



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:03 PM UTC

PDB ID : 3IAS / pdb_00003ias
Title : Crystal structure of the hydrophilic domain of respiratory complex I from *Thermus thermophilus*, oxidized, 4 mol/ASU, re-refined to 3.15 angstrom resolution
Authors : Sazanov, L.A.; Berrisford, J.M.
Deposited on : 2009-07-14
Resolution : 3.15 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

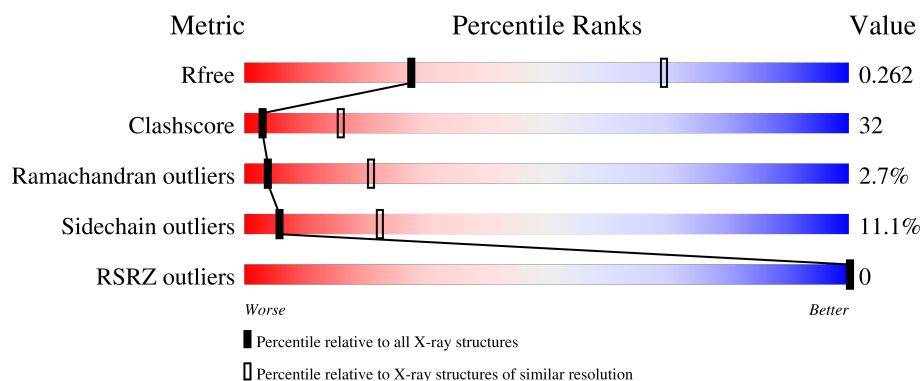
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

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



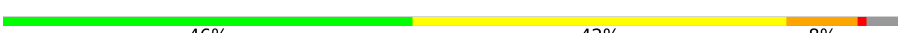
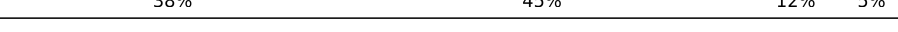
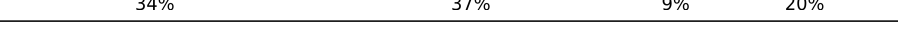
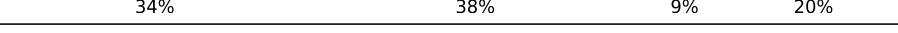
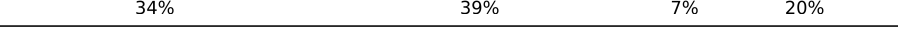
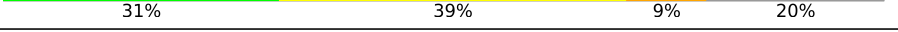
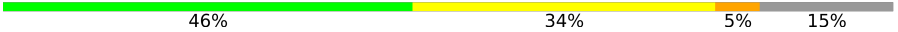
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	438	49% 42% 8%
1	A	438	49% 43% 8%
1	J	438	48% 43% 8%
1	S	438	49% 42% 8%

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Mol	Chain	Length	Quality of chain
2	2	181	 52% 38% 7% ..
2	B	181	 55% 36% 7% ..
2	K	181	 53% 37% 7% ..
2	T	181	 52% 38% 8% ..
3	3	783	 46% 42% 8% ..
3	C	783	 46% 42% 8% ..
3	L	783	 46% 42% 8% ..
3	U	783	 45% 42% 8% .
4	4	409	 37% 44% 11% 8%
4	D	409	 37% 44% 11% 8%
4	M	409	 38% 44% 10% 8%
4	V	409	 35% 48% 9% 8%
5	5	207	 41% 42% 12% 5%
5	E	207	 40% 43% 12% 5%
5	N	207	 41% 43% 11% 5%
5	W	207	 38% 45% 12% 5%
6	6	181	 34% 37% 9% 20%
6	F	181	 34% 38% 9% 20%
6	O	181	 34% 39% 7% 20%
6	X	181	 31% 39% 9% 20%
7	9	182	 45% 34% 6% 15%
7	G	182	 47% 33% 5% 15%
7	P	182	 45% 35% 5% 15%
7	Y	182	 46% 34% 5% 15%
8	7	129	 59% 34% 5% ..

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Mol	Chain	Length	Quality of chain
8	H	129	
8	Q	129	
8	Z	129	

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
9	SF4	6	182	-	-	X	-
9	SF4	F	182	-	-	X	-
9	SF4	O	182	-	-	X	-
9	SF4	X	182	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 75028 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 NADH-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			
1	A	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			
1	J	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			
1	S	437	Total	C	N	O	S	0	0	0
			3417	2180	595	624	18			

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			
2	B	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			
2	K	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			
2	T	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			
3	C	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			
3	L	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			
3	U	754	Total	C	N	O	S	0	0	0
			5880	3743	1055	1051	31			

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	377	Total	C	N	O	S	0	0	0
			3011	1941	510	549	11			
4	D	377	Total	C	N	O	S	0	0	0
			3011	1941	510	549	11			
4	M	377	Total	C	N	O	S	0	0	0
			3011	1941	510	549	11			
4	V	377	Total	C	N	O	S	0	0	0
			3011	1941	510	549	11			

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	5	196	Total	C	N	O	S	0	0	0
			1607	1043	273	288	3			
5	E	196	Total	C	N	O	S	0	0	0
			1607	1043	273	288	3			
5	N	196	Total	C	N	O	S	0	0	0
			1607	1043	273	288	3			
5	W	196	Total	C	N	O	S	0	0	0
			1607	1043	273	288	3			

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	6	145	Total	C	N	O	S	0	0	0
			1113	706	196	198	13			
6	F	145	Total	C	N	O	S	0	0	0
			1113	706	196	198	13			
6	O	145	Total	C	N	O	S	0	0	0
			1113	706	196	198	13			
6	X	145	Total	C	N	O	S	0	0	0
			1113	706	196	198	13			

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	9	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			
7	G	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			
7	P	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			

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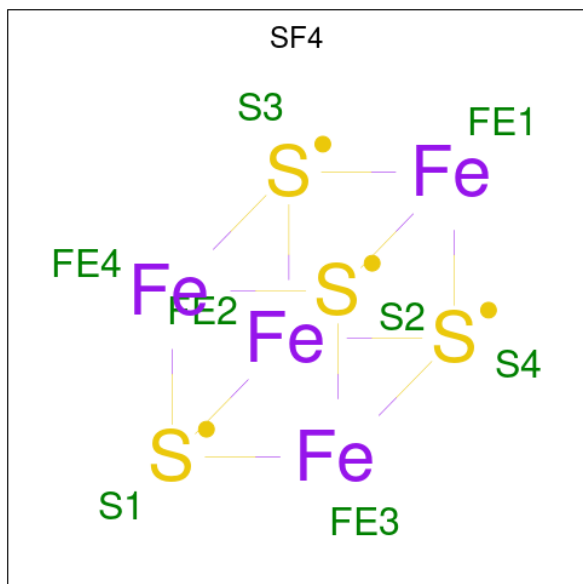
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Y	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			
8	H	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			
8	Q	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			
8	Z	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	1	1	Total	Fe	S	0	0
			8	4	4		
9	3	1	Total	Fe	S	0	0
			8	4	4		
9	3	1	Total	Fe	S	0	0
			8	4	4		
9	3	1	Total	Fe	S	0	0
			8	4	4		

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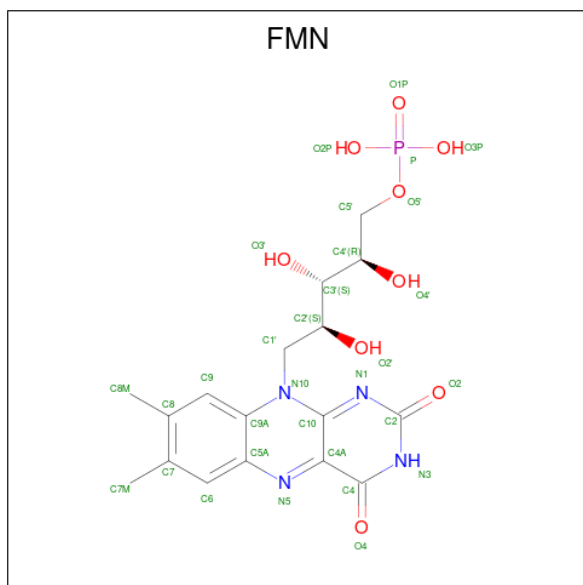
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	6	1	Total 8	Fe 4	S 4	0	0
9	9	1	Total 8	Fe 4	S 4	0	0
9	9	1	Total 8	Fe 4	S 4	0	0
9	A	1	Total 8	Fe 4	S 4	0	0
9	C	1	Total 8	Fe 4	S 4	0	0
9	C	1	Total 8	Fe 4	S 4	0	0
9	C	1	Total 8	Fe 4	S 4	0	0
9	F	1	Total 8	Fe 4	S 4	0	0
9	G	1	Total 8	Fe 4	S 4	0	0
9	G	1	Total 8	Fe 4	S 4	0	0
9	J	1	Total 8	Fe 4	S 4	0	0
9	L	1	Total 8	Fe 4	S 4	0	0
9	L	1	Total 8	Fe 4	S 4	0	0
9	L	1	Total 8	Fe 4	S 4	0	0
9	O	1	Total 8	Fe 4	S 4	0	0
9	P	1	Total 8	Fe 4	S 4	0	0
9	P	1	Total 8	Fe 4	S 4	0	0
9	S	1	Total 8	Fe 4	S 4	0	0
9	U	1	Total 8	Fe 4	S 4	0	0
9	U	1	Total 8	Fe 4	S 4	0	0
9	U	1	Total 8	Fe 4	S 4	0	0

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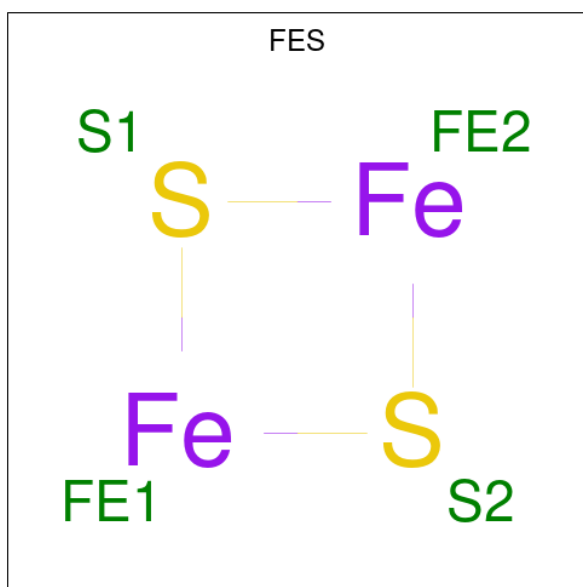
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	X	1	Total 8	Fe 4	S 4	0	0
9	Y	1	Total 8	Fe 4	S 4	0	0
9	Y	1	Total 8	Fe 4	S 4	0	0

- Molecule 10 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	1	1	Total 31	C 17	N 4	O 9	P 1	0	0
10	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
10	J	1	Total 31	C 17	N 4	O 9	P 1	0	0
10	S	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	2	1	Total	Fe	S	0	0
			4	2	2		
11	3	1	Total	Fe	S	0	0
			4	2	2		
11	B	1	Total	Fe	S	0	0
			4	2	2		
11	C	1	Total	Fe	S	0	0
			4	2	2		
11	K	1	Total	Fe	S	0	0
			4	2	2		
11	L	1	Total	Fe	S	0	0
			4	2	2		
11	T	1	Total	Fe	S	0	0
			4	2	2		
11	U	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	2	1	Total	Ca	0	0
			1	1		
12	3	2	Total	Ca	0	0
			2	2		
12	9	1	Total	Ca	0	0
			1	1		
12	B	1	Total	Ca	0	0
			1	1		

