



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:29 PM UTC

PDB ID : 1I50 / pdb_00001i50
Title : RNA POLYMERASE II CRYSTAL FORM II AT 2.8 A RESOLUTION
Authors : Cramer, P.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2001-02-23
Resolution : 2.80 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

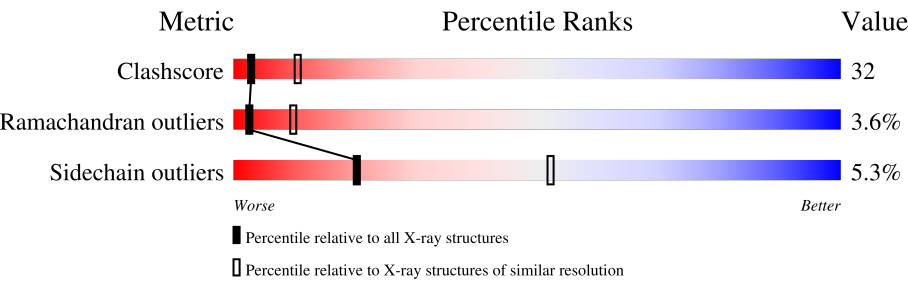
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1733	41%34%7%18%
2	B	1224	46%37%5%11%
3	C	318	41%37%6%16%
4	E	215	51%45%. .
5	F	155	23%28%. .46%
6	H	146	30%49%10%. 9%
7	I	122	51%43%6%. .
8	J	70	47%41%. . 7%

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Mol	Chain	Length	Quality of chain
9	K	120	52% 37% 7% 5%
10	L	70	16% 36% 11% • 34%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28366 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 DNA-DIRECTED RNA POLYMERASE II LARGEST SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1419	Total	C	N	O	S	0	0	0
			11154	7023	1952	2118	61			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1094	Total	C	N	O	S	0	0	0
			8711	5525	1519	1614	53			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE.

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	122	Total	C	N	O	S	0	0	0
			997	613	182	191	11			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Zn	0	0
			2	2		
11	B	1	Total	Zn	0	0
			1	1		
11	C	1	Total	Zn	0	0
			1	1		
11	I	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	J	1	Total 1	Zn 1	0	0
11	L	1	Total 1	Zn 1	0	0

- Molecule 12 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total 1	Mn 1	0	0

- Molecule 13 is water.

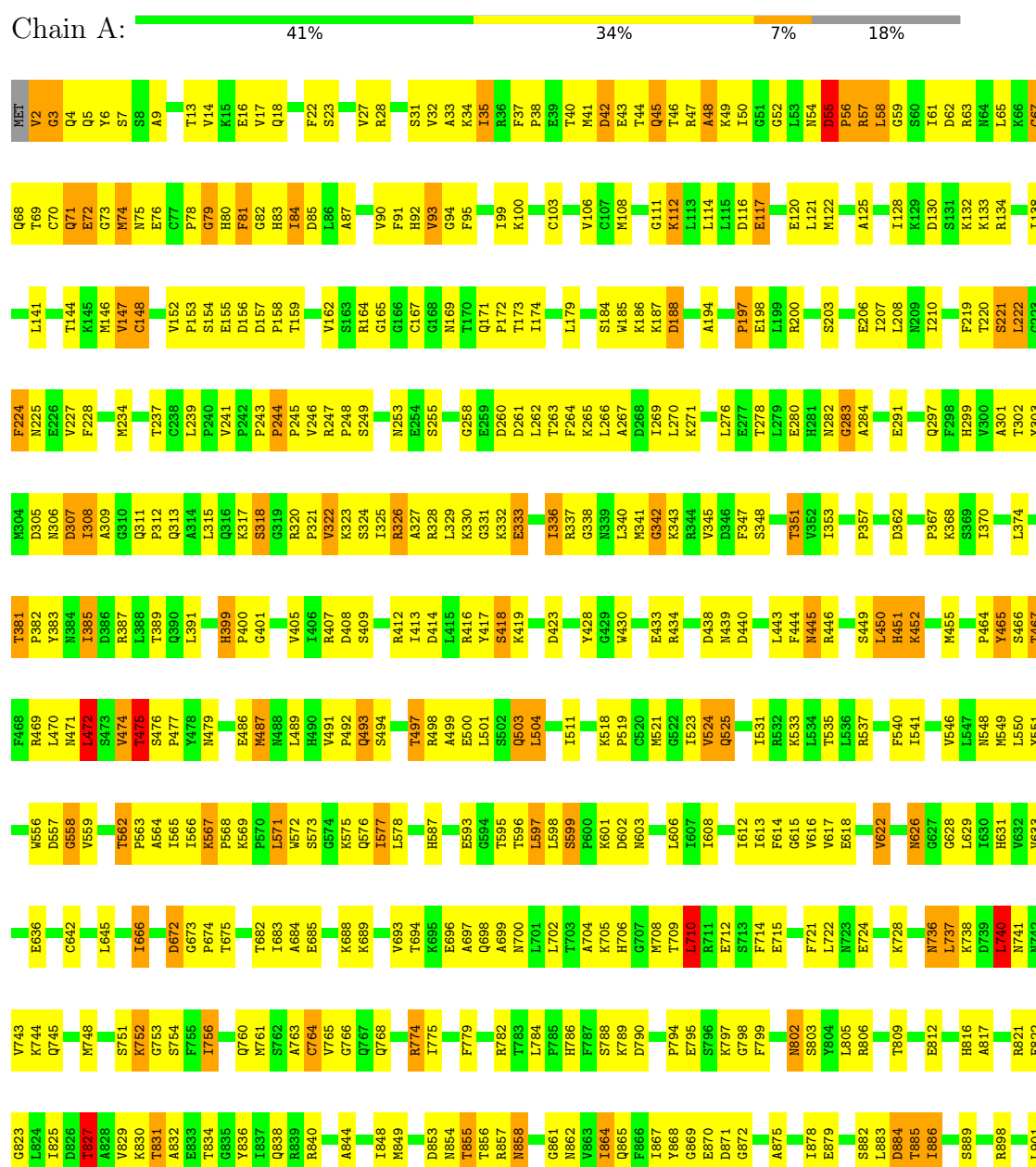
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	35	Total 35	O 35	0	0
13	B	23	Total 23	O 23	0	0
13	C	4	Total 4	O 4	0	0
13	E	7	Total 7	O 7	0	0
13	F	5	Total 5	O 5	0	0
13	I	2	Total 2	O 2	0	0
13	K	2	Total 2	O 2	0	0

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. 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. 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.

Note EDS was not executed.

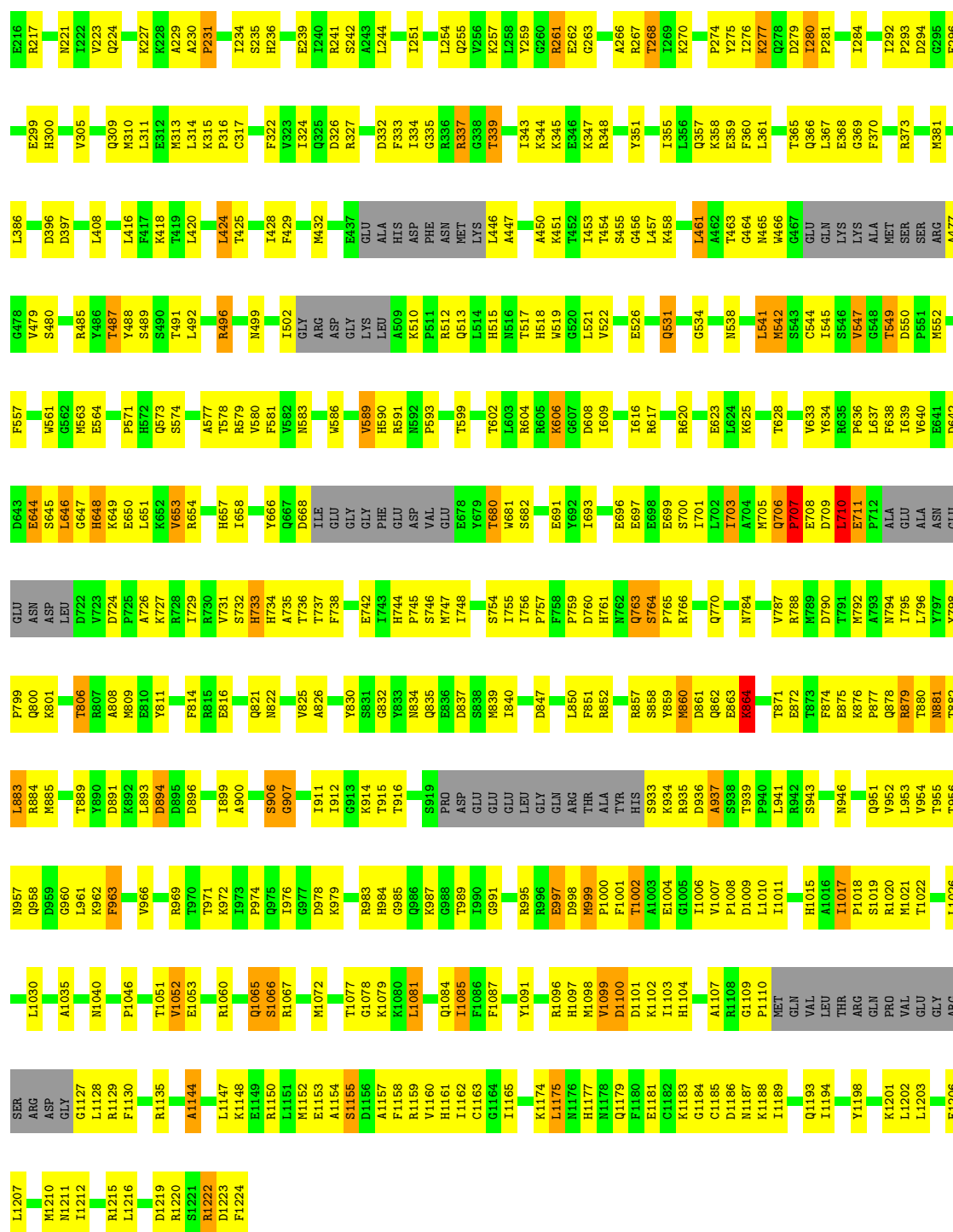
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT

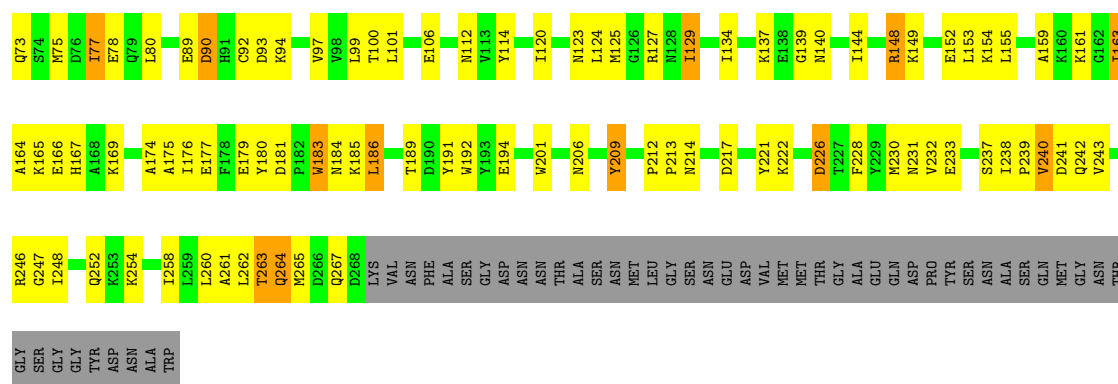




Response	Percentage
Yes, the U.S. is responsible	46%
No, the U.S. is not responsible	37%
Don't know	5%
Refuse to answer	11%



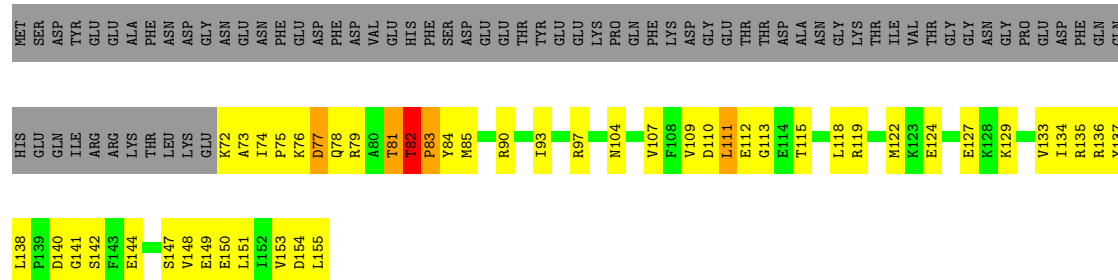




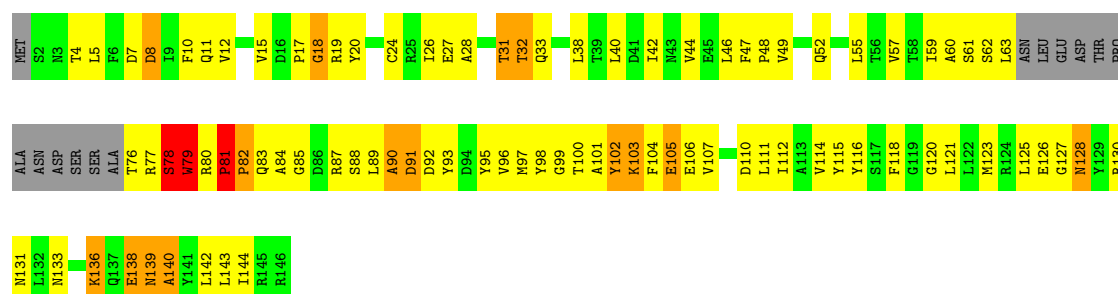
- Molecule 4: DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE



- Molecule 5: DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE

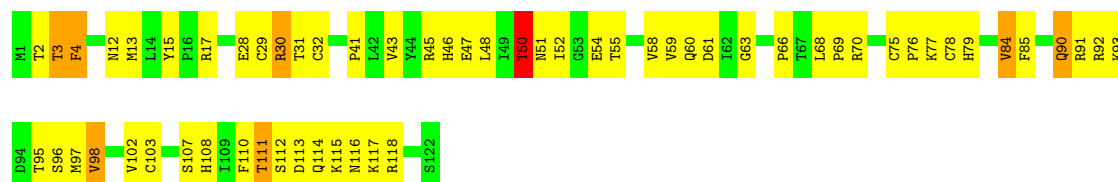


• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE



• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE

Chain I: 



• Molecule 8: DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE

Chain J: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.70Å 223.00Å 376.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28366	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.50	2/11352 (0.0%)	1.05	69/15352 (0.4%)
2	B	0.54	2/8882 (0.0%)	1.04	55/11976 (0.5%)
3	C	0.47	0/2133	1.01	13/2891 (0.4%)
4	E	0.44	0/1796	0.97	6/2416 (0.2%)
5	F	0.49	0/691	1.00	4/933 (0.4%)
6	H	1.15	1/1086 (0.1%)	1.56	12/1470 (0.8%)
7	I	0.43	0/1016	0.96	4/1365 (0.3%)
8	J	0.51	0/541	1.03	3/727 (0.4%)
9	K	0.44	0/937	0.85	0/1265
10	L	0.47	0/366	0.94	2/485 (0.4%)
All	All	0.54	5/28800 (0.0%)	1.05	168/38880 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
6	H	0	3
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	79	TRP	C-N	-35.47	0.72	1.33
2	B	707	PRO	C-N	-19.28	1.08	1.34
2	B	710	LEU	C-N	-8.77	1.17	1.33
1	A	3	GLY	C-N	-8.28	1.22	1.33
1	A	487	MET	SD-CE	-5.52	1.65	1.79

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	78	SER	O-C-N	-38.14	71.87	122.59
2	B	707	PRO	O-C-N	-16.41	101.05	122.22
6	H	78	SER	CA-C-N	15.98	152.06	121.54
6	H	78	SER	C-N-CA	15.98	152.06	121.54
6	H	102	TYR	N-CA-C	-11.80	99.24	112.57
1	A	333	GLU	N-CA-C	-10.79	100.66	114.04
1	A	399	HIS	CA-C-N	-10.60	106.59	119.84
1	A	399	HIS	C-N-CA	-10.60	106.59	119.84
2	B	707	PRO	CA-C-N	9.99	134.66	120.28
2	B	707	PRO	C-N-CA	9.99	134.66	120.28
1	A	1155	ASP	CA-C-N	9.92	130.06	119.05
1	A	1155	ASP	C-N-CA	9.92	130.06	119.05
1	A	1222	ASN	N-CA-C	-9.75	101.07	113.16
6	H	81	PRO	N-CA-C	9.13	121.83	110.70
1	A	827	THR	N-CA-C	-8.14	102.38	111.82
2	B	710	LEU	O-C-N	7.96	132.56	122.37
1	A	222	LEU	N-CA-C	-7.82	98.25	110.36
4	E	171	LYS	N-CA-C	-7.70	99.43	110.59
2	B	1085	ILE	N-CA-C	7.57	118.76	108.17
1	A	221	SER	N-CA-C	-7.57	103.31	112.54
1	A	999	VAL	N-CA-C	-7.57	105.77	111.90
6	H	31	THR	N-CA-C	-7.55	100.56	110.53
2	B	825	VAL	N-CA-C	7.53	118.71	108.17
3	C	10	ILE	N-CA-C	7.44	119.05	109.30
2	B	937	ALA	N-CA-C	-7.42	96.80	108.90
6	H	92	ASP	N-CA-C	-7.37	104.68	112.93
2	B	1184	GLY	N-CA-C	-7.31	106.14	115.42
1	A	779	PHE	N-CA-C	-7.30	100.01	110.59
3	C	39	ALA	N-CA-C	7.29	123.72	114.31
1	A	798	GLY	N-CA-C	7.29	126.49	115.63
1	A	475	THR	N-CA-C	7.20	118.91	111.14
1	A	280	GLU	N-CA-C	-7.19	104.38	113.43
1	A	564	ALA	N-CA-C	-7.17	104.50	113.18
2	B	736	THR	N-CA-C	-7.17	101.67	113.50
2	B	280	ILE	N-CA-C	7.15	115.68	107.89
1	A	524	VAL	N-CA-C	7.13	117.52	108.82
6	H	136	LYS	N-CA-C	-7.04	101.92	112.54
6	H	103	LYS	N-CA-C	6.98	120.97	110.64
3	C	40	GLU	N-CA-C	6.98	121.48	112.41
1	A	1270	ASN	N-CA-C	6.86	120.13	111.69
2	B	1144	ALA	N-CA-C	6.79	118.48	111.14
1	A	491	VAL	N-CA-C	6.77	114.25	107.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1009	ASP	N-CA-C	-6.77	104.99	113.18
2	B	1078	GLY	N-CA-C	-6.68	106.73	114.69
2	B	510	LYS	CA-C-N	6.64	127.17	119.47
2	B	510	LYS	C-N-CA	6.64	127.17	119.47
2	B	1223	ASP	N-CA-C	-6.60	105.98	112.97
7	I	84	VAL	N-CA-C	-6.55	98.19	108.86
2	B	851	PHE	N-CA-C	6.54	121.03	113.38
4	E	205	SER	N-CA-C	-6.53	100.55	109.95
1	A	224	PHE	N-CA-C	6.48	119.64	110.50
2	B	680	THR	N-CA-C	6.43	118.31	109.18
2	B	418	LYS	N-CA-C	-6.43	103.90	111.03
1	A	998	LEU	N-CA-C	6.40	119.67	109.24
2	B	837	ASP	N-CA-C	6.40	120.39	112.58
1	A	472	LEU	N-CA-C	6.36	118.21	111.28
2	B	172	ILE	N-CA-C	6.34	117.43	108.36
10	L	58	LYS	N-CA-C	6.24	124.09	110.80
1	A	3	GLY	CA-C-N	6.23	133.44	121.54
1	A	3	GLY	C-N-CA	6.23	133.44	121.54
3	C	55	THR	N-CA-C	-6.22	104.85	112.88
5	F	83	PRO	N-CA-C	-6.15	105.63	114.18
2	B	200	GLY	N-CA-C	6.12	125.12	115.08
2	B	1019	SER	N-CA-C	6.12	118.91	111.82
2	B	606	LYS	N-CA-C	-6.08	104.00	112.45
1	A	740	LEU	N-CA-C	-6.07	104.95	112.90
6	H	57	VAL	N-CA-C	6.07	116.59	107.80
1	A	158	PRO	N-CA-C	-6.05	106.17	113.98
1	A	244	PRO	N-CA-C	6.01	118.03	110.70
3	C	191	TYR	N-CA-C	5.99	118.89	109.96
8	J	9	SER	N-CA-C	5.99	118.70	111.40
2	B	864	LYS	N-CA-C	5.95	123.48	110.80
1	A	764	CYS	N-CA-C	5.93	118.66	110.35
5	F	77	ASP	N-CA-C	-5.91	101.25	110.42
1	A	336	ILE	N-CA-C	-5.90	105.96	113.22
1	A	155	GLU	N-CA-C	-5.89	106.14	113.15
2	B	763	GLN	N-CA-C	-5.88	101.58	110.28
2	B	277	LYS	N-CA-C	5.79	121.08	113.20
2	B	1066	SER	N-CA-C	5.78	123.11	110.80
1	A	452	LYS	N-CA-C	-5.76	105.14	111.82
2	B	1001	PHE	N-CA-C	5.76	118.44	109.52
1	A	493	GLN	N-CA-C	5.75	120.45	113.38
3	C	7	GLN	N-CA-C	5.75	118.25	108.02
1	A	81	PHE	N-CA-C	5.74	119.27	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	176	SER	N-CA-C	-5.72	103.15	110.53
2	B	99	LYS	N-CA-C	-5.72	101.72	110.07
3	C	183	TRP	N-CA-C	-5.72	99.21	108.41
1	A	802	ASN	N-CA-C	5.71	118.26	110.55
2	B	102	VAL	N-CA-C	5.67	117.77	108.97
2	B	703	ILE	N-CA-C	5.67	116.47	108.36
3	C	247	GLY	N-CA-C	-5.65	105.94	112.50
1	A	173	THR	N-CA-C	-5.65	99.98	108.96
7	I	90	GLN	N-CA-C	-5.64	103.08	110.53
2	B	711	GLU	O-C-N	5.62	126.89	121.28
1	A	474	VAL	N-CA-C	-5.60	107.02	112.29
2	B	1052	VAL	N-CA-C	-5.59	105.07	110.72
1	A	55	ASP	N-CA-C	5.58	122.15	109.81
1	A	234	MET	N-CA-C	-5.58	106.32	113.01
1	A	524	VAL	CB-CA-C	-5.56	103.55	111.34
1	A	884	ASP	N-CA-C	5.54	117.00	111.07
2	B	609	ILE	N-CA-C	-5.51	100.40	108.11
2	B	111	ALA	N-CA-C	-5.50	101.02	109.76
2	B	424	LEU	N-CA-C	-5.49	105.84	112.54
2	B	894	ASP	N-CA-C	-5.49	102.07	110.14
1	A	898	ARG	N-CA-C	5.48	118.13	109.96
2	B	1175	LEU	N-CA-C	5.47	118.00	111.71
1	A	1341	ILE	N-CA-C	5.46	116.23	110.72
1	A	864	ILE	N-CA-C	-5.45	106.49	111.67
1	A	1154	TYR	N-CA-C	-5.43	98.92	108.20
1	A	169	ASN	N-CA-C	5.42	117.94	110.35
1	A	1343	ALA	N-CA-C	-5.42	105.54	111.82
1	A	960	ILE	N-CA-C	5.41	116.04	110.36
2	B	733	HIS	N-CA-C	5.41	120.55	113.20
1	A	117	GLU	N-CA-C	-5.38	106.49	113.16
2	B	1081	LEU	N-CA-C	-5.38	101.51	110.17
2	B	292	ILE	N-CA-C	5.36	120.45	108.88
1	A	1311	VAL	N-CA-C	5.35	115.99	108.17
1	A	710	LEU	N-CA-C	-5.35	104.50	111.02
2	B	202	TYR	N-CA-C	5.34	116.77	109.18
4	E	32	GLN	N-CA-C	-5.33	105.41	112.34
2	B	764	SER	N-CA-C	5.31	120.16	113.25
1	A	1162	VAL	N-CA-C	-5.31	105.85	113.07
1	A	766	GLY	N-CA-C	5.29	119.32	111.76
5	F	82	THR	N-CA-C	5.28	116.35	109.64
2	B	748	ILE	N-CA-C	-5.28	105.17	112.50
1	A	578	LEU	N-CA-C	-5.27	105.53	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	700	SER	N-CA-C	5.27	119.34	113.02
3	C	262	LEU	N-CA-C	-5.26	105.54	111.28
7	I	50	THR	N-CA-C	5.26	118.25	110.46
1	A	1156	PRO	N-CA-C	5.25	120.82	113.53
7	I	111	THR	N-CA-C	5.22	117.12	109.24
1	A	326	ARG	N-CA-C	-5.21	105.60	111.28
2	B	943	SER	N-CA-C	5.19	117.61	111.33
3	C	148	ARG	N-CA-C	-5.19	102.84	110.52
2	B	327	ARG	N-CA-C	5.17	117.31	111.11
8	J	3	VAL	CA-C-N	-5.17	114.46	119.78
8	J	3	VAL	C-N-CA	-5.17	114.46	119.78
2	B	542	MET	N-CA-C	5.15	118.59	112.72
1	A	1171	GLN	N-CA-C	-5.15	105.31	111.03
1	A	1038	THR	N-CA-C	-5.15	102.84	110.46
2	B	896	ASP	N-CA-C	-5.14	106.78	113.16
1	A	405	VAL	N-CA-C	-5.14	100.91	108.11
2	B	832	GLY	N-CA-C	-5.13	108.58	114.69
1	A	3	GLY	O-C-N	-5.12	116.04	122.70
1	A	562	THR	CA-C-N	5.12	125.11	119.89
1	A	562	THR	C-N-CA	5.12	125.11	119.89
1	A	227	VAL	CB-CA-C	-5.11	106.39	111.30
3	C	226	ASP	N-CA-C	-5.11	101.92	109.18
10	L	68	GLU	N-CA-C	-5.11	102.72	110.28
6	H	10	PHE	N-CA-C	5.09	117.89	109.85
1	A	322	VAL	N-CA-C	5.08	116.31	108.44
1	A	1389	PHE	N-CA-C	-5.08	106.59	112.89
2	B	574	SER	CA-C-N	5.07	124.85	119.28
2	B	574	SER	C-N-CA	5.07	124.85	119.28
1	A	471	ASN	N-CA-C	-5.07	102.78	110.28
3	C	267	GLN	CB-CA-C	-5.06	109.25	116.34
1	A	1021	LEU	N-CA-C	-5.05	105.85	111.36
1	A	886	ILE	N-CA-C	5.05	119.51	112.50
6	H	79	TRP	O-C-N	-5.05	115.88	122.59
2	B	205	ILE	N-CA-C	5.04	115.10	107.80
5	F	153	VAL	N-CA-C	5.02	113.98	106.85
1	A	318	SER	N-CA-C	-5.01	106.33	112.90
1	A	1192	LEU	N-CA-C	5.01	116.58	108.41
4	E	72	PHE	CA-C-N	5.01	126.11	119.84
4	E	72	PHE	C-N-CA	5.01	126.11	119.84
3	C	21	ILE	CB-CA-C	-5.01	105.53	111.09
1	A	120	GLU	N-CA-C	5.01	116.82	111.36
4	E	20	LYS	N-CA-C	-5.00	105.73	111.14

