2.73	0.42
2:F:506:THR:HG22	2:F:507:ILE:N	2.34	0.42
1:A:69:MET:HE1	1:A:114:HIS:HB2	1.98	0.42
2:B:271:TRP:CE3	2:B:272:ILE:HG12	2.54	0.42
2:B:298:LEU:HD23	2:B:298:LEU:HA	1.85	0.42
2:B:321:LEU:O	2:B:324:TYR:N	2.53	0.42
1:D:49:LEU:HD11	1:D:51:ALA:O	2.20	0.42
1:D:145:ILE:HD11	1:D:202:TRP:HB3	2.01	0.42
1:E:40:PHE:CE2	2:F:168:SER:HB2	2.52	0.42
1:E:72:ASN:HD22	1:E:72:ASN:HA	1.71	0.42
2:F:220:ALA:HB3	2:F:234:TRP:CE3	2.54	0.42
2:G:215:LEU:HD13	2:G:452:TYR:HE1	1.85	0.42
2:G:271:TRP:CE3	2:G:272:ILE:HG12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:206:GLN:OE1	1:H:251:ASN:O	2.38	0.42
1:H:301:SER:O	1:H:302:ASP:C	2.62	0.42
2:B:143:ARG:HH11	2:B:143:ARG:HG3	1.84	0.42
2:B:302:ASP:HA	2:C:304:VAL:HG21	2.01	0.42
2:B:318:LEU:C	2:B:320:VAL:N	2.77	0.42
2:B:462:THR:O	2:B:463:ARG:HD2	2.19	0.42
1:D:192:LYS:HD3	1:D:204:GLU:OE1	2.19	0.42
1:D:245:CYS:SG	1:D:246:ASP:N	2.92	0.42
1:D:283:ASP:C	1:D:285:LYS:N	2.78	0.42
2:F:263:GLU:HB2	2:G:320:VAL:HG21	2.02	0.42
2:F:522:THR:HG21	2:F:526:ILE:CD1	2.50	0.42
2:G:318:LEU:C	2:G:320:VAL:N	2.77	0.42
2:G:343:TRP:HZ3	2:G:350:ILE:CG2	2.30	0.42
2:G:375:LEU:HB3	2:G:379:PHE:CD1	2.54	0.42
2:G:435:TYR:CE2	2:G:454:ILE:HD11	2.55	0.42
1:H:258:LEU:HD13	1:H:297:TRP:CB	2.50	0.42
1:A:49:LEU:HD11	1:A:51:ALA:O	2.19	0.41
1:A:247:ASP:OD1	1:A:248:ALA:N	2.53	0.41
2:B:148:TYR:CE1	2:B:149:THR:O	2.73	0.41
2:B:329:ASP:HB3	2:B:332:ILE:HD13	2.02	0.41
2:B:432:GLU:OE1	2:B:466:SER:N	2.49	0.41
2:C:236:LEU:HD23	2:C:421:ILE:HG21	2.02	0.41
2:C:280:ILE:O	2:C:281:GLU:C	2.62	0.41
1:D:77:CYS:HA	1:D:83:VAL:HG22	2.01	0.41
1:D:189:ASN:OD1	1:D:213:ASP:C	2.64	0.41
1:E:49:LEU:HD11	1:E:51:ALA:O	2.19	0.41
1:E:214:TRP:O	1:E:235:SER:CB	2.56	0.41
1:E:230:THR:O	1:E:231:ILE:HG13	2.20	0.41
2:G:329:ASP:HB3	2:G:332:ILE:HD13	2.02	0.41
2:G:399:LEU:O	2:G:400:GLU:C	2.62	0.41
2:G:494:SER:OG	2:G:506:THR:HG21	2.20	0.41
1:H:257:LEU:HD12	1:H:258:LEU:N	2.35	0.41
1:H:258:LEU:HD13	1:H:297:TRP:CG	2.55	0.41
1:H:287:THR:O	1:H:288:LEU:HD23	2.19	0.41
1:A:194:TRP:CD1	1:A:194:TRP:N	2.88	0.41