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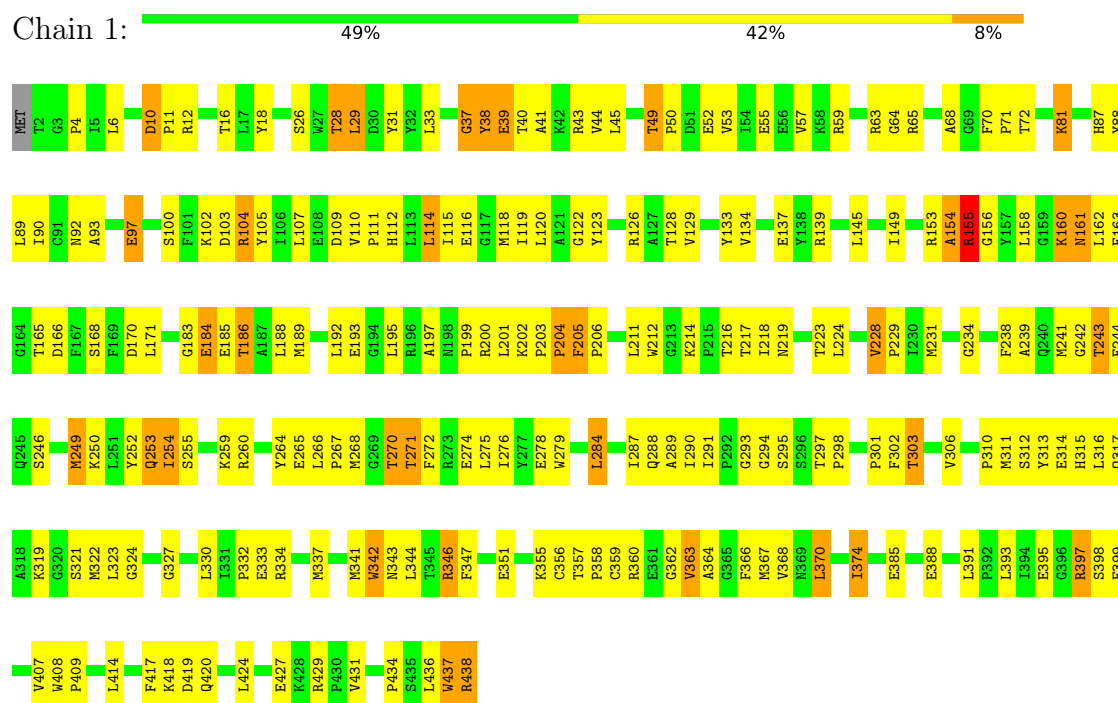
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total 1	Ca 1	0	0
12	G	1	Total 1	Ca 1	0	0
12	H	1	Total 1	Ca 1	0	0
12	K	1	Total 1	Ca 1	0	0
12	L	2	Total 2	Ca 2	0	0
12	P	1	Total 1	Ca 1	0	0
12	T	1	Total 1	Ca 1	0	0
12	U	1	Total 1	Ca 1	0	0
12	Y	1	Total 1	Ca 1	0	0
12	Z	1	Total 1	Ca 1	0	0

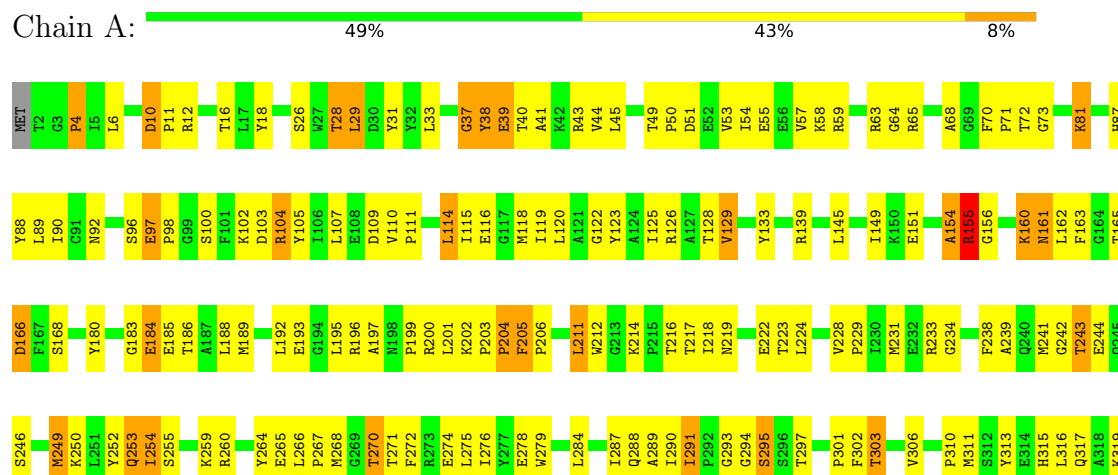
3 Residue-property plots

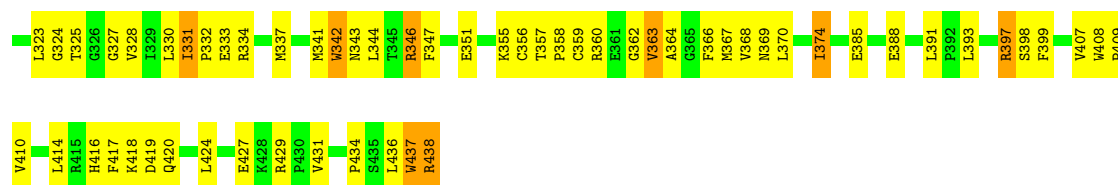
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NADH-quinone oxidoreductase subunit 1

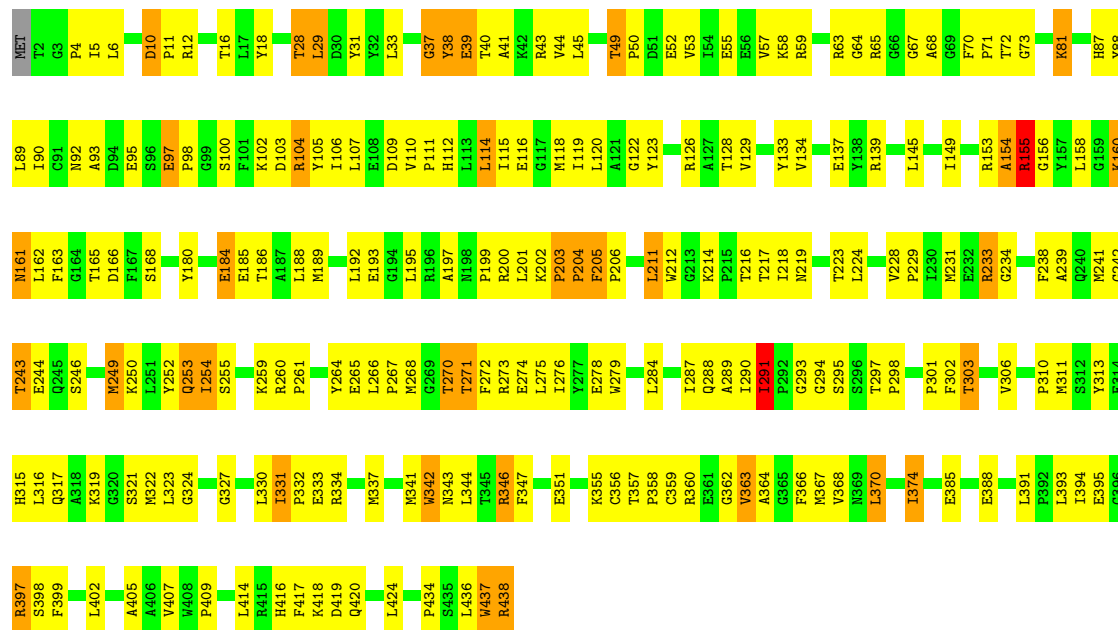


• Molecule 1: NADH-quinone oxidoreductase subunit 1

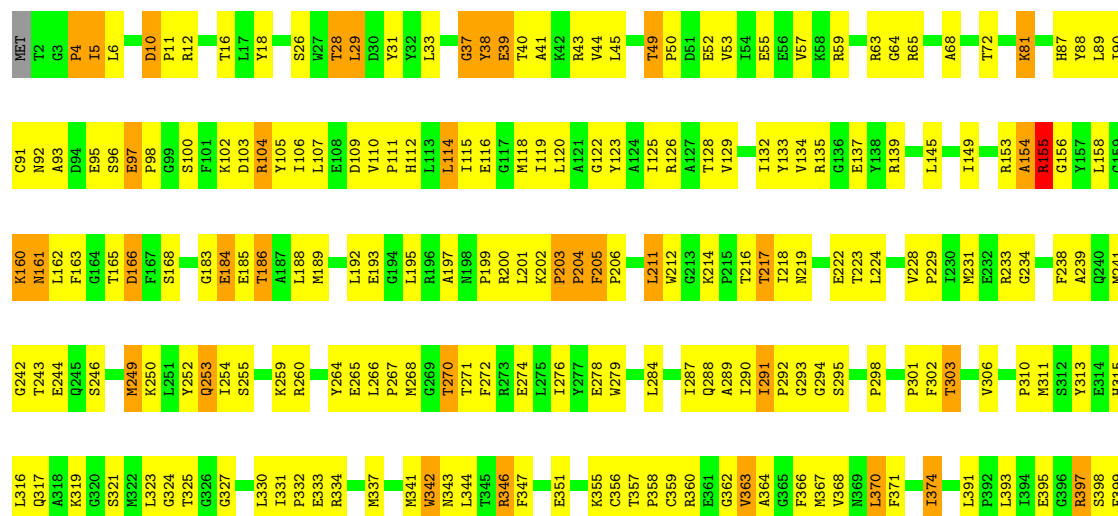




• Molecule 1: NADH-quinone oxidoreductase subunit 1



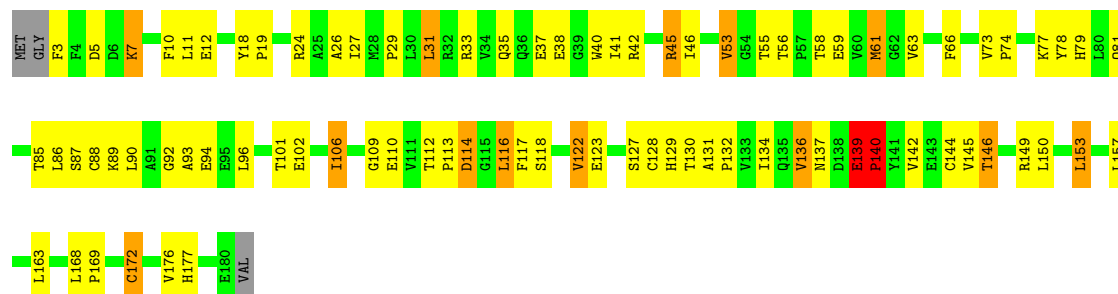
• Molecule 1: NADH-quinone oxidoreductase subunit 1





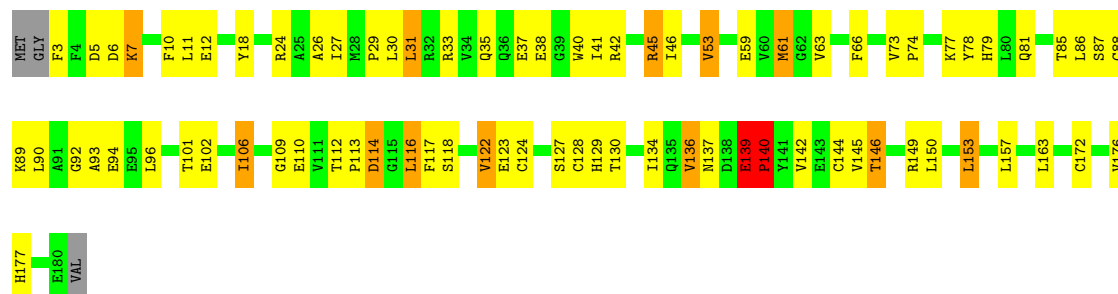
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2: 52% 38% 7% ..



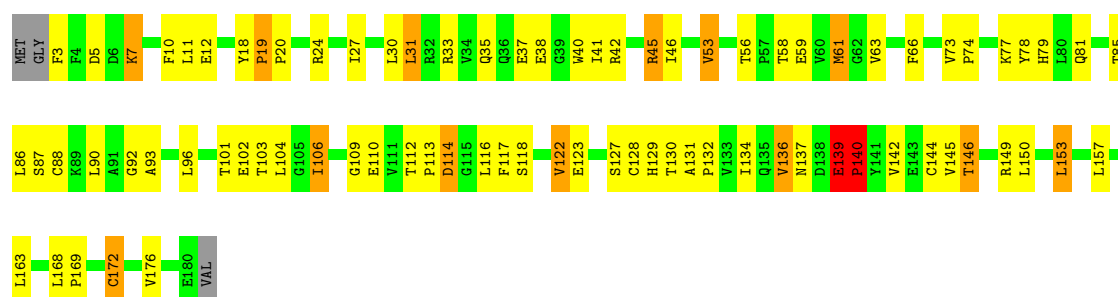
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain B: 55% 36% 7% ..



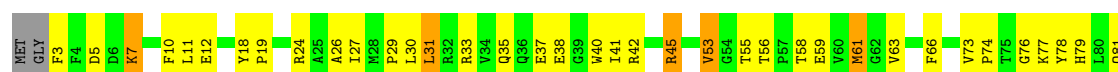
• Molecule 2: NADH-quinone oxidoreductase subunit 2

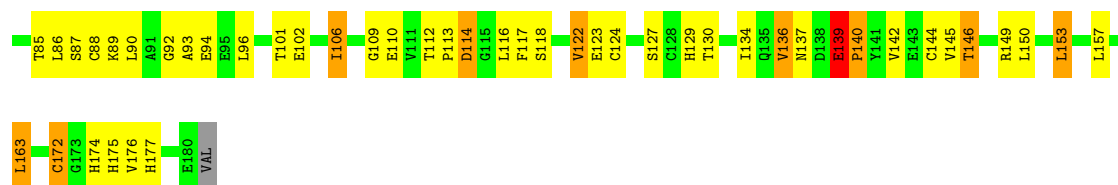
Chain K: 53% 37% 7% ..