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	707	PRO	Mainchain
2	B	710	LEU	Mainchain
6	H	78	SER	Peptide,Mainchain
6	H	79	TRP	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11154	0	11223	804	0
2	B	8711	0	8735	557	0
3	C	2095	0	2051	144	0
4	E	1760	0	1788	95	0
5	F	679	0	701	54	0
6	H	1068	0	1038	125	0
7	I	997	0	956	72	0
8	J	532	0	542	50	0
9	K	919	0	929	64	0
10	L	364	0	387	69	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	0	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	1	0	0	0	0
13	A	35	0	0	2	0
13	B	23	0	0	2	0
13	C	4	0	0	0	0
13	E	7	0	0	1	0
13	F	5	0	0	0	0
13	I	2	0	0	0	0
13	K	2	0	0	0	0
All	All	28366	0	28350	1833	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 32.

All (1833) 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)
6:H:79:TRP:C	6:H:80:ARG:CA	1.90	1.45
2:B:708:GLU:O	2:B:711:GLU:HG3	1.20	1.34
6:H:79:TRP:CA	6:H:80:ARG:N	1.94	1.29
6:H:79:TRP:O	6:H:80:ARG:N	1.67	1.26
3:C:56:THR:HG23	3:C:58:LEU:H	1.14	1.13
1:A:855:THR:HG21	1:A:857:ARG:HE	1.02	1.11
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.32	1.10
1:A:308:ILE:HG22	1:A:309:ALA:H	1.14	1.09
1:A:47:ARG:HH12	1:A:255:SER:HA	1.17	1.09
1:A:672:ASP:HB2	1:A:736:ASN:HD21	0.94	1.08
1:A:901:LEU:H	1:A:926:GLN:NE2	1.51	1.08
1:A:1161:THR:HG22	1:A:1163:ILE:H	0.98	1.08
1:A:1383:SER:HB3	1:A:1387:HIS:NE2	1.69	1.08
2:B:955:THR:HG22	2:B:956:THR:H	1.11	1.08
2:B:710:LEU:CD2	2:B:738:PHE:CD1	2.38	1.07
1:A:345:VAL:HG21	2:B:1129:ARG:HA	1.33	1.07
1:A:1394:THR:HG22	1:A:1395:GLY:H	1.14	1.06
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.35	1.06
7:I:111:THR:HG22	7:I:113:ASP:H	1.16	1.06
1:A:974:ASP:HB2	6:H:136:LYS:HZ3	1.15	1.06
2:B:800:GLN:HB3	8:J:52:THR:CG2	1.84	1.05
2:B:871:THR:HG22	2:B:872:GLU:H	1.21	1.05
1:A:470:LEU:HD11	1:A:487:MET:HE1	1.12	1.04
2:B:542:MET:HG3	2:B:747:MET:HE3	1.36	1.04
3:C:148:ARG:HH12	8:J:64:ASN:HA	1.16	1.04
6:H:79:TRP:O	6:H:80:ARG:CA	1.98	1.03
1:A:672:ASP:HB2	1:A:736:ASN:ND2	1.72	1.03
2:B:542:MET:HE2	2:B:747:MET:HG3	1.40	1.03
1:A:264:PHE:HB3	1:A:315:LEU:HD22	1.39	1.03
1:A:313:GLN:HG2	1:A:322:VAL:HB	1.36	1.03
2:B:29:ASP:HB3	2:B:658:ILE:CD1	1.88	1.02
3:C:148:ARG:NH1	8:J:64:ASN:HA	1.73	1.02
1:A:444:PHE:HE2	1:A:470:LEU:HD21	1.26	1.01
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.76	1.01
2:B:708:GLU:O	2:B:711:GLU:CG	2.08	1.01
6:H:130:ARG:HA	6:H:133:ASN:HD22	1.24	1.00
1:A:524:VAL:HG12	1:A:525:GLN:H	1.24	1.00
9:K:65:HIS:HD2	9:K:67:PHE:H	1.10	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:79:TRP:O	6:H:80:ARG:HA	1.62	0.99
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.45	0.99
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.45	0.99
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.40	0.98
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.45	0.98
1:A:3:GLY:O	1:A:5:GLN:N	1.98	0.97
1:A:597:LEU:H	1:A:597:LEU:HD12	1.28	0.96
1:A:1161:THR:HG22	1:A:1163:ILE:N	1.80	0.95
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.46	0.95
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.31	0.95
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.31	0.95
1:A:567:LYS:HB3	6:H:96:VAL:H	1.30	0.95
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.49	0.95
1:A:444:PHE:CE2	1:A:470:LEU:HD21	2.00	0.95
1:A:901:LEU:H	1:A:926:GLN:HE21	1.05	0.95
1:A:913:LEU:HD11	1:A:981:LEU:O	1.68	0.94
1:A:855:THR:HG21	1:A:857:ARG:NE	1.84	0.93
2:B:737:THR:HG21	7:I:66:PRO:O	1.67	0.93
2:B:710:LEU:HD21	2:B:738:PHE:CD1	2.04	0.92
2:B:710:LEU:CD2	2:B:738:PHE:HD1	1.78	0.92
1:A:49:LYS:HD3	1:A:55:ASP:HB2	1.49	0.92
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.49	0.92
1:A:524:VAL:HG12	1:A:525:GLN:N	1.81	0.91
2:B:244:LEU:HD11	2:B:366:GLN:HE21	1.34	0.91
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.52	0.91
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.52	0.90
2:B:806:THR:HG22	2:B:809:MET:H	1.34	0.90
1:A:1446:ASP:HB2	5:F:133:VAL:HG23	1.52	0.90
2:B:654:ARG:H	2:B:657:HIS:HD2	1.14	0.90
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.18	0.90
5:F:111:LEU:HD12	5:F:111:LEU:H	1.34	0.90
4:E:78:LEU:HD23	4:E:107:THR:HB	1.54	0.89
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.53	0.89
1:A:672:ASP:CB	1:A:736:ASN:HD21	1.84	0.89
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.51	0.89
1:A:903:ASN:ND2	1:A:905:ASP:H	1.70	0.89
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.56	0.88
9:K:47:ARG:HB3	9:K:47:ARG:HH11	1.38	0.88
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.03	0.88
1:A:704:ALA:HB2	1:A:710:LEU:HD12	1.53	0.88
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.52	0.88
5:F:81:THR:CG2	5:F:136:ARG:HH11	1.87	0.87
1:A:567:LYS:HB3	6:H:96:VAL:N	1.90	0.86
1:A:374:LEU:HD23	2:B:1107:ALA:HB2	1.57	0.86
1:A:855:THR:CG2	1:A:857:ARG:HE	1.87	0.86
2:B:889:THR:HG22	2:B:891:ASP:H	1.39	0.86
1:A:302:THR:HG21	1:A:312:PRO:CG	2.05	0.86
1:A:42:ASP:OD1	1:A:47:ARG:HG2	1.76	0.86
2:B:955:THR:HG22	2:B:956:THR:N	1.91	0.85
7:I:98:VAL:HG21	7:I:113:ASP:HB2	1.56	0.85
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	1.74	0.85
1:A:1094:VAL:HG12	1:A:1095:THR:H	1.41	0.85
6:H:105:GLU:O	6:H:107:VAL:HG23	1.75	0.85
2:B:705:MET:HE3	2:B:742:GLU:HG3	1.57	0.85
2:B:955:THR:HG23	10:L:54:ARG:O	1.77	0.85
10:L:38:LEU:HG	10:L:39:SER:H	1.41	0.85
6:H:103:LYS:HG2	6:H:115:TYR:H	1.41	0.84
1:A:381:THR:HG23	1:A:383:TYR:H	1.42	0.84
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.58	0.84
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.58	0.84
1:A:40:THR:HG22	1:A:41:MET:HG3	1.60	0.84
1:A:47:ARG:NH1	1:A:255:SER:HA	1.93	0.84
10:L:46:VAL:HG13	10:L:56:LEU:HD12	1.59	0.84
1:A:32:VAL:HB	1:A:57:ARG:HD2	1.60	0.83
2:B:25:ILE:HD12	2:B:653:VAL:HB	1.60	0.83
1:A:844:ALA:HB2	1:A:1384:VAL:HG13	1.59	0.83
6:H:15:VAL:HG22	6:H:26:ILE:HG12	1.59	0.83
2:B:731:VAL:HG12	2:B:732:SER:H	1.42	0.83
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	1.77	0.83
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.42	0.83
1:A:903:ASN:C	1:A:903:ASN:HD22	1.86	0.83
2:B:879:ARG:HE	2:B:885:MET:HE2	1.43	0.82
7:I:45:ARG:HG2	7:I:45:ARG:HH11	1.44	0.82
7:I:50:THR:H	7:I:92:ARG:HH12	1.26	0.82
2:B:365:THR:HG22	2:B:367:LEU:H	1.43	0.82
2:B:464:GLY:O	2:B:477:ALA:HB3	1.78	0.82
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.77	0.82
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.58	0.82
1:A:503:GLN:HE21	5:F:90:ARG:NH2	1.76	0.82
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.61	0.82
1:A:1336:MET:HE3	1:A:1381:LEU:HG	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:103:LYS:HG2	6:H:115:TYR:N	1.94	0.82
1:A:903:ASN:HD22	1:A:905:ASP:H	1.25	0.82
1:A:1383:SER:HB3	1:A:1387:HIS:CE1	2.14	0.82
1:A:982:THR:HG22	1:A:984:LYS:H	1.44	0.82
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.62	0.82
8:J:64:ASN:HB3	8:J:65:PRO:HD3	1.60	0.82
1:A:470:LEU:HD11	1:A:487:MET:CE	2.05	0.82
1:A:849:MET:HE3	1:A:1063:MET:SD	2.19	0.82
2:B:277:LYS:N	2:B:277:LYS:HD2	1.93	0.82
6:H:79:TRP:C	6:H:80:ARG:N	0.72	0.82
2:B:583:ASN:HD21	2:B:628:THR:HB	1.45	0.81
2:B:979:LYS:HE3	2:B:987:LYS:HD2	1.62	0.81
2:B:1051:THR:HG22	2:B:1053:GLU:N	1.94	0.81
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.63	0.81
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.10	0.81
1:A:597:LEU:HD12	1:A:597:LEU:N	1.96	0.81
1:A:399:HIS:O	1:A:401:GLY:N	2.14	0.81
2:B:130:VAL:HG12	2:B:131:ASP:H	1.45	0.81
1:A:33:ALA:O	1:A:83:HIS:HB3	1.82	0.80
2:B:1153:GLU:HG2	2:B:1154:ALA:H	1.47	0.80
1:A:567:LYS:NZ	6:H:46:LEU:HB2	1.97	0.80
1:A:1124:HIS:HB3	1:A:1130:GLN:OE1	1.81	0.80
1:A:500:GLU:OE2	1:A:1438:THR:HG21	1.81	0.79
3:C:265:MET:HE1	9:K:19:LEU:HB2	1.61	0.79
6:H:130:ARG:HA	6:H:133:ASN:ND2	1.96	0.79
1:A:313:GLN:HG2	1:A:322:VAL:CB	2.12	0.79
3:C:22:LEU:HD12	3:C:230:MET:HE3	1.65	0.79
1:A:55:ASP:H	1:A:56:PRO:HD2	1.47	0.79
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.65	0.79
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.65	0.79
1:A:63:ARG:HA	1:A:74:MET:HE2	1.65	0.78
6:H:103:LYS:HG3	6:H:115:TYR:O	1.82	0.78
3:C:7:GLN:HG2	9:K:104:ASN:ND2	1.98	0.78
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.63	0.78
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.64	0.78
6:H:100:THR:OG1	6:H:138:GLU:HG3	1.84	0.78
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.65	0.78
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.66	0.78
1:A:587:HIS:CE1	1:A:969:GLN:HG2	2.18	0.78
2:B:914:LYS:HB3	2:B:937:ALA:O	1.83	0.78
1:A:565:ILE:HG21	1:A:567:LYS:HE2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:531:GLN:CD	2:B:531:GLN:H	1.92	0.77
1:A:1398:MET:HG3	1:A:1426:GLU:HG2	1.66	0.77
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.18	0.77
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.66	0.77
1:A:179:LEU:HD21	1:A:308:ILE:HD13	1.66	0.77
2:B:705:MET:CE	2:B:742:GLU:HG3	2.15	0.77
1:A:524:VAL:CG1	1:A:525:GLN:H	1.95	0.77
1:A:317:LYS:HD3	1:A:321:PRO:HD2	1.65	0.77
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.66	0.77
2:B:199:MET:HE3	2:B:492:LEU:HD23	1.67	0.77
3:C:66:ARG:NH2	8:J:3:VAL:O	2.18	0.77
1:A:596:THR:HG22	1:A:597:LEU:H	1.50	0.77
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.67	0.77
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.67	0.77
1:A:1400:CYS:HB3	1:A:1405:THR:OG1	1.85	0.76
6:H:125:LEU:C	6:H:130:ARG:HH12	1.93	0.76
4:E:94:LYS:HG3	4:E:123:LEU:HD11	1.66	0.76
2:B:25:ILE:CD1	2:B:653:VAL:HB	2.16	0.76
2:B:98:THR:HG21	2:B:101:MET:HE2	1.67	0.76
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.85	0.76
1:A:1394:THR:HG22	1:A:1395:GLY:N	1.94	0.76
1:A:869:GLY:O	4:E:204:THR:HG21	1.83	0.76
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.01	0.76
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.16	0.76
5:F:76:LYS:O	5:F:79:ARG:HD2	1.86	0.76
9:K:29:ASN:HD21	9:K:79:GLU:HA	1.48	0.75
1:A:974:ASP:CB	6:H:136:LYS:HZ3	1.96	0.75
2:B:268:THR:HG21	2:B:270:LYS:HE3	1.69	0.75
1:A:353:ILE:HG21	1:A:487:MET:CE	2.16	0.75
1:A:849:MET:HE1	1:A:1436:ILE:HA	1.68	0.75
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.68	0.75
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.50	0.75
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.33	0.75
1:A:1376:THR:HG22	4:E:212:ARG:HH22	1.50	0.75
5:F:109:VAL:HG12	5:F:110:ASP:N	2.00	0.75
1:A:666:ILE:HD12	2:B:1030:LEU:HD22	1.68	0.75
3:C:124:LEU:O	3:C:127:ARG:HG2	1.86	0.75
1:A:1376:THR:CG2	4:E:212:ARG:HH22	2.00	0.75
3:C:214:ASN:HB2	3:C:217:ASP:OD2	1.87	0.75
2:B:955:THR:CG2	2:B:956:THR:H	1.95	0.75
5:F:81:THR:HG22	5:F:136:ARG:HH11	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:VAL:HG11	8:J:60:PHE:CB	2.17	0.74
1:A:768:GLN:HE21	1:A:816:HIS:HA	1.52	0.74
2:B:235:SER:HA	2:B:261:ARG:HH21	1.50	0.74
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.52	0.74
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.70	0.74
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.52	0.74
5:F:147:SER:OG	5:F:150:GLU:HG3	1.88	0.74
9:K:65:HIS:CD2	9:K:67:PHE:H	2.01	0.74
1:A:613:ILE:HD13	6:H:102:TYR:HB3	1.69	0.74
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.03	0.73
4:E:100:ILE:HD13	4:E:108:GLY:HA3	1.70	0.73
1:A:345:VAL:HA	2:B:1150:ARG:HH12	1.52	0.73
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.70	0.73
1:A:225:ASN:ND2	1:A:228:PHE:HD1	1.86	0.73
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.69	0.73
2:B:954:VAL:O	10:L:55:ILE:O	2.07	0.73
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.68	0.73
6:H:100:THR:HG23	6:H:138:GLU:HA	1.69	0.73
1:A:225:ASN:HD21	1:A:228:PHE:HD1	1.36	0.73
2:B:563:MET:CE	2:B:580:VAL:HB	2.19	0.73
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.68	0.73
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.52	0.73
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.23	0.73
2:B:205:ILE:HD13	2:B:461:LEU:HB3	1.71	0.73
1:A:308:ILE:HG22	1:A:309:ALA:N	1.96	0.73
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.19	0.72
3:C:261:ALA:O	3:C:265:MET:HB2	1.89	0.72
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.24	0.72
1:A:741:ASN:HD22	1:A:744:LYS:H	1.34	0.72
2:B:871:THR:HG22	2:B:872:GLU:N	2.02	0.72
3:C:242:GLN:HE21	3:C:246:ARG:HH21	1.36	0.72
1:A:907:THR:HG22	1:A:908:LEU:H	1.54	0.72
6:H:103:LYS:HD3	6:H:114:VAL:HB	1.70	0.72
2:B:680:THR:HG22	2:B:682:SER:H	1.53	0.72
1:A:114:LEU:HD22	1:A:171:GLN:NE2	2.04	0.72
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.54	0.72
9:K:113:THR:O	9:K:114:LEU:HB2	1.90	0.72
1:A:573:SER:HB3	1:A:576:GLN:HG3	1.72	0.72
2:B:205:ILE:CD1	2:B:461:LEU:HB3	2.20	0.72
1:A:760:GLN:HB2	2:B:1021:MET:HE1	1.71	0.72
1:A:32:VAL:HG11	1:A:68:GLN:HE22	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:LYS:HD2	2:B:1015:HIS:O	1.89	0.71
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.72	0.71
1:A:705:LYS:HB2	1:A:708:MET:HE3	1.71	0.71
10:L:51:CYS:HB3	10:L:53:HIS:CD2	2.25	0.71
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.37	0.71
1:A:72:GLU:HB3	1:A:76:GLU:HB2	1.71	0.71
5:F:119:ARG:HA	5:F:122:MET:HE3	1.72	0.71
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.20	0.71
2:B:345:LYS:HA	2:B:348:ARG:NH1	2.06	0.71
1:A:122:MET:HE1	1:A:138:ILE:HG23	1.73	0.71
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.20	0.71
9:K:47:ARG:HB3	9:K:47:ARG:NH1	2.05	0.71
1:A:5:GLN:OE1	2:B:1175:LEU:HD12	1.91	0.71
1:A:1336:MET:HE1	1:A:1381:LEU:N	2.05	0.71
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.20	0.71
3:C:22:LEU:HD12	3:C:230:MET:CE	2.20	0.71
2:B:710:LEU:HD23	2:B:738:PHE:CD1	2.24	0.70
1:A:55:ASP:O	1:A:57:ARG:N	2.24	0.70
2:B:800:GLN:CB	8:J:52:THR:HG22	2.18	0.70
2:B:550:ASP:OD2	2:B:552:MET:HE2	1.91	0.70
2:B:244:LEU:HD11	2:B:366:GLN:NE2	2.04	0.70
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.72	0.70
1:A:975:HIS:ND1	1:A:1036:ARG:HG3	2.05	0.70
2:B:69:LEU:HD21	2:B:425:THR:HG23	1.73	0.70
1:A:1146:VAL:HG12	1:A:1197:LEU:HD22	1.74	0.70
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.07	0.70
1:A:565:ILE:CG2	1:A:567:LYS:HE2	2.21	0.70
2:B:731:VAL:HG12	2:B:732:SER:N	2.06	0.70
8:J:48:ARG:NH2	8:J:49:MET:HE1	2.07	0.70
2:B:654:ARG:H	2:B:657:HIS:CD2	2.04	0.70
3:C:56:THR:CG2	3:C:58:LEU:H	2.00	0.70
2:B:563:MET:HE2	2:B:580:VAL:HB	1.73	0.69
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.74	0.69
9:K:18:LYS:HZ2	9:K:38:GLU:HG2	1.56	0.69
1:A:329:LEU:O	1:A:333:GLU:N	2.25	0.69
1:A:849:MET:HE2	1:A:1061:GLY:HA2	1.72	0.69
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.73	0.69
4:E:155:ARG:HD2	4:E:194:GLU:OE2	1.92	0.69
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.21	0.69
10:L:60:ARG:HG2	10:L:61:THR:H	1.58	0.69
1:A:80:HIS:O	1:A:243:PRO:HB3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.74	0.69
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.74	0.69
2:B:1153:GLU:HG2	2:B:1154:ALA:N	2.06	0.69
3:C:20:PHE:HE1	3:C:22:LEU:HG	1.55	0.69
10:L:55:ILE:O	10:L:56:LEU:HB2	1.91	0.69
1:A:901:LEU:N	1:A:926:GLN:NE2	2.35	0.69
2:B:956:THR:HA	2:B:961:LEU:O	1.93	0.69
10:L:61:THR:HG21	10:L:63:ARG:HD3	1.74	0.69
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.72	0.69
1:A:55:ASP:N	1:A:56:PRO:HD2	2.05	0.69
1:A:302:THR:HG21	1:A:312:PRO:HG2	1.75	0.69
1:A:345:VAL:HG11	2:B:1128:LEU:O	1.93	0.69
2:B:120:ARG:HD2	2:B:955:THR:HG21	1.75	0.69
7:I:4:PHE:HE1	7:I:13:MET:HE2	1.58	0.69
7:I:63:GLY:O	7:I:70:ARG:NH2	2.26	0.69
1:A:61:ILE:HG22	1:A:62:ASP:H	1.57	0.69
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.74	0.69
2:B:864:LYS:HD3	2:B:871:THR:HA	1.75	0.69
3:C:174:ALA:O	8:J:10:CYS:HB2	1.93	0.69
1:A:313:GLN:HE21	1:A:322:VAL:HG12	1.58	0.69
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.75	0.69
5:F:111:LEU:HD12	5:F:111:LEU:N	2.07	0.68
2:B:872:GLU:HG2	2:B:916:THR:OG1	1.94	0.68
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.74	0.68
2:B:130:VAL:HG12	2:B:131:ASP:N	2.08	0.68
6:H:104:PHE:O	6:H:106:GLU:N	2.25	0.68
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.19	0.68
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.74	0.68
1:A:1111:MET:HE3	1:A:1114:PRO:HG3	1.74	0.68
5:F:77:ASP:O	5:F:78:GLN:HB2	1.92	0.68
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.59	0.68
5:F:109:VAL:HG12	5:F:110:ASP:H	1.58	0.68
8:J:44:TYR:HA	8:J:47:ARG:HG3	1.74	0.68
2:B:680:THR:CG2	2:B:681:TRP:N	2.56	0.68
2:B:839:MET:CE	2:B:1010:LEU:HD11	2.24	0.68
1:A:911:SER:O	1:A:978:PRO:HB3	1.94	0.68
1:A:974:ASP:HB2	6:H:136:LYS:NZ	2.00	0.68
2:B:1162:ILE:HD11	2:B:1216:LEU:HD12	1.75	0.68
3:C:258:ILE:HD13	9:K:35:PHE:HE2	1.58	0.68
1:A:23:SER:O	1:A:27:VAL:HG23	1.94	0.67
1:A:1390:ASN:O	1:A:1391:ARG:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:GLY:C	3:C:24:ASN:HD22	2.00	0.67
7:I:98:VAL:HG21	7:I:113:ASP:CB	2.23	0.67
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.29	0.67
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.58	0.67
6:H:103:LYS:HZ1	6:H:114:VAL:HG23	1.60	0.67
1:A:1395:GLY:C	1:A:1397:LEU:H	2.02	0.67
2:B:120:ARG:CZ	10:L:54:ARG:HD2	2.25	0.67
1:A:470:LEU:CD1	1:A:487:MET:HE1	2.06	0.67
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.76	0.67
1:A:1128:GLN:O	1:A:1132:LYS:HG3	1.94	0.67
1:A:567:LYS:HZ2	6:H:46:LEU:HB2	1.58	0.67
2:B:235:SER:HA	2:B:261:ARG:NH2	2.08	0.67
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.25	0.67
2:B:311:LEU:HB3	7:I:4:PHE:CZ	2.29	0.67
3:C:39:ALA:O	3:C:163:ILE:HG23	1.95	0.67
1:A:714:PHE:HB2	7:I:97:MET:HE1	1.77	0.67
2:B:879:ARG:HB3	2:B:883:LEU:CD2	2.25	0.67
1:A:317:LYS:HD3	1:A:321:PRO:CD	2.25	0.67
1:A:1113:THR:O	1:A:1113:THR:HG22	1.93	0.67
2:B:550:ASP:OD1	2:B:552:MET:HG3	1.94	0.67
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.77	0.67
2:B:651:LEU:HD11	2:B:707:PRO:HB3	1.77	0.67
8:J:2:ILE:HD11	8:J:57:ILE:CD1	2.25	0.67
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.21	0.66
5:F:127:GLU:O	5:F:129:LYS:HG3	1.96	0.66
1:A:128:ILE:HG22	1:A:130:ASP:H	1.59	0.66
1:A:597:LEU:H	1:A:597:LEU:CD1	2.04	0.66
2:B:172:ILE:CD1	2:B:178:ASN:HD22	2.08	0.66
2:B:1072:MET:HE1	2:B:1087:PHE:CD1	2.30	0.66
5:F:82:THR:HG22	5:F:84:TYR:H	1.60	0.66
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.76	0.66
4:E:117:THR:HG22	4:E:119:SER:H	1.60	0.66
7:I:47:GLU:OE1	7:I:50:THR:HG23	1.96	0.66
2:B:103:ASN:HB2	2:B:169:ARG:NH2	2.10	0.66
2:B:193:LYS:HD2	2:B:787:VAL:HG11	1.78	0.66
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.76	0.66
6:H:87:ARG:O	6:H:89:LEU:HG	1.95	0.66
6:H:11:GLN:NE2	6:H:52:GLN:HA	2.10	0.66
1:A:92:HIS:HD2	1:A:94:GLY:H	1.42	0.66
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.78	0.66
3:C:22:LEU:HD21	9:K:101:LEU:HD21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.31	0.66
6:H:125:LEU:HB3	6:H:130:ARG:NH1	2.10	0.66
7:I:17:ARG:HG3	7:I:28:GLU:CD	2.21	0.66
1:A:1341:ILE:HD11	1:A:1376:THR:HG23	1.78	0.65
2:B:120:ARG:HH12	10:L:54:ARG:NH1	1.93	0.65
1:A:44:THR:O	1:A:45:GLN:HB2	1.97	0.65
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.77	0.65
1:A:247:ARG:HH11	1:A:263:THR:HG23	1.62	0.65
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.77	0.65
1:A:1269:GLU:OE2	2:B:263:GLY:HA3	1.96	0.65
1:A:1383:SER:CB	1:A:1387:HIS:NE2	2.54	0.65
3:C:8:VAL:HG21	9:K:105:PHE:HB2	1.78	0.65
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.77	0.65
1:A:320:ARG:N	1:A:321:PRO:HD3	2.12	0.65
1:A:1111:MET:HB2	1:A:1114:PRO:HG3	1.78	0.65
4:E:204:THR:HG22	4:E:205:SER:N	2.12	0.65
1:A:31:SER:CB	1:A:83:HIS:HB2	2.26	0.65
1:A:472:LEU:O	1:A:475:THR:HB	1.97	0.65
1:A:595:THR:OG1	1:A:603:ASN:HB3	1.96	0.65
2:B:35:SER:O	2:B:39:ARG:HG3	1.97	0.65
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.61	0.65
1:A:901:LEU:HD13	1:A:919:ILE:HG23	1.77	0.65
2:B:322:PHE:HZ	7:I:30:ARG:HB2	1.62	0.65
2:B:801:LYS:O	8:J:52:THR:HG23	1.97	0.65
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.59	0.65
10:L:49:LYS:O	10:L:50:ASP:HB2	1.95	0.65
1:A:705:LYS:O	1:A:708:MET:HB2	1.97	0.64
1:A:1132:LYS:HE2	1:A:1284:MET:HE1	1.78	0.64
2:B:54:PHE:HA	2:B:58:THR:HB	1.79	0.64
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.62	0.64
1:A:567:LYS:CB	1:A:568:PRO:CD	2.71	0.64
1:A:1206:ASP:HB2	1:A:1274:ARG:HH12	1.61	0.64
2:B:1198:TYR:CE1	2:B:1201:LYS:HD3	2.32	0.64
6:H:126:GLU:N	6:H:130:ARG:HH12	1.95	0.64
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.79	0.64
6:H:103:LYS:CD	6:H:114:VAL:HB	2.27	0.64
1:A:13:THR:HB	1:A:1432:GLN:NE2	2.13	0.64
1:A:768:GLN:NE2	1:A:816:HIS:HA	2.11	0.64
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.28	0.64
10:L:58:LYS:O	10:L:58:LYS:HD3	1.98	0.64
4:E:127:ILE:HD11	4:E:132:ILE:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.95	0.64
1:A:907:THR:HG22	1:A:908:LEU:N	2.12	0.64
1:A:1167:GLU:O	1:A:1171:GLN:HG3	1.98	0.64
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.28	0.64
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.96	0.64
4:E:112:TYR:CE1	4:E:115:ASN:HA	2.33	0.64
5:F:118:LEU:HG	5:F:122:MET:HE2	1.79	0.64
1:A:1295:THR:HB	1:A:1297:GLU:OE1	1.97	0.64
2:B:120:ARG:NH2	10:L:54:ARG:HD2	2.12	0.64
7:I:4:PHE:CE1	7:I:13:MET:HE2	2.33	0.64
1:A:112:LYS:HZ1	1:A:165:GLY:H	1.46	0.64
1:A:709:THR:HG21	7:I:93:LYS:O	1.98	0.64
4:E:158:SER:O	4:E:162:ARG:HG3	1.98	0.64
1:A:666:ILE:HG12	2:B:1026:LEU:HB3	1.80	0.63
2:B:784:ASN:OD1	2:B:788:ARG:HD2	1.97	0.63
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.63	0.63
2:B:616:ILE:HD11	2:B:696:GLU:HB3	1.80	0.63
2:B:644:GLU:HG3	2:B:654:ARG:NH2	2.13	0.63
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.28	0.63
9:K:46:ILE:HG22	9:K:50:LEU:HD12	1.80	0.63
1:A:184:SER:HA	1:A:198:GLU:O	1.98	0.63
1:A:313:GLN:NE2	1:A:322:VAL:HG12	2.13	0.63
8:J:2:ILE:HG12	8:J:57:ILE:HG21	1.80	0.63