1:A:230:THR:O	1:A:231:ILE:HG13	2.20	0.41
1:A:293:VAL:O	1:A:293:VAL:HG12	2.20	0.41
1:D:197:GLU:O	1:D:198:GLU:CB	2.68	0.41
1:D:234:CYS:HB3	1:D:268:VAL:HG21	2.02	0.41
1:E:47:GLN:OE1	2:F:166:GLY:CA	2.68	0.41
2:F:321:LEU:O	2:F:324:TYR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:451:TRP:CE2	2:F:493:VAL:HG13	2.55	0.41
2:F:522:THR:C	2:F:523:ASN:CG	2.86	0.41
2:F:525:HIS:ND1	2:F:525:HIS:N	2.67	0.41
2:G:199:ILE:CG2	2:G:200:GLU:N	2.83	0.41
2:G:546:ARG:HH11	2:G:546:ARG:HG3	1.86	0.41
1:A:77:CYS:SG	1:A:106:VAL:O	2.67	0.41
1:A:183:ALA:O	1:A:184:SER:CB	2.67	0.41
1:A:241:PHE:CD2	1:A:257:LEU:HA	2.54	0.41
2:B:202:ARG:HG2	2:B:209:GLN:HB2	2.02	0.41
2:B:381:TRP:HA	2:B:384:LEU:HD12	2.01	0.41
2:B:451:TRP:HZ2	2:B:496:PHE:CD1	2.38	0.41
2:C:148:TYR:HB2	1:D:266:TRP:CD2	2.55	0.41
2:C:246:TYR:CD2	2:C:248:TYR:O	2.73	0.41
2:C:460:ASN:C	2:C:462:THR:H	2.28	0.41
2:C:530:LEU:O	2:C:531:LYS:C	2.62	0.41
2:F:432:GLU:OE1	2:F:466:SER:HB3	2.20	0.41
2:G:435:TYR:O	2:G:436:LYS:C	2.61	0.41
1:H:258:LEU:HD13	1:H:297:TRP:HB2	2.02	0.41
1:H:264:VAL:CG1	1:H:265:VAL:N	2.82	0.41
2:B:220:ALA:HB3	2:B:234:TRP:CE3	2.54	0.41
2:C:381:TRP:H	2:C:381:TRP:CD1	2.37	0.41
2:C:480:GLN:OE1	2:C:480:GLN:CA	2.66	0.41
2:C:495:CYS:C	2:C:497:LEU:N	2.77	0.41
1:D:194:TRP:CD1	1:D:194:TRP:N	2.88	0.41
1:E:77:CYS:HA	1:E:83:VAL:HG22	2.01	0.41
2:F:307:SER:O	2:F:308:LYS:C	2.63	0.41
2:G:143:ARG:HB2	1:H:216:ARG:NH2	2.35	0.41
2:G:269:THR:O	2:G:273:VAL:HG23	2.20	0.41
2:G:280:ILE:O	2:G:281:GLU:C	2.63	0.41
2:G:340:LEU:HD21	2:G:358:TYR:HB3	2.02	0.41
2:G:375:LEU:HB3	2:G:379:PHE:HD1	1.85	0.41
1:A:266:TRP:CZ3	2:B:144:PHE:CD2	3.08	0.41
2:B:166:GLY:O	2:B:167:LYS:C	2.62	0.41
2:C:289:ASN:O	2:C:291:ILE:N	2.53	0.41
2:C:546:ARG:HG3	2:C:546:ARG:HH11	1.86	0.41
1:E:283:ASP:C	1:E:285:LYS:N	2.79	0.41
2:F:522:THR:HG21	2:F:526:ILE:HD12	2.03	0.41
2:F:546:ARG:HH11	2:F:546:ARG:HG3	1.85	0.41
2:G:291:ILE:CD1	2:G:351:ASP:OD2	2.65	0.41
2:G:343:TRP:HZ3	2:G:350:ILE:CB	2.34	0.41
1:A:271:SER:HB2	2:B:153:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:PHE:HE2	2:B:449:PHE:CE1	2.38	0.41