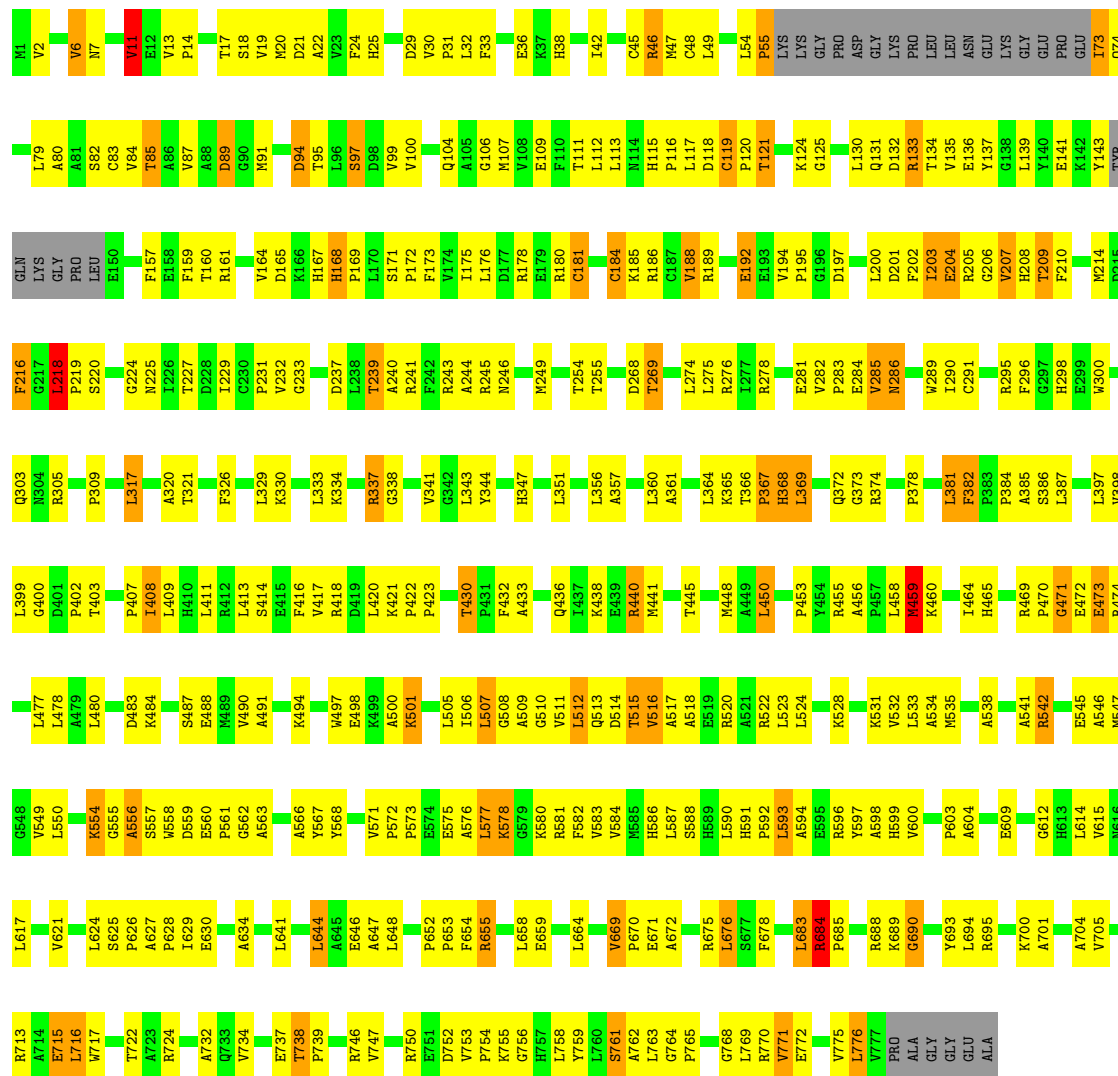
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain T: 52% 38% 8% ..



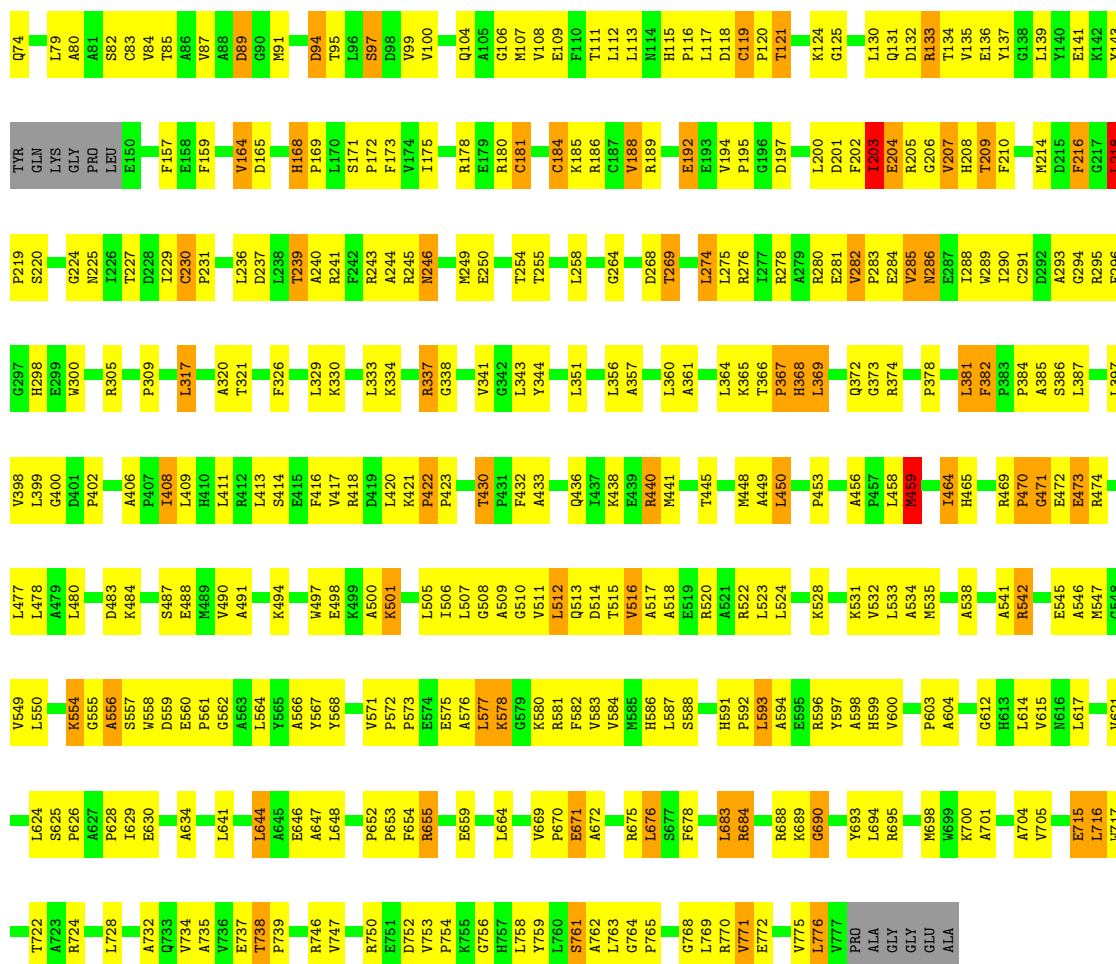


• Molecule 3: NADH-quinone oxidoreductase subunit 3



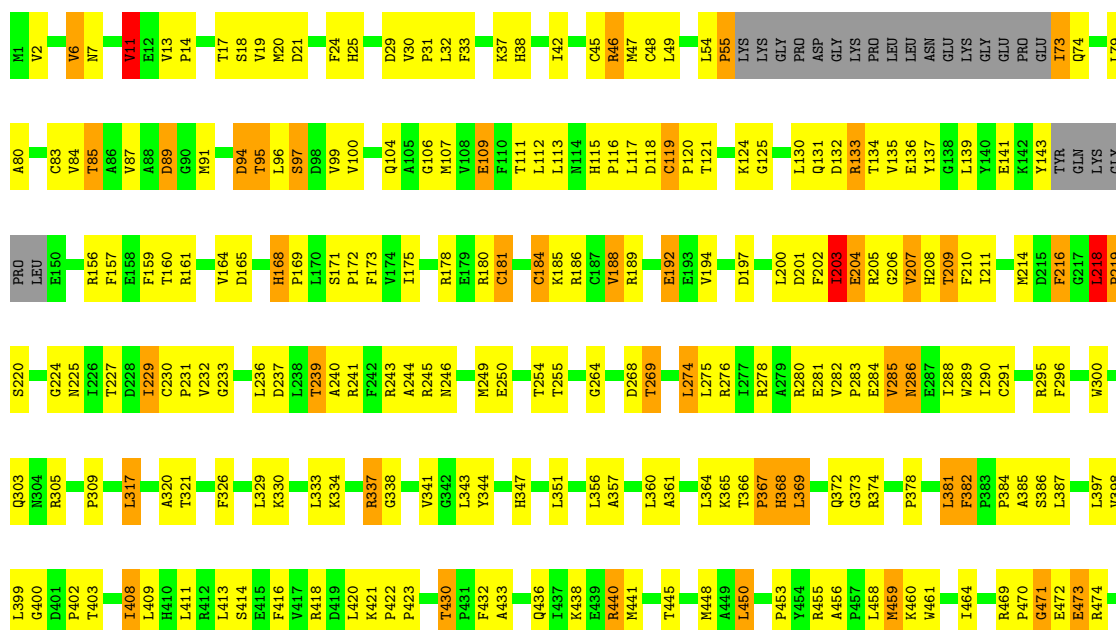
• Molecule 3: NADH-quinone oxidoreductase subunit 3