1:A:472:LEU:HD13	2:B:835:GLN:NE2	2.14	0.63
1:A:666:ILE:HD11	2:B:1030:LEU:HB2	1.80	0.63
3:C:7:GLN:HG2	9:K:104:ASN:HD22	1.63	0.63
6:H:103:LYS:NZ	6:H:114:VAL:HG23	2.13	0.63
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.32	0.63
3:C:52:GLU:HA	10:L:64:LEU:CD2	2.28	0.63
8:J:2:ILE:HG22	8:J:3:VAL:N	2.13	0.63
3:C:134:ILE:HG21	3:C:139:GLY:HA2	1.80	0.63
6:H:4:THR:HA	6:H:60:ALA:HA	1.79	0.63
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.62	0.63
1:A:134:ARG:HD2	1:A:221:SER:O	1.97	0.63
1:A:317:LYS:CD	1:A:321:PRO:HD2	2.28	0.63
1:A:329:LEU:HA	1:A:332:LYS:HB2	1.81	0.63
7:I:50:THR:HG22	7:I:51:ASN:H	1.63	0.63
8:J:2:ILE:HD11	8:J:57:ILE:HD13	1.80	0.63
1:A:825:ILE:HD13	2:B:512:ARG:HG3	1.81	0.63
1:A:878:ILE:CG2	1:A:955:PRO:HB2	2.29	0.62
5:F:81:THR:HG22	5:F:136:ARG:NH1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:38:LEU:O	10:L:39:SER:HB2	1.99	0.62
1:A:32:VAL:HG11	1:A:68:GLN:NE2	2.13	0.62
1:A:322:VAL:HG22	1:A:323:LYS:N	2.14	0.62
1:A:566:ILE:O	1:A:567:LYS:O	2.17	0.62
1:A:1206:ASP:HB2	1:A:1274:ARG:NH1	2.14	0.62
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.14	0.62
6:H:82:PRO:O	6:H:84:ALA:N	2.32	0.62
7:I:45:ARG:HG2	7:I:45:ARG:NH1	2.11	0.62
1:A:601:LYS:HD2	1:A:603:ASN:ND2	2.13	0.62
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	1.99	0.62
10:L:30:ILE:HG22	10:L:31:CYS:N	2.14	0.62
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.97	0.62
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.81	0.62
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.80	0.62
9:K:18:LYS:NZ	9:K:38:GLU:HG2	2.14	0.62
1:A:853:ASP:O	1:A:854:ASN:HB2	1.99	0.62
1:A:1080:THR:O	1:A:1081:LEU:HG	1.99	0.62
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.82	0.62
4:E:54:GLN:CB	4:E:57:MET:HE3	2.29	0.62
6:H:12:VAL:HG13	6:H:26:ILE:HG23	1.81	0.62
9:K:18:LYS:HZ2	9:K:38:GLU:CG	2.13	0.62
2:B:294:ASP:H	7:I:12:ASN:ND2	1.97	0.62
2:B:322:PHE:CZ	7:I:30:ARG:HB2	2.35	0.62
6:H:89:LEU:C	6:H:91:ASP:H	2.07	0.62
2:B:35:SER:HA	2:B:811:TYR:HE2	1.65	0.62
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.47	0.62
1:A:56:PRO:O	1:A:57:ARG:HG3	2.00	0.61
1:A:1398:MET:CG	1:A:1426:GLU:HG2	2.28	0.61
2:B:164:LYS:O	2:B:165:VAL:HB	2.00	0.61
2:B:210:LYS:HE3	2:B:480:SER:OG	2.00	0.61
2:B:1165:ILE:CD1	2:B:1187:ASN:HD21	2.13	0.61
8:J:48:ARG:HG2	8:J:48:ARG:HH11	1.63	0.61
1:A:203:SER:OG	1:A:206:GLU:HG3	2.00	0.61
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.15	0.61
2:B:46:GLN:HG3	2:B:47:GLN:H	1.66	0.61
2:B:234:ILE:HD13	2:B:257:LYS:HD3	1.80	0.61
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	1.82	0.61
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.65	0.61
2:B:251:ILE:O	2:B:251:ILE:HG22	2.00	0.61
2:B:276:ILE:HD13	2:B:334:ILE:HG23	1.82	0.61
2:B:1008:PRO:HB3	2:B:1087:PHE:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:GLN:HE21	3:C:75:MET:H	1.47	0.61
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.80	0.61
1:A:187:LYS:HB2	1:A:194:ALA:HB1	1.81	0.61
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.82	0.61
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.14	0.61
5:F:111:LEU:O	5:F:113:GLY:N	2.31	0.61
7:I:103:CYS:O	7:I:107:SER:HA	2.01	0.61
9:K:12:LEU:HD11	9:K:18:LYS:HE2	1.82	0.61
1:A:387:ARG:O	1:A:391:LEU:HG	2.01	0.61
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.66	0.61
2:B:602:THR:HG22	2:B:606:LYS:HE3	1.82	0.61
1:A:302:THR:HG21	1:A:312:PRO:HG3	1.80	0.61
1:A:1064:VAL:HG13	13:A:3010:HOH:O	2.00	0.61
3:C:179:GLU:HG3	3:C:180:TYR:N	2.15	0.61
4:E:28:TYR:CZ	4:E:78:LEU:HG	2.36	0.61
4:E:65:THR:O	4:E:69:ILE:HG13	2.01	0.61
1:A:883:LEU:O	1:A:886:ILE:HG22	2.01	0.61
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.82	0.61
7:I:4:PHE:H	7:I:4:PHE:HD2	1.48	0.61
1:A:345:VAL:HG12	2:B:1150:ARG:HH22	1.65	0.61
2:B:577:ALA:HB1	2:B:589:VAL:HG13	1.82	0.61
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.82	0.61
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.83	0.61
6:H:5:LEU:HD22	6:H:133:ASN:O	2.00	0.61
7:I:2:THR:O	7:I:3:THR:C	2.44	0.61
7:I:95:THR:HG22	7:I:96:SER:N	2.15	0.61
1:A:78:PRO:O	1:A:79:GLY:O	2.19	0.60
1:A:597:LEU:HD23	6:H:104:PHE:CD1	2.35	0.60
3:C:137:LYS:H	3:C:137:LYS:HD2	1.65	0.60
1:A:345:VAL:CG1	2:B:1150:ARG:HH22	2.13	0.60
1:A:682:THR:HG21	1:A:728:LYS:HG3	1.83	0.60
1:A:689:LYS:O	1:A:693:VAL:HG23	2.01	0.60
2:B:879:ARG:HB3	2:B:883:LEU:HD23	1.83	0.60
1:A:903:ASN:HD22	1:A:905:ASP:N	1.97	0.60
1:A:1265:ASN:HD21	2:B:263:GLY:C	2.09	0.60
2:B:542:MET:CE	2:B:747:MET:HG3	2.24	0.60
2:B:680:THR:HG22	2:B:681:TRP:N	2.16	0.60
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.37	0.60
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.27	0.60
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.01	0.60
2:B:1181:GLU:CG	2:B:1188:LYS:HE2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ARG:O	1:A:48:ALA:HB2	2.00	0.60
2:B:706:GLN:NE2	2:B:709:ASP:OD2	2.34	0.60
6:H:97:MET:HE3	6:H:142:LEU:HD23	1.84	0.60
10:L:68:GLU:H	10:L:68:GLU:CD	2.10	0.60
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.84	0.60
1:A:466:SER:O	1:A:467:THR:HG23	2.02	0.60
1:A:541:ILE:HD12	1:A:541:ILE:N	2.17	0.60
1:A:751:SER:O	1:A:752:LYS:O	2.19	0.60
1:A:849:MET:CE	1:A:1437:GLY:H	2.14	0.60
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.16	0.60
4:E:43:LYS:O	4:E:47:CYS:HB2	2.02	0.60
10:L:51:CYS:C	10:L:53:HIS:H	2.10	0.60
8:J:14:VAL:HG13	8:J:50:ILE:HD11	1.84	0.60
1:A:901:LEU:N	1:A:926:GLN:HE21	1.88	0.60
2:B:884:ARG:O	2:B:936:ASP:CB	2.50	0.60
1:A:79:GLY:HA3	1:A:245:PRO:HG3	1.84	0.59
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.83	0.59
2:B:1127:GLY:O	2:B:1128:LEU:HB3	2.01	0.59
6:H:103:LYS:HZ2	6:H:114:VAL:C	2.08	0.59
10:L:53:HIS:C	10:L:55:ILE:H	2.10	0.59
1:A:116:ASP:OD2	1:A:164:ARG:HD2	2.02	0.59
1:A:1064:VAL:CG1	1:A:1370:LEU:HD22	2.32	0.59
1:A:1077:THR:HG22	1:A:1077:THR:O	2.02	0.59
2:B:62:ILE:O	2:B:65:GLU:HG2	2.03	0.59
2:B:899:ILE:HG22	2:B:900:ALA:N	2.17	0.59
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.83	0.59
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.02	0.59
1:A:1363:VAL:HB	1:A:1368:MET:HE2	1.84	0.59
3:C:52:GLU:HG2	10:L:64:LEU:HD11	1.84	0.59
5:F:81:THR:HB	5:F:144:GLU:OE1	2.03	0.59
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.37	0.59
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.29	0.59
1:A:443:LEU:HG	1:A:455:MET:HE2	1.85	0.59
1:A:1215:ARG:HA	1:A:1218:GLN:HE21	1.67	0.59
2:B:710:LEU:HD22	2:B:738:PHE:HD1	1.63	0.59
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.50	0.59
10:L:51:CYS:O	10:L:53:HIS:N	2.36	0.59
1:A:499:ALA:O	1:A:503:GLN:HB2	2.03	0.59
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.42	0.59
2:B:229:ALA:C	2:B:231:PRO:HD2	2.28	0.59
6:H:26:ILE:CD1	6:H:49:VAL:HG11	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:CYS:O	1:A:68:GLN:HB2	2.01	0.59
1:A:844:ALA:CB	1:A:1384:VAL:HG13	2.29	0.59
2:B:549:THR:O	2:B:628:THR:HG22	2.02	0.59
3:C:6:PRO:HG3	3:C:25:VAL:HG12	1.84	0.59
3:C:31:ASN:O	3:C:35:ARG:HG3	2.03	0.59
3:C:56:THR:HG23	3:C:58:LEU:N	2.00	0.59
5:F:109:VAL:CG1	5:F:110:ASP:N	2.66	0.59
1:A:903:ASN:ND2	1:A:903:ASN:C	2.57	0.59
1:A:1096:SER:O	1:A:1099:PRO:HG2	2.02	0.59
2:B:168:GLY:H	2:B:450:ALA:HB1	1.68	0.59
2:B:416:LEU:O	2:B:420:LEU:HG	2.02	0.59
1:A:2:VAL:HG21	2:B:1157:ALA:O	2.02	0.59
1:A:92:HIS:CD2	1:A:94:GLY:H	2.21	0.59
1:A:249:SER:HB2	1:A:258:GLY:O	2.02	0.59
1:A:332:LYS:HD3	2:B:1206:GLU:OE2	2.02	0.59
2:B:357:GLN:NE2	2:B:368:GLU:HG2	2.17	0.59
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.83	0.59
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.42	0.59
7:I:115:LYS:O	7:I:117:LYS:HG3	2.03	0.59
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.38	0.59
1:A:324:SER:O	1:A:328:ARG:HG3	2.03	0.59
2:B:63:ILE:CG1	2:B:95:ILE:HD11	2.33	0.59
1:A:596:THR:HG22	1:A:597:LEU:N	2.18	0.58
1:A:774:ARG:HH11	1:A:774:ARG:HG3	1.67	0.58
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.33	0.58
1:A:58:LEU:HD22	1:A:80:HIS:O	2.03	0.58
1:A:567:LYS:HZ3	6:H:95:TYR:HE1	1.51	0.58
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.02	0.58
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.51	0.58
3:C:17:ASN:HD22	3:C:17:ASN:N	2.01	0.58
6:H:110:ASP:O	6:H:128:ASN:ND2	2.36	0.58
1:A:353:ILE:HG21	1:A:487:MET:HE2	1.85	0.58
1:A:503:GLN:HE21	5:F:90:ARG:HH22	1.47	0.58
2:B:324:ILE:HD11	2:B:333:PHE:CD1	2.38	0.58
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.33	0.58
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.67	0.58
2:B:882:THR:HB	2:B:934:LYS:O	2.02	0.58
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.39	0.58
1:A:494:SER:OG	1:A:497:THR:HB	2.04	0.58
1:A:525:GLN:NE2	1:A:752:LYS:HE3	2.17	0.58
1:A:1333:ILE:O	1:A:1337:GLU:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:365:THR:HG22	2:B:367:LEU:N	2.17	0.58
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.86	0.58
4:E:4:GLU:O	4:E:6:GLU:N	2.37	0.58
10:L:27:LEU:HD13	10:L:37:LYS:CD	2.32	0.58
4:E:124:VAL:HB	4:E:125:PRO:CD	2.33	0.58
6:H:40:LEU:CD1	6:H:123:MET:HB2	2.34	0.58
1:A:243:PRO:C	1:A:245:PRO:HD2	2.29	0.58
1:A:264:PHE:HB2	1:A:315:LEU:HD13	1.85	0.58
5:F:81:THR:HG21	5:F:136:ARG:HH11	1.67	0.58
1:A:1124:HIS:CB	1:A:1130:GLN:OE1	2.52	0.58
2:B:193:LYS:CD	2:B:787:VAL:HG11	2.34	0.58
4:E:5:ASN:HA	4:E:8:ASN:HB3	1.84	0.58
1:A:283:GLY:O	1:A:284:ALA:HB2	2.04	0.58
1:A:598:LEU:HG	6:H:115:TYR:HE2	1.69	0.58
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.33	0.58
1:A:867:ILE:HD11	1:A:999:VAL:HG11	1.85	0.58
2:B:120:ARG:HD2	2:B:955:THR:CG2	2.33	0.58
2:B:477:ALA:HB1	2:B:479:VAL:HG23	1.85	0.58
2:B:542:MET:CG	2:B:747:MET:HE3	2.25	0.58
2:B:640:VAL:O	2:B:640:VAL:HG12	2.02	0.58
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.33	0.58
1:A:423:ASP:CG	1:A:423:ASP:O	2.46	0.58
1:A:724:GLU:O	1:A:728:LYS:HG2	2.04	0.58
1:A:774:ARG:HB2	1:A:797:LYS:HG2	1.85	0.58
1:A:901:LEU:HA	1:A:907:THR:HG23	1.86	0.58
3:C:16:ASP:C	3:C:17:ASN:HD22	2.11	0.58
7:I:59:VAL:HG12	7:I:61:ASP:H	1.68	0.58
10:L:33:GLU:HB2	10:L:53:HIS:CD2	2.38	0.58
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.43	0.57
1:A:1285:MET:HG3	1:A:1307:GLU:OE1	2.03	0.57
2:B:979:LYS:CE	2:B:987:LYS:HD2	2.32	0.57
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.85	0.57
6:H:26:ILE:HD13	6:H:49:VAL:HG11	1.86	0.57
1:A:65:LEU:HD22	1:A:72:GLU:O	2.04	0.57
1:A:848:ILE:HD13	1:A:864:ILE:HD13	1.87	0.57
1:A:144:THR:O	1:A:146:MET:HG3	2.04	0.57
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.19	0.57
2:B:754:SER:O	2:B:806:THR:HG21	2.04	0.57
2:B:707:PRO:O	2:B:708:GLU:C	2.45	0.57
2:B:760:ASP:OD1	2:B:761:HIS:HD2	1.87	0.57
6:H:62:SER:O	6:H:63:LEU:C	2.46	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:51:ASN:O	7:I:54:GLU:HG3	2.04	0.57
10:L:34:CYS:HB3	10:L:51:CYS:SG	2.44	0.57
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.85	0.57
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.19	0.57
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.39	0.57
1:A:70:CYS:O	1:A:72:GLU:HG3	2.04	0.57
1:A:187:LYS:O	1:A:188:ASP:HB2	2.04	0.57
2:B:357:GLN:HE21	2:B:368:GLU:HG2	1.69	0.57
5:F:109:VAL:CG1	5:F:110:ASP:H	2.17	0.57
1:A:1446:ASP:OD2	1:A:1448:GLU:HB2	2.04	0.57
1:A:112:LYS:NZ	1:A:165:GLY:H	2.02	0.57
1:A:486:GLU:OE2	2:B:1102:LYS:HB3	2.05	0.57
1:A:567:LYS:NZ	6:H:95:TYR:HE1	2.02	0.57
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.86	0.57
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.87	0.57
2:B:876:LYS:HE2	2:B:893:LEU:O	2.05	0.57
8:J:14:VAL:CG1	8:J:50:ILE:HD11	2.35	0.57
1:A:598:LEU:O	1:A:599:SER:C	2.47	0.57
4:E:13:TRP:CE3	4:E:39:LEU:HD13	2.40	0.57
1:A:33:ALA:HB2	1:A:56:PRO:HB2	1.87	0.57
1:A:629:LEU:O	1:A:633:VAL:HG23	2.04	0.57
2:B:863:GLU:O	2:B:864:LYS:O	2.23	0.57
2:B:999:MET:HE2	2:B:1011:ILE:CD1	2.30	0.57
5:F:79:ARG:HH22	5:F:150:GLU:CD	2.13	0.57
6:H:87:ARG:O	6:H:89:LEU:N	2.37	0.57
1:A:714:PHE:CB	7:I:97:MET:HE1	2.34	0.56
1:A:1277:GLU:H	1:A:1277:GLU:CD	2.13	0.56
2:B:130:VAL:CG2	2:B:167:ILE:HD12	2.35	0.56
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.86	0.56
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.05	0.56
2:B:640:VAL:HG22	2:B:651:LEU:HD22	1.87	0.56
2:B:1022:THR:HG23	2:B:1022:THR:O	2.05	0.56
1:A:33:ALA:CB	1:A:56:PRO:HB2	2.35	0.56
1:A:34:LYS:HE3	1:A:85:ASP:OD2	2.05	0.56
1:A:537:ARG:NH1	6:H:120:GLY:O	2.37	0.56
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.20	0.56
2:B:709:ASP:C	2:B:711:GLU:H	2.12	0.56
2:B:830:TYR:CE1	2:B:1000:PRO:HB3	2.40	0.56
4:E:120:ALA:O	4:E:123:LEU:HB2	2.05	0.56
6:H:138:GLU:HG2	6:H:139:ASN:N	2.20	0.56
1:A:69:THR:O	1:A:71:GLN:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.87	0.56
1:A:697:ALA:HB2	1:A:702:LEU:CD1	2.35	0.56
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.38	0.56
1:A:1064:VAL:HG12	1:A:1370:LEU:CD2	2.36	0.56
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.20	0.56
2:B:642:ASP:CB	2:B:649:LYS:HG2	2.23	0.56
2:B:1165:ILE:HD12	2:B:1187:ASN:HD21	1.69	0.56
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.87	0.56
6:H:7:ASP:O	6:H:8:ASP:HB2	2.04	0.56
6:H:95:TYR:HE2	6:H:97:MET:HE2	1.69	0.56
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.87	0.56
1:A:49:LYS:HD3	1:A:55:ASP:CB	2.30	0.56
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.88	0.56
2:B:46:GLN:HG3	2:B:47:GLN:N	2.21	0.56
1:A:1318:THR:HG21	4:E:11:ARG:HH12	1.71	0.56
1:A:1395:GLY:O	1:A:1397:LEU:N	2.37	0.56
2:B:120:ARG:NH1	10:L:54:ARG:NH1	2.53	0.56
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.21	0.56
10:L:27:LEU:HD13	10:L:37:LYS:HD3	1.88	0.56
1:A:28:ARG:HG2	1:A:83:HIS:CE1	2.40	0.56
1:A:313:GLN:HE21	1:A:322:VAL:N	2.04	0.56
1:A:595:THR:HG23	1:A:599:SER:HB3	1.86	0.56
1:A:1394:THR:CG2	1:A:1398:MET:HB2	2.35	0.56
2:B:98:THR:HG21	2:B:101:MET:CE	2.34	0.56
2:B:915:THR:HG21	2:B:934:LYS:HG2	1.87	0.56
3:C:54:ASN:OD1	3:C:56:THR:HG22	2.06	0.56
4:E:88:VAL:HG13	4:E:92:THR:HB	1.88	0.56
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.87	0.56
1:A:1402:PHE:C	1:A:1404:GLU:H	2.13	0.56
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.06	0.56
2:B:1165:ILE:HD12	2:B:1187:ASN:ND2	2.20	0.56
2:B:230:ALA:N	2:B:231:PRO:HD2	2.20	0.56
1:A:100:LYS:HE3	1:A:174:ILE:O	2.06	0.56
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.88	0.56
3:C:175:ALA:O	3:C:176:ILE:HG12	2.06	0.56
5:F:111:LEU:H	5:F:111:LEU:CD1	2.13	0.56
10:L:30:ILE:HG22	10:L:31:CYS:H	1.71	0.56
2:B:864:LYS:CG	2:B:871:THR:HG23	2.36	0.55
2:B:1103:ILE:HG22	2:B:1103:ILE:O	2.05	0.55
2:B:1165:ILE:CG1	2:B:1187:ASN:HD21	2.20	0.55
3:C:167:HIS:HD2	3:C:169:LYS:H	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:75:PRO:O	5:F:77:ASP:O	2.24	0.55
1:A:469:ARG:NH2	2:B:991:GLY:O	2.38	0.55
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.88	0.55
2:B:953:LEU:HD21	2:B:955:THR:OG1	2.06	0.55
1:A:269:ILE:HD11	1:A:303:TYR:HB2	1.87	0.55
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.32	0.55
1:A:489:LEU:HD23	1:A:489:LEU:C	2.30	0.55
2:B:602:THR:O	2:B:606:LYS:HG3	2.07	0.55
2:B:884:ARG:O	2:B:885:MET:HG2	2.07	0.55
2:B:1051:THR:CG2	2:B:1052:VAL:N	2.69	0.55
1:A:305:ASP:HB3	1:A:326:ARG:CZ	2.37	0.55
1:A:337:ARG:HH22	1:A:1403:GLU:HA	1.72	0.55
1:A:699:ALA:HB1	7:I:114:GLN:NE2	2.21	0.55
1:A:317:LYS:HD3	1:A:321:PRO:CG	2.37	0.55
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.34	0.55
2:B:561:TRP:O	2:B:590:HIS:HE1	1.90	0.55
6:H:103:LYS:HZ2	6:H:115:TYR:N	2.04	0.55
2:B:809:MET:HG2	2:B:814:PHE:HB3	1.88	0.55
5:F:72:LYS:N	5:F:142:SER:HA	2.21	0.55
1:A:714:PHE:CG	7:I:97:MET:HE1	2.41	0.55
1:A:805:LEU:HD11	2:B:1052:VAL:HG21	1.87	0.55
1:A:1431:GLY:HA2	2:B:1152:MET:HE2	1.87	0.55
2:B:120:ARG:HH22	10:L:54:ARG:HH11	1.55	0.55
6:H:85:GLY:O	6:H:89:LEU:HD21	2.06	0.55
1:A:308:ILE:CG2	1:A:309:ALA:H	1.99	0.55
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.88	0.55
2:B:25:ILE:HD12	2:B:653:VAL:CB	2.35	0.55
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.22	0.55
1:A:345:VAL:HG12	1:A:348:SER:OG	2.06	0.55
1:A:567:LYS:NZ	6:H:95:TYR:CE1	2.75	0.55
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.06	0.55
1:A:541:ILE:HG12	1:A:549:MET:HE1	1.89	0.54
1:A:1094:VAL:HG12	1:A:1095:THR:N	2.18	0.54
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.89	0.54
2:B:707:PRO:O	2:B:709:ASP:N	2.39	0.54
5:F:111:LEU:C	5:F:113:GLY:H	2.15	0.54
9:K:38:GLU:OE1	9:K:42:LEU:HD22	2.07	0.54
1:A:313:GLN:HB3	1:A:320:ARG:C	2.33	0.54
1:A:601:LYS:HD2	1:A:603:ASN:HD22	1.71	0.54
1:A:862:ASN:OD1	4:E:174:GLN:HA	2.08	0.54
1:A:1146:VAL:HG11	1:A:1202:MET:SD	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:SER:O	2:B:106:ASP:HB2	2.07	0.54
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.07	0.54
2:B:311:LEU:HB3	7:I:4:PHE:HZ	1.69	0.54
9:K:29:ASN:ND2	9:K:79:GLU:HA	2.21	0.54
1:A:540:PHE:C	1:A:541:ILE:HD12	2.32	0.54
2:B:230:ALA:HA	2:B:261:ARG:NH1	2.22	0.54
2:B:884:ARG:O	2:B:936:ASP:HB2	2.06	0.54
3:C:56:THR:HG23	3:C:57:VAL:N	2.23	0.54
6:H:100:THR:HG23	6:H:138:GLU:CA	2.36	0.54
6:H:101:ALA:C	6:H:103:LYS:H	2.15	0.54
10:L:38:LEU:O	10:L:39:SER:CB	2.55	0.54
1:A:683:ILE:HD11	1:A:764:CYS:HB2	1.90	0.54
2:B:604:ARG:NH2	2:B:697:GLU:OE1	2.41	0.54
2:B:1135:ARG:HG3	2:B:1147:LEU:HD22	1.89	0.54
3:C:258:ILE:HD13	9:K:35:PHE:CE2	2.40	0.54
6:H:123:MET:HE1	6:H:142:LEU:CD1	2.36	0.54
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.89	0.54
8:J:64:ASN:HB3	8:J:65:PRO:CD	2.34	0.54
10:L:27:LEU:HD13	10:L:37:LYS:HG2	1.89	0.54
1:A:49:LYS:CD	1:A:55:ASP:HB2	2.30	0.54
1:A:523:ILE:HD12	1:A:622:VAL:HG22	1.88	0.54
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.40	0.54
2:B:515:HIS:HD2	2:B:517:THR:H	1.54	0.54
4:E:116:ILE:HG22	4:E:117:THR:N	2.21	0.54
1:A:614:PHE:CD1	1:A:614:PHE:C	2.86	0.54
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.90	0.54
1:A:1438:THR:HG22	2:B:1144:ALA:H	1.73	0.54
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.43	0.54
6:H:12:VAL:HA	6:H:28:ALA:HB2	1.89	0.54
6:H:96:VAL:HG13	6:H:143:LEU:CD2	2.37	0.54
7:I:84:VAL:HG12	7:I:102:VAL:HB	1.88	0.54
2:B:1051:THR:HG22	2:B:1052:VAL:N	2.22	0.54
4:E:9:ILE:HD11	4:E:51:GLY:O	2.07	0.54
1:A:47:ARG:O	1:A:48:ALA:CB	2.56	0.54
2:B:1165:ILE:HG13	2:B:1187:ASN:HD21	1.73	0.54
10:L:27:LEU:HG	10:L:27:LEU:O	2.07	0.54
1:A:562:THR:HB	6:H:98:TYR:HE2	1.72	0.54
1:A:608:ILE:HD12	1:A:613:ILE:HD12	1.90	0.54
1:A:871:ASP:CB	4:E:204:THR:HG23	2.36	0.54
2:B:351:TYR:CE2	2:B:355:ILE:HD11	2.43	0.54
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1162:ILE:HD13	2:B:1216:LEU:HB2	1.90	0.54
1:A:343:LYS:O	1:A:345:VAL:HG23	2.07	0.53
1:A:1199:ARG:HG3	1:A:1236:LEU:HD11	1.88	0.53
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.72	0.53
2:B:766:ARG:NH1	2:B:985:GLY:O	2.40	0.53
3:C:165:LYS:O	9:K:6:ARG:NH1	2.41	0.53
1:A:1341:ILE:CD1	1:A:1376:THR:HG23	2.37	0.53
2:B:461:LEU:HD12	2:B:466:TRP:HH2	1.72	0.53
2:B:549:THR:O	2:B:628:THR:CG2	2.56	0.53
4:E:5:ASN:O	4:E:9:ILE:HG13	2.09	0.53
6:H:103:LYS:HE2	6:H:116:TYR:CE2	2.44	0.53
1:A:765:VAL:HG23	1:A:802:ASN:O	2.09	0.53
2:B:332:ASP:OD2	2:B:345:LYS:HG3	2.08	0.53
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.43	0.53
1:A:32:VAL:HG23	1:A:33:ALA:H	1.73	0.53
1:A:264:PHE:HB3	1:A:315:LEU:CD2	2.27	0.53
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.44	0.53
2:B:515:HIS:H	2:B:518:HIS:CD2	2.27	0.53
4:E:31:THR:C	4:E:33:GLU:N	2.65	0.53
1:A:32:VAL:HB	1:A:57:ARG:CB	2.39	0.53
1:A:417:TYR:O	1:A:418:SER:HB2	2.08	0.53
1:A:535:THR:O	1:A:575:LYS:HE3	2.09	0.53
1:A:626:ASN:O	1:A:631:HIS:CD2	2.62	0.53
10:L:34:CYS:C	10:L:36:SER:H	2.17	0.53
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.90	0.53
2:B:63:ILE:HD13	2:B:95:ILE:HD11	1.91	0.53
2:B:199:MET:CE	2:B:491:THR:HG22	2.38	0.53
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.44	0.53
1:A:1390:ASN:O	1:A:1391:ARG:CB	2.56	0.53
1:A:1394:THR:HG22	1:A:1398:MET:HB2	1.91	0.53
2:B:63:ILE:HB	2:B:95:ILE:HD11	1.91	0.53
3:C:183:TRP:O	3:C:185:LYS:N	2.39	0.53
4:E:177:ARG:HD3	4:E:215:MET:HE2	1.90	0.53
5:F:97:ARG:NE	5:F:124:GLU:OE1	2.40	0.53
6:H:103:LYS:HZ3	6:H:115:TYR:C	2.16	0.53
10:L:38:LEU:HG	10:L:39:SER:N	2.19	0.53
1:A:328:ARG:HD3	1:A:332:LYS:HZ1	1.74	0.53
1:A:853:ASP:OD1	1:A:855:THR:HB	2.09	0.53
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.15	0.53
2:B:680:THR:HG22	2:B:682:SER:N	2.22	0.53
3:C:148:ARG:HD2	8:J:61:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:43:ARG:O	8:J:47:ARG:HG3	2.09	0.53
10:L:38:LEU:HD22	10:L:56:LEU:HD21	1.91	0.53
2:B:463:THR:HG21	2:B:465:ASN:OD1	2.09	0.53
2:B:798:TYR:CD2	8:J:4:PRO:HG3	2.44	0.53
1:A:305:ASP:OD1	1:A:326:ARG:HB2	2.09	0.53
2:B:199:MET:HE3	2:B:492:LEU:CD2	2.38	0.53
2:B:1081:LEU:CD1	2:B:1085:ILE:HD11	2.39	0.53
10:L:43:THR:HG22	10:L:43:THR:O	2.09	0.53
1:A:1166:ASP:HA	1:A:1169:ILE:HG22	1.91	0.52
1:A:1438:THR:HG22	2:B:1144:ALA:CB	2.40	0.52
2:B:365:THR:HG22	2:B:366:GLN:N	2.24	0.52
4:E:159:ASP:HA	4:E:162:ARG:NH1	2.23	0.52
4:E:200:ARG:HD2	13:E:221:HOH:O	2.10	0.52
7:I:2:THR:O	7:I:2:THR:HG22	2.09	0.52
10:L:26:THR:HG22	10:L:27:LEU:N	2.23	0.52
1:A:525:GLN:HE21	1:A:752:LYS:HE3	1.73	0.52
1:A:551:TYR:CE2	9:K:62:LYS:HE2	2.45	0.52
1:A:694:THR:O	1:A:698:GLN:HG3	2.08	0.52
1:A:973:ILE:HD11	1:A:1041:ALA:CB	2.40	0.52
1:A:1199:ARG:HA	1:A:1202:MET:HB2	1.91	0.52
1:A:1398:MET:O	1:A:1399:ARG:C	2.52	0.52
2:B:1077:THR:HG22	2:B:1079:LYS:N	2.21	0.52
3:C:258:ILE:CD1	9:K:42:LEU:HD21	2.39	0.52
4:E:4:GLU:O	4:E:5:ASN:C	2.52	0.52
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.09	0.52
1:A:303:TYR:CZ	1:A:325:ILE:HD11	2.44	0.52
1:A:1111:MET:CE	1:A:1114:PRO:HA	2.39	0.52
1:A:1394:THR:HA	1:A:1398:MET:HE3	1.92	0.52
6:H:31:THR:O	6:H:32:THR:HB	2.08	0.52