2:B:247:PRO:HG2	2:B:248:TYR:H	1.85	0.41
2:B:366:PHE:O	2:B:373:LYS:HG3	2.21	0.41
2:B:445:LEU:HD23	2:B:445:LEU:HA	1.89	0.41
2:C:481:LEU:HA	2:C:484:ALA:HB3	2.02	0.41
1:D:182:PHE:CD1	1:D:182:PHE:C	2.97	0.41
2:F:329:ASP:HB3	2:F:332:ILE:HD13	2.03	0.41
2:G:512:MET:HA	2:G:540:ALA:CB	2.50	0.41
1:H:196:GLU:HB3	1:H:202:TRP:CE2	2.55	0.41
1:A:18:ASP:OD2	1:A:62:GLN:HG2	2.21	0.41
2:B:269:THR:O	2:B:273:VAL:HG23	2.21	0.41
2:B:307:SER:O	2:B:308:LYS:C	2.64	0.41
2:C:154:SER:OG	2:C:158:MET:HB2	2.20	0.41
2:C:244:VAL:HG12	2:C:260:LEU:HD22	2.03	0.41
2:C:318:LEU:C	2:C:320:VAL:N	2.77	0.41
2:C:474:THR:HG23	2:C:493:VAL:CG1	2.51	0.41
2:C:551:TYR:HD2	2:C:552:LEU:HD23	1.85	0.41
1:D:183:ALA:H	1:D:220:TRP:CD1	2.38	0.41
1:E:21:MET:HA	1:E:28:LEU:HD12	2.01	0.41
2:F:399:LEU:O	2:F:400:GLU:C	2.62	0.41
2:G:307:SER:O	2:G:308:LYS:C	2.64	0.41
2:G:366:PHE:O	2:G:373:LYS:HG3	2.21	0.41
2:G:493:VAL:O	2:G:494:SER:C	2.63	0.41
1:H:195:LYS:HD2	1:H:195:LYS:C	2.45	0.41
2:B:139:MET:O	2:B:144:PHE:HB2	2.21	0.41
2:B:145:THR:CG2	2:B:146:ALA:N	2.84	0.41
2:B:384:LEU:O	2:B:385:LEU:C	2.62	0.41
2:B:399:LEU:HD23	2:B:425:TYR:OH	2.20	0.41
2:C:208:PRO:CB	2:C:530:LEU:O	2.69	0.41
2:C:343:TRP:CE3	2:C:349:SER:HB3	2.56	0.41
2:C:372:LEU:C	2:C:374:GLU:N	2.78	0.41
1:D:21:MET:HA	1:D:28:LEU:HD12	2.01	0.41
2:F:252:ASN:O	2:F:255:VAL:N	2.49	0.41
2:F:291:ILE:HG22	2:F:353:ASN:CB	2.50	0.41
2:F:316:GLY:O	2:F:319:SER:N	2.54	0.41
2:F:372:LEU:C	2:F:374:GLU:N	2.78	0.41
2:G:213:SER:HB3	2:G:459:PHE:CD2	2.56	0.41
2:G:521:SER:C	2:G:523:ASN:H	2.28	0.41
1:H:240:VAL:HB	1:H:258:LEU:HB3	2.03	0.41
1:A:226:LEU:HD12	1:A:228:THR:H	1.86	0.41
1:A:241:PHE:HE2	1:A:257:LEU:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:GLY:O	2:B:319:SER:N	2.54	0.41
2:B:370:PHE:HD2	2:B:370:PHE:HA	1.75	0.41
2:B:371:SER:HG	2:B:373:LYS:H	1.66	0.41
2:B:380:SER:O	2:B:383:CYS:N	2.50	0.41
2:B:442:THR:CG2	2:B:444:ALA:CB	2.99	0.41
2:B:532:ILE:HG23	2:B:533:PRO:CD	2.51	0.41
2:C:152:LYS:NZ	1:D:18:ASP:OD2	2.50	0.41
2:C:153:PHE:HA	2:C:158:MET:O	2.21	0.41