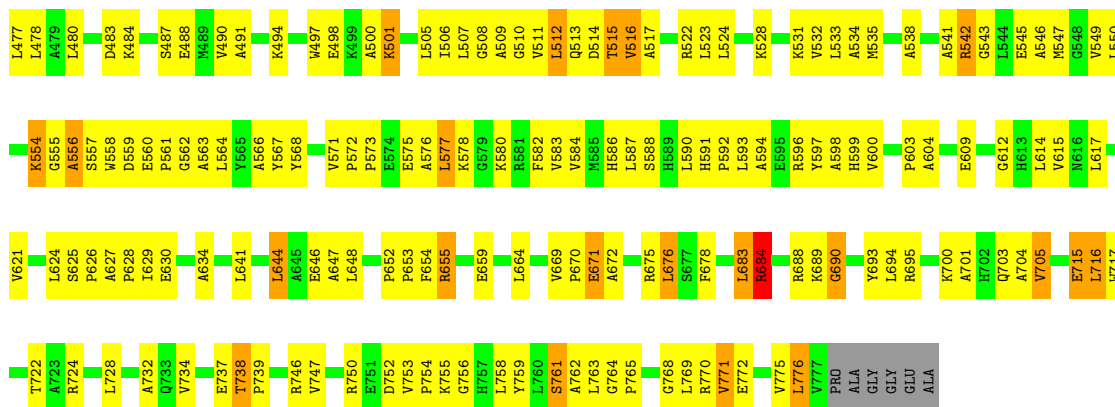




● Molecule 3: NADH-quinone oxidoreductase subunit 3

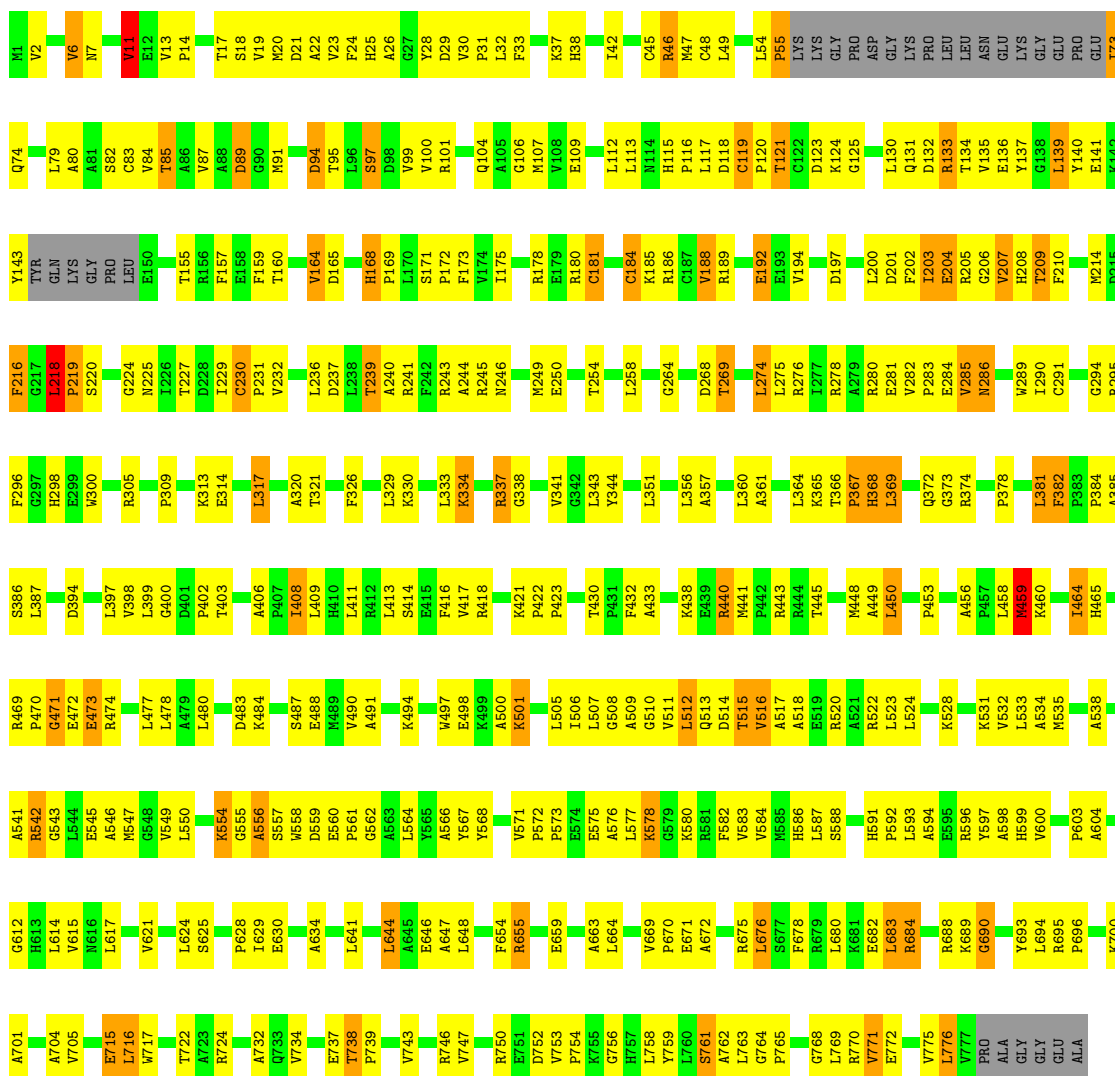
Chain L: 46% 42% 8%



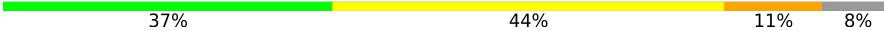


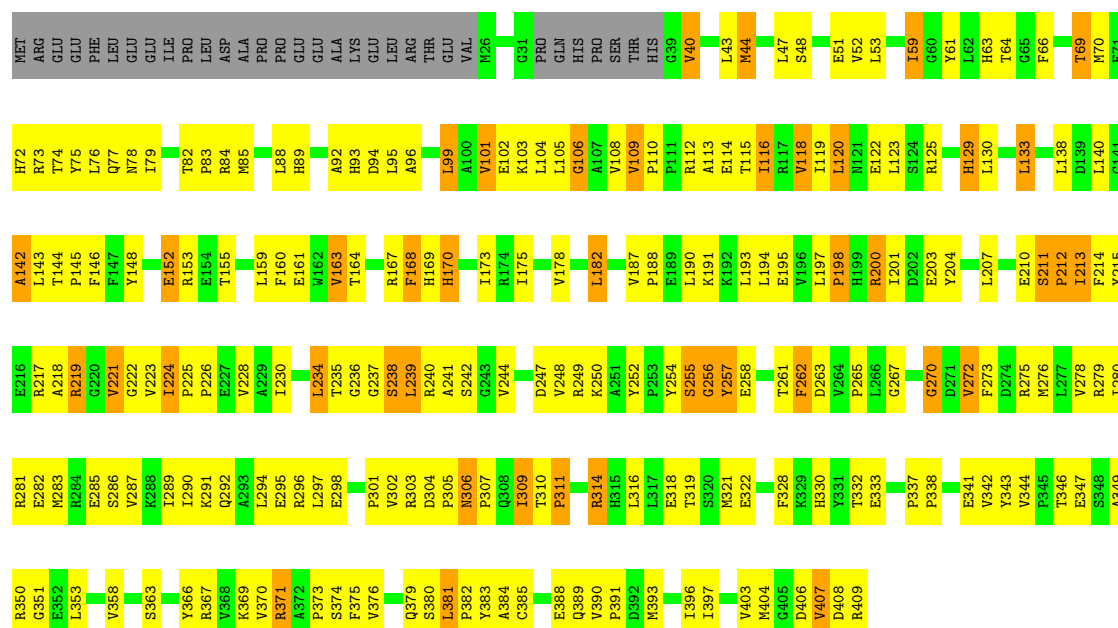
• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain U: 45% 42% 8%

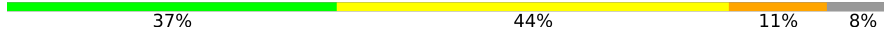


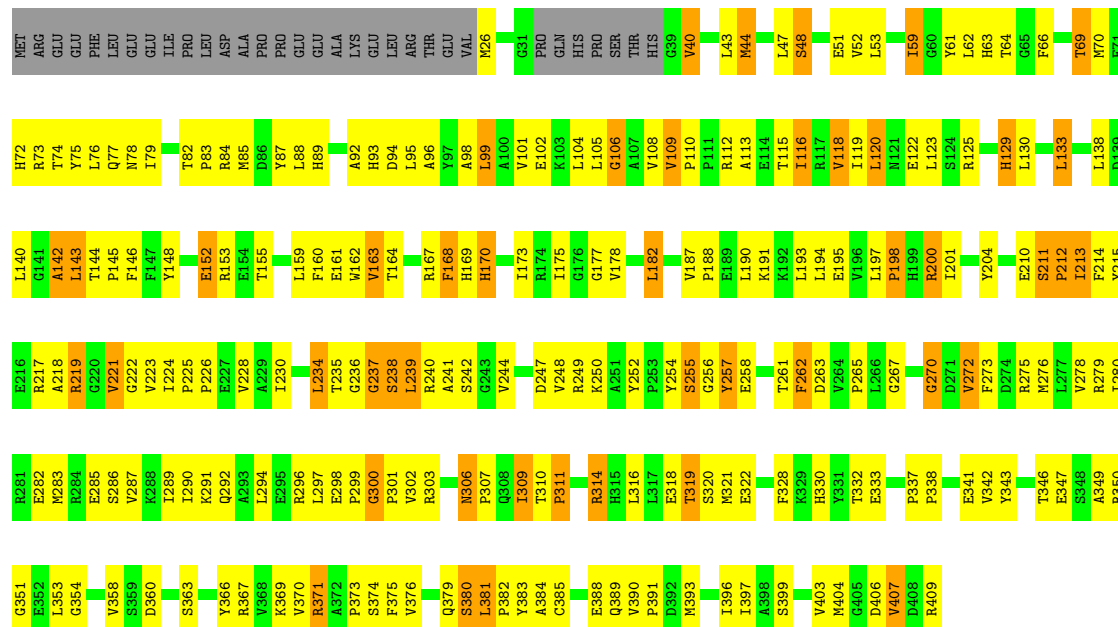
• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain 4: 

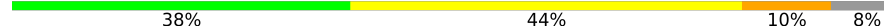


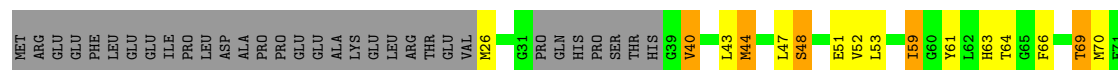
• Molecule 4: NADH-quinone oxidoreductase subunit 4

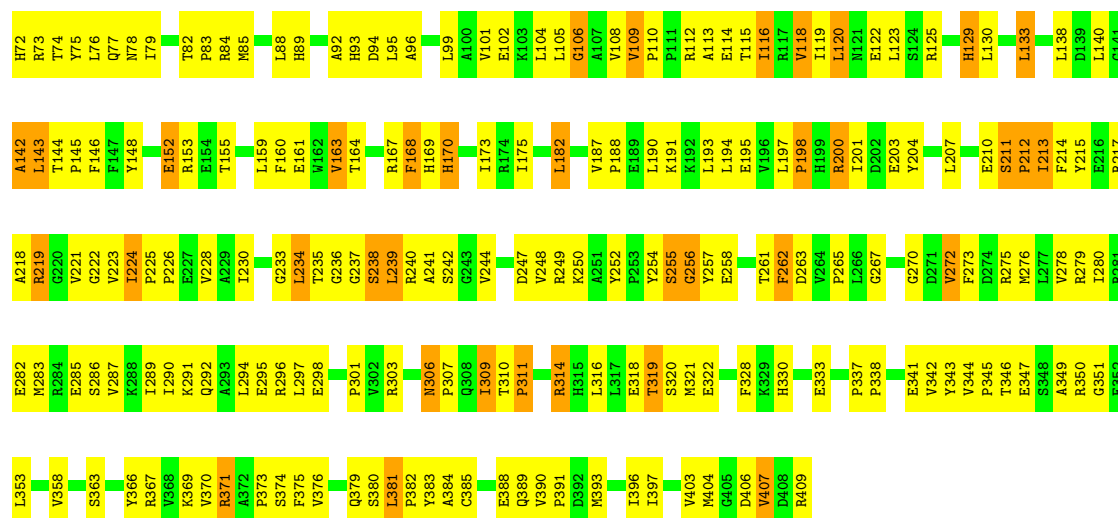
Chain D: 



• Molecule 4: NADH-quinone oxidoreductase subunit 4

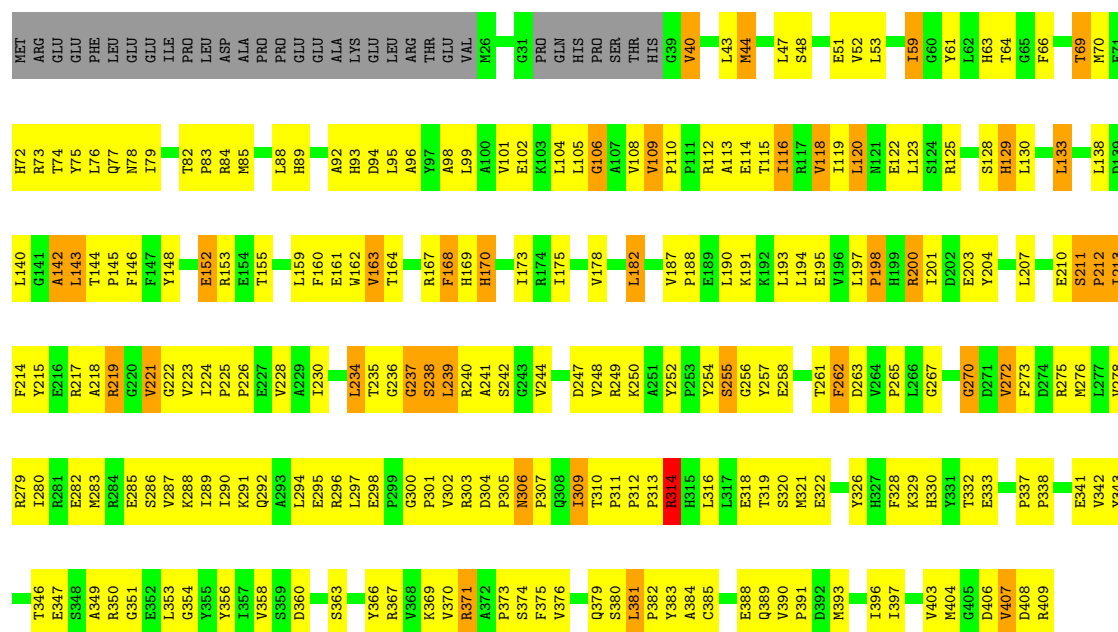
Chain M: 





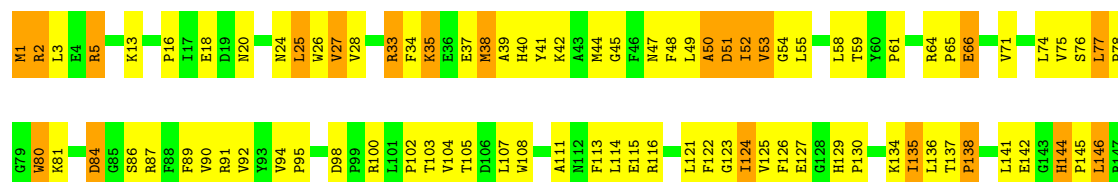
• Molecule 4: NADH-quinone oxidoreductase subunit 4

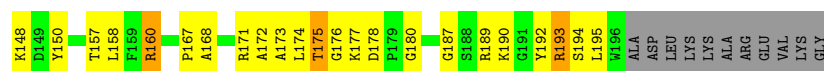
Chain V: 35% 48% 9% 8%



• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain 5: 41% 42% 12% 5%





• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain E: 40% 43% 12% 5%



• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain N: 41% 43% 11% 5%



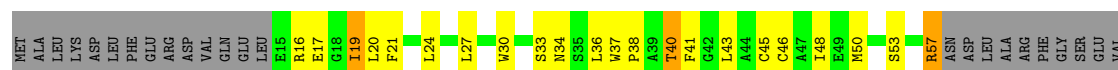
• Molecule 5: NADH-quinone oxidoreductase subunit 5