7:I:31:THR:HG22	7:I:32:CYS:N	2.23	0.52
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.91	0.52
1:A:65:LEU:O	1:A:71:GLN:HA	2.08	0.52
1:A:500:GLU:O	1:A:504:LEU:HB2	2.10	0.52
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.44	0.52
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.44	0.52
1:A:1147:THR:HB	7:I:48:LEU:HD12	1.91	0.52
1:A:1438:THR:CG2	2:B:1144:ALA:HB3	2.39	0.52
9:K:47:ARG:HD3	9:K:59:ALA:O	2.10	0.52
2:B:545:ILE:HG12	2:B:633:VAL:HG22	1.90	0.52
2:B:1153:GLU:CG	2:B:1154:ALA:H	2.21	0.52
1:A:982:THR:HG22	1:A:983:ILE:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LYS:O	1:A:988:LEU:HB2	2.09	0.52
2:B:18:PHE:N	2:B:18:PHE:CD2	2.76	0.52
2:B:653:VAL:HG22	13:B:3026:HOH:O	2.10	0.52
2:B:976:ILE:O	2:B:1099:VAL:HG21	2.09	0.52
3:C:152:GLU:OE2	3:C:154:LYS:HE3	2.09	0.52
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.91	0.52
2:B:731:VAL:CG1	2:B:732:SER:H	2.19	0.52
3:C:73:GLN:HE21	3:C:75:MET:N	2.07	0.52
1:A:32:VAL:HG23	1:A:33:ALA:N	2.24	0.52
2:B:953:LEU:HD23	2:B:953:LEU:C	2.34	0.52
6:H:96:VAL:HG22	6:H:143:LEU:HD22	1.92	0.52
1:A:262:LEU:O	1:A:266:LEU:HG	2.10	0.52
1:A:870:GLU:HG2	4:E:208:TYR:CD2	2.45	0.52
2:B:35:SER:HA	2:B:811:TYR:CE2	2.42	0.52
2:B:680:THR:HG23	2:B:681:TRP:H	1.75	0.52
2:B:862:GLN:O	2:B:914:LYS:HE3	2.10	0.52
7:I:29:CYS:SG	7:I:31:THR:HB	2.50	0.52
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.45	0.52
2:B:254:LEU:CD2	2:B:381:MET:HE1	2.37	0.52
2:B:299:GLU:HG2	2:B:571:PRO:CG	2.40	0.52
2:B:351:TYR:O	2:B:355:ILE:HG13	2.11	0.52
1:A:438:ASP:O	1:A:439:ASN:HB2	2.09	0.51
6:H:76:THR:O	6:H:76:THR:HG22	2.10	0.51
1:A:636:GLU:OE1	1:A:966:ASN:ND2	2.42	0.51
1:A:834:THR:HG21	1:A:1077:THR:HA	1.93	0.51
6:H:59:ILE:O	6:H:60:ALA:HB3	2.11	0.51
6:H:130:ARG:HA	6:H:133:ASN:HB2	1.93	0.51
1:A:567:LYS:HZ1	6:H:46:LEU:HB2	1.75	0.51
1:A:682:THR:CG2	1:A:728:LYS:HE3	2.41	0.51
1:A:753:GLY:O	1:A:754:SER:HB3	2.11	0.51
2:B:120:ARG:NH2	10:L:54:ARG:HH11	2.09	0.51
5:F:93:ILE:HD13	5:F:148:VAL:HG22	1.92	0.51
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.93	0.51
1:A:260:ASP:OD1	1:A:261:ASP:N	2.44	0.51
1:A:317:LYS:HD3	1:A:321:PRO:HG2	1.93	0.51
1:A:666:ILE:CD1	2:B:1030:LEU:HB2	2.39	0.51
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	1.92	0.51
1:A:1341:ILE:HD12	1:A:1379:GLY:C	2.35	0.51
2:B:101:MET:HB2	2:B:110:HIS:O	2.10	0.51
2:B:199:MET:HE2	2:B:491:THR:HG22	1.93	0.51
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.45	0.51
1:A:903:ASN:ND2	1:A:905:ASP:N	2.51	0.51
1:A:998:LEU:HD12	1:A:1001:ARG:NH1	2.26	0.51
2:B:542:MET:HE2	2:B:747:MET:CG	2.26	0.51
2:B:852:ARG:NH2	10:L:70:ARG:O	2.40	0.51
2:B:874:PHE:O	2:B:875:GLU:HG3	2.11	0.51
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.40	0.51
2:B:1065:GLN:HE22	2:B:1067:ARG:CB	2.23	0.51
1:A:642:CYS:O	1:A:645:LEU:HB3	2.11	0.51
1:A:849:MET:HE1	1:A:1437:GLY:H	1.74	0.51
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.10	0.51
2:B:118:ARG:NH1	2:B:204:ILE:HD11	2.26	0.51
2:B:906:SER:O	2:B:907:GLY:C	2.53	0.51
1:A:337:ARG:O	1:A:341:MET:HG3	2.11	0.51
1:A:768:GLN:NE2	1:A:816:HIS:ND1	2.59	0.51
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.91	0.51
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.75	0.51
2:B:894:ASP:OD2	10:L:58:LYS:NZ	2.44	0.51
3:C:57:VAL:HG11	8:J:60:PHE:HB2	1.91	0.51
1:A:596:THR:HG22	1:A:597:LEU:HD12	1.93	0.51
1:A:1447:GLU:OE1	1:A:1447:GLU:HA	2.11	0.51
2:B:199:MET:HG2	2:B:200:GLY:N	2.25	0.51
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.92	0.51
1:A:535:THR:O	1:A:535:THR:HG22	2.10	0.51
1:A:682:THR:CG2	1:A:728:LYS:HG3	2.40	0.51
1:A:710:LEU:HD23	7:I:96:SER:HA	1.93	0.51
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	1.93	0.51
8:J:48:ARG:CZ	8:J:49:MET:HE1	2.40	0.51
9:K:82:ASP:OD1	9:K:84:LYS:N	2.41	0.51
1:A:57:ARG:C	1:A:68:GLN:HE21	2.19	0.51
1:A:328:ARG:HD3	1:A:332:LYS:NZ	2.26	0.51
1:A:329:LEU:C	1:A:331:GLY:H	2.18	0.51
2:B:515:HIS:CD2	2:B:517:THR:H	2.29	0.51
10:L:48:CYS:SG	10:L:49:LYS:N	2.84	0.51
1:A:597:LEU:HD23	6:H:104:PHE:CG	2.46	0.50
1:A:1366:ARG:HG2	1:A:1366:ARG:HH11	1.76	0.50
2:B:43:LEU:HD11	2:B:811:TYR:O	2.11	0.50
4:E:90:VAL:HG13	4:E:91:LYS:N	2.25	0.50
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.93	0.50
10:L:27:LEU:HD13	10:L:37:LYS:CG	2.39	0.50
1:A:37:PHE:HD1	1:A:50:ILE:HG21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:THR:HG23	1:A:306:ASN:OD1	2.12	0.50
2:B:416:LEU:HD11	2:B:466:TRP:CE2	2.46	0.50
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.92	0.50
2:B:1099:VAL:O	2:B:1101:ASP:N	2.44	0.50
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.46	0.50
1:A:146:MET:O	1:A:147:VAL:HG23	2.10	0.50
1:A:524:VAL:CG1	1:A:525:GLN:N	2.52	0.50
1:A:672:ASP:OD1	1:A:674:PRO:HD2	2.11	0.50
2:B:794:ASN:C	2:B:795:ILE:HD12	2.36	0.50
3:C:43:THR:HG22	3:C:44:LEU:N	2.26	0.50
4:E:71:LYS:O	4:E:73:PRO:HD3	2.11	0.50
1:A:1402:PHE:O	1:A:1404:GLU:N	2.44	0.50
2:B:172:ILE:HD11	2:B:178:ASN:HD22	1.75	0.50
2:B:259:TYR:O	2:B:267:ARG:HG2	2.11	0.50
2:B:557:PHE:HZ	2:B:599:THR:HG21	1.77	0.50
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.41	0.50
3:C:25:VAL:HG23	3:C:228:PHE:HE1	1.77	0.50
4:E:93:MET:O	4:E:97:VAL:HG23	2.11	0.50
9:K:103:THR:HG22	9:K:104:ASN:N	2.26	0.50
1:A:709:THR:HB	1:A:712:GLU:HG3	1.93	0.50
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.11	0.50
9:K:113:THR:O	9:K:114:LEU:CB	2.58	0.50
1:A:265:LYS:NZ	1:A:302:THR:HB	2.27	0.50
1:A:823:GLY:O	1:A:827:THR:HB	2.12	0.50
3:C:263:THR:C	3:C:265:MET:H	2.19	0.50
5:F:77:ASP:O	5:F:78:GLN:CB	2.60	0.50
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.41	0.50
1:A:315:LEU:C	1:A:317:LYS:H	2.19	0.50
1:A:1336:MET:HE1	1:A:1381:LEU:H	1.75	0.50
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.47	0.50
1:A:78:PRO:O	1:A:79:GLY:C	2.55	0.50
1:A:225:ASN:ND2	1:A:228:PHE:CD1	2.75	0.50
1:A:337:ARG:HG2	1:A:341:MET:HE2	1.93	0.50
1:A:345:VAL:HG13	2:B:1150:ARG:HH12	1.76	0.50
1:A:385:ILE:HG13	1:A:428:TYR:HE2	1.77	0.50
1:A:697:ALA:HB1	7:I:97:MET:HE3	1.94	0.50
3:C:258:ILE:HD12	9:K:42:LEU:HD21	1.94	0.50
1:A:244:PRO:N	1:A:245:PRO:HD2	2.26	0.50
1:A:503:GLN:NE2	5:F:90:ARG:HH22	2.10	0.50
1:A:736:ASN:O	1:A:737:LEU:C	2.55	0.50
2:B:98:THR:HG22	2:B:99:LYS:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:LYS:O	2:B:165:VAL:CB	2.60	0.50
2:B:241:ARG:CG	2:B:251:ILE:HG23	2.42	0.50
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.93	0.50
1:A:185:TRP:HZ3	1:A:200:ARG:HG2	1.76	0.49
1:A:282:ASN:O	1:A:283:GLY:O	2.30	0.49
1:A:973:ILE:HD11	1:A:1041:ALA:HB2	1.94	0.49
1:A:1095:THR:HG22	1:A:1100:ARG:HB2	1.94	0.49
1:A:1187:GLN:CG	1:A:1188:GLN:H	2.25	0.49
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.45	0.49
2:B:1158:PHE:CE2	2:B:1160:VAL:HG22	2.47	0.49
2:B:1183:LYS:C	2:B:1185:CYS:H	2.20	0.49
3:C:186:LEU:N	3:C:186:LEU:CD1	2.75	0.49
6:H:103:LYS:CG	6:H:115:TYR:O	2.58	0.49
1:A:357:PRO:HA	13:A:3038:HOH:O	2.12	0.49
1:A:440:ASP:OD1	1:A:498:ARG:NH2	2.45	0.49
1:A:849:MET:HE2	1:A:1061:GLY:CA	2.40	0.49
1:A:1391:ARG:NH2	1:A:1417:GLU:HG3	2.27	0.49
2:B:130:VAL:HG21	2:B:167:ILE:HD12	1.92	0.49
2:B:911:ILE:HG23	2:B:966:VAL:HG11	1.94	0.49
1:A:327:ALA:HA	1:A:330:LYS:HD2	1.93	0.49
1:A:511:ILE:HA	1:A:521:MET:HE3	1.94	0.49
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.47	0.49
2:B:315:LYS:N	2:B:316:PRO:HD2	2.26	0.49
2:B:826:ALA:HB2	2:B:1087:PHE:CE1	2.47	0.49
3:C:51:VAL:O	10:L:64:LEU:HD22	2.11	0.49
4:E:96:PHE:CE2	4:E:110:PHE:HB2	2.46	0.49
6:H:118:PHE:HB2	6:H:121:LEU:HB2	1.94	0.49
10:L:46:VAL:O	10:L:54:ARG:HA	2.12	0.49
1:A:741:ASN:ND2	1:A:743:VAL:HB	2.27	0.49
1:A:756:ILE:O	1:A:760:GLN:HG3	2.13	0.49
1:A:831:THR:HG22	1:A:832:ALA:N	2.26	0.49
1:A:1277:GLU:CD	1:A:1277:GLU:N	2.71	0.49
2:B:60:GLN:O	2:B:63:ILE:HG22	2.13	0.49
3:C:93:ASP:O	3:C:127:ARG:NH2	2.46	0.49
3:C:265:MET:CE	9:K:19:LEU:HB2	2.38	0.49
7:I:15:TYR:N	7:I:15:TYR:CD1	2.81	0.49
8:J:48:ARG:O	8:J:52:THR:HB	2.13	0.49
9:K:24:ASP:OD2	9:K:74:ARG:NH1	2.43	0.49
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.43	0.49
1:A:806:ARG:HH12	2:B:729:ILE:HD11	1.77	0.49
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1385:THR:O	1:A:1386:ARG:HG2	2.12	0.49
2:B:223:VAL:O	2:B:224:GLN:HG3	2.12	0.49
2:B:492:LEU:O	2:B:496:ARG:HG3	2.12	0.49
2:B:680:THR:CG2	2:B:681:TRP:H	2.25	0.49
2:B:884:ARG:O	2:B:936:ASP:HB3	2.12	0.49
2:B:906:SER:HA	2:B:946:ASN:HB2	1.94	0.49
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.42	0.49
7:I:59:VAL:CG1	7:I:60:GLN:N	2.75	0.49
1:A:31:SER:OG	1:A:83:HIS:HB2	2.11	0.49
1:A:90:VAL:HG13	1:A:297:GLN:NE2	2.28	0.49
1:A:381:THR:HG21	1:A:383:TYR:HD1	1.77	0.49
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.95	0.49
1:A:704:ALA:HB2	1:A:710:LEU:CD1	2.33	0.49
2:B:174:LEU:O	2:B:200:GLY:O	2.29	0.49
2:B:1135:ARG:HG3	2:B:1147:LEU:CD2	2.42	0.49
3:C:57:VAL:O	3:C:57:VAL:CG1	2.61	0.49
5:F:109:VAL:HG13	5:F:127:GLU:OE1	2.11	0.49
1:A:362:ASP:OD2	1:A:362:ASP:N	2.46	0.49
1:A:466:SER:C	1:A:467:THR:HG23	2.38	0.49
1:A:673:GLY:N	1:A:674:PRO:HD2	2.28	0.49
2:B:99:LYS:HB3	2:B:180:TYR:CZ	2.47	0.49
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.95	0.49
2:B:645:SER:O	2:B:647:GLY:N	2.45	0.49
2:B:756:ILE:O	2:B:759:PRO:HD3	2.13	0.49
2:B:906:SER:CB	2:B:946:ASN:HB2	2.43	0.49
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.78	0.49
7:I:50:THR:HG22	7:I:51:ASN:N	2.27	0.49
10:L:39:SER:O	10:L:40:LEU:HD23	2.13	0.49
1:A:57:ARG:HB3	1:A:68:GLN:NE2	2.28	0.49
1:A:878:ILE:HG21	1:A:955:PRO:HB2	1.93	0.49
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.47	0.49
2:B:862:GLN:NE2	2:B:963:PHE:CE1	2.81	0.49
2:B:1065:GLN:NE2	2:B:1067:ARG:HB2	2.23	0.49
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.48	0.49
3:C:260:LEU:HD12	3:C:260:LEU:O	2.12	0.49
4:E:93:MET:HG3	4:E:97:VAL:HG23	1.95	0.49
5:F:107:VAL:HG12	5:F:109:VAL:H	1.75	0.49
5:F:154:ASP:O	5:F:155:LEU:HD23	2.12	0.49
10:L:60:ARG:HG2	10:L:61:THR:N	2.25	0.49
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.95	0.49
2:B:296:GLU:O	2:B:300:HIS:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:HIS:O	2:B:735:ALA:N	2.46	0.49
1:A:32:VAL:HG22	1:A:81:PHE:O	2.12	0.49
1:A:32:VAL:CB	1:A:57:ARG:HD2	2.39	0.49
1:A:73:GLY:C	1:A:75:ASN:H	2.20	0.49
2:B:999:MET:HA	2:B:999:MET:HE3	1.95	0.49
3:C:89:GLU:O	3:C:90:ASP:CB	2.60	0.49
3:C:239:PRO:O	3:C:242:GLN:HB2	2.12	0.49
1:A:829:VAL:O	1:A:830:LYS:C	2.56	0.48
1:A:1102:LYS:HG2	1:A:1106:ASN:ND2	2.28	0.48
2:B:604:ARG:HH22	2:B:697:GLU:CD	2.21	0.48
2:B:792:MET:SD	2:B:857:ARG:NH2	2.86	0.48
2:B:821:GLN:OE1	2:B:850:LEU:HD12	2.13	0.48
2:B:877:PRO:O	2:B:878:GLN:HG3	2.12	0.48
10:L:61:THR:HG21	10:L:63:ARG:CD	2.40	0.48
1:A:56:PRO:O	1:A:57:ARG:CG	2.61	0.48
1:A:264:PHE:CD1	1:A:315:LEU:HB3	2.48	0.48
2:B:311:LEU:HB3	7:I:4:PHE:CE2	2.48	0.48
1:A:550:LEU:HD13	1:A:556:TRP:CZ2	2.48	0.48
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.95	0.48
1:A:282:ASN:C	1:A:283:GLY:O	2.57	0.48
1:A:326:ARG:O	1:A:330:LYS:HG3	2.13	0.48
1:A:559:VAL:HA	6:H:78:SER:HB3	1.96	0.48
1:A:971:PHE:O	1:A:972:HIS:C	2.55	0.48
1:A:1111:MET:HE1	1:A:1114:PRO:HA	1.96	0.48
1:A:1147:THR:HB	7:I:48:LEU:CD1	2.43	0.48
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.24	0.48
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.93	0.48
2:B:69:LEU:CD2	2:B:425:THR:HG23	2.42	0.48
2:B:816:GLU:O	8:J:56:LEU:HD21	2.14	0.48
3:C:20:PHE:CE1	3:C:22:LEU:HG	2.43	0.48
9:K:45:LEU:HG	9:K:94:ILE:HD13	1.94	0.48
1:A:264:PHE:CB	1:A:315:LEU:HD13	2.43	0.48
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	3.01	0.48
1:A:1169:ILE:O	1:A:1173:HIS:CD2	2.67	0.48
2:B:648:HIS:CD2	2:B:648:HIS:N	2.79	0.48
10:L:32:ALA:HB2	10:L:55:ILE:CG2	2.43	0.48
1:A:5:GLN:CG	1:A:6:TYR:H	2.26	0.48
1:A:535:THR:HG22	1:A:575:LYS:HE2	1.95	0.48
1:A:602:ASP:O	1:A:615:GLY:HA2	2.13	0.48
1:A:1171:GLN:C	1:A:1173:HIS:H	2.21	0.48
2:B:864:LYS:HD3	2:B:871:THR:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:THR:O	3:C:55:THR:HG22	2.14	0.48
6:H:4:THR:O	6:H:5:LEU:HD23	2.13	0.48
6:H:103:LYS:NZ	6:H:114:VAL:CG2	2.76	0.48
1:A:41:MET:O	1:A:42:ASP:HB2	2.13	0.48
1:A:345:VAL:HA	2:B:1150:ARG:NH1	2.23	0.48
1:A:763:ALA:O	1:A:803:SER:HB3	2.13	0.48
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.13	0.48
2:B:98:THR:HG22	2:B:99:LYS:N	2.28	0.48
2:B:199:MET:HG2	2:B:200:GLY:H	1.78	0.48
2:B:957:ASN:OD1	2:B:958:GLN:N	2.33	0.48
3:C:209:TYR:N	3:C:209:TYR:CD1	2.82	0.48
5:F:81:THR:HG21	5:F:136:ARG:CD	2.43	0.48
1:A:13:THR:CB	1:A:1432:GLN:NE2	2.77	0.48
1:A:313:GLN:HG2	1:A:322:VAL:CG1	2.43	0.48
1:A:492:PRO:HB2	1:A:497:THR:CG2	2.44	0.48
1:A:1386:ARG:HG3	1:A:1386:ARG:O	2.13	0.48
2:B:806:THR:HG22	2:B:809:MET:N	2.14	0.48
2:B:1098:MET:O	2:B:1099:VAL:C	2.57	0.48
3:C:57:VAL:CG1	8:J:60:PHE:HB3	2.43	0.48
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.38	0.48
4:E:129:PRO:O	4:E:130:ALA:C	2.56	0.48
8:J:2:ILE:HD11	8:J:57:ILE:HD12	1.96	0.48
1:A:596:THR:C	1:A:598:LEU:H	2.22	0.48
1:A:672:ASP:H	1:A:736:ASN:ND2	2.11	0.48
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.96	0.48
2:B:755:ILE:CG2	2:B:755:ILE:O	2.62	0.48
3:C:5:GLY:O	3:C:24:ASN:ND2	2.40	0.48
4:E:114:ASN:O	4:E:115:ASN:HB3	2.14	0.48
6:H:31:THR:O	6:H:32:THR:CB	2.61	0.48
6:H:138:GLU:O	6:H:139:ASN:C	2.56	0.48
1:A:857:ARG:HD3	1:A:861:GLY:O	2.13	0.48
1:A:1217:LYS:C	1:A:1219:THR:H	2.22	0.48
2:B:880:THR:O	2:B:882:THR:N	2.38	0.48
2:B:1202:LEU:O	2:B:1206:GLU:HG3	2.14	0.48
4:E:79:TRP:HB2	4:E:105:PHE:CE1	2.49	0.48
8:J:2:ILE:CG2	8:J:3:VAL:N	2.77	0.48
1:A:50:ILE:C	1:A:52:GLY:H	2.21	0.47
1:A:84:ILE:CG2	1:A:239:LEU:O	2.62	0.47
1:A:858:ASN:C	1:A:858:ASN:HD22	2.21	0.47
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.49	0.47
1:A:1146:VAL:O	1:A:1146:VAL:CG1	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1277:GLU:O	1:A:1278:ASN:CB	2.61	0.47
6:H:89:LEU:C	6:H:91:ASP:N	2.72	0.47
1:A:476:SER:N	1:A:477:PRO:HD2	2.29	0.47
1:A:858:ASN:HD21	1:A:862:ASN:H	1.62	0.47
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.49	0.47
2:B:1162:ILE:HD12	2:B:1194:ILE:HD13	1.95	0.47
8:J:12:LYS:NZ	8:J:17:LYS:NZ	2.63	0.47
1:A:329:LEU:HD23	1:A:332:LYS:HB2	1.96	0.47
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.14	0.47
2:B:879:ARG:HB3	2:B:883:LEU:HD22	1.93	0.47
3:C:53:THR:O	3:C:153:LEU:HA	2.13	0.47
4:E:38:PRO:HG2	4:E:41:ASP:OD2	2.14	0.47
4:E:88:VAL:HG21	4:E:110:PHE:HZ	1.79	0.47
4:E:94:LYS:CG	4:E:123:LEU:HD11	2.41	0.47
1:A:35:ILE:HG23	1:A:52:GLY:O	2.15	0.47
1:A:84:ILE:HG22	1:A:241:VAL:HG23	1.96	0.47
1:A:919:ILE:HD13	1:A:983:ILE:CD1	2.45	0.47
1:A:1111:MET:HE2	1:A:1331:SER:HB2	1.97	0.47
2:B:579:ARG:HG3	2:B:581:PHE:HE1	1.79	0.47
6:H:103:LYS:HZ2	6:H:114:VAL:CB	2.27	0.47
1:A:446:ARG:HB2	1:A:487:MET:SD	2.54	0.47
2:B:454:THR:O	2:B:458:LYS:HB2	2.15	0.47
2:B:710:LEU:HD23	2:B:738:PHE:CE1	2.49	0.47
3:C:120:ILE:HD13	3:C:124:LEU:HD11	1.96	0.47
3:C:185:LYS:HD2	3:C:213:PRO:HD3	1.96	0.47
1:A:982:THR:HG22	1:A:984:LYS:N	2.23	0.47
1:A:1067:LEU:HD13	13:B:3028:HOH:O	2.13	0.47
2:B:268:THR:CG2	2:B:270:LYS:HE3	2.43	0.47
2:B:616:ILE:CD1	2:B:696:GLU:HG3	2.44	0.47
2:B:650:GLU:HG2	2:B:654:ARG:NH1	2.29	0.47
3:C:43:THR:CG2	3:C:44:LEU:N	2.78	0.47
6:H:63:LEU:C	6:H:90:ALA:CB	2.87	0.47
6:H:81:PRO:CB	6:H:82:PRO:CD	2.92	0.47
8:J:36:LEU:HB2	8:J:47:ARG:HH21	1.80	0.47
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.96	0.47
1:A:606:LEU:HD11	1:A:608:ILE:HD11	1.96	0.47
1:A:696:GLU:OE2	1:A:702:LEU:HD23	2.15	0.47
2:B:100:PRO:HA	2:B:125:SER:O	2.15	0.47
2:B:915:THR:HG22	2:B:916:THR:N	2.30	0.47
4:E:93:MET:HG3	4:E:97:VAL:CG2	2.43	0.47
6:H:125:LEU:HB3	6:H:130:ARG:CZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:111:THR:CG2	7:I:112:SER:N	2.77	0.47
8:J:32:GLU:CD	8:J:32:GLU:H	2.22	0.47
1:A:1402:PHE:C	1:A:1404:GLU:N	2.72	0.47
2:B:175:ARG:HB3	2:B:175:ARG:HH11	1.78	0.47
2:B:408:LEU:HD11	2:B:545:ILE:HD12	1.96	0.47
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.95	0.47
4:E:88:VAL:HG21	4:E:110:PHE:CZ	2.50	0.47
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.15	0.47
1:A:329:LEU:HD21	2:B:1203:LEU:HD13	1.97	0.47
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.96	0.47
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.96	0.47
2:B:221:ASN:OD1	2:B:242:SER:HA	2.15	0.47
9:K:24:ASP:HB3	9:K:30:ALA:HB3	1.96	0.47
1:A:264:PHE:O	1:A:267:ALA:HB3	2.15	0.47
1:A:329:LEU:HD21	2:B:1203:LEU:CD1	2.45	0.47
2:B:126:SER:OG	2:B:172:ILE:HD12	2.15	0.47
3:C:25:VAL:HG23	3:C:228:PHE:CE1	2.50	0.47
7:I:69:PRO:HG2	7:I:85:PHE:O	2.15	0.47
1:A:761:MET:O	1:A:803:SER:HB2	2.15	0.46
2:B:172:ILE:HD11	2:B:178:ASN:ND2	2.31	0.46
1:A:114:LEU:HD13	1:A:171:GLN:OE1	2.15	0.46
1:A:130:ASP:CB	1:A:133:LYS:HB2	2.40	0.46
1:A:399:HIS:C	1:A:401:GLY:N	2.73	0.46
1:A:1391:ARG:HB3	1:A:1392:SER:H	1.59	0.46
2:B:130:VAL:CG1	2:B:131:ASP:H	2.22	0.46
2:B:357:GLN:OE1	2:B:358:LYS:HE3	2.16	0.46
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.97	0.46
2:B:882:THR:C	2:B:884:ARG:H	2.23	0.46
2:B:1004:GLU:HA	3:C:177:GLU:HG2	1.98	0.46
1:A:17:VAL:HA	2:B:1215:ARG:O	2.15	0.46
1:A:122:MET:HE1	1:A:138:ILE:CG2	2.44	0.46
1:A:567:LYS:HZ1	6:H:46:LEU:HD12	1.81	0.46
1:A:879:GLU:CD	1:A:962:ARG:HH22	2.23	0.46
2:B:1148:LYS:HE3	2:B:1152:MET:HE1	1.97	0.46
1:A:48:ALA:C	1:A:49:LYS:HG3	2.40	0.46
1:A:569:LYS:HE3	3:C:221:TYR:O	2.15	0.46
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.80	0.46
1:A:1171:GLN:O	1:A:1173:HIS:N	2.48	0.46
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.78	0.46
2:B:98:THR:O	2:B:126:SER:HB3	2.16	0.46
2:B:130:VAL:CG1	2:B:131:ASP:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:ALA:O	8:J:10:CYS:O	2.33	0.46
6:H:103:LYS:HZ2	6:H:114:VAL:HB	1.80	0.46
1:A:103:CYS:SG	1:A:207:ILE:HD12	2.56	0.46
1:A:318:SER:O	1:A:320:ARG:HG3	2.15	0.46
1:A:562:THR:HB	6:H:98:TYR:CE2	2.50	0.46
1:A:964:ILE:HD13	1:A:1035:TYR:CE1	2.49	0.46
1:A:982:THR:O	1:A:985:ASP:HB2	2.15	0.46
2:B:104:GLU:CD	10:L:54:ARG:CZ	2.89	0.46
2:B:284:ILE:HD13	2:B:324:ILE:HD12	1.96	0.46
7:I:113:ASP:O	7:I:116:ASN:CG	2.59	0.46
1:A:157:ASP:C	1:A:159:THR:N	2.71	0.46
1:A:571:LEU:HD22	6:H:46:LEU:HD11	1.98	0.46
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.97	0.46
1:A:47:ARG:HH12	1:A:255:SER:CA	2.07	0.46
1:A:164:ARG:O	1:A:165:GLY:C	2.59	0.46
1:A:322:VAL:CG2	1:A:323:LYS:N	2.78	0.46
1:A:326:ARG:CG	1:A:1406:VAL:HG21	2.42	0.46
1:A:1139:GLU:HG3	1:A:1280:GLU:O	2.15	0.46
2:B:731:VAL:CG1	2:B:732:SER:N	2.78	0.46
2:B:806:THR:HG22	2:B:809:MET:HB2	1.97	0.46
2:B:859:TYR:N	2:B:859:TYR:CD1	2.84	0.46
7:I:55:THR:O	7:I:58:VAL:HG23	2.15	0.46
7:I:90:GLN:O	7:I:91:ARG:HD3	2.15	0.46
10:L:48:CYS:HB3	10:L:51:CYS:O	2.16	0.46
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.46	0.46
1:A:817:ALA:HA	2:B:764:SER:OG	2.15	0.46
1:A:1113:THR:N	1:A:1114:PRO:HD3	2.31	0.46
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.98	0.46
2:B:63:ILE:CB	2:B:95:ILE:HD11	2.45	0.46
2:B:309:GLN:HE22	7:I:50:THR:HG21	1.81	0.46
2:B:1185:CYS:O	2:B:1186:ASP:HB2	2.15	0.46
5:F:82:THR:HG22	5:F:83:PRO:HD2	1.97	0.46
6:H:139:ASN:O	6:H:140:ALA:HB2	2.15	0.46
1:A:1161:THR:HG21	1:A:1239:ARG:NH2	2.31	0.46
1:A:1162:VAL:HG11	7:I:41:PRO:HG3	1.97	0.46
1:A:1169:ILE:O	1:A:1173:HIS:HD2	1.99	0.46
1:A:1256:GLU:O	1:A:1258:HIS:N	2.49	0.46
2:B:18:PHE:O	2:B:19:GLU:HB2	2.16	0.46
2:B:1103:ILE:O	2:B:1104:HIS:C	2.59	0.46
3:C:57:VAL:O	3:C:57:VAL:HG12	2.16	0.46
10:L:34:CYS:O	10:L:36:SER:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLN:HG2	1:A:6:TYR:H	1.80	0.46
1:A:93:VAL:HG13	1:A:301:ALA:CB	2.43	0.46
1:A:246:VAL:O	1:A:328:ARG:NH1	2.45	0.46
1:A:445:ASN:HD21	1:A:449:SER:HB3	1.79	0.46
2:B:365:THR:CG2	2:B:367:LEU:H	2.21	0.46
2:B:1002:THR:HG21	2:B:1006:ILE:HB	1.98	0.46
2:B:1065:GLN:HG3	2:B:1065:GLN:O	2.15	0.46
5:F:140:ASP:OD1	5:F:140:ASP:C	2.59	0.46
6:H:112:ILE:HD12	6:H:131:ASN:HD21	1.81	0.46
1:A:381:THR:HG23	1:A:383:TYR:N	2.20	0.45
1:A:1111:MET:CE	1:A:1331:SER:HB2	2.45	0.45
1:A:1446:ASP:CG	1:A:1448:GLU:HB2	2.41	0.45
2:B:108:VAL:HG12	2:B:109:THR:N	2.30	0.45
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.98	0.45
2:B:708:GLU:O	2:B:711:GLU:CD	2.59	0.45
3:C:52:GLU:HA	10:L:64:LEU:HD21	1.97	0.45
5:F:81:THR:CG2	5:F:82:THR:N	2.79	0.45
9:K:61:TYR:HA	9:K:72:LYS:O	2.16	0.45
1:A:108:MET:HA	1:A:210:ILE:HD13	1.98	0.45
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.17	0.45
2:B:104:GLU:CG	10:L:54:ARG:NH1	2.79	0.45
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.51	0.45
2:B:241:ARG:HG2	2:B:251:ILE:HG23	1.97	0.45
2:B:735:ALA:HB3	2:B:738:PHE:CE1	2.52	0.45
2:B:1100:ASP:HA	2:B:1103:ILE:CD1	2.45	0.45
4:E:14:ARG:O	4:E:17:ARG:HB3	2.15	0.45
4:E:64:PRO:HG2	4:E:75:MET:O	2.16	0.45
5:F:134:ILE:HD12	5:F:151:LEU:CD1	2.46	0.45
1:A:633:VAL:HG21	1:A:645:LEU:HD22	1.97	0.45
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.74	0.45
2:B:424:LEU:O	2:B:428:ILE:HG13	2.16	0.45
2:B:914:LYS:O	2:B:937:ALA:O	2.33	0.45
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.81	0.45
6:H:32:THR:HG22	6:H:33:GLN:N	2.31	0.45
6:H:103:LYS:HE2	6:H:116:TYR:CZ	2.51	0.45
9:K:111:LEU:N	9:K:111:LEU:HD23	2.31	0.45
1:A:45:GLN:O	1:A:47:ARG:N	2.49	0.45
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.97	0.45
1:A:345:VAL:HG13	2:B:1150:ARG:NH1	2.31	0.45
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.51	0.45
1:A:715:GLU:OE1	1:A:774:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.33	0.45
2:B:326:ASP:C	2:B:326:ASP:OD2	2.59	0.45
2:B:451:LYS:HE2	2:B:455:SER:OG	2.16	0.45
2:B:1035:ALA:HB1	2:B:1040:ASN:O	2.16	0.45
4:E:5:ASN:O	4:E:9:ILE:N	2.48	0.45
4:E:202:SER:O	4:E:205:SER:O	2.33	0.45
7:I:51:ASN:HB2	7:I:118:ARG:NH1	2.31	0.45
9:K:103:THR:O	9:K:104:ASN:C	2.59	0.45
1:A:32:VAL:CG2	1:A:58:LEU:HD23	2.47	0.45
