



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:35 AM EDT

PDB ID : 1M1Y / pdb_00001m1y
Title : Chemical Crosslink of Nitrogenase MoFe Protein and Fe Protein
Authors : Schmid, B.; Einsle, O.; Chiu, H.J.; Willing, A.; Yoshida, M.; Howard, J.B.;
Rees, D.C.
Deposited on : 2002-06-20
Resolution : 3.20 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
Mogul	:	2022.3.0, CSD as543be (2022)
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)	:	2.50

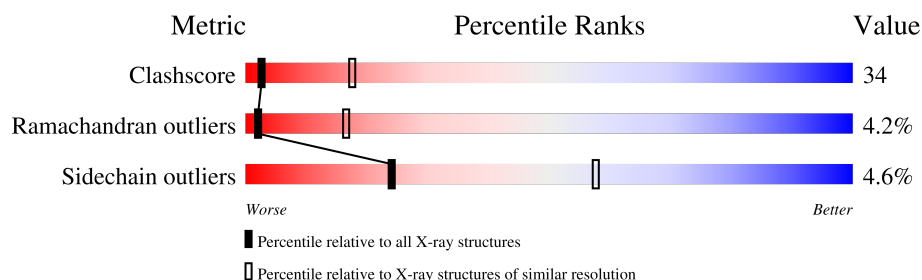
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

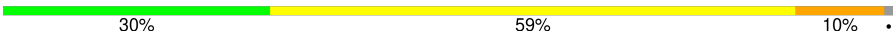
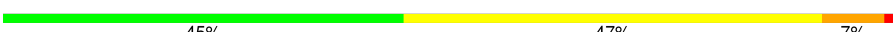
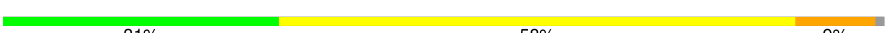
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	491	45% 45% 7% .
1	C	491	44% 47% 6% .
1	I	491	45% 47% 5% .
1	K	491	46% 46% 6% .
2	B	522	48% 46% 6%
2	D	522	45% 49% 5%
2	J	522	45% 49% 6%
2	L	522	47% 47% 6%

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Mol	Chain	Length	Quality of chain
3	E	289	
3	F	289	
3	G	289	
3	H	289	
3	M	289	
3	N	289	
3	O	289	
3	P	289	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CFM	A	6496	-	-	X	-
5	CFM	C	7496	-	-	X	-
6	CLF	A	6498	-	-	X	-
6	CLF	K	9498	-	-	X	-
8	SF4	E	290	-	-	X	-
8	SF4	G	1290	-	-	X	-
8	SF4	N	2290	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 49464 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 Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3790	2410	646	709	25			
1	C	477	Total	C	N	O	S	0	0	0
			3790	2410	646	709	25			
1	I	477	Total	C	N	O	S	0	0	0
			3790	2410	646	709	25			
1	K	477	Total	C	N	O	S	0	0	0
			3790	2410	646	709	25			

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	J	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	L	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			

- Molecule 3 is a protein called nitrogenase IRON protein 1.

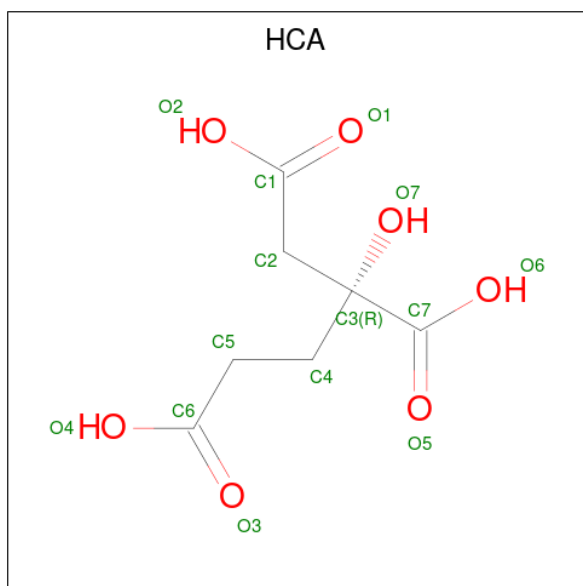
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	286	Total	C	N	O	S	0	0	0
			2161	1349	366	425	21			
3	F	289	Total	C	N	O	S	0	0	0
			2186	1364	369	432	21			
3	G	286	Total	C	N	O	S	0	0	0
			2161	1349	366	425	21			
3	H	289	Total	C	N	O	S	0	0	0
			2186	1364	369	432	21			

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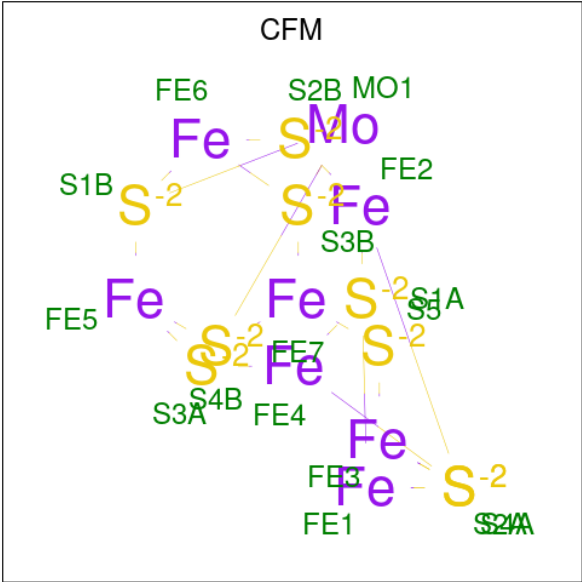
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	286	Total	C	N	O	S	0	0	0
			2161	1349	366	425	21			
3	N	289	Total	C	N	O	S	0	0	0
			2186	1364	369	432	21			
3	O	286	Total	C	N	O	S	0	0	0
			2161	1349	366	425	21			
3	P	289	Total	C	N	O	S	0	0	0
			2186	1364	369	432	21			

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$).



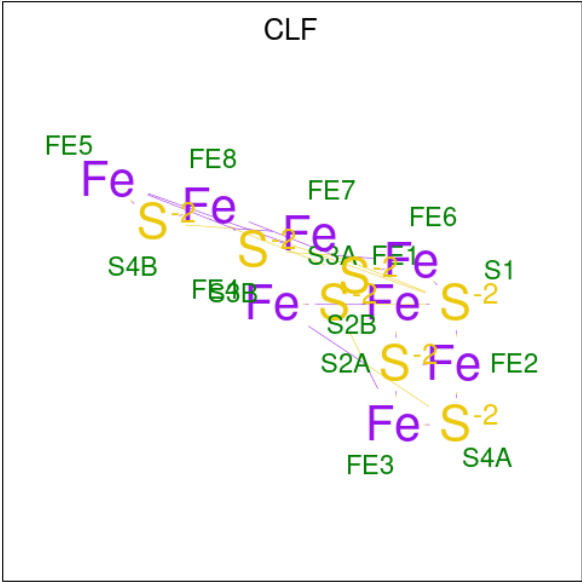
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	7	7		
4	C	1	Total	C	O	0	0
			14	7	7		
4	I	1	Total	C	O	0	0
			14	7	7		
4	K	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is FE-MO-S CLUSTER (CCD ID: CFM) (formula: Fe_7MoS_9).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	I	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	K	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 6 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe₈S₇).

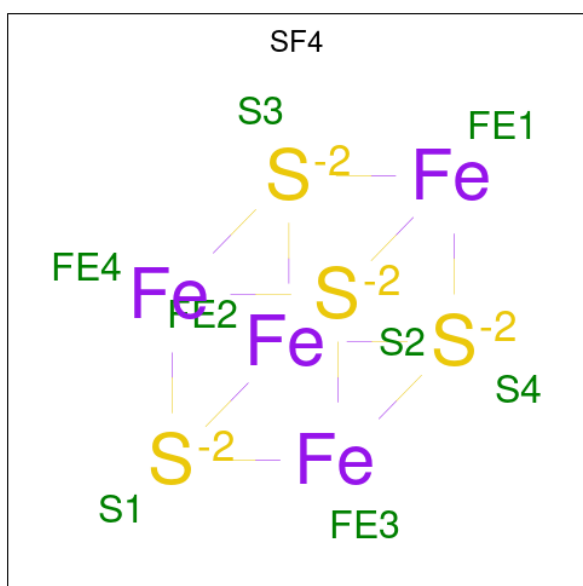


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			15	8	7		
6	D	1	Total	Fe	S	0	0
			15	8	7		
6	J	1	Total	Fe	S	0	0
			15	8	7		
6	K	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	D	1	Total	Ca	0	0
			1	1		
7	J	1	Total	Ca	0	0
			1	1		
7	L	1	Total	Ca	0	0
			1	1		

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	Fe	S	0	0
			8	4	4		
8	G	1	Total	Fe	S	0	0
			8	4	4		

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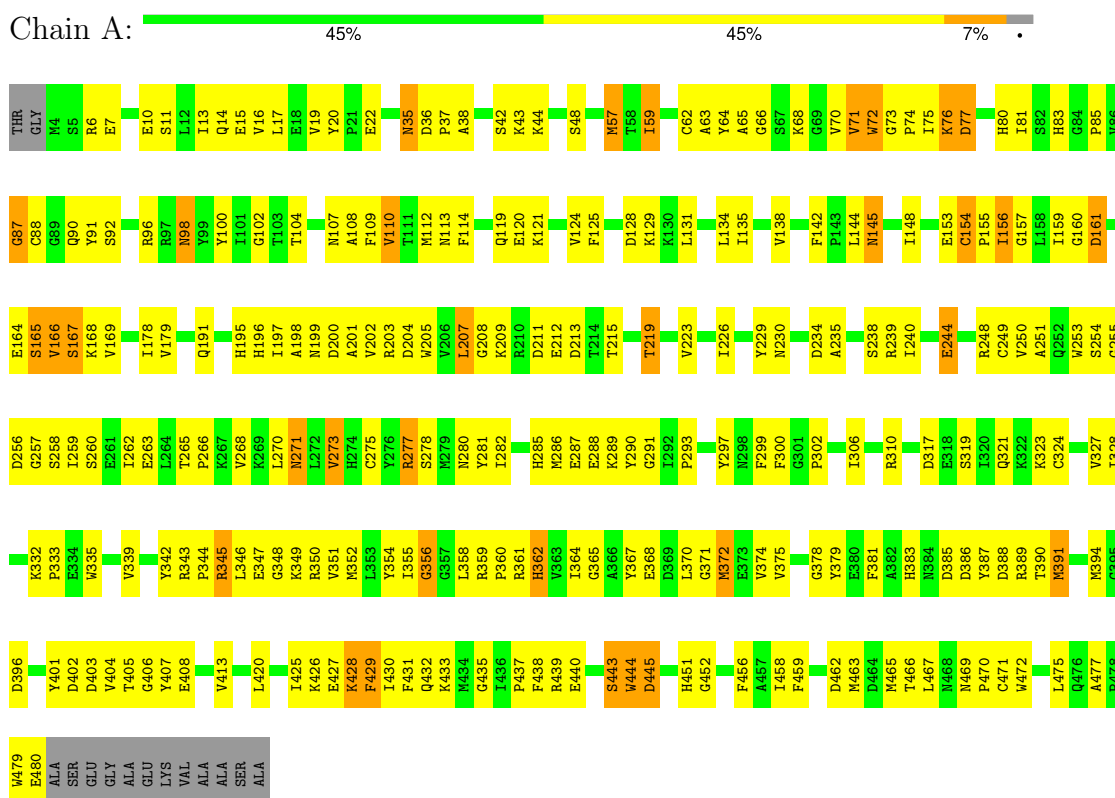
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	N	1	Total	Fe	S	0	0
			8	4	4		
8	P	1	Total	Fe	S	0	0
			8	4	4		

3 Residue-property plots

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

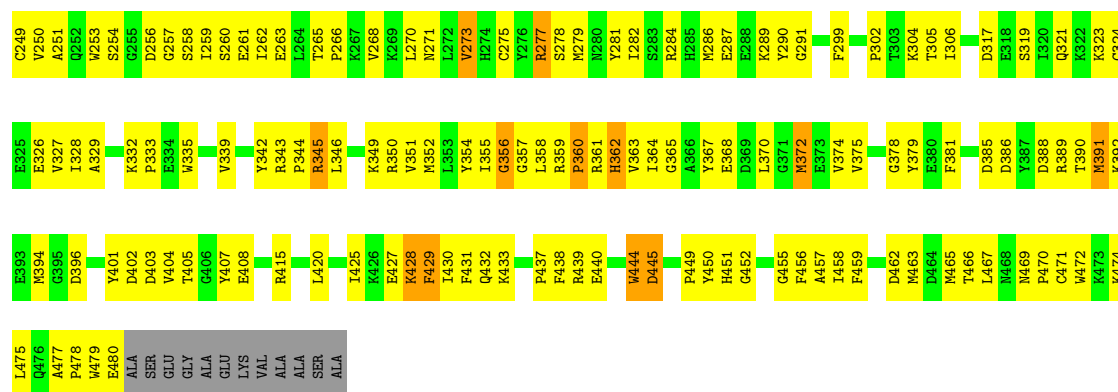
Note EDS was not executed.

• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



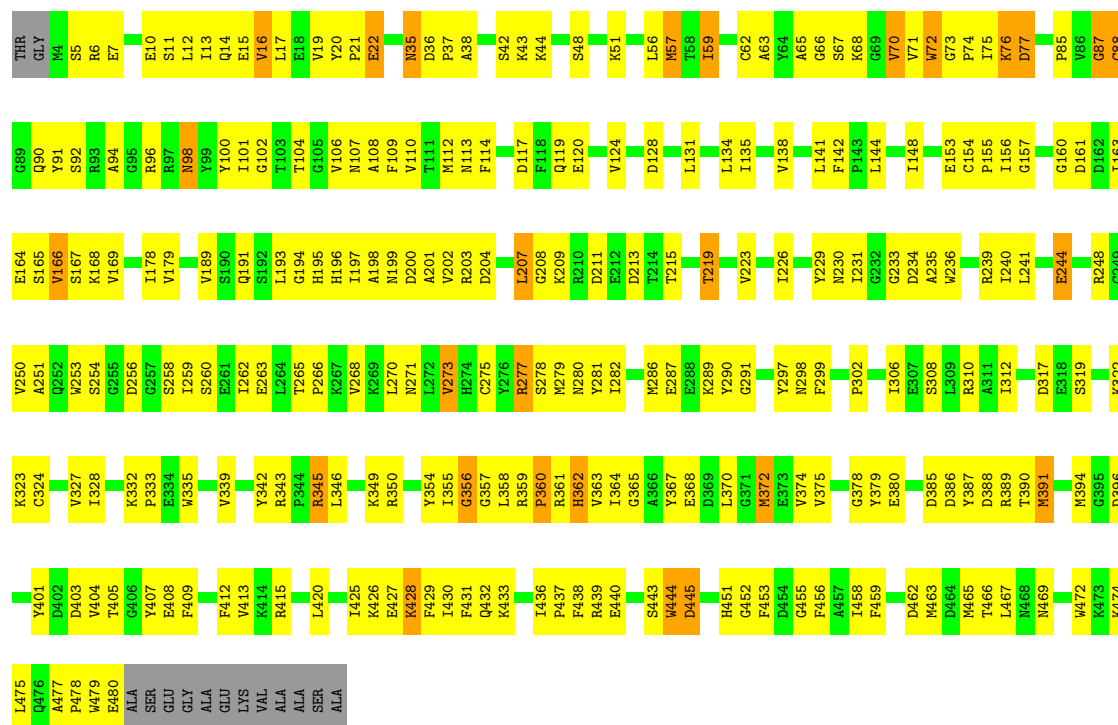
• Molecule 1: Nitrogenase molybdenum-iron protein alpha chain





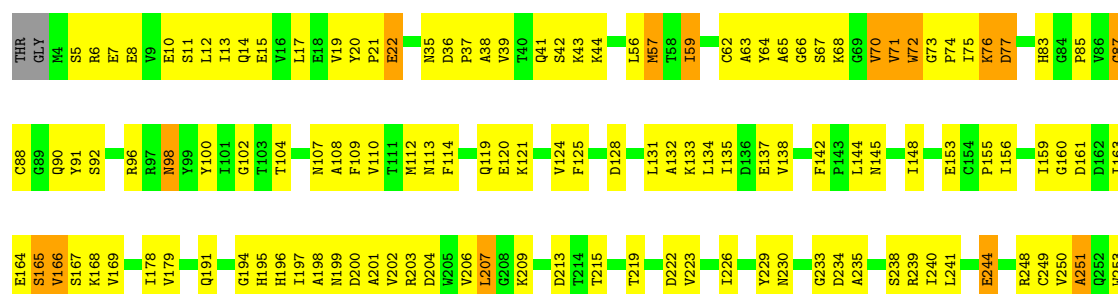
● Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

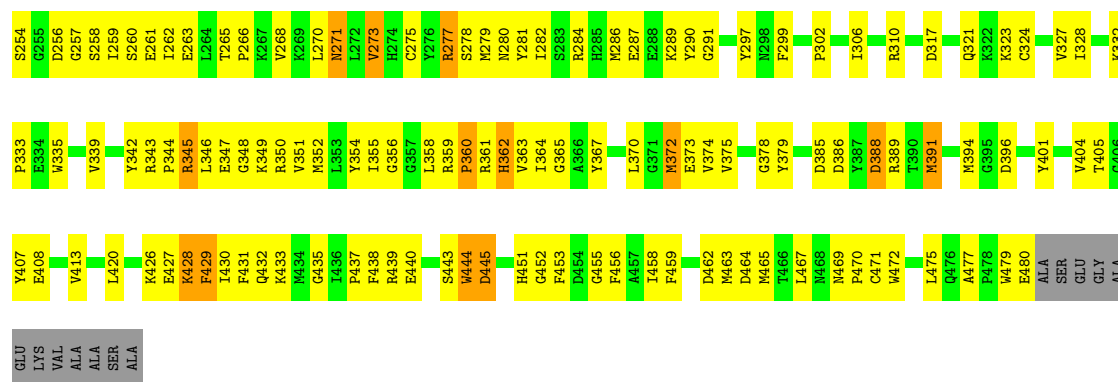
Chain I: 45% 47% 5% .



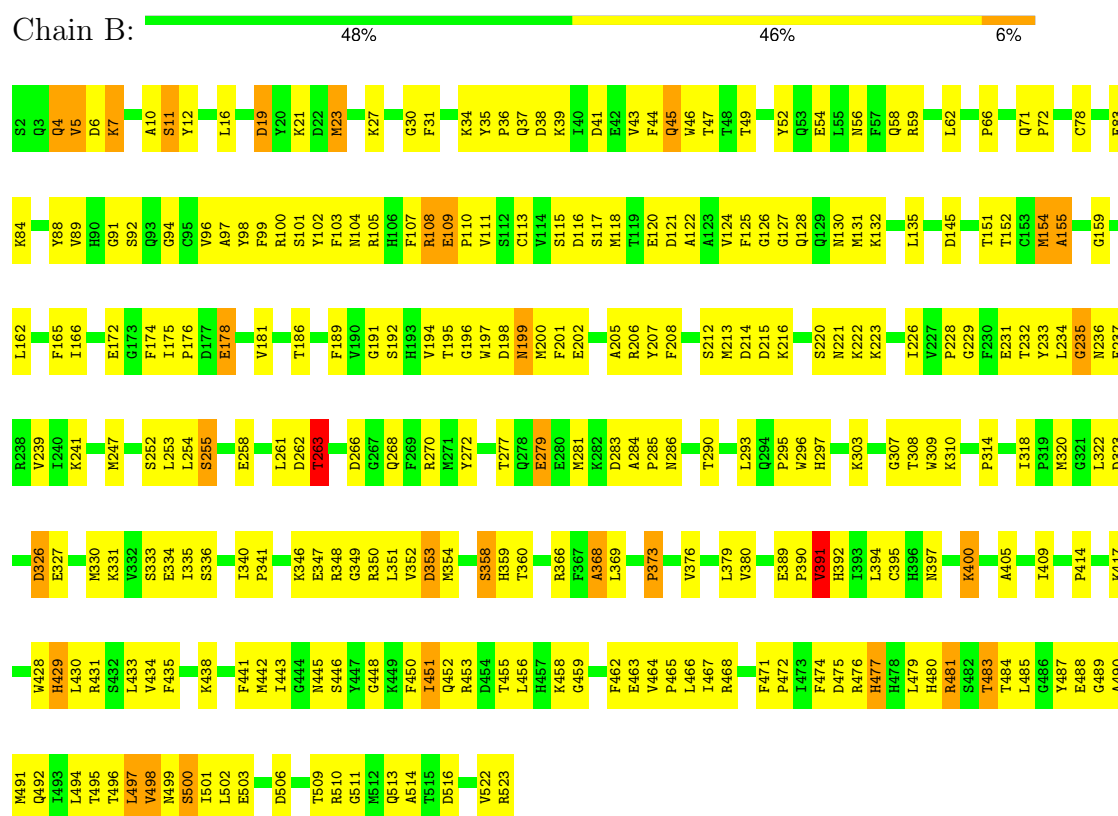
● Molecule 1: Nitrogenase molybdenum-iron protein alpha chain

Chain K: 46% 46% 6% .



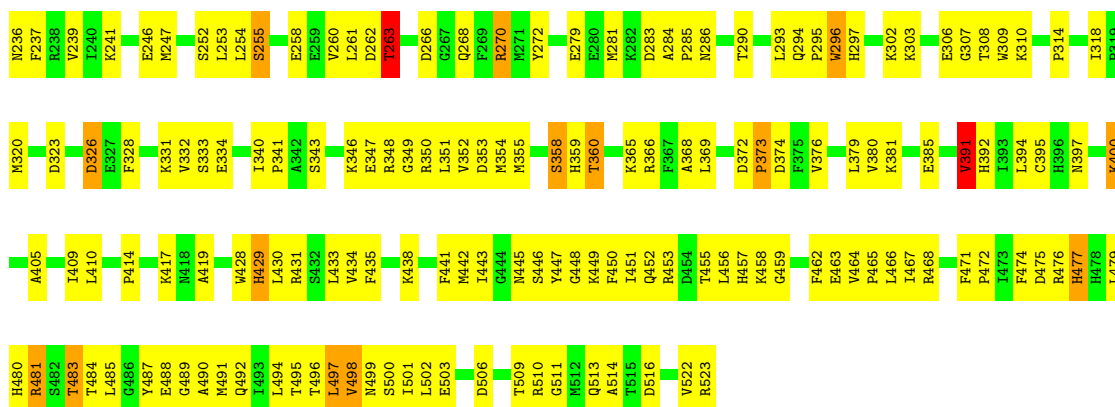


• Molecule 2: Nitrogenase molybdenum-iron protein beta chain



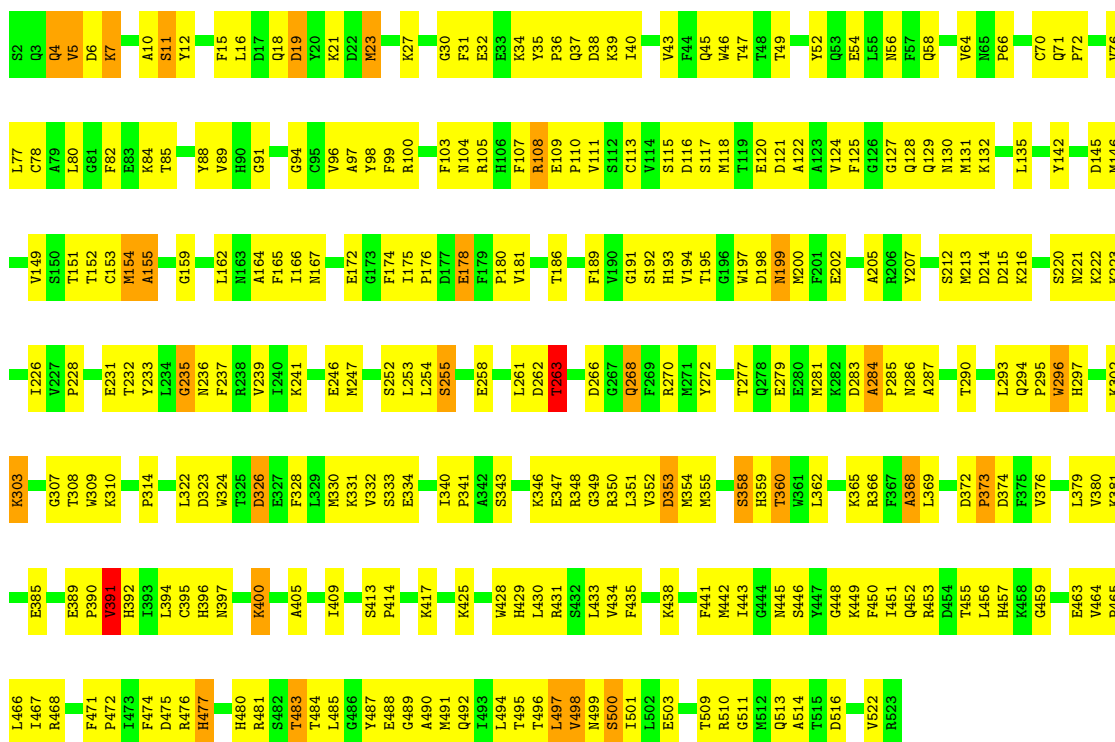
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain





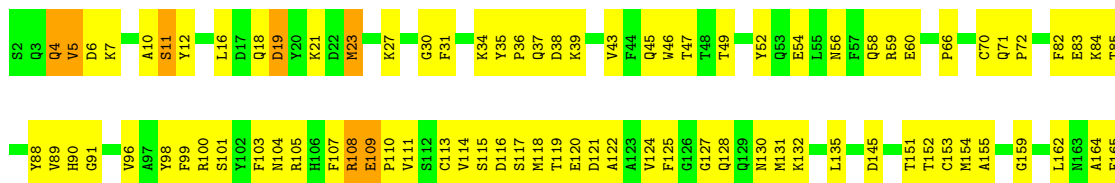
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

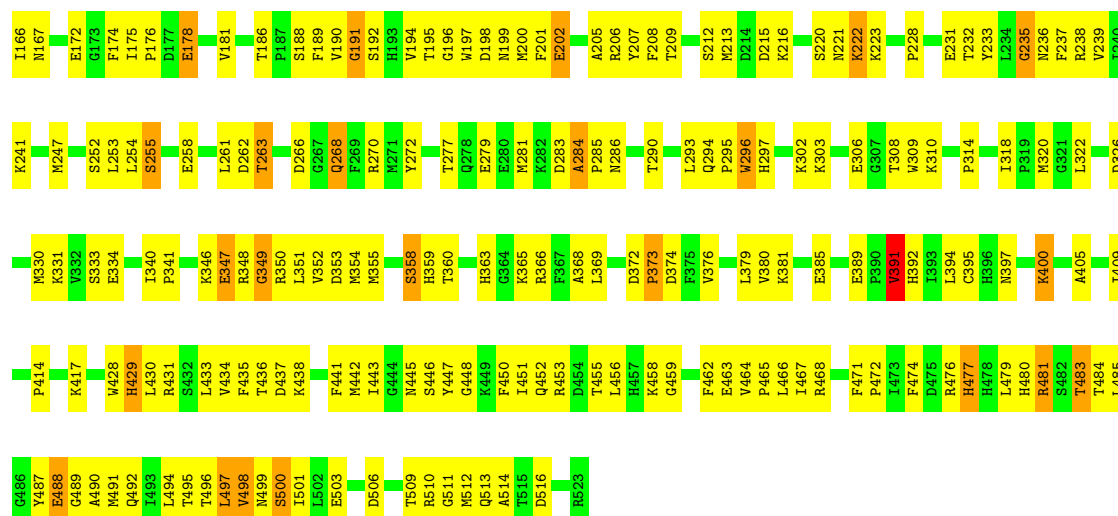
Chain J: 45% 49% 6%



• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

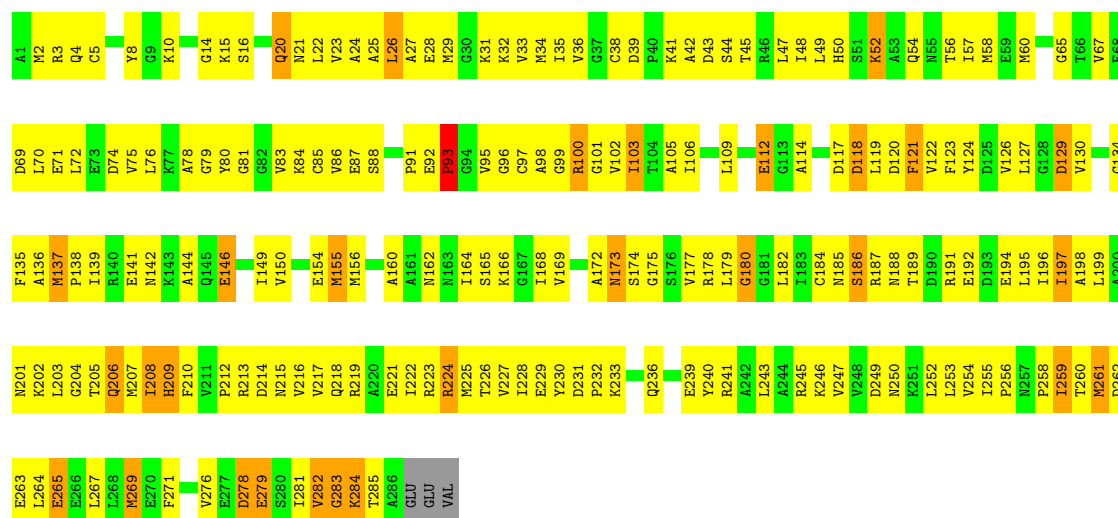
Chain L: 47% 47% 6%





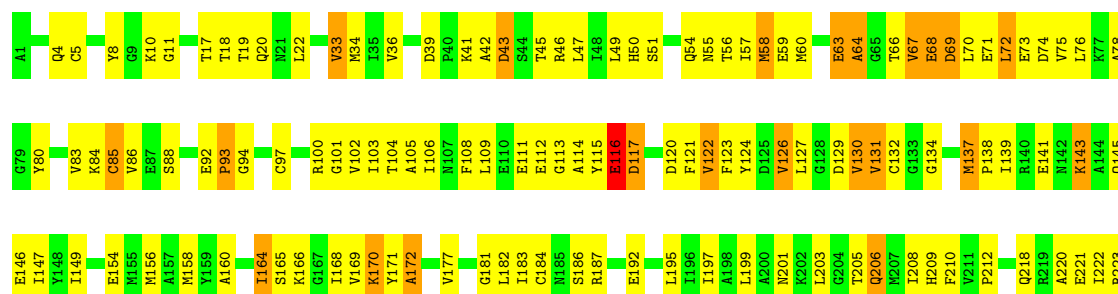
• Molecule 3: nitrogenase IRON protein 1

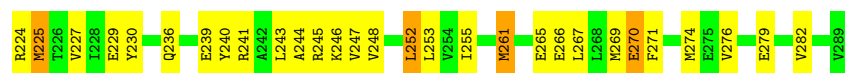
Chain E: 30% 59% 10%



• Molecule 3: nitrogenase IRON protein 1

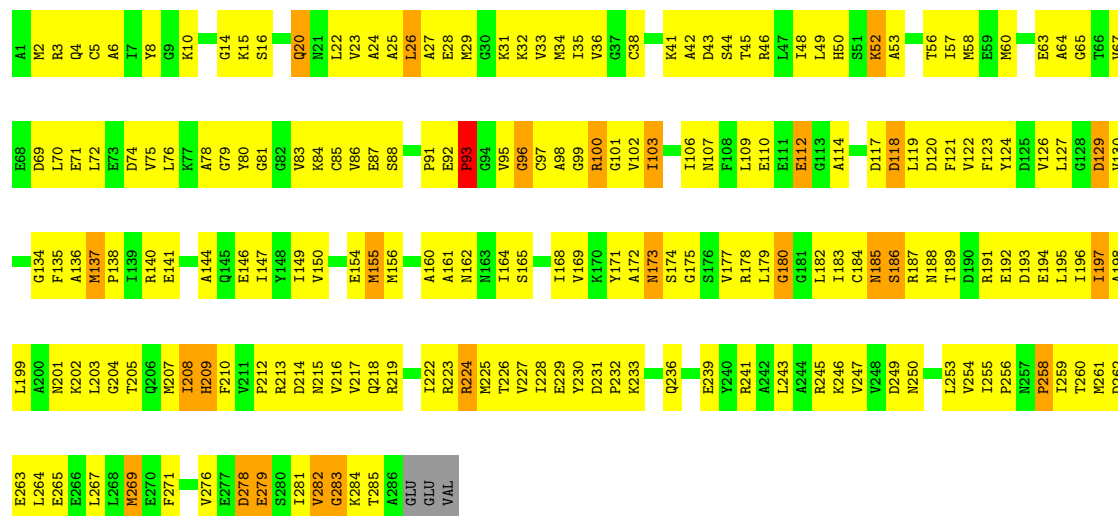
Chain F: 46% 45% 9%





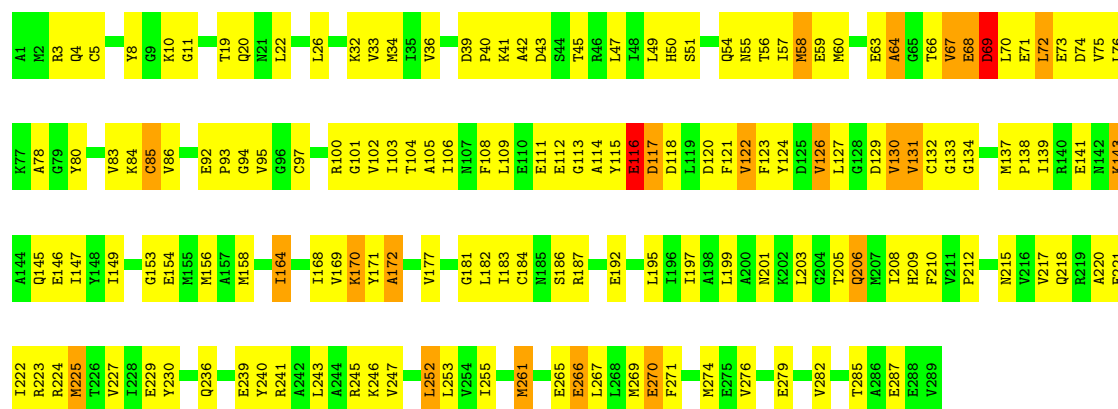
• Molecule 3: nitrogenase IRON protein 1

Chain G: 29% 61% 9%



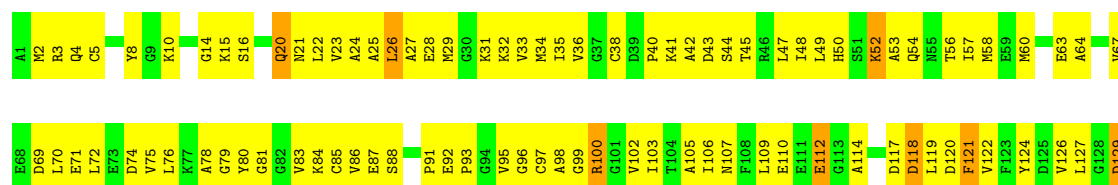
• Molecule 3: nitrogenase IRON protein 1

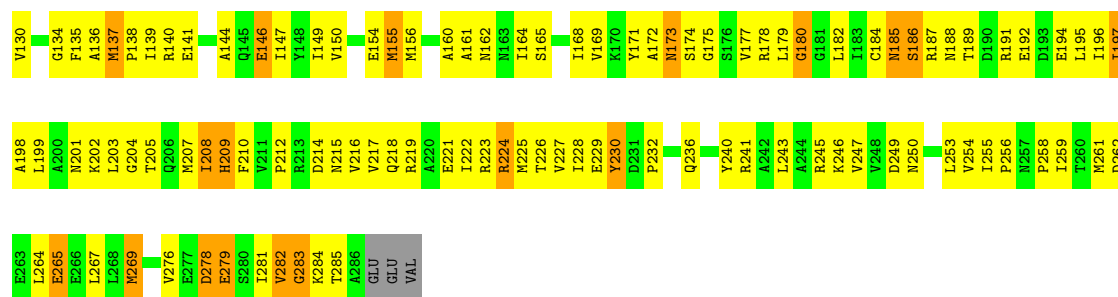
Chain H: 45% 47% 7%



• Molecule 3: nitrogenase IRON protein 1

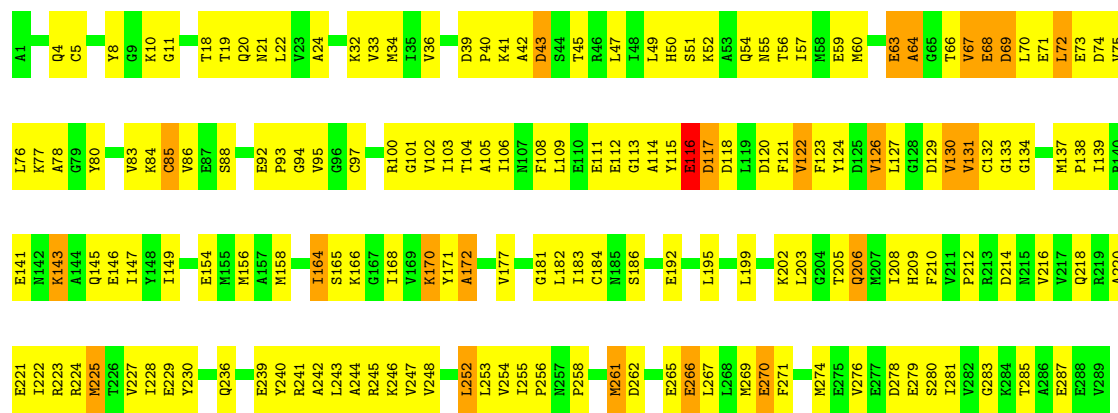
Chain M: 31% 58% 9%





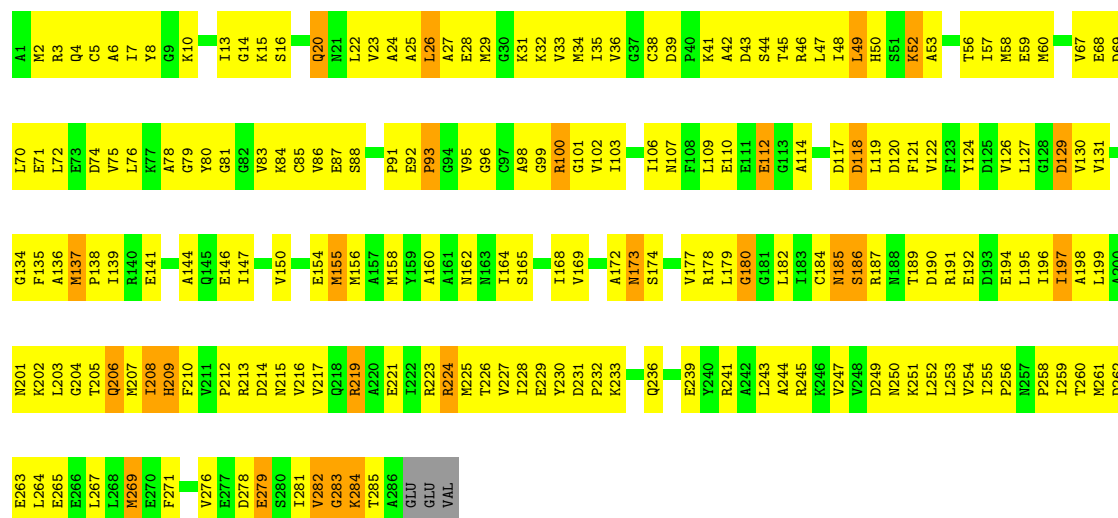
• Molecule 3: nitrogenase IRON protein 1

Chain N: 41% 51% 8%



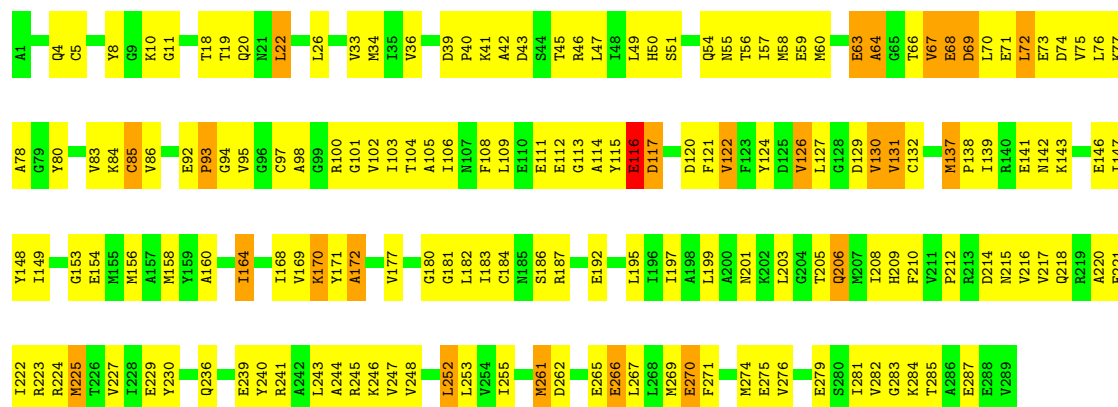
• Molecule 3: nitrogenase IRON protein 1

Chain O: 30% 60% 9%



• Molecule 3: nitrogenase IRON protein 1

Chain P: 42% 50% 8%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.27Å 214.94Å 320.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20	Depositor
% Data completeness (in resolution range)	81.1 (50.00-3.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.329	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	49464	wwPDB-VP
Average B, all atoms (Å ²)	62.0	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: HCA, CA, SF4, CLF, CFM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.66	0/3878	1.03	23/5229 (0.4%)
1	C	0.52	0/3878	1.00	20/5229 (0.4%)
1	I	0.54	0/3878	1.00	18/5229 (0.3%)
1	K	0.52	0/3878	1.00	18/5229 (0.3%)
2	B	0.71	0/4280	1.03	21/5786 (0.4%)
2	D	0.64	0/4280	1.02	24/5786 (0.4%)
2	J	0.60	0/4280	1.01	21/5786 (0.4%)
2	L	0.64	0/4280	1.01	21/5786 (0.4%)
3	E	0.49	0/2185	0.99	9/2943 (0.3%)
3	F	0.53	0/2210	0.98	8/2975 (0.3%)
3	G	0.50	0/2185	0.98	7/2943 (0.2%)
3	H	0.50	0/2210	0.96	10/2975 (0.3%)
3	M	0.56	0/2185	1.00	7/2943 (0.2%)
3	N	0.53	0/2210	0.99	10/2975 (0.3%)
3	O	0.51	0/2185	0.99	10/2943 (0.3%)
3	P	0.55	0/2210	0.99	8/2975 (0.3%)
All	All	0.58	0/50212	1.00	235/67732 (0.3%)

There are no bond length outliers.