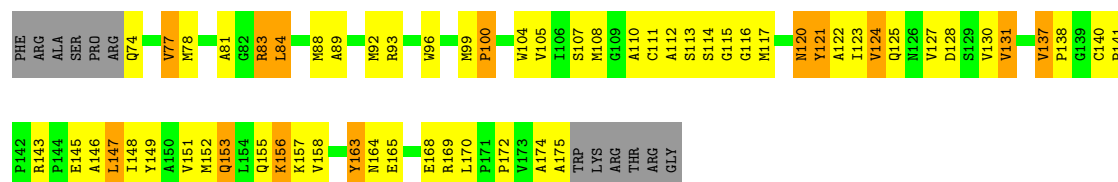
Chain W: 38% 45% 12% 5%



• Molecule 6: NADH-quinone oxidoreductase subunit 6

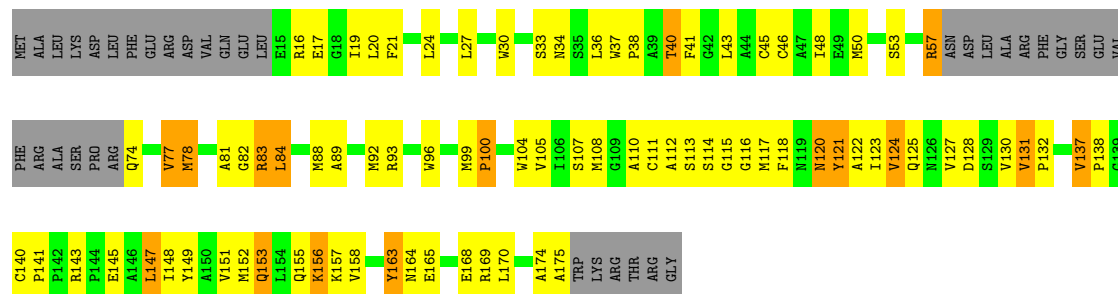
Chain 6: 34% 37% 9% 20%





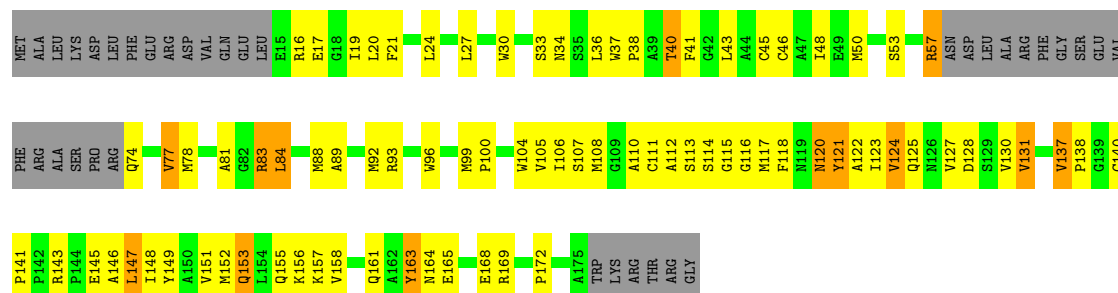
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain F: 34% 38% 9% 20%



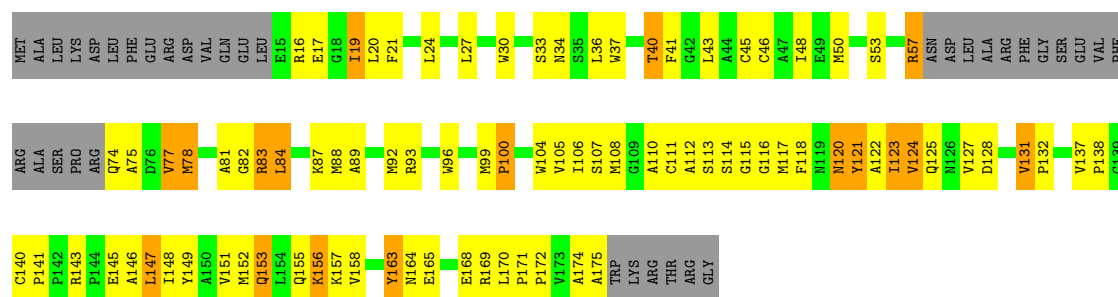
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain O: 34% 39% 7% 20%



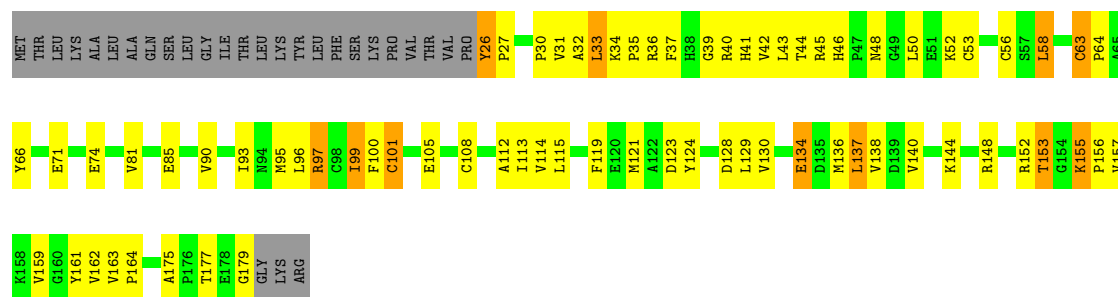
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain X: 31% 39% 9% 20%

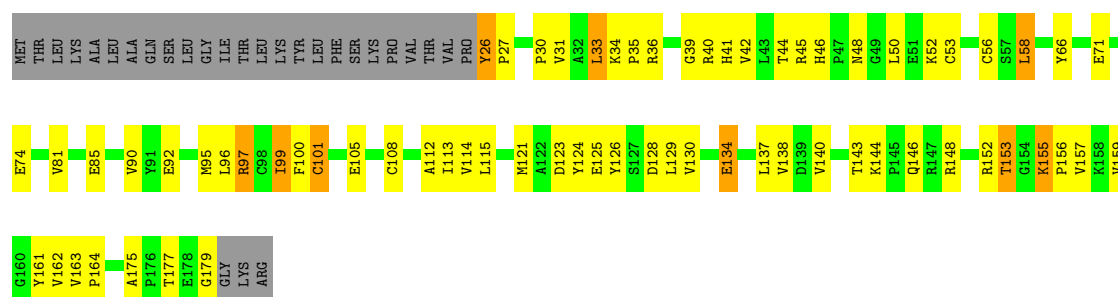


• Molecule 7: NADH-quinone oxidoreductase subunit 9

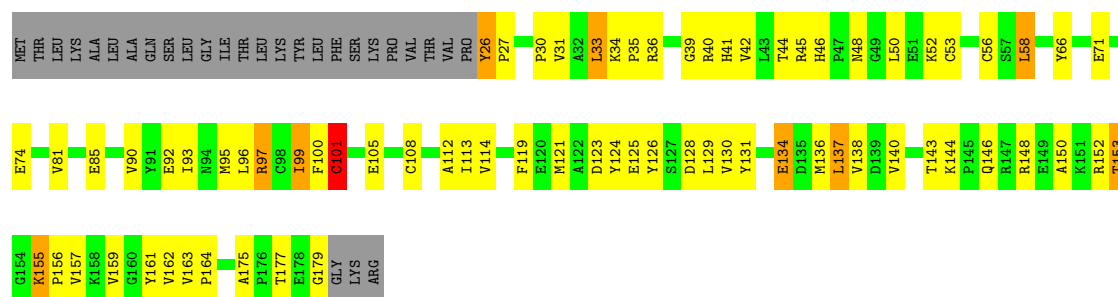
Chain 9: 45% 34% 6% 15%



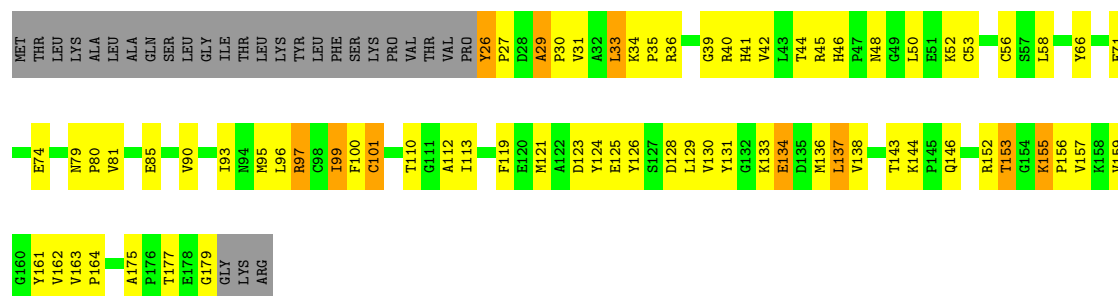
- Molecule 7: NADH-quinone oxidoreductase subunit 9



- Molecule 7: NADH-quinone oxidoreductase subunit 9

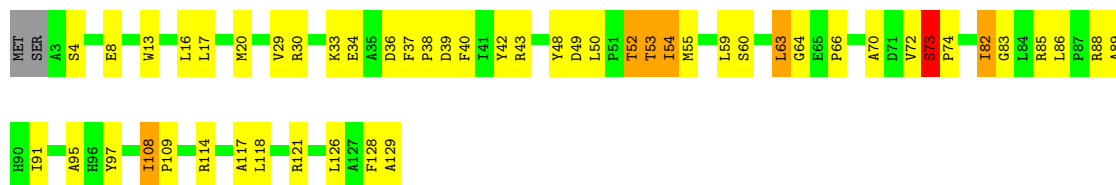


- Molecule 7: NADH-quinone oxidoreductase subunit 9



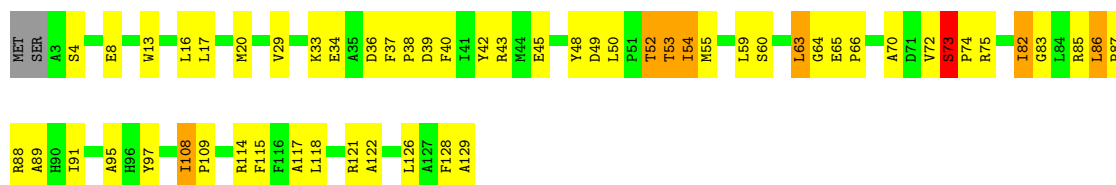
- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7:  59% 34% 5% ..



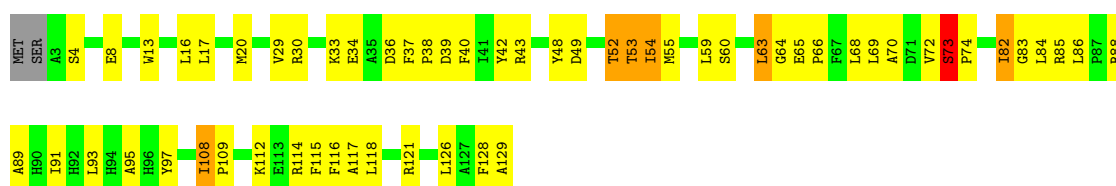
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain H:  55% 37% 5% ..



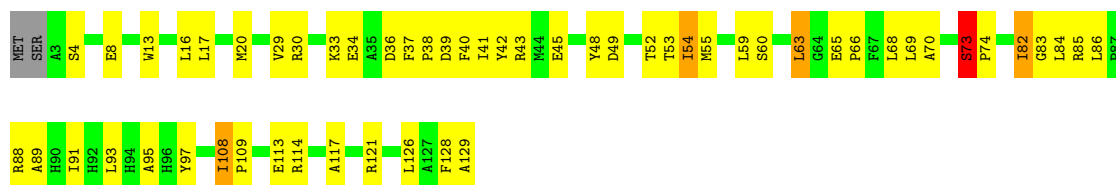
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain Q:  53% 40% 5% ..



• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain Z:  56% 39%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.08Å 266.11Å 201.73Å 90.00° 104.71° 90.00°	Depositor
Resolution (Å)	29.98 – 3.15 29.98 – 3.15	Depositor EDS
% Data completeness (in resolution range)	82.5 (29.98-3.15) 82.5 (29.98-3.15)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.237 , 0.270 0.232 , 0.262	Depositor DCC
R_{free} test set	4194 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	75028	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, CA, FES, SF4

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	1	0.55	0/3506	0.93	6/4745 (0.1%)
1	A	0.51	0/3506	0.94	8/4745 (0.2%)
1	J	0.57	0/3506	0.93	9/4745 (0.2%)
1	S	0.50	0/3506	0.94	6/4745 (0.1%)
2	2	0.55	0/1439	0.97	9/1953 (0.5%)
2	B	0.49	0/1439	0.95	6/1953 (0.3%)
2	K	0.55	0/1439	0.95	11/1953 (0.6%)
2	T	0.52	0/1439	0.95	9/1953 (0.5%)
3	3	0.54	0/6019	0.98	24/8163 (0.3%)
3	C	0.51	0/6019	0.98	27/8163 (0.3%)
3	L	0.50	0/6019	0.97	21/8163 (0.3%)
3	U	0.51	0/6019	0.97	22/8163 (0.3%)
4	4	0.52	0/3089	0.94	12/4197 (0.3%)
4	D	0.52	0/3089	0.94	9/4197 (0.2%)
4	M	0.56	0/3089	0.95	11/4197 (0.3%)
4	V	0.50	0/3089	0.94	8/4197 (0.2%)
5	5	0.50	0/1656	1.00	11/2246 (0.5%)
5	E	0.48	0/1656	1.03	12/2246 (0.5%)
5	N	0.51	0/1656	1.03	13/2246 (0.6%)
5	W	0.46	0/1656	1.01	13/2246 (0.6%)
6	6	0.57	0/1137	1.01	5/1542 (0.3%)
6	F	0.59	0/1137	1.01	5/1542 (0.3%)
6	O	0.55	0/1137	0.99	3/1542 (0.2%)
6	X	0.53	0/1137	0.99	3/1542 (0.2%)
7	9	0.57	0/1224	0.96	4/1663 (0.2%)
7	G	0.57	0/1224	0.97	2/1663 (0.1%)
7	P	0.55	0/1224	0.97	3/1663 (0.2%)
7	Y	0.52	0/1224	0.97	4/1663 (0.2%)
8	7	0.51	0/1059	0.97	5/1429 (0.3%)
8	H	0.50	0/1059	0.96	7/1429 (0.5%)
8	Q	0.51	0/1059	0.96	5/1429 (0.3%)
8	Z	0.48	0/1059	0.94	6/1429 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.52	0/76516	0.96	299/103752 (0.3%)

There are no bond length outliers.