1:A:106:VAL:HG22	1:A:111:GLY:HA2	1.99	0.45
1:A:805:LEU:CD1	2:B:1052:VAL:HG21	2.47	0.45
1:A:858:ASN:C	1:A:858:ASN:ND2	2.74	0.45
1:A:1015:VAL:CG1	1:A:1015:VAL:O	2.63	0.45
3:C:17:ASN:HA	3:C:232:VAL:O	2.16	0.45
4:E:19:VAL:HG11	4:E:80:VAL:HG11	1.96	0.45
4:E:31:THR:C	4:E:33:GLU:H	2.24	0.45
4:E:204:THR:CG2	4:E:205:SER:N	2.76	0.45
1:A:92:HIS:CD2	1:A:92:HIS:C	2.94	0.45
1:A:167:CYS:O	1:A:167:CYS:SG	2.75	0.45
1:A:382:PRO:HD2	5:F:104:ASN:OD1	2.16	0.45
1:A:994:GLN:HG2	1:A:1019:CYS:SG	2.56	0.45
1:A:1146:VAL:HG12	1:A:1146:VAL:O	2.16	0.45
1:A:1336:MET:HE1	1:A:1380:GLY:HA2	1.98	0.45
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.64	0.45
2:B:254:LEU:HD23	2:B:361:LEU:HD21	1.99	0.45
6:H:62:SER:O	6:H:63:LEU:O	2.34	0.45
6:H:105:GLU:H	6:H:105:GLU:CD	2.24	0.45
10:L:25:ALA:O	10:L:26:THR:HB	2.16	0.45
1:A:806:ARG:NH1	2:B:729:ILE:HD11	2.31	0.45
2:B:169:ARG:N	2:B:454:THR:OG1	2.49	0.45
3:C:40:GLU:OE2	3:C:254:LYS:NZ	2.47	0.45
3:C:78:GLU:C	3:C:80:LEU:H	2.24	0.45
4:E:114:ASN:OD1	4:E:115:ASN:N	2.50	0.45
6:H:12:VAL:HA	6:H:28:ALA:CB	2.46	0.45
6:H:26:ILE:CD1	6:H:42:ILE:HD12	2.31	0.45
6:H:89:LEU:O	6:H:91:ASP:N	2.49	0.45
1:A:220:THR:O	1:A:222:LEU:O	2.35	0.45
1:A:239:LEU:C	1:A:239:LEU:HD23	2.42	0.45
1:A:92:HIS:HE1	2:B:1210:MET:O	2.00	0.45
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.98	0.45
1:A:35:ILE:CD1	1:A:241:VAL:HG21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:C	1:A:141:LEU:HD21	2.41	0.45
1:A:157:ASP:C	1:A:159:THR:H	2.26	0.45
1:A:1079:MET:SD	1:A:1359:ASP:OD2	2.75	0.45
2:B:227:LYS:HD3	2:B:236:HIS:CE1	2.51	0.45
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.31	0.45
3:C:8:VAL:HG21	9:K:105:PHE:CB	2.45	0.45
6:H:100:THR:HG22	6:H:101:ALA:N	2.32	0.45
7:I:45:ARG:NH1	7:I:45:ARG:CG	2.77	0.45
1:A:63:ARG:CA	1:A:74:MET:HE2	2.39	0.44
1:A:95:PHE:O	1:A:99:ILE:HG13	2.17	0.44
1:A:185:TRP:O	1:A:186:LYS:HB2	2.17	0.44
1:A:278:THR:O	1:A:278:THR:HG22	2.17	0.44
1:A:307:ASP:C	1:A:308:ILE:HG13	2.43	0.44
1:A:535:THR:CG2	1:A:575:LYS:HE2	2.47	0.44
1:A:1127:ASP:C	1:A:1129:GLU:N	2.74	0.44
1:A:1281:ARG:HD2	1:A:1309:ASP:CG	2.43	0.44
1:A:1336:MET:CE	1:A:1380:GLY:HA2	2.48	0.44
2:B:1222:ARG:C	2:B:1224:PHE:H	2.23	0.44
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.99	0.44
4:E:147:HIS:CD2	4:E:149:LEU:H	2.35	0.44
6:H:130:ARG:CA	6:H:133:ASN:HD22	2.12	0.44
1:A:44:THR:O	1:A:45:GLN:CB	2.65	0.44
1:A:511:ILE:O	1:A:519:PRO:HA	2.17	0.44
1:A:1152:ILE:HA	1:A:1192:LEU:O	2.18	0.44
2:B:235:SER:OG	2:B:236:HIS:HD2	2.00	0.44
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.51	0.44
2:B:860:MET:O	2:B:861:ASP:HB2	2.17	0.44
2:B:1099:VAL:C	2:B:1101:ASP:H	2.25	0.44
7:I:111:THR:CG2	7:I:113:ASP:H	2.06	0.44
8:J:2:ILE:HG22	8:J:3:VAL:H	1.82	0.44
1:A:684:ALA:O	1:A:688:LYS:HG3	2.17	0.44
2:B:102:VAL:HG22	2:B:112:LEU:HD13	2.00	0.44
2:B:502:ILE:O	2:B:502:ILE:HG22	2.16	0.44
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.51	0.44
2:B:899:ILE:HG22	2:B:900:ALA:H	1.81	0.44
2:B:1162:ILE:HG22	2:B:1163:CYS:O	2.18	0.44
2:B:1162:ILE:CD1	2:B:1216:LEU:HD12	2.46	0.44
1:A:67:CYS:O	1:A:70:CYS:SG	2.76	0.44
2:B:280:ILE:HA	2:B:281:PRO:HD2	1.89	0.44
3:C:99:LEU:HD12	3:C:99:LEU:N	2.32	0.44
3:C:148:ARG:HG2	3:C:149:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:79:ARG:HB3	5:F:144:GLU:OE1	2.18	0.44
7:I:115:LYS:O	7:I:116:ASN:C	2.60	0.44
9:K:68:PHE:CD1	9:K:68:PHE:N	2.86	0.44
1:A:5:GLN:HG2	1:A:6:TYR:N	2.33	0.44
1:A:794:PRO:HG2	1:A:795:GLU:OE2	2.17	0.44
2:B:25:ILE:HD13	2:B:658:ILE:HD11	1.99	0.44
2:B:879:ARG:NE	2:B:885:MET:HE2	2.22	0.44
3:C:34:ARG:NH1	3:C:35:ARG:HG2	2.32	0.44
3:C:97:VAL:HB	3:C:159:ALA:HB3	1.99	0.44
10:L:53:HIS:C	10:L:55:ILE:N	2.75	0.44
1:A:55:ASP:C	1:A:57:ARG:N	2.75	0.44
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.99	0.44
1:A:1260:LEU:HD12	1:A:1260:LEU:HA	1.85	0.44
1:A:1422:ARG:HA	1:A:1435:PRO:CG	2.48	0.44
2:B:726:ALA:CB	2:B:1051:THR:HG21	2.35	0.44
2:B:916:THR:O	2:B:935:ARG:HB2	2.17	0.44
3:C:42:PRO:HB3	3:C:161:LYS:HE3	1.98	0.44
6:H:79:TRP:HA	6:H:80:ARG:N	2.15	0.44
7:I:4:PHE:CD2	7:I:4:PHE:N	2.81	0.44
9:K:7:PHE:CD1	9:K:7:PHE:C	2.95	0.44
1:A:672:ASP:H	1:A:736:ASN:HD21	1.63	0.44
1:A:1001:ARG:O	1:A:1002:GLY:C	2.61	0.44
1:A:1111:MET:HE3	1:A:1114:PRO:CG	2.45	0.44
2:B:549:THR:CG2	2:B:550:ASP:N	2.80	0.44
2:B:936:ASP:OD1	2:B:936:ASP:C	2.60	0.44
2:B:1160:VAL:CG1	2:B:1161:HIS:N	2.80	0.44
3:C:214:ASN:HB2	3:C:217:ASP:CG	2.43	0.44
1:A:34:LYS:HG3	1:A:83:HIS:CD2	2.53	0.44
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.00	0.44
1:A:313:GLN:HB3	1:A:321:PRO:C	2.42	0.44
1:A:412:ARG:NH2	1:A:433:GLU:OE2	2.50	0.44
1:A:775:ILE:O	1:A:797:LYS:HE3	2.17	0.44
1:A:1204:ASP:OD1	1:A:1204:ASP:C	2.61	0.44
1:A:1328:TYR:CG	1:A:1329:THR:N	2.85	0.44
2:B:360:PHE:O	2:B:361:LEU:C	2.61	0.44
2:B:756:ILE:HG12	2:B:770:GLN:HG2	1.98	0.44
3:C:22:LEU:HD23	3:C:22:LEU:HA	1.87	0.44
4:E:159:ASP:HA	4:E:162:ARG:HH11	1.82	0.44
9:K:108:GLU:O	9:K:112:GLN:HG2	2.18	0.44
1:A:709:THR:HG22	1:A:710:LEU:N	2.33	0.44
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:620:ARG:NH1	7:I:68:LEU:HD21	2.33	0.44
2:B:724:ASP:HB3	2:B:727:LYS:HG3	1.99	0.44
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.51	0.44
1:A:5:GLN:CG	1:A:6:TYR:N	2.81	0.43
1:A:41:MET:HG2	1:A:48:ALA:O	2.18	0.43
1:A:179:LEU:HD21	1:A:308:ILE:CD1	2.43	0.43
1:A:1138:ILE:CG2	1:A:1279:ILE:HG21	2.47	0.43
2:B:357:GLN:O	2:B:357:GLN:HG2	2.17	0.43
4:E:156:LEU:HD21	4:E:197:LYS:HB2	2.00	0.43
1:A:114:LEU:HD13	1:A:171:GLN:NE2	2.33	0.43
1:A:329:LEU:C	1:A:331:GLY:N	2.75	0.43
1:A:789:LYS:O	1:A:790:ASP:HB2	2.18	0.43
1:A:868:TYR:CZ	1:A:1366:ARG:HD3	2.53	0.43
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.17	0.43
2:B:293:PRO:HA	7:I:12:ASN:HD21	1.82	0.43
2:B:420:LEU:HD11	2:B:456:GLY:HA3	1.98	0.43
2:B:526:GLU:HG2	2:B:526:GLU:O	2.18	0.43
2:B:796:LEU:HD12	2:B:796:LEU:HA	1.87	0.43
2:B:1020:ARG:O	2:B:1021:MET:HB2	2.18	0.43
2:B:1154:ALA:O	2:B:1155:SER:C	2.60	0.43
3:C:134:ILE:CG2	3:C:139:GLY:HA2	2.48	0.43
7:I:50:THR:CB	7:I:92:ARG:HH22	2.31	0.43
1:A:43:GLU:O	1:A:44:THR:HB	2.17	0.43
1:A:90:VAL:HG12	1:A:91:PHE:O	2.19	0.43
1:A:854:ASN:HD22	1:A:1000:LEU:HD23	1.82	0.43
1:A:1394:THR:CG2	1:A:1395:GLY:N	2.65	0.43
2:B:487:THR:HG22	2:B:489:SER:N	2.33	0.43
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.18	0.43
3:C:124:LEU:HD22	3:C:129:ILE:HG22	2.01	0.43
5:F:93:ILE:CD1	5:F:148:VAL:HG22	2.49	0.43
6:H:103:LYS:CE	6:H:116:TYR:CZ	3.02	0.43
1:A:705:LYS:O	1:A:706:HIS:C	2.61	0.43
1:A:709:THR:HB	1:A:712:GLU:H	1.83	0.43
1:A:760:GLN:HB2	2:B:1021:MET:CE	2.44	0.43
1:A:1100:ARG:HD2	1:A:1100:ARG:O	2.18	0.43
3:C:100:THR:HG22	3:C:101:LEU:N	2.34	0.43
3:C:242:GLN:O	3:C:243:VAL:C	2.62	0.43
4:E:86:PRO:HA	4:E:113:GLN:HB2	2.00	0.43
6:H:27:GLU:HA	6:H:38:LEU:O	2.17	0.43
7:I:103:CYS:HB3	7:I:108:HIS:H	1.83	0.43
9:K:7:PHE:HA	9:K:10:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:CYS:HB3	1:A:167:CYS:O	2.19	0.43
1:A:246:VAL:O	1:A:248:PRO:HD3	2.19	0.43
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.54	0.43
1:A:1295:THR:O	1:A:1295:THR:HG22	2.17	0.43
2:B:339:THR:HG23	2:B:343:ILE:HB	2.01	0.43
2:B:623:GLU:OE1	2:B:625:LYS:HE3	2.18	0.43
2:B:1181:GLU:CD	2:B:1188:LYS:HE2	2.43	0.43
5:F:111:LEU:C	5:F:113:GLY:N	2.73	0.43
9:K:90:ALA:O	9:K:94:ILE:HG13	2.19	0.43
1:A:172:PRO:HB3	1:A:185:TRP:CZ2	2.54	0.43
1:A:598:LEU:HG	6:H:115:TYR:CE2	2.52	0.43
1:A:738:LYS:HZ1	3:C:194:GLU:C	2.26	0.43
1:A:914:GLU:HB2	1:A:979:SER:O	2.19	0.43
2:B:63:ILE:CD1	2:B:95:ILE:HD11	2.49	0.43
2:B:463:THR:HG21	2:B:465:ASN:CG	2.44	0.43
2:B:636:PRO:HA	2:B:691:GLU:O	2.19	0.43
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.49	0.43
7:I:55:THR:O	7:I:55:THR:CG2	2.65	0.43
1:A:219:PHE:CD1	1:A:219:PHE:C	2.97	0.43
1:A:626:ASN:O	1:A:631:HIS:HD2	2.00	0.43
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.18	0.43
1:A:1421:CYS:HA	1:A:1426:GLU:OE1	2.19	0.43
2:B:29:ASP:HB3	2:B:658:ILE:HD12	1.91	0.43
2:B:952:VAL:HB	10:L:58:LYS:CB	2.46	0.43
6:H:17:PRO:O	6:H:18:GLY:C	2.61	0.43
9:K:1:MET:HG3	9:K:2:ASN:N	2.33	0.43
10:L:61:THR:HB	10:L:63:ARG:HG2	2.00	0.43
1:A:535:THR:HG22	1:A:616:VAL:HA	2.01	0.43
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.32	0.43
1:A:1220:PHE:O	1:A:1221:LYS:C	2.62	0.43
2:B:227:LYS:NZ	2:B:236:HIS:HE1	2.17	0.43
2:B:638:PHE:CE2	2:B:653:VAL:HG21	2.54	0.43
4:E:45:LYS:HG2	4:E:45:LYS:O	2.18	0.43
6:H:99:GLY:N	6:H:118:PHE:CD2	2.87	0.43
7:I:95:THR:CG2	7:I:96:SER:N	2.79	0.43
8:J:48:ARG:HG3	8:J:49:MET:N	2.33	0.43
9:K:30:ALA:HB2	9:K:76:GLN:HG3	2.01	0.43
1:A:49:LYS:HB3	1:A:55:ASP:HB2	2.00	0.43
1:A:84:ILE:CG2	1:A:241:VAL:HG23	2.48	0.43
1:A:557:ASP:N	1:A:557:ASP:OD1	2.51	0.43
1:A:786:HIS:HE1	2:B:742:GLU:OE2	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:ASP:OD2	2:B:515:HIS:HE1	2.01	0.43
4:E:28:TYR:CE2	4:E:78:LEU:HG	2.54	0.43
4:E:45:LYS:HE2	4:E:46:TYR:CZ	2.54	0.43
4:E:58:MET:O	4:E:59:SER:C	2.62	0.43
6:H:11:GLN:HE22	6:H:52:GLN:HA	1.80	0.43
6:H:47:PHE:CD2	6:H:47:PHE:O	2.71	0.43
1:A:69:THR:HB	2:B:1174:LYS:HE2	2.01	0.43
1:A:261:ASP:O	1:A:264:PHE:HB2	2.19	0.43
1:A:347:PHE:H	2:B:1107:ALA:HA	1.84	0.43
1:A:565:ILE:HG23	1:A:567:LYS:HE2	2.00	0.43
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.18	0.43
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.19	0.43
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.19	0.43
2:B:487:THR:CG2	2:B:488:TYR:N	2.82	0.43
3:C:179:GLU:HG3	3:C:180:TYR:H	1.82	0.43
5:F:76:LYS:C	5:F:79:ARG:HD2	2.41	0.43
5:F:140:ASP:OD1	5:F:141:GLY:N	2.51	0.43
6:H:111:LEU:HB3	6:H:127:GLY:O	2.18	0.43
9:K:63:VAL:HG22	9:K:63:VAL:O	2.19	0.43
10:L:46:VAL:HG13	10:L:56:LEU:CD1	2.40	0.43
10:L:49:LYS:HA	10:L:49:LYS:HD3	1.77	0.43
1:A:907:THR:CG2	1:A:908:LEU:N	2.81	0.42
1:A:946:VAL:CG2	4:E:201:LYS:HD2	2.48	0.42
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.19	0.42
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.54	0.42
2:B:1127:GLY:O	2:B:1128:LEU:CB	2.65	0.42
5:F:81:THR:HG21	5:F:136:ARG:HD3	2.01	0.42
6:H:123:MET:HE1	6:H:142:LEU:HD11	1.99	0.42
7:I:59:VAL:HG12	7:I:60:GLN:N	2.33	0.42
8:J:12:LYS:HZ1	8:J:17:LYS:NZ	2.16	0.42
1:A:54:ASN:O	1:A:55:ASP:HB2	2.18	0.42
1:A:313:GLN:HB3	1:A:321:PRO:N	2.34	0.42
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.52	0.42
1:A:557:ASP:O	1:A:559:VAL:N	2.53	0.42
2:B:108:VAL:CG1	2:B:109:THR:N	2.82	0.42
2:B:858:SER:HA	2:B:966:VAL:O	2.20	0.42
8:J:57:ILE:HA	8:J:60:PHE:CD2	2.54	0.42
10:L:30:ILE:O	10:L:56:LEU:HA	2.19	0.42
1:A:311:GLN:O	1:A:313:GLN:HG3	2.20	0.42
1:A:834:THR:HG21	1:A:1077:THR:CA	2.49	0.42
2:B:276:ILE:HG23	2:B:337:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:645:SER:O	2:B:646:LEU:C	2.61	0.42
2:B:757:PRO:HG2	2:B:984:HIS:HE1	1.85	0.42
2:B:872:GLU:HA	2:B:915:THR:O	2.18	0.42
4:E:55:ARG:HB2	4:E:84:ASP:OD2	2.20	0.42
4:E:71:LYS:C	4:E:73:PRO:HD3	2.44	0.42
6:H:142:LEU:O	6:H:143:LEU:HD23	2.18	0.42
9:K:28:PRO:O	9:K:29:ASN:HB2	2.20	0.42
9:K:56:VAL:HA	9:K:77:THR:HG22	2.00	0.42
1:A:31:SER:HB2	1:A:83:HIS:HB2	2.00	0.42
1:A:407:ARG:O	1:A:408:ASP:C	2.63	0.42
1:A:740:LEU:N	1:A:740:LEU:CD1	2.82	0.42
1:A:871:ASP:CG	4:E:204:THR:HG23	2.45	0.42
1:A:879:GLU:O	1:A:955:PRO:HA	2.20	0.42
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.84	0.42
1:A:1395:GLY:C	1:A:1397:LEU:N	2.69	0.42
2:B:969:ARG:HB3	2:B:969:ARG:NH1	2.33	0.42
3:C:265:MET:HE1	9:K:19:LEU:CB	2.42	0.42
6:H:24:CYS:SG	6:H:44:VAL:HG21	2.60	0.42
8:J:48:ARG:HH11	8:J:48:ARG:CG	2.31	0.42
10:L:61:THR:CG2	10:L:63:ARG:HG2	2.50	0.42
1:A:324:SER:H	1:A:327:ALA:HB3	1.84	0.42
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	2.02	0.42
1:A:1258:HIS:O	1:A:1262:LYS:HG3	2.20	0.42
1:A:1434:ALA:O	1:A:1436:ILE:N	2.46	0.42
2:B:899:ILE:CG2	2:B:900:ALA:N	2.81	0.42
4:E:136:ASN:O	4:E:137:GLU:C	2.62	0.42
5:F:85:MET:HE2	5:F:93:ILE:HD12	2.01	0.42
6:H:93:TYR:CD1	6:H:93:TYR:N	2.87	0.42
1:A:44:THR:O	1:A:44:THR:HG22	2.19	0.42
1:A:114:LEU:HD13	1:A:171:GLN:CD	2.44	0.42
1:A:367:PRO:HB3	1:A:465:TYR:O	2.19	0.42
1:A:699:ALA:O	1:A:700:ASN:HB3	2.20	0.42
1:A:1015:VAL:HG13	1:A:1019:CYS:SG	2.60	0.42
1:A:1215:ARG:CA	1:A:1218:GLN:HG2	2.50	0.42
1:A:1259:MET:O	1:A:1263:ILE:HG13	2.19	0.42
2:B:63:ILE:O	2:B:63:ILE:HG23	2.19	0.42
2:B:972:LYS:HD3	2:B:1098:MET:SD	2.59	0.42
2:B:978:ASP:O	2:B:989:THR:HA	2.20	0.42
2:B:1177:HIS:HB3	2:B:1179:GLN:HE21	1.83	0.42
3:C:44:LEU:CG	3:C:159:ALA:HB1	2.49	0.42
3:C:51:VAL:HG12	10:L:60:ARG:HH12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:98:ILE:O	4:E:102:GLU:HG3	2.20	0.42
7:I:111:THR:HG22	7:I:112:SER:N	2.34	0.42
8:J:36:LEU:HD11	8:J:51:LEU:HB2	2.01	0.42
1:A:130:ASP:C	1:A:132:LYS:N	2.74	0.42
1:A:486:GLU:OE1	2:B:1102:LYS:HD3	2.20	0.42
1:A:492:PRO:HG3	1:A:501:LEU:HD12	2.02	0.42
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.84	0.42
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.34	0.42
5:F:138:LEU:HD12	5:F:142:SER:OG	2.19	0.42
6:H:55:LEU:HD22	6:H:144:ILE:CG2	2.50	0.42
7:I:15:TYR:CZ	7:I:30:ARG:HD2	2.54	0.42
10:L:30:ILE:CG2	10:L:31:CYS:N	2.82	0.42
1:A:68:GLN:O	1:A:69:THR:HB	2.20	0.42
1:A:535:THR:CG2	1:A:616:VAL:HA	2.49	0.42
1:A:884:ASP:OD2	1:A:1030:ARG:NH2	2.50	0.42
1:A:1145:SER:HB2	1:A:1205:LYS:NZ	2.34	0.42
2:B:446:LEU:O	2:B:447:ALA:HB3	2.20	0.42
2:B:496:ARG:NH2	2:B:541:LEU:HA	2.34	0.42
2:B:847:ASP:O	3:C:65:HIS:HE1	2.02	0.42
2:B:877:PRO:C	2:B:878:GLN:HG3	2.45	0.42
2:B:881:ASN:HB2	2:B:933:SER:OG	2.20	0.42
3:C:114:TYR:HB3	3:C:140:ASN:O	2.20	0.42
3:C:179:GLU:CG	3:C:180:TYR:N	2.82	0.42
4:E:58:MET:O	4:E:59:SER:O	2.38	0.42
1:A:225:ASN:OD1	1:A:225:ASN:C	2.63	0.42
1:A:368:LYS:HE3	1:A:368:LYS:HB2	1.66	0.42
1:A:795:GLU:CD	1:A:795:GLU:H	2.27	0.42
1:A:856:THR:HB	1:A:865:GLN:HB2	2.01	0.42
1:A:1336:MET:HE1	1:A:1380:GLY:C	2.44	0.42
1:A:1342:GLU:CG	4:E:198:ILE:HD13	2.49	0.42
1:A:1401:SER:O	1:A:1402:PHE:HB2	2.20	0.42
2:B:89:GLU:N	2:B:135:ARG:O	2.53	0.42
2:B:125:SER:HA	2:B:171:PRO:HA	2.01	0.42
2:B:512:ARG:HB2	2:B:534:GLY:HA3	2.02	0.42
1:A:49:LYS:HB3	1:A:55:ASP:CB	2.49	0.42
1:A:475:THR:HG22	1:A:476:SER:N	2.34	0.42
1:A:836:TYR:O	1:A:840:ARG:HG2	2.20	0.42
1:A:946:VAL:HG22	4:E:201:LYS:CD	2.49	0.42
1:A:1394:THR:HA	1:A:1398:MET:CE	2.50	0.42
1:A:1410:PHE:HD2	2:B:1212:ILE:CD1	2.33	0.42
1:A:1434:ALA:C	1:A:1436:ILE:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:MET:O	2:B:313:MET:HB2	2.20	0.42
2:B:571:PRO:C	2:B:573:GLN:N	2.77	0.42
2:B:863:GLU:CD	2:B:962:LYS:HD2	2.45	0.42
3:C:64:ALA:HA	3:C:67:LEU:HD12	2.01	0.42
3:C:71:PRO:O	3:C:72:LEU:HD23	2.19	0.42
7:I:75:CYS:O	7:I:77:LYS:N	2.53	0.42
10:L:34:CYS:C	10:L:36:SER:N	2.77	0.42
1:A:40:THR:O	1:A:41:MET:HB2	2.20	0.41
1:A:125:ALA:O	1:A:134:ARG:HG3	2.20	0.41
2:B:863:GLU:OE1	2:B:962:LYS:HD2	2.20	0.41
5:F:74:ILE:HG23	5:F:75:PRO:HD2	2.01	0.41
6:H:18:GLY:O	6:H:20:TYR:N	2.52	0.41
1:A:329:LEU:O	1:A:333:GLU:HG2	2.20	0.41
2:B:181:LEU:HD22	2:B:189:LEU:HD23	2.01	0.41
2:B:239:GLU:HG2	2:B:255:GLN:HG2	2.02	0.41
2:B:274:PRO:HG3	2:B:359:GLU:HB3	2.01	0.41
2:B:335:GLY:O	2:B:339:THR:HB	2.20	0.41
3:C:263:THR:HG22	3:C:264:GLN:N	2.34	0.41
4:E:144:ILE:HG13	4:E:145:THR:N	2.34	0.41
7:I:17:ARG:HG3	7:I:28:GLU:OE1	2.20	0.41
7:I:75:CYS:C	7:I:77:LYS:H	2.27	0.41
8:J:5:VAL:HG12	8:J:6:ARG:HG2	2.02	0.41
8:J:23:ASN:O	8:J:24:LEU:C	2.63	0.41
1:A:450:LEU:CB	1:A:838:GLN:NE2	2.83	0.41
1:A:914:GLU:C	1:A:916:GLY:H	2.29	0.41
1:A:1121:GLU:HG3	1:A:1122:PRO:HD2	2.02	0.41
1:A:1163:ILE:HA	1:A:1164:PRO:HD2	1.90	0.41
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.20	0.41
1:A:1199:ARG:CG	1:A:1236:LEU:HD11	2.50	0.41
2:B:92:PHE:CD2	2:B:132:VAL:HG22	2.56	0.41
2:B:314:LEU:O	2:B:317:CYS:HB2	2.20	0.41
2:B:324:ILE:HD11	2:B:333:PHE:CG	2.55	0.41
1:A:336:ILE:O	1:A:336:ILE:HG22	2.20	0.41
1:A:340:LEU:HD13	1:A:1399:ARG:HA	2.02	0.41
1:A:451:HIS:CG	1:A:1074:GLU:HG3	2.55	0.41
1:A:465:TYR:CE2	9:K:4:PRO:HD2	2.54	0.41
1:A:531:ILE:HG23	1:A:617:VAL:O	2.21	0.41
3:C:112:ASN:CB	3:C:114:TYR:CE1	3.04	0.41
3:C:166:GLU:HG2	10:L:70:ARG:NH1	2.35	0.41
3:C:186:LEU:N	3:C:186:LEU:HD12	2.36	0.41
3:C:237:SER:O	3:C:238:ILE:HG13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.50	0.41
4:E:62:ALA:O	4:E:77:SER:HB2	2.20	0.41
9:K:76:GLN:HE21	9:K:76:GLN:HB3	1.69	0.41
1:A:82:GLY:HA3	1:A:241:VAL:HB	2.02	0.41
1:A:112:LYS:NZ	1:A:164:ARG:HB2	2.35	0.41
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	2.02	0.41
1:A:751:SER:O	1:A:752:LYS:C	2.64	0.41
1:A:1111:MET:HE3	1:A:1111:MET:HB2	1.90	0.41
2:B:344:LYS:H	2:B:347:LYS:HE3	1.85	0.41
2:B:457:LEU:O	2:B:458:LYS:C	2.64	0.41
2:B:549:THR:HG22	2:B:628:THR:CG2	2.51	0.41
4:E:50:MET:HE3	4:E:50:MET:O	2.20	0.41
4:E:98:ILE:HG22	4:E:102:GLU:OE1	2.20	0.41
1:A:548:ASN:HA	9:K:60:ALA:HB1	2.01	0.41
1:A:1391:ARG:O	1:A:1392:SER:HB3	2.21	0.41
2:B:274:PRO:O	2:B:275:TYR:HB2	2.21	0.41
6:H:100:THR:HG23	6:H:138:GLU:CB	2.50	0.41
9:K:18:LYS:O	9:K:19:LEU:HD23	2.20	0.41
1:A:267:ALA:O	1:A:271:LYS:HG3	2.20	0.41
1:A:548:ASN:ND2	9:K:47:ARG:HH21	2.19	0.41
1:A:849:MET:HE1	1:A:1437:GLY:N	2.35	0.41
2:B:365:THR:CG2	2:B:366:GLN:N	2.84	0.41
2:B:564:GLU:OE2	2:B:591:ARG:NE	2.47	0.41
4:E:40:GLU:OE1	4:E:43:LYS:HD2	2.21	0.41
6:H:17:PRO:HB3	6:H:24:CYS:SG	2.61	0.41
7:I:43:VAL:O	7:I:43:VAL:HG12	2.20	0.41
1:A:262:LEU:HD11	1:A:328:ARG:HD2	2.03	0.41
1:A:853:ASP:CG	1:A:855:THR:HB	2.46	0.41
1:A:901:LEU:HG	1:A:929:LEU:HD12	2.03	0.41
1:A:1187:GLN:HG3	1:A:1188:GLN:N	2.34	0.41
1:A:1422:ARG:HA	1:A:1435:PRO:HG3	2.03	0.41
1:A:1448:GLU:O	1:A:1449:SER:C	2.64	0.41
2:B:174:LEU:HD22	2:B:202:TYR:CZ	2.56	0.41
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.35	0.41
1:A:16:GLU:HG3	2:B:1220:ARG:HA	2.03	0.41
1:A:32:VAL:HB	1:A:57:ARG:HB3	2.03	0.41
1:A:774:ARG:CB	1:A:797:LYS:HG2	2.51	0.41
1:A:1171:GLN:C	1:A:1173:HIS:N	2.79	0.41
1:A:1318:THR:CG2	4:E:11:ARG:HH12	2.34	0.41
1:A:1384:VAL:O	1:A:1386:ARG:N	2.48	0.41
2:B:174:LEU:HD22	2:B:202:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:429:PHE:HA	2:B:432:MET:HE3	2.02	0.41
2:B:666:TYR:C	2:B:668:ASP:H	2.29	0.41
2:B:744:HIS:CD2	2:B:746:SER:H	2.38	0.41
2:B:806:THR:HG23	2:B:808:ALA:H	1.86	0.41
2:B:1084:GLN:HE22	3:C:192:TRP:N	2.16	0.41
2:B:1109:GLY:H	2:B:1110:PRO:HD2	1.85	0.41
2:B:1148:LYS:HG3	2:B:1152:MET:CE	2.51	0.41
3:C:33:LEU:HG	3:C:37:MET:HE2	2.02	0.41
3:C:238:ILE:HG23	3:C:242:GLN:HB2	2.02	0.41
3:C:248:ILE:HD13	9:K:101:LEU:HD13	2.03	0.41
3:C:252:GLN:HE22	9:K:99:GLY:HA2	1.86	0.41
4:E:28:TYR:CE1	4:E:75:MET:HE2	2.56	0.41
4:E:40:GLU:OE1	4:E:40:GLU:HA	2.21	0.41
4:E:116:ILE:CG2	4:E:117:THR:N	2.84	0.41
8:J:12:LYS:NZ	8:J:17:LYS:HZ2	2.19	0.41
1:A:834:THR:CG2	1:A:1077:THR:OG1	2.69	0.41
1:A:1394:THR:CA	1:A:1398:MET:HE3	2.50	0.41
2:B:519:TRP:CD1	2:B:519:TRP:C	2.99	0.41
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.49	0.41
2:B:784:ASN:O	2:B:788:ARG:HG3	2.21	0.41
2:B:787:VAL:O	2:B:787:VAL:HG12	2.19	0.41
3:C:8:VAL:HG11	9:K:105:PHE:CD1	2.56	0.41
5:F:85:MET:HB2	5:F:151:LEU:HB3	2.03	0.41
5:F:109:VAL:HG22	5:F:129:LYS:HD2	2.03	0.41
1:A:269:ILE:HD11	1:A:303:TYR:CB	2.50	0.40
1:A:338:GLY:HA2	1:A:341:MET:HE3	2.02	0.40
1:A:1221:LYS:HD2	1:A:1223:ASP:OD2	2.21	0.40
2:B:549:THR:HG22	2:B:628:THR:HG23	2.03	0.40
2:B:589:VAL:CG1	2:B:590:HIS:N	2.83	0.40
2:B:862:GLN:HB3	2:B:863:GLU:H	1.59	0.40
2:B:872:GLU:OE2	2:B:914:LYS:HE2	2.21	0.40
2:B:914:LYS:CB	2:B:937:ALA:O	2.63	0.40
2:B:1222:ARG:H	2:B:1222:ARG:HG3	1.63	0.40
3:C:114:TYR:CD1	3:C:114:TYR:N	2.90	0.40
3:C:180:TYR:CD1	3:C:180:TYR:C	2.99	0.40
10:L:26:THR:CG2	10:L:27:LEU:N	2.84	0.40
1:A:565:ILE:CG2	1:A:567:LYS:HG2	2.43	0.40
1:A:872:GLY:O	1:A:1058:VAL:HG12	2.21	0.40
2:B:89:GLU:HB2	2:B:137:TYR:CD1	2.57	0.40
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.55	0.40
2:B:911:ILE:HD11	2:B:941:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1153:GLU:CG	2:B:1154:ALA:N	2.78	0.40
6:H:106:GLU:O	6:H:107:VAL:C	2.62	0.40
7:I:75:CYS:HB3	7:I:110:PHE:CE2	2.56	0.40
1:A:219:PHE:O	1:A:224:PHE:HB2	2.22	0.40
1:A:342:GLY:HA3	2:B:1130:PHE:O	2.22	0.40
1:A:685:GLU:HA	1:A:688:LYS:HD2	2.04	0.40
3:C:106:GLU:O	3:C:149:LYS:HE3	2.22	0.40
4:E:100:ILE:CD1	4:E:108:GLY:HA3	2.45	0.40
6:H:26:ILE:HD11	6:H:49:VAL:HG11	2.03	0.40
8:J:52:THR:HG22	8:J:52:THR:O	2.21	0.40
1:A:7:SER:C	1:A:9:ALA:H	2.28	0.40
1:A:247:ARG:HD2	1:A:263:THR:OG1	2.21	0.40
1:A:577:ILE:H	1:A:577:ILE:HG12	1.49	0.40
1:A:782:ARG:NH2	2:B:699:GLU:O	2.54	0.40
1:A:1199:ARG:NH2	1:A:1233:ASP:O	2.55	0.40
2:B:53:GLN:HG2	2:B:547:VAL:HG13	2.03	0.40
2:B:284:ILE:CD1	2:B:324:ILE:HD12	2.51	0.40
2:B:542:MET:HE2	2:B:747:MET:CE	2.52	0.40
2:B:889:THR:HG21	2:B:891:ASP:OD2	2.21	0.40
3:C:70:ILE:HD11	3:C:144:ILE:HG12	2.03	0.40
4:E:197:LYS:HG3	4:E:211:TYR:CE2	2.57	0.40
6:H:111:LEU:HD22	6:H:127:GLY:O	2.21	0.40
7:I:78:CYS:SG	7:I:103:CYS:SG	3.19	0.40
1:A:825:ILE:CD1	2:B:512:ARG:HG3	2.49	0.40
1:A:1216:ILE:O	1:A:1219:THR:HB	2.21	0.40
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.62	0.40
1:A:1433:MET:HE2	1:A:1439:GLY:CA	2.51	0.40
2:B:305:VAL:O	2:B:305:VAL:HG12	2.21	0.40
2:B:429:PHE:HA	2:B:432:MET:CE	2.52	0.40
3:C:221:TYR:HD1	3:C:222:LYS:HG3	1.85	0.40
4:E:20:LYS:NZ	4:E:34:GLU:CD	2.79	0.40
10:L:34:CYS:SG	10:L:51:CYS:SG	3.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1411/1733 (81%)	1203 (85%)	149 (11%)	59 (4%)	2	7
2	B	1074/1224 (88%)	953 (89%)	100 (9%)	21 (2%)	6	21
3	C	264/318 (83%)	228 (86%)	30 (11%)	6 (2%)	5	18
4	E	213/215 (99%)	184 (86%)	24 (11%)	5 (2%)	5	18
5	F	82/155 (53%)	74 (90%)	6 (7%)	2 (2%)	4	17
6	H	129/146 (88%)	83 (64%)	28 (22%)	18 (14%)	0	0
7	I	120/122 (98%)	103 (86%)	14 (12%)	3 (2%)	4	16
8	J	63/70 (90%)	58 (92%)	4 (6%)	1 (2%)	7	27
9	K	112/120 (93%)	101 (90%)	11 (10%)	0	100	100
10	L	44/70 (63%)	21 (48%)	13 (30%)	10 (23%)	0	0
All	All	3512/4173 (84%)	3008 (86%)	379 (11%)	125 (4%)	2	10