2:C:269:THR:O	2:C:273:VAL:HG23	2.20	0.41
2:C:316:GLY:O	2:C:319:SER:N	2.54	0.41
2:C:366:PHE:O	2:C:373:LYS:HG3	2.21	0.41
1:D:18:ASP:OD2	1:D:62:GLN:HG2	2.21	0.41
1:E:15:MET:HG3	2:F:162:LYS:HZ2	1.83	0.41
1:E:18:ASP:OD2	1:E:62:GLN:HG2	2.21	0.41
1:E:40:PHE:CD1	1:E:40:PHE:N	2.89	0.41
2:F:139:MET:O	2:F:144:PHE:HB2	2.20	0.41
2:F:155:THR:HG22	2:F:513:ARG:HD3	2.03	0.41
2:F:166:GLY:O	2:F:167:LYS:C	2.62	0.41
2:F:209:GLN:HG2	2:F:497:LEU:O	2.21	0.41
2:F:236:LEU:HD22	2:F:418:ILE:HG22	2.02	0.41
2:F:318:LEU:C	2:F:320:VAL:N	2.77	0.41
2:F:381:TRP:HA	2:F:384:LEU:HD12	2.02	0.41
2:F:435:TYR:O	2:F:436:LYS:C	2.62	0.41
2:G:153:PHE:CE2	1:H:271:SER:HB3	2.56	0.41
2:G:352:LYS:HE2	2:G:356:LYS:HE3	2.03	0.41
1:H:191:ILE:HD13	1:H:233:SER:HB3	2.03	0.41
1:A:283:ASP:C	1:A:285:LYS:N	2.78	0.41
2:C:244:VAL:CG1	2:C:260:LEU:HD22	2.51	0.41
1:D:132:LEU:CD2	1:D:142:VAL:HG13	2.51	0.41
1:E:53:LEU:HD23	1:E:53:LEU:H	1.80	0.41
2:F:445:LEU:CD2	2:F:449:PHE:CD2	2.98	0.41
2:G:372:LEU:C	2:G:374:GLU:N	2.78	0.41
2:G:381:TRP:CH2	2:G:382:LEU:HD13	2.56	0.41
1:H:18:ASP:OD2	1:H:62:GLN:HG2	2.20	0.41
1:H:293:VAL:O	1:H:293:VAL:HG12	2.21	0.41
2:B:191:ASP:OD1	2:B:529:ARG:NH1	2.54	0.40
2:C:202:ARG:HG2	2:C:209:GLN:HB2	2.02	0.40
2:C:343:TRP:HZ3	2:C:349:SER:CB	2.33	0.40
1:D:102:HIS:NE2	1:D:130:SER:HB3	2.29	0.40
1:E:303:VAL:HG12	1:E:304:ASN:N	2.37	0.40
2:F:432:GLU:OE1	2:F:466:SER:N	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:467:LYS:HA	2:G:498:ASN:ND2	2.36	0.40
1:A:132:LEU:CD2	1:A:142:VAL:HG13	2.51	0.40
2:B:177:THR:HG22	2:B:179:LEU:HD23	1.98	0.40
2:C:218:LYS:HG2	2:C:238:SER:HG	1.83	0.40
2:C:307:SER:O	2:C:308:LYS:C	2.64	0.40
2:C:329:ASP:HB3	2:C:332:ILE:HD13	2.03	0.40
2:C:530:LEU:HB2	2:C:532:ILE:HG12	2.03	0.40
1:D:226:LEU:HD12	1:D:228:THR:H	1.87	0.40
1:D:230:THR:O	1:D:231:ILE:HG13	2.20	0.40
1:D:240:VAL:O	1:D:258:LEU:CB	2.69	0.40
2:F:210:ILE:HD13	2:F:496:PHE:CG	2.56	0.40
2:F:366:PHE:O	2:F:373:LYS:HG3	2.21	0.40
2:G:153:PHE:HA	2:G:158:MET:O	2.21	0.40
1:H:21:MET:HA	1:H:28:LEU:HD12	2.02	0.40
1:H:194:TRP:CD1	1:H:194:TRP:N	2.88	0.40