All (299) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	184	CYS	N-CA-C	-10.00	98.11	110.41
3	3	184	CYS	N-CA-C	-9.44	98.80	110.41
3	L	184	CYS	N-CA-C	-9.39	98.86	110.41
3	C	430	THR	CA-C-N	9.35	129.11	119.76
3	C	430	THR	C-N-CA	9.35	129.11	119.76
3	3	430	THR	CA-C-N	9.35	129.11	119.76
3	3	430	THR	C-N-CA	9.35	129.11	119.76
3	3	216	PHE	N-CA-C	9.23	121.34	111.28
3	C	184	CYS	N-CA-C	-9.22	99.07	110.41
3	L	430	THR	CA-C-N	9.12	128.88	119.76
3	L	430	THR	C-N-CA	9.12	128.88	119.76
3	L	14	PRO	CA-C-N	8.98	128.31	118.97
3	L	14	PRO	C-N-CA	8.98	128.31	118.97
3	C	14	PRO	CA-C-N	8.96	128.29	118.97
3	C	14	PRO	C-N-CA	8.96	128.29	118.97
3	3	14	PRO	CA-C-N	8.94	128.27	118.97
3	3	14	PRO	C-N-CA	8.94	128.27	118.97
3	U	430	THR	CA-C-N	8.91	128.67	119.76
3	U	430	THR	C-N-CA	8.91	128.67	119.76
3	U	216	PHE	N-CA-C	8.72	120.78	111.28
3	L	216	PHE	N-CA-C	8.60	120.65	111.28
3	C	216	PHE	N-CA-C	8.58	120.63	111.28
5	N	190	LYS	N-CA-C	-8.33	102.14	113.30
3	U	14	PRO	CA-C-N	8.26	127.56	118.97
3	U	14	PRO	C-N-CA	8.26	127.56	118.97
3	U	168	HIS	CA-C-N	8.25	128.74	119.83
3	U	168	HIS	C-N-CA	8.25	128.74	119.83
3	L	168	HIS	CA-C-N	8.19	128.67	119.83
3	L	168	HIS	C-N-CA	8.19	128.67	119.83
5	E	190	LYS	N-CA-C	-8.05	102.51	113.30
5	W	77	LEU	CA-C-N	7.98	128.17	119.87
5	W	77	LEU	C-N-CA	7.98	128.17	119.87
5	N	144	HIS	CA-C-N	7.96	127.24	118.97
5	N	144	HIS	C-N-CA	7.96	127.24	118.97
2	2	139	GLU	CA-C-N	7.88	129.68	119.84
2	2	139	GLU	C-N-CA	7.88	129.68	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	190	LYS	N-CA-C	-7.81	102.83	113.30
3	L	55	PRO	CB-CA-C	-7.64	95.58	110.10
4	M	306	ASN	CA-C-N	7.50	127.54	119.28
4	M	306	ASN	C-N-CA	7.50	127.54	119.28
4	M	309	ILE	CB-CA-C	-7.46	102.56	110.62
4	M	238	SER	N-CA-C	-7.43	103.34	113.30
5	5	144	HIS	CA-C-N	7.34	126.61	118.97
5	5	144	HIS	C-N-CA	7.34	126.61	118.97
4	D	306	ASN	CA-C-N	7.34	127.36	119.28
4	D	306	ASN	C-N-CA	7.34	127.36	119.28
2	K	139	GLU	CA-C-N	7.33	129.00	119.84
2	K	139	GLU	C-N-CA	7.33	129.00	119.84
5	N	77	LEU	CA-C-N	7.32	127.95	120.04
5	N	77	LEU	C-N-CA	7.32	127.95	120.04
3	C	55	PRO	CB-CA-C	-7.29	96.24	110.10
5	E	144	HIS	CA-C-N	7.29	126.55	118.97
5	E	144	HIS	C-N-CA	7.29	126.55	118.97
3	U	55	PRO	CB-CA-C	-7.27	96.28	110.10
3	3	55	PRO	CB-CA-C	-7.27	96.28	110.10
2	T	139	GLU	CA-C-N	7.26	128.92	119.84
2	T	139	GLU	C-N-CA	7.26	128.92	119.84
5	N	94	VAL	CA-C-N	7.26	128.91	119.84
5	N	94	VAL	C-N-CA	7.26	128.91	119.84
4	V	238	SER	N-CA-C	-7.23	104.06	113.17
3	3	168	HIS	CA-C-N	7.19	128.32	119.98
3	3	168	HIS	C-N-CA	7.19	128.32	119.98
5	E	77	LEU	CA-C-N	7.19	127.80	120.04
5	E	77	LEU	C-N-CA	7.19	127.80	120.04
5	W	190	LYS	N-CA-C	-7.17	103.69	113.30
4	4	306	ASN	CA-C-N	7.16	127.16	119.28
4	4	306	ASN	C-N-CA	7.16	127.16	119.28
8	7	4	SER	N-CA-C	-7.15	104.17	113.17
3	C	168	HIS	CA-C-N	7.12	127.52	119.83
3	C	168	HIS	C-N-CA	7.12	127.52	119.83
2	B	139	GLU	CA-C-N	7.10	128.72	119.84
2	B	139	GLU	C-N-CA	7.10	128.72	119.84
4	4	238	SER	N-CA-C	-7.07	104.26	113.17
8	Q	4	SER	N-CA-C	-6.98	104.38	113.17
5	5	77	LEU	CA-C-N	6.90	127.50	120.04
5	5	77	LEU	C-N-CA	6.90	127.50	120.04
1	1	97	GLU	CA-C-N	6.89	127.30	119.93
1	1	97	GLU	C-N-CA	6.89	127.30	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ILE	CA-C-N	6.84	128.39	119.84
1	A	291	ILE	C-N-CA	6.84	128.39	119.84
4	D	238	SER	N-CA-C	-6.82	104.58	113.17
4	V	306	ASN	CA-C-N	6.73	126.68	119.28
4	V	306	ASN	C-N-CA	6.73	126.68	119.28
8	H	4	SER	N-CA-C	-6.71	104.72	113.17
5	E	94	VAL	CA-C-N	6.71	128.22	119.84
5	E	94	VAL	C-N-CA	6.71	128.22	119.84
5	W	94	VAL	CA-C-N	6.65	128.15	119.84
5	W	94	VAL	C-N-CA	6.65	128.15	119.84
1	S	291	ILE	CA-C-N	6.49	127.95	119.84
1	S	291	ILE	C-N-CA	6.49	127.95	119.84
5	E	64	ARG	CA-C-N	6.41	127.86	119.84
5	E	64	ARG	C-N-CA	6.41	127.86	119.84
1	S	97	GLU	CA-C-N	6.41	126.79	119.93
1	S	97	GLU	C-N-CA	6.41	126.79	119.93
8	Z	4	SER	N-CA-C	-6.40	105.11	113.17
3	3	218	LEU	CA-C-N	6.39	127.83	119.84
3	3	218	LEU	C-N-CA	6.39	127.83	119.84
5	5	94	VAL	CA-C-N	6.38	127.81	119.84
5	5	94	VAL	C-N-CA	6.38	127.81	119.84
8	7	108	ILE	N-CA-C	6.38	114.12	108.63
3	L	421	LYS	CA-C-N	6.31	126.88	120.38
3	L	421	LYS	C-N-CA	6.31	126.88	120.38
4	D	300	GLY	CA-C-N	6.27	126.45	120.31
4	D	300	GLY	C-N-CA	6.27	126.45	120.31
2	B	18	TYR	CA-C-N	6.26	126.83	120.38
2	B	18	TYR	C-N-CA	6.26	126.83	120.38
4	4	309	ILE	CB-CA-C	-6.24	103.88	110.62
2	2	19	PRO	CA-C-N	6.20	125.76	119.19
2	2	19	PRO	C-N-CA	6.20	125.76	119.19
3	C	459	MET	N-CA-C	-6.18	105.70	113.18
5	W	64	ARG	CA-C-N	6.18	127.57	119.84
5	W	64	ARG	C-N-CA	6.18	127.57	119.84
6	O	120	ASN	N-CA-C	6.15	116.39	108.34
1	1	205	PHE	N-CA-C	6.14	118.91	110.01
1	J	291	ILE	CA-C-N	6.10	127.47	119.84
1	J	291	ILE	C-N-CA	6.10	127.47	119.84
6	X	170	LEU	CA-C-N	6.09	126.65	120.38
6	X	170	LEU	C-N-CA	6.09	126.65	120.38
2	2	18	TYR	CA-C-N	6.08	126.64	120.38
2	2	18	TYR	C-N-CA	6.08	126.64	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	18	TYR	CA-C-N	6.04	126.61	120.38
2	T	18	TYR	C-N-CA	6.04	126.61	120.38
1	J	205	PHE	N-CA-C	6.00	118.71	110.01
6	6	120	ASN	N-CA-C	5.99	116.18	108.34
3	U	421	LYS	CA-C-N	5.94	126.50	120.38
3	U	421	LYS	C-N-CA	5.94	126.50	120.38
3	3	421	LYS	CA-C-N	5.93	126.49	120.38
3	3	421	LYS	C-N-CA	5.93	126.49	120.38
3	C	421	LYS	CA-C-N	5.92	126.48	120.38
3	C	421	LYS	C-N-CA	5.92	126.48	120.38
3	U	459	MET	N-CA-C	-5.86	106.09	113.18
1	A	205	PHE	N-CA-C	5.86	118.50	110.01
5	N	64	ARG	CA-C-N	5.86	127.16	119.84
5	N	64	ARG	C-N-CA	5.86	127.16	119.84
5	5	64	ARG	CA-C-N	5.85	127.15	119.84
5	5	64	ARG	C-N-CA	5.85	127.15	119.84
4	M	256	GLY	N-CA-C	-5.84	107.11	115.64
4	4	311	PRO	CA-C-N	5.83	126.39	120.38
4	4	311	PRO	C-N-CA	5.83	126.39	120.38
3	C	218	LEU	CA-C-N	5.81	127.10	119.84
3	C	218	LEU	C-N-CA	5.81	127.10	119.84
5	5	124	ILE	N-CA-C	5.80	116.50	108.84
1	S	205	PHE	N-CA-C	5.80	118.42	110.01
5	N	124	ILE	N-CA-C	5.78	116.46	108.84
5	5	94	VAL	N-CA-C	5.76	113.25	107.55
1	A	331	ILE	CA-C-N	5.74	126.22	120.14
1	A	331	ILE	C-N-CA	5.74	126.22	120.14
5	E	124	ILE	N-CA-C	5.73	116.41	108.84
4	D	309	ILE	CB-CA-C	-5.73	104.43	110.62