All (235) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	76	LYS	N-CA-C	10.47	123.97	111.82
2	B	391	VAL	N-CA-C	10.04	120.86	110.62
1	A	76	LYS	N-CA-C	10.03	123.46	111.82
2	L	391	VAL	N-CA-C	9.91	120.73	110.72
2	J	391	VAL	N-CA-C	9.85	120.67	110.72
1	C	76	LYS	N-CA-C	9.74	123.12	111.82
1	I	76	LYS	N-CA-C	9.73	123.11	111.82
2	D	391	VAL	N-CA-C	9.69	120.51	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	30	GLY	N-CA-C	8.89	122.81	112.50
1	C	191	GLN	N-CA-C	-8.85	102.62	113.50
1	K	90	GLN	N-CA-C	8.72	120.87	111.36
2	B	30	GLY	N-CA-C	8.59	122.88	112.49
1	I	90	GLN	N-CA-C	8.58	120.41	111.14
1	A	90	GLN	N-CA-C	8.47	120.59	111.36
2	J	30	GLY	N-CA-C	8.43	122.69	112.49
1	C	90	GLN	N-CA-C	8.36	120.47	111.36
1	K	191	GLN	N-CA-C	-8.36	102.87	113.23
1	C	71	VAL	N-CA-C	8.28	119.53	111.67
1	I	191	GLN	N-CA-C	-8.16	103.47	113.50
2	L	30	GLY	N-CA-C	7.93	122.09	112.49
1	A	191	GLN	N-CA-C	-7.86	103.48	113.23
2	B	438	LYS	N-CA-C	7.70	120.57	109.48
2	L	438	LYS	N-CA-C	7.67	120.53	109.48
1	A	71	VAL	N-CA-C	7.65	118.94	111.67
2	L	108	ARG	N-CA-C	-7.38	101.80	111.02
2	D	488	GLU	N-CA-C	-7.37	102.94	110.97
1	K	71	VAL	N-CA-C	7.37	118.67	111.67
2	B	326	ASP	N-CA-C	-7.30	103.01	110.97
2	J	488	GLU	N-CA-C	-7.22	103.10	110.97
2	B	108	ARG	N-CA-C	-7.14	101.39	111.24
2	D	438	LYS	N-CA-C	7.09	119.69	109.48
2	J	326	ASP	N-CA-C	-7.05	103.28	110.97
2	L	109	GLU	N-CA-C	-7.05	101.88	108.22
2	J	368	ALA	N-CA-C	-6.86	97.16	108.76
2	L	326	ASP	N-CA-C	-6.75	103.61	110.97
2	L	429	HIS	N-CA-C	-6.67	103.93	111.14
2	B	477	HIS	N-CA-C	6.66	120.31	109.59
3	H	126	VAL	N-CA-C	6.66	117.47	107.75
2	D	368	ALA	N-CA-C	-6.65	97.52	108.76
2	J	108	ARG	N-CA-C	-6.65	102.07	111.24
2	L	368	ALA	N-CA-C	-6.63	97.55	108.76
2	J	438	LYS	N-CA-C	6.62	121.16	109.58
2	L	488	GLU	N-CA-C	-6.59	103.20	111.11
3	F	114	ALA	N-CA-C	-6.55	105.27	113.20
1	C	70	VAL	N-CA-C	6.52	117.52	111.45
3	H	120	ASP	N-CA-C	-6.51	105.47	113.41
1	A	72	TRP	N-CA-C	6.50	118.24	111.03
2	J	429	HIS	N-CA-C	-6.49	103.83	111.03
2	D	214	ASP	N-CA-C	6.48	118.14	111.14
2	D	326	ASP	N-CA-C	-6.48	103.91	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	26	LEU	N-CA-C	6.40	117.91	111.07
2	B	429	HIS	N-CA-C	-6.39	103.94	111.03
2	B	488	GLU	N-CA-C	-6.37	103.25	111.02
1	K	72	TRP	N-CA-C	6.36	118.09	111.03
2	D	108	ARG	N-CA-C	-6.30	102.55	111.24
2	L	477	HIS	N-CA-C	6.27	119.92	109.95
2	B	16	LEU	N-CA-C	-6.25	105.69	113.38
1	I	104	THR	N-CA-C	6.25	119.28	109.96
3	E	103	ILE	N-CA-C	-6.24	104.43	110.42
2	D	429	HIS	N-CA-C	-6.20	103.83	111.40
2	J	477	HIS	N-CA-C	6.20	119.56	109.59
2	B	368	ALA	N-CA-C	-6.19	98.29	108.76
1	I	273	VAL	N-CA-C	6.18	117.02	107.99
2	D	477	HIS	N-CA-C	6.17	119.52	109.59
3	F	120	ASP	N-CA-C	-6.16	105.90	113.41
1	A	110	VAL	N-CA-C	-6.14	106.77	111.62
3	P	114	ALA	N-CA-C	-6.13	105.78	113.20
3	N	120	ASP	N-CA-C	-6.12	105.95	113.41
3	G	265	GLU	N-CA-C	-6.11	104.69	111.71
3	N	108	PHE	N-CA-C	-6.09	104.27	111.03
1	A	104	THR	N-CA-C	6.08	119.03	109.96
1	C	244	GLU	N-CA-C	-6.06	105.14	112.54
3	H	114	ALA	N-CA-C	-6.06	105.85	113.18
3	M	265	GLU	N-CA-C	-6.05	104.75	111.71
3	F	108	PHE	N-CA-C	-6.03	104.63	111.14
1	I	72	TRP	N-CA-C	6.02	117.65	111.14
3	E	269	MET	N-CA-C	-6.02	105.77	113.23
3	P	120	ASP	N-CA-C	-5.97	106.12	113.41
2	J	16	LEU	N-CA-C	-5.96	106.05	113.38
2	B	481	ARG	N-CA-C	-5.93	105.69	113.17
2	D	16	LEU	N-CA-C	-5.93	106.09	113.38
1	A	348	GLY	N-CA-C	5.91	123.21	115.47
1	A	429	PHE	N-CA-C	5.90	118.67	111.82
1	K	244	GLU	N-CA-C	-5.90	105.34	112.54
2	B	109	GLU	N-CA-C	-5.84	102.96	108.22
1	I	179	VAL	N-CA-C	5.84	114.39	107.73
2	D	358	SER	N-CA-C	5.82	117.88	110.61
1	A	121	LYS	N-CA-C	5.81	118.56	111.82
2	D	263	THR	N-CA-C	-5.81	102.45	109.83
2	B	263	THR	N-CA-C	-5.79	102.47	109.83
3	H	108	PHE	N-CA-C	-5.79	104.60	111.03
1	K	104	THR	N-CA-C	5.78	118.58	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	16	LEU	N-CA-C	-5.78	106.27	113.38
3	H	69	ASP	N-CA-C	-5.78	105.33	112.90
3	P	108	PHE	N-CA-C	-5.78	104.62	111.03
3	F	126	VAL	N-CA-C	5.77	116.17	107.75
3	G	269	MET	N-CA-C	-5.74	106.11	113.23
3	G	112	GLU	N-CA-C	-5.74	106.18	112.72
1	A	179	VAL	N-CA-C	5.70	114.23	107.73
1	C	154	CYS	N-CA-C	5.69	122.39	109.81
1	I	279	MET	N-CA-C	5.68	119.32	111.71
3	O	265	GLU	N-CA-C	-5.68	105.18	111.71
1	C	104	THR	N-CA-C	5.67	118.41	109.96
3	M	149	ILE	N-CA-C	5.67	116.48	108.36
1	C	179	VAL	N-CA-C	5.66	114.18	107.73
3	M	26	LEU	N-CA-C	5.66	117.12	111.07
1	A	273	VAL	N-CA-C	5.65	116.25	107.99
2	L	294	GLN	CA-C-N	5.65	125.12	119.24
2	L	294	GLN	C-N-CA	5.65	125.12	119.24
2	L	500	SER	N-CA-C	-5.64	105.13	111.28
3	N	114	ALA	N-CA-C	-5.64	106.37	113.20
2	L	114	VAL	N-CA-C	5.63	116.95	108.96
3	F	164	ILE	N-CA-C	-5.60	105.07	110.72
3	E	149	ILE	N-CA-C	5.58	116.34	108.36
3	N	126	VAL	N-CA-C	5.58	115.92	108.11
1	I	244	GLU	N-CA-C	-5.58	105.74	112.54
2	D	294	GLN	CA-C-N	5.57	125.04	119.24
2	D	294	GLN	C-N-CA	5.57	125.04	119.24
2	J	353	ASP	N-CA-C	-5.56	104.23	111.02
1	K	179	VAL	N-CA-C	5.55	114.06	107.73
1	K	70	VAL	N-CA-C	5.55	116.61	111.45
3	N	164	ILE	N-CA-C	-5.54	105.12	110.72
2	J	358	SER	N-CA-C	5.54	117.53	110.61
3	G	103	ILE	N-CA-C	-5.54	105.10	110.42
1	A	57	MET	N-CA-C	5.53	118.74	111.28
1	K	56	LEU	N-CA-C	5.52	119.65	113.02
3	F	63	GLU	N-CA-C	-5.52	103.94	111.56
2	B	214	ASP	N-CA-C	5.51	117.09	111.14
1	A	156	ILE	N-CA-C	5.51	115.71	110.42
3	P	126	VAL	N-CA-C	5.50	115.81	108.11
2	J	214	ASP	N-CA-C	5.49	117.06	111.14
1	C	56	LEU	N-CA-C	5.48	119.60	113.02
1	K	57	MET	N-CA-C	5.48	118.68	111.28
2	J	307	GLY	N-CA-C	5.47	118.85	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	22	LEU	N-CA-C	-5.47	105.01	110.97
1	C	205	TRP	N-CA-C	5.47	120.83	113.72
1	K	280	ASN	N-CA-C	-5.47	105.48	111.82
3	O	112	GLU	N-CA-C	-5.46	105.93	112.59
2	B	358	SER	N-CA-C	5.46	117.43	110.61
3	E	26	LEU	N-CA-C	5.46	116.92	110.97
2	D	506	ASP	N-CA-C	-5.45	105.26	111.14
1	I	70	VAL	N-CA-C	5.44	116.51	111.45
2	D	438	LYS	CA-C-N	5.44	126.64	119.84
2	D	438	LYS	C-N-CA	5.44	126.64	119.84
1	K	273	VAL	N-CA-C	5.44	115.93	107.99
3	N	143	LYS	N-CA-C	-5.44	106.65	113.72
3	P	95	VAL	N-CA-C	5.44	115.68	107.80
2	L	506	ASP	N-CA-C	-5.43	105.28	111.14
3	E	265	GLU	N-CA-C	-5.42	105.48	111.71
2	J	149	VAL	N-CA-C	5.41	115.75	108.17
1	A	205	TRP	N-CA-C	5.40	120.54	113.30
1	A	280	ASN	N-CA-C	-5.40	105.55	111.82
3	M	147	ILE	N-CA-C	5.40	114.52	106.85
1	A	244	GLU	N-CA-C	-5.40	105.79	112.38
2	J	263	THR	N-CA-C	-5.38	103.00	109.83
3	E	206	GLN	N-CA-C	5.38	116.82	109.18
3	P	164	ILE	N-CA-C	-5.37	105.48	110.53
3	H	63	GLU	N-CA-C	-5.36	104.02	110.88
1	I	280	ASN	N-CA-C	-5.36	105.60	111.82
3	F	33	VAL	N-CA-C	5.35	117.34	108.99
3	O	206	GLN	N-CA-C	5.35	116.78	109.18
2	D	307	GLY	N-CA-C	5.35	118.70	112.50
3	N	95	VAL	N-CA-C	5.34	115.55	107.80
1	K	121	LYS	N-CA-C	5.34	118.02	111.82
2	L	358	SER	N-CA-C	5.34	117.29	110.61
3	G	149	ILE	N-CA-C	5.34	116.00	108.36
1	K	348	GLY	N-CA-C	5.34	122.46	115.47
1	A	443	SER	N-CA-C	5.33	118.90	112.93
1	I	154	CYS	N-CA-C	5.32	121.57	109.81
1	C	72	TRP	N-CA-C	5.31	116.92	111.03
1	K	429	PHE	N-CA-C	5.30	117.97	111.82
1	I	251	ALA	N-CA-C	5.30	117.12	109.07
2	L	347	GLU	N-CA-C	-5.29	104.76	111.11
1	C	156	ILE	N-CA-C	5.29	115.73	110.23
1	C	429	PHE	N-CA-C	5.28	117.94	111.82
3	N	133	GLY	N-CA-C	-5.28	108.12	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	396	HIS	N-CA-C	5.27	117.71	111.33
2	J	294	GLN	CA-C-N	5.26	124.71	119.24
2	J	294	GLN	C-N-CA	5.26	124.71	119.24
1	K	388	ASP	N-CA-C	-5.25	105.20	111.03
2	L	438	LYS	CA-C-N	5.25	126.41	119.84
2	L	438	LYS	C-N-CA	5.25	126.41	119.84
3	H	95	VAL	N-CA-C	5.24	115.40	107.75
3	E	112	GLU	N-CA-C	-5.24	106.12	112.88
3	G	26	LEU	N-CA-C	5.23	116.67	110.97
2	L	481	ARG	N-CA-C	-5.21	106.69	113.16
3	N	254	VAL	N-CA-C	5.21	115.18	108.82
3	E	39	ASP	N-CA-C	-5.20	103.51	110.07
3	E	121	PHE	N-CA-C	5.20	117.59	109.52
1	K	251	ALA	N-CA-C	5.20	116.71	108.96
2	B	353	ASP	N-CA-C	-5.19	104.69	111.02
1	I	48	SER	N-CA-C	5.19	115.90	108.74
2	B	506	ASP	N-CA-C	-5.18	105.53	111.07
3	P	63	GLU	N-CA-C	-5.17	104.26	110.88
1	A	251	ALA	N-CA-C	5.16	116.92	109.07
1	A	390	THR	N-CA-C	5.16	116.76	111.03
1	C	279	MET	N-CA-C	5.16	118.62	111.71
1	I	57	MET	N-CA-C	5.15	118.24	111.28
3	H	143	LYS	N-CA-C	-5.15	107.03	113.72
1	C	121	LYS	N-CA-C	5.15	117.79	111.82
3	N	63	GLU	N-CA-C	-5.13	104.20	110.61
1	A	48	SER	N-CA-C	5.13	115.82	108.74
1	A	154	CYS	N-CA-C	5.12	121.14	109.81
3	O	219	ARG	N-CA-C	-5.11	107.59	113.88
2	D	481	ARG	N-CA-C	-5.11	106.83	113.16
2	J	302	LYS	N-CA-C	-5.10	104.99	111.11
1	C	128	ASP	N-CA-C	-5.10	105.84	111.71
3	G	147	ILE	N-CA-C	5.10	114.09	106.85
2	D	227	VAL	CA-C-N	5.09	124.71	119.56
2	D	227	VAL	C-N-CA	5.09	124.71	119.56
3	M	121	PHE	N-CA-C	5.09	117.42	109.52
2	J	500	SER	N-CA-C	-5.09	105.73	111.28
1	I	16	VAL	N-CA-C	5.08	115.31	110.53
3	H	133	GLY	N-CA-C	-5.08	108.36	114.66
1	I	322	LYS	N-CA-C	-5.08	105.21	111.40
1	C	124	VAL	N-CA-C	5.07	115.22	110.30
3	H	164	ILE	N-CA-C	-5.07	105.60	110.72
1	C	273	VAL	N-CA-C	5.06	115.38	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	39	ASP	N-CA-C	-5.06	103.69	110.07
3	M	112	GLU	N-CA-C	-5.05	106.43	112.59
2	B	336	SER	N-CA-C	5.05	116.86	111.36
2	B	307	GLY	N-CA-C	5.05	118.79	112.73
3	F	143	LYS	N-CA-C	-5.04	107.17	113.72
3	O	39	ASP	CA-C-N	5.04	124.83	119.28
3	O	39	ASP	C-N-CA	5.04	124.83	119.28
2	D	12	TYR	N-CA-C	-5.04	102.53	110.14
1	C	48	SER	N-CA-C	5.04	115.69	108.74
3	O	269	MET	N-CA-C	-5.03	106.99	113.23
2	B	500	SER	N-CA-C	-5.03	105.80	111.28
1	I	56	LEU	N-CA-C	5.02	119.05	113.02
2	D	109	GLU	N-CA-C	-5.02	103.70	108.22
3	M	269	MET	N-CA-C	-5.01	107.01	113.23
1	A	16	VAL	N-CA-C	5.01	115.24	110.53
3	O	147	ILE	N-CA-C	5.01	113.96	106.85
2	B	323	ASP	N-CA-C	5.00	121.45	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3790	0	3732	244	0
1	C	3790	0	3732	240	0
1	I	3790	0	3731	247	0
1	K	3790	0	3730	227	0
2	B	4174	0	4088	259	0
2	D	4174	0	4088	262	0
2	J	4174	0	4089	265	0
2	L	4174	0	4089	264	0
3	E	2161	0	2176	209	0
3	F	2186	0	2197	168	0
3	G	2161	0	2176	209	0
3	H	2186	0	2197	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	2161	0	2176	216	0
3	N	2186	0	2197	184	0
3	O	2161	0	2176	217	0
3	P	2186	0	2197	183	0
4	A	14	0	6	1	0
4	C	14	0	6	1	0
4	I	14	0	6	1	0
4	K	14	0	6	1	0
5	A	17	0	0	7	0
5	C	17	0	0	5	0
5	I	17	0	0	3	0
5	K	17	0	0	3	0
6	A	15	0	0	6	0
6	D	15	0	0	2	0
6	J	15	0	0	3	0
6	K	15	0	0	4	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
7	L	1	0	0	0	0
8	E	8	0	0	2	0
8	G	8	0	0	2	0
8	N	8	0	0	5	0
8	P	8	0	0	0	0
All	All	49464	0	48795	3329	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 34.