1:H:223:SER:C	1:H:225:GLY:H	2.29	0.40
1:H:283:ASP:C	1:H:285:LYS:N	2.78	0.40
2:B:158:MET:HE2	2:B:158:MET:HB3	2.01	0.40
2:B:199:ILE:CG2	2:B:208:PRO:HB2	2.52	0.40
2:B:217:PHE:CZ	2:B:453:LEU:HD23	2.56	0.40
2:C:502:ALA:O	2:C:503:ALA:C	2.65	0.40
1:D:223:SER:C	1:D:225:GLY:N	2.80	0.40
2:F:460:ASN:C	2:F:462:THR:H	2.28	0.40
2:G:261:LYS:HG3	2:G:262:LYS:N	2.36	0.40
2:G:316:GLY:O	2:G:319:SER:N	2.54	0.40
2:G:451:TRP:CE2	2:G:493:VAL:HG13	2.56	0.40
1:H:230:THR:O	1:H:231:ILE:HG13	2.20	0.40
1:A:113:PRO:HB3	1:A:161:ALA:HB2	2.00	0.40
2:B:161:THR:O	2:B:171:SER:N	2.55	0.40
2:B:372:LEU:C	2:B:374:GLU:N	2.78	0.40
2:B:381:TRP:CD2	2:B:412:LEU:HD22	2.56	0.40
2:B:480:GLN:OE1	2:B:483:PHE:HD1	2.05	0.40
2:C:177:THR:CG2	2:C:179:LEU:H	2.16	0.40
2:C:198:THR:HB	2:C:212:GLU:HB2	2.03	0.40
2:C:241:PHE:CD2	2:C:457:LEU:HD21	2.57	0.40
2:C:261:LYS:HG3	2:C:262:LYS:N	2.36	0.40
2:C:442:THR:CG2	2:C:444:ALA:CB	2.99	0.40
1:D:113:PRO:HB2	1:D:161:ALA:HB2	2.03	0.40
1:E:194:TRP:CD1	1:E:194:TRP:N	2.89	0.40
1:E:221:ALA:HA	1:E:270:TRP:CD1	2.56	0.40
2:F:145:THR:CG2	2:F:146:ALA:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:198:THR:HB	2:F:212:GLU:HB2	2.03	0.40
2:F:261:LYS:HG3	2:F:262:LYS:N	2.36	0.40
2:F:276:ILE:HD13	2:F:383:CYS:CA	2.39	0.40
2:F:371:SER:HG	2:F:373:LYS:H	1.67	0.40
2:F:384:LEU:O	2:F:385:LEU:C	2.62	0.40
2:G:272:ILE:H	2:G:272:ILE:HG13	1.67	0.40
1:H:18:ASP:OD1	1:H:19:ALA:N	2.55	0.40
1:H:226:LEU:HD12	1:H:228:THR:H	1.87	0.40
1:A:283:ASP:O	1:A:284:ASN:HB2	2.22	0.40
2:B:177:THR:HG21	2:B:484:ALA:HB2	2.03	0.40
2:B:198:THR:HB	2:B:212:GLU:HB2	2.04	0.40
2:B:261:LYS:HG3	2:B:262:LYS:N	2.36	0.40
2:C:202:ARG:HA	2:C:202:ARG:HD3	1.55	0.40
2:F:174:ARG:NH2	2:F:485:GLN:OE1	2.46	0.40
2:G:175:LEU:CD2	2:G:483:PHE:HE2	2.34	0.40
2:G:202:ARG:HG2	2:G:209:GLN:HB2	2.02	0.40
1:H:102:HIS:NE2	1:H:130:SER:HB3	2.29	0.40
1:H:223:SER:C	1:H:225:GLY:N	2.80	0.40
1:H:283:ASP:O	1:H:284:ASN:HB2	2.22	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 X-ray entries followed by that with respect to entries of similar resolution.