8	Z	73	SER	CA-C-N	5.73	125.73	119.89
8	Z	73	SER	C-N-CA	5.73	125.73	119.89
3	C	422	PRO	CA-C-N	5.68	126.00	119.92
3	C	422	PRO	C-N-CA	5.68	126.00	119.92
3	C	230	CYS	CA-C-N	5.67	126.05	119.47
3	C	230	CYS	C-N-CA	5.67	126.05	119.47
4	V	309	ILE	CB-CA-C	-5.67	104.49	110.62
6	F	170	LEU	CA-C-N	5.67	126.22	120.38
6	F	170	LEU	C-N-CA	5.67	126.22	120.38
8	H	73	SER	CA-C-N	5.66	125.67	119.90
8	H	73	SER	C-N-CA	5.66	125.67	119.90
3	U	218	LEU	CA-C-N	5.62	126.86	119.84
3	U	218	LEU	C-N-CA	5.62	126.86	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	291	ILE	CA-C-N	5.61	126.86	119.84
1	1	291	ILE	C-N-CA	5.61	126.86	119.84
8	Q	73	SER	CA-C-N	5.61	125.61	119.89
8	Q	73	SER	C-N-CA	5.61	125.61	119.89
6	X	120	ASN	N-CA-C	5.60	115.67	108.34
3	L	218	LEU	CA-C-N	5.59	126.83	119.84
3	L	218	LEU	C-N-CA	5.59	126.83	119.84
3	3	459	MET	N-CA-C	-5.59	106.42	113.18
5	E	94	VAL	N-CA-C	5.58	113.08	107.55
6	F	120	ASN	N-CA-C	5.58	115.64	108.34
2	K	18	TYR	CA-C-N	5.57	126.12	120.38
2	K	18	TYR	C-N-CA	5.57	126.12	120.38
2	2	172	CYS	N-CA-C	5.56	117.48	108.26
2	T	73	VAL	CA-C-N	5.56	126.78	119.84
2	T	73	VAL	C-N-CA	5.56	126.78	119.84
3	L	764	GLY	CA-C-N	5.55	126.78	119.84
3	L	764	GLY	C-N-CA	5.55	126.78	119.84
4	4	298	GLU	CA-C-N	5.54	126.76	119.84
4	4	298	GLU	C-N-CA	5.54	126.76	119.84
5	N	104	VAL	N-CA-C	-5.52	107.35	112.43
7	Y	29	ALA	CA-C-N	5.49	125.49	119.89
7	Y	29	ALA	C-N-CA	5.49	125.49	119.89
2	2	73	VAL	CA-C-N	5.47	126.68	119.84
2	2	73	VAL	C-N-CA	5.47	126.68	119.84
4	M	311	PRO	CA-C-N	5.47	126.01	120.38
4	M	311	PRO	C-N-CA	5.47	126.01	120.38
1	A	97	GLU	CA-C-N	5.45	125.77	119.93
1	A	97	GLU	C-N-CA	5.45	125.77	119.93
5	W	94	VAL	N-CA-C	5.45	112.94	107.55
3	3	184	CYS	CA-C-N	-5.44	113.94	122.65
3	3	184	CYS	C-N-CA	-5.44	113.94	122.65
7	9	155	LYS	CA-C-N	5.43	126.63	119.84
7	9	155	LYS	C-N-CA	5.43	126.63	119.84
6	6	170	LEU	CA-C-N	5.41	125.95	120.38
6	6	170	LEU	C-N-CA	5.41	125.95	120.38
4	V	298	GLU	CA-C-N	5.41	126.61	119.84
4	V	298	GLU	C-N-CA	5.41	126.61	119.84
4	D	257	TYR	N-CA-C	-5.41	105.78	112.38
4	D	311	PRO	CA-C-N	5.41	125.95	120.38
4	D	311	PRO	C-N-CA	5.41	125.95	120.38
5	E	104	VAL	N-CA-C	-5.39	107.47	112.43
3	U	764	GLY	CA-C-N	5.39	126.58	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	764	GLY	C-N-CA	5.39	126.58	119.84
3	3	566	ALA	N-CA-C	5.38	117.58	109.23
7	P	155	LYS	CA-C-N	5.38	126.57	119.84
7	P	155	LYS	C-N-CA	5.38	126.57	119.84
2	K	73	VAL	CA-C-N	5.38	126.56	119.84
2	K	73	VAL	C-N-CA	5.38	126.56	119.84
1	J	331	ILE	CA-C-N	5.36	125.82	120.14
1	J	331	ILE	C-N-CA	5.36	125.82	120.14
5	W	104	VAL	N-CA-C	-5.36	107.50	112.43
3	C	246	ASN	N-CA-C	5.35	117.87	111.71
4	M	298	GLU	CA-C-N	5.33	126.51	119.84
4	M	298	GLU	C-N-CA	5.33	126.51	119.84
2	T	19	PRO	CA-C-N	5.33	124.84	119.19
2	T	19	PRO	C-N-CA	5.33	124.84	119.19
8	Z	30	ARG	N-CA-C	5.32	117.94	109.96
3	C	11	VAL	N-CA-C	5.32	116.32	108.45
3	U	566	ALA	N-CA-C	5.31	117.47	109.23
7	G	155	LYS	CA-C-N	5.31	126.48	119.84
7	G	155	LYS	C-N-CA	5.31	126.48	119.84
1	J	97	GLU	CA-C-N	5.30	126.47	119.84
1	J	97	GLU	C-N-CA	5.30	126.47	119.84
5	W	62	ASP	CA-C-N	5.30	125.29	119.89
5	W	62	ASP	C-N-CA	5.30	125.29	119.89
8	H	108	ILE	N-CA-C	5.29	113.18	108.63
4	M	224	ILE	CA-C-N	5.29	125.83	120.38
4	M	224	ILE	C-N-CA	5.29	125.83	120.38
3	C	764	GLY	CA-C-N	5.29	126.45	119.84
3	C	764	GLY	C-N-CA	5.29	126.45	119.84
6	F	137	VAL	CA-C-N	5.27	125.25	120.03
6	F	137	VAL	C-N-CA	5.27	125.25	120.03
6	O	137	VAL	CA-C-N	5.26	125.55	119.92
6	O	137	VAL	C-N-CA	5.26	125.55	119.92
3	3	684	ARG	CA-C-N	5.25	125.25	120.21
3	3	684	ARG	C-N-CA	5.25	125.25	120.21
2	K	19	PRO	CA-C-N	5.25	124.76	119.19
2	K	19	PRO	C-N-CA	5.25	124.76	119.19
3	3	11	VAL	N-CA-C	5.25	116.22	108.45
1	J	137	GLU	N-CA-C	-5.23	107.27	113.97
6	6	137	VAL	CA-C-N	5.22	125.51	119.92
6	6	137	VAL	C-N-CA	5.22	125.51	119.92
8	7	73	SER	CA-C-N	5.22	125.22	119.89
8	7	73	SER	C-N-CA	5.22	125.22	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	11	VAL	N-CA-C	5.21	116.16	108.45
4	4	224	ILE	CA-C-N	5.20	125.74	120.38
4	4	224	ILE	C-N-CA	5.20	125.74	120.38
3	L	566	ALA	N-CA-C	5.20	117.29	109.23
1	1	137	GLU	N-CA-C	-5.20	107.32	113.97
1	S	5	ILE	N-CA-C	5.20	116.20	108.46
4	V	300	GLY	CA-C-N	5.20	125.40	120.31
4	V	300	GLY	C-N-CA	5.20	125.40	120.31
7	9	63	CYS	CA-C-N	5.19	125.65	120.04
7	9	63	CYS	C-N-CA	5.19	125.65	120.04
2	T	172	CYS	N-CA-C	5.17	116.84	108.26
7	Y	155	LYS	CA-C-N	5.17	126.30	119.84
7	Y	155	LYS	C-N-CA	5.17	126.30	119.84
3	U	406	ALA	CA-C-N	5.17	126.30	119.84
3	U	406	ALA	C-N-CA	5.17	126.30	119.84
2	K	56	THR	CA-C-N	5.16	124.95	119.28
2	K	56	THR	C-N-CA	5.16	124.95	119.28
1	A	129	VAL	N-CA-C	5.15	115.33	108.27
8	Z	45	GLU	N-CA-C	-5.14	106.51	112.89
5	N	94	VAL	N-CA-C	5.14	112.64	107.55
1	J	5	ILE	N-CA-C	5.13	116.11	108.46
3	3	669	VAL	CA-C-N	5.11	126.22	119.84
3	3	669	VAL	C-N-CA	5.11	126.22	119.84
3	C	566	ALA	N-CA-C	5.11	117.15	109.23
2	K	172	CYS	N-CA-C	5.10	116.72	108.26
3	L	684	ARG	CA-C-N	5.10	125.10	120.21
3	L	684	ARG	C-N-CA	5.10	125.10	120.21
4	4	257	TYR	N-CA-C	-5.09	106.17	112.38
4	4	256	GLY	N-CA-C	-5.09	108.21	115.64
8	Q	108	ILE	N-CA-C	5.09	113.01	108.63
2	B	73	VAL	CA-C-N	5.09	126.20	119.84
2	B	73	VAL	C-N-CA	5.09	126.20	119.84
3	U	11	VAL	N-CA-C	5.08	115.97	108.45
3	C	282	VAL	CA-C-N	5.08	125.36	119.47
3	C	282	VAL	C-N-CA	5.08	125.36	119.47
8	H	86	LEU	CA-C-N	5.06	125.00	119.78
8	H	86	LEU	C-N-CA	5.06	125.00	119.78
3	U	230	CYS	CA-C-N	5.06	125.34	119.47
3	U	230	CYS	C-N-CA	5.06	125.34	119.47
3	L	230	CYS	CA-C-N	5.06	125.34	119.47
3	L	230	CYS	C-N-CA	5.06	125.34	119.47
3	3	764	GLY	CA-C-N	5.05	126.16	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	764	GLY	C-N-CA	5.05	126.16	119.84
8	7	30	ARG	N-CA-C	5.05	117.53	109.96
5	N	172	ALA	N-CA-C	-5.04	107.30	113.50
8	Z	108	ILE	N-CA-C	5.04	112.96	108.63
8	H	45	GLU	N-CA-C	-5.03	106.66	112.89
7	P	101	CYS	N-CA-C	-5.03	107.28	113.41
5	W	144	HIS	CA-C-N	5.03	126.12	119.84
5	W	144	HIS	C-N-CA	5.03	126.12	119.84
8	Q	30	ARG	N-CA-C	5.02	117.48	109.96
3	C	406	ALA	CA-C-N	5.01	126.11	119.84
3	C	406	ALA	C-N-CA	5.01	126.11	119.84