All (3329) 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)
2:B:400:LYS:HZ2	3:F:112:GLU:CD	1.21	1.43
2:B:400:LYS:NZ	3:F:112:GLU:CD	1.81	1.39
2:B:96:VAL:HG21	2:B:115:SER:HB2	1.32	1.11
2:D:96:VAL:HG21	2:D:115:SER:HB2	1.35	1.08
2:L:96:VAL:HG21	2:L:115:SER:HB2	1.34	1.08
3:O:52:LYS:H	3:O:52:LYS:HD3	1.20	1.06
3:F:137:MET:HB3	3:F:138:PRO:HD3	1.37	1.06
2:J:96:VAL:HG21	2:J:115:SER:HB2	1.34	1.06
3:G:52:LYS:H	3:G:52:LYS:HD3	1.19	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:52:LYS:HD3	3:E:52:LYS:H	1.20	1.02
3:G:189:THR:HB	3:G:192:GLU:HB2	1.37	1.02
3:M:52:LYS:H	3:M:52:LYS:HD3	1.22	1.01
3:H:137:MET:HB3	3:H:138:PRO:HD3	1.42	1.01
2:J:477:HIS:H	2:L:499:ASN:HD21	1.03	1.01
3:H:60:MET:HE1	3:H:75:VAL:HG13	1.38	1.00
3:N:137:MET:HB3	3:N:138:PRO:HD3	1.42	1.00
3:N:60:MET:HE1	3:N:75:VAL:HG13	1.43	1.00
3:F:60:MET:HE1	3:F:75:VAL:HG13	1.43	0.99
3:E:189:THR:HB	3:E:192:GLU:HB2	1.44	0.99
3:P:137:MET:HB3	3:P:138:PRO:HD3	1.46	0.98
3:G:162:ASN:HD21	3:G:259:ILE:HG12	1.27	0.97
3:M:162:ASN:HD21	3:M:259:ILE:HG12	1.29	0.96
1:A:88:CYS:HG	6:A:6498:CLF:FE4	0.70	0.96
3:G:259:ILE:HD11	3:G:264:LEU:HG	1.49	0.94
3:M:189:THR:HB	3:M:192:GLU:HB2	1.49	0.94
3:H:50:HIS:O	3:H:224:ARG:HD3	1.68	0.94
3:O:189:THR:HB	3:O:192:GLU:HB2	1.50	0.94
3:N:76:LEU:HD11	3:N:84:LYS:HB3	1.49	0.93
3:G:91:PRO:HA	3:G:100:ARG:HH22	1.31	0.93
3:M:91:PRO:HA	3:M:100:ARG:HH22	1.33	0.93
3:M:281:ILE:HG22	3:N:223:ARG:HD2	1.51	0.93
3:O:91:PRO:HA	3:O:100:ARG:HH22	1.30	0.93
3:P:60:MET:HE1	3:P:75:VAL:HG13	1.51	0.92
3:E:76:LEU:HD11	3:E:84:LYS:HB3	1.51	0.92
3:M:76:LEU:HD11	3:M:84:LYS:HB3	1.52	0.92
3:N:50:HIS:O	3:N:224:ARG:HD3	1.70	0.92
3:E:162:ASN:HD21	3:E:259:ILE:HG12	1.30	0.91
2:J:499:ASN:HD21	2:L:477:HIS:H	1.13	0.91
3:E:259:ILE:HD11	3:E:264:LEU:HG	1.52	0.91
1:A:275:CYS:HG	5:A:6496:CFM:FE1	0.78	0.91
1:A:88:CYS:SG	6:A:6498:CLF:FE4	1.63	0.91
3:E:91:PRO:HA	3:E:100:ARG:HH22	1.34	0.90
3:F:206:GLN:HG2	3:F:252:LEU:HD22	1.52	0.90
3:P:206:GLN:HG2	3:P:252:LEU:HD22	1.52	0.89
1:I:88:CYS:HG	6:J:8498:CLF:FE4	0.83	0.89
1:K:88:CYS:HG	6:K:9498:CLF:FE4	0.61	0.89
2:B:477:HIS:H	2:D:499:ASN:HD21	1.13	0.88
3:F:50:HIS:O	3:F:224:ARG:HD3	1.74	0.88
1:A:433:LYS:HE3	2:B:263:THR:HG23	1.54	0.88
3:O:259:ILE:HD11	3:O:264:LEU:HG	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:203:ARG:HD2	1:I:204:ASP:OD1	1.73	0.88
3:O:162:ASN:HD21	3:O:259:ILE:HG12	1.37	0.88
2:D:400:LYS:NZ	3:H:112:GLU:CD	2.32	0.88
2:B:400:LYS:HZ3	3:F:112:GLU:CD	1.77	0.87
3:N:241:ARG:HB3	3:N:245:ARG:HH12	1.36	0.87
3:H:127:LEU:HD21	3:H:129:ASP:HB2	1.56	0.87
3:M:32:LYS:HB3	3:M:119:LEU:HD12	1.57	0.87
3:P:50:HIS:O	3:P:224:ARG:HD3	1.73	0.87
3:F:241:ARG:HB3	3:F:245:ARG:HH12	1.37	0.87
1:I:433:LYS:HE3	2:J:263:THR:HG23	1.56	0.86
3:P:127:LEU:HD21	3:P:129:ASP:HB2	1.56	0.86
3:H:206:GLN:HG2	3:H:252:LEU:HD22	1.58	0.86
3:N:206:GLN:HG2	3:N:252:LEU:HD22	1.58	0.86
3:N:127:LEU:HD21	3:N:129:ASP:HB2	1.55	0.86
1:K:203:ARG:HD2	1:K:204:ASP:OD1	1.75	0.86
3:M:259:ILE:HD11	3:M:264:LEU:HG	1.55	0.85
1:C:433:LYS:HE3	2:D:263:THR:HG23	1.56	0.85
3:F:127:LEU:HD21	3:F:129:ASP:HB2	1.59	0.85
3:O:32:LYS:HB3	3:O:119:LEU:HD12	1.59	0.85
2:B:128:GLN:HE22	2:B:165:PHE:HA	1.42	0.85
3:E:32:LYS:HB3	3:E:119:LEU:HD12	1.58	0.85
3:P:76:LEU:HD11	3:P:84:LYS:HB3	1.58	0.85
2:J:128:GLN:HE22	2:J:165:PHE:HA	1.42	0.84
3:O:76:LEU:HD11	3:O:84:LYS:HB3	1.58	0.84
2:D:128:GLN:HE22	2:D:165:PHE:HA	1.42	0.84
1:K:42:SER:HA	1:K:391:MET:HE1	1.60	0.84
2:B:499:ASN:HD21	2:D:477:HIS:H	1.19	0.84
1:K:433:LYS:HE3	2:L:263:THR:HG23	1.59	0.83
3:F:76:LEU:HD11	3:F:84:LYS:HB3	1.57	0.83
1:A:203:ARG:HD2	1:A:204:ASP:OD1	1.78	0.83
2:J:178:GLU:H	2:J:178:GLU:CD	1.87	0.83
3:M:160:ALA:O	3:M:164:ILE:HG13	1.79	0.82
3:H:76:LEU:HD11	3:H:84:LYS:HB3	1.59	0.82
3:M:223:ARG:HG2	3:N:281:ILE:HD12	1.60	0.82
1:K:88:CYS:SG	6:K:9498:CLF:FE4	1.72	0.82
3:M:136:ALA:HB1	3:N:94:GLY:HA2	1.61	0.82
2:B:23:MET:HE2	2:B:23:MET:O	1.78	0.81
3:G:162:ASN:ND2	3:G:259:ILE:HG12	1.94	0.81
3:M:41:LYS:HG3	3:N:156:MET:HE1	1.61	0.81
3:G:32:LYS:HB3	3:G:119:LEU:HD12	1.60	0.81
3:H:241:ARG:HB3	3:H:245:ARG:HH12	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:ARG:HD2	1:C:204:ASP:OD1	1.81	0.81
2:J:23:MET:HE2	2:J:23:MET:O	1.80	0.81
2:J:118:MET:HE3	2:J:127:GLY:HA3	1.61	0.81
2:L:466:LEU:HD12	2:L:467:ILE:N	1.96	0.81
3:E:197:ILE:HG23	3:E:207:MET:HB3	1.63	0.81
1:I:120:GLU:O	1:I:124:VAL:HG23	1.81	0.80
3:O:160:ALA:O	3:O:164:ILE:HG13	1.81	0.80
3:O:285:THR:HG21	3:P:230:TYR:CE1	2.15	0.80
3:P:241:ARG:HB3	3:P:245:ARG:HH12	1.45	0.80
2:B:178:GLU:H	2:B:178:GLU:CD	1.89	0.80
1:A:88:CYS:SG	6:A:6498:CLF:FE5	1.73	0.80
2:D:452:GLN:OE1	2:D:465:PRO:HA	1.82	0.80
3:G:267:LEU:HD23	3:G:267:LEU:O	1.82	0.80
1:I:74:PRO:HB2	1:I:254:SER:HB2	1.64	0.80
3:E:267:LEU:O	3:E:267:LEU:HD23	1.82	0.80
3:G:76:LEU:HD11	3:G:84:LYS:HB3	1.64	0.80
2:B:394:LEU:HD23	2:B:395:CYS:N	1.97	0.79
3:E:160:ALA:O	3:E:164:ILE:HG13	1.80	0.79
1:K:74:PRO:HB2	1:K:254:SER:HB2	1.62	0.79
2:B:510:ARG:CZ	2:D:452:GLN:HE21	1.96	0.79
3:F:141:GLU:HB3	3:F:143:LYS:HE2	1.65	0.79
2:J:466:LEU:HD12	2:J:467:ILE:N	1.97	0.79
2:B:452:GLN:OE1	2:B:465:PRO:HA	1.83	0.79
2:D:400:LYS:HZ2	3:H:112:GLU:CD	1.89	0.79
1:A:250:VAL:HG13	2:B:31:PHE:CD1	2.18	0.79
2:D:466:LEU:HD12	2:D:467:ILE:N	1.98	0.79
1:I:389:ARG:HG3	1:I:389:ARG:HH11	1.48	0.79
2:D:178:GLU:H	2:D:178:GLU:CD	1.91	0.79
3:G:197:ILE:HG23	3:G:207:MET:HB3	1.66	0.78
3:F:225:MET:HE2	3:F:230:TYR:HA	1.66	0.78
3:E:225:MET:HE3	3:E:229:GLU:OE1	1.82	0.78
3:M:162:ASN:ND2	3:M:259:ILE:HG12	1.97	0.78
3:M:197:ILE:HG23	3:M:207:MET:HB3	1.62	0.78
2:D:376:VAL:O	2:D:380:VAL:HG23	1.83	0.78
1:A:120:GLU:O	1:A:124:VAL:HG23	1.83	0.78
2:L:128:GLN:HE22	2:L:165:PHE:HA	1.46	0.78
3:O:197:ILE:HG23	3:O:207:MET:HB3	1.65	0.78
2:B:118:MET:HE3	2:B:127:GLY:HA3	1.66	0.77
2:L:452:GLN:OE1	2:L:465:PRO:HA	1.84	0.77
1:A:74:PRO:HB2	1:A:254:SER:HB2	1.67	0.77
2:B:358:SER:HB3	2:D:477:HIS:ND1	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:96:VAL:CG2	2:D:115:SER:HB2	2.12	0.77
3:O:223:ARG:HD3	3:P:281:ILE:O	1.85	0.77
3:E:162:ASN:ND2	3:E:259:ILE:HG12	1.99	0.77
2:B:376:VAL:O	2:B:380:VAL:HG23	1.85	0.77
2:D:394:LEU:HD23	2:D:395:CYS:N	2.00	0.76
3:F:182:LEU:O	3:F:208:ILE:HG22	1.86	0.76
1:K:120:GLU:O	1:K:124:VAL:HG23	1.84	0.76
3:G:160:ALA:O	3:G:164:ILE:HG13	1.86	0.76
3:G:52:LYS:HD3	3:G:52:LYS:N	2.00	0.76
2:J:394:LEU:HD23	2:J:395:CYS:N	2.01	0.76
3:O:162:ASN:ND2	3:O:259:ILE:HG12	2.00	0.76
3:E:103:ILE:HG13	3:E:137:MET:HG3	1.68	0.76
3:F:137:MET:HB3	3:F:138:PRO:CD	2.15	0.75
2:J:452:GLN:OE1	2:J:465:PRO:HA	1.85	0.75
2:L:118:MET:HE3	2:L:127:GLY:HA3	1.67	0.75
1:A:335:TRP:O	1:A:339:VAL:HG23	1.86	0.75
2:B:96:VAL:CG2	2:B:115:SER:HB2	2.15	0.75
3:H:41:LYS:O	3:H:41:LYS:HD3	1.85	0.75
3:N:158:MET:HE1	3:N:195:LEU:HD11	1.67	0.75
3:E:76:LEU:CD1	3:E:84:LYS:HB3	2.16	0.75
1:I:42:SER:HA	1:I:391:MET:HE1	1.69	0.75
3:G:103:ILE:HG13	3:G:137:MET:HG3	1.67	0.75
3:H:139:ILE:HG23	3:H:177:VAL:HG21	1.66	0.75
3:N:141:GLU:HB3	3:N:143:LYS:HE2	1.66	0.75
3:M:76:LEU:CD1	3:M:84:LYS:HB3	2.17	0.75
1:C:120:GLU:O	1:C:124:VAL:HG23	1.85	0.74
3:M:136:ALA:CB	3:N:94:GLY:HA2	2.16	0.74
1:C:250:VAL:HG13	2:D:31:PHE:CD1	2.21	0.74
2:J:96:VAL:CG2	2:J:115:SER:HB2	2.15	0.74
3:H:182:LEU:O	3:H:208:ILE:HG22	1.86	0.74
2:L:394:LEU:HD23	2:L:395:CYS:N	2.03	0.74
1:A:88:CYS:HB2	1:A:153:GLU:OE2	1.88	0.74
3:G:127:LEU:HD11	3:G:129:ASP:HB2	1.68	0.74
3:O:52:LYS:HD3	3:O:52:LYS:N	2.01	0.74
3:O:48:ILE:HG22	3:O:49:LEU:HD23	1.69	0.74
1:C:74:PRO:HB2	1:C:254:SER:HB2	1.68	0.74
3:M:103:ILE:HG13	3:M:137:MET:HG3	1.68	0.74
2:J:510:ARG:CZ	2:L:452:GLN:HE21	2.01	0.74
3:M:127:LEU:HD11	3:M:129:ASP:HB2	1.70	0.74
3:O:225:MET:HE3	3:O:229:GLU:OE1	1.88	0.74
2:D:23:MET:HE2	2:D:23:MET:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:208:ILE:O	3:E:209:HIS:HB2	1.87	0.73
3:O:91:PRO:HA	3:O:100:ARG:NH2	2.03	0.73
3:M:4:GLN:HA	3:M:122:VAL:HB	1.69	0.73
3:M:267:LEU:O	3:M:267:LEU:HD23	1.87	0.73
1:K:335:TRP:O	1:K:339:VAL:HG23	1.88	0.73
3:N:139:ILE:HG23	3:N:177:VAL:HG21	1.68	0.73
3:O:267:LEU:HD23	3:O:267:LEU:O	1.88	0.73
3:F:139:ILE:HG23	3:F:177:VAL:HG21	1.70	0.73
3:G:136:ALA:CB	3:H:94:GLY:HA2	2.18	0.73
2:J:192:SER:OG	2:J:194:VAL:HG22	1.88	0.73
1:I:230:ASN:HA	1:I:235:ALA:H	1.53	0.73
1:C:335:TRP:O	1:C:339:VAL:HG23	1.89	0.73
2:L:23:MET:HE2	2:L:23:MET:O	1.89	0.73
3:P:139:ILE:HG23	3:P:177:VAL:HG21	1.70	0.73
1:A:19:VAL:HG11	1:A:407:TYR:CE2	2.23	0.73
3:E:45:THR:CG2	3:E:85:CYS:HB3	2.19	0.73
3:H:225:MET:HE2	3:H:230:TYR:HA	1.71	0.73
3:O:136:ALA:CB	3:P:94:GLY:HA2	2.19	0.73
3:E:127:LEU:HD11	3:E:129:ASP:HB2	1.71	0.73
2:L:96:VAL:CG2	2:L:115:SER:HB2	2.13	0.73
3:N:41:LYS:O	3:N:41:LYS:HD3	1.88	0.73
1:C:57:MET:HE2	2:D:113:CYS:H	1.52	0.72
3:P:41:LYS:O	3:P:41:LYS:HD3	1.89	0.72
2:J:477:HIS:ND1	2:L:358:SER:HB3	2.03	0.72
1:K:59:ILE:H	1:K:59:ILE:HD12	1.54	0.72
1:C:230:ASN:HA	1:C:235:ALA:H	1.54	0.72
1:K:275:CYS:HA	1:K:358:LEU:HD22	1.70	0.72
3:H:141:GLU:HB3	3:H:143:LYS:HE2	1.70	0.72
1:I:88:CYS:HB2	1:I:153:GLU:OE2	1.90	0.72
3:N:147:ILE:HG21	3:N:168:ILE:HD11	1.71	0.72
3:P:225:MET:HE2	3:P:230:TYR:HA	1.71	0.72
3:M:91:PRO:HA	3:M:100:ARG:NH2	2.04	0.72
3:G:91:PRO:HA	3:G:100:ARG:NH2	2.05	0.72
3:G:225:MET:HE3	3:G:229:GLU:OE1	1.89	0.72
1:I:335:TRP:O	1:I:339:VAL:HG23	1.90	0.72
1:K:59:ILE:HD12	1:K:59:ILE:N	2.04	0.72
2:J:452:GLN:HE21	2:L:510:ARG:CZ	2.02	0.72
3:M:225:MET:HE3	3:M:229:GLU:OE1	1.90	0.72
3:O:186:SER:HB2	3:O:212:PRO:HA	1.71	0.72
1:C:226:ILE:O	1:C:273:VAL:HA	1.90	0.72
1:C:275:CYS:HA	1:C:358:LEU:HD22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:466:LEU:HD12	2:B:467:ILE:N	2.05	0.72
3:N:54:GLN:HE22	3:N:86:VAL:HA	1.55	0.72
1:C:339:VAL:O	1:C:343:ARG:HB3	1.90	0.71
3:G:4:GLN:HA	3:G:122:VAL:HB	1.71	0.71
1:K:19:VAL:HG11	1:K:407:TYR:CE2	2.25	0.71
3:M:135:PHE:HZ	3:N:130:VAL:HG11	1.53	0.71
3:N:208:ILE:HD11	3:N:246:LYS:HB3	1.70	0.71
3:N:208:ILE:O	3:N:246:LYS:HD3	1.89	0.71
1:A:230:ASN:HA	1:A:235:ALA:H	1.55	0.71
2:B:205:ALA:HA	2:B:281:MET:HE1	1.72	0.71
2:L:466:LEU:HD12	2:L:467:ILE:H	1.53	0.71
3:O:49:LEU:HD11	3:O:85:CYS:HB2	1.72	0.71
3:O:127:LEU:HD11	3:O:129:ASP:HB2	1.71	0.71
3:M:49:LEU:HD21	3:M:85:CYS:SG	2.30	0.71
3:O:49:LEU:HD21	3:O:85:CYS:SG	2.29	0.71
3:O:103:ILE:HG13	3:O:137:MET:HG3	1.72	0.71
1:C:13:ILE:O	1:C:17:LEU:HG	1.90	0.71
3:F:41:LYS:O	3:F:41:LYS:HD3	1.91	0.71
2:J:376:VAL:O	2:J:380:VAL:HG23	1.90	0.71
3:P:158:MET:HE1	3:P:195:LEU:HD11	1.71	0.71
3:G:41:LYS:HG3	3:H:156:MET:HE1	1.71	0.71
3:E:45:THR:HG21	3:E:85:CYS:HB3	1.74	0.70
1:I:239:ARG:NE	2:J:23:MET:HE1	2.06	0.70
2:B:213:MET:HE1	2:B:309:TRP:HA	1.74	0.70
1:C:346:LEU:O	1:C:349:LYS:HG2	1.91	0.70
2:D:118:MET:HE3	2:D:127:GLY:HA3	1.73	0.70
3:G:2:MET:HA	3:G:120:ASP:O	1.91	0.70
3:G:48:ILE:HG22	3:G:49:LEU:HD23	1.71	0.70
1:C:42:SER:HA	1:C:391:MET:HE1	1.73	0.70
1:K:226:ILE:O	1:K:273:VAL:HA	1.92	0.70
1:A:389:ARG:HG3	1:A:389:ARG:HH11	1.55	0.70
1:I:250:VAL:HG13	2:J:31:PHE:CD1	2.26	0.70
3:M:45:THR:CG2	3:M:85:CYS:HB3	2.21	0.70
3:E:91:PRO:HA	3:E:100:ARG:NH2	2.05	0.70
3:N:225:MET:HE2	3:N:230:TYR:HA	1.73	0.70
1:A:35:ASN:ND2	1:A:36:ASP:H	1.90	0.70
1:C:19:VAL:HG11	1:C:407:TYR:CE2	2.26	0.70
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.26	0.70
3:G:45:THR:CG2	3:G:85:CYS:HB3	2.20	0.70
3:H:10:LYS:HG2	3:H:11:GLY:N	2.07	0.70
1:A:59:ILE:H	1:A:59:ILE:HD12	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:48:ILE:HG22	3:M:49:LEU:HD23	1.73	0.69
3:E:71:GLU:HB3	3:E:74:ASP:OD1	1.92	0.69
2:J:494:LEU:O	2:J:498:VAL:HG12	1.92	0.69
1:A:68:LYS:C	1:A:68:LYS:HD3	2.17	0.69
1:A:42:SER:HA	1:A:391:MET:HE1	1.73	0.69
3:O:15:LYS:NZ	3:O:127:LEU:HA	2.08	0.69
2:J:213:MET:HE1	2:J:309:TRP:HA	1.74	0.69
1:A:289:LYS:O	1:A:289:LYS:HG2	1.91	0.69
3:E:76:LEU:HD11	3:E:84:LYS:CB	2.23	0.69
3:H:8:TYR:HB3	3:H:164:ILE:HD13	1.74	0.69
1:I:19:VAL:HG11	1:I:407:TYR:CE2	2.28	0.69
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.28	0.69
2:D:466:LEU:HD12	2:D:467:ILE:H	1.57	0.69
3:F:208:ILE:HD11	3:F:246:LYS:HB3	1.75	0.69
3:G:208:ILE:O	3:G:209:HIS:HB2	1.92	0.69
1:I:234:ASP:HB3	1:I:451:HIS:ND1	2.08	0.69
1:I:339:VAL:O	1:I:343:ARG:HB3	1.93	0.69
3:M:165:SER:HB3	3:M:256:PRO:HB2	1.72	0.69
2:B:205:ALA:HA	2:B:281:MET:CE	2.22	0.69
3:E:4:GLN:HA	3:E:122:VAL:HB	1.75	0.69
3:P:72:LEU:C	3:P:72:LEU:HD22	2.17	0.69
2:B:231:GLU:CD	2:B:236:ASN:HD22	2.01	0.69
2:D:400:LYS:HZ3	3:H:112:GLU:CD	2.00	0.69
2:J:231:GLU:CD	2:J:236:ASN:HD22	2.01	0.69
2:L:178:GLU:H	2:L:178:GLU:CD	2.00	0.69
1:A:367:TYR:HD1	1:A:372:MET:HG2	1.58	0.68
3:H:137:MET:HB3	3:H:138:PRO:CD	2.22	0.68
1:I:68:LYS:C	1:I:68:LYS:HD3	2.18	0.68
3:M:49:LEU:HD11	3:M:85:CYS:HB2	1.75	0.68
3:O:76:LEU:CD1	3:O:84:LYS:HB3	2.23	0.68
2:B:477:HIS:ND1	2:D:358:SER:HB3	2.08	0.68
3:F:208:ILE:O	3:F:246:LYS:HD3	1.93	0.68
2:L:213:MET:HE1	2:L:309:TRP:HA	1.74	0.68
1:K:339:VAL:O	1:K:343:ARG:HB3	1.92	0.68
2:B:468:ARG:HH11	2:B:468:ARG:HG3	1.58	0.68
3:E:99:GLY:HA3	3:E:134:GLY:HA2	1.76	0.68
1:K:77:ASP:OD2	1:K:258:SER:HB2	1.93	0.68
3:E:49:LEU:HD11	3:E:85:CYS:HB2	1.76	0.68
3:E:92:GLU:OE1	3:F:170:LYS:HE3	1.94	0.68
3:F:147:ILE:HG21	3:F:168:ILE:HD11	1.74	0.68
3:G:127:LEU:HD13	3:G:129:ASP:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:33:VAL:HG12	3:H:34:MET:N	2.08	0.68
1:I:275:CYS:HA	1:I:358:LEU:HD22	1.75	0.68
3:N:8:TYR:HB3	3:N:164:ILE:HD13	1.76	0.68
2:B:511:GLY:O	2:B:516:ASP:HB3	1.93	0.68
3:E:48:ILE:HG22	3:E:49:LEU:HD23	1.74	0.68
1:K:354:TYR:CZ	1:K:404:VAL:HG12	2.29	0.68
3:P:141:GLU:HB3	3:P:143:LYS:HE2	1.76	0.68
3:P:182:LEU:O	3:P:208:ILE:HG22	1.93	0.68
3:O:165:SER:HB3	3:O:256:PRO:HB2	1.76	0.68
1:C:68:LYS:C	1:C:68:LYS:HD3	2.19	0.67
3:E:52:LYS:HD3	3:E:52:LYS:N	2.01	0.67
1:A:35:ASN:HD22	1:A:36:ASP:H	1.41	0.67
3:G:49:LEU:HD11	3:G:85:CYS:HB2	1.74	0.67
3:M:184:CYS:HG	3:M:210:PHE:HE1	1.39	0.67
2:B:220:SER:OG	2:B:286:ASN:HB3	1.94	0.67
2:B:452:GLN:HE21	2:D:510:ARG:CZ	2.07	0.67
3:E:96:GLY:HA3	3:E:100:ARG:NH1	2.08	0.67
2:J:178:GLU:CD	2:J:178:GLU:N	2.51	0.67
2:J:205:ALA:HA	2:J:281:MET:CE	2.25	0.67
3:H:184:CYS:HG	3:H:210:PHE:HE1	1.42	0.67
3:P:33:VAL:HG12	3:P:34:MET:N	2.08	0.67
1:C:113:ASN:HD22	2:D:66:PRO:CD	2.07	0.67
2:D:178:GLU:CD	2:D:178:GLU:N	2.52	0.67
3:H:223:ARG:HB3	3:H:225:MET:HG2	1.77	0.67
3:N:212:PRO:HG2	3:N:236:GLN:OE1	1.95	0.67
3:O:4:GLN:HA	3:O:122:VAL:HB	1.74	0.67
1:K:230:ASN:HA	1:K:235:ALA:H	1.57	0.67
3:E:197:ILE:HG23	3:E:207:MET:CB	2.24	0.67
3:G:165:SER:HB3	3:G:256:PRO:HB2	1.77	0.67
3:N:102:VAL:HG12	3:N:106:ILE:HD11	1.76	0.67
3:O:197:ILE:HG23	3:O:207:MET:CB	2.25	0.67
1:C:88:CYS:HB2	1:C:153:GLU:OE2	1.95	0.67
3:E:186:SER:HB2	3:E:212:PRO:HA	1.75	0.67
3:G:228:ILE:O	3:G:232:PRO:HG3	1.95	0.67
1:I:355:ILE:HG22	1:I:356:GLY:H	1.59	0.67
2:J:205:ALA:HA	2:J:281:MET:HE1	1.77	0.67
1:K:13:ILE:O	1:K:17:LEU:HG	1.95	0.67
3:M:127:LEU:HD13	3:M:129:ASP:H	1.59	0.67
3:O:45:THR:CG2	3:O:85:CYS:HB3	2.25	0.67
3:G:186:SER:HB2	3:G:212:PRO:HA	1.77	0.67
1:I:253:TRP:CZ2	1:I:262:ILE:HG23	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:466:LEU:HD12	2:J:467:ILE:H	1.56	0.67
2:B:43:VAL:O	2:B:46:TRP:HB3	1.95	0.66
3:P:208:ILE:O	3:P:246:LYS:HD3	1.95	0.66
2:B:178:GLU:CD	2:B:178:GLU:N	2.50	0.66
3:F:33:VAL:HG12	3:F:34:MET:N	2.08	0.66
3:N:47:LEU:HD22	3:N:225:MET:O	1.96	0.66
2:L:91:GLY:HA3	2:L:152:THR:OG1	1.95	0.66
3:M:99:GLY:HA3	3:M:134:GLY:HA2	1.77	0.66
3:N:182:LEU:O	3:N:208:ILE:HG22	1.95	0.66
1:K:66:GLY:O	1:K:70:VAL:HB	1.95	0.66
3:M:186:SER:HB2	3:M:212:PRO:HA	1.75	0.66
3:O:127:LEU:HD13	3:O:129:ASP:H	1.61	0.66
1:A:59:ILE:HD12	1:A:59:ILE:N	2.11	0.66
2:J:151:THR:HG23	2:J:162:LEU:HD11	1.77	0.66
2:J:358:SER:HB3	2:L:477:HIS:ND1	2.10	0.66
1:K:367:TYR:HD1	1:K:372:MET:HG2	1.61	0.66
1:A:239:ARG:NE	2:B:23:MET:HE1	2.10	0.66
3:F:236:GLN:O	3:F:239:GLU:HB2	1.96	0.66
1:I:367:TYR:HD1	1:I:372:MET:HG2	1.60	0.66
2:L:400:LYS:HZ2	3:P:112:GLU:CD	2.03	0.66
3:M:197:ILE:HG23	3:M:207:MET:CB	2.25	0.66
3:M:208:ILE:O	3:M:209:HIS:HB2	1.94	0.66
1:C:35:ASN:ND2	1:C:36:ASP:H	1.93	0.66
3:G:2:MET:HE3	3:G:122:VAL:HG21	1.78	0.66
3:G:182:LEU:HD12	3:G:196:ILE:HG22	1.78	0.66
3:H:208:ILE:O	3:H:246:LYS:HD3	1.95	0.66
3:N:10:LYS:HG2	3:N:11:GLY:N	2.10	0.66
3:N:137:MET:HB3	3:N:138:PRO:CD	2.22	0.66
3:O:169:VAL:HG23	3:O:256:PRO:HG2	1.77	0.66
2:D:213:MET:HE1	2:D:309:TRP:HA	1.77	0.66
3:N:223:ARG:HB3	3:N:225:MET:HG2	1.77	0.66
3:E:169:VAL:HG23	3:E:256:PRO:HG2	1.77	0.66
3:H:67:VAL:C	3:H:69:ASP:H	2.03	0.66
3:M:223:ARG:HG2	3:N:281:ILE:CD1	2.24	0.66
2:B:295:PRO:O	2:B:297:HIS:N	2.29	0.66
1:C:35:ASN:HD22	1:C:36:ASP:H	1.43	0.66
3:G:76:LEU:CD1	3:G:84:LYS:HB3	2.26	0.66
2:J:373:PRO:HD3	2:J:397:ASN:OD1	1.96	0.66
3:P:67:VAL:C	3:P:69:ASP:H	2.04	0.66
1:A:253:TRP:CZ2	1:A:262:ILE:HG23	2.31	0.65
3:E:165:SER:HB3	3:E:256:PRO:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:49:LEU:HD21	3:G:85:CYS:SG	2.35	0.65
3:G:72:LEU:HD13	3:G:112:GLU:CB	2.26	0.65
1:I:226:ILE:O	1:I:273:VAL:HA	1.95	0.65
1:K:389:ARG:HH11	1:K:389:ARG:HG3	1.61	0.65
3:M:86:VAL:HG21	3:M:109:LEU:HD11	1.78	0.65
3:O:20:GLN:NE2	3:O:48:ILE:HG12	2.11	0.65
3:H:54:GLN:HE22	3:H:86:VAL:HA	1.61	0.65
3:M:52:LYS:HD3	3:M:52:LYS:N	2.05	0.65
3:H:147:ILE:HG21	3:H:168:ILE:HD11	1.78	0.65
2:L:231:GLU:CD	2:L:236:ASN:HD22	2.05	0.65
2:B:247:MET:HE3	2:B:341:PRO:HD2	1.78	0.65
1:I:275:CYS:HB3	1:I:278:SER:OG	1.97	0.65
3:E:228:ILE:O	3:E:232:PRO:HG3	1.96	0.65
3:G:197:ILE:HG23	3:G:207:MET:CB	2.27	0.65
3:H:158:MET:HE1	3:H:195:LEU:HD11	1.79	0.65
1:K:35:ASN:ND2	1:K:36:ASP:H	1.94	0.65
3:N:127:LEU:CD2	3:N:129:ASP:HB2	2.27	0.65
3:P:137:MET:HB3	3:P:138:PRO:CD	2.24	0.65
3:P:147:ILE:HG21	3:P:168:ILE:HD11	1.79	0.65
3:E:20:GLN:NE2	3:E:48:ILE:HG12	2.11	0.65
1:I:439:ARG:HH12	1:I:465:MET:HE3	1.61	0.65
1:A:87:GLY:HA3	6:A:6498:CLF:S2B	2.36	0.65
1:C:59:ILE:N	1:C:59:ILE:HD12	2.11	0.65
3:F:54:GLN:HE22	3:F:86:VAL:HA	1.62	0.65
2:J:91:GLY:HA3	2:J:152:THR:OG1	1.97	0.65
3:M:92:GLU:OE1	3:N:170:LYS:HE3	1.97	0.65
3:F:67:VAL:C	3:F:69:ASP:H	2.05	0.65
3:G:52:LYS:H	3:G:52:LYS:CD	2.03	0.65
3:G:45:THR:HG21	3:G:85:CYS:HB3	1.80	0.64
1:C:275:CYS:HB3	1:C:278:SER:OG	1.97	0.64
2:D:23:MET:HE2	2:D:23:MET:C	2.23	0.64
2:J:70:CYS:SG	2:J:72:PRO:HG2	2.37	0.64
2:D:247:MET:HE1	2:D:340:ILE:HG12	1.79	0.64
2:J:236:ASN:HB3	2:J:485:LEU:HD12	1.80	0.64
1:K:57:MET:HE2	2:L:113:CYS:H	1.61	0.64
3:O:192:GLU:O	3:O:196:ILE:HG12	1.98	0.64
1:C:234:ASP:HB3	1:C:451:HIS:ND1	2.13	0.64
2:D:509:THR:O	2:D:516:ASP:HA	1.97	0.64
3:E:2:MET:HA	3:E:120:ASP:O	1.98	0.64
1:I:13:ILE:O	1:I:17:LEU:HG	1.96	0.64
1:I:66:GLY:O	1:I:70:VAL:HB	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:151:THR:HG23	2:L:162:LEU:HD11	1.79	0.64
1:I:35:ASN:ND2	1:I:36:ASP:H	1.96	0.64
3:M:2:MET:HE3	3:M:122:VAL:HG21	1.80	0.64
3:O:52:LYS:H	3:O:52:LYS:CD	2.04	0.64
2:B:91:GLY:HA3	2:B:152:THR:OG1	1.98	0.64
2:B:477:HIS:H	2:D:499:ASN:ND2	1.93	0.64
3:E:52:LYS:HB3	3:E:224:ARG:NH1	2.13	0.64
3:E:284:LYS:C	3:E:284:LYS:HD3	2.22	0.64
3:F:47:LEU:HD22	3:F:225:MET:O	1.97	0.64
3:N:67:VAL:C	3:N:69:ASP:H	2.05	0.64
1:A:19:VAL:HG13	1:A:20:TYR:N	2.12	0.64
3:O:33:VAL:HG22	3:O:121:PHE:HB2	1.80	0.64
2:B:213:MET:CE	2:B:309:TRP:HA	2.28	0.64
1:C:389:ARG:HH11	1:C:389:ARG:HG3	1.63	0.64
3:E:241:ARG:HG2	3:E:245:ARG:NH1	2.12	0.64
1:K:275:CYS:HB3	1:K:278:SER:OG	1.98	0.64
2:L:205:ALA:HA	2:L:281:MET:HE1	1.80	0.64
3:O:208:ILE:O	3:O:209:HIS:HB2	1.97	0.64
1:A:405:THR:HG23	1:A:408:GLU:CD	2.23	0.64
3:M:182:LEU:HD12	3:M:196:ILE:HG22	1.80	0.64
3:P:10:LYS:HG2	3:P:11:GLY:N	2.12	0.64
1:C:239:ARG:NE	2:D:23:MET:HE1	2.13	0.63
2:D:494:LEU:O	2:D:498:VAL:HG12	1.98	0.63
3:M:215:ASN:O	3:M:219:ARG:HG3	1.97	0.63
1:A:199:ASN:OD1	1:A:281:TYR:HB2	1.98	0.63
2:B:247:MET:CE	2:B:340:ILE:HA	2.28	0.63
2:D:205:ALA:HA	2:D:281:MET:CE	2.28	0.63
3:F:158:MET:HE1	3:F:195:LEU:HD11	1.79	0.63
3:H:269:MET:HB3	3:H:274:MET:HE2	1.79	0.63
1:C:355:ILE:HG22	1:C:356:GLY:H	1.61	0.63
3:F:10:LYS:HG2	3:F:11:GLY:N	2.12	0.63
2:L:376:VAL:O	2:L:380:VAL:HG23	1.98	0.63
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.81	0.63
2:D:192:SER:OG	2:D:194:VAL:HG22	1.99	0.63
3:E:191:ARG:HE	3:E:194:GLU:CD	2.07	0.63
3:E:278:ASP:CB	3:E:281:ILE:HD12	2.29	0.63
2:J:103:PHE:CB	2:J:111:VAL:HG21	2.28	0.63
3:M:76:LEU:HD11	3:M:84:LYS:CB	2.25	0.63
3:P:100:ARG:HD3	3:P:101:GLY:N	2.14	0.63
3:E:15:LYS:NZ	3:E:127:LEU:HA	2.13	0.63
3:E:136:ALA:CB	3:F:94:GLY:HA2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:285:THR:HG21	3:F:230:TYR:CE1	2.34	0.63
3:G:278:ASP:CB	3:G:281:ILE:HD12	2.28	0.63
1:I:59:ILE:HD12	1:I:59:ILE:N	2.12	0.63
1:I:199:ASN:OD1	1:I:281:TYR:HB2	1.97	0.63
1:K:250:VAL:HG13	2:L:31:PHE:CD1	2.33	0.63
3:M:192:GLU:O	3:M:196:ILE:HG12	1.99	0.63
3:M:228:ILE:O	3:M:232:PRO:HG3	1.98	0.63
3:O:155:MET:CG	3:O:156:MET:HE2	2.29	0.63
3:P:56:THR:OG1	3:P:59:GLU:HG3	1.98	0.63
1:A:66:GLY:O	1:A:70:VAL:HB	1.98	0.63
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.81	0.63
1:C:289:LYS:HG2	1:C:289:LYS:O	1.97	0.63
3:O:278:ASP:CB	3:O:281:ILE:HD12	2.28	0.63
1:K:234:ASP:HB3	1:K:451:HIS:ND1	2.13	0.63
3:N:33:VAL:HG12	3:N:34:MET:N	2.13	0.63
3:P:86:VAL:HG21	3:P:109:LEU:HD11	1.81	0.63
1:C:59:ILE:HD12	1:C:59:ILE:H	1.64	0.63
3:H:86:VAL:HG21	3:H:109:LEU:HD11	1.81	0.63
3:P:103:ILE:HG23	3:P:104:THR:N	2.13	0.63
2:D:205:ALA:HA	2:D:281:MET:HE1	1.81	0.63
1:I:332:LYS:HA	1:I:335:TRP:NE1	2.13	0.63
2:L:205:ALA:HA	2:L:281:MET:CE	2.29	0.63
3:O:185:ASN:HD22	3:O:185:ASN:N	1.96	0.63
2:B:23:MET:HE2	2:B:23:MET:C	2.23	0.62
2:J:23:MET:HE2	2:J:23:MET:C	2.24	0.62
1:K:477:ALA:HB3	1:K:480:GLU:HG2	1.80	0.62
3:O:96:GLY:HA3	3:O:100:ARG:NH1	2.13	0.62
1:A:234:ASP:HB3	1:A:451:HIS:ND1	2.15	0.62
2:B:466:LEU:HD12	2:B:467:ILE:H	1.64	0.62
3:F:115:TYR:O	3:F:117:ASP:N	2.32	0.62
1:K:88:CYS:HB2	1:K:153:GLU:OE2	1.98	0.62
1:K:289:LYS:HG2	1:K:289:LYS:O	1.97	0.62
2:L:247:MET:HE1	2:L:340:ILE:HG12	1.80	0.62
3:P:54:GLN:HE22	3:P:86:VAL:HA	1.64	0.62
1:C:75:ILE:H	1:C:75:ILE:HD12	1.63	0.62
2:J:477:HIS:H	2:L:499:ASN:ND2	1.86	0.62
3:O:217:VAL:HG22	3:O:227:VAL:HG21	1.80	0.62
3:E:127:LEU:HD13	3:E:129:ASP:H	1.62	0.62
3:E:192:GLU:O	3:E:196:ILE:HG12	1.99	0.62
3:G:225:MET:HE2	3:G:230:TYR:N	2.13	0.62
1:K:68:LYS:C	1:K:68:LYS:HD3	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:2:MET:HA	3:M:120:ASP:O	1.99	0.62
3:M:15:LYS:NZ	3:M:127:LEU:HA	2.15	0.62
3:M:155:MET:CG	3:M:156:MET:HE2	2.29	0.62
3:O:285:THR:HG21	3:P:230:TYR:HE1	1.61	0.62
2:D:233:TYR:HD1	2:D:484:THR:HG23	1.64	0.62
1:I:77:ASP:OD2	1:I:258:SER:HB2	2.00	0.62
3:O:137:MET:HE3	3:O:141:GLU:HG3	1.80	0.62
3:P:223:ARG:HB3	3:P:225:MET:HG2	1.80	0.62
3:E:194:GLU:HA	3:E:197:ILE:HG13	1.81	0.62
3:E:215:ASN:O	3:E:219:ARG:HG3	1.99	0.62
2:J:235:GLY:C	2:J:483:THR:HG23	2.23	0.62
2:J:247:MET:HE3	2:J:341:PRO:HD2	1.80	0.62
3:P:47:LEU:HD22	3:P:225:MET:O	1.99	0.62
1:A:76:LYS:O	1:A:108:ALA:HA	2.00	0.62
1:C:76:LYS:O	1:C:108:ALA:HA	2.00	0.62
1:A:306:ILE:HG23	1:A:328:ILE:HD13	1.81	0.62
3:H:47:LEU:HD22	3:H:225:MET:O	1.99	0.62
1:I:286:MET:O	1:I:290:TYR:HB2	2.00	0.62
1:K:355:ILE:HG22	1:K:356:GLY:H	1.64	0.62
1:C:57:MET:CE	2:D:113:CYS:H	2.13	0.62
3:E:56:THR:HG22	3:E:87:GLU:HB3	1.82	0.62
3:F:8:TYR:HB3	3:F:164:ILE:HD13	1.80	0.62
1:I:59:ILE:HD12	1:I:59:ILE:H	1.65	0.62
2:L:494:LEU:O	2:L:498:VAL:HG12	2.00	0.62
3:O:99:GLY:HA3	3:O:134:GLY:HA2	1.80	0.62
1:A:91:TYR:HB2	2:B:98:TYR:CD1	2.35	0.62
1:A:226:ILE:O	1:A:273:VAL:HA	2.00	0.62
1:A:277:ARG:NH1	1:A:386:ASP:OD2	2.31	0.62
2:B:235:GLY:C	2:B:483:THR:HG23	2.25	0.62
2:J:295:PRO:O	2:J:297:HIS:N	2.32	0.62
2:L:400:LYS:HG3	3:P:111:GLU:HG2	1.82	0.62
3:M:278:ASP:CB	3:M:281:ILE:HD12	2.29	0.62
1:A:275:CYS:HB3	1:A:278:SER:OG	2.00	0.61
3:F:223:ARG:HB3	3:F:225:MET:HG2	1.81	0.61
1:K:76:LYS:O	1:K:108:ALA:HA	2.00	0.61
1:A:339:VAL:O	1:A:343:ARG:HB3	2.00	0.61
1:C:367:TYR:HD1	1:C:372:MET:HG2	1.64	0.61
3:G:136:ALA:HB1	3:H:94:GLY:HA2	1.82	0.61
2:L:431:ARG:O	2:L:434:VAL:HG22	2.00	0.61
3:M:29:MET:O	3:M:29:MET:HG2	2.00	0.61
3:O:2:MET:HA	3:O:120:ASP:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:127:LEU:HD12	3:E:135:PHE:CE2	2.36	0.61
3:P:218:GLN:O	3:P:222:ILE:HG13	2.01	0.61
2:D:91:GLY:HA3	2:D:152:THR:OG1	2.01	0.61
3:F:100:ARG:O	3:F:103:ILE:HG22	2.00	0.61
1:K:75:ILE:H	1:K:75:ILE:HD12	1.65	0.61
3:M:5:CYS:SG	3:M:146:GLU:HG3	2.40	0.61
3:P:115:TYR:O	3:P:117:ASP:N	2.33	0.61
2:D:220:SER:OG	2:D:286:ASN:HB3	2.00	0.61
2:J:494:LEU:O	2:J:494:LEU:HD23	2.01	0.61
1:K:332:LYS:HA	1:K:335:TRP:NE1	2.16	0.61
2:L:178:GLU:CD	2:L:178:GLU:N	2.58	0.61
2:L:241:LYS:HE3	2:L:253:LEU:HD23	1.83	0.61
3:M:241:ARG:HG2	3:M:245:ARG:NH1	2.15	0.61
3:O:76:LEU:HD11	3:O:84:LYS:CB	2.30	0.61
3:P:127:LEU:CD2	3:P:129:ASP:HB2	2.30	0.61
3:P:208:ILE:HG23	3:P:209:HIS:N	2.16	0.61
3:E:184:CYS:HB2	3:E:196:ILE:HG13	1.83	0.61
3:G:96:GLY:HA3	3:G:100:ARG:NH1	2.14	0.61
3:G:212:PRO:HG2	3:G:236:GLN:OE1	2.01	0.61
3:G:284:LYS:HD3	3:G:284:LYS:C	2.26	0.61
3:P:184:CYS:HG	3:P:210:PHE:HE1	1.47	0.61
1:C:19:VAL:HG13	1:C:20:TYR:N	2.15	0.61
3:O:284:LYS:HD3	3:O:284:LYS:C	2.26	0.61
1:A:355:ILE:HG22	1:A:356:GLY:H	1.65	0.61
1:C:332:LYS:N	1:C:333:PRO:HD2	2.15	0.61
3:E:52:LYS:H	3:E:52:LYS:CD	2.04	0.61
3:G:256:PRO:C	3:G:258:PRO:HD3	2.26	0.61
1:I:277:ARG:NH1	1:I:386:ASP:OD2	2.33	0.61
3:F:64:ALA:HB1	3:F:69:ASP:HB2	1.83	0.61
3:F:102:VAL:HG12	3:F:106:ILE:HD11	1.81	0.61
3:H:100:ARG:C	3:H:100:ARG:HD3	2.26	0.61
1:I:57:MET:HE2	2:J:113:CYS:H	1.65	0.61
3:E:15:LYS:HG3	3:E:150:VAL:HG21	1.83	0.61
3:G:15:LYS:NZ	3:G:127:LEU:HA	2.16	0.61
1:I:479:TRP:HE3	2:L:330:MET:HE3	1.66	0.61
1:K:35:ASN:ND2	1:K:391:MET:HG2	2.16	0.61
2:L:132:LYS:HD3	2:L:174:PHE:CE2	2.36	0.61
3:M:15:LYS:HG3	3:M:150:VAL:HG21	1.83	0.61
3:M:52:LYS:H	3:M:52:LYS:CD	2.07	0.61
3:O:5:CYS:SG	3:O:146:GLU:HG3	2.41	0.61
3:F:195:LEU:HD13	3:F:271:PHE:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:162:ASN:HD21	3:G:259:ILE:CG1	2.08	0.60
1:I:35:ASN:HD22	1:I:36:ASP:H	1.48	0.60
1:K:131:LEU:O	1:K:135:ILE:HG13	2.00	0.60
3:M:33:VAL:HG22	3:M:121:PHE:HB2	1.82	0.60
3:O:225:MET:HE2	3:O:230:TYR:N	2.16	0.60
2:D:247:MET:CE	2:D:340:ILE:HA	2.30	0.60
3:F:100:ARG:HD3	3:F:101:GLY:N	2.15	0.60
3:G:155:MET:CG	3:G:156:MET:HE2	2.31	0.60
1:C:332:LYS:HA	1:C:335:TRP:NE1	2.16	0.60
3:E:182:LEU:HD12	3:E:196:ILE:HG22	1.83	0.60
3:E:256:PRO:C	3:E:258:PRO:HD3	2.26	0.60
1:I:332:LYS:N	1:I:333:PRO:HD2	2.15	0.60
2:J:236:ASN:O	2:J:237:PHE:C	2.43	0.60
1:K:20:TYR:OH	1:K:408:GLU:HG3	2.02	0.60
3:O:182:LEU:HD12	3:O:196:ILE:HG22	1.82	0.60
3:P:19:THR:O	3:P:22:LEU:HB3	2.02	0.60
1:A:13:ILE:O	1:A:17:LEU:HG	2.02	0.60
2:D:468:ARG:HG3	2:D:468:ARG:HH11	1.66	0.60
3:G:71:GLU:HB3	3:G:74:ASP:OD1	2.00	0.60
3:G:184:CYS:HB2	3:G:196:ILE:HG13	1.83	0.60
3:H:127:LEU:HD23	3:H:129:ASP:H	1.66	0.60
3:H:236:GLN:O	3:H:239:GLU:HB2	2.01	0.60
3:N:115:TYR:O	3:N:117:ASP:N	2.34	0.60
1:A:477:ALA:HB3	1:A:480:GLU:HG2	1.82	0.60
2:B:330:MET:HE3	1:C:479:TRP:HE3	1.67	0.60
1:C:96:ARG:NH2	5:C:7496:CFM:S5	2.72	0.60
2:D:372:ASP:O	2:D:376:VAL:HG23	2.01	0.60
3:E:29:MET:O	3:E:29:MET:HG2	2.02	0.60
3:H:102:VAL:HG12	3:H:106:ILE:HD11	1.84	0.60
2:J:132:LYS:HD3	2:J:174:PHE:CE2	2.36	0.60
2:J:247:MET:CE	2:J:340:ILE:HA	2.31	0.60
3:M:72:LEU:HD13	3:M:112:GLU:CB	2.32	0.60
2:D:213:MET:CE	2:D:309:TRP:HA	2.31	0.60
1:K:239:ARG:NE	2:L:23:MET:HE1	2.16	0.60
2:L:118:MET:HA	2:L:130:ASN:ND2	2.16	0.60
2:D:235:GLY:C	2:D:483:THR:HG23	2.27	0.60
3:F:212:PRO:HG2	3:F:236:GLN:OE1	2.00	0.60
3:G:192:GLU:O	3:G:196:ILE:HG12	2.02	0.60
3:H:115:TYR:O	3:H:117:ASP:N	2.35	0.60
3:H:212:PRO:HG2	3:H:236:GLN:OE1	2.02	0.60
1:I:346:LEU:O	1:I:349:LYS:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:199:ASN:OD1	1:K:281:TYR:HB2	2.01	0.60
1:K:253:TRP:CZ2	1:K:262:ILE:HG23	2.37	0.60
1:K:356:GLY:HA3	5:K:9496:CFM:S1B	2.42	0.60
1:A:35:ASN:ND2	1:A:36:ASP:N	2.49	0.60
1:C:229:TYR:CE2	5:C:7496:CFM:S2A	2.94	0.60
1:C:286:MET:O	1:C:290:TYR:HB2	2.02	0.60
2:J:220:SER:OG	2:J:286:ASN:HB3	2.02	0.60
1:K:439:ARG:HH12	1:K:465:MET:HE3	1.66	0.60
3:M:20:GLN:NE2	3:M:48:ILE:HG12	2.17	0.60
3:M:169:VAL:HG23	3:M:256:PRO:HG2	1.83	0.60
3:O:22:LEU:HD11	3:O:243:LEU:HG	1.83	0.60
1:C:477:ALA:HB3	1:C:480:GLU:HG2	1.83	0.60
3:E:33:VAL:HG22	3:E:121:PHE:HB2	1.84	0.60
3:H:127:LEU:CD2	3:H:129:ASP:HB2	2.30	0.60
2:L:441:PHE:CE2	2:L:501:ILE:HG12	2.37	0.60
1:A:266:PRO:HB3	1:A:290:TYR:CE1	2.37	0.60
1:A:332:LYS:HA	1:A:335:TRP:NE1	2.17	0.60
2:B:468:ARG:HG3	2:B:468:ARG:NH1	2.16	0.60
2:D:132:LYS:HD3	2:D:174:PHE:CE2	2.36	0.60
3:F:103:ILE:HG23	3:F:104:THR:N	2.16	0.60
1:K:324:CYS:O	1:K:328:ILE:HG13	2.01	0.60
2:D:118:MET:HA	2:D:130:ASN:ND2	2.17	0.59
3:E:199:LEU:HB2	3:E:267:LEU:HD11	1.84	0.59
1:K:35:ASN:HD22	1:K:36:ASP:H	1.49	0.59
2:L:233:TYR:HD1	2:L:484:THR:HG23	1.65	0.59
3:M:45:THR:HG21	3:M:85:CYS:HB3	1.84	0.59
3:N:86:VAL:HG21	3:N:109:LEU:HD11	1.82	0.59
1:A:131:LEU:O	1:A:135:ILE:HG13	2.02	0.59
1:I:356:GLY:HA3	5:I:8496:CFM:S1B	2.41	0.59
2:L:236:ASN:O	2:L:237:PHE:C	2.44	0.59
3:M:265:GLU:OE1	3:N:52:LYS:HD3	2.02	0.59
3:N:19:THR:O	3:N:22:LEU:HB3	2.02	0.59
3:O:223:ARG:O	3:O:225:MET:N	2.35	0.59
1:A:350:ARG:HB3	1:A:375:VAL:CG1	2.32	0.59
2:B:270:ARG:HG3	2:B:270:ARG:HH11	1.67	0.59
2:D:347:GLU:OE1	2:D:487:TYR:HB2	2.01	0.59
3:E:99:GLY:HA3	3:E:134:GLY:CA	2.32	0.59
3:E:185:ASN:HD22	3:E:185:ASN:N	2.00	0.59
3:M:281:ILE:CG2	3:N:223:ARG:HD2	2.30	0.59
3:N:33:VAL:HG22	3:N:121:PHE:HB2	1.84	0.59
3:P:267:LEU:O	3:P:270:GLU:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ASP:OD2	1:A:215:THR:HG23	2.02	0.59
1:C:223:VAL:HG12	1:C:270:LEU:HB3	1.84	0.59
1:C:356:GLY:HA3	5:C:7496:CFM:S1B	2.42	0.59
3:G:41:LYS:HB3	3:G:43:ASP:OD1	2.03	0.59
3:M:225:MET:HE2	3:M:230:TYR:N	2.17	0.59
3:N:267:LEU:O	3:N:270:GLU:HG3	2.02	0.59
2:B:118:MET:HA	2:B:130:ASN:ND2	2.17	0.59
1:C:355:ILE:HB	1:C:360:PRO:HD3	1.85	0.59
3:H:195:LEU:HD13	3:H:271:PHE:CD2	2.37	0.59
3:O:72:LEU:HD13	3:O:112:GLU:CB	2.32	0.59
2:B:236:ASN:O	2:B:239:VAL:HG12	2.03	0.59
2:D:10:ALA:O	2:D:11:SER:C	2.45	0.59
3:F:267:LEU:O	3:F:270:GLU:HG3	2.02	0.59
2:J:431:ARG:O	2:J:434:VAL:HG22	2.02	0.59
1:K:42:SER:CA	1:K:391:MET:HE1	2.30	0.59
4:K:9494:HCA:O2	4:K:9494:HCA:O7	2.19	0.59
3:O:71:GLU:HB3	3:O:74:ASP:OD1	2.03	0.59
2:B:247:MET:HE1	2:B:340:ILE:HG12	1.84	0.59
3:E:155:MET:CG	3:E:156:MET:HE2	2.32	0.59
3:G:35:ILE:HD12	3:G:48:ILE:HG13	1.85	0.59
2:J:88:TYR:OH	2:J:116:ASP:HB3	2.02	0.59
1:K:346:LEU:O	1:K:349:LYS:HG2	2.03	0.59
3:M:284:LYS:C	3:M:284:LYS:HD3	2.27	0.59
2:B:233:TYR:HD1	2:B:484:THR:HG23	1.68	0.59
1:I:35:ASN:ND2	1:I:391:MET:HG2	2.18	0.59
1:I:354:TYR:CZ	1:I:404:VAL:HG12	2.38	0.59
1:K:35:ASN:ND2	1:K:36:ASP:N	2.51	0.59
1:K:223:VAL:HG12	1:K:270:LEU:HB3	1.83	0.59
3:M:202:LYS:HD3	3:M:267:LEU:HD12	1.84	0.59
1:A:57:MET:HE2	2:B:113:CYS:H	1.68	0.59
1:C:35:ASN:ND2	1:C:36:ASP:N	2.51	0.59
1:C:131:LEU:O	1:C:135:ILE:HG13	2.03	0.59
2:J:270:ARG:HG3	2:J:270:ARG:NH1	2.18	0.59
2:L:499:ASN:O	2:L:503:GLU:HB2	2.02	0.59
3:N:103:ILE:HG23	3:N:104:THR:N	2.18	0.59
3:P:76:LEU:HA	3:P:86:VAL:HG12	1.85	0.59
1:A:356:GLY:HA3	5:A:6496:CFM:S1B	2.42	0.59
1:I:19:VAL:HG13	1:I:20:TYR:N	2.16	0.59
2:J:372:ASP:O	2:J:376:VAL:HG23	2.03	0.59
2:L:220:SER:OG	2:L:286:ASN:HB3	2.03	0.59
2:L:235:GLY:C	2:L:483:THR:HG23	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:72:LEU:HD22	3:N:72:LEU:C	2.28	0.59
3:N:100:ARG:C	3:N:100:ARG:HD3	2.28	0.59
3:P:105:ALA:O	3:P:109:LEU:HG	2.03	0.59
1:A:77:ASP:OD2	1:A:258:SER:HB2	2.01	0.58
3:E:284:LYS:HD3	3:E:285:THR:N	2.18	0.58
1:I:239:ARG:NH1	2:J:27:LYS:HD2	2.18	0.58
2:L:247:MET:CE	2:L:340:ILE:HA	2.33	0.58
3:M:127:LEU:HD12	3:M:135:PHE:CE2	2.38	0.58
3:P:236:GLN:O	3:P:239:GLU:HB2	2.03	0.58
2:B:431:ARG:HG2	2:B:431:ARG:HH11	1.68	0.58
2:B:494:LEU:HD23	2:B:494:LEU:O	2.03	0.58
3:G:52:LYS:HB3	3:G:224:ARG:NH1	2.18	0.58
1:I:479:TRP:CZ2	2:L:340:ILE:HG21	2.37	0.58
1:K:65:ALA:O	1:K:70:VAL:HG23	2.04	0.58
1:K:332:LYS:N	1:K:333:PRO:HD2	2.18	0.58
2:L:23:MET:HE2	2:L:23:MET:C	2.28	0.58
2:L:346:LYS:O	2:L:347:GLU:C	2.45	0.58
2:B:270:ARG:HG3	2:B:270:ARG:NH1	2.18	0.58
2:D:151:THR:HG23	2:D:162:LEU:HD11	1.84	0.58
2:D:431:ARG:O	2:D:434:VAL:HG22	2.03	0.58
1:I:131:LEU:O	1:I:135:ILE:HG13	2.03	0.58
2:D:373:PRO:HD3	2:D:397:ASN:OD1	2.03	0.58
3:H:208:ILE:HD11	3:H:246:LYS:HB3	1.84	0.58
1:I:195:HIS:O	1:I:198:ALA:HB3	2.04	0.58
3:N:56:THR:OG1	3:N:59:GLU:HG3	2.04	0.58
3:O:45:THR:HG21	3:O:85:CYS:HB3	1.84	0.58
3:O:86:VAL:HG21	3:O:109:LEU:HD11	1.86	0.58
3:P:199:LEU:HD23	3:P:199:LEU:C	2.28	0.58
1:A:75:ILE:H	1:A:75:ILE:HD12	1.69	0.58
1:C:20:TYR:OH	1:C:408:GLU:HG3	2.04	0.58
3:E:217:VAL:HG22	3:E:227:VAL:HG21	1.85	0.58
2:J:270:ARG:HG3	2:J:270:ARG:HH11	1.67	0.58
2:J:494:LEU:HD23	2:J:494:LEU:C	2.28	0.58
3:N:243:LEU:O	3:N:247:VAL:HG23	2.04	0.58
3:P:80:TYR:CD2	3:P:229:GLU:HG3	2.39	0.58
3:P:100:ARG:HD3	3:P:100:ARG:C	2.28	0.58
2:B:400:LYS:HD2	3:F:112:GLU:HG3	1.84	0.58
1:C:6:ARG:NH2	1:C:396:ASP:OD2	2.37	0.58
1:C:66:GLY:O	1:C:70:VAL:HB	2.03	0.58
2:D:231:GLU:CD	2:D:236:ASN:HD22	2.12	0.58
3:F:199:LEU:HD23	3:F:199:LEU:C	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:72:LEU:HD13	3:G:112:GLU:HB2	1.86	0.58
1:K:306:ILE:HG23	1:K:328:ILE:HD13	1.85	0.58
3:N:64:ALA:HB1	3:N:69:ASP:HB2	1.86	0.58
3:N:206:GLN:CG	3:N:252:LEU:HD22	2.31	0.58
1:A:71:VAL:O	1:A:74:PRO:HD2	2.03	0.58
2:B:132:LYS:HD3	2:B:174:PHE:CE2	2.38	0.58
2:B:192:SER:OG	2:B:194:VAL:HG22	2.03	0.58
2:B:431:ARG:O	2:B:434:VAL:HG22	2.03	0.58
1:C:306:ILE:HG23	1:C:328:ILE:HD13	1.86	0.58
2:D:70:CYS:SG	2:D:72:PRO:HG2	2.44	0.58
3:F:184:CYS:HG	3:F:210:PHE:HE1	1.52	0.58
3:G:29:MET:O	3:G:29:MET:HG2	2.04	0.58
3:G:194:GLU:HA	3:G:197:ILE:HG13	1.85	0.58
1:I:289:LYS:O	1:I:289:LYS:HG2	2.02	0.58
1:K:467:LEU:O	1:K:467:LEU:HD23	2.03	0.58
2:L:103:PHE:CB	2:L:111:VAL:HG21	2.33	0.58
3:M:256:PRO:C	3:M:258:PRO:HD3	2.29	0.58
3:N:76:LEU:HA	3:N:86:VAL:HG12	1.86	0.58
2:B:494:LEU:O	2:B:498:VAL:HG12	2.04	0.58
2:D:56:ASN:HD21	2:D:428:TRP:CD1	2.21	0.58
2:D:511:GLY:O	2:D:516:ASP:HB3	2.04	0.58
3:F:149:ILE:HB	3:F:182:LEU:HD22	1.85	0.58
3:G:217:VAL:HG22	3:G:227:VAL:HG21	1.83	0.58
2:J:4:GLN:O	2:J:6:ASP:N	2.37	0.58
1:K:19:VAL:HG13	1:K:20:TYR:N	2.18	0.58
3:O:225:MET:SD	3:P:283:GLY:HA2	2.44	0.58
3:E:86:VAL:HG21	3:E:109:LEU:HD11	1.86	0.58
2:J:489:GLY:O	2:J:490:ALA:C	2.47	0.58
1:K:266:PRO:HB3	1:K:290:TYR:CE1	2.39	0.58
2:L:373:PRO:HD3	2:L:397:ASN:OD1	2.04	0.58
3:M:165:SER:HB3	3:M:256:PRO:CB	2.33	0.58
3:M:217:VAL:HG22	3:M:227:VAL:HG21	1.86	0.58
3:O:52:LYS:HB3	3:O:224:ARG:NH1	2.18	0.58
3:O:256:PRO:C	3:O:258:PRO:HD3	2.29	0.58
1:A:100:TYR:C	1:A:100:TYR:CD2	2.82	0.58
2:D:346:LYS:O	2:D:347:GLU:C	2.45	0.58
3:G:243:LEU:O	3:G:247:VAL:HG23	2.03	0.58
3:N:60:MET:HE1	3:N:75:VAL:CG1	2.28	0.58
3:P:208:ILE:HD11	3:P:246:LYS:HB3	1.85	0.58
1:C:465:MET:O	1:C:469:ASN:HB2	2.04	0.57
2:D:468:ARG:HG3	2:D:468:ARG:NH1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:76:LEU:HA	3:F:86:VAL:HG12	1.85	0.57
3:F:206:GLN:CG	3:F:252:LEU:HD22	2.29	0.57
3:M:185:ASN:HD22	3:M:185:ASN:N	2.01	0.57
3:M:199:LEU:HB2	3:M:267:LEU:HD11	1.86	0.57
3:O:92:GLU:OE2	3:P:170:LYS:HE3	2.04	0.57
1:A:65:ALA:O	1:A:70:VAL:HG23	2.04	0.57
2:B:497:LEU:O	2:B:500:SER:N	2.36	0.57
2:D:43:VAL:O	2:D:46:TRP:HB3	2.02	0.57
3:M:96:GLY:HA3	3:M:100:ARG:NH1	2.19	0.57
3:M:155:MET:HG3	3:M:156:MET:HE2	1.85	0.57
1:A:467:LEU:HD23	1:A:467:LEU:O	2.03	0.57
2:B:455:THR:OG1	2:B:463:GLU:HA	2.05	0.57
2:D:128:GLN:NE2	2:D:165:PHE:HA	2.18	0.57
3:E:182:LEU:O	3:E:208:ILE:HG22	2.03	0.57
3:E:224:ARG:HG3	3:F:282:VAL:HG13	1.86	0.57
3:G:199:LEU:HB2	3:G:267:LEU:HD11	1.86	0.57
3:H:103:ILE:HG23	3:H:104:THR:N	2.18	0.57
3:N:236:GLN:O	3:N:239:GLU:HB2	2.03	0.57
3:O:41:LYS:HB3	3:O:43:ASP:OD1	2.05	0.57
2:B:236:ASN:O	2:B:237:PHE:C	2.47	0.57
2:D:88:TYR:OH	2:D:116:ASP:HB3	2.04	0.57
3:H:56:THR:OG1	3:H:59:GLU:HG3	2.03	0.57
2:J:46:TRP:O	2:J:49:THR:HG23	2.04	0.57
2:J:451:ILE:O	2:J:455:THR:HG23	2.04	0.57
2:L:494:LEU:HD23	2:L:494:LEU:C	2.28	0.57
3:O:8:TYR:HB3	3:O:164:ILE:HD13	1.86	0.57
3:P:195:LEU:HD13	3:P:271:PHE:CD2	2.39	0.57
2:D:236:ASN:HB3	2:D:485:LEU:HD12	1.86	0.57
3:E:225:MET:HE2	3:E:230:TYR:N	2.19	0.57
3:G:33:VAL:HG22	3:G:121:PHE:HB2	1.86	0.57
3:G:33:VAL:O	3:G:83:VAL:HG13	2.04	0.57
1:I:467:LEU:HD23	1:I:467:LEU:O	2.04	0.57
2:J:213:MET:CE	2:J:309:TRP:HA	2.34	0.57
1:K:213:ASP:OD2	1:K:215:THR:HG23	2.04	0.57
3:M:95:VAL:HG22	3:N:171:TYR:OH	2.05	0.57
3:M:135:PHE:CZ	3:N:130:VAL:HG11	2.37	0.57
3:F:253:LEU:H	3:F:253:LEU:HD22	1.70	0.57