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	46	THR
1	A	48	ALA
1	A	55	ASP
1	A	56	PRO
1	A	79	GLY
1	A	84	ILE
1	A	464	PRO
1	A	465	TYR
1	A	567	LYS
1	A	626	ASN
1	A	752	LYS
1	A	1391	ARG
1	A	1393	ASN
2	B	646	LEU
2	B	864	LYS
2	B	879	ARG
2	B	881	ASN
2	B	1099	VAL
3	C	4	GLU

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Mol	Chain	Res	Type
3	C	90	ASP
3	C	184	ASN
4	E	4	GLU
4	E	5	ASN
6	H	19	ARG
6	H	79	TRP
6	H	81	PRO
6	H	83	GLN
6	H	88	SER
6	H	138	GLU
10	L	39	SER
1	A	57	ARG
1	A	67	CYS
1	A	74	MET
1	A	418	SER
1	A	558	GLY
1	A	1172	LEU
1	A	1257	ASP
1	A	1392	SER
1	A	1396	ALA
1	A	1399	ARG
1	A	1403	GLU
2	B	165	VAL
2	B	734	HIS
2	B	907	GLY
2	B	1066	SER
2	B	1100	ASP
2	B	1155	SER
2	B	1222	ARG
3	C	263	THR
4	E	3	GLN
4	E	50	MET
4	E	59	SER
5	F	73	ALA
6	H	18	GLY
6	H	78	SER
6	H	82	PRO
6	H	90	ALA
6	H	105	GLU
6	H	128	ASN
6	H	140	ALA
10	L	52	GLY