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	281/316 (89%)	231 (82%)	42 (15%)	8 (3%)	4	21
1	D	279/316 (88%)	226 (81%)	43 (15%)	10 (4%)	2	16
1	E	281/316 (89%)	231 (82%)	43 (15%)	7 (2%)	4	23
1	H	279/316 (88%)	228 (82%)	43 (15%)	8 (3%)	3	20
2	B	421/442 (95%)	336 (80%)	68 (16%)	17 (4%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	416/442 (94%)	330 (79%)	73 (18%)	13 (3%)	3	19
2	F	421/442 (95%)	337 (80%)	65 (15%)	19 (4%)	2	12
2	G	416/442 (94%)	330 (79%)	73 (18%)	13 (3%)	3	19
All	All	2794/3032 (92%)	2249 (80%)	450 (16%)	95 (3%)	3	17

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	ASN
2	B	164	ILE
2	B	371	SER
2	B	428	ASN
2	B	520	ALA
2	B	523	ASN
2	C	371	SER
2	C	395	ASP
2	C	428	ASN
2	C	520	ALA
2	C	523	ASN
2	F	164	ILE
2	F	371	SER
2	F	428	ASN
2	F	520	ALA
2	F	523	ASN
2	G	371	SER
2	G	428	ASN
2	G	496	PHE
2	G	520	ALA
2	G	523	ASN
1	H	249	SER
1	A	114	HIS
2	B	178	GLU
2	B	247	PRO
2	B	346	GLY
2	B	499	ASP
2	B	526	ILE
2	C	526	ILE
1	D	114	HIS
1	D	250	SER
1	E	114	HIS
2	F	178	GLU

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Mol	Chain	Res	Type
2	F	346	GLY
2	F	394	ILE
2	F	499	ASP
2	F	526	ILE
2	G	500	ASP
2	G	526	ILE
1	H	114	HIS
1	A	184	SER
2	B	157	SER
2	B	447	VAL
2	C	393	GLN
2	C	447	VAL
1	D	184	SER
1	E	184	SER
2	F	157	SER
2	F	447	VAL
2	F	486	LEU
2	G	395	ASP
2	G	447	VAL
1	H	184	SER
1	A	55	GLY
2	B	182	LYS
2	B	431	THR
2	C	182	LYS
2	C	431	THR
1	D	55	GLY
1	D	198	GLU
1	E	55	GLY
2	F	182	LYS
2	F	431	THR
2	G	182	LYS
2	G	431	THR
1	H	55	GLY
1	A	68	PRO
2	C	250	THR
1	D	68	PRO
1	D	247	ASP
1	E	68	PRO
2	F	247	PRO
2	F	393	GLN
2	G	524	ASP
1	H	68	PRO

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Mol	Chain	Res	Type
2	B	226	LYS
2	C	226	LYS
2	C	290	GLU
2	F	226	LYS
2	G	346	GLY
2	B	172	ILE
2	F	172	ILE
1	A	129	ILE
1	A	176	PRO
2	B	347	GLY
1	D	129	ILE
1	D	176	PRO
1	E	129	ILE
1	E	176	PRO
1	H	129	ILE
1	H	176	PRO
1	D	224	ILE
1	A	224	ILE
1	E	224	ILE
1	H	224	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 X-ray entries followed by that with respect to entries of similar resolution.