3:H:102:VAL:O	3:H:106:ILE:HG13	2.05	0.57
1:I:420:LEU:HD23	1:I:420:LEU:C	2.29	0.57
2:J:153:CYS:SG	6:J:8498:CLF:S2B	3.03	0.57
2:L:235:GLY:O	2:L:483:THR:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:494:LEU:O	2:L:494:LEU:HD23	2.04	0.57
3:O:35:ILE:HD12	3:O:48:ILE:HG13	1.87	0.57
3:O:215:ASN:O	3:O:219:ARG:HG3	2.05	0.57
2:B:494:LEU:HD23	2:B:494:LEU:C	2.29	0.57
3:G:86:VAL:HG21	3:G:109:LEU:HD11	1.85	0.57
2:L:451:ILE:O	2:L:455:THR:HG23	2.03	0.57
3:P:245:ARG:HH11	3:P:245:ARG:HG3	1.68	0.57
2:B:509:THR:O	2:B:516:ASP:HA	2.05	0.57
1:C:77:ASP:OD2	1:C:258:SER:HB2	2.05	0.57
2:D:236:ASN:O	2:D:237:PHE:C	2.48	0.57
3:F:86:VAL:HG21	3:F:109:LEU:HD11	1.85	0.57
1:I:71:VAL:O	1:I:74:PRO:HD2	2.05	0.57
2:L:236:ASN:HB3	2:L:485:LEU:HD12	1.87	0.57
3:M:50:HIS:CE1	3:N:283:GLY:HA2	2.39	0.57
1:A:57:MET:CE	2:B:113:CYS:H	2.18	0.57
3:E:164:ILE:O	3:E:168:ILE:HG13	2.03	0.57
3:F:100:ARG:HD3	3:F:100:ARG:C	2.30	0.57
3:G:20:GLN:NE2	3:G:48:ILE:HG12	2.20	0.57
2:L:213:MET:CE	2:L:309:TRP:HA	2.35	0.57
3:M:202:LYS:HE3	3:M:259:ILE:HG21	1.86	0.57
2:D:247:MET:HE3	2:D:341:PRO:HD2	1.86	0.57
3:G:15:LYS:HG3	3:G:150:VAL:HG21	1.86	0.57
3:H:267:LEU:O	3:H:270:GLU:HG3	2.04	0.57
1:I:76:LYS:O	1:I:108:ALA:HA	2.05	0.57
2:J:405:ALA:O	2:J:409:ILE:HG13	2.05	0.57
1:K:7:GLU:HA	1:K:10:GLU:OE1	2.05	0.57
1:K:420:LEU:HD23	1:K:420:LEU:C	2.29	0.57
1:K:427:GLU:O	1:K:428:LYS:C	2.48	0.57
2:L:489:GLY:O	2:L:490:ALA:C	2.48	0.57
1:A:59:ILE:HD13	1:A:354:TYR:CE2	2.40	0.56
1:A:96:ARG:NH2	5:A:6496:CFM:S5	2.72	0.56
2:J:43:VAL:O	2:J:46:TRP:HB3	2.04	0.56
2:J:235:GLY:O	2:J:483:THR:HG23	2.04	0.56
3:O:212:PRO:HG2	3:O:236:GLN:OE1	2.05	0.56
3:O:223:ARG:NE	3:P:281:ILE:HB	2.20	0.56
1:A:480:GLU:HA	1:A:480:GLU:OE2	2.05	0.56
2:B:10:ALA:O	2:B:11:SER:C	2.48	0.56
2:D:441:PHE:CE2	2:D:501:ILE:HG12	2.40	0.56
2:D:494:LEU:O	2:D:494:LEU:HD23	2.05	0.56
3:E:22:LEU:HD11	3:E:243:LEU:HG	1.87	0.56
3:G:185:ASN:HD22	3:G:185:ASN:N	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:480:GLU:HA	1:K:480:GLU:OE2	2.05	0.56
3:M:49:LEU:HD23	3:M:79:GLY:HA3	1.86	0.56
3:P:183:ILE:HG12	3:P:208:ILE:CG2	2.35	0.56
1:A:144:LEU:HD22	2:B:35:TYR:CD1	2.40	0.56
1:A:374:VAL:HG12	1:A:394:MET:HE1	1.86	0.56
2:B:96:VAL:HA	2:B:99:PHE:CD2	2.41	0.56
2:B:445:ASN:HB2	2:B:472:PRO:O	2.05	0.56
2:D:262:ASP:CG	2:D:481:ARG:HH12	2.14	0.56
3:E:2:MET:HE3	3:E:122:VAL:HG21	1.86	0.56
3:F:56:THR:OG1	3:F:59:GLU:HG3	2.05	0.56
3:G:202:LYS:HD3	3:G:267:LEU:HD12	1.87	0.56
1:I:306:ILE:HG23	1:I:328:ILE:HD13	1.85	0.56
1:K:144:LEU:HD22	2:L:35:TYR:CD1	2.40	0.56
1:K:350:ARG:HB3	1:K:375:VAL:CG1	2.35	0.56
2:L:497:LEU:O	2:L:500:SER:N	2.38	0.56
3:M:5:CYS:SG	3:M:146:GLU:HB2	2.45	0.56
3:O:228:ILE:O	3:O:232:PRO:HG3	2.04	0.56
3:P:80:TYR:HD2	3:P:229:GLU:HG3	1.70	0.56
1:A:7:GLU:HA	1:A:10:GLU:OE1	2.05	0.56
1:A:286:MET:O	1:A:290:TYR:HB2	2.06	0.56
2:B:236:ASN:HB3	2:B:485:LEU:HD12	1.87	0.56
2:B:499:ASN:ND2	2:D:477:HIS:H	1.98	0.56
1:C:35:ASN:ND2	1:C:391:MET:HG2	2.19	0.56
2:D:295:PRO:O	2:D:297:HIS:N	2.39	0.56
3:E:10:LYS:HG2	3:E:10:LYS:O	2.05	0.56
3:E:49:LEU:HD21	3:E:85:CYS:SG	2.45	0.56
3:G:99:GLY:HA3	3:G:134:GLY:HA2	1.86	0.56
3:H:19:THR:O	3:H:22:LEU:HB3	2.05	0.56
1:I:324:CYS:O	1:I:328:ILE:HG13	2.05	0.56
3:M:194:GLU:HA	3:M:197:ILE:HG13	1.87	0.56
2:B:4:GLN:O	2:B:6:ASP:N	2.37	0.56
1:C:7:GLU:HA	1:C:10:GLU:OE1	2.06	0.56
2:L:452:GLN:OE1	2:L:466:LEU:N	2.39	0.56
3:N:183:ILE:HG12	3:N:208:ILE:CG2	2.36	0.56
3:P:8:TYR:HB3	3:P:164:ILE:HD13	1.88	0.56
1:C:429:PHE:CZ	2:D:108:ARG:HA	2.39	0.56
3:F:72:LEU:HD22	3:F:72:LEU:C	2.30	0.56
3:G:169:VAL:HG23	3:G:256:PRO:HG2	1.86	0.56
3:G:218:GLN:O	3:G:222:ILE:HG13	2.06	0.56
1:I:477:ALA:HB3	1:I:480:GLU:HG2	1.87	0.56
2:J:247:MET:HE3	2:J:340:ILE:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:499:ASN:ND2	2:L:477:HIS:H	1.94	0.56
1:K:428:LYS:O	1:K:432:GLN:HG3	2.06	0.56
3:M:52:LYS:HB3	3:M:224:ARG:NH1	2.21	0.56
3:M:137:MET:HE3	3:M:141:GLU:HG3	1.87	0.56
3:M:164:ILE:O	3:M:168:ILE:HG13	2.06	0.56
3:O:127:LEU:HD12	3:O:135:PHE:CE2	2.41	0.56
2:B:431:ARG:NH1	2:B:435:PHE:HE2	2.03	0.56
2:B:513:GLN:HE21	1:C:102:GLY:HA2	1.70	0.56
1:C:209:LYS:HD3	1:C:263:GLU:OE2	2.06	0.56
1:C:354:TYR:CE1	1:C:404:VAL:HG12	2.41	0.56
2:D:497:LEU:O	2:D:500:SER:N	2.39	0.56
3:G:78:ALA:HA	3:G:83:VAL:O	2.06	0.56
3:H:57:ILE:HA	3:H:60:MET:CE	2.36	0.56
3:H:199:LEU:HD23	3:H:199:LEU:C	2.30	0.56
3:M:35:ILE:HD12	3:M:48:ILE:HG13	1.87	0.56
3:N:57:ILE:HA	3:N:60:MET:CE	2.35	0.56
3:N:105:ALA:O	3:N:109:LEU:HG	2.06	0.56
3:P:100:ARG:O	3:P:103:ILE:HG22	2.06	0.56
2:B:197:TRP:O	2:B:198:ASP:C	2.49	0.56
1:C:213:ASP:OD2	1:C:215:THR:HG23	2.06	0.56
3:H:218:GLN:O	3:H:222:ILE:HG13	2.04	0.56
1:I:113:ASN:HD22	2:J:66:PRO:CD	2.19	0.56
1:A:359:ARG:NH1	1:A:444:TRP:CH2	2.74	0.56
2:B:71:GLN:N	2:B:72:PRO:HD2	2.21	0.56
3:G:279:GLU:O	3:G:282:VAL:HG22	2.06	0.56
2:J:103:PHE:HB2	2:J:111:VAL:HG21	1.87	0.56
2:L:247:MET:HE3	2:L:341:PRO:HD2	1.86	0.56
3:N:97:CYS:HA	8:N:2290:SF4:S4	2.46	0.56
1:A:323:LYS:O	1:A:327:VAL:HG23	2.07	0.56
2:B:59:ARG:HH22	2:B:429:HIS:CE1	2.24	0.56
3:E:223:ARG:O	3:E:225:MET:N	2.39	0.56
3:G:56:THR:HG22	3:G:87:GLU:HB3	1.87	0.56
1:I:223:VAL:HG12	1:I:270:LEU:HB3	1.88	0.56
1:I:265:THR:O	1:I:268:VAL:HG22	2.05	0.56
2:J:132:LYS:HD3	2:J:174:PHE:HE2	1.71	0.56
2:L:391:VAL:HG23	2:L:392:HIS:CG	2.41	0.56
2:L:400:LYS:CG	3:P:111:GLU:HG2	2.36	0.56
2:L:400:LYS:NZ	3:P:112:GLU:CD	2.63	0.56
3:M:99:GLY:HA3	3:M:134:GLY:CA	2.35	0.56
3:M:184:CYS:HB2	3:M:196:ILE:HG13	1.87	0.56
1:A:428:LYS:O	1:A:432:GLN:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:VAL:HG11	2:D:40:ILE:HG23	1.88	0.55
3:F:19:THR:O	3:F:22:LEU:HB3	2.07	0.55
3:H:76:LEU:HA	3:H:86:VAL:HG12	1.87	0.55
2:J:118:MET:HA	2:J:130:ASN:ND2	2.21	0.55
2:J:346:LYS:O	2:J:347:GLU:C	2.46	0.55
1:K:14:GLN:HA	1:K:14:GLN:HE21	1.71	0.55
1:K:71:VAL:O	1:K:74:PRO:HD2	2.07	0.55
3:M:71:GLU:HB3	3:M:74:ASP:OD1	2.06	0.55
3:M:127:LEU:HB3	3:M:135:PHE:CE1	2.41	0.55
3:M:212:PRO:HG2	3:M:236:GLN:OE1	2.06	0.55
3:N:45:THR:CG2	3:N:85:CYS:HB2	2.35	0.55
3:N:206:GLN:HG2	3:N:252:LEU:CD2	2.33	0.55
3:O:155:MET:HG3	3:O:156:MET:HE2	1.87	0.55
3:O:165:SER:HB3	3:O:256:PRO:CB	2.35	0.55
3:P:212:PRO:HG2	3:P:236:GLN:OE1	2.06	0.55
1:A:14:GLN:HA	1:A:14:GLN:HE21	1.71	0.55
2:B:46:TRP:O	2:B:49:THR:HG23	2.07	0.55
2:D:165:PHE:HD1	2:D:165:PHE:H	1.53	0.55
2:D:236:ASN:O	2:D:239:VAL:HG12	2.06	0.55
3:F:212:PRO:HG2	3:F:236:GLN:HE22	1.71	0.55
3:G:57:ILE:HG13	3:G:75:VAL:HG11	1.88	0.55
3:G:223:ARG:O	3:G:225:MET:N	2.40	0.55
3:H:227:VAL:HG21	3:H:240:TYR:HE2	1.71	0.55
1:I:266:PRO:HB3	1:I:290:TYR:CE1	2.41	0.55
2:L:308:THR:O	2:L:310:LYS:HG2	2.07	0.55
3:M:144:ALA:O	3:M:177:VAL:HG22	2.06	0.55
3:M:179:LEU:HD23	3:M:205:THR:HB	1.87	0.55
3:O:194:GLU:HA	3:O:197:ILE:HG13	1.87	0.55
1:C:87:GLY:HA3	6:D:7498:CLF:S2B	2.46	0.55
1:C:265:THR:O	1:C:268:VAL:HG22	2.06	0.55
3:G:76:LEU:HD11	3:G:84:LYS:CB	2.34	0.55
3:G:224:ARG:HG3	3:H:282:VAL:HG13	1.88	0.55
2:J:247:MET:HE1	2:J:340:ILE:HG12	1.88	0.55
1:K:14:GLN:HA	1:K:14:GLN:NE2	2.20	0.55
3:O:78:ALA:HB2	3:O:84:LYS:HD3	1.88	0.55
3:O:164:ILE:O	3:O:168:ILE:HG13	2.06	0.55
2:B:103:PHE:CB	2:B:111:VAL:HG21	2.36	0.55
1:C:427:GLU:O	1:C:428:LYS:C	2.49	0.55
3:F:206:GLN:HG2	3:F:252:LEU:CD2	2.31	0.55
3:G:127:LEU:HB3	3:G:135:PHE:CE1	2.42	0.55
3:G:127:LEU:HD12	3:G:135:PHE:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:208:ILE:HG23	3:H:209:HIS:N	2.21	0.55
1:I:229:TYR:CE2	5:I:8496:CFM:S2A	3.00	0.55
2:L:103:PHE:HB2	2:L:111:VAL:HG21	1.88	0.55
2:L:511:GLY:O	2:L:516:ASP:HB3	2.07	0.55
3:O:225:MET:HE2	3:O:230:TYR:CA	2.37	0.55
3:P:57:ILE:HA	3:P:60:MET:CE	2.37	0.55
2:B:452:GLN:OE1	2:B:466:LEU:N	2.35	0.55
1:C:428:LYS:O	1:C:432:GLN:HG3	2.06	0.55
3:E:281:ILE:HG22	3:F:223:ARG:HD2	1.88	0.55
3:H:183:ILE:HG12	3:H:208:ILE:CG2	2.36	0.55
1:I:193:LEU:O	1:I:197:ILE:HG13	2.07	0.55
2:J:165:PHE:H	2:J:165:PHE:HD1	1.53	0.55
1:K:405:THR:HG23	1:K:408:GLU:CD	2.30	0.55
1:A:223:VAL:HG12	1:A:270:LEU:HB3	1.88	0.55
3:E:5:CYS:SG	3:E:146:GLU:HG3	2.47	0.55
3:E:137:MET:HE3	3:E:141:GLU:HG3	1.89	0.55
3:G:225:MET:HE2	3:G:230:TYR:CA	2.37	0.55
3:H:10:LYS:HG2	3:H:11:GLY:H	1.69	0.55
2:L:43:VAL:O	2:L:46:TRP:HB3	2.06	0.55
2:L:352:VAL:O	2:L:353:ASP:C	2.49	0.55
3:M:78:ALA:HB2	3:M:84:LYS:HD3	1.88	0.55
3:N:245:ARG:HH11	3:N:245:ARG:HG3	1.70	0.55
1:C:199:ASN:OD1	1:C:281:TYR:HB2	2.06	0.55
1:C:480:GLU:HA	1:C:480:GLU:OE2	2.06	0.55
2:D:228:PRO:HA	2:D:293:LEU:HD12	1.89	0.55
2:D:270:ARG:HH11	2:D:270:ARG:HG3	1.71	0.55
2:D:455:THR:OG1	2:D:463:GLU:HA	2.06	0.55
3:G:215:ASN:O	3:G:219:ARG:HG3	2.06	0.55
3:H:199:LEU:HD23	3:H:203:LEU:HD23	1.88	0.55
1:I:35:ASN:ND2	1:I:36:ASP:N	2.55	0.55
3:P:71:GLU:HG3	3:P:72:LEU:HD13	1.88	0.55
2:B:96:VAL:HA	2:B:99:PHE:HD2	1.72	0.55
1:C:282:ILE:O	1:C:286:MET:HG3	2.07	0.55
2:D:431:ARG:HG2	2:D:431:ARG:HH11	1.70	0.55
3:E:72:LEU:HD13	3:E:112:GLU:CB	2.36	0.55
3:G:78:ALA:HB2	3:G:84:LYS:HD3	1.88	0.55
3:G:155:MET:HG3	3:G:156:MET:HE2	1.87	0.55
2:J:10:ALA:O	2:J:11:SER:C	2.49	0.55
3:M:56:THR:HG22	3:M:87:GLU:HB3	1.89	0.55
3:M:243:LEU:O	3:M:247:VAL:HG23	2.07	0.55
3:N:205:THR:OG1	3:N:206:GLN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:45:THR:CG2	3:P:85:CYS:HB2	2.36	0.55
3:P:56:THR:O	3:P:60:MET:HE2	2.07	0.55
3:P:102:VAL:HG12	3:P:106:ILE:HD11	1.89	0.55
3:P:253:LEU:N	3:P:253:LEU:HD22	2.22	0.55
1:A:266:PRO:HB3	1:A:290:TYR:CD1	2.42	0.55
2:B:308:THR:O	2:B:310:LYS:HG2	2.07	0.55
2:D:247:MET:HE3	2:D:340:ILE:HA	1.89	0.55
3:E:35:ILE:HD12	3:E:48:ILE:HG13	1.88	0.55
3:F:78:ALA:HA	3:F:83:VAL:O	2.06	0.55
3:H:72:LEU:C	3:H:72:LEU:HD22	2.32	0.55
1:I:355:ILE:HB	1:I:360:PRO:HD3	1.88	0.55
1:I:389:ARG:HG3	1:I:389:ARG:NH1	2.21	0.55
2:L:165:PHE:HD1	2:L:165:PHE:H	1.54	0.55
3:O:47:LEU:HD21	3:O:221:GLU:HG2	1.89	0.55
3:O:67:VAL:C	3:O:69:ASP:H	2.14	0.55
3:P:36:VAL:HG22	3:P:86:VAL:HG22	1.88	0.55
3:P:160:ALA:O	3:P:164:ILE:HG13	2.07	0.55
1:A:427:GLU:O	1:A:428:LYS:C	2.49	0.55
1:A:429:PHE:CZ	2:B:108:ARG:HA	2.42	0.55
2:B:373:PRO:HD3	2:B:397:ASN:OD1	2.07	0.55
2:D:456:LEU:O	2:D:459:GLY:N	2.40	0.55
3:F:127:LEU:CD2	3:F:129:ASP:HB2	2.34	0.55
3:F:127:LEU:HD23	3:F:129:ASP:H	1.71	0.55
3:G:191:ARG:HE	3:G:194:GLU:CD	2.14	0.55
2:L:430:LEU:HD12	2:L:433:LEU:HD12	1.89	0.55
3:N:209:HIS:HB3	3:N:243:LEU:HD13	1.88	0.55
3:N:244:ALA:O	3:N:248:VAL:HG23	2.07	0.55
3:P:154:GLU:OE1	3:P:156:MET:HB2	2.07	0.55
2:B:235:GLY:O	2:B:483:THR:HG23	2.08	0.54
1:C:266:PRO:HB3	1:C:290:TYR:CE1	2.42	0.54
3:E:214:ASP:HB3	3:E:216:VAL:HG12	1.88	0.54
3:F:33:VAL:CG1	3:F:34:MET:N	2.69	0.54
2:J:414:PRO:O	2:J:417:LYS:HG3	2.07	0.54
2:L:71:GLN:HB3	2:L:186:THR:HB	1.88	0.54
3:N:269:MET:HB3	3:N:274:MET:HE2	1.88	0.54
1:A:167:SER:O	1:A:168:LYS:C	2.50	0.54
1:A:332:LYS:N	1:A:333:PRO:HD2	2.22	0.54
2:D:451:ILE:O	2:D:455:THR:HG23	2.07	0.54
2:D:489:GLY:O	2:D:490:ALA:C	2.50	0.54
3:G:164:ILE:O	3:G:168:ILE:HG13	2.07	0.54
2:J:221:ASN:ND2	2:J:286:ASN:C	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:91:TYR:HB2	2:L:98:TYR:CD1	2.42	0.54
1:K:265:THR:O	1:K:268:VAL:HG22	2.07	0.54
2:L:441:PHE:HE2	2:L:501:ILE:HG12	1.72	0.54
3:M:16:SER:O	3:M:20:GLN:HG2	2.07	0.54
3:O:194:GLU:HA	3:O:197:ILE:CG1	2.37	0.54
1:A:458:ILE:O	1:A:459:PHE:C	2.50	0.54
3:E:218:GLN:O	3:E:222:ILE:HG13	2.07	0.54
3:E:279:GLU:O	3:E:282:VAL:HG22	2.07	0.54
1:I:62:CYS:HB3	2:J:94:GLY:HA3	1.90	0.54
1:K:355:ILE:HB	1:K:360:PRO:HD3	1.89	0.54
3:N:149:ILE:HB	3:N:182:LEU:HD22	1.88	0.54
1:A:14:GLN:HA	1:A:14:GLN:NE2	2.22	0.54
2:D:96:VAL:HA	2:D:99:PHE:CD2	2.42	0.54
3:E:8:TYR:HB3	3:E:164:ILE:HD13	1.89	0.54
3:H:71:GLU:OE2	3:H:112:GLU:HG2	2.08	0.54
3:H:212:PRO:HG2	3:H:236:GLN:HE22	1.72	0.54
1:I:359:ARG:O	1:I:363:VAL:HG22	2.07	0.54
1:K:350:ARG:HB3	1:K:375:VAL:HG13	1.88	0.54
3:M:279:GLU:O	3:M:282:VAL:HG22	2.07	0.54
2:B:366:ARG:HG2	2:B:366:ARG:HH11	1.72	0.54
1:C:405:THR:HG23	1:C:408:GLU:CD	2.33	0.54
3:F:253:LEU:HD22	3:F:253:LEU:N	2.22	0.54
3:H:33:VAL:CG1	3:H:34:MET:N	2.70	0.54
2:J:4:GLN:HB3	2:J:6:ASP:OD1	2.07	0.54
2:J:497:LEU:O	2:J:500:SER:N	2.41	0.54
1:K:359:ARG:O	1:K:363:VAL:HG22	2.07	0.54
2:L:10:ALA:O	2:L:11:SER:C	2.50	0.54
2:L:431:ARG:HG2	2:L:431:ARG:HH11	1.72	0.54
3:M:40:PRO:HG2	3:N:130:VAL:CG1	2.37	0.54
3:M:60:MET:HB3	3:M:70:LEU:HD21	1.89	0.54
3:M:72:LEU:HD13	3:M:112:GLU:HB2	1.90	0.54
3:O:92:GLU:CD	3:P:170:LYS:HE3	2.32	0.54
1:A:350:ARG:HB3	1:A:375:VAL:HG13	1.89	0.54
1:A:354:TYR:CE1	1:A:404:VAL:HG12	2.42	0.54
1:C:92:SER:HB3	2:D:98:TYR:CE1	2.43	0.54
2:D:235:GLY:O	2:D:483:THR:HG23	2.08	0.54
3:E:155:MET:HG3	3:E:156:MET:HE2	1.89	0.54
3:H:100:ARG:HD3	3:H:101:GLY:N	2.23	0.54
1:I:427:GLU:O	1:I:430:ILE:N	2.38	0.54
2:J:128:GLN:NE2	2:J:165:PHE:HA	2.19	0.54
3:M:186:SER:CB	3:M:212:PRO:HA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:195:LEU:HD13	3:N:271:PHE:CD2	2.43	0.54
3:N:208:ILE:HG23	3:N:209:HIS:N	2.23	0.54
3:O:162:ASN:HD21	3:O:259:ILE:CG1	2.15	0.54
3:O:182:LEU:O	3:O:208:ILE:HG22	2.08	0.54
2:D:494:LEU:HD23	2:D:494:LEU:C	2.33	0.54
3:E:103:ILE:HG13	3:E:137:MET:CG	2.36	0.54
3:G:8:TYR:HB3	3:G:164:ILE:HD13	1.88	0.54
3:G:202:LYS:HE3	3:G:259:ILE:HG21	1.89	0.54
3:H:172:ALA:HB1	3:H:255:ILE:HG12	1.89	0.54
1:I:427:GLU:O	1:I:428:LYS:C	2.50	0.54
3:M:225:MET:HE2	3:M:230:TYR:CA	2.36	0.54
2:B:59:ARG:NH2	2:B:429:HIS:CE1	2.76	0.54
2:B:128:GLN:NE2	2:B:165:PHE:HA	2.18	0.54
2:B:347:GLU:OE1	2:B:487:TYR:HB2	2.08	0.54
1:C:378:GLY:HA3	1:C:401:TYR:CD2	2.42	0.54
2:D:46:TRP:O	2:D:49:THR:HG23	2.06	0.54
3:G:5:CYS:SG	3:G:146:GLU:HG3	2.47	0.54
3:G:50:HIS:HE1	3:G:229:GLU:OE1	1.90	0.54
2:J:509:THR:O	2:J:516:ASP:HA	2.08	0.54
3:N:100:ARG:HH11	3:N:100:ARG:HG3	1.73	0.54
3:N:102:VAL:O	3:N:106:ILE:HG13	2.07	0.54
1:A:265:THR:O	1:A:268:VAL:HG22	2.08	0.54
2:B:510:ARG:CZ	2:D:452:GLN:NE2	2.70	0.54
2:D:132:LYS:HD3	2:D:174:PHE:HE2	1.73	0.54
3:F:269:MET:HB3	3:F:274:MET:HE2	1.90	0.54
3:G:241:ARG:HG2	3:G:245:ARG:NH1	2.23	0.54
2:J:352:VAL:O	2:J:353:ASP:C	2.51	0.54
2:L:124:VAL:HG23	2:L:125:PHE:N	2.23	0.54
3:M:178:ARG:HB2	3:M:253:LEU:HB3	1.90	0.54
3:O:184:CYS:HB2	3:O:196:ILE:HG13	1.89	0.54
3:O:281:ILE:HG22	3:P:223:ARG:HD2	1.90	0.54
2:B:100:ARG:O	2:B:104:ASN:ND2	2.41	0.54
2:B:128:GLN:HA	2:B:165:PHE:CD2	2.43	0.54
2:D:103:PHE:CB	2:D:111:VAL:HG21	2.38	0.54
3:E:50:HIS:HE1	3:E:229:GLU:OE1	1.91	0.54
3:E:194:GLU:HA	3:E:197:ILE:CG1	2.38	0.54
1:I:239:ARG:NH2	2:J:27:LYS:HB2	2.23	0.54
1:K:87:GLY:HA3	6:K:9498:CLF:S2B	2.48	0.54
1:K:286:MET:O	1:K:290:TYR:HB2	2.08	0.54
6:K:9498:CLF:S2B	2:L:153:CYS:SG	3.05	0.54
2:L:192:SER:OG	2:L:194:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:22:LEU:HD11	3:M:243:LEU:HG	1.90	0.54
3:N:184:CYS:HB3	3:N:210:PHE:HD1	1.72	0.54
3:O:92:GLU:OE1	3:P:170:LYS:HE3	2.08	0.54
3:O:202:LYS:HD3	3:O:267:LEU:HD12	1.88	0.54
2:B:56:ASN:HD21	2:B:428:TRP:CD1	2.26	0.53
2:B:405:ALA:O	2:B:409:ILE:HG13	2.08	0.53
2:D:468:ARG:HD2	2:D:476:ARG:HG3	1.90	0.53
3:G:144:ALA:O	3:G:177:VAL:HG22	2.08	0.53
1:I:350:ARG:HB3	1:I:375:VAL:CG1	2.38	0.53
2:L:270:ARG:HG3	2:L:270:ARG:NH1	2.24	0.53
3:N:56:THR:O	3:N:60:MET:HE2	2.08	0.53
3:O:72:LEU:HD13	3:O:112:GLU:HB2	1.91	0.53
1:A:92:SER:HB3	2:B:98:TYR:HE1	1.74	0.53
2:B:489:GLY:O	2:B:490:ALA:C	2.51	0.53
2:D:359:HIS:CG	2:D:360:THR:N	2.76	0.53
3:F:33:VAL:HG22	3:F:121:PHE:HB2	1.89	0.53
3:F:243:LEU:O	3:F:247:VAL:HG23	2.08	0.53
3:G:49:LEU:HD23	3:G:79:GLY:HA3	1.91	0.53
3:G:214:ASP:HB3	3:G:216:VAL:HG12	1.91	0.53
3:H:154:GLU:OE1	3:H:156:MET:HB2	2.08	0.53
1:I:465:MET:O	1:I:469:ASN:HB2	2.08	0.53
1:K:209:LYS:HD3	1:K:263:GLU:OE2	2.07	0.53
2:L:88:TYR:OH	2:L:116:ASP:HB3	2.08	0.53
2:L:394:LEU:CD1	2:L:430:LEU:HB2	2.38	0.53
3:O:103:ILE:HG13	3:O:137:MET:CG	2.38	0.53
3:P:20:GLN:HE22	3:P:47:LEU:H	1.57	0.53
2:B:450:PHE:O	2:B:451:ILE:C	2.52	0.53
1:C:75:ILE:HD12	1:C:75:ILE:N	2.22	0.53
1:C:277:ARG:NH1	1:C:386:ASP:OD2	2.39	0.53
3:E:165:SER:HB3	3:E:256:PRO:CB	2.38	0.53
3:F:45:THR:CG2	3:F:85:CYS:HB2	2.38	0.53
3:F:183:ILE:HG12	3:F:208:ILE:CG2	2.37	0.53
3:G:137:MET:HE3	3:G:141:GLU:HG3	1.89	0.53
2:J:233:TYR:HD1	2:J:484:THR:HG23	1.73	0.53
2:L:236:ASN:O	2:L:239:VAL:HG12	2.08	0.53
3:N:71:GLU:OE2	3:N:112:GLU:HG2	2.08	0.53
3:O:95:VAL:HG12	3:O:96:GLY:N	2.22	0.53
3:P:33:VAL:CG1	3:P:34:MET:N	2.70	0.53
3:P:100:ARG:HH11	3:P:100:ARG:HG3	1.74	0.53
3:P:149:ILE:HB	3:P:182:LEU:CD2	2.38	0.53
2:B:431:ARG:NH1	2:B:435:PHE:CE2	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ARG:NH2	2:D:27:LYS:HB2	2.23	0.53
1:C:350:ARG:HB3	1:C:375:VAL:CG1	2.38	0.53
1:K:266:PRO:HB3	1:K:290:TYR:CD1	2.43	0.53
1:A:317:ASP:O	1:A:321:GLN:HG3	2.09	0.53
1:C:350:ARG:HB3	1:C:375:VAL:HG13	1.90	0.53
1:I:7:GLU:HA	1:I:10:GLU:OE1	2.08	0.53
2:J:132:LYS:HB3	2:J:174:PHE:CE2	2.43	0.53
2:J:513:GLN:HE21	1:K:102:GLY:HA2	1.74	0.53
3:N:149:ILE:HB	3:N:182:LEU:CD2	2.38	0.53
3:O:186:SER:HB3	3:O:213:ARG:HG3	1.91	0.53
3:P:36:VAL:HG22	3:P:86:VAL:CG2	2.38	0.53
2:B:340:ILE:HG21	1:C:479:TRP:CZ2	2.43	0.53
1:C:359:ARG:NH1	1:C:444:TRP:CH2	2.77	0.53
3:H:253:LEU:H	3:H:253:LEU:HD22	1.73	0.53
1:K:203:ARG:HA	1:K:207:LEU:HB2	1.90	0.53
3:M:38:CYS:CB	3:M:126:VAL:HG22	2.39	0.53
2:B:468:ARG:HD2	2:B:476:ARG:HG3	1.89	0.53
3:E:267:LEU:HD23	3:E:267:LEU:C	2.33	0.53
1:I:75:ILE:HD12	1:I:75:ILE:H	1.73	0.53
1:K:66:GLY:HA2	1:K:70:VAL:HG21	1.90	0.53
3:M:8:TYR:HB3	3:M:164:ILE:HD13	1.91	0.53
3:O:99:GLY:HA3	3:O:134:GLY:CA	2.38	0.53
1:C:259:ILE:HG23	1:C:260:SER:N	2.23	0.53
2:D:441:PHE:HE2	2:D:501:ILE:HG12	1.72	0.53
1:I:96:ARG:NH2	5:I:8496:CFM:S5	2.75	0.53
1:I:203:ARG:HA	1:I:207:LEU:HB2	1.90	0.53
2:J:103:PHE:HB3	2:J:111:VAL:HG21	1.90	0.53
2:L:414:PRO:O	2:L:417:LYS:HG3	2.09	0.53
3:N:100:ARG:HD3	3:N:101:GLY:N	2.23	0.53
3:O:191:ARG:HE	3:O:194:GLU:CD	2.15	0.53
3:P:33:VAL:HG22	3:P:121:PHE:HB2	1.91	0.53
2:B:88:TYR:OH	2:B:116:ASP:HB3	2.08	0.53
2:B:346:LYS:O	2:B:347:GLU:C	2.50	0.53
3:E:178:ARG:HB2	3:E:253:LEU:HB3	1.91	0.53
3:F:20:GLN:HE22	3:F:47:LEU:H	1.54	0.53
3:G:194:GLU:HA	3:G:197:ILE:CG1	2.39	0.53
2:J:236:ASN:O	2:J:239:VAL:HG12	2.08	0.53
2:L:128:GLN:HA	2:L:165:PHE:CD2	2.43	0.53
2:L:270:ARG:HG3	2:L:270:ARG:HH11	1.74	0.53
3:M:26:LEU:C	3:M:31:LYS:HB2	2.34	0.53
3:N:100:ARG:O	3:N:103:ILE:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:134:GLY:N	8:N:2290:SF4:S2	2.81	0.53
3:N:206:GLN:HG2	3:N:252:LEU:HD13	1.91	0.53
3:P:10:LYS:HG2	3:P:11:GLY:H	1.72	0.53
3:P:269:MET:HB3	3:P:274:MET:HE2	1.91	0.53
1:A:35:ASN:ND2	1:A:391:MET:HG2	2.24	0.53
3:G:34:MET:HG3	3:G:84:LYS:O	2.09	0.53
3:N:124:TYR:O	3:N:126:VAL:HG23	2.09	0.53
3:O:186:SER:CB	3:O:212:PRO:HA	2.38	0.53
3:P:49:LEU:C	3:P:51:SER:H	2.17	0.53
2:B:241:LYS:HE3	2:B:253:LEU:HD23	1.91	0.52
1:C:96:ARG:HD3	1:C:98:ASN:OD1	2.09	0.52
2:D:96:VAL:HA	2:D:99:PHE:HD2	1.74	0.52
3:E:20:GLN:HE21	3:E:48:ILE:HG12	1.72	0.52
1:I:91:TYR:HB2	2:J:98:TYR:CD1	2.44	0.52
2:J:450:PHE:O	2:J:451:ILE:C	2.51	0.52
3:N:199:LEU:HD23	3:N:199:LEU:C	2.34	0.52
3:O:2:MET:HE3	3:O:122:VAL:HG21	1.91	0.52
3:O:36:VAL:HA	3:O:86:VAL:HG23	1.91	0.52
3:P:253:LEU:HD22	3:P:253:LEU:H	1.74	0.52
1:A:102:GLY:HA2	2:D:513:GLN:HE21	1.74	0.52
3:F:208:ILE:HG23	3:F:209:HIS:N	2.24	0.52
3:G:267:LEU:HD23	3:G:267:LEU:C	2.34	0.52
3:H:253:LEU:HD22	3:H:253:LEU:N	2.24	0.52
1:I:240:ILE:O	1:I:244:GLU:HG3	2.10	0.52
2:J:347:GLU:OE1	2:J:487:TYR:HB2	2.08	0.52
2:L:366:ARG:HG2	2:L:366:ARG:HH11	1.74	0.52
3:M:194:GLU:HA	3:M:197:ILE:CG1	2.40	0.52
3:O:15:LYS:HG3	3:O:150:VAL:HG21	1.90	0.52
3:O:165:SER:HA	3:O:168:ILE:HD12	1.91	0.52
1:A:42:SER:CA	1:A:391:MET:HE1	2.40	0.52
1:C:239:ARG:NH1	2:D:27:LYS:HD2	2.23	0.52
3:F:199:LEU:HD23	3:F:203:LEU:HD23	1.91	0.52
3:F:267:LEU:HD22	3:F:271:PHE:HE2	1.74	0.52
3:O:56:THR:HG22	3:O:87:GLU:HB3	1.91	0.52
3:E:72:LEU:HD13	3:E:112:GLU:HB2	1.91	0.52
3:H:100:ARG:O	3:H:103:ILE:HG22	2.10	0.52
2:J:197:TRP:O	2:J:198:ASP:C	2.51	0.52
1:K:125:PHE:CZ	3:P:142:ASN:ND2	2.77	0.52
1:K:239:ARG:NH1	2:L:27:LYS:HD2	2.25	0.52
1:A:389:ARG:HG3	1:A:389:ARG:NH1	2.24	0.52
3:E:144:ALA:O	3:E:177:VAL:HG22	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:212:PRO:HG2	3:E:236:GLN:OE1	2.09	0.52
3:F:66:THR:H	3:F:69:ASP:CG	2.17	0.52
3:H:100:ARG:HH11	3:H:100:ARG:HG3	1.73	0.52
1:I:36:ASP:OD1	1:I:38:ALA:HB3	2.09	0.52
1:I:87:GLY:HA3	6:J:8498:CLF:S2B	2.49	0.52
2:J:71:GLN:N	2:J:72:PRO:HD2	2.24	0.52
1:A:196:HIS:O	1:A:197:ILE:C	2.50	0.52
1:A:324:CYS:O	1:A:328:ILE:HG13	2.10	0.52
2:B:348:ARG:O	2:B:351:LEU:N	2.43	0.52
1:C:42:SER:CA	1:C:391:MET:HE1	2.40	0.52
1:C:113:ASN:HD22	2:D:66:PRO:HD2	1.72	0.52
2:D:221:ASN:ND2	2:D:286:ASN:C	2.68	0.52
2:D:452:GLN:OE1	2:D:466:LEU:N	2.41	0.52
3:E:32:LYS:HG2	3:E:118:ASP:O	2.10	0.52
3:E:36:VAL:HB	3:E:124:TYR:CD1	2.45	0.52
3:H:223:ARG:O	3:H:224:ARG:HB2	2.08	0.52
1:K:59:ILE:HD13	1:K:354:TYR:CE2	2.44	0.52
3:N:253:LEU:H	3:N:253:LEU:HD22	1.73	0.52
3:P:127:LEU:HD23	3:P:127:LEU:C	2.35	0.52
1:A:59:ILE:HG23	1:A:426:LYS:HD2	1.92	0.52
1:A:92:SER:HB3	2:B:98:TYR:CE1	2.45	0.52
1:A:113:ASN:HD22	2:B:66:PRO:CD	2.23	0.52
1:A:148:ILE:O	1:A:178:ILE:HA	2.09	0.52
2:D:283:ASP:O	2:D:284:ALA:C	2.52	0.52
1:K:277:ARG:NH1	1:K:386:ASP:OD2	2.42	0.52
2:L:46:TRP:O	2:L:49:THR:HG23	2.09	0.52
2:L:71:GLN:N	2:L:72:PRO:HD2	2.25	0.52
3:N:36:VAL:HG22	3:N:86:VAL:HG22	1.91	0.52
3:O:223:ARG:O	3:O:224:ARG:C	2.52	0.52
3:O:284:LYS:HD3	3:O:285:THR:N	2.25	0.52
3:P:127:LEU:HD23	3:P:129:ASP:H	1.75	0.52
2:D:241:LYS:HE3	2:D:253:LEU:HD23	1.91	0.52
3:F:57:ILE:HA	3:F:60:MET:CE	2.40	0.52
2:J:441:PHE:CE2	2:J:501:ILE:HG12	2.45	0.52
3:M:214:ASP:HB3	3:M:216:VAL:HG12	1.91	0.52
2:B:391:VAL:HG23	2:B:392:HIS:CG	2.44	0.52
1:C:12:LEU:HD13	1:C:415:ARG:NH1	2.24	0.52
1:C:437:PRO:HA	1:C:472:TRP:CZ2	2.44	0.52
2:D:71:GLN:N	2:D:72:PRO:HD2	2.25	0.52
2:D:92:SER:OG	6:D:7498:CLF:S2A	2.62	0.52
3:H:71:GLU:HG3	3:H:72:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:245:ARG:HH11	3:H:245:ARG:HG3	1.75	0.52
1:I:92:SER:HB3	2:J:98:TYR:CE1	2.45	0.52
2:J:54:GLU:O	2:J:58:GLN:HG3	2.10	0.52
2:L:405:ALA:O	2:L:409:ILE:HG13	2.10	0.52
3:M:198:ALA:O	3:M:202:LYS:HG3	2.09	0.52
3:M:269:MET:SD	3:M:276:VAL:HA	2.50	0.52
3:O:214:ASP:HB3	3:O:216:VAL:HG12	1.92	0.52
1:C:137:GLU:OE2	2:D:59:ARG:HA	2.11	0.52
3:F:80:TYR:HD2	3:F:229:GLU:HG3	1.75	0.52
3:F:172:ALA:HB1	3:F:255:ILE:HG12	1.92	0.52
3:G:249:ASP:O	3:G:250:ASN:C	2.52	0.52
3:H:20:GLN:HE22	3:H:47:LEU:H	1.58	0.52
3:H:64:ALA:HB1	3:H:69:ASP:HB2	1.91	0.52
2:J:262:ASP:CG	2:J:481:ARG:HH12	2.18	0.52
2:J:314:PRO:HB3	2:J:331:LYS:HE2	1.92	0.52
1:K:57:MET:CE	2:L:113:CYS:H	2.23	0.52
1:K:226:ILE:HB	1:K:273:VAL:HG22	1.91	0.52
2:L:445:ASN:HB2	2:L:472:PRO:O	2.10	0.52
2:B:295:PRO:C	2:B:297:HIS:H	2.18	0.51
2:D:109:GLU:HG3	2:D:261:LEU:O	2.10	0.51
3:H:186:SER:HB2	3:H:212:PRO:HA	1.91	0.51
1:I:474:LYS:HB3	2:L:322:LEU:HD21	1.92	0.51
2:J:232:THR:HG21	2:J:471:PHE:CD1	2.45	0.51
3:M:50:HIS:HE1	3:M:229:GLU:OE1	1.92	0.51
1:A:355:ILE:HB	1:A:360:PRO:HD3	1.92	0.51
2:B:19:ASP:O	2:B:23:MET:HB2	2.11	0.51
2:B:314:PRO:HB3	2:B:331:LYS:HE2	1.92	0.51
2:B:352:VAL:O	2:B:353:ASP:C	2.52	0.51
1:C:467:LEU:HD23	1:C:467:LEU:O	2.11	0.51
2:D:247:MET:CE	2:D:340:ILE:HG12	2.40	0.51
3:E:249:ASP:O	3:E:250:ASN:C	2.52	0.51
1:I:114:PHE:HE2	1:I:142:PHE:CE2	2.29	0.51
2:J:96:VAL:HA	2:J:99:PHE:CD2	2.46	0.51
1:K:100:TYR:C	1:K:100:TYR:CD2	2.88	0.51
2:L:262:ASP:CG	2:L:481:ARG:HH12	2.18	0.51
2:L:295:PRO:O	2:L:297:HIS:N	2.43	0.51
3:N:145:GLN:NE2	3:N:145:GLN:HA	2.24	0.51
3:N:218:GLN:O	3:N:222:ILE:HG13	2.11	0.51
3:N:269:MET:HA	3:N:274:MET:O	2.11	0.51
2:B:450:PHE:O	2:B:453:ARG:N	2.44	0.51
2:D:430:LEU:HD12	2:D:433:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:80:TYR:CD2	3:F:229:GLU:HG3	2.45	0.51
3:G:154:GLU:OE2	3:G:155:MET:HB3	2.10	0.51
3:G:155:MET:HG2	3:G:156:MET:HE2	1.93	0.51
1:I:107:ASN:HD21	2:J:34:LYS:HE2	1.76	0.51
1:I:196:HIS:O	1:I:197:ILE:C	2.50	0.51
1:I:428:LYS:O	1:I:432:GLN:HG3	2.09	0.51
2:J:348:ARG:O	2:J:349:GLY:C	2.51	0.51
1:K:96:ARG:NH2	5:K:9496:CFM:S5	2.74	0.51
1:K:367:TYR:O	1:K:372:MET:HB2	2.10	0.51
1:K:462:ASP:O	1:K:463:MET:C	2.53	0.51
2:L:4:GLN:O	2:L:6:ASP:N	2.44	0.51
2:B:71:GLN:HB3	2:B:186:THR:HB	1.92	0.51
2:B:441:PHE:CE2	2:B:501:ILE:HG12	2.45	0.51
1:C:36:ASP:OD1	1:C:38:ALA:HB3	2.10	0.51
1:C:196:HIS:O	1:C:197:ILE:C	2.53	0.51
4:C:7494:HCA:O2	4:C:7494:HCA:O7	2.29	0.51
2:D:4:GLN:O	2:D:6:ASP:N	2.43	0.51
2:D:89:VAL:HG12	2:D:152:THR:HG23	1.92	0.51
2:D:135:LEU:HB3	2:D:175:ILE:HD13	1.93	0.51
3:E:27:ALA:HB1	3:E:81:GLY:O	2.10	0.51
3:E:127:LEU:HD13	3:E:127:LEU:C	2.36	0.51
3:F:92:GLU:O	3:F:93:PRO:C	2.53	0.51
1:I:478:PRO:HB2	2:L:330:MET:CE	2.40	0.51
2:J:56:ASN:HD21	2:J:428:TRP:CD1	2.28	0.51
1:K:75:ILE:HD12	1:K:75:ILE:N	2.25	0.51
2:L:509:THR:O	2:L:516:ASP:HA	2.11	0.51
3:O:26:LEU:O	3:O:31:LYS:HB2	2.10	0.51
3:O:155:MET:HG2	3:O:156:MET:HE2	1.92	0.51
3:P:199:LEU:HD23	3:P:203:LEU:HD23	1.92	0.51
2:B:430:LEU:HD12	2:B:433:LEU:HD12	1.91	0.51
2:D:391:VAL:HG23	2:D:392:HIS:CG	2.45	0.51
3:G:72:LEU:HD13	3:G:112:GLU:HB3	1.90	0.51
1:K:92:SER:HB3	2:L:98:TYR:CE1	2.45	0.51
1:K:378:GLY:HA3	1:K:401:TYR:CD2	2.46	0.51
1:K:465:MET:O	1:K:469:ASN:HB2	2.09	0.51
2:L:283:ASP:O	2:L:284:ALA:C	2.54	0.51
3:N:127:LEU:HD23	3:N:129:ASP:H	1.75	0.51
2:B:165:PHE:H	2:B:165:PHE:HD1	1.58	0.51
2:B:232:THR:HG21	2:B:471:PHE:CD1	2.46	0.51
1:C:100:TYR:C	1:C:100:TYR:CD2	2.89	0.51
2:D:308:THR:O	2:D:310:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:49:LEU:HD23	3:E:79:GLY:HA3	1.91	0.51
3:E:179:LEU:HG	3:E:180:GLY:H	1.76	0.51
3:E:179:LEU:HD23	3:E:205:THR:HB	1.92	0.51
3:E:223:ARG:O	3:E:224:ARG:C	2.53	0.51
3:F:71:GLU:OE2	3:F:112:GLU:HG2	2.10	0.51
1:I:144:LEU:HG	2:J:43:VAL:HG21	1.93	0.51
2:L:84:LYS:HA	2:L:272:TYR:CD1	2.45	0.51
3:N:10:LYS:HG2	3:N:11:GLY:H	1.72	0.51
3:N:208:ILE:CD1	3:N:246:LYS:HB3	2.37	0.51
1:A:440:GLU:HG3	1:A:445:ASP:OD2	2.11	0.51
1:C:203:ARG:HA	1:C:207:LEU:HB2	1.93	0.51
3:E:26:LEU:C	3:E:31:LYS:HB2	2.35	0.51
3:E:99:GLY:HA3	3:E:134:GLY:O	2.11	0.51
3:F:10:LYS:HG2	3:F:11:GLY:H	1.74	0.51
3:G:103:ILE:HG13	3:G:137:MET:CG	2.37	0.51
3:H:56:THR:O	3:H:60:MET:HE2	2.09	0.51
2:J:47:THR:HA	2:J:52:TYR:CG	2.46	0.51
2:J:431:ARG:HG2	2:J:431:ARG:HH11	1.76	0.51
1:K:107:ASN:HD21	2:L:34:LYS:HE2	1.75	0.51
2:L:468:ARG:HG3	2:L:468:ARG:HH11	1.76	0.51
3:M:32:LYS:HG2	3:M:118:ASP:O	2.10	0.51
3:N:154:GLU:OE1	3:N:156:MET:HB2	2.10	0.51
3:O:130:VAL:HG23	3:O:130:VAL:O	2.11	0.51
3:O:136:ALA:HB1	3:P:94:GLY:HA2	1.90	0.51
1:C:57:MET:CE	2:D:113:CYS:N	2.73	0.51
1:C:324:CYS:O	1:C:328:ILE:HG13	2.10	0.51
1:C:359:ARG:O	1:C:363:VAL:HG22	2.11	0.51
2:D:366:ARG:HG2	2:D:366:ARG:HH11	1.76	0.51
2:D:379:LEU:HD21	2:D:443:ILE:HG21	1.93	0.51
1:I:134:LEU:HD23	1:I:134:LEU:C	2.35	0.51
2:J:452:GLN:OE1	2:J:466:LEU:N	2.42	0.51
2:L:348:ARG:O	2:L:349:GLY:C	2.54	0.51
3:O:223:ARG:HG2	3:P:281:ILE:HG13	1.92	0.51
3:P:209:HIS:HB3	3:P:243:LEU:HD13	1.92	0.51
2:B:103:PHE:HB2	2:B:111:VAL:HG21	1.91	0.51
1:C:226:ILE:HB	1:C:273:VAL:HG22	1.93	0.51
1:C:239:ARG:CZ	2:D:27:LYS:HB2	2.41	0.51
1:C:253:TRP:CZ2	1:C:262:ILE:HG23	2.46	0.51
3:E:27:ALA:HA	3:E:31:LYS:O	2.10	0.51
1:K:167:SER:O	1:K:168:LYS:C	2.54	0.51
1:K:359:ARG:NH1	1:K:444:TRP:CH2	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:90:HIS:ND1	2:L:116:ASP:OD2	2.28	0.51
3:P:244:ALA:O	3:P:248:VAL:HG23	2.11	0.51
1:A:68:LYS:C	1:A:68:LYS:CD	2.84	0.51
1:C:156:ILE:HG22	1:C:157:GLY:N	2.26	0.51
1:C:345:ARG:HG2	1:C:345:ARG:HH11	1.75	0.51
3:E:198:ALA:O	3:E:202:LYS:HG3	2.11	0.51
3:G:281:ILE:HG22	3:H:223:ARG:HD2	1.92	0.51
3:G:285:THR:HG21	3:H:230:TYR:CE1	2.46	0.51
3:H:45:THR:CG2	3:H:85:CYS:HB2	2.40	0.51
3:H:124:TYR:O	3:H:126:VAL:HG23	2.11	0.51
1:I:100:TYR:C	1:I:100:TYR:CD2	2.88	0.51
2:J:241:LYS:HE3	2:J:253:LEU:HD23	1.93	0.51
1:K:287:GLU:O	1:K:291:GLY:HA2	2.11	0.51
3:M:204:GLY:O	3:M:254:VAL:HG21	2.11	0.51
3:M:223:ARG:O	3:M:225:MET:N	2.44	0.51
3:N:227:VAL:HG21	3:N:240:TYR:HE2	1.75	0.51
1:A:346:LEU:O	1:A:349:LYS:HG2	2.11	0.50
2:B:221:ASN:ND2	2:B:286:ASN:C	2.69	0.50
2:B:228:PRO:HA	2:B:293:LEU:HD12	1.92	0.50
2:J:475:ASP:O	2:J:476:ARG:NH1	2.37	0.50
1:K:36:ASP:OD1	1:K:38:ALA:HB3	2.11	0.50
2:L:89:VAL:HG12	2:L:152:THR:HG23	1.93	0.50
2:L:96:VAL:HA	2:L:99:PHE:CD2	2.46	0.50
3:M:26:LEU:O	3:M:31:LYS:HB2	2.11	0.50
3:O:32:LYS:HG2	3:O:118:ASP:O	2.10	0.50
2:D:270:ARG:HG3	2:D:270:ARG:NH1	2.23	0.50
3:E:57:ILE:HG13	3:E:75:VAL:HG11	1.92	0.50
3:E:225:MET:HE2	3:E:230:TYR:CA	2.41	0.50
3:F:50:HIS:CE1	3:F:229:GLU:OE1	2.64	0.50
3:F:50:HIS:HE1	3:F:229:GLU:OE1	1.94	0.50
3:F:149:ILE:HB	3:F:182:LEU:CD2	2.40	0.50
3:G:99:GLY:HA3	3:G:134:GLY:O	2.12	0.50
3:G:165:SER:HB3	3:G:256:PRO:CB	2.40	0.50
3:G:178:ARG:HB2	3:G:253:LEU:HB3	1.93	0.50
2:L:19:ASP:O	2:L:23:MET:HB2	2.12	0.50
2:B:109:GLU:HG3	2:B:261:LEU:O	2.11	0.50
2:D:405:ALA:O	2:D:409:ILE:HG13	2.11	0.50
2:D:499:ASN:O	2:D:503:GLU:HB2	2.12	0.50
3:F:245:ARG:HH11	3:F:245:ARG:HG3	1.76	0.50
3:N:33:VAL:CG1	3:N:34:MET:N	2.74	0.50
3:O:20:GLN:HE21	3:O:48:ILE:HG12	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:67:VAL:C	3:G:69:ASP:H	2.20	0.50
3:H:184:CYS:HB3	3:H:210:PHE:HD1	1.76	0.50
1:I:437:PRO:HA	1:I:472:TRP:CZ2	2.46	0.50
3:M:27:ALA:HB1	3:M:81:GLY:O	2.12	0.50
3:O:29:MET:O	3:O:29:MET:HG2	2.10	0.50
1:A:367:TYR:CD1	1:A:372:MET:HG2	2.44	0.50
1:A:433:LYS:HE2	2:B:110:PRO:HD3	1.94	0.50
1:A:437:PRO:HA	1:A:472:TRP:CZ2	2.47	0.50
2:B:215:ASP:OD2	2:B:216:LYS:HE3	2.12	0.50
1:C:42:SER:O	1:C:44:LYS:N	2.45	0.50
3:E:136:ALA:HB1	3:F:94:GLY:HA2	1.92	0.50
3:E:186:SER:CB	3:E:212:PRO:HA	2.41	0.50
3:E:202:LYS:HE3	3:E:259:ILE:HG21	1.94	0.50
3:F:205:THR:OG1	3:F:206:GLN:N	2.37	0.50
3:F:266:GLU:O	3:F:270:GLU:HB3	2.12	0.50
3:G:182:LEU:O	3:G:208:ILE:HG22	2.10	0.50
3:H:265:GLU:HB3	3:H:274:MET:HE1	1.94	0.50
1:I:479:TRP:CD2	2:L:340:ILE:HD12	2.46	0.50
1:K:66:GLY:HA2	1:K:70:VAL:CG2	2.41	0.50
3:N:4:GLN:HA	3:N:122:VAL:HG13	1.94	0.50
3:N:71:GLU:HG3	3:N:72:LEU:HD13	1.93	0.50
3:O:127:LEU:HD13	3:O:127:LEU:C	2.36	0.50
3:O:194:GLU:HA	3:O:197:ILE:HD11	1.92	0.50
3:F:39:ASP:OD2	3:F:41:LYS:HB3	2.12	0.50
3:G:22:LEU:HD11	3:G:243:LEU:HG	1.93	0.50
3:G:186:SER:CB	3:G:212:PRO:HA	2.42	0.50
3:H:33:VAL:HG22	3:H:121:PHE:HB2	1.92	0.50
1:I:20:TYR:OH	1:I:408:GLU:HG3	2.12	0.50
1:I:209:LYS:HD3	1:I:263:GLU:OE2	2.10	0.50
1:I:367:TYR:O	1:I:372:MET:HB2	2.12	0.50
1:K:354:TYR:CE1	1:K:404:VAL:HG12	2.46	0.50
1:K:385:ASP:HA	1:K:388:ASP:OD2	2.11	0.50
2:L:132:LYS:HD3	2:L:174:PHE:HE2	1.74	0.50
2:L:221:ASN:ND2	2:L:286:ASN:C	2.70	0.50
2:L:347:GLU:OE1	2:L:487:TYR:HB2	2.11	0.50
3:M:155:MET:HG2	3:M:156:MET:HE2	1.93	0.50
3:M:187:ARG:HB3	3:M:187:ARG:NH1	2.27	0.50
3:P:214:ASP:OD1	3:P:216:VAL:HG12	2.11	0.50
1:A:42:SER:O	1:A:44:LYS:N	2.44	0.50
1:C:317:ASP:O	1:C:321:GLN:HG3	2.11	0.50
2:D:302:LYS:HE2	2:D:306:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:128:GLN:HA	2:J:165:PHE:CD2	2.47	0.50
2:J:135:LEU:HB3	2:J:175:ILE:HD13	1.94	0.50
2:L:4:GLN:HB3	2:L:6:ASP:OD1	2.12	0.50
3:O:241:ARG:HG2	3:O:245:ARG:NH1	2.27	0.50
3:P:45:THR:HG21	3:P:85:CYS:HB2	1.93	0.50
1:A:203:ARG:HA	1:A:207:LEU:HB2	1.94	0.50
2:B:94:GLY:O	2:B:97:ALA:HB3	2.12	0.50
1:C:439:ARG:HH12	1:C:465:MET:HE3	1.77	0.50
3:E:67:VAL:C	3:E:69:ASP:H	2.20	0.50
3:E:127:LEU:HB3	3:E:135:PHE:CE1	2.47	0.50
3:G:16:SER:O	3:G:20:GLN:HG2	2.11	0.50
1:I:239:ARG:HE	2:J:23:MET:HE1	1.76	0.50
1:K:317:ASP:O	1:K:321:GLN:HG3	2.12	0.50
2:L:197:TRP:O	2:L:198:ASP:C	2.55	0.50
3:M:249:ASP:O	3:M:250:ASN:C	2.55	0.50
3:O:249:ASP:O	3:O:250:ASN:C	2.55	0.50
3:P:186:SER:HB2	3:P:212:PRO:HA	1.92	0.50
1:A:19:VAL:CG1	1:A:20:TYR:N	2.75	0.50
2:J:71:GLN:HB3	2:J:186:THR:HB	1.94	0.50
1:K:42:SER:O	1:K:44:LYS:N	2.45	0.50
1:K:345:ARG:HG2	1:K:345:ARG:HH11	1.77	0.50
2:L:206:ARG:O	2:L:208:PHE:N	2.45	0.50
3:M:182:LEU:O	3:M:208:ILE:HG22	2.12	0.50
3:O:154:GLU:OE2	3:O:155:MET:HB3	2.11	0.50
1:A:259:ILE:HG23	1:A:260:SER:N	2.26	0.49
2:B:221:ASN:OD1	2:B:223:LYS:HB2	2.12	0.49
2:B:369:LEU:CD1	2:B:376:VAL:HG13	2.42	0.49
2:B:497:LEU:O	2:B:498:VAL:C	2.55	0.49
2:D:10:ALA:O	2:D:12:TYR:N	2.45	0.49
2:D:279:GLU:H	2:D:279:GLU:CD	2.18	0.49
2:D:450:PHE:O	2:D:451:ILE:C	2.55	0.49
3:F:56:THR:O	3:F:60:MET:HE2	2.12	0.49
3:H:56:THR:C	3:H:60:MET:HE2	2.37	0.49
1:I:332:LYS:HA	1:I:335:TRP:CD1	2.47	0.49
2:J:78:CYS:HB2	2:J:197:TRP:CD1	2.47	0.49
1:K:85:PRO:CD	1:K:155:PRO:HG2	2.42	0.49
3:M:172:ALA:HB1	3:M:255:ILE:HD13	1.94	0.49
3:M:191:ARG:HE	3:M:194:GLU:CD	2.20	0.49
3:N:20:GLN:HE22	3:N:47:LEU:H	1.59	0.49
3:P:5:CYS:SG	3:P:146:GLU:HB2	2.51	0.49
3:P:122:VAL:O	3:P:122:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:LYS:HA	1:A:438:PHE:CD1	2.47	0.49
2:B:499:ASN:O	2:B:503:GLU:HB2	2.12	0.49
1:C:59:ILE:HD13	1:C:354:TYR:CE2	2.47	0.49
2:D:233:TYR:CD1	2:D:484:THR:HG23	2.46	0.49
3:F:244:ALA:O	3:F:248:VAL:HG23	2.13	0.49
3:G:199:LEU:HD23	3:G:199:LEU:C	2.37	0.49
3:N:78:ALA:HA	3:N:83:VAL:O	2.12	0.49
3:N:265:GLU:HB3	3:N:274:MET:HE1	1.92	0.49
1:A:165:SER:O	1:A:166:VAL:C	2.54	0.49
1:C:465:MET:HG3	1:C:466:THR:N	2.26	0.49
2:D:54:GLU:O	2:D:58:GLN:HG3	2.12	0.49
3:E:34:MET:HG3	3:E:84:LYS:O	2.12	0.49
3:E:155:MET:HG2	3:E:156:MET:HE2	1.94	0.49
3:G:57:ILE:CG1	3:G:75:VAL:HG11	2.43	0.49
3:G:91:PRO:HB3	3:G:98:ALA:HA	1.94	0.49
1:I:239:ARG:CZ	2:J:27:LYS:HB2	2.42	0.49
2:J:497:LEU:O	2:J:498:VAL:C	2.55	0.49
3:N:47:LEU:HD21	3:N:221:GLU:HA	1.93	0.49
1:C:230:ASN:OD1	1:C:233:GLY:HA2	2.13	0.49
1:C:420:LEU:HD23	1:C:420:LEU:C	2.37	0.49
2:D:314:PRO:HB3	2:D:331:LYS:HE2	1.95	0.49
3:F:4:GLN:HA	3:F:122:VAL:HG13	1.95	0.49
3:F:103:ILE:HG23	3:F:104:THR:H	1.77	0.49
3:G:95:VAL:HG12	3:G:96:GLY:N	2.26	0.49
3:G:97:CYS:SG	3:G:134:GLY:HA2	2.52	0.49
1:I:354:TYR:CE1	1:I:404:VAL:HG12	2.47	0.49
2:J:468:ARG:HD2	2:J:476:ARG:HG3	1.93	0.49
2:J:511:GLY:O	2:J:516:ASP:HB3	2.13	0.49
2:L:56:ASN:HD21	2:L:428:TRP:CD1	2.31	0.49
2:L:124:VAL:HG23	2:L:125:PHE:CD2	2.48	0.49
1:A:195:HIS:O	1:A:198:ALA:HB3	2.13	0.49
3:E:162:ASN:HD21	3:E:259:ILE:CG1	2.15	0.49
3:H:149:ILE:HB	3:H:182:LEU:HD22	1.93	0.49
1:I:361:ARG:HG3	1:I:362:HIS:N	2.27	0.49
2:L:47:THR:HA	2:L:52:TYR:CG	2.47	0.49
2:L:297:HIS:O	2:L:297:HIS:CD2	2.65	0.49
2:L:458:LYS:HG2	2:L:462:PHE:CD2	2.48	0.49
3:N:172:ALA:HB1	3:N:255:ILE:HG12	1.94	0.49
3:O:27:ALA:HB1	3:O:81:GLY:O	2.13	0.49
3:P:39:ASP:OD2	3:P:41:LYS:HB3	2.12	0.49
1:C:266:PRO:HB3	1:C:290:TYR:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:PHE:CZ	5:C:7496:CFM:S2B	3.05	0.49
2:D:124:VAL:HG23	2:D:125:PHE:CD2	2.47	0.49
3:F:127:LEU:HD23	3:F:127:LEU:C	2.37	0.49
3:H:49:LEU:C	3:H:51:SER:H	2.19	0.49
1:I:345:ARG:HG2	1:I:345:ARG:HH11	1.77	0.49
2:L:431:ARG:NH1	2:L:435:PHE:HE2	2.11	0.49
2:L:495:THR:O	2:L:496:THR:C	2.55	0.49
3:M:99:GLY:HA3	3:M:134:GLY:O	2.12	0.49
3:N:45:THR:HG21	3:N:85:CYS:HB2	1.94	0.49
3:N:214:ASP:OD1	3:N:216:VAL:HG12	2.13	0.49
3:O:179:LEU:HG	3:O:180:GLY:H	1.76	0.49
3:O:267:LEU:HD23	3:O:267:LEU:C	2.38	0.49
1:C:327:VAL:O	1:C:328:ILE:C	2.56	0.49
2:D:352:VAL:O	2:D:353:ASP:C	2.53	0.49
1:K:240:ILE:O	1:K:244:GLU:HG3	2.13	0.49
1:K:259:ILE:HG23	1:K:260:SER:N	2.28	0.49
2:L:59:ARG:NH2	2:L:429:HIS:CE1	2.81	0.49
2:L:128:GLN:NE2	2:L:165:PHE:HA	2.23	0.49
2:L:348:ARG:O	2:L:351:LEU:N	2.46	0.49
3:M:41:LYS:HB3	3:M:43:ASP:OD1	2.13	0.49
3:M:67:VAL:C	3:M:69:ASP:H	2.20	0.49
3:O:199:LEU:HB2	3:O:267:LEU:HD11	1.94	0.49
1:A:119:GLN:O	1:A:120:GLU:C	2.55	0.49
2:B:262:ASP:OD2	2:D:350:ARG:HD3	2.13	0.49
2:B:348:ARG:O	2:B:349:GLY:C	2.56	0.49
2:B:458:LYS:HG2	2:B:462:PHE:CD2	2.47	0.49
2:B:495:THR:O	2:B:496:THR:C	2.53	0.49
1:C:167:SER:O	1:C:168:LYS:C	2.55	0.49
3:E:26:LEU:O	3:E:31:LYS:HB2	2.13	0.49
1:I:96:ARG:HD3	1:I:98:ASN:OD1	2.12	0.49
2:J:430:LEU:HD12	2:J:433:LEU:HD12	1.93	0.49
2:J:452:GLN:NE2	2:L:510:ARG:CZ	2.74	0.49
2:L:369:LEU:C	2:L:369:LEU:HD12	2.38	0.49
3:M:88:SER:HB3	3:M:102:VAL:HG22	1.94	0.49
3:M:130:VAL:HG23	3:M:130:VAL:O	2.12	0.49
3:O:57:ILE:HG13	3:O:75:VAL:HG11	1.93	0.49
3:O:279:GLU:O	3:O:282:VAL:HG22	2.13	0.49
3:P:47:LEU:HD21	3:P:221:GLU:HA	1.94	0.49
3:P:184:CYS:HB3	3:P:210:PHE:HD1	1.77	0.49
3:P:206:GLN:CG	3:P:252:LEU:HD22	2.34	0.49
2:B:333:SER:O	2:B:334:GLU:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:ARG:HB2	2:B:487:TYR:CE2	2.48	0.49
1:C:14:GLN:HA	1:C:14:GLN:NE2	2.28	0.49
2:D:194:VAL:HG23	2:D:195:THR:N	2.27	0.49
3:E:95:VAL:HG12	3:E:96:GLY:N	2.27	0.49
3:F:181:GLY:HA2	3:F:205:THR:OG1	2.12	0.49
3:F:197:ILE:O	3:F:201:ASN:ND2	2.46	0.49
3:F:212:PRO:HG2	3:F:236:GLN:NE2	2.27	0.49
1:I:6:ARG:NH2	1:I:396:ASP:OD2	2.46	0.49
1:I:57:MET:CE	2:J:113:CYS:H	2.26	0.49
2:J:94:GLY:O	2:J:97:ALA:HB3	2.13	0.49
3:M:27:ALA:HA	3:M:31:LYS:O	2.13	0.49