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Mol	Chain	Res	Type
10	L	59	ALA
1	A	45	GLN
1	A	72	GLU
1	A	148	CYS
1	A	885	THR
1	A	1221	LYS
1	A	1386	ARG
1	A	1402	PHE
2	B	883	LEU
3	C	206	ASN
6	H	32	THR
6	H	139	ASN
7	I	3	THR
10	L	35	SER
10	L	64	LEU
1	A	58	LEU
1	A	188	ASP
1	A	253	ASN
1	A	283	GLY
1	A	307	ASP
1	A	342	GLY
1	A	599	SER
1	A	737	LEU
1	A	958	VAL
1	A	1278	ASN
1	A	1385	THR
2	B	266	ALA
5	F	112	GLU
6	H	8	ASP
6	H	77	ARG
7	I	76	PRO
7	I	79	HIS
10	L	37	LYS
10	L	54	ARG
1	A	35	ILE
1	A	42	ASP
1	A	197	PRO
1	A	525	GLN
1	A	593	GLU
1	A	628	GLY
1	A	736	ASN
1	A	1097	GLY

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Mol	Chain	Res	Type
1	A	1122	PRO
2	B	21	GLU
2	B	90	ILE
2	B	262	GLU
2	B	369	GLY
2	B	906	SER
3	C	264	GLN
6	H	61	SER
8	J	26	GLN
10	L	27	LEU
10	L	50	ASP
10	L	56	LEU
1	A	308	ILE
1	A	409	SER
1	A	419	LYS
1	A	1094	VAL
1	A	147	VAL
1	A	1437	GLY
2	B	231	PRO
2	B	1017	ILE
1	A	1114	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1239/1520 (82%)	1164 (94%)	75 (6%)	17	46
2	B	950/1061 (90%)	903 (95%)	47 (5%)	22	55
3	C	234/274 (85%)	222 (95%)	12 (5%)	21	54
4	E	197/197 (100%)	192 (98%)	5 (2%)	42	76
5	F	74/137 (54%)	69 (93%)	5 (7%)	14	42
6	H	117/128 (91%)	116 (99%)	1 (1%)	70	89
7	I	116/116 (100%)	111 (96%)	5 (4%)	26	60
8	J	60/65 (92%)	56 (93%)	4 (7%)	15	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	K	99/102 (97%)	90 (91%)	9 (9%)	9	28
10	L	40/57 (70%)	36 (90%)	4 (10%)	7	24
All	All	3126/3657 (86%)	2959 (95%)	167 (5%)	20	52