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	240/267 (90%)	221 (92%)	19 (8%)	11	39
1	D	238/267 (89%)	220 (92%)	18 (8%)	12	41
1	E	240/267 (90%)	221 (92%)	19 (8%)	11	39
1	H	238/267 (89%)	221 (93%)	17 (7%)	13	43
2	B	386/403 (96%)	348 (90%)	38 (10%)	7	30
2	C	384/403 (95%)	351 (91%)	33 (9%)	10	36
2	F	386/403 (96%)	345 (89%)	41 (11%)	6	27
2	G	384/403 (95%)	347 (90%)	37 (10%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2496/2680 (93%)	2274 (91%)	222 (9%)	9 34

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ILE
1	A	53	LEU
1	A	70	TYR
1	A	83	VAL
1	A	86	TRP
1	A	113	PRO
1	A	184	SER
1	A	193	LEU
1	A	201	GLN
1	A	220	TRP
1	A	226	LEU
1	A	242	ILE
1	A	244	THR
1	A	271	SER
1	A	280	SER
1	A	283	ASP
1	A	287	THR
1	A	298	VAL
1	A	300	ILE
2	B	133	ASP
2	B	141	GLU
2	B	142	ARG
2	B	158	MET
2	B	159	LEU
2	B	160	LEU
2	B	163	ASP
2	B	164	ILE
2	B	167	LYS
2	B	179	LEU
2	B	202	ARG
2	B	209	GLN
2	B	223	TYR
2	B	228	SER
2	B	255	VAL
2	B	267	ARG
2	B	282	GLU
2	B	299	LEU

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Mol	Chain	Res	Type
2	B	321	LEU
2	B	339	GLN
2	B	365	PRO
2	B	370	PHE
2	B	378	GLU
2	B	395	ASP
2	B	401	SER
2	B	412	LEU
2	B	418	ILE
2	B	421	ILE
2	B	431	THR
2	B	453	LEU
2	B	455	GLN
2	B	466	SER
2	B	470	SER
2	B	489	HIS
2	B	505	ASP
2	B	515	ILE
2	B	532	ILE
2	B	550	ASN
2	C	132	ILE
2	C	133	ASP
2	C	138	ILE
2	C	139	MET
2	C	150	PHE
2	C	164	ILE
2	C	175	LEU
2	C	202	ARG
2	C	209	GLN
2	C	223	TYR
2	C	228	SER
2	C	255	VAL
2	C	267	ARG
2	C	282	GLU
2	C	299	LEU
2	C	321	LEU
2	C	339	GLN
2	C	365	PRO
2	C	370	PHE
2	C	378	GLU
2	C	401	SER
2	C	418	ILE

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Mol	Chain	Res	Type
2	C	421	ILE
2	C	431	THR
2	C	453	LEU
2	C	455	GLN
2	C	466	SER
2	C	470	SER
2	C	492	PHE
2	C	495	CYS
2	C	505	ASP
2	C	515	ILE
2	C	550	ASN
1	D	41	ASP
1	D	53	LEU
1	D	70	TYR
1	D	83	VAL
1	D	86	TRP
1	D	113	PRO
1	D	184	SER
1	D	193	LEU
1	D	220	TRP
1	D	226	LEU
1	D	246	ASP
1	D	271	SER
1	D	280	SER
1	D	283	ASP
1	D	287	THR
1	D	296	GLN
1	D	299	CYS
1	D	301	SER
1	E	41	ASP
1	E	53	LEU
1	E	70	TYR
1	E	83	VAL
1	E	86	TRP
1	E	113	PRO
1	E	184	SER
1	E	193	LEU
1	E	201	GLN
1	E	220	TRP
1	E	226	LEU
1	E	244	THR
1	E	252	THR

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Mol	Chain	Res	Type
1	E	271	SER
1	E	280	SER
1	E	283	ASP
1	E	287	THR
1	E	298	VAL
1	E	300	ILE
2	F	133	ASP
2	F	141	GLU
2	F	142	ARG
2	F	158	MET
2	F	159	LEU
2	F	160	LEU
2	F	163	ASP
2	F	164	ILE
2	F	167	LYS
2	F	179	LEU
2	F	202	ARG
2	F	209	GLN
2	F	223	TYR