3:M:97:CYS:SG	3:M:134:GLY:HA2	2.53	0.49
3:M:284:LYS:HD3	3:M:285:THR:N	2.27	0.49
3:N:49:LEU:C	3:N:51:SER:H	2.19	0.49
1:A:327:VAL:O	1:A:328:ILE:C	2.55	0.49
3:E:202:LYS:HD3	3:E:267:LEU:HD12	1.95	0.49
3:E:208:ILE:O	3:E:208:ILE:HG12	2.12	0.49
3:F:124:TYR:O	3:F:126:VAL:HG23	2.13	0.49
2:J:279:GLU:H	2:J:279:GLU:CD	2.18	0.49
1:K:458:ILE:O	1:K:459:PHE:C	2.55	0.49
2:L:222:LYS:HD2	2:L:222:LYS:N	2.28	0.49
3:O:204:GLY:O	3:O:254:VAL:HG21	2.13	0.49
3:O:208:ILE:O	3:O:208:ILE:HG12	2.13	0.49
1:A:465:MET:HG3	1:A:466:THR:N	2.27	0.48
2:D:71:GLN:HB3	2:D:186:THR:HB	1.95	0.48
2:D:103:PHE:HB2	2:D:111:VAL:HG21	1.94	0.48
3:F:71:GLU:HG3	3:F:72:LEU:HD13	1.94	0.48
3:G:184:CYS:HG	3:G:210:PHE:HE1	1.50	0.48
1:I:462:ASP:O	1:I:463:MET:C	2.55	0.48
2:J:353:ASP:O	2:J:354:MET:C	2.56	0.48
2:J:366:ARG:HG2	2:J:366:ARG:HH11	1.78	0.48
1:K:6:ARG:NH2	1:K:396:ASP:OD2	2.46	0.48
1:K:374:VAL:HG12	1:K:394:MET:HE1	1.95	0.48
2:L:124:VAL:HG23	2:L:125:PHE:H	1.78	0.48
2:L:455:THR:OG1	2:L:463:GLU:HA	2.12	0.48
3:O:72:LEU:HD13	3:O:112:GLU:HB3	1.94	0.48
3:P:206:GLN:HG2	3:P:252:LEU:CD2	2.34	0.48
2:B:10:ALA:O	2:B:12:TYR:N	2.46	0.48
2:B:59:ARG:NH2	2:B:429:HIS:NE2	2.61	0.48
2:B:369:LEU:C	2:B:369:LEU:HD12	2.38	0.48
2:B:451:ILE:O	2:B:455:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:GLU:OE2	2:D:60:GLU:N	2.43	0.48
1:C:381:PHE:HZ	5:C:7496:CFM:S2B	2.35	0.48
2:D:108:ARG:CZ	2:D:477:HIS:CD2	2.97	0.48
2:D:124:VAL:HG23	2:D:125:PHE:N	2.28	0.48
3:F:154:GLU:OE1	3:F:156:MET:HB2	2.13	0.48
1:K:196:HIS:O	1:K:197:ILE:C	2.56	0.48
2:L:18:GLN:O	2:L:21:LYS:HB2	2.12	0.48
2:L:228:PRO:HA	2:L:293:LEU:HD12	1.94	0.48
3:O:5:CYS:SG	3:O:146:GLU:HB2	2.52	0.48
3:O:56:THR:OG1	3:O:59:GLU:HG3	2.13	0.48
3:O:80:TYR:HE1	3:O:229:GLU:HG3	1.78	0.48
3:O:202:LYS:HE3	3:O:259:ILE:HG21	1.93	0.48
2:B:89:VAL:HG12	2:B:152:THR:HG23	1.95	0.48
2:B:107:PHE:HD1	2:B:480:HIS:CD2	2.32	0.48
2:B:297:HIS:CD2	2:B:297:HIS:O	2.66	0.48
1:C:91:TYR:HB2	2:D:98:TYR:CD1	2.48	0.48
2:D:27:LYS:NZ	2:D:32:GLU:OE2	2.47	0.48
3:E:72:LEU:HD11	3:E:114:ALA:HB2	1.94	0.48
3:G:5:CYS:SG	3:G:146:GLU:HB2	2.53	0.48
3:G:269:MET:SD	3:G:276:VAL:HA	2.53	0.48
3:H:130:VAL:O	3:H:131:VAL:C	2.56	0.48
1:I:213:ASP:OD2	1:I:215:THR:HG23	2.13	0.48
1:I:480:GLU:HA	1:I:480:GLU:OE2	2.13	0.48
2:J:283:ASP:O	2:J:284:ALA:C	2.55	0.48
3:M:41:LYS:HG3	3:N:156:MET:CE	2.40	0.48
3:M:91:PRO:HB3	3:M:98:ALA:HA	1.94	0.48
3:M:172:ALA:HB1	3:M:255:ILE:CD1	2.43	0.48
3:P:55:ASN:HD22	3:P:77:LYS:NZ	2.11	0.48
2:B:47:THR:HA	2:B:52:TYR:CG	2.48	0.48
2:B:283:ASP:O	2:B:284:ALA:C	2.56	0.48
2:D:394:LEU:CD1	2:D:430:LEU:HB2	2.43	0.48
3:F:4:GLN:HG2	3:F:122:VAL:HG11	1.95	0.48
3:G:207:MET:O	3:G:209:HIS:N	2.46	0.48
1:I:42:SER:CA	1:I:391:MET:HE1	2.42	0.48
2:L:100:ARG:O	2:L:104:ASN:ND2	2.47	0.48
2:L:135:LEU:HB3	2:L:175:ILE:HD13	1.95	0.48
3:O:26:LEU:C	3:O:31:LYS:HB2	2.37	0.48
3:P:78:ALA:HA	3:P:83:VAL:O	2.14	0.48
1:A:71:VAL:C	1:A:74:PRO:HD2	2.38	0.48
1:A:439:ARG:HH12	1:A:465:MET:HE3	1.79	0.48
2:B:279:GLU:H	2:B:279:GLU:CD	2.18	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:TRP:CE3	1:C:444:TRP:HA	2.49	0.48
2:D:47:THR:HA	2:D:52:TYR:CG	2.48	0.48
3:E:154:GLU:OE2	3:E:155:MET:HB3	2.13	0.48
3:G:80:TYR:HE1	3:G:229:GLU:HG3	1.77	0.48
3:H:39:ASP:OD2	3:H:41:LYS:HB3	2.13	0.48
3:H:50:HIS:CE1	3:H:229:GLU:OE1	2.67	0.48
3:H:71:GLU:HG3	3:H:72:LEU:CD1	2.44	0.48
3:H:206:GLN:HG2	3:H:252:LEU:CD2	2.39	0.48
3:H:261:MET:O	3:H:265:GLU:HG3	2.13	0.48
1:I:66:GLY:HA2	1:I:70:VAL:HG21	1.95	0.48
3:M:135:PHE:O	3:M:138:PRO:HD2	2.12	0.48
3:M:184:CYS:SG	3:M:210:PHE:CE1	3.01	0.48
3:N:36:VAL:HG22	3:N:86:VAL:CG2	2.43	0.48
3:P:205:THR:OG1	3:P:206:GLN:N	2.38	0.48
1:A:370:LEU:O	1:A:372:MET:N	2.47	0.48
1:A:465:MET:O	1:A:469:ASN:HB2	2.14	0.48
2:B:35:TYR:O	2:B:36:PRO:C	2.55	0.48
1:C:92:SER:HB3	2:D:98:TYR:HE1	1.78	0.48
1:C:289:LYS:HE3	1:C:290:TYR:OH	2.13	0.48
3:G:36:VAL:HB	3:G:124:TYR:CD1	2.48	0.48
3:H:209:HIS:HB3	3:H:243:LEU:HD13	1.94	0.48
1:I:14:GLN:HA	1:I:14:GLN:NE2	2.29	0.48
2:J:228:PRO:HA	2:J:293:LEU:HD12	1.96	0.48
2:J:455:THR:OG1	2:J:463:GLU:HA	2.13	0.48
2:J:468:ARG:HH11	2:J:468:ARG:HG3	1.78	0.48
1:K:66:GLY:C	1:K:70:VAL:HB	2.38	0.48
1:K:323:LYS:O	1:K:327:VAL:HG23	2.14	0.48
2:L:120:GLU:C	2:L:122:ALA:H	2.21	0.48
2:L:279:GLU:H	2:L:279:GLU:CD	2.22	0.48
3:M:223:ARG:CG	3:N:281:ILE:HD12	2.35	0.48
3:O:225:MET:HE2	3:O:230:TYR:HA	1.96	0.48
1:A:425:ILE:O	1:A:425:ILE:HG13	2.13	0.48
2:B:36:PRO:O	2:B:37:GLN:C	2.56	0.48
2:B:199:ASN:O	2:B:200:MET:C	2.57	0.48
2:B:233:TYR:CD1	2:B:484:THR:HG23	2.48	0.48
2:B:369:LEU:HD11	2:B:376:VAL:HG13	1.95	0.48
3:F:105:ALA:O	3:F:109:LEU:HG	2.13	0.48
3:F:186:SER:HA	3:F:192:GLU:OE1	2.14	0.48
2:J:266:ASP:OD2	2:J:270:ARG:NH2	2.46	0.48
2:J:295:PRO:C	2:J:297:HIS:H	2.21	0.48
3:M:36:VAL:HB	3:M:124:TYR:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:95:VAL:HG12	3:M:96:GLY:N	2.29	0.48
3:M:107:ASN:HA	3:M:110:GLU:OE1	2.13	0.48
3:N:253:LEU:HD22	3:N:253:LEU:N	2.28	0.48
3:O:49:LEU:HD23	3:O:79:GLY:HA3	1.96	0.48
1:A:66:GLY:HA2	1:A:70:VAL:HG21	1.95	0.48
3:E:20:GLN:OE1	3:E:44:SER:C	2.57	0.48
3:F:100:ARG:HH11	3:F:100:ARG:HG3	1.79	0.48
3:F:265:GLU:HB3	3:F:274:MET:HE1	1.95	0.48
3:G:32:LYS:HG2	3:G:118:ASP:O	2.13	0.48
3:G:208:ILE:O	3:G:208:ILE:HG12	2.13	0.48
1:I:42:SER:O	1:I:44:LYS:N	2.46	0.48
2:J:100:ARG:O	2:J:104:ASN:ND2	2.46	0.48
1:K:361:ARG:HG3	1:K:362:HIS:N	2.28	0.48
1:K:428:LYS:HA	1:K:438:PHE:CD1	2.49	0.48
3:M:57:ILE:HD12	3:M:105:ALA:CB	2.44	0.48
3:O:178:ARG:HB2	3:O:253:LEU:HB3	1.95	0.48
3:P:56:THR:C	3:P:60:MET:HE2	2.39	0.48
3:P:59:GLU:O	3:P:63:GLU:HG3	2.13	0.48
3:P:71:GLU:OE2	3:P:112:GLU:HG2	2.13	0.48
3:P:103:ILE:CG2	3:P:104:THR:N	2.75	0.48
1:A:360:PRO:HB2	1:A:379:TYR:CE2	2.49	0.48
2:B:472:PRO:HB2	2:B:474:PHE:CZ	2.49	0.48
1:C:71:VAL:O	1:C:74:PRO:HD2	2.14	0.48
2:D:37:GLN:HG3	2:D:41:ASP:OD1	2.14	0.48
2:D:445:ASN:HB2	2:D:472:PRO:O	2.13	0.48
3:E:38:CYS:CB	3:E:126:VAL:HG22	2.43	0.48
3:F:269:MET:HA	3:F:274:MET:O	2.14	0.48
3:G:106:ILE:HD12	3:G:137:MET:HE1	1.95	0.48
3:H:212:PRO:HG2	3:H:236:GLN:NE2	2.29	0.48
1:I:350:ARG:HB3	1:I:375:VAL:HG13	1.96	0.48
1:I:444:TRP:CE3	1:I:444:TRP:HA	2.49	0.48
1:K:71:VAL:HG13	1:K:279:MET:HE3	1.96	0.48
2:L:164:ALA:O	2:L:165:PHE:C	2.56	0.48
2:L:431:ARG:NH1	2:L:435:PHE:CE2	2.82	0.48
2:L:450:PHE:O	2:L:451:ILE:C	2.56	0.48
3:M:127:LEU:HD13	3:M:127:LEU:C	2.39	0.48
3:P:130:VAL:O	3:P:132:CYS:N	2.47	0.48
3:P:245:ARG:HG3	3:P:245:ARG:NH1	2.27	0.48
1:A:20:TYR:OH	1:A:408:GLU:HG3	2.14	0.48
1:A:75:ILE:HD12	1:A:75:ILE:N	2.28	0.48
1:C:119:GLN:O	1:C:120:GLU:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:TYR:O	2:D:36:PRO:C	2.57	0.48
3:E:33:VAL:O	3:E:83:VAL:HG13	2.14	0.48
3:E:207:MET:O	3:E:209:HIS:N	2.47	0.48
3:F:184:CYS:HB3	3:F:210:PHE:HD1	1.79	0.48
3:G:175:GLY:O	3:G:178:ARG:NH2	2.46	0.48
3:H:105:ALA:O	3:H:109:LEU:HG	2.14	0.48
1:I:75:ILE:HD12	1:I:75:ILE:N	2.29	0.48
1:I:239:ARG:HE	2:J:23:MET:CE	2.27	0.48
1:I:439:ARG:NH1	1:I:465:MET:HE3	2.28	0.48
2:J:354:MET:O	2:J:355:MET:C	2.56	0.48
1:K:134:LEU:HD23	1:K:138:VAL:CG2	2.44	0.48
2:L:103:PHE:HB3	2:L:111:VAL:HG21	1.96	0.48
3:P:131:VAL:O	3:P:131:VAL:HG12	2.14	0.48
1:C:65:ALA:O	1:C:70:VAL:HG23	2.14	0.47
1:C:144:LEU:HG	2:D:43:VAL:HG21	1.95	0.47
1:C:360:PRO:HB2	1:C:379:TYR:CE2	2.49	0.47
2:D:107:PHE:HD1	2:D:480:HIS:CD2	2.32	0.47
3:E:99:GLY:HA3	3:E:134:GLY:C	2.39	0.47
3:E:184:CYS:CB	3:E:196:ILE:HG13	2.44	0.47
3:F:97:CYS:O	3:F:100:ARG:HB3	2.13	0.47
3:G:42:ALA:HA	3:G:87:GLU:OE1	2.13	0.47
3:G:72:LEU:HD11	3:G:114:ALA:HB2	1.96	0.47
1:I:21:PRO:O	1:I:22:GLU:C	2.57	0.47
1:I:155:PRO:HG3	2:J:153:CYS:HB3	1.95	0.47
1:I:389:ARG:HH11	1:I:389:ARG:CG	2.20	0.47
2:J:348:ARG:O	2:J:351:LEU:N	2.47	0.47
1:K:113:ASN:HD22	2:L:66:PRO:CD	2.27	0.47
2:L:468:ARG:HG3	2:L:468:ARG:NH1	2.28	0.47
3:M:20:GLN:HE21	3:M:48:ILE:HG12	1.77	0.47
3:M:72:LEU:HD13	3:M:112:GLU:HB3	1.95	0.47
3:P:71:GLU:C	3:P:73:GLU:N	2.72	0.47
3:P:220:ALA:HB1	3:P:225:MET:O	2.14	0.47
3:P:243:LEU:O	3:P:247:VAL:HG23	2.14	0.47
1:A:98:ASN:ND2	1:A:98:ASN:H	2.12	0.47
1:A:368:GLU:C	1:A:370:LEU:H	2.22	0.47
1:C:144:LEU:HD22	2:D:35:TYR:CD1	2.50	0.47
2:D:128:GLN:HA	2:D:165:PHE:CD2	2.49	0.47
3:E:36:VAL:HA	3:E:86:VAL:HG23	1.95	0.47
3:F:34:MET:HA	3:F:84:LYS:O	2.13	0.47
2:J:297:HIS:CD2	2:J:297:HIS:O	2.67	0.47
3:O:137:MET:HE2	3:O:137:MET:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:179:LEU:HD23	3:O:205:THR:HB	1.96	0.47
3:O:243:LEU:O	3:O:247:VAL:HG23	2.14	0.47
2:B:4:GLN:C	2:B:6:ASP:N	2.72	0.47
2:B:475:ASP:O	2:B:476:ARG:NH1	2.40	0.47
1:C:19:VAL:CG1	1:C:20:TYR:N	2.77	0.47
2:D:414:PRO:O	2:D:417:LYS:HG3	2.13	0.47
3:E:47:LEU:HD21	3:E:221:GLU:HG2	1.96	0.47
3:G:38:CYS:HB2	3:G:126:VAL:HA	1.96	0.47
1:I:66:GLY:HA2	1:I:70:VAL:CG2	2.45	0.47
1:I:66:GLY:C	1:I:70:VAL:HB	2.39	0.47
1:I:102:GLY:HA2	2:L:513:GLN:HE21	1.79	0.47
1:K:429:PHE:CZ	2:L:108:ARG:HA	2.49	0.47
1:K:437:PRO:HA	1:K:472:TRP:CZ2	2.50	0.47
2:L:247:MET:CE	2:L:340:ILE:HG12	2.41	0.47
2:L:491:MET:O	2:L:492:GLN:C	2.56	0.47
3:M:162:ASN:HD21	3:M:259:ILE:CG1	2.12	0.47
3:M:225:MET:HE2	3:M:230:TYR:HA	1.96	0.47
2:B:394:LEU:HD23	2:B:394:LEU:C	2.38	0.47
1:C:332:LYS:HA	1:C:335:TRP:CD1	2.49	0.47
3:G:10:LYS:HG2	3:G:10:LYS:O	2.13	0.47
3:G:86:VAL:HG11	3:G:109:LEU:HD21	1.97	0.47
3:H:149:ILE:HB	3:H:182:LEU:CD2	2.44	0.47
1:I:62:CYS:O	1:I:63:ALA:C	2.56	0.47
2:J:132:LYS:HB3	2:J:174:PHE:CD2	2.50	0.47
2:L:254:LEU:O	2:L:255:SER:CB	2.63	0.47
2:L:391:VAL:HG23	2:L:392:HIS:CD2	2.49	0.47
2:L:394:LEU:HD23	2:L:394:LEU:C	2.40	0.47
3:N:239:GLU:O	3:N:242:ALA:HB3	2.14	0.47
3:O:230:TYR:O	3:P:285:THR:HB	2.14	0.47
3:P:149:ILE:HB	3:P:182:LEU:HD22	1.96	0.47
3:P:181:GLY:HA2	3:P:205:THR:OG1	2.14	0.47
1:A:405:THR:HG23	1:A:408:GLU:OE2	2.15	0.47
2:B:84:LYS:HA	2:B:272:TYR:CD1	2.49	0.47
2:B:322:LEU:HD21	1:C:474:LYS:HB3	1.97	0.47
1:C:101:ILE:HG12	1:C:236:TRP:CZ2	2.49	0.47
1:C:351:VAL:HG13	1:C:420:LEU:HD23	1.97	0.47
1:C:433:LYS:HE2	2:D:110:PRO:HD3	1.96	0.47
2:D:120:GLU:C	2:D:122:ALA:H	2.22	0.47
3:E:187:ARG:HB3	3:E:187:ARG:NH1	2.29	0.47
3:E:214:ASP:CG	3:E:216:VAL:HG12	2.40	0.47
3:F:5:CYS:SG	3:F:146:GLU:HB2	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:36:VAL:HG22	3:F:86:VAL:HG22	1.96	0.47
3:H:197:ILE:O	3:H:201:ASN:ND2	2.48	0.47
1:I:167:SER:O	1:I:168:LYS:C	2.57	0.47
1:I:428:LYS:HA	1:I:438:PHE:CD1	2.50	0.47
2:J:283:ASP:C	2:J:285:PRO:HD2	2.39	0.47
2:J:391:VAL:HG23	2:J:392:HIS:CG	2.49	0.47
2:J:495:THR:O	2:J:496:THR:C	2.57	0.47
1:K:229:TYR:CE2	5:K:9496:CFM:S2A	3.07	0.47
1:K:339:VAL:HG12	1:K:343:ARG:HB2	1.97	0.47
3:M:57:ILE:HG13	3:M:75:VAL:HG11	1.95	0.47
3:N:186:SER:HB2	3:N:212:PRO:HA	1.96	0.47
3:N:212:PRO:HG2	3:N:236:GLN:HE22	1.78	0.47
3:P:49:LEU:O	3:P:50:HIS:HB2	2.14	0.47
1:A:420:LEU:HD23	1:A:420:LEU:C	2.40	0.47
1:C:68:LYS:C	1:C:68:LYS:CD	2.87	0.47
1:C:430:ILE:HG22	1:C:431:PHE:N	2.30	0.47
1:C:444:TRP:HA	1:C:444:TRP:HE3	1.80	0.47
3:F:80:TYR:CD1	3:F:80:TYR:C	2.92	0.47
3:G:26:LEU:C	3:G:31:LYS:HB2	2.39	0.47
3:G:198:ALA:O	3:G:202:LYS:HG3	2.14	0.47
3:G:216:VAL:HG22	3:G:227:VAL:HG13	1.97	0.47
2:J:109:GLU:HG3	2:J:261:LEU:O	2.14	0.47
2:J:254:LEU:O	2:J:255:SER:CB	2.63	0.47
2:L:96:VAL:HA	2:L:99:PHE:HD2	1.80	0.47
2:L:233:TYR:CD1	2:L:484:THR:HG23	2.48	0.47
3:O:231:ASP:OD1	3:O:233:LYS:HB2	2.15	0.47
1:A:209:LYS:HD3	1:A:263:GLU:OE2	2.14	0.47
1:A:345:ARG:HG2	1:A:345:ARG:HH11	1.79	0.47
2:B:200:MET:O	2:B:201:PHE:C	2.57	0.47
2:B:277:THR:HB	2:B:279:GLU:OE2	2.15	0.47
1:C:14:GLN:HA	1:C:14:GLN:HE21	1.78	0.47
1:C:62:CYS:HB3	2:D:94:GLY:HA3	1.95	0.47
1:C:114:PHE:HE2	1:C:142:PHE:CE2	2.33	0.47
1:C:427:GLU:O	1:C:430:ILE:N	2.43	0.47
2:D:318:ILE:HG12	2:D:320:MET:HG3	1.96	0.47
3:F:131:VAL:O	3:F:131:VAL:HG12	2.15	0.47
3:G:92:GLU:OE1	3:H:170:LYS:HE3	2.15	0.47
3:G:179:LEU:HD23	3:G:205:THR:HB	1.96	0.47
3:G:187:ARG:HB3	3:G:187:ARG:NH1	2.29	0.47
3:H:5:CYS:HB2	3:H:123:PHE:CE1	2.50	0.47
3:H:5:CYS:O	3:H:123:PHE:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:36:PRO:O	2:J:37:GLN:C	2.58	0.47
2:J:96:VAL:HA	2:J:99:PHE:HD2	1.79	0.47
1:K:163:ILE:O	1:K:164:GLU:C	2.58	0.47
1:K:413:VAL:HG21	1:K:431:PHE:CE1	2.50	0.47
2:L:54:GLU:O	2:L:58:GLN:HG3	2.15	0.47
3:O:20:GLN:OE1	3:O:44:SER:C	2.58	0.47
3:O:72:LEU:HD11	3:O:114:ALA:HB2	1.97	0.47
3:P:64:ALA:HB1	3:P:69:ASP:HB2	1.95	0.47
3:P:115:TYR:O	3:P:116:GLU:C	2.57	0.47
3:P:214:ASP:CG	3:P:216:VAL:HG12	2.39	0.47
2:B:368:ALA:O	2:B:442:MET:HA	2.15	0.47
2:D:222:LYS:HD2	2:D:222:LYS:N	2.30	0.47
3:E:204:GLY:O	3:E:254:VAL:HG21	2.14	0.47
3:F:261:MET:O	3:F:265:GLU:HG3	2.15	0.47
3:G:26:LEU:O	3:G:31:LYS:HB2	2.15	0.47
3:G:225:MET:HE2	3:G:230:TYR:HA	1.97	0.47
1:I:259:ILE:HG23	1:I:260:SER:N	2.28	0.47
2:J:277:THR:HB	2:J:279:GLU:OE2	2.15	0.47
1:K:427:GLU:O	1:K:430:ILE:N	2.48	0.47
1:K:444:TRP:CE3	1:K:444:TRP:HA	2.50	0.47
1:K:458:ILE:HD13	2:L:10:ALA:HA	1.96	0.47
2:L:84:LYS:HB2	2:L:145:ASP:HB2	1.96	0.47
2:L:318:ILE:HG23	2:L:318:ILE:O	2.14	0.47
3:N:245:ARG:HG3	3:N:245:ARG:NH1	2.30	0.47
3:P:66:THR:H	3:P:69:ASP:CG	2.23	0.47
3:P:274:MET:HG2	3:P:275:GLU:N	2.29	0.47
2:B:247:MET:HE2	2:B:340:ILE:HA	1.96	0.47
3:F:102:VAL:O	3:F:106:ILE:HG13	2.15	0.47
3:G:192:GLU:O	3:G:195:LEU:HB3	2.14	0.47
1:I:14:GLN:HA	1:I:14:GLN:HE21	1.80	0.47
2:J:89:VAL:HG12	2:J:152:THR:HG23	1.96	0.47
2:J:330:MET:HE3	1:K:479:TRP:HE3	1.79	0.47
2:J:333:SER:O	2:J:334:GLU:C	2.58	0.47
2:J:350:ARG:HD3	2:L:262:ASP:OD2	2.14	0.47
3:M:208:ILE:O	3:M:208:ILE:HG12	2.15	0.47
3:N:76:LEU:HD21	3:N:84:LYS:HD3	1.97	0.47
3:N:134:GLY:HA3	8:N:2290:SF4:S2	2.55	0.47
1:A:144:LEU:HG	2:B:43:VAL:HG21	1.97	0.47
1:A:344:PRO:C	1:A:346:LEU:H	2.23	0.47
1:C:364:ILE:O	1:C:365:GLY:C	2.55	0.47
1:C:428:LYS:HA	1:C:438:PHE:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:442:MET:HG3	2:D:464:VAL:HG12	1.97	0.47
3:E:86:VAL:HG11	3:E:109:LEU:HD21	1.97	0.47
3:E:172:ALA:HB1	3:E:255:ILE:HD13	1.97	0.47
3:F:218:GLN:O	3:F:222:ILE:HG13	2.14	0.47
3:G:223:ARG:O	3:G:224:ARG:C	2.57	0.47
1:I:19:VAL:CG1	1:I:20:TYR:N	2.78	0.47
1:I:360:PRO:HB2	1:I:379:TYR:CE2	2.50	0.47
1:I:444:TRP:HA	1:I:444:TRP:HE3	1.79	0.47
2:J:268:GLN:HE21	2:J:268:GLN:HB2	1.49	0.47
2:J:340:ILE:HG21	1:K:479:TRP:CZ2	2.50	0.47
2:J:452:GLN:HE21	2:L:510:ARG:NH1	2.13	0.47
2:L:109:GLU:HG3	2:L:261:LEU:O	2.15	0.47
2:L:221:ASN:OD1	2:L:223:LYS:HB2	2.14	0.47
3:M:127:LEU:HD12	3:M:135:PHE:CZ	2.50	0.47
3:N:50:HIS:CE1	3:N:229:GLU:OE1	2.68	0.47
3:O:194:GLU:HA	3:O:197:ILE:CD1	2.45	0.47
3:O:224:ARG:HG3	3:P:282:VAL:HG13	1.97	0.47
3:P:34:MET:HA	3:P:84:LYS:O	2.14	0.47
3:P:71:GLU:HG3	3:P:72:LEU:CD1	2.45	0.47
1:A:134:LEU:HD23	1:A:134:LEU:C	2.40	0.46
1:A:229:TYR:CE2	5:A:6496:CFM:S2A	3.08	0.46
1:C:458:ILE:HD13	2:D:10:ALA:HA	1.97	0.46
2:D:166:ILE:HD13	2:D:181:VAL:HG12	1.96	0.46
2:D:353:ASP:O	2:D:354:MET:C	2.58	0.46
3:E:199:LEU:HD23	3:E:199:LEU:C	2.40	0.46
3:G:130:VAL:HG23	3:G:130:VAL:O	2.15	0.46
1:I:71:VAL:C	1:I:74:PRO:HD2	2.40	0.46
1:I:119:GLN:O	1:I:120:GLU:C	2.58	0.46
1:I:200:ASP:O	1:I:201:ALA:C	2.58	0.46
2:J:18:GLN:O	2:J:21:LYS:HB2	2.16	0.46
2:J:468:ARG:HG3	2:J:468:ARG:NH1	2.30	0.46
2:J:510:ARG:CZ	2:L:452:GLN:NE2	2.73	0.46
1:K:367:TYR:CD1	1:K:372:MET:HG2	2.47	0.46
2:L:365:LYS:HE2	2:L:501:ILE:HD13	1.97	0.46
3:M:283:GLY:O	3:N:225:MET:SD	2.73	0.46
3:O:60:MET:HB3	3:O:70:LEU:HD21	1.97	0.46
3:O:285:THR:HG23	3:P:223:ARG:HH21	1.80	0.46
2:B:124:VAL:HG23	2:B:125:PHE:N	2.30	0.46
2:B:498:VAL:HG13	2:B:499:ASN:N	2.30	0.46
2:D:497:LEU:O	2:D:498:VAL:C	2.58	0.46
3:G:20:GLN:OE1	3:G:44:SER:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:27:ALA:HB1	3:G:81:GLY:O	2.15	0.46
3:H:67:VAL:C	3:H:69:ASP:N	2.72	0.46
1:I:429:PHE:CZ	2:J:108:ARG:HA	2.50	0.46
1:I:465:MET:HG3	1:I:466:THR:N	2.29	0.46
1:K:389:ARG:HG3	1:K:389:ARG:NH1	2.29	0.46
2:L:59:ARG:HH22	2:L:429:HIS:CE1	2.33	0.46
3:M:80:TYR:HE1	3:M:229:GLU:HG3	1.79	0.46
3:N:214:ASP:CG	3:N:216:VAL:HG12	2.40	0.46
3:P:92:GLU:O	3:P:93:PRO:C	2.57	0.46
1:A:114:PHE:HE2	1:A:142:PHE:CE2	2.33	0.46
1:A:239:ARG:HG2	2:B:23:MET:SD	2.55	0.46
2:B:124:VAL:HG23	2:B:125:PHE:H	1.80	0.46
2:B:262:ASP:CG	2:B:481:ARG:HH12	2.24	0.46
2:B:452:GLN:NE2	2:D:510:ARG:CZ	2.78	0.46
1:C:319:SER:O	1:C:323:LYS:HG3	2.15	0.46
2:D:254:LEU:O	2:D:255:SER:CB	2.63	0.46
3:E:5:CYS:SG	3:E:146:GLU:HB2	2.55	0.46
3:E:78:ALA:HB2	3:E:84:LYS:HD3	1.97	0.46
3:E:106:ILE:HD12	3:E:137:MET:HE1	1.97	0.46
3:F:49:LEU:O	3:F:50:HIS:HB2	2.14	0.46
1:I:134:LEU:HD23	1:I:138:VAL:HG23	1.97	0.46
2:J:445:ASN:HB2	2:J:472:PRO:O	2.15	0.46
1:K:433:LYS:HE2	2:L:110:PRO:HD3	1.96	0.46
2:L:400:LYS:NZ	3:P:111:GLU:OE1	2.48	0.46
3:M:42:ALA:HA	3:M:87:GLU:OE1	2.15	0.46
3:P:172:ALA:HB1	3:P:255:ILE:HG12	1.95	0.46
1:A:85:PRO:CD	1:A:155:PRO:HG2	2.45	0.46
3:E:243:LEU:O	3:E:247:VAL:HG23	2.16	0.46
3:F:130:VAL:O	3:F:132:CYS:N	2.48	0.46
3:F:227:VAL:HG21	3:F:240:TYR:HE2	1.81	0.46
3:G:216:VAL:HG11	3:G:236:GLN:HB3	1.98	0.46
1:I:282:ILE:O	1:I:286:MET:HG3	2.15	0.46
4:I:8494:HCA:O2	4:I:8494:HCA:O7	2.32	0.46
2:J:19:ASP:O	2:J:23:MET:HB2	2.15	0.46
2:J:262:ASP:OD2	2:L:350:ARG:HD3	2.14	0.46
1:K:360:PRO:HB2	1:K:379:TYR:CE2	2.50	0.46
2:L:381:LYS:O	2:L:385:GLU:HG3	2.15	0.46
3:M:216:VAL:HG11	3:M:236:GLN:HB3	1.96	0.46
3:N:5:CYS:HB2	3:N:123:PHE:CE1	2.51	0.46
3:N:5:CYS:O	3:N:123:PHE:HA	2.16	0.46
3:N:66:THR:H	3:N:69:ASP:CG	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:76:LEU:HD13	3:P:86:VAL:HG13	1.96	0.46
3:P:80:TYR:CD1	3:P:80:TYR:C	2.93	0.46
3:P:197:ILE:O	3:P:201:ASN:ND2	2.49	0.46
1:A:135:ILE:O	1:A:138:VAL:HB	2.15	0.46
1:A:381:PHE:HZ	5:A:6496:CFM:S2B	2.38	0.46
3:H:127:LEU:HD23	3:H:127:LEU:C	2.41	0.46
1:I:148:ILE:O	1:I:178:ILE:HA	2.15	0.46
1:K:155:PRO:O	1:K:159:ILE:HG12	2.15	0.46
2:L:247:MET:HE2	2:L:340:ILE:HA	1.96	0.46
2:L:372:ASP:O	2:L:376:VAL:HG23	2.15	0.46
3:N:71:GLU:HG3	3:N:72:LEU:CD1	2.45	0.46
3:O:136:ALA:HB2	3:P:94:GLY:HA2	1.97	0.46
3:P:266:GLU:O	3:P:270:GLU:HB3	2.16	0.46
2:B:118:MET:HE3	2:B:127:GLY:CA	2.43	0.46
2:B:118:MET:HA	2:B:130:ASN:HD22	1.80	0.46
2:B:254:LEU:O	2:B:255:SER:CB	2.63	0.46
1:C:299:PHE:HB3	1:C:452:GLY:H	1.80	0.46
2:D:381:LYS:O	2:D:385:GLU:HG3	2.16	0.46
3:E:16:SER:O	3:E:20:GLN:HG2	2.16	0.46
3:F:71:GLU:HG3	3:F:72:LEU:CD1	2.46	0.46
3:H:60:MET:HE1	3:H:75:VAL:CG1	2.28	0.46
3:H:78:ALA:HA	3:H:83:VAL:O	2.16	0.46
3:H:80:TYR:CD2	3:H:229:GLU:HG3	2.51	0.46
1:I:458:ILE:O	1:I:459:PHE:C	2.58	0.46
1:K:71:VAL:C	1:K:74:PRO:HD2	2.40	0.46
1:K:230:ASN:OD1	1:K:233:GLY:HA2	2.16	0.46
3:N:181:GLY:HA2	3:N:205:THR:OG1	2.16	0.46
1:A:479:TRP:CZ2	2:D:340:ILE:HG21	2.51	0.46
1:C:21:PRO:O	1:C:22:GLU:C	2.58	0.46
2:D:354:MET:O	2:D:355:MET:C	2.58	0.46
3:E:117:ASP:O	3:E:118:ASP:C	2.59	0.46
3:H:186:SER:CB	3:H:212:PRO:HA	2.46	0.46
1:I:253:TRP:HA	1:I:254:SER:HA	1.67	0.46
2:J:4:GLN:C	2:J:6:ASP:N	2.73	0.46
2:J:295:PRO:HG2	2:J:296:TRP:H	1.81	0.46
1:K:327:VAL:O	1:K:328:ILE:C	2.59	0.46
2:L:266:ASP:OD2	2:L:270:ARG:NH2	2.48	0.46
2:L:314:PRO:HB3	2:L:331:LYS:HE2	1.97	0.46
3:M:154:GLU:OE2	3:M:155:MET:HB3	2.15	0.46
1:A:255:GLY:O	1:A:256:ASP:C	2.58	0.46
1:A:462:ASP:O	1:A:463:MET:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:LEU:CD1	2:B:430:LEU:HB2	2.46	0.46
2:D:295:PRO:C	2:D:297:HIS:H	2.24	0.46
3:E:60:MET:HE1	3:E:74:ASP:O	2.16	0.46
3:G:14:GLY:O	3:G:15:LYS:C	2.58	0.46
3:G:231:ASP:OD1	3:G:233:LYS:HB2	2.16	0.46
1:I:266:PRO:HB3	1:I:290:TYR:CD1	2.51	0.46
2:J:70:CYS:SG	2:J:72:PRO:CG	3.04	0.46
1:K:470:PRO:O	1:K:471:CYS:C	2.59	0.46
3:M:5:CYS:O	3:M:124:TYR:HD2	1.98	0.46
3:M:179:LEU:HG	3:M:180:GLY:H	1.79	0.46
3:M:218:GLN:O	3:M:222:ILE:HG13	2.15	0.46
3:P:33:VAL:CG1	3:P:34:MET:H	2.29	0.46
2:B:359:HIS:CG	2:B:360:THR:N	2.84	0.46
2:B:431:ARG:HG2	2:B:431:ARG:NH1	2.31	0.46
1:C:11:SER:O	1:C:15:GLU:HG3	2.15	0.46
2:D:102:TYR:OH	2:D:472:PRO:HG3	2.16	0.46
2:D:284:ALA:HB3	2:D:285:PRO:HD3	1.98	0.46
3:E:194:GLU:HA	3:E:197:ILE:CD1	2.46	0.46
3:E:194:GLU:HA	3:E:197:ILE:HD11	1.97	0.46
3:F:45:THR:HG21	3:F:85:CYS:HB2	1.97	0.46
3:G:188:ASN:N	3:G:188:ASN:HD22	2.13	0.46
3:G:284:LYS:HD3	3:G:285:THR:N	2.31	0.46
3:H:205:THR:OG1	3:H:206:GLN:N	2.41	0.46
1:I:164:GLU:H	1:I:164:GLU:CD	2.24	0.46
2:J:4:GLN:O	2:J:5:VAL:C	2.59	0.46
2:J:215:ASP:OD2	2:J:216:LYS:HE3	2.16	0.46
2:L:107:PHE:O	2:L:108:ARG:C	2.58	0.46
2:L:353:ASP:O	2:L:354:MET:C	2.57	0.46
2:L:450:PHE:O	2:L:453:ARG:N	2.48	0.46
3:M:60:MET:HE1	3:M:74:ASP:O	2.16	0.46
3:M:106:ILE:HD12	3:M:137:MET:HE1	1.97	0.46
3:N:134:GLY:CA	8:N:2290:SF4:S2	3.04	0.46
3:N:266:GLU:O	3:N:270:GLU:HB3	2.16	0.46
2:B:4:GLN:O	2:B:5:VAL:C	2.57	0.46
2:B:452:GLN:HE21	2:D:510:ARG:NH1	2.14	0.46
1:C:66:GLY:HA2	1:C:70:VAL:HG21	1.97	0.46
1:C:76:LYS:HG2	1:C:257:GLY:O	2.16	0.46
3:G:186:SER:HB3	3:G:213:ARG:HG3	1.98	0.46
3:H:47:LEU:HD21	3:H:221:GLU:HA	1.98	0.46
1:I:428:LYS:HA	1:I:438:PHE:CE1	2.51	0.46
1:K:364:ILE:O	1:K:365:GLY:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:296:TRP:HB2	2:L:374:ASP:OD1	2.16	0.46
3:M:194:GLU:HA	3:M:197:ILE:HD11	1.98	0.46
3:N:39:ASP:OD1	3:N:127:LEU:HD12	2.16	0.46
3:N:56:THR:C	3:N:60:MET:HE2	2.41	0.46
3:N:80:TYR:CD2	3:N:229:GLU:HG3	2.51	0.46
1:A:62:CYS:O	1:A:63:ALA:C	2.57	0.45
1:A:351:VAL:HG12	1:A:352:MET:N	2.31	0.45
1:A:361:ARG:HG3	1:A:362:HIS:N	2.30	0.45
2:B:222:LYS:N	2:B:222:LYS:HD2	2.30	0.45
3:E:269:MET:SD	3:E:276:VAL:HA	2.56	0.45
3:F:47:LEU:HD21	3:F:221:GLU:HA	1.96	0.45
3:H:97:CYS:O	3:H:100:ARG:HB3	2.15	0.45
3:H:186:SER:HA	3:H:192:GLU:OE1	2.16	0.45
1:I:275:CYS:HB3	1:I:278:SER:HG	1.79	0.45
2:J:221:ASN:OD1	2:J:223:LYS:HB2	2.16	0.45
2:J:510:ARG:NH1	2:L:452:GLN:HE21	2.14	0.45
1:K:114:PHE:HE2	1:K:142:PHE:CE2	2.34	0.45
3:M:86:VAL:HG11	3:M:109:LEU:HD21	1.98	0.45
3:M:282:VAL:HA	3:N:223:ARG:HG3	1.98	0.45
3:N:54:GLN:HG2	3:N:55:ASN:N	2.32	0.45
3:P:67:VAL:N	3:P:69:ASP:OD2	2.48	0.45
1:A:66:GLY:C	1:A:70:VAL:HB	2.41	0.45
1:A:91:TYR:CB	2:B:98:TYR:HD1	2.29	0.45
1:C:361:ARG:HG3	1:C:362:HIS:N	2.31	0.45
2:D:200:MET:O	2:D:201:PHE:C	2.59	0.45
3:E:127:LEU:HD12	3:E:135:PHE:CZ	2.50	0.45
3:G:179:LEU:HG	3:G:180:GLY:H	1.81	0.45
3:H:66:THR:H	3:H:69:ASP:CG	2.23	0.45
1:I:433:LYS:HE3	2:J:263:THR:CG2	2.39	0.45
2:J:233:TYR:CD1	2:J:484:THR:HG23	2.51	0.45
2:J:247:MET:CE	2:J:340:ILE:HG12	2.45	0.45
2:L:107:PHE:HD1	2:L:480:HIS:CD2	2.34	0.45
2:L:442:MET:HG3	2:L:464:VAL:HG12	1.99	0.45
3:M:92:GLU:CD	3:N:170:LYS:HE3	2.40	0.45
3:N:115:TYR:O	3:N:116:GLU:C	2.60	0.45
3:O:207:MET:O	3:O:209:HIS:N	2.49	0.45
3:P:33:VAL:HG12	3:P:34:MET:H	1.81	0.45
3:P:208:ILE:HG23	3:P:209:HIS:H	1.81	0.45
1:A:107:ASN:HD21	2:B:34:LYS:HE2	1.81	0.45
1:A:427:GLU:O	1:A:430:ILE:N	2.48	0.45
2:B:522:VAL:HA	2:D:474:PHE:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:GLY:HA2	1:C:70:VAL:CG2	2.46	0.45
1:C:134:LEU:C	1:C:134:LEU:HD23	2.41	0.45
1:C:148:ILE:O	1:C:178:ILE:HA	2.16	0.45
3:E:42:ALA:HA	3:E:87:GLU:OE1	2.15	0.45
3:E:172:ALA:HB1	3:E:255:ILE:CD1	2.46	0.45
3:H:206:GLN:CG	3:H:252:LEU:HD22	2.38	0.45
1:I:113:ASN:HD22	2:J:66:PRO:HD2	1.80	0.45
2:L:35:TYR:O	2:L:36:PRO:C	2.60	0.45
3:M:32:LYS:CB	3:M:119:LEU:HA	2.46	0.45
3:M:38:CYS:HB2	3:M:126:VAL:HG22	1.98	0.45
3:M:47:LEU:HD21	3:M:221:GLU:HG2	1.98	0.45
3:O:187:ARG:HB3	3:O:187:ARG:NH1	2.32	0.45
3:P:223:ARG:O	3:P:224:ARG:HB2	2.16	0.45
1:A:239:ARG:CZ	1:A:249:CYS:SG	3.05	0.45
1:A:444:TRP:HA	1:A:444:TRP:CE3	2.51	0.45
2:B:330:MET:CE	1:C:478:PRO:HB2	2.46	0.45
2:B:456:LEU:O	2:B:459:GLY:N	2.50	0.45
2:D:36:PRO:O	2:D:37:GLN:C	2.58	0.45
2:D:495:THR:O	2:D:496:THR:C	2.58	0.45
3:F:57:ILE:HG22	3:F:58:MET:N	2.31	0.45
3:H:130:VAL:O	3:H:132:CYS:N	2.50	0.45
3:H:206:GLN:HG2	3:H:252:LEU:HD13	1.97	0.45
3:H:220:ALA:HB1	3:H:225:MET:O	2.16	0.45
2:J:166:ILE:HD13	2:J:181:VAL:HG12	1.97	0.45
1:K:134:LEU:HD23	1:K:134:LEU:C	2.42	0.45
1:K:195:HIS:O	1:K:198:ALA:HB3	2.17	0.45
2:L:153:CYS:SG	2:L:188:SER:CB	3.04	0.45
3:M:165:SER:HA	3:M:168:ILE:HD12	1.97	0.45
3:P:4:GLN:HG2	3:P:122:VAL:HG11	1.98	0.45
2:B:479:LEU:HA	2:B:479:LEU:HD23	1.83	0.45
3:E:195:LEU:HA	3:E:271:PHE:CE2	2.52	0.45
3:F:208:ILE:CD1	3:F:246:LYS:HB3	2.44	0.45
1:I:134:LEU:HD23	1:I:138:VAL:CG2	2.46	0.45
2:J:354:MET:SD	2:J:491:MET:HG2	2.56	0.45
2:J:446:SER:C	2:J:448:GLY:N	2.71	0.45
1:K:332:LYS:HA	1:K:335:TRP:CD1	2.52	0.45
2:L:153:CYS:SG	2:L:188:SER:HB2	2.57	0.45
3:M:40:PRO:HG2	3:N:130:VAL:HG12	1.97	0.45
3:N:76:LEU:HD13	3:N:86:VAL:HG13	1.98	0.45
3:O:91:PRO:HB3	3:O:98:ALA:HA	1.98	0.45
3:O:192:GLU:O	3:O:195:LEU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:TYR:HB2	2:B:236:ASN:ND2	2.32	0.45
2:B:340:ILE:HD12	1:C:479:TRP:CD2	2.51	0.45
1:C:144:LEU:HD11	2:D:43:VAL:HG21	1.97	0.45
1:C:165:SER:O	1:C:166:VAL:C	2.60	0.45
1:C:339:VAL:HG12	1:C:343:ARG:HB2	1.99	0.45
1:C:368:GLU:C	1:C:370:LEU:H	2.24	0.45
2:D:78:CYS:HB2	2:D:197:TRP:CD1	2.51	0.45
2:D:103:PHE:HB3	2:D:111:VAL:HG21	1.99	0.45
3:E:260:THR:OG1	3:E:263:GLU:HG3	2.17	0.45
3:F:64:ALA:CB	3:F:69:ASP:HB2	2.46	0.45
3:G:88:SER:HB3	3:G:102:VAL:HG22	1.98	0.45
3:H:45:THR:HG21	3:H:85:CYS:HB2	1.99	0.45
3:H:103:ILE:HG23	3:H:104:THR:H	1.79	0.45
1:I:413:VAL:HG21	1:I:431:PHE:CE1	2.51	0.45
2:J:82:PHE:HB2	2:J:85:THR:OG1	2.17	0.45
2:J:107:PHE:HD1	2:J:480:HIS:CD2	2.35	0.45
2:J:400:LYS:HZ3	3:N:112:GLU:CD	2.25	0.45
1:K:119:GLN:O	1:K:120:GLU:C	2.58	0.45
1:K:310:ARG:HA	1:K:324:CYS:SG	2.56	0.45
2:L:283:ASP:C	2:L:285:PRO:HD2	2.42	0.45
2:L:333:SER:O	2:L:334:GLU:C	2.60	0.45
3:O:10:LYS:O	3:O:10:LYS:HG2	2.16	0.45
3:P:130:VAL:O	3:P:131:VAL:C	2.59	0.45
3:P:227:VAL:HG21	3:P:240:TYR:HE2	1.81	0.45
1:A:144:LEU:HD22	2:B:35:TYR:CE1	2.52	0.45
1:A:239:ARG:NH1	2:B:27:LYS:HD2	2.32	0.45
2:B:197:TRP:CZ3	2:B:229:GLY:HA2	2.52	0.45
3:E:191:ARG:HG2	3:E:194:GLU:OE2	2.17	0.45
1:I:231:ILE:HG13	1:I:359:ARG:HH22	1.82	0.45
1:I:439:ARG:HD3	1:I:466:THR:OG1	2.16	0.45
1:I:440:GLU:HG3	1:I:445:ASP:OD2	2.16	0.45
2:J:199:ASN:O	2:J:200:MET:C	2.57	0.45
1:K:256:ASP:CG	1:K:256:ASP:O	2.60	0.45
2:L:4:GLN:O	2:L:5:VAL:C	2.60	0.45
2:L:19:ASP:OD1	2:L:19:ASP:N	2.42	0.45
3:M:102:VAL:O	3:M:106:ILE:HG13	2.16	0.45
3:M:192:GLU:O	3:M:195:LEU:HB3	2.16	0.45
3:O:33:VAL:O	3:O:83:VAL:HG13	2.17	0.45
1:A:6:ARG:NH2	1:A:396:ASP:OD2	2.50	0.45
1:A:364:ILE:O	1:A:365:GLY:C	2.59	0.45
2:B:54:GLU:O	2:B:58:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:VAL:C	1:C:74:PRO:HD2	2.41	0.45
2:D:132:LYS:HB3	2:D:174:PHE:CE2	2.52	0.45
3:E:91:PRO:HB3	3:E:98:ALA:HA	1.99	0.45
3:G:117:ASP:O	3:G:118:ASP:C	2.60	0.45
1:I:405:THR:HG23	1:I:408:GLU:CD	2.41	0.45
2:J:379:LEU:HD21	2:J:443:ILE:HG21	1.99	0.45
2:J:394:LEU:CD1	2:J:430:LEU:HB2	2.47	0.45
2:J:499:ASN:O	2:J:503:GLU:HB2	2.17	0.45
1:K:199:ASN:O	1:K:200:ASP:C	2.59	0.45
1:K:299:PHE:HB3	1:K:452:GLY:H	1.81	0.45
1:K:444:TRP:HA	1:K:444:TRP:HE3	1.80	0.45
2:L:36:PRO:O	2:L:37:GLN:C	2.58	0.45
3:O:260:THR:OG1	3:O:263:GLU:HG3	2.17	0.45
1:A:367:TYR:O	1:A:372:MET:HB2	2.17	0.45
1:A:402:ASP:O	1:A:403:ASP:C	2.60	0.45
6:A:6498:CLF:S2A	2:B:92:SER:OG	2.67	0.45
2:B:206:ARG:O	2:B:208:PHE:N	2.50	0.45
1:C:160:GLY:O	1:C:161:ASP:C	2.58	0.45
1:C:433:LYS:HE3	2:D:263:THR:CG2	2.38	0.45
2:D:221:ASN:OD1	2:D:223:LYS:HB2	2.16	0.45
3:E:278:ASP:OD1	3:E:281:ILE:HB	2.16	0.45
3:F:56:THR:C	3:F:60:MET:HE2	2.42	0.45
3:G:27:ALA:HA	3:G:31:LYS:O	2.17	0.45
3:H:145:GLN:NE2	3:H:145:GLN:HA	2.31	0.45
1:K:108:ALA:C	1:K:109:PHE:CG	2.94	0.45
1:K:148:ILE:O	1:K:178:ILE:HA	2.17	0.45
1:K:165:SER:O	1:K:166:VAL:C	2.60	0.45
1:K:440:GLU:HG3	1:K:445:ASP:OD2	2.17	0.45
2:L:119:THR:HB	2:L:120:GLU:H	1.68	0.45
3:M:14:GLY:O	3:M:15:LYS:C	2.59	0.45
3:M:20:GLN:OE1	3:M:44:SER:C	2.60	0.45
3:M:76:LEU:HD13	3:M:86:VAL:HG13	1.99	0.45
3:N:34:MET:HA	3:N:84:LYS:O	2.16	0.45
3:N:130:VAL:O	3:N:132:CYS:N	2.50	0.45
3:P:186:SER:CB	3:P:212:PRO:HA	2.47	0.45
1:A:253:TRP:HA	1:A:254:SER:HA	1.69	0.45
1:A:299:PHE:HB3	1:A:452:GLY:H	1.81	0.45
1:A:428:LYS:HA	1:A:438:PHE:CE1	2.52	0.45
1:A:470:PRO:O	1:A:471:CYS:C	2.58	0.45
4:A:6494:HCA:O7	4:A:6494:HCA:O2	2.32	0.45
2:B:100:ARG:C	2:B:104:ASN:ND2	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:414:PRO:O	2:B:417:LYS:HG3	2.16	0.45
1:C:240:ILE:HG23	1:C:241:LEU:N	2.31	0.45
2:D:410:LEU:HD22	2:D:419:ALA:CB	2.47	0.45
3:E:88:SER:HB3	3:E:102:VAL:HG22	1.98	0.45
3:H:57:ILE:HG22	3:H:58:MET:N	2.32	0.45
1:I:160:GLY:O	1:I:161:ASP:C	2.60	0.45
1:I:226:ILE:HB	1:I:273:VAL:HG22	1.98	0.45
1:K:342:TYR:O	1:K:343:ARG:C	2.59	0.45
1:K:430:ILE:HG22	1:K:431:PHE:N	2.32	0.45
2:L:442:MET:HG3	2:L:464:VAL:CG1	2.47	0.45
3:N:50:HIS:HE1	3:N:229:GLU:OE1	2.00	0.45
3:N:220:ALA:HB1	3:N:225:MET:O	2.16	0.45
1:A:271:ASN:HD22	1:A:271:ASN:HA	1.63	0.44
1:A:317:ASP:OD1	1:A:319:SER:HB3	2.17	0.44
1:A:332:LYS:HA	1:A:335:TRP:CD1	2.52	0.44
2:B:84:LYS:HB2	2:B:145:ASP:HB2	1.99	0.44
2:B:103:PHE:HB3	2:B:111:VAL:HG21	1.99	0.44
2:D:197:TRP:O	2:D:198:ASP:C	2.59	0.44
2:D:226:ILE:O	2:D:253:LEU:HD12	2.18	0.44
3:E:278:ASP:CG	3:E:281:ILE:HD12	2.42	0.44
3:G:99:GLY:HA3	3:G:134:GLY:CA	2.47	0.44
3:G:173:ASN:C	3:G:173:ASN:HD22	2.25	0.44
1:I:231:ILE:HG13	1:I:359:ARG:NH2	2.32	0.44
2:J:10:ALA:O	2:J:12:TYR:N	2.50	0.44
2:J:359:HIS:CG	2:J:360:THR:N	2.85	0.44
1:K:200:ASP:O	1:K:201:ALA:C	2.60	0.44
3:M:33:VAL:O	3:M:83:VAL:HG13	2.17	0.44
3:M:34:MET:HG3	3:M:84:LYS:O	2.18	0.44
1:A:239:ARG:NE	1:A:249:CYS:SG	2.90	0.44
3:E:41:LYS:HB3	3:E:43:ASP:OD1	2.17	0.44
3:F:115:TYR:O	3:F:116:GLU:C	2.58	0.44
3:F:122:VAL:HG13	3:F:122:VAL:O	2.16	0.44
3:G:5:CYS:HB2	3:G:123:PHE:CD1	2.52	0.44
3:H:33:VAL:CG1	3:H:34:MET:H	2.31	0.44
3:H:169:VAL:O	3:H:171:TYR:N	2.51	0.44
1:I:364:ILE:O	1:I:365:GLY:C	2.60	0.44
1:K:110:VAL:C	1:K:112:MET:H	2.25	0.44
2:L:379:LEU:HD21	2:L:443:ILE:HG21	1.98	0.44
3:N:186:SER:CB	3:N:212:PRO:HA	2.47	0.44
3:O:36:VAL:HB	3:O:124:TYR:CD1	2.52	0.44
2:B:21:LYS:HE2	2:B:21:LYS:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:LEU:HD21	2:B:443:ILE:HG21	1.99	0.44
2:B:391:VAL:HG23	2:B:392:HIS:CD2	2.52	0.44
1:C:239:ARG:NE	1:C:249:CYS:SG	2.90	0.44
2:D:262:ASP:OD1	2:D:481:ARG:NH1	2.49	0.44
3:E:80:TYR:HE1	3:E:229:GLU:HG3	1.82	0.44
3:E:130:VAL:HG23	3:E:130:VAL:O	2.17	0.44
3:E:165:SER:HA	3:E:168:ILE:HD12	1.99	0.44
3:G:41:LYS:O	3:G:42:ALA:HB3	2.16	0.44
3:G:60:MET:HB3	3:G:70:LEU:HD21	1.98	0.44
3:G:172:ALA:HB1	3:G:255:ILE:CD1	2.47	0.44
3:G:173:ASN:C	3:G:173:ASN:ND2	2.75	0.44
3:G:184:CYS:CB	3:G:196:ILE:HG13	2.47	0.44
3:H:41:LYS:HD3	3:H:41:LYS:C	2.43	0.44
3:H:132:CYS:SG	3:H:134:GLY:N	2.88	0.44
3:H:181:GLY:HA2	3:H:205:THR:OG1	2.17	0.44
2:J:124:VAL:HG23	2:J:125:PHE:CD2	2.52	0.44
2:J:308:THR:O	2:J:310:LYS:HG2	2.18	0.44
1:K:144:LEU:HD22	2:L:35:TYR:CE1	2.51	0.44
1:K:439:ARG:HG3	1:K:463:MET:HE1	1.99	0.44
2:L:4:GLN:C	2:L:6:ASP:N	2.74	0.44
2:L:132:LYS:HB3	2:L:174:PHE:CE2	2.52	0.44
3:M:207:MET:O	3:M:209:HIS:N	2.51	0.44
3:N:278:ASP:OD2	3:N:280:SER:OG	2.34	0.44
1:A:36:ASP:OD1	1:A:38:ALA:HB3	2.18	0.44
1:A:57:MET:CE	2:B:113:CYS:N	2.80	0.44
2:B:105:ARG:HD3	2:D:522:VAL:HG21	1.99	0.44
2:B:318:ILE:HG12	2:B:320:MET:HG3	1.99	0.44
1:C:42:SER:C	1:C:44:LYS:N	2.74	0.44
1:C:164:GLU:CD	1:C:164:GLU:H	2.25	0.44
1:C:195:HIS:O	1:C:198:ALA:HB3	2.17	0.44
1:C:240:ILE:O	1:C:244:GLU:HG3	2.17	0.44
2:D:4:GLN:O	2:D:5:VAL:C	2.60	0.44
2:D:4:GLN:HB3	2:D:6:ASP:OD1	2.17	0.44
2:D:266:ASP:OD2	2:D:270:ARG:NH2	2.50	0.44
3:E:139:ILE:HG23	3:E:177:VAL:HG11	1.98	0.44
3:E:283:GLY:O	3:F:225:MET:SD	2.75	0.44
3:F:67:VAL:C	3:F:69:ASP:N	2.74	0.44
3:G:127:LEU:HD13	3:G:127:LEU:C	2.41	0.44
3:H:266:GLU:O	3:H:270:GLU:HB3	2.17	0.44
1:I:387:TYR:O	1:I:390:THR:HB	2.18	0.44
2:J:151:THR:CG2	2:J:162:LEU:HD11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:144:LEU:HG	2:L:43:VAL:HG21	2.00	0.44
1:K:160:GLY:O	1:K:161:ASP:C	2.61	0.44
1:K:164:GLU:CD	1:K:164:GLU:H	2.25	0.44
1:K:297:TYR:HD2	1:K:299:PHE:CE1	2.36	0.44
2:L:82:PHE:HB2	2:L:85:THR:OG1	2.18	0.44
3:N:132:CYS:SG	3:N:134:GLY:N	2.91	0.44
3:N:202:LYS:N	3:N:202:LYS:HD2	2.33	0.44
3:P:47:LEU:HD22	3:P:225:MET:C	2.42	0.44
1:A:72:TRP:CZ2	1:A:202:VAL:HG22	2.53	0.44
1:A:346:LEU:O	1:A:347:GLU:C	2.60	0.44
1:C:437:PRO:HG3	1:C:472:TRP:CE2	2.53	0.44
1:C:440:GLU:HG3	1:C:445:ASP:OD2	2.16	0.44
2:D:199:ASN:O	2:D:200:MET:C	2.59	0.44
2:D:232:THR:HG21	2:D:471:PHE:CD1	2.52	0.44
3:F:76:LEU:HD13	3:F:86:VAL:HG13	1.99	0.44
3:G:20:GLN:HE21	3:G:48:ILE:HG12	1.81	0.44
3:H:71:GLU:C	3:H:73:GLU:N	2.73	0.44
3:H:215:ASN:C	3:H:217:VAL:N	2.74	0.44
1:I:59:ILE:HG23	1:I:426:LYS:HD2	1.99	0.44
1:I:230:ASN:OD1	1:I:233:GLY:HA2	2.18	0.44
1:I:298:ASN:C	1:I:298:ASN:OD1	2.59	0.44
2:J:108:ARG:CZ	2:J:477:HIS:CD2	3.00	0.44
2:J:194:VAL:HG23	2:J:195:THR:N	2.32	0.44
2:J:365:LYS:HE2	2:J:501:ILE:HD13	2.00	0.44
2:J:389:GLU:O	2:J:391:VAL:N	2.51	0.44
2:L:37:GLN:O	2:L:39:LYS:N	2.50	0.44
2:L:196:GLY:O	2:L:197:TRP:C	2.61	0.44
2:L:472:PRO:HB2	2:L:474:PHE:CZ	2.52	0.44
3:N:41:LYS:HD3	3:N:41:LYS:C	2.43	0.44
3:N:97:CYS:O	3:N:100:ARG:HB3	2.16	0.44
3:N:103:ILE:HG23	3:N:104:THR:H	1.83	0.44
3:O:23:VAL:C	3:O:25:ALA:N	2.73	0.44
3:O:43:ASP:HB3	3:O:46:ARG:CZ	2.47	0.44
3:O:78:ALA:HA	3:O:83:VAL:O	2.17	0.44
3:O:185:ASN:N	3:O:185:ASN:ND2	2.64	0.44
3:P:4:GLN:HA	3:P:122:VAL:HG13	1.99	0.44
1:A:302:PRO:HD3	1:A:456:PHE:CG	2.52	0.44
1:A:361:ARG:HB3	1:A:379:TYR:OH	2.17	0.44
1:A:444:TRP:HA	1:A:444:TRP:HE3	1.81	0.44
2:B:442:MET:SD	2:B:451:ILE:HG21	2.58	0.44
1:C:51:LYS:HA	1:C:189:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ALA:O	1:C:67:SER:N	2.51	0.44
1:C:389:ARG:HG3	1:C:389:ARG:NH1	2.31	0.44
2:D:233:TYR:HB2	2:D:236:ASN:ND2	2.33	0.44
2:D:475:ASP:O	2:D:476:ARG:NH1	2.42	0.44
3:F:212:PRO:HG2	3:F:236:GLN:CD	2.43	0.44
3:G:165:SER:HA	3:G:168:ILE:HD12	2.00	0.44
1:I:374:VAL:HG12	1:I:394:MET:HE1	2.00	0.44
2:J:369:LEU:CD1	2:J:376:VAL:HG13	2.48	0.44
3:M:99:GLY:HA3	3:M:134:GLY:C	2.42	0.44
3:N:5:CYS:SG	3:N:146:GLU:HB2	2.57	0.44
3:N:131:VAL:CG2	3:N:164:ILE:HG12	2.48	0.44
3:O:27:ALA:HA	3:O:31:LYS:O	2.17	0.44
3:O:201:ASN:C	3:O:203:LEU:N	2.76	0.44
3:P:97:CYS:O	3:P:100:ARG:HB3	2.17	0.44
1:A:208:GLY:HA2	1:A:211:ASP:OD1	2.17	0.44
1:A:226:ILE:HB	1:A:273:VAL:HG22	1.98	0.44
2:B:78:CYS:HB2	2:B:197:TRP:CD1	2.53	0.44
2:B:247:MET:CE	2:B:340:ILE:HG12	2.47	0.44
1:C:144:LEU:CG	2:D:43:VAL:HG21	2.48	0.44
1:C:323:LYS:O	1:C:327:VAL:HG23	2.17	0.44
1:C:475:LEU:H	1:C:475:LEU:HD12	1.82	0.44
2:D:124:VAL:HG23	2:D:125:PHE:H	1.81	0.44
3:E:23:VAL:C	3:E:25:ALA:N	2.73	0.44
3:F:103:ILE:CG2	3:F:104:THR:N	2.80	0.44
3:F:245:ARG:HG3	3:F:245:ARG:NH1	2.33	0.44
3:G:23:VAL:C	3:G:25:ALA:N	2.72	0.44
3:G:38:CYS:CB	3:G:126:VAL:HG22	2.48	0.44
3:H:131:VAL:HG21	3:H:164:ILE:HG12	1.99	0.44
1:I:165:SER:O	1:I:166:VAL:C	2.59	0.44
2:J:120:GLU:C	2:J:122:ALA:H	2.25	0.44
2:J:368:ALA:O	2:J:442:MET:HA	2.18	0.44
1:K:85:PRO:HD3	1:K:155:PRO:HG2	1.98	0.44
2:L:166:ILE:HD13	2:L:181:VAL:HG12	2.00	0.44
3:N:4:GLN:HG2	3:N:122:VAL:HG11	1.99	0.44
3:N:71:GLU:C	3:N:73:GLU:N	2.76	0.44
3:N:212:PRO:HG2	3:N:236:GLN:NE2	2.32	0.44
3:O:24:ALA:HB2	3:O:226:THR:HG21	1.99	0.44
1:A:42:SER:C	1:A:44:LYS:N	2.76	0.44
2:B:107:PHE:O	2:B:108:ARG:C	2.60	0.44
2:B:135:LEU:HB3	2:B:175:ILE:HD13	2.00	0.44
1:C:108:ALA:C	1:C:109:PHE:CG	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:GLU:O	1:C:329:ALA:HB3	2.17	0.44
1:C:462:ASP:O	1:C:463:MET:C	2.59	0.44
2:D:94:GLY:O	2:D:97:ALA:HB3	2.17	0.44
2:D:348:ARG:HB2	2:D:487:TYR:CE2	2.52	0.44
2:D:442:MET:HG3	2:D:464:VAL:CG1	2.47	0.44
3:E:60:MET:HB3	3:E:70:LEU:HD21	2.00	0.44
3:E:186:SER:HB3	3:E:213:ARG:HG3	2.00	0.44
3:F:60:MET:HE1	3:F:75:VAL:CG1	2.30	0.44
3:G:260:THR:OG1	3:G:263:GLU:HG3	2.18	0.44
2:J:221:ASN:HD21	2:J:287:ALA:N	2.16	0.44
2:J:222:LYS:N	2:J:222:LYS:HD2	2.33	0.44
3:M:199:LEU:C	3:M:199:LEU:HD23	2.43	0.44
3:N:186:SER:HA	3:N:192:GLU:OE1	2.18	0.44
3:O:32:LYS:CB	3:O:119:LEU:HA	2.47	0.44
3:O:42:ALA:HA	3:O:87:GLU:OE1	2.17	0.44
3:P:103:ILE:HG23	3:P:104:THR:H	1.81	0.44
2:B:353:ASP:O	2:B:354:MET:C	2.61	0.44
1:C:346:LEU:HD22	1:C:372:MET:HE1	2.00	0.44
1:C:351:VAL:HG12	1:C:352:MET:N	2.32	0.44
2:D:85:THR:HA	2:D:146:MET:O	2.18	0.44
3:F:186:SER:HB2	3:F:212:PRO:HA	2.00	0.44
3:H:5:CYS:SG	3:H:146:GLU:HB2	2.58	0.44
3:H:127:LEU:HD23	3:H:129:ASP:N	2.32	0.44
1:I:59:ILE:HD13	1:I:354:TYR:CE2	2.52	0.44
1:I:339:VAL:HG12	1:I:343:ARG:HB2	1.99	0.44
2:J:37:GLN:O	2:J:39:LYS:N	2.51	0.44
2:J:100:ARG:C	2:J:104:ASN:ND2	2.76	0.44
2:J:118:MET:HE3	2:J:127:GLY:CA	2.39	0.44
2:J:295:PRO:C	2:J:297:HIS:N	2.76	0.44
2:L:10:ALA:O	2:L:12:TYR:N	2.50	0.44
2:L:70:CYS:SG	2:L:72:PRO:HG2	2.58	0.44
2:L:199:ASN:O	2:L:200:MET:C	2.60	0.44
3:M:10:LYS:O	3:M:10:LYS:HG2	2.17	0.44
3:M:117:ASP:O	3:M:118:ASP:C	2.61	0.44