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	22	PHE
1	A	71	GLN
1	A	93	VAL
1	A	112	LYS
1	A	117	GLU
1	A	156	ASP
1	A	197	PRO
1	A	208	LEU
1	A	237	THR
1	A	291	GLU
1	A	351	THR
1	A	381	THR
1	A	385	ILE
1	A	389	THR
1	A	434	ARG
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	452	LYS
1	A	467	THR
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	479	ASN
1	A	493	GLN
1	A	497	THR
1	A	503	GLN
1	A	504	LEU
1	A	571	LEU
1	A	577	ILE
1	A	597	LEU
1	A	612	ILE
1	A	618	GLU

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Mol	Chain	Res	Type
1	A	622	VAL
1	A	666	ILE
1	A	672	ASP
1	A	710	LEU
1	A	740	LEU
1	A	756	ILE
1	A	774	ARG
1	A	788	SER
1	A	821	ARG
1	A	822	GLU
1	A	827	THR
1	A	831	THR
1	A	855	THR
1	A	858	ASN
1	A	882	SER
1	A	885	THR
1	A	903	ASN
1	A	919	ILE
1	A	920	LEU
1	A	948	VAL
1	A	1015	VAL
1	A	1030	ARG
1	A	1064	VAL
1	A	1118	VAL
1	A	1122	PRO
1	A	1129	GLU
1	A	1165	GLU
1	A	1255	GLU
1	A	1264	GLU
1	A	1297	GLU
1	A	1318	THR
1	A	1325	THR
1	A	1364	ASN
1	A	1376	THR
1	A	1385	THR
1	A	1415	SER
1	A	1419	ASP
1	A	1425	SER
1	A	1426	GLU
1	A	1436	ILE
1	A	1438	THR
2	B	18	PHE

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Mol	Chain	Res	Type
2	B	63	ILE
2	B	98	THR
2	B	102	VAL
2	B	175	ARG
2	B	178	ASN
2	B	183	GLU
2	B	194	GLU
2	B	199	MET
2	B	217	ARG
2	B	261	ARG
2	B	268	THR
2	B	337	ARG
2	B	339	THR
2	B	461	LEU
2	B	485	ARG
2	B	487	THR
2	B	496	ARG
2	B	513	GLN
2	B	522	VAL
2	B	531	GLN
2	B	541	LEU
2	B	547	VAL
2	B	549	THR
2	B	578	THR
2	B	589	VAL
2	B	644	GLU
2	B	648	HIS
2	B	653	VAL
2	B	706	GLN
2	B	806	THR
2	B	860	MET
2	B	939	THR
2	B	951	GLN
2	B	963	PHE
2	B	974	PRO
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1060	ARG
2	B	1065	GLN
2	B	1159	ARG

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Mol	Chain	Res	Type
2	B	1189	ILE
2	B	1193	GLN
2	B	1211	ASN
2	B	1219	ASP
3	C	17	ASN
3	C	26	ASP
3	C	56	THR
3	C	77	ILE
3	C	129	ILE
3	C	163	ILE
3	C	186	LEU
3	C	189	THR
3	C	209	TYR
3	C	226	ASP
3	C	233	GLU
3	C	240	VAL
4	E	81	GLU
4	E	104	ASN
4	E	123	LEU
4	E	149	LEU
4	E	204	THR
5	F	81	THR
5	F	82	THR
5	F	111	LEU
5	F	115	THR
5	F	149	GLU
6	H	91	ASP
7	I	4	PHE
7	I	30	ARG
7	I	50	THR
7	I	52	ILE
7	I	98	VAL
8	J	1	MET
8	J	3	VAL
8	J	22	LEU
8	J	48	ARG
9	K	6	ARG
9	K	11	LEU
9	K	47	ARG
9	K	63	VAL
9	K	73	LEU
9	K	101	LEU

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Mol	Chain	Res	Type
9	K	103	THR
9	K	111	LEU
9	K	114	LEU
10	L	42	ARG
10	L	50	ASP
10	L	61	THR
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	68	GLN
1	A	71	GLN
1	A	83	HIS
1	A	92	HIS
1	A	118	HIS
1	A	256	GLN
1	A	287	HIS
1	A	299	HIS
1	A	313	GLN
1	A	339	ASN
1	A	390	GLN
1	A	394	ASN
1	A	397	ASN
1	A	445	ASN
1	A	479	ASN
1	A	493	GLN
1	A	503	GLN
1	A	517	ASN
1	A	589	GLN
1	A	603	ASN
1	A	611	GLN
1	A	626	ASN
1	A	631	HIS
1	A	660	ASN
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN

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Mol	Chain	Res	Type
1	A	786	HIS
1	A	851	HIS
1	A	854	ASN
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	994	GLN
1	A	1033	GLN
1	A	1040	GLN
1	A	1078	GLN
1	A	1128	GLN
1	A	1140	HIS
1	A	1173	HIS
1	A	1218	GLN
1	A	1265	ASN
1	A	1364	ASN
1	A	1378	GLN
1	A	1432	GLN
2	B	46	GLN
2	B	60	GLN
2	B	178	ASN
2	B	215	GLN
2	B	224	GLN
2	B	236	HIS
2	B	300	HIS
2	B	366	GLN
2	B	383	ASN
2	B	415	GLN
2	B	465	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	587	HIS
2	B	590	HIS
2	B	648	HIS
2	B	657	HIS
2	B	706	GLN
2	B	744	HIS
2	B	761	HIS
2	B	763	GLN

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Mol	Chain	Res	Type
2	B	786	ASN
2	B	862	GLN
2	B	1015	HIS
2	B	1062	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1176	ASN
2	B	1179	GLN
2	B	1187	ASN
2	B	1193	GLN
3	C	17	ASN
3	C	24	ASN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	242	GLN
3	C	252	GLN
4	E	3	GLN
4	E	63	ASN
4	E	104	ASN
4	E	106	GLN
4	E	147	HIS
6	H	11	GLN
6	H	133	ASN
7	I	12	ASN
7	I	51	ASN
7	I	89	GLN
7	I	108	HIS
7	I	114	GLN
8	J	64	ASN
9	K	29	ASN
9	K	65	HIS
9	K	76	GLN
9	K	89	ASN
9	K	110	ASN
10	L	53	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
6	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	710:LEU	C	711:GLU	N	1.16

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	707:PRO	C	708:GLU	N	1.08
1	H	79:TRP	C	80:ARG	N	0.72

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.