2	F	228	SER
2	F	255	VAL
2	F	267	ARG
2	F	282	GLU
2	F	299	LEU
2	F	321	LEU
2	F	339	GLN
2	F	365	PRO
2	F	370	PHE
2	F	378	GLU
2	F	379	PHE
2	F	393	GLN
2	F	397	TYR
2	F	401	SER
2	F	412	LEU
2	F	418	ILE
2	F	421	ILE
2	F	431	THR
2	F	453	LEU
2	F	455	GLN
2	F	466	SER
2	F	470	SER
2	F	486	LEU

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Mol	Chain	Res	Type
2	F	489	HIS
2	F	497	LEU
2	F	505	ASP
2	F	515	ILE
2	F	550	ASN
2	G	132	ILE
2	G	133	ASP
2	G	138	ILE
2	G	139	MET
2	G	150	PHE
2	G	164	ILE
2	G	175	LEU
2	G	202	ARG
2	G	209	GLN
2	G	223	TYR
2	G	228	SER
2	G	244	VAL
2	G	255	VAL
2	G	267	ARG
2	G	282	GLU
2	G	299	LEU
2	G	321	LEU
2	G	339	GLN
2	G	365	PRO
2	G	370	PHE
2	G	378	GLU
2	G	380	SER
2	G	401	SER
2	G	412	LEU
2	G	414	TYR
2	G	418	ILE
2	G	421	ILE
2	G	431	THR
2	G	453	LEU
2	G	455	GLN
2	G	466	SER
2	G	470	SER
2	G	494	SER
2	G	495	CYS
2	G	505	ASP
2	G	515	ILE
2	G	550	ASN

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Mol	Chain	Res	Type
1	H	53	LEU
1	H	70	TYR
1	H	83	VAL
1	H	86	TRP
1	H	113	PRO
1	H	184	SER
1	H	193	LEU
1	H	195	LYS
1	H	220	TRP
1	H	226	LEU
1	H	246	ASP
1	H	271	SER
1	H	280	SER
1	H	283	ASP
1	H	287	THR
1	H	296	GLN
1	H	301	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	97	HIS
1	A	114	HIS
1	A	275	ASN
1	A	296	GLN
2	B	232	ASN
2	B	328	ASN
2	B	341	GLN
2	B	353	ASN
2	B	386	ASN
2	B	448	GLN
2	B	455	GLN
2	B	487	HIS
2	B	523	ASN
2	C	134	ASN
2	C	328	ASN
2	C	341	GLN
2	C	455	GLN
2	C	487	HIS
1	D	47	GLN
1	D	62	GLN

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Mol	Chain	Res	Type
1	D	72	ASN
1	D	97	HIS
1	D	114	HIS
1	E	17	HIS
1	E	97	HIS
1	E	107	ASN
1	E	114	HIS
1	E	154	ASN
1	E	275	ASN
2	F	232	ASN
2	F	328	ASN
2	F	341	GLN
2	F	386	ASN
2	F	393	GLN
2	F	455	GLN
2	F	523	ASN
2	G	134	ASN
2	G	328	ASN
2	G	341	GLN
2	G	353	ASN
2	G	386	ASN
2	G	455	GLN
2	G	498	ASN
1	H	47	GLN
1	H	97	HIS
1	H	114	HIS
1	H	206	GLN
1	H	296	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	285/316 (90%)	-0.50	0 100 100	79, 129, 189, 200	0
1	D	283/316 (89%)	-0.25	0 100 100	119, 185, 200, 200	0
1	E	285/316 (90%)	-0.49	0 100 100	70, 128, 189, 200	0
1	H	283/316 (89%)	-0.45	0 100 100	108, 174, 200, 200	0
2	B	423/442 (95%)	-0.63	0 100 100	70, 134, 189, 200	0
2	C	420/442 (95%)	-0.62	0 100 100	99, 150, 195, 200	0
2	F	423/442 (95%)	-0.67	0 100 100	70, 142, 193, 200	0
2	G	420/442 (95%)	-0.64	0 100 100	92, 151, 197, 200	0
All	All	2822/3032 (93%)	-0.55	0 100 100	70, 149, 200, 200	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.