3:M:161:ALA:HA	3:M:164:ILE:HD12	2.00	0.44
3:M:216:VAL:HG22	3:M:227:VAL:HG13	1.99	0.44
3:O:223:ARG:NH1	3:P:284:LYS:O	2.46	0.44
3:O:269:MET:SD	3:O:276:VAL:HA	2.58	0.44
3:P:169:VAL:O	3:P:171:TYR:N	2.51	0.44
1:A:287:GLU:O	1:A:291:GLY:HA2	2.18	0.43
1:A:342:TYR:O	1:A:343:ARG:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:PHE:O	1:C:457:ALA:C	2.61	0.43
1:C:475:LEU:HD12	1:C:475:LEU:N	2.33	0.43
3:E:14:GLY:O	3:E:15:LYS:C	2.61	0.43
3:E:92:GLU:CD	3:F:170:LYS:HE3	2.42	0.43
3:F:49:LEU:C	3:F:51:SER:H	2.26	0.43
3:H:50:HIS:HE1	3:H:229:GLU:OE1	2.01	0.43
3:H:67:VAL:N	3:H:69:ASP:OD2	2.49	0.43
1:I:72:TRP:CZ2	1:I:202:VAL:HG22	2.53	0.43
1:I:289:LYS:HE3	1:I:290:TYR:OH	2.18	0.43
1:K:63:ALA:O	1:K:64:TYR:C	2.60	0.43
1:K:251:ALA:HB2	1:K:261:GLU:O	2.19	0.43
1:K:271:ASN:HD22	1:K:271:ASN:HA	1.56	0.43
2:L:200:MET:O	2:L:201:PHE:C	2.60	0.43
2:L:497:LEU:O	2:L:498:VAL:C	2.60	0.43
3:M:184:CYS:CB	3:M:196:ILE:HG13	2.48	0.43
3:N:47:LEU:HD22	3:N:225:MET:C	2.43	0.43
3:N:60:MET:CE	3:N:75:VAL:HG22	2.47	0.43
3:O:131:VAL:HG12	3:P:94:GLY:H	1.82	0.43
3:P:40:PRO:HD2	3:P:127:LEU:HD13	1.99	0.43
3:P:50:HIS:CE1	3:P:229:GLU:OE1	2.71	0.43
1:A:156:ILE:HG22	1:A:157:GLY:N	2.33	0.43
1:A:275:CYS:SG	5:A:6496:CFM:S1A	3.16	0.43
1:A:310:ARG:HA	1:A:324:CYS:SG	2.58	0.43
1:A:368:GLU:C	1:A:370:LEU:N	2.76	0.43
1:A:430:ILE:HG22	1:A:431:PHE:N	2.33	0.43
2:B:196:GLY:O	2:B:197:TRP:C	2.60	0.43
2:B:226:ILE:O	2:B:253:LEU:HD12	2.19	0.43
2:B:330:MET:O	2:B:333:SER:HB3	2.18	0.43
1:C:42:SER:C	1:C:44:LYS:H	2.27	0.43
1:C:253:TRP:HA	1:C:254:SER:HA	1.63	0.43
1:C:374:VAL:HG12	1:C:394:MET:HE1	1.99	0.43
3:E:173:ASN:N	3:E:173:ASN:HD22	2.16	0.43
3:G:32:LYS:CB	3:G:119:LEU:HA	2.47	0.43
3:G:91:PRO:O	3:G:93:PRO:HD3	2.18	0.43
2:J:76:VAL:O	2:J:77:LEU:C	2.61	0.43
1:K:21:PRO:O	1:K:22:GLU:C	2.62	0.43
1:K:359:ARG:N	1:K:360:PRO:CD	2.81	0.43
3:O:34:MET:HG3	3:O:84:LYS:O	2.18	0.43
3:O:107:ASN:HA	3:O:110:GLU:OE1	2.18	0.43
3:O:117:ASP:O	3:O:118:ASP:C	2.60	0.43
3:O:144:ALA:O	3:O:177:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:71:GLU:C	3:P:73:GLU:H	2.26	0.43
1:A:359:ARG:N	1:A:360:PRO:CD	2.80	0.43
2:B:37:GLN:HG3	2:B:41:ASP:OD1	2.17	0.43
2:B:132:LYS:HD3	2:B:174:PHE:HE2	1.83	0.43
1:C:98:ASN:ND2	1:C:98:ASN:H	2.16	0.43
1:C:239:ARG:HG2	2:D:23:MET:SD	2.58	0.43
3:E:225:MET:HE2	3:E:230:TYR:HA	2.00	0.43
3:G:134:GLY:HA3	8:G:1290:SF4:S1	2.58	0.43
2:J:71:GLN:OE1	2:J:186:THR:HA	2.18	0.43
2:J:456:LEU:O	2:J:459:GLY:N	2.51	0.43
1:K:42:SER:C	1:K:44:LYS:N	2.77	0.43
3:P:66:THR:N	3:P:69:ASP:OD1	2.51	0.43
1:A:85:PRO:HD3	1:A:155:PRO:HG2	2.00	0.43
1:A:154:CYS:SG	6:A:6498:CLF:S2A	3.16	0.43
1:C:144:LEU:CD1	2:D:43:VAL:HG21	2.49	0.43
1:C:385:ASP:HA	1:C:388:ASP:OD2	2.17	0.43
1:C:425:ILE:O	1:C:425:ILE:HG13	2.17	0.43
2:D:215:ASP:OD2	2:D:216:LYS:HE3	2.18	0.43
2:D:348:ARG:O	2:D:349:GLY:C	2.57	0.43
3:E:207:MET:C	3:E:209:HIS:H	2.26	0.43
3:G:48:ILE:HG22	3:G:79:GLY:HA3	1.99	0.43
3:G:57:ILE:HG12	3:G:75:VAL:HG21	1.99	0.43
3:G:204:GLY:O	3:G:254:VAL:HG21	2.19	0.43
3:G:212:PRO:HG3	3:G:239:GLU:HG3	2.01	0.43
3:H:33:VAL:HG12	3:H:34:MET:H	1.82	0.43
3:H:80:TYR:CD1	3:H:80:TYR:C	2.97	0.43
3:H:187:ARG:HB2	3:H:192:GLU:OE2	2.18	0.43
3:H:269:MET:HA	3:H:274:MET:O	2.18	0.43
1:I:163:ILE:O	1:I:164:GLU:C	2.60	0.43
1:I:427:GLU:O	1:I:429:PHE:N	2.52	0.43
1:I:474:LYS:HB3	2:L:322:LEU:CD2	2.49	0.43
2:J:146:MET:HA	2:J:180:PRO:HG2	2.00	0.43
3:M:267:LEU:HD23	3:M:267:LEU:C	2.43	0.43
3:N:103:ILE:CG2	3:N:104:THR:N	2.81	0.43
3:P:261:MET:O	3:P:265:GLU:HG3	2.18	0.43
1:A:160:GLY:O	1:A:161:ASP:C	2.61	0.43
2:B:102:TYR:OH	2:B:472:PRO:HG3	2.19	0.43
2:B:120:GLU:C	2:B:122:ALA:H	2.26	0.43
2:B:131:MET:HG2	2:B:165:PHE:HB3	2.01	0.43
2:B:266:ASP:OD2	2:B:270:ARG:NH2	2.51	0.43
2:B:283:ASP:C	2:B:285:PRO:HD2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:ASP:OD1	1:C:319:SER:HB3	2.18	0.43
1:C:361:ARG:HB3	1:C:379:TYR:OH	2.18	0.43
2:D:4:GLN:C	2:D:6:ASP:N	2.76	0.43
3:E:57:ILE:CG1	3:E:75:VAL:HG11	2.49	0.43
3:F:223:ARG:O	3:F:224:ARG:HB2	2.19	0.43
3:G:24:ALA:HB2	3:G:226:THR:HG21	2.01	0.43
3:H:4:GLN:HG2	3:H:122:VAL:HG11	2.00	0.43
3:H:4:GLN:HA	3:H:122:VAL:HG13	1.99	0.43
3:H:34:MET:HA	3:H:84:LYS:O	2.17	0.43
1:I:73:GLY:N	1:I:74:PRO:CD	2.82	0.43
1:I:144:LEU:CG	2:J:43:VAL:HG21	2.48	0.43
1:I:208:GLY:HA2	1:I:211:ASP:OD1	2.19	0.43
2:J:441:PHE:HE2	2:J:501:ILE:HG12	1.82	0.43
1:K:137:GLU:OE2	2:L:59:ARG:HA	2.18	0.43
1:K:302:PRO:HD3	1:K:456:PHE:CG	2.54	0.43
1:K:346:LEU:O	1:K:347:GLU:C	2.62	0.43
2:L:164:ALA:O	2:L:167:ASN:N	2.52	0.43
2:L:261:LEU:HD23	2:L:261:LEU:HA	1.81	0.43
3:N:131:VAL:HG21	3:N:164:ILE:HG12	2.00	0.43
3:N:223:ARG:O	3:N:224:ARG:HB2	2.17	0.43
3:N:285:THR:C	3:N:287:GLU:H	2.26	0.43
3:O:10:LYS:O	3:O:13:ILE:HG12	2.18	0.43
3:O:135:PHE:O	3:O:138:PRO:HD2	2.19	0.43
3:P:45:THR:O	3:P:46:ARG:C	2.62	0.43
1:A:212:GLU:HB3	2:L:279:GLU:HB3	2.01	0.43
1:A:350:ARG:HB3	1:A:375:VAL:HG11	1.98	0.43
1:A:379:TYR:HD1	1:A:387:TYR:CE1	2.36	0.43
2:B:350:ARG:HD3	2:D:262:ASP:OD2	2.18	0.43
1:C:134:LEU:HD23	1:C:138:VAL:CG2	2.49	0.43
2:D:37:GLN:O	2:D:39:LYS:N	2.52	0.43
3:E:214:ASP:CB	3:E:216:VAL:HG12	2.48	0.43
1:I:106:VAL:HG11	2:J:40:ILE:HG23	2.01	0.43
1:I:287:GLU:O	1:I:291:GLY:HA2	2.18	0.43
2:J:164:ALA:O	2:J:167:ASN:N	2.52	0.43
2:J:228:PRO:HD2	2:J:254:LEU:O	2.19	0.43
2:J:428:TRP:O	2:J:431:ARG:HB3	2.18	0.43
1:K:42:SER:CB	1:K:391:MET:HE1	2.49	0.43
2:L:284:ALA:HB3	2:L:285:PRO:HD3	2.01	0.43
3:M:72:LEU:HD11	3:M:114:ALA:HB2	1.99	0.43
3:M:278:ASP:HB2	3:M:281:ILE:HD12	1.99	0.43
3:N:100:ARG:HG3	3:N:100:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:212:PRO:HG2	3:N:236:GLN:CD	2.42	0.43
1:A:282:ILE:O	1:A:286:MET:HG3	2.18	0.43
2:B:442:MET:HE1	2:B:451:ILE:HG22	1.99	0.43
2:B:474:PHE:HB3	2:D:522:VAL:HA	1.99	0.43
1:C:193:LEU:O	1:C:197:ILE:HG13	2.19	0.43
1:C:339:VAL:O	1:C:343:ARG:CB	2.63	0.43
2:D:216:LYS:HA	2:D:286:ASN:HD21	1.83	0.43
2:D:296:TRP:HB2	2:D:374:ASP:OD1	2.18	0.43
2:D:359:HIS:O	2:D:360:THR:C	2.62	0.43
1:I:11:SER:O	1:I:15:GLU:HG3	2.18	0.43
1:I:342:TYR:O	1:I:343:ARG:C	2.61	0.43
1:I:357:GLY:HA2	1:I:379:TYR:HD2	1.83	0.43
2:J:84:LYS:HD2	2:J:145:ASP:OD2	2.19	0.43
1:K:453:PHE:C	1:K:455:GLY:N	2.76	0.43
2:L:215:ASP:OD2	2:L:216:LYS:HE3	2.18	0.43
2:L:389:GLU:O	2:L:391:VAL:N	2.51	0.43
2:L:446:SER:C	2:L:448:GLY:N	2.75	0.43
1:A:73:GLY:N	1:A:74:PRO:CD	2.81	0.43
1:A:80:HIS:O	1:A:114:PHE:HB2	2.18	0.43
1:A:98:ASN:ND2	1:A:98:ASN:N	2.65	0.43
2:B:4:GLN:O	2:B:7:LYS:N	2.48	0.43
2:B:101:SER:HA	2:B:104:ASN:HD22	1.84	0.43
2:D:197:TRP:CZ3	2:D:229:GLY:HA2	2.54	0.43
3:E:216:VAL:HG11	3:E:236:GLN:HB3	2.01	0.43
3:G:137:MET:HB3	3:G:138:PRO:HD3	2.00	0.43
3:H:92:GLU:O	3:H:93:PRO:C	2.62	0.43
1:I:219:THR:HG23	1:I:248:ARG:NH2	2.33	0.43
1:I:327:VAL:O	1:I:328:ILE:C	2.62	0.43
1:K:370:LEU:O	1:K:372:MET:N	2.52	0.43
3:M:60:MET:HE1	3:M:74:ASP:HB3	1.99	0.43
3:N:21:ASN:O	3:N:24:ALA:HB3	2.19	0.43
3:O:191:ARG:O	3:O:192:GLU:C	2.62	0.43
3:O:278:ASP:HB2	3:O:281:ILE:HD12	2.00	0.43
1:A:35:ASN:HD22	1:A:36:ASP:N	2.09	0.43
1:A:129:LYS:HE3	1:A:129:LYS:HB2	1.88	0.43
1:A:235:ALA:O	1:A:238:SER:N	2.50	0.43
1:A:433:LYS:HE3	2:B:263:THR:CG2	2.37	0.43
2:B:71:GLN:OE1	2:B:186:THR:HA	2.18	0.43
1:C:367:TYR:O	1:C:372:MET:HB2	2.18	0.43
1:C:405:THR:HG23	1:C:408:GLU:OE2	2.18	0.43
2:D:59:ARG:HH22	2:D:429:HIS:CE1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:ARG:O	2:D:208:PHE:N	2.51	0.43
2:D:431:ARG:O	2:D:434:VAL:CG2	2.66	0.43
3:E:38:CYS:HB2	3:E:126:VAL:HG22	2.01	0.43
3:E:184:CYS:HG	3:E:210:PHE:HE1	1.62	0.43
3:F:165:SER:O	3:F:166:LYS:C	2.61	0.43
3:F:187:ARG:HB2	3:F:192:GLU:OE2	2.19	0.43
3:G:127:LEU:HD12	3:G:135:PHE:CZ	2.54	0.43
1:I:85:PRO:CD	1:I:155:PRO:HG2	2.49	0.43
1:I:98:ASN:ND2	1:I:98:ASN:H	2.16	0.43
1:I:199:ASN:O	1:I:200:ASP:C	2.62	0.43
2:J:154:MET:O	2:J:155:ALA:C	2.61	0.43
2:J:394:LEU:HD23	2:J:394:LEU:C	2.42	0.43
2:J:522:VAL:HG21	2:L:105:ARG:HD3	1.99	0.43
1:K:72:TRP:O	1:K:73:GLY:C	2.60	0.43
1:K:137:GLU:OE2	2:L:60:GLU:N	2.45	0.43
2:L:84:LYS:HD2	2:L:145:ASP:OD2	2.18	0.43
2:L:101:SER:HA	2:L:104:ASN:HD22	1.84	0.43
3:M:21:ASN:HB3	3:M:240:TYR:CD1	2.54	0.43
2:B:88:TYR:CE2	2:B:135:LEU:HD23	2.54	0.43
2:B:213:MET:HE2	2:B:308:THR:HG22	2.00	0.43
2:B:247:MET:HE3	2:B:340:ILE:HA	1.98	0.43
2:B:389:GLU:O	2:B:391:VAL:N	2.52	0.43
1:C:75:ILE:H	1:C:75:ILE:CD1	2.32	0.43
1:C:343:ARG:N	1:C:344:PRO:CD	2.82	0.43
2:D:118:MET:HA	2:D:130:ASN:HD22	1.82	0.43
2:D:431:ARG:NH1	2:D:435:PHE:HE2	2.16	0.43
3:E:41:LYS:HG3	3:F:156:MET:HE1	2.01	0.43
3:F:33:VAL:CG1	3:F:34:MET:H	2.31	0.43
3:F:60:MET:CE	3:F:75:VAL:HG22	2.48	0.43
3:F:209:HIS:HB3	3:F:243:LEU:HD13	2.00	0.43
3:H:111:GLU:C	3:H:113:GLY:H	2.26	0.43
1:I:420:LEU:CD1	1:I:467:LEU:HD12	2.48	0.43
1:I:458:ILE:HD13	2:J:10:ALA:HA	2.00	0.43
2:J:77:LEU:O	2:J:80:LEU:HB2	2.19	0.43
2:J:164:ALA:O	2:J:165:PHE:C	2.61	0.43
1:K:134:LEU:HD23	1:K:138:VAL:HG23	2.00	0.43
1:K:239:ARG:NE	1:K:249:CYS:SG	2.92	0.43
2:L:100:ARG:C	2:L:104:ASN:ND2	2.77	0.43
2:L:322:LEU:HB3	2:L:385:GLU:OE2	2.19	0.43
3:M:184:CYS:SG	3:M:210:PHE:HE1	2.37	0.43
3:N:116:GLU:OE1	3:N:116:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:111:GLU:C	3:P:113:GLY:H	2.27	0.43
3:P:208:ILE:CG2	3:P:209:HIS:N	2.81	0.43
1:A:66:GLY:HA2	1:A:70:VAL:CG2	2.49	0.42
2:B:4:GLN:HB3	2:B:6:ASP:OD1	2.18	0.42
2:B:108:ARG:CZ	2:B:477:HIS:CD2	3.02	0.42
2:B:154:MET:O	2:B:155:ALA:C	2.61	0.42
1:C:110:VAL:C	1:C:112:MET:H	2.27	0.42
1:C:284:ARG:HG2	1:C:284:ARG:HH11	1.84	0.42
1:C:346:LEU:HB3	1:C:372:MET:SD	2.59	0.42
2:D:4:GLN:O	2:D:7:LYS:N	2.50	0.42
2:D:246:GLU:OE2	2:D:343:SER:HB2	2.19	0.42
3:E:137:MET:HB3	3:E:138:PRO:HD3	2.01	0.42
3:F:116:GLU:OE1	3:F:116:GLU:N	2.52	0.42
3:F:220:ALA:HB1	3:F:225:MET:O	2.18	0.42
3:G:214:ASP:CG	3:G:216:VAL:HG12	2.44	0.42
3:G:246:LYS:O	3:G:250:ASN:HB2	2.19	0.42
3:H:80:TYR:HD2	3:H:229:GLU:HG3	1.83	0.42
3:H:169:VAL:C	3:H:171:TYR:N	2.76	0.42
3:H:212:PRO:HG2	3:H:236:GLN:CD	2.44	0.42
3:H:285:THR:C	3:H:287:GLU:H	2.27	0.42
1:I:310:ARG:C	1:I:312:ILE:N	2.75	0.42
1:I:475:LEU:H	1:I:475:LEU:HD12	1.84	0.42
2:J:35:TYR:O	2:J:36:PRO:C	2.62	0.42
1:K:206:VAL:O	1:K:207:LEU:C	2.62	0.42
1:K:235:ALA:O	1:K:238:SER:N	2.52	0.42
1:K:351:VAL:HG12	1:K:352:MET:N	2.33	0.42
2:L:201:PHE:O	2:L:202:GLU:C	2.62	0.42
3:O:50:HIS:HE1	3:O:229:GLU:OE1	2.01	0.42
3:P:39:ASP:OD1	3:P:127:LEU:HD12	2.19	0.42
1:A:200:ASP:O	1:A:201:ALA:C	2.60	0.42
2:B:475:ASP:C	2:B:476:ARG:HG2	2.44	0.42
1:C:223:VAL:HG23	1:C:249:CYS:HA	2.00	0.42
2:D:44:PHE:O	2:D:45:GLN:C	2.62	0.42
2:D:59:ARG:NH2	2:D:429:HIS:CE1	2.87	0.42
2:D:348:ARG:O	2:D:351:LEU:N	2.53	0.42
8:E:290:SF4:S2	3:F:134:GLY:N	2.92	0.42
3:F:36:VAL:HG22	3:F:86:VAL:CG2	2.49	0.42
3:F:206:GLN:HG2	3:F:252:LEU:HD13	2.02	0.42
3:G:278:ASP:CG	3:G:281:ILE:HD12	2.44	0.42
3:H:54:GLN:HG2	3:H:55:ASN:N	2.34	0.42
1:I:359:ARG:N	1:I:360:PRO:CD	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:131:MET:HG2	2:J:165:PHE:HB3	2.00	0.42
2:J:491:MET:O	2:J:492:GLN:C	2.62	0.42
1:K:98:ASN:ND2	1:K:98:ASN:H	2.17	0.42
1:K:370:LEU:C	1:K:372:MET:N	2.77	0.42
2:L:369:LEU:HD11	2:L:376:VAL:HG13	2.01	0.42
3:M:23:VAL:C	3:M:25:ALA:N	2.75	0.42
3:M:223:ARG:O	3:M:224:ARG:C	2.61	0.42
3:O:6:ALA:C	3:O:7:ILE:HD13	2.43	0.42
3:O:202:LYS:HE3	3:O:202:LYS:HB3	1.94	0.42
3:P:100:ARG:HG3	3:P:100:ARG:NH1	2.33	0.42
1:A:285:HIS:O	1:A:288:GLU:N	2.52	0.42
2:B:221:ASN:OD1	2:B:223:LYS:N	2.51	0.42
2:D:431:ARG:HG2	2:D:431:ARG:NH1	2.35	0.42
3:E:54:GLN:NE2	3:E:75:VAL:O	2.52	0.42
3:H:36:VAL:HG22	3:H:86:VAL:CG2	2.49	0.42
3:H:245:ARG:HG3	3:H:245:ARG:NH1	2.33	0.42
1:I:57:MET:CE	2:J:113:CYS:N	2.82	0.42
1:I:346:LEU:HD22	1:I:372:MET:HE1	2.01	0.42
1:I:425:ILE:C	1:I:427:GLU:H	2.27	0.42
1:I:436:ILE:O	1:I:437:PRO:C	2.61	0.42
1:I:475:LEU:HD12	1:I:475:LEU:N	2.35	0.42
1:K:11:SER:O	1:K:15:GLU:HG3	2.19	0.42
1:K:62:CYS:O	1:K:63:ALA:C	2.61	0.42
1:K:76:LYS:HG2	1:K:257:GLY:O	2.18	0.42
1:K:145:ASN:OD1	1:K:145:ASN:C	2.63	0.42
3:N:127:LEU:HD23	3:N:127:LEU:C	2.44	0.42
3:N:256:PRO:O	3:N:258:PRO:HD3	2.19	0.42
3:O:184:CYS:HG	3:O:210:PHE:HE1	1.62	0.42
3:P:116:GLU:OE1	3:P:116:GLU:N	2.53	0.42
1:A:72:TRP:C	1:A:74:PRO:HD2	2.45	0.42
2:B:37:GLN:O	2:B:39:LYS:N	2.53	0.42
2:B:502:LEU:HD22	2:B:523:ARG:HD2	2.00	0.42
1:C:357:GLY:HA2	1:C:379:TYR:HD2	1.84	0.42
2:D:164:ALA:O	2:D:165:PHE:C	2.63	0.42
2:D:445:ASN:OD1	2:D:447:TYR:HB2	2.19	0.42
3:E:201:ASN:C	3:E:203:LEU:N	2.76	0.42
3:F:43:ASP:OD1	3:F:43:ASP:N	2.51	0.42
3:F:54:GLN:HG2	3:F:55:ASN:N	2.33	0.42
3:G:201:ASN:C	3:G:203:LEU:N	2.75	0.42
3:G:278:ASP:HB2	3:G:281:ILE:HD12	2.00	0.42
3:H:115:TYR:O	3:H:116:GLU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:131:VAL:CG2	3:H:164:ILE:HG12	2.49	0.42
1:I:88:CYS:CB	1:I:153:GLU:OE2	2.64	0.42
1:I:354:TYR:OH	1:I:380:GLU:HA	2.19	0.42
1:K:19:VAL:CG1	1:K:20:TYR:N	2.81	0.42
1:K:98:ASN:HD22	1:K:98:ASN:C	2.26	0.42
1:K:405:THR:OG1	1:K:408:GLU:HG3	2.19	0.42
3:N:80:TYR:CD1	3:N:80:TYR:C	2.98	0.42
3:O:14:GLY:O	3:O:15:LYS:C	2.62	0.42
3:O:16:SER:O	3:O:20:GLN:HG2	2.19	0.42
3:O:88:SER:HB3	3:O:102:VAL:HG22	2.01	0.42
1:C:287:GLU:O	1:C:291:GLY:HA2	2.20	0.42
1:C:470:PRO:O	1:C:471:CYS:C	2.60	0.42
3:G:78:ALA:HA	3:G:83:VAL:C	2.45	0.42
1:I:12:LEU:HD13	1:I:415:ARG:NH1	2.34	0.42
1:I:451:HIS:O	1:I:455:GLY:HA3	2.20	0.42
2:J:413:SER:HA	2:J:414:PRO:HD3	1.92	0.42
1:K:68:LYS:C	1:K:68:LYS:CD	2.91	0.42
2:L:59:ARG:NH2	2:L:429:HIS:NE2	2.67	0.42
2:L:194:VAL:HG23	2:L:195:THR:N	2.34	0.42
2:L:221:ASN:HD22	2:L:286:ASN:HB2	1.84	0.42
2:L:445:ASN:OD1	2:L:447:TYR:HB2	2.20	0.42
3:M:3:ARG:NH1	3:M:121:PHE:HZ	2.16	0.42
3:M:54:GLN:NE2	3:M:75:VAL:O	2.52	0.42
3:M:60:MET:CB	3:M:70:LEU:HD21	2.50	0.42
3:O:3:ARG:NH1	3:O:121:PHE:HZ	2.16	0.42
3:O:195:LEU:HA	3:O:271:PHE:CE2	2.54	0.42
3:O:243:LEU:O	3:O:244:ALA:C	2.62	0.42
1:A:63:ALA:O	1:A:64:TYR:C	2.62	0.42
2:B:491:MET:O	2:B:492:GLN:C	2.63	0.42
1:C:239:ARG:CZ	1:C:249:CYS:SG	3.07	0.42
1:C:359:ARG:N	1:C:360:PRO:CD	2.82	0.42
1:C:364:ILE:HD11	1:C:394:MET:SD	2.60	0.42
2:D:502:LEU:HD22	2:D:523:ARG:HD2	2.00	0.42
3:E:142:ASN:HD21	3:E:175:GLY:HA3	1.85	0.42
3:F:71:GLU:C	3:F:73:GLU:N	2.77	0.42
3:G:100:ARG:HE	3:G:101:GLY:N	2.18	0.42
3:G:173:ASN:HD22	3:G:173:ASN:N	2.18	0.42
3:G:207:MET:C	3:G:209:HIS:H	2.27	0.42
1:I:359:ARG:NH1	1:I:444:TRP:CH2	2.88	0.42
2:J:84:LYS:HA	2:J:272:TYR:CD1	2.54	0.42
2:L:451:ILE:HD12	2:L:451:ILE:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:80:TYR:HD2	3:N:229:GLU:HG3	1.85	0.42
3:O:198:ALA:O	3:O:202:LYS:HG3	2.19	0.42
3:P:71:GLU:O	3:P:73:GLU:N	2.53	0.42
3:P:72:LEU:C	3:P:72:LEU:CD2	2.88	0.42
2:B:450:PHE:O	2:B:452:GLN:N	2.53	0.42
1:C:358:LEU:HD11	1:C:362:HIS:CE1	2.55	0.42
2:D:164:ALA:O	2:D:167:ASN:N	2.53	0.42
2:D:456:LEU:O	2:D:457:HIS:C	2.62	0.42
3:E:78:ALA:HA	3:E:83:VAL:O	2.20	0.42
3:F:145:GLN:NE2	3:F:145:GLN:HA	2.34	0.42
1:I:156:ILE:HG22	1:I:157:GLY:N	2.34	0.42
2:J:324:TRP:CZ2	2:J:381:LYS:HD3	2.55	0.42
2:J:326:ASP:OD1	2:J:487:TYR:OH	2.34	0.42
1:K:42:SER:C	1:K:44:LYS:H	2.27	0.42
2:L:268:GLN:HE21	2:L:268:GLN:HB2	1.53	0.42
2:L:348:ARG:HB2	2:L:487:TYR:CE2	2.54	0.42
3:M:201:ASN:C	3:M:203:LEU:N	2.77	0.42
3:M:207:MET:C	3:M:209:HIS:H	2.27	0.42
3:N:92:GLU:O	3:N:93:PRO:C	2.62	0.42
3:O:283:GLY:O	3:P:225:MET:SD	2.77	0.42
3:P:54:GLN:HG2	3:P:55:ASN:N	2.34	0.42
1:A:253:TRP:CZ3	1:A:282:ILE:HG12	2.55	0.42
1:A:255:GLY:C	1:A:257:GLY:N	2.74	0.42
1:C:427:GLU:O	1:C:429:PHE:N	2.53	0.42
2:D:369:LEU:C	2:D:369:LEU:HD12	2.44	0.42
2:D:479:LEU:HD23	2:D:479:LEU:HA	1.77	0.42
3:E:187:ARG:O	3:E:188:ASN:HB2	2.20	0.42
3:H:32:LYS:NZ	3:H:118:ASP:HB2	2.35	0.42
1:I:194:GLY:O	1:I:195:HIS:C	2.62	0.42
1:I:370:LEU:C	1:I:372:MET:H	2.28	0.42
2:J:37:GLN:O	2:J:40:ILE:N	2.52	0.42
1:K:439:ARG:HG3	1:K:463:MET:CE	2.50	0.42
2:L:108:ARG:CZ	2:L:477:HIS:CD2	3.02	0.42
2:L:238:ARG:O	2:L:239:VAL:C	2.60	0.42
3:N:32:LYS:NZ	3:N:118:ASP:HB2	2.35	0.42
3:N:39:ASP:OD2	3:N:41:LYS:HB3	2.19	0.42
3:N:64:ALA:CB	3:N:69:ASP:HB2	2.49	0.42
3:O:49:LEU:HD23	3:O:49:LEU:N	2.34	0.42
3:O:184:CYS:C	3:O:185:ASN:HD22	2.28	0.42
1:A:68:LYS:HD3	1:A:68:LYS:O	2.20	0.42
1:A:70:VAL:O	1:A:96:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASN:OD1	1:A:145:ASN:C	2.62	0.42
1:A:300:PHE:CD2	1:A:362:HIS:HB3	2.54	0.42
1:A:358:LEU:HD11	1:A:362:HIS:CE1	2.54	0.42
1:C:256:ASP:CG	1:C:256:ASP:O	2.62	0.42
1:C:342:TYR:O	1:C:343:ARG:C	2.63	0.42
1:C:455:GLY:O	1:C:456:PHE:C	2.62	0.42
2:D:56:ASN:OD1	2:D:59:ARG:NH2	2.41	0.42
2:D:333:SER:O	2:D:334:GLU:C	2.62	0.42
3:E:5:CYS:HB2	3:E:123:PHE:CD1	2.54	0.42
3:E:134:GLY:HA3	8:E:290:SF4:S1	2.60	0.42
3:E:261:MET:O	3:E:265:GLU:HG3	2.20	0.42
3:H:36:VAL:HG22	3:H:86:VAL:HG22	2.02	0.42
3:H:66:THR:N	3:H:69:ASP:OD1	2.53	0.42
2:J:221:ASN:C	2:J:222:LYS:HD2	2.45	0.42
2:J:254:LEU:O	2:J:255:SER:HB3	2.20	0.42
2:J:296:TRP:HB2	2:J:374:ASP:OD1	2.20	0.42
2:J:322:LEU:HB3	2:J:385:GLU:OE2	2.20	0.42
1:K:132:ALA:O	1:K:133:LYS:C	2.63	0.42
1:K:343:ARG:HB3	1:K:344:PRO:HD3	2.02	0.42
2:L:232:THR:HG21	2:L:471:PHE:CD1	2.55	0.42
2:L:436:THR:OG1	2:L:437:ASP:N	2.53	0.42
3:O:67:VAL:C	3:O:69:ASP:N	2.77	0.42
3:O:173:ASN:C	3:O:173:ASN:ND2	2.78	0.42
3:O:184:CYS:CB	3:O:196:ILE:HG13	2.49	0.42
3:P:41:LYS:HD3	3:P:41:LYS:C	2.45	0.42
3:P:153:GLY:O	3:P:154:GLU:HB2	2.20	0.42
3:P:186:SER:HA	3:P:192:GLU:OE1	2.20	0.42
3:P:215:ASN:C	3:P:217:VAL:N	2.77	0.42
1:A:270:LEU:CD1	1:A:293:PRO:HG2	2.50	0.42
2:B:166:ILE:HD13	2:B:181:VAL:HG12	2.02	0.42
2:B:441:PHE:HE2	2:B:501:ILE:HG12	1.85	0.42
1:C:332:LYS:N	1:C:333:PRO:CD	2.82	0.42
1:C:402:ASP:O	1:C:403:ASP:C	2.63	0.42
1:C:425:ILE:C	1:C:427:GLU:H	2.27	0.42
2:D:201:PHE:O	2:D:202:GLU:C	2.63	0.42
2:D:221:ASN:C	2:D:222:LYS:HD2	2.44	0.42
2:D:491:MET:O	2:D:492:GLN:C	2.61	0.42
3:E:217:VAL:HA	3:E:227:VAL:CG2	2.50	0.42
3:G:136:ALA:HB2	3:H:94:GLY:HA2	2.01	0.42
3:G:184:CYS:SG	3:G:210:PHE:CE1	3.04	0.42
3:G:193:ASP:HB3	3:G:210:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:72:TRP:O	1:I:73:GLY:C	2.63	0.42
1:I:368:GLU:C	1:I:370:LEU:H	2.27	0.42
1:I:425:ILE:O	1:I:425:ILE:HG13	2.20	0.42
2:L:118:MET:HA	2:L:130:ASN:HD22	1.84	0.42
3:M:38:CYS:HB2	3:M:126:VAL:HA	2.02	0.42
3:N:33:VAL:CG1	3:N:34:MET:H	2.33	0.42
3:O:60:MET:HE1	3:O:74:ASP:O	2.20	0.42
3:P:269:MET:HA	3:P:274:MET:O	2.20	0.42
1:A:72:TRP:C	1:A:74:PRO:CD	2.93	0.41
1:A:76:LYS:HG2	1:A:257:GLY:O	2.19	0.41
1:A:230:ASN:OD1	1:A:235:ALA:HB3	2.20	0.41
1:A:385:ASP:HA	1:A:388:ASP:OD2	2.19	0.41
2:B:234:LEU:O	2:B:236:ASN:N	2.52	0.41
1:C:39:VAL:HG12	1:C:41:GLN:H	1.85	0.41
1:C:200:ASP:O	1:C:201:ALA:C	2.62	0.41
3:G:3:ARG:NH1	3:G:121:PHE:HZ	2.18	0.41
3:G:107:ASN:HA	3:G:110:GLU:OE1	2.20	0.41
3:G:184:CYS:SG	3:G:210:PHE:HE1	2.43	0.41
1:I:42:SER:C	1:I:44:LYS:H	2.28	0.41
1:I:51:LYS:HA	1:I:189:VAL:HG11	2.01	0.41
1:I:63:ALA:O	1:I:67:SER:N	2.52	0.41
1:I:443:SER:C	1:I:445:ASP:N	2.77	0.41
2:J:84:LYS:HB2	2:J:145:ASP:HB2	2.01	0.41
2:J:391:VAL:HG23	2:J:392:HIS:CD2	2.54	0.41
1:K:467:LEU:HD23	1:K:467:LEU:C	2.44	0.41
2:L:302:LYS:HE2	2:L:306:GLU:OE1	2.20	0.41
3:M:76:LEU:CD1	3:M:86:VAL:HG13	2.50	0.41
3:N:57:ILE:HG13	3:N:75:VAL:HG11	2.01	0.41
3:N:111:GLU:C	3:N:113:GLY:H	2.28	0.41
3:N:165:SER:O	3:N:166:LYS:C	2.63	0.41
3:P:50:HIS:HE1	3:P:229:GLU:OE1	2.03	0.41
1:A:240:ILE:O	1:A:244:GLU:HG3	2.20	0.41
1:A:378:GLY:HA3	1:A:401:TYR:CD2	2.54	0.41
1:A:381:PHE:CZ	5:A:6496:CFM:S2B	3.13	0.41
2:B:359:HIS:O	2:B:360:THR:C	2.62	0.41
2:B:446:SER:C	2:B:448:GLY:N	2.77	0.41
1:C:142:PHE:HE1	2:D:428:TRP:CZ2	2.38	0.41
1:C:259:ILE:CG2	1:C:260:SER:N	2.83	0.41
1:C:370:LEU:C	1:C:372:MET:N	2.78	0.41
1:C:405:THR:OG1	1:C:408:GLU:HG3	2.20	0.41
1:C:458:ILE:O	1:C:459:PHE:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:458:LYS:HG2	2:D:462:PHE:CD2	2.55	0.41
3:E:38:CYS:HB2	3:E:126:VAL:HA	2.01	0.41
3:F:34:MET:O	3:F:122:VAL:HA	2.20	0.41
3:G:172:ALA:HB1	3:G:255:ILE:HD13	2.01	0.41
3:H:100:ARG:HG3	3:H:100:ARG:NH1	2.34	0.41
1:I:350:ARG:HB3	1:I:375:VAL:HG11	2.00	0.41
1:I:467:LEU:HD23	1:I:467:LEU:C	2.45	0.41
2:J:442:MET:HG3	2:J:464:VAL:CG1	2.50	0.41
2:J:442:MET:HG3	2:J:464:VAL:HG12	2.01	0.41
2:J:452:GLN:O	2:J:453:ARG:C	2.62	0.41
1:K:59:ILE:HG23	1:K:426:LYS:HD2	2.02	0.41
1:K:155:PRO:HG3	2:L:153:CYS:HB3	2.01	0.41
3:M:134:GLY:HA3	8:N:2290:SF4:S1	2.60	0.41
3:M:246:LYS:O	3:M:250:ASN:HB2	2.20	0.41
3:O:139:ILE:HG23	3:O:177:VAL:HG11	2.01	0.41
3:O:207:MET:C	3:O:209:HIS:H	2.27	0.41
1:A:42:SER:HB3	1:A:391:MET:CE	2.50	0.41
1:A:219:THR:HG23	1:A:248:ARG:NH2	2.36	0.41
2:B:326:ASP:O	2:B:327:GLU:C	2.63	0.41
2:D:19:ASP:O	2:D:23:MET:HB2	2.19	0.41
2:D:260:VAL:O	2:D:260:VAL:HG22	2.19	0.41
2:D:431:ARG:NH1	2:D:435:PHE:CE2	2.88	0.41
3:E:24:ALA:HB2	3:E:226:THR:HG21	2.02	0.41
3:G:140:ARG:HG3	3:G:171:TYR:CE1	2.56	0.41
3:H:40:PRO:HD2	3:H:127:LEU:HD13	2.03	0.41
3:H:49:LEU:O	3:H:50:HIS:HB2	2.20	0.41
1:I:68:LYS:C	1:I:68:LYS:CD	2.87	0.41
2:J:64:VAL:HG12	2:J:428:TRP:HB2	2.02	0.41
2:J:118:MET:HA	2:J:130:ASN:HD22	1.82	0.41
2:L:221:ASN:C	2:L:222:LYS:HD2	2.45	0.41
2:L:318:ILE:HG12	2:L:320:MET:HG3	2.01	0.41
2:L:394:LEU:HD13	2:L:430:LEU:HB2	2.01	0.41
2:L:431:ARG:O	2:L:434:VAL:CG2	2.67	0.41
2:L:479:LEU:HD23	2:L:479:LEU:HA	1.85	0.41
3:M:32:LYS:HB2	3:M:119:LEU:HA	2.01	0.41
3:M:139:ILE:HG23	3:M:177:VAL:HG11	2.02	0.41
3:N:199:LEU:HD23	3:N:203:LEU:HD23	2.02	0.41
3:O:74:ASP:OD1	3:O:74:ASP:N	2.53	0.41
3:O:199:LEU:C	3:O:199:LEU:HD23	2.46	0.41
3:O:216:VAL:HG11	3:O:236:GLN:HB3	2.02	0.41
1:A:239:ARG:HE	2:B:23:MET:HE1	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:475:ASP:O	2:B:476:ARG:HG2	2.20	0.41
1:C:70:VAL:O	1:C:96:ARG:NH1	2.53	0.41
2:D:234:LEU:O	2:D:236:ASN:N	2.54	0.41
3:E:5:CYS:O	3:E:124:TYR:HD2	2.02	0.41
3:F:20:GLN:HE22	3:F:47:LEU:N	2.17	0.41
3:F:160:ALA:O	3:F:164:ILE:HG13	2.20	0.41
3:G:195:LEU:HA	3:G:271:PHE:CE2	2.54	0.41
8:G:1290:SF4:S2	3:H:134:GLY:N	2.93	0.41
3:H:76:LEU:HD13	3:H:86:VAL:HG13	2.03	0.41
1:I:16:VAL:HG21	1:I:412:PHE:CE1	2.55	0.41
1:I:141:LEU:HB3	2:J:52:TYR:OH	2.19	0.41
1:I:297:TYR:HD2	1:I:299:PHE:CE1	2.38	0.41
1:I:302:PRO:HD3	1:I:456:PHE:CG	2.55	0.41
1:I:378:GLY:HA3	1:I:401:TYR:CD2	2.55	0.41
1:I:433:LYS:HE2	2:J:110:PRO:HD3	2.01	0.41
2:J:369:LEU:C	2:J:369:LEU:HD12	2.46	0.41
2:L:209:THR:O	2:L:213:MET:HG2	2.20	0.41
2:L:277:THR:HB	2:L:279:GLU:OE2	2.20	0.41
3:M:40:PRO:HG2	3:N:130:VAL:HG11	2.00	0.41
3:O:22:LEU:HD13	3:O:243:LEU:HD23	2.02	0.41
3:P:26:LEU:HD12	3:P:26:LEU:HA	1.82	0.41
1:A:72:TRP:O	1:A:73:GLY:C	2.63	0.41
1:A:142:PHE:HE1	2:B:428:TRP:CZ2	2.39	0.41
2:B:83:GLU:O	2:B:84:LYS:C	2.64	0.41
2:B:441:PHE:CD1	2:B:465:PRO:HB2	2.55	0.41
1:C:305:THR:O	1:C:306:ILE:C	2.63	0.41
2:D:82:PHE:O	2:D:83:GLU:C	2.64	0.41
2:D:129:GLN:C	2:D:131:MET:N	2.77	0.41
3:E:23:VAL:O	3:E:24:ALA:C	2.62	0.41
3:E:97:CYS:SG	3:E:134:GLY:HA2	2.61	0.41
3:E:231:ASP:OD1	3:E:233:LYS:HB2	2.20	0.41
3:F:111:GLU:C	3:F:113:GLY:H	2.28	0.41
1:I:57:MET:HB3	2:J:142:TYR:OH	2.20	0.41
1:I:370:LEU:C	1:I:372:MET:N	2.78	0.41
1:I:370:LEU:O	1:I:372:MET:N	2.53	0.41
2:J:431:ARG:NH1	2:J:435:PHE:HE2	2.18	0.41
1:K:137:GLU:CD	2:L:60:GLU:H	2.29	0.41
2:L:456:LEU:O	2:L:459:GLY:N	2.52	0.41
2:L:487:TYR:O	2:L:488:GLU:C	2.63	0.41
3:M:41:LYS:HD3	3:M:41:LYS:O	2.20	0.41
3:M:173:ASN:C	3:M:173:ASN:ND2	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:194:GLU:HA	3:M:197:ILE:CD1	2.50	0.41
3:O:191:ARG:HG2	3:O:194:GLU:OE2	2.20	0.41
3:O:194:GLU:O	3:O:197:ILE:HG13	2.21	0.41
3:P:124:TYR:O	3:P:126:VAL:HG23	2.21	0.41
1:A:42:SER:C	1:A:44:LYS:H	2.27	0.41
1:A:110:VAL:C	1:A:112:MET:H	2.28	0.41
2:B:44:PHE:O	2:B:45:GLN:C	2.61	0.41
2:B:122:ALA:HB1	2:B:126:GLY:O	2.21	0.41
1:C:302:PRO:HD3	1:C:456:PHE:CG	2.56	0.41
1:C:370:LEU:O	1:C:372:MET:N	2.53	0.41
2:D:379:LEU:HD21	2:D:443:ILE:CG2	2.51	0.41
2:D:450:PHE:O	2:D:453:ARG:N	2.54	0.41
3:E:72:LEU:HD13	3:E:112:GLU:HB3	2.03	0.41
3:E:192:GLU:O	3:E:195:LEU:HB3	2.20	0.41
3:F:267:LEU:HD22	3:F:271:PHE:CE2	2.54	0.41
3:H:153:GLY:O	3:H:154:GLU:HB2	2.19	0.41
1:I:42:SER:C	1:I:44:LYS:N	2.77	0.41
1:I:317:ASP:OD1	1:I:319:SER:HB3	2.20	0.41
1:I:465:MET:HB2	2:L:363:HIS:CD2	2.56	0.41
2:J:450:PHE:O	2:J:452:GLN:N	2.53	0.41
1:K:370:LEU:C	1:K:372:MET:H	2.29	0.41
2:L:354:MET:O	2:L:355:MET:C	2.64	0.41
3:O:15:LYS:HZ2	3:O:127:LEU:HA	1.82	0.41
3:O:99:GLY:HA3	3:O:134:GLY:O	2.20	0.41
3:P:187:ARG:HB2	3:P:192:GLU:OE2	2.21	0.41
1:A:81:ILE:HD13	1:A:114:PHE:HB3	2.03	0.41
1:A:155:PRO:O	1:A:159:ILE:HG12	2.20	0.41
1:A:239:ARG:HE	2:B:23:MET:CE	2.34	0.41
1:A:297:TYR:HD2	1:A:299:PHE:CE1	2.38	0.41
1:A:351:VAL:HG13	1:A:420:LEU:HD23	2.03	0.41
1:A:435:GLY:HA3	1:A:475:LEU:HD22	2.03	0.41
2:B:494:LEU:C	2:B:494:LEU:CD2	2.93	0.41
2:D:351:LEU:HD12	2:D:351:LEU:O	2.21	0.41
2:D:369:LEU:HD11	2:D:376:VAL:HG13	2.02	0.41
3:E:166:LYS:HG2	3:E:258:PRO:HB3	2.02	0.41
3:E:173:ASN:ND2	3:E:173:ASN:C	2.77	0.41
3:E:246:LYS:O	3:E:250:ASN:HB2	2.21	0.41
3:F:20:GLN:NE2	3:F:47:LEU:HB2	2.36	0.41
3:G:32:LYS:HB2	3:G:119:LEU:HA	2.01	0.41
3:G:76:LEU:HD13	3:G:86:VAL:HG13	2.02	0.41
3:H:122:VAL:HG13	3:H:122:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:76:LYS:HZ1	2:J:32:GLU:CD	2.29	0.41
1:I:240:ILE:HG23	1:I:241:LEU:N	2.34	0.41
1:I:332:LYS:N	1:I:333:PRO:CD	2.82	0.41
1:I:409:PHE:O	1:I:413:VAL:HG23	2.21	0.41
2:J:127:GLY:C	2:J:129:GLN:N	2.79	0.41
2:J:303:LYS:HB2	2:J:303:LYS:NZ	2.35	0.41
2:J:328:PHE:O	2:J:332:VAL:HG23	2.20	0.41
2:J:330:MET:O	2:J:333:SER:N	2.54	0.41
1:K:57:MET:CE	2:L:113:CYS:N	2.84	0.41
1:K:240:ILE:HG23	1:K:241:LEU:N	2.34	0.41
1:K:284:ARG:HG2	1:K:284:ARG:HH11	1.85	0.41
3:M:185:ASN:N	3:M:185:ASN:ND2	2.68	0.41
3:N:130:VAL:O	3:N:131:VAL:C	2.63	0.41
3:O:86:VAL:HG11	3:O:109:LEU:HD21	2.03	0.41
3:O:106:ILE:HD12	3:O:137:MET:HE1	2.03	0.41
3:O:190:ASP:C	3:O:192:GLU:H	2.28	0.41
3:P:103:ILE:CG2	3:P:104:THR:H	2.34	0.41
1:A:11:SER:O	1:A:15:GLU:HG3	2.21	0.41
1:A:124:VAL:HG12	1:A:125:PHE:CD1	2.56	0.41
1:A:289:LYS:HE3	1:A:290:TYR:OH	2.20	0.41
1:A:443:SER:C	1:A:445:ASP:N	2.78	0.41
2:B:331:LYS:O	2:B:335:ILE:HG13	2.21	0.41
1:C:428:LYS:HA	1:C:438:PHE:CE1	2.55	0.41
2:D:365:LYS:HE2	2:D:501:ILE:HD13	2.03	0.41
2:D:369:LEU:CD1	2:D:376:VAL:HG13	2.51	0.41
3:E:3:ARG:NH1	3:E:121:PHE:HZ	2.19	0.41
3:E:102:VAL:O	3:E:106:ILE:HG13	2.20	0.41
3:F:67:VAL:N	3:F:69:ASP:OD2	2.52	0.41
3:H:243:LEU:O	3:H:247:VAL:HG23	2.21	0.41
1:I:144:LEU:HD11	2:J:43:VAL:HG21	2.02	0.41
1:I:239:ARG:HG2	2:J:23:MET:SD	2.60	0.41
1:I:299:PHE:HB3	1:I:452:GLY:H	1.85	0.41
1:I:323:LYS:O	1:I:327:VAL:HG23	2.21	0.41
2:J:64:VAL:CG1	2:J:428:TRP:HB2	2.51	0.41
2:J:124:VAL:HG23	2:J:125:PHE:N	2.36	0.41
2:J:246:GLU:OE2	2:J:343:SER:HB2	2.20	0.41
2:J:323:ASP:O	2:J:326:ASP:HB2	2.20	0.41
2:J:350:ARG:O	2:J:351:LEU:C	2.63	0.41
1:K:194:GLY:O	1:K:195:HIS:C	2.64	0.41
1:K:219:THR:HG23	1:K:248:ARG:NH2	2.36	0.41
1:K:428:LYS:HA	1:K:438:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:233:TYR:HB2	2:L:236:ASN:ND2	2.36	0.41
2:L:295:PRO:C	2:L:297:HIS:H	2.28	0.41
2:L:306:GLU:O	2:L:310:LYS:HA	2.21	0.41
3:M:175:GLY:O	3:M:178:ARG:NH2	2.48	0.41
3:P:148:TYR:CE1	3:P:180:GLY:HA3	2.56	0.41
1:A:164:GLU:H	1:A:164:GLU:CD	2.28	0.41
1:A:203:ARG:NH1	1:A:204:ASP:OD1	2.54	0.41
1:A:239:ARG:NH2	2:B:27:LYS:HB2	2.36	0.41
1:A:370:LEU:C	1:A:372:MET:H	2.28	0.41
1:A:370:LEU:C	1:A:372:MET:N	2.77	0.41
1:A:444:TRP:CE3	1:A:444:TRP:CA	3.04	0.41
2:B:394:LEU:HD13	2:B:430:LEU:HB2	2.02	0.41
1:C:62:CYS:O	1:C:63:ALA:C	2.63	0.41
1:C:155:PRO:HG3	2:D:153:CYS:HB3	2.01	0.41
1:C:368:GLU:C	1:C:370:LEU:N	2.78	0.41
2:D:209:THR:O	2:D:213:MET:HG2	2.20	0.41
2:D:293:LEU:O	2:D:318:ILE:HA	2.21	0.41
2:D:359:HIS:CG	2:D:360:THR:H	2.38	0.41
3:E:21:ASN:HB3	3:E:240:TYR:CD1	2.55	0.41
3:E:32:LYS:CB	3:E:119:LEU:HA	2.50	0.41
3:E:92:GLU:O	3:E:93:PRO:C	2.63	0.41
3:F:45:THR:O	3:F:46:ARG:C	2.63	0.41
3:F:59:GLU:O	3:F:63:GLU:HG3	2.21	0.41
3:F:66:THR:N	3:F:69:ASP:OD1	2.54	0.41
3:F:127:LEU:HD23	3:F:129:ASP:N	2.36	0.41
3:F:169:VAL:C	3:F:171:TYR:N	2.79	0.41
3:G:43:ASP:HB3	3:G:46:ARG:CZ	2.50	0.41
1:I:92:SER:HB3	2:J:98:TYR:HE1	1.83	0.41
1:I:108:ALA:C	1:I:109:PHE:CG	2.98	0.41
1:I:110:VAL:C	1:I:112:MET:H	2.29	0.41
1:I:144:LEU:HD22	2:J:35:TYR:CD1	2.56	0.41
1:I:256:ASP:O	1:I:256:ASP:CG	2.63	0.41
1:I:339:VAL:O	1:I:343:ARG:CB	2.65	0.41
1:I:389:ARG:NH1	1:I:389:ARG:CG	2.78	0.41
2:J:457:HIS:ND1	2:L:512:MET:HB3	2.35	0.41
1:K:133:LYS:O	1:K:134:LEU:C	2.64	0.41
1:K:339:VAL:O	1:K:343:ARG:CB	2.65	0.41
2:L:228:PRO:HD2	2:L:254:LEU:O	2.21	0.41
2:L:369:LEU:CD1	2:L:376:VAL:HG13	2.51	0.41
2:L:512:MET:O	2:L:513:GLN:C	2.64	0.41
3:M:50:HIS:CE1	3:M:229:GLU:OE1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:212:PRO:HG2	3:M:236:GLN:HE22	1.86	0.41
3:N:33:VAL:HG12	3:N:34:MET:H	1.85	0.41
3:N:242:ALA:O	3:N:246:LYS:HG3	2.20	0.41
3:O:4:GLN:HG2	3:O:122:VAL:HG21	2.03	0.41
3:O:57:ILE:CG1	3:O:75:VAL:HG11	2.50	0.41
3:O:127:LEU:HB3	3:O:135:PHE:CE1	2.56	0.41
3:O:158:MET:HE1	3:O:195:LEU:HG	2.03	0.41
3:O:172:ALA:HB1	3:O:255:ILE:HD13	2.02	0.41
3:O:173:ASN:N	3:O:173:ASN:HD22	2.18	0.41
3:P:169:VAL:C	3:P:171:TYR:N	2.78	0.41
1:A:351:VAL:HG22	1:A:420:LEU:HD22	2.03	0.41
2:B:389:GLU:O	2:B:391:VAL:HG13	2.21	0.41
1:C:85:PRO:CD	1:C:155:PRO:HG2	2.51	0.41
2:D:394:LEU:HD23	2:D:394:LEU:C	2.45	0.41
3:F:5:CYS:O	3:F:123:PHE:HA	2.21	0.41
3:G:6:ALA:HB1	3:G:8:TYR:HE1	1.86	0.41
3:H:3:ARG:HH21	3:H:146:GLU:CD	2.29	0.41
3:H:103:ILE:CG2	3:H:104:THR:N	2.82	0.41
1:I:100:TYR:CE1	1:I:110:VAL:HB	2.56	0.41
1:I:385:ASP:HA	1:I:388:ASP:OD2	2.20	0.41
1:I:453:PHE:C	1:I:455:GLY:N	2.77	0.41
1:I:465:MET:CG	1:I:466:THR:N	2.84	0.41
2:J:283:ASP:O	2:J:285:PRO:N	2.54	0.41
2:J:340:ILE:HD12	1:K:479:TRP:CD2	2.56	0.41
1:K:39:VAL:HG12	1:K:41:GLN:H	1.86	0.41
1:K:83:HIS:CD2	1:K:156:ILE:HG12	2.56	0.41
1:K:435:GLY:CA	1:K:475:LEU:HD22	2.51	0.41
3:N:228:ILE:HD13	3:N:228:ILE:HA	1.93	0.41
3:O:38:CYS:CB	3:O:126:VAL:HG22	2.51	0.41
3:O:100:ARG:HE	3:O:101:GLY:N	2.18	0.41
3:O:127:LEU:HD12	3:O:135:PHE:CZ	2.56	0.41
3:P:57:ILE:HG22	3:P:58:MET:N	2.36	0.41
3:P:97:CYS:O	3:P:98:ALA:C	2.64	0.41
3:P:285:THR:C	3:P:287:GLU:H	2.28	0.41
1:A:83:HIS:CD2	1:A:156:ILE:HG12	2.55	0.40
1:A:383:HIS:O	1:A:386:ASP:HB2	2.20	0.40
2:D:297:HIS:CD2	2:D:297:HIS:O	2.74	0.40
2:D:449:LYS:HE3	2:D:449:LYS:HB2	1.90	0.40
3:F:49:LEU:O	3:F:50:HIS:CB	2.70	0.40
3:H:208:ILE:HG23	3:H:209:HIS:H	1.86	0.40
1:I:101:ILE:HG12	1:I:236:TRP:CZ2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:265:THR:N	1:I:266:PRO:CD	2.84	0.40
2:J:450:PHE:C	2:J:452:GLN:N	2.76	0.40
2:L:131:MET:HG2	2:L:165:PHE:HB3	2.03	0.40
3:M:36:VAL:HA	3:M:86:VAL:HG23	2.02	0.40
3:O:206:GLN:OE1	3:O:252:LEU:HD23	2.21	0.40
3:O:212:PRO:HG3	3:O:239:GLU:HG3	2.02	0.40
3:O:282:VAL:HG23	3:O:283:GLY:N	2.37	0.40
1:A:59:ILE:N	1:A:59:ILE:CD1	2.80	0.40
1:A:413:VAL:HG21	1:A:431:PHE:CE1	2.56	0.40
1:C:251:ALA:HB2	1:C:261:GLU:O	2.22	0.40
1:C:390:THR:O	1:C:392:LYS:N	2.54	0.40
2:D:84:LYS:HB2	2:D:145:ASP:HB2	2.03	0.40
2:D:84:LYS:HA	2:D:272:TYR:CD1	2.56	0.40
2:D:295:PRO:C	2:D:297:HIS:N	2.80	0.40
2:D:309:TRP:O	2:D:310:LYS:HB2	2.22	0.40
2:D:318:ILE:HG23	2:D:318:ILE:O	2.21	0.40
2:D:323:ASP:O	2:D:326:ASP:HB2	2.22	0.40
2:D:446:SER:C	2:D:448:GLY:N	2.77	0.40
3:F:41:LYS:HD3	3:F:41:LYS:C	2.47	0.40
3:G:63:GLU:HB3	3:G:64:ALA:H	1.73	0.40
3:G:199:LEU:HD23	3:G:199:LEU:O	2.21	0.40
3:H:26:LEU:HD12	3:H:26:LEU:HA	1.84	0.40
1:I:65:ALA:O	1:I:70:VAL:HG23	2.22	0.40
2:J:105:ARG:HB3	2:J:474:PHE:CD1	2.56	0.40
1:K:73:GLY:N	1:K:74:PRO:CD	2.83	0.40
1:K:253:TRP:HA	1:K:254:SER:HA	1.65	0.40
1:K:344:PRO:C	1:K:346:LEU:H	2.29	0.40
1:K:350:ARG:HA	1:K:373:GLU:O	2.21	0.40
2:L:295:PRO:C	2:L:297:HIS:N	2.79	0.40
2:L:468:ARG:HD2	2:L:476:ARG:HG3	2.01	0.40
3:M:26:LEU:HB3	3:M:31:LYS:HB2	2.04	0.40
3:M:57:ILE:HG12	3:M:75:VAL:HG21	2.03	0.40
3:M:140:ARG:HG3	3:M:171:TYR:CE1	2.56	0.40
3:M:187:ARG:O	3:M:188:ASN:HB2	2.21	0.40
3:N:55:ASN:HD22	3:N:77:LYS:NZ	2.19	0.40
3:N:261:MET:O	3:N:265:GLU:HG3	2.20	0.40
3:O:184:CYS:SG	3:O:210:PHE:CE1	3.11	0.40
3:O:251:LYS:HE3	3:O:251:LYS:HB3	1.92	0.40
3:P:76:LEU:CD1	3:P:86:VAL:HG13	2.51	0.40
3:P:199:LEU:CD2	3:P:203:LEU:HD23	2.51	0.40
1:A:199:ASN:O	1:A:200:ASP:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ARG:N	1:A:344:PRO:CD	2.85	0.40
1:A:444:TRP:O	1:A:445:ASP:C	2.64	0.40
1:A:462:ASP:HA	1:A:465:MET:HE2	2.03	0.40
2:B:59:ARG:HD3	2:B:62:LEU:HD23	2.03	0.40
2:B:194:VAL:HG23	2:B:195:THR:N	2.36	0.40
2:B:351:LEU:HD12	2:B:351:LEU:O	2.21	0.40
2:B:442:MET:HG3	2:B:464:VAL:HG12	2.04	0.40
1:C:107:ASN:HD21	2:D:34:LYS:HE2	1.86	0.40
1:C:275:CYS:HB3	1:C:278:SER:HG	1.84	0.40
1:C:304:LYS:HD3	1:C:304:LYS:HA	1.95	0.40
3:E:57:ILE:HD12	3:E:105:ALA:CB	2.51	0.40
3:F:199:LEU:O	3:F:203:LEU:HD23	2.20	0.40
3:G:183:ILE:HG12	3:G:208:ILE:CG2	2.52	0.40
1:I:308:SER:O	1:I:312:ILE:HG13	2.21	0.40
1:I:403:ASP:CG	1:I:403:ASP:O	2.64	0.40
2:J:21:LYS:HE2	2:J:21:LYS:HB3	1.87	0.40
2:J:71:GLN:HA	2:J:193:HIS:HA	2.04	0.40
2:J:226:ILE:O	2:J:253:LEU:HD12	2.21	0.40
1:K:222:ASP:HA	1:K:248:ARG:O	2.21	0.40
1:K:339:VAL:CG1	1:K:343:ARG:HB2	2.50	0.40
1:K:358:LEU:HD11	1:K:362:HIS:CE1	2.56	0.40
2:L:190:VAL:O	2:L:191:GLY:O	2.40	0.40
3:M:63:GLU:HB3	3:M:64:ALA:H	1.75	0.40
3:M:195:LEU:HD12	3:M:267:LEU:CD2	2.51	0.40
3:M:229:GLU:O	3:N:285:THR:HG22	2.22	0.40
3:N:40:PRO:HD2	3:N:127:LEU:HD13	2.03	0.40
3:P:206:GLN:HG2	3:P:252:LEU:HD13	2.03	0.40
1:A:405:THR:O	1:A:406:GLY:C	2.64	0.40
2:B:135:LEU:HD23	2:B:135:LEU:HA	1.91	0.40
1:C:66:GLY:C	1:C:70:VAL:HB	2.46	0.40
1:C:206:VAL:O	1:C:207:LEU:C	2.64	0.40
1:C:444:TRP:CE3	1:C:444:TRP:CA	3.04	0.40
2:D:70:CYS:SG	2:D:72:PRO:CG	3.09	0.40
2:D:328:PHE:O	2:D:332:VAL:HG23	2.21	0.40
3:E:173:ASN:HD22	3:E:173:ASN:C	2.28	0.40
3:E:206:GLN:OE1	3:E:252:LEU:HD23	2.21	0.40
3:E:212:PRO:HG3	3:E:239:GLU:HG3	2.04	0.40
3:F:17:THR:O	3:F:18:THR:C	2.65	0.40
3:G:36:VAL:HA	3:G:86:VAL:HG23	2.02	0.40
3:G:60:MET:HE1	3:G:74:ASP:HB3	2.03	0.40
3:G:102:VAL:O	3:G:106:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:278:ASP:OD1	3:G:281:ILE:HB	2.22	0.40
3:G:283:GLY:O	3:H:225:MET:SD	2.79	0.40
3:H:199:LEU:CD2	3:H:203:LEU:HD23	2.50	0.40
1:I:297:TYR:HD2	1:I:299:PHE:CD1	2.40	0.40
2:J:359:HIS:O	2:J:362:LEU:N	2.55	0.40
2:J:425:LYS:HA	2:J:425:LYS:HD3	1.96	0.40
1:K:63:ALA:O	1:K:67:SER:N	2.53	0.40
1:K:72:TRP:CZ2	1:K:202:VAL:HG22	2.57	0.40
1:K:124:VAL:HG12	1:K:125:PHE:CD1	2.56	0.40
1:K:253:TRP:CZ3	1:K:282:ILE:HG12	2.56	0.40
1:K:443:SER:C	1:K:445:ASP:N	2.78	0.40
2:L:21:LYS:HE2	2:L:21:LYS:HB3	1.92	0.40
3:N:59:GLU:O	3:N:63:GLU:HG3	2.21	0.40
3:O:41:LYS:O	3:O:42:ALA:HB3	2.21	0.40
1:A:113:ASN:HD22	2:B:66:PRO:HD2	1.86	0.40
1:C:208:GLY:HA2	1:C:211:ASP:OD1	2.21	0.40
1:C:449:PRO:O	1:C:450:TYR:HD1	2.05	0.40
2:D:221:ASN:O	2:D:222:LYS:HB2	2.22	0.40
3:E:22:LEU:HD13	3:E:243:LEU:HD23	2.03	0.40
3:E:79:GLY:O	3:E:80:TYR:C	2.65	0.40
3:E:100:ARG:HE	3:E:101:GLY:N	2.20	0.40
3:E:202:LYS:HE3	3:E:202:LYS:HB3	1.90	0.40
3:G:50:HIS:CE1	3:G:229:GLU:OE1	2.72	0.40
3:G:161:ALA:HA	3:G:164:ILE:HD12	2.03	0.40
1:I:12:LEU:O	1:I:13:ILE:C	2.65	0.40
1:I:346:LEU:HB3	1:I:372:MET:SD	2.61	0.40
2:J:4:GLN:O	2:J:7:LYS:N	2.51	0.40
2:J:449:LYS:HE3	2:J:449:LYS:HB2	1.91	0.40
2:J:494:LEU:C	2:J:494:LEU:CD2	2.94	0.40
1:K:8:GLU:O	1:K:11:SER:HB3	2.21	0.40
1:K:12:LEU:O	1:K:13:ILE:C	2.64	0.40
2:L:71:GLN:OE1	2:L:186:THR:HA	2.22	0.40
2:L:83:GLU:O	2:L:84:LYS:C	2.63	0.40
2:L:348:ARG:O	2:L:350:ARG:N	2.54	0.40
2:L:359:HIS:CG	2:L:360:THR:N	2.90	0.40
3:M:24:ALA:HB2	3:M:226:THR:HG21	2.02	0.40
3:N:43:ASP:N	3:N:43:ASP:OD1	2.54	0.40
3:O:214:ASP:CG	3:O:216:VAL:HG12	2.47	0.40
3:O:216:VAL:HG22	3:O:227:VAL:HG13	2.03	0.40
3:P:221:GLU:O	3:P:224:ARG:N	2.48	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	475/491 (97%)	364 (77%)	96 (20%)	15 (3%)	3	21
1	C	475/491 (97%)	358 (75%)	102 (22%)	15 (3%)	3	21
1	I	475/491 (97%)	357 (75%)	104 (22%)	14 (3%)	3	24
1	K	475/491 (97%)	364 (77%)	99 (21%)	12 (2%)	4	27
2	B	520/522 (100%)	423 (81%)	74 (14%)	23 (4%)	2	15
2	D	520/522 (100%)	417 (80%)	82 (16%)	21 (4%)	2	17
2	J	520/522 (100%)	421 (81%)	74 (14%)	25 (5%)	2	14
2	L	520/522 (100%)	423 (81%)	75 (14%)	22 (4%)	2	16
3	E	284/289 (98%)	219 (77%)	50 (18%)	15 (5%)	1	12
3	F	287/289 (99%)	228 (79%)	43 (15%)	16 (6%)	1	11
3	G	284/289 (98%)	221 (78%)	47 (16%)	16 (6%)	1	11
3	H	287/289 (99%)	224 (78%)	50 (17%)	13 (4%)	2	15
3	M	284/289 (98%)	223 (78%)	47 (16%)	14 (5%)	1	13
3	N	287/289 (99%)	230 (80%)	44 (15%)	13 (4%)	2	15
3	O	284/289 (98%)	221 (78%)	48 (17%)	15 (5%)	1	12
3	P	287/289 (99%)	228 (79%)	45 (16%)	14 (5%)	1	13
All	All	6264/6364 (98%)	4921 (79%)	1080 (17%)	263 (4%)	2	16

All (263) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
2	B	296	TRP
1	C	22	GLU
3	E	118	ASP
3	E	208	ILE
3	E	224	ARG

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Mol	Chain	Res	Type
3	E	282	VAL
3	F	131	VAL
3	G	118	ASP
3	G	208	ILE
3	G	224	ARG
3	G	282	VAL
3	H	131	VAL
1	I	22	GLU
2	J	296	TRP
1	K	22	GLU
3	M	118	ASP
3	M	208	ILE
3	M	224	ARG
3	M	282	VAL
3	N	131	VAL
3	O	118	ASP
3	O	208	ILE
3	O	224	ARG
3	O	282	VAL
3	P	131	VAL
1	A	43	LYS
1	A	87	GLY
1	A	207	LEU
1	A	345	ARG
2	B	5	VAL
2	B	38	ASP
2	B	117	SER
2	B	159	GLY
2	B	207	TYR
1	C	43	LYS
1	C	87	GLY
1	C	391	MET
1	C	428	LYS
2	D	5	VAL
2	D	38	ASP
2	D	117	SER
2	D	159	GLY
2	D	207	TYR
2	D	212	SER
2	D	296	TRP
3	E	283	GLY
3	F	43	ASP

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Mol	Chain	Res	Type
3	F	67	VAL
3	F	116	GLU
3	F	279	GLU
3	G	283	GLY
3	H	43	ASP
3	H	67	VAL
3	H	116	GLU
3	H	170	LYS
3	H	279	GLU
1	I	43	LYS
1	I	87	GLY
1	I	345	ARG
1	I	428	LYS
2	J	5	VAL
2	J	38	ASP
2	J	117	SER
2	J	159	GLY
2	J	207	TYR
1	K	43	LYS
1	K	87	GLY
1	K	428	LYS
2	L	5	VAL
2	L	38	ASP
2	L	117	SER
2	L	121	ASP
2	L	159	GLY
2	L	207	TYR
2	L	296	TRP
3	N	43	ASP
3	N	67	VAL
3	N	116	GLU
3	N	117	ASP
3	N	279	GLU
3	O	155	MET
3	O	283	GLY
3	P	43	ASP
3	P	67	VAL
3	P	116	GLU
3	P	117	ASP
3	P	172	ALA
3	P	279	GLU
1	A	428	LYS

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Mol	Chain	Res	Type
2	B	11	SER
2	B	121	ASP
2	B	212	SER
2	B	235	GLY
2	B	255	SER
2	B	497	LEU
1	C	207	LEU
1	C	345	ARG
2	D	11	SER
2	D	15	PHE
2	D	121	ASP
2	D	235	GLY
2	D	255	SER
3	E	93	PRO
3	E	155	MET
3	E	209	HIS
3	E	284	LYS
3	F	88	SER
3	F	117	ASP
3	F	170	LYS
3	F	172	ALA
3	G	93	PRO
3	G	155	MET
3	G	180	GLY
3	G	186	SER
3	G	209	HIS
3	G	279	GLU
3	H	64	ALA
3	H	117	ASP
1	I	94	ALA
1	I	207	LEU
1	I	391	MET
2	J	11	SER
2	J	121	ASP
2	J	155	ALA
2	J	176	PRO
2	J	255	SER
2	J	497	LEU
1	K	207	LEU
1	K	345	ARG
1	K	391	MET
2	L	11	SER

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Mol	Chain	Res	Type
2	L	189	PHE
2	L	191	GLY
2	L	212	SER
2	L	255	SER
3	M	93	PRO
3	M	155	MET
3	M	180	GLY
3	M	186	SER
3	M	209	HIS
3	M	279	GLU
3	N	64	ALA
3	N	170	LYS
3	N	172	ALA
3	O	68	GLU
3	O	93	PRO
3	O	279	GLU
3	O	284	LYS
3	P	170	LYS
2	B	176	PRO
2	B	189	PHE
1	C	94	ALA
2	D	189	PHE
3	E	180	GLY
3	E	186	SER
3	E	279	GLU
3	G	174	SER
3	H	42	ALA
3	H	58	MET
3	H	68	GLU
3	H	172	ALA
1	I	117	ASP
2	J	15	PHE
2	J	154	MET
2	J	212	SER
2	J	235	GLY
2	J	498	VAL
2	J	514	ALA
1	K	165	SER
1	K	464	ASP
2	L	155	ALA
2	L	176	PRO
2	L	497	LEU

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Mol	Chain	Res	Type
2	L	514	ALA
3	M	174	SER
3	N	42	ALA
3	N	68	GLU
3	N	88	SER
3	O	174	SER
3	O	180	GLY
3	O	186	SER
3	O	209	HIS
3	P	64	ALA
1	A	35	ASN
1	A	165	SER
1	A	166	VAL
1	A	391	MET
2	B	154	MET
2	B	155	ALA
2	B	199	ASN
2	B	514	ALA
1	C	99	TYR
2	D	155	ALA
2	D	497	LEU
2	D	514	ALA
3	E	174	SER
3	F	58	MET
3	F	64	ALA
3	F	68	GLU
1	I	35	ASN
1	I	356	GLY
2	J	199	ASN
2	J	360	THR
2	L	154	MET
3	M	53	ALA
3	M	230	TYR
3	M	283	GLY
3	O	53	ALA
3	P	42	ALA
3	P	68	GLU
1	A	167	SER
1	A	169	VAL
2	B	191	GLY
2	B	373	PRO
2	B	498	VAL

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Mol	Chain	Res	Type
1	C	117	ASP
2	D	154	MET
2	D	176	PRO
2	D	360	THR
3	F	42	ALA
3	G	53	ALA
2	J	189	PHE
2	J	373	PRO
1	K	169	VAL
2	L	373	PRO
1	A	371	GLY
1	C	169	VAL
3	F	93	PRO
3	G	65	GLY
1	K	166	VAL
1	C	160	GLY
2	D	498	VAL
3	F	137	MET
2	J	284	ALA
2	J	390	PRO
1	K	37	PRO
3	P	93	PRO
1	A	37	PRO
1	A	356	GLY
1	C	37	PRO
1	C	166	VAL
2	D	373	PRO
3	E	259	ILE
3	G	258	PRO
3	H	130	VAL
2	L	349	GLY
2	L	498	VAL
3	P	137	MET
2	B	390	PRO
2	B	451	ILE
1	C	356	GLY
3	E	65	GLY
3	F	130	VAL
1	I	166	VAL
1	I	169	VAL
2	J	191	GLY
2	L	284	ALA

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Mol	Chain	Res	Type
3	N	130	VAL
3	P	130	VAL
3	G	96	GLY
1	I	37	PRO
2	L	235	GLY

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	407/414 (98%)	393 (97%)	14 (3%)	32	64
1	C	407/414 (98%)	394 (97%)	13 (3%)	34	65
1	I	407/414 (98%)	393 (97%)	14 (3%)	32	64
1	K	407/414 (98%)	395 (97%)	12 (3%)	37	67
2	B	454/454 (100%)	436 (96%)	18 (4%)	28	61
2	D	454/454 (100%)	436 (96%)	18 (4%)	28	61
2	J	454/454 (100%)	437 (96%)	17 (4%)	30	63
2	L	454/454 (100%)	436 (96%)	18 (4%)	28	61
3	E	230/233 (99%)	216 (94%)	14 (6%)	17	49
3	F	233/233 (100%)	219 (94%)	14 (6%)	17	50
3	G	230/233 (99%)	216 (94%)	14 (6%)	17	49
3	H	233/233 (100%)	218 (94%)	15 (6%)	16	48
3	M	230/233 (99%)	216 (94%)	14 (6%)	17	49
3	N	233/233 (100%)	216 (93%)	17 (7%)	13	43
3	O	230/233 (99%)	216 (94%)	14 (6%)	17	49
3	P	233/233 (100%)	216 (93%)	17 (7%)	13	43
All	All	5296/5336 (99%)	5053 (95%)	243 (5%)	24	58

All (243) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	77	ASP
1	A	98	ASN
1	A	109	PHE
1	A	128	ASP
1	A	145	ASN
1	A	161	ASP
1	A	219	THR
1	A	271	ASN
1	A	277	ARG
1	A	362	HIS
1	A	372	MET
1	A	444	TRP
1	A	445	ASP
2	B	4	GLN
2	B	7	LYS
2	B	19	ASP
2	B	23	MET
2	B	45	GLN
2	B	172	GLU
2	B	178	GLU
2	B	202	GLU
2	B	252	SER
2	B	258	GLU
2	B	263	THR
2	B	268	GLN
2	B	279	GLU
2	B	290	THR
2	B	303	LYS
2	B	391	VAL
2	B	400	LYS
2	B	483	THR
1	C	59	ILE
1	C	77	ASP
1	C	88	CYS
1	C	98	ASN
1	C	128	ASP
1	C	219	THR
1	C	271	ASN
1	C	277	ARG
1	C	360	PRO
1	C	362	HIS
1	C	372	MET

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Mol	Chain	Res	Type
1	C	444	TRP
1	C	445	ASP
2	D	4	GLN
2	D	7	LYS
2	D	19	ASP
2	D	23	MET
2	D	45	GLN
2	D	172	GLU
2	D	178	GLU
2	D	202	GLU
2	D	252	SER
2	D	258	GLU
2	D	263	THR
2	D	268	GLN
2	D	270	ARG
2	D	290	THR
2	D	303	LYS
2	D	391	VAL
2	D	400	LYS
2	D	483	THR
3	E	20	GLN
3	E	28	GLU
3	E	52	LYS
3	E	58	MET
3	E	93	PRO
3	E	100	ARG
3	E	129	ASP
3	E	137	MET
3	E	146	GLU
3	E	173	ASN
3	E	197	ILE
3	E	261	MET
3	E	262	ASP
3	E	278	ASP
3	F	68	GLU
3	F	69	ASP
3	F	70	LEU
3	F	72	LEU
3	F	74	ASP
3	F	85	CYS
3	F	116	GLU
3	F	122	VAL

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Mol	Chain	Res	Type
3	F	206	GLN
3	F	225	MET
3	F	252	LEU
3	F	261	MET
3	F	270	GLU
3	F	276	VAL
3	G	20	GLN
3	G	28	GLU
3	G	52	LYS
3	G	58	MET
3	G	93	PRO
3	G	100	ARG
3	G	129	ASP
3	G	137	MET
3	G	173	ASN
3	G	185	ASN
3	G	197	ILE
3	G	261	MET
3	G	262	ASP
3	G	278	ASP
3	H	68	GLU
3	H	69	ASP
3	H	70	LEU
3	H	72	LEU
3	H	74	ASP
3	H	85	CYS
3	H	116	GLU
3	H	122	VAL
3	H	206	GLN
3	H	225	MET
3	H	252	LEU
3	H	261	MET
3	H	266	GLU
3	H	270	GLU
3	H	276	VAL
1	I	5	SER
1	I	59	ILE
1	I	77	ASP
1	I	88	CYS
1	I	98	ASN
1	I	128	ASP
1	I	219	THR

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Mol	Chain	Res	Type
1	I	271	ASN
1	I	277	ARG
1	I	360	PRO
1	I	362	HIS
1	I	372	MET
1	I	444	TRP
1	I	445	ASP
2	J	4	GLN
2	J	7	LYS
2	J	19	ASP
2	J	23	MET
2	J	45	GLN
2	J	172	GLU
2	J	178	GLU
2	J	202	GLU
2	J	252	SER
2	J	258	GLU
2	J	263	THR
2	J	268	GLN
2	J	290	THR
2	J	303	LYS
2	J	391	VAL
2	J	400	LYS
2	J	483	THR
1	K	5	SER
1	K	59	ILE
1	K	77	ASP
1	K	98	ASN
1	K	128	ASP
1	K	271	ASN
1	K	277	ARG
1	K	360	PRO
1	K	362	HIS
1	K	372	MET
1	K	444	TRP
1	K	445	ASP
2	L	4	GLN
2	L	7	LYS
2	L	19	ASP
2	L	23	MET
2	L	45	GLN
2	L	172	GLU

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Mol	Chain	Res	Type
2	L	178	GLU
2	L	202	GLU
2	L	222	LYS
2	L	252	SER
2	L	258	GLU
2	L	263	THR
2	L	268	GLN
2	L	290	THR
2	L	303	LYS
2	L	391	VAL
2	L	400	LYS
2	L	483	THR
3	M	20	GLN
3	M	28	GLU
3	M	52	LYS
3	M	58	MET
3	M	100	ARG
3	M	129	ASP
3	M	137	MET
3	M	146	GLU
3	M	173	ASN
3	M	185	ASN
3	M	197	ILE
3	M	261	MET
3	M	262	ASP
3	M	278	ASP
3	N	18	THR
3	N	68	GLU
3	N	69	ASP
3	N	70	LEU
3	N	72	LEU
3	N	74	ASP
3	N	85	CYS
3	N	116	GLU
3	N	122	VAL
3	N	206	GLN
3	N	225	MET
3	N	252	LEU
3	N	261	MET
3	N	262	ASP
3	N	266	GLU
3	N	270	GLU

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Mol	Chain	Res	Type
3	N	276	VAL
3	O	20	GLN
3	O	28	GLU
3	O	49	LEU
3	O	52	LYS
3	O	58	MET
3	O	93	PRO
3	O	100	ARG
3	O	129	ASP
3	O	137	MET
3	O	173	ASN
3	O	185	ASN
3	O	197	ILE
3	O	261	MET
3	O	262	ASP
3	P	18	THR
3	P	68	GLU
3	P	69	ASP
3	P	70	LEU
3	P	72	LEU
3	P	74	ASP
3	P	85	CYS
3	P	116	GLU
3	P	122	VAL
3	P	206	GLN
3	P	225	MET
3	P	252	LEU
3	P	261	MET
3	P	262	ASP
3	P	266	GLU
3	P	270	GLU
3	P	276	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	31	HIS
1	A	35	ASN
1	A	49	ASN
1	A	53	GLN
1	A	98	ASN

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Mol	Chain	Res	Type
1	A	107	ASN
1	A	113	ASN
1	A	432	GLN
2	B	37	GLN
2	B	45	GLN
2	B	104	ASN
2	B	128	GLN
2	B	137	ASN
2	B	225	ASN
2	B	268	GLN
2	B	278	GLN
2	B	286	ASN
2	B	499	ASN
2	B	513	GLN
2	B	519	HIS
1	C	14	GLN
1	C	31	HIS
1	C	35	ASN
1	C	49	ASN
1	C	53	GLN
1	C	107	ASN
1	C	113	ASN
1	C	271	ASN
1	C	432	GLN
2	D	37	GLN
2	D	45	GLN
2	D	104	ASN
2	D	128	GLN
2	D	225	ASN
2	D	268	GLN
2	D	278	GLN
2	D	286	ASN
2	D	478	HIS
2	D	499	ASN
2	D	513	GLN
2	D	519	HIS
3	E	50	HIS
3	E	107	ASN
3	E	142	ASN
3	E	162	ASN
3	E	173	ASN
3	E	185	ASN

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Mol	Chain	Res	Type
3	E	188	ASN
3	E	236	GLN
3	F	20	GLN
3	F	50	HIS
3	F	54	GLN
3	F	55	ASN
3	F	142	ASN
3	F	145	GLN
3	F	162	ASN
3	F	185	ASN
3	F	201	ASN
3	F	206	GLN
3	G	50	HIS
3	G	107	ASN
3	G	142	ASN
3	G	162	ASN
3	G	173	ASN
3	G	185	ASN
3	G	188	ASN
3	G	236	GLN
3	H	20	GLN
3	H	50	HIS
3	H	55	ASN
3	H	145	GLN
3	H	162	ASN
3	H	185	ASN
3	H	201	ASN
1	I	14	GLN
1	I	35	ASN
1	I	49	ASN
1	I	53	GLN
1	I	98	ASN
1	I	107	ASN
1	I	113	ASN
1	I	271	ASN
1	I	432	GLN
2	J	37	GLN
2	J	45	GLN
2	J	71	GLN
2	J	104	ASN
2	J	128	GLN
2	J	137	ASN

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Mol	Chain	Res	Type
2	J	225	ASN
2	J	268	GLN
2	J	278	GLN
2	J	286	ASN
2	J	478	HIS
2	J	499	ASN
2	J	513	GLN
2	J	519	HIS
1	K	14	GLN
1	K	31	HIS
1	K	35	ASN
1	K	49	ASN
1	K	53	GLN
1	K	107	ASN
1	K	113	ASN
1	K	362	HIS
1	K	432	GLN
2	L	37	GLN
2	L	45	GLN
2	L	104	ASN
2	L	128	GLN
2	L	137	ASN
2	L	168	ASN
2	L	225	ASN
2	L	268	GLN
2	L	278	GLN
2	L	286	ASN
2	L	294	GLN
2	L	478	HIS
2	L	499	ASN
2	L	513	GLN
2	L	519	HIS
3	M	4	GLN
3	M	50	HIS
3	M	54	GLN
3	M	107	ASN
3	M	142	ASN
3	M	162	ASN
3	M	173	ASN
3	M	185	ASN
3	M	188	ASN
3	M	209	HIS

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Mol	Chain	Res	Type
3	M	236	GLN
3	N	20	GLN
3	N	50	HIS
3	N	54	GLN
3	N	55	ASN
3	N	142	ASN
3	N	145	GLN
3	N	162	ASN
3	N	201	ASN
3	N	206	GLN
3	N	250	ASN
3	O	4	GLN
3	O	50	HIS
3	O	107	ASN
3	O	142	ASN
3	O	162	ASN
3	O	173	ASN
3	O	185	ASN
3	O	188	ASN
3	O	209	HIS
3	O	236	GLN
3	P	20	GLN
3	P	50	HIS
3	P	55	ASN
3	P	142	ASN
3	P	145	GLN
3	P	162	ASN
3	P	185	ASN
3	P	201	ASN
3	P	206	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CLF	K	9498	2,1	0,24,24	-	-	-		
5	CFM	I	8496	4,1	0,24,24	-	-	-		
8	SF4	E	290	3	0,12,12	-	-	-		
4	HCA	K	9494	5	13,13,13	1.96	4 (30%)	15,18,18	1.38	2 (13%)
4	HCA	A	6494	5	13,13,13	2.37	3 (23%)	15,18,18	1.48	4 (26%)
4	HCA	C	7494	5	13,13,13	1.98	3 (23%)	15,18,18	1.34	2 (13%)
5	CFM	C	7496	4,1	0,24,24	-	-	-		
5	CFM	K	9496	4,1	0,24,24	-	-	-		
6	CLF	D	7498	2,1	0,24,24	-	-	-		
8	SF4	G	1290	3	0,12,12	-	-	-		
8	SF4	N	2290	3	0,12,12	-	-	-		
8	SF4	P	3290	3	0,12,12	-	-	-		
6	CLF	A	6498	2,1	0,24,24	-	-	-		
5	CFM	A	6496	4,1	0,24,24	-	-	-		
4	HCA	I	8494	5	13,13,13	1.77	4 (30%)	15,18,18	1.20	0
6	CLF	J	8498	2,1	0,24,24	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLF	K	9498	2,1	-	-	0/12/10/10
8	SF4	E	290	3	-	-	0/6/5/5
4	HCA	K	9494	5	-	6/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HCA	A	6494	5	-	6/17/17/17	-
4	HCA	C	7494	5	-	7/17/17/17	-
6	CLF	D	7498	2,1	-	-	0/12/10/10
8	SF4	G	1290	3	-	-	0/6/5/5
8	SF4	N	2290	3	-	-	0/6/5/5
8	SF4	P	3290	3	-	-	0/6/5/5
6	CLF	A	6498	2,1	-	-	0/12/10/10
4	HCA	I	8494	5	-	7/17/17/17	-
6	CLF	J	8498	2,1	-	-	0/12/10/10

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	6494	HCA	C3-C7	-5.57	1.47	1.53
4	C	7494	HCA	O7-C3	5.15	1.53	1.43
4	K	9494	HCA	O7-C3	4.68	1.52	1.43
4	A	6494	HCA	C2-C3	-4.10	1.48	1.54
4	A	6494	HCA	O7-C3	3.68	1.50	1.43
4	I	8494	HCA	O7-C3	3.65	1.50	1.43
4	K	9494	HCA	C2-C3	-2.89	1.50	1.54
4	C	7494	HCA	C3-C7	-2.83	1.50	1.53
4	I	8494	HCA	C5-C6	2.67	1.56	1.50
4	K	9494	HCA	C3-C7	-2.19	1.51	1.53
4	C	7494	HCA	C5-C6	2.08	1.55	1.50
4	K	9494	HCA	C5-C6	2.08	1.55	1.50
4	I	8494	HCA	C3-C7	-2.05	1.51	1.53
4	I	8494	HCA	C2-C3	-2.02	1.51	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	6494	HCA	O6-C7-C3	2.62	118.16	113.14
4	K	9494	HCA	O6-C7-C3	2.57	118.08	113.14
4	C	7494	HCA	C2-C3-C7	-2.44	104.64	110.03
4	C	7494	HCA	O6-C7-C3	2.35	117.64	113.14
4	A	6494	HCA	O5-C7-C3	-2.03	118.16	122.09
4	K	9494	HCA	C2-C3-C7	-2.03	105.56	110.03
4	A	6494	HCA	O7-C3-C7	-2.02	106.10	108.96
4	A	6494	HCA	O3-C6-C5	-2.01	116.70	123.09

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	6494	HCA	C2-C3-C4-C5
4	A	6494	HCA	C7-C3-C4-C5
4	A	6494	HCA	O7-C3-C4-C5
4	C	7494	HCA	C2-C3-C4-C5
4	C	7494	HCA	C7-C3-C4-C5
4	C	7494	HCA	O7-C3-C4-C5
4	I	8494	HCA	C2-C3-C4-C5
4	I	8494	HCA	C7-C3-C4-C5
4	I	8494	HCA	O7-C3-C4-C5
4	K	9494	HCA	C2-C3-C4-C5
4	K	9494	HCA	C7-C3-C4-C5
4	K	9494	HCA	O7-C3-C4-C5
4	I	8494	HCA	O2-C1-C2-C3
4	A	6494	HCA	O1-C1-C2-C3
4	C	7494	HCA	O2-C1-C2-C3
4	A	6494	HCA	O2-C1-C2-C3
4	I	8494	HCA	O1-C1-C2-C3
4	K	9494	HCA	O1-C1-C2-C3
4	K	9494	HCA	O2-C1-C2-C3
4	C	7494	HCA	O1-C1-C2-C3
4	K	9494	HCA	C4-C5-C6-O4
4	C	7494	HCA	C4-C5-C6-O4
4	A	6494	HCA	C4-C5-C6-O4
4	C	7494	HCA	C4-C5-C6-O3
4	I	8494	HCA	C4-C5-C6-O3
4	I	8494	HCA	C4-C5-C6-O4

There are no ring outliers.

15 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	9498	CLF	4	0
5	I	8496	CFM	3	0
8	E	290	SF4	2	0
4	K	9494	HCA	1	0
4	A	6494	HCA	1	0
4	C	7494	HCA	1	0
5	C	7496	CFM	5	0
5	K	9496	CFM	3	0
6	D	7498	CLF	2	0
8	G	1290	SF4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	2290	SF4	5	0
6	A	6498	CLF	6	0
5	A	6496	CFM	7	0
4	I	8494	HCA	1	0
6	J	8498	CLF	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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.