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	1	3417	0	3388	211	0
1	A	3417	0	3388	217	0
1	J	3417	0	3388	218	0
1	S	3417	0	3388	205	0
2	2	1406	0	1373	75	0
2	B	1406	0	1373	79	0
2	K	1406	0	1373	77	0
2	T	1406	0	1373	79	0
3	3	5880	0	5911	370	0
3	C	5880	0	5911	370	0
3	L	5880	0	5911	373	0
3	U	5880	0	5911	386	0
4	4	3011	0	3000	271	0
4	D	3011	0	3000	288	0
4	M	3011	0	3000	263	0
4	V	3011	0	3000	290	0
5	5	1607	0	1574	112	0
5	E	1607	0	1574	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	1607	0	1574	110	0
5	W	1607	0	1574	131	0
6	6	1113	0	1121	111	0
6	F	1113	0	1121	111	0
6	O	1113	0	1121	110	0
6	X	1113	0	1121	116	0
7	9	1193	0	1160	77	0
7	G	1193	0	1160	77	0
7	P	1193	0	1160	77	0
7	Y	1193	0	1160	74	0
8	7	1031	0	1029	50	0
8	H	1031	0	1029	58	0
8	Q	1031	0	1029	55	0
8	Z	1031	0	1029	50	0
9	1	8	0	0	0	0
9	3	24	0	0	3	0
9	6	8	0	0	2	0
9	9	16	0	0	2	0
9	A	8	0	0	1	0
9	C	24	0	0	1	0
9	F	8	0	0	3	0
9	G	16	0	0	2	0
9	J	8	0	0	0	0
9	L	24	0	0	3	0
9	O	8	0	0	2	0
9	P	16	0	0	2	0
9	S	8	0	0	0	0
9	U	24	0	0	2	0
9	X	8	0	0	3	0
9	Y	16	0	0	0	0
10	1	31	0	19	7	0
10	A	31	0	19	6	0
10	J	31	0	19	8	0
10	S	31	0	19	6	0
11	2	4	0	0	1	0
11	3	4	0	0	0	0
11	B	4	0	0	1	0
11	C	4	0	0	1	0
11	K	4	0	0	1	0
11	L	4	0	0	0	0
11	T	4	0	0	1	0
11	U	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	2	1	0	0	0	0
12	3	2	0	0	0	0
12	9	1	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	G	1	0	0	0	0
12	H	1	0	0	0	0
12	K	1	0	0	0	0
12	L	2	0	0	0	0
12	P	1	0	0	0	0
12	T	1	0	0	0	0
12	U	1	0	0	0	0
12	Y	1	0	0	0	0
12	Z	1	0	0	0	0
All	All	75028	0	74300	4758	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (4758) 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)
4:D:188:PRO:HB3	3:U:724:ARG:CD	1.63	1.27
3:C:46:ARG:HG2	3:C:46:ARG:HH11	1.05	1.19
3:C:474:ARG:NH2	3:C:516:VAL:HG21	1.62	1.13
6:X:145:GLU:HG2	7:Y:31:VAL:HG21	1.31	1.11
4:D:188:PRO:CB	3:U:724:ARG:HD2	1.81	1.11
3:3:46:ARG:HG2	3:3:46:ARG:HH11	0.98	1.10
3:U:474:ARG:NH2	3:U:516:VAL:HG21	1.67	1.09
3:L:474:ARG:NH2	3:L:516:VAL:HG21	1.67	1.09
5:5:5:ARG:HH11	5:5:5:ARG:HG3	1.17	1.07
5:W:121:LEU:HB3	5:W:146:LEU:HB2	1.36	1.06
3:L:46:ARG:HG2	3:L:46:ARG:HH11	0.94	1.05
3:3:474:ARG:NH2	3:3:516:VAL:HG21	1.71	1.04
5:N:5:ARG:HG3	5:N:5:ARG:HH11	1.19	1.03
5:5:121:LEU:HB3	5:5:146:LEU:HB2	1.39	1.02
5:E:5:ARG:HH11	5:E:5:ARG:HG3	1.22	1.02
7:Y:41:HIS:HB3	7:Y:113:ILE:HD11	1.42	1.02
5:N:121:LEU:HB3	5:N:146:LEU:HB2	1.38	1.02
7:P:41:HIS:HB3	7:P:113:ILE:HD11	1.42	1.02
3:U:46:ARG:HG2	3:U:46:ARG:HH11	0.93	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:5:ARG:HH11	5:W:5:ARG:HG3	1.19	1.02
5:E:121:LEU:HB3	5:E:146:LEU:HB2	1.42	1.01
4:D:72:HIS:O	4:D:73:ARG:HD2	1.60	1.01
4:V:72:HIS:O	4:V:73:ARG:HD2	1.60	1.01
1:1:185:GLU:HB2	1:1:218:ILE:HD12	1.38	1.01
4:M:350:ARG:HE	4:M:403:VAL:HG23	1.22	1.00
1:S:293:GLY:HA3	1:S:324:GLY:H	1.24	1.00
1:1:293:GLY:HA3	1:1:324:GLY:H	1.26	1.00
4:M:72:HIS:O	4:M:73:ARG:HD2	1.60	1.00
3:C:117:LEU:N	4:D:321:MET:HE1	1.76	1.00
3:U:501:LYS:H	3:U:501:LYS:HD2	1.24	1.00
4:D:350:ARG:HE	4:D:403:VAL:HG23	1.27	1.00
1:J:293:GLY:HA3	1:J:324:GLY:H	1.26	0.99
4:M:129:HIS:CE1	4:M:349:ALA:HB1	1.97	0.99
7:9:41:HIS:HB3	7:9:113:ILE:HD11	1.44	0.99
4:4:72:HIS:O	4:4:73:ARG:HD2	1.61	0.99
3:U:117:LEU:N	4:V:321:MET:HE1	1.77	0.98
3:3:117:LEU:N	4:4:321:MET:HE1	1.77	0.98
1:A:293:GLY:HA3	1:A:324:GLY:H	1.27	0.98
3:3:87:VAL:HA	3:3:91:MET:HE1	1.45	0.98
3:L:501:LYS:H	3:L:501:LYS:HD2	1.26	0.98
6:6:145:GLU:HG2	7:9:31:VAL:HG21	1.45	0.98
5:E:193:ARG:HG2	5:E:193:ARG:HH11	1.27	0.98
5:W:145:PRO:HA	5:W:150:TYR:CD2	1.99	0.98
3:3:501:LYS:H	3:3:501:LYS:HD2	1.27	0.97
3:U:46:ARG:HG2	3:U:46:ARG:NH1	1.72	0.97
3:C:501:LYS:H	3:C:501:LYS:HD2	1.28	0.97
4:V:350:ARG:HE	4:V:403:VAL:HG23	1.28	0.97
1:S:437:TRP:HB3	2:T:92:GLY:HA3	1.46	0.97
4:V:254:TYR:HD1	4:V:255:SER:H	1.12	0.96
6:F:145:GLU:HG2	7:G:31:VAL:HG21	1.47	0.95
1:1:437:TRP:HB3	2:2:92:GLY:HA3	1.47	0.95
3:L:715:GLU:H	3:L:761:SER:HB2	1.31	0.95
6:O:145:GLU:HG2	7:P:31:VAL:HG21	1.48	0.95
3:3:715:GLU:H	3:3:761:SER:HB2	1.31	0.95
7:G:41:HIS:HB3	7:G:113:ILE:HD11	1.45	0.95
1:S:185:GLU:HB2	1:S:218:ILE:HD12	1.49	0.95
2:B:31:LEU:HD12	2:B:41:ILE:HD13	1.48	0.94
4:4:350:ARG:HE	4:4:403:VAL:HG23	1.28	0.94
3:L:136:GLU:HG2	5:N:189:ARG:HG2	1.48	0.94
2:T:31:LEU:HD12	2:T:41:ILE:HD13	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:212:PRO:HG2	4:V:213:ILE:HD12	1.50	0.94
5:N:42:LYS:HB3	5:N:107:LEU:HD13	1.46	0.94
4:D:188:PRO:HB3	3:U:724:ARG:HD2	0.95	0.93
4:D:212:PRO:HG2	4:D:213:ILE:HD12	1.50	0.93
5:W:42:LYS:HB3	5:W:107:LEU:HD13	1.50	0.93
4:D:129:HIS:CE1	4:D:349:ALA:HB1	2.02	0.93
5:N:145:PRO:HA	5:N:150:TYR:CD2	2.03	0.93
2:2:31:LEU:HD12	2:2:41:ILE:HD13	1.51	0.93
5:5:145:PRO:HA	5:5:150:TYR:CD2	2.02	0.93
3:L:87:VAL:HA	3:L:91:MET:HE1	1.47	0.93
5:5:42:LYS:HB3	5:5:107:LEU:HD13	1.48	0.93
5:W:193:ARG:HH11	5:W:193:ARG:HG2	1.28	0.93
5:E:42:LYS:HB3	5:E:107:LEU:HD13	1.50	0.93
3:3:509:ALA:HB1	3:3:768:GLY:HA3	1.52	0.93
6:6:19:ILE:HD11	1:J:271:THR:HG21	1.51	0.93
4:D:225:PRO:HG2	4:D:228:VAL:HB	1.51	0.92
2:K:31:LEU:HD12	2:K:41:ILE:HD13	1.50	0.92
3:L:117:LEU:N	4:M:321:MET:HE1	1.83	0.92
4:4:254:TYR:HD1	4:4:255:SER:H	1.14	0.92
3:C:87:VAL:HA	3:C:91:MET:HE1	1.48	0.92
5:N:193:ARG:HG2	5:N:193:ARG:HH11	1.31	0.92
5:5:193:ARG:HG2	5:5:193:ARG:HH11	1.33	0.92
3:3:655:ARG:HB2	3:3:655:ARG:HH11	1.35	0.92
3:L:561:PRO:HB3	3:L:576:ALA:HA	1.48	0.92
5:E:175:THR:HG23	5:E:178:ASP:HB2	1.51	0.92
4:M:254:TYR:HD1	4:M:255:SER:H	1.15	0.92
4:4:367:ARG:NH1	4:4:369:LYS:HB2	1.85	0.92
4:4:129:HIS:CE1	4:4:349:ALA:HB1	2.03	0.92
3:3:561:PRO:HB3	3:3:576:ALA:HA	1.49	0.92
3:C:715:GLU:H	3:C:761:SER:HB2	1.34	0.92
1:A:185:GLU:HB2	1:A:218:ILE:HD12	1.49	0.92
3:C:509:ALA:HB1	3:C:768:GLY:HA3	1.52	0.91
5:E:145:PRO:HA	5:E:150:TYR:CD2	2.04	0.91
3:U:715:GLU:H	3:U:761:SER:HB2	1.32	0.91
3:U:561:PRO:HB3	3:U:576:ALA:HA	1.52	0.91
4:4:212:PRO:HG2	4:4:213:ILE:HD12	1.50	0.91
7:P:40:ARG:HB2	7:P:121:MET:HE1	1.52	0.91
4:V:367:ARG:NH1	4:V:369:LYS:HB2	1.86	0.91
3:3:46:ARG:HG2	3:3:46:ARG:NH1	1.77	0.91
3:3:413:LEU:HD13	3:3:448:MET:HE1	1.50	0.91
3:L:46:ARG:HG2	3:L:46:ARG:NH1	1.73	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:185:GLU:HB2	1:J:218:ILE:HD12	1.50	0.90
6:X:163:TYR:HE1	7:Y:152:ARG:HD2	1.35	0.90
4:D:254:TYR:HD1	4:D:255:SER:H	1.14	0.90
3:L:509:ALA:HB1	3:L:768:GLY:HA3	1.53	0.90
4:V:318:GLU:HB2	8:Z:39:ASP:HA	1.52	0.90
6:6:108:MET:HE1	6:6:147:LEU:HG	1.54	0.90
3:C:117:LEU:H	4:D:321:MET:HE1	1.35	0.90
5:W:175:THR:HG23	5:W:178:ASP:HB2	1.54	0.90
3:U:738:THR:HG22	3:U:739:PRO:HD2	1.54	0.89
4:V:254:TYR:CE2	4:V:346:THR:HA	2.06	0.89
1:S:90:ILE:HD11	1:S:211:LEU:HD22	1.53	0.89
3:U:655:ARG:HH11	3:U:655:ARG:HB2	1.37	0.89
6:X:108:MET:HE1	6:X:147:LEU:HG	1.52	0.89
3:U:87:VAL:HA	3:U:91:MET:HE1	1.54	0.89
3:C:136:GLU:HG2	5:E:189:ARG:HG2	1.54	0.89
4:V:225:PRO:HG2	4:V:228:VAL:HB	1.54	0.89
1:A:437:TRP:HB3	2:B:92:GLY:HA3	1.54	0.89
3:C:561:PRO:HB3	3:C:576:ALA:HA	1.54	0.88
5:5:175:THR:HG23	5:5:178:ASP:HB2	1.54	0.88
6:F:108:MET:HE1	6:F:147:LEU:HG	1.56	0.88
3:L:655:ARG:HB2	3:L:655:ARG:HH11	1.38	0.88
7:9:40:ARG:HB2	7:9:121:MET:HE1	1.54	0.88
4:M:225:PRO:HG2	4:M:228:VAL:HB	1.51	0.88
4:V:129:HIS:CE1	4:V:349:ALA:HB1	2.09	0.88
4:4:225:PRO:HG2	4:4:228:VAL:HB	1.52	0.88
7:Y:33:LEU:HD11	7:Y:161:TYR:HB2	1.55	0.88
1:J:437:TRP:HB3	2:K:92:GLY:HA3	1.56	0.88
4:M:367:ARG:NH1	4:M:369:LYS:HB2	1.88	0.88
5:W:26:TRP:NE1	5:W:91:ARG:HH21	1.71	0.88
3:L:413:LEU:HD13	3:L:448:MET:HE1	1.53	0.88
3:L:738:THR:HG22	3:L:739:PRO:HD2	1.56	0.88
4:M:212:PRO:HG2	4:M:213:ILE:HD12	1.53	0.88
7:G:40:ARG:HB2	7:G:121:MET:HE1	1.56	0.87
3:3:117:LEU:H	4:4:321:MET:HE1	1.36	0.87
5:N:42:LYS:HD3	5:N:107:LEU:HD22	1.55	0.87
3:C:55:PRO:HG3	3:C:74:GLN:N	1.90	0.87
3:C:738:THR:HG22	3:C:739:PRO:HD2	1.56	0.87
3:U:509:ALA:HB1	3:U:768:GLY:HA3	1.54	0.87
3:C:655:ARG:HB2	3:C:655:ARG:HH11	1.40	0.87
6:X:81:ALA:HA	6:X:108:MET:HB3	1.57	0.87
6:O:108:MET:HE1	6:O:147:LEU:HG	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:413:LEU:HD13	3:C:448:MET:HE1	1.56	0.87
7:Y:40:ARG:HB2	7:Y:121:MET:HE1	1.53	0.87
3:3:738:THR:HG22	3:3:739:PRO:HD2	1.57	0.86
5:W:103:THR:HG22	5:W:126:PHE:HB3	1.57	0.86
3:C:46:ARG:HG2	3:C:46:ARG:NH1	1.84	0.86
4:D:318:GLU:HB2	8:H:39:ASP:HA	1.57	0.86
2:B:139:GLU:HB2	2:B:140:PRO:HD2	1.56	0.86
1:J:90:ILE:HD11	1:J:211:LEU:HD22	1.55	0.86
4:4:314:ARG:HG2	4:4:314:ARG:HH11	1.40	0.86
3:U:55:PRO:HG3	3:U:74:GLN:N	1.90	0.86
2:2:139:GLU:HB2	2:2:140:PRO:HD2	1.56	0.86
1:S:16:THR:HG21	1:S:229:PRO:HB3	1.57	0.86
6:6:19:ILE:HD11	1:J:271:THR:CG2	2.06	0.85
6:X:163:TYR:CE1	7:Y:152:ARG:HD2	2.10	0.85
3:U:413:LEU:HD13	3:U:448:MET:HE1	1.56	0.85
5:5:103:THR:HG22	5:5:126:PHE:HB3	1.56	0.85
1:A:90:ILE:HD11	1:A:211:LEU:HD22	1.57	0.85
5:E:103:THR:HG22	5:E:126:PHE:HB3	1.56	0.85
3:L:55:PRO:HG3	3:L:74:GLN:N	1.90	0.85
6:X:145:GLU:HG2	7:Y:31:VAL:CG2	2.05	0.85
5:W:5:ARG:HG3	5:W:5:ARG:NH1	1.88	0.85
3:3:136:GLU:HG2	5:5:189:ARG:HG2	1.57	0.85
3:L:538:ALA:HB3	3:L:541:ALA:HB2	1.56	0.85
3:U:136:GLU:HG2	5:W:189:ARG:HG2	1.58	0.85
3:L:694:LEU:HB3	3:L:762:ALA:HB2	1.57	0.85
4:M:254:TYR:CE2	4:M:346:THR:HA	2.12	0.85
5:N:103:THR:HG22	5:N:126:PHE:HB3	1.57	0.85
3:U:117:LEU:H	4:V:321:MET:HE1	1.37	0.85
3:3:55:PRO:HG3	3:3:74:GLN:N	1.92	0.85
4:D:61:TYR:HB3	6:F:88:MET:HE2	1.58	0.85
5:E:193:ARG:HH11	5:E:193:ARG:CG	1.90	0.84
7:G:33:LEU:HD11	7:G:161:TYR:HB2	1.58	0.84
3:3:244:ALA:HB3	3:3:249:MET:HE2	1.59	0.84
5:N:5:ARG:HG3	5:N:5:ARG:NH1	1.88	0.84
2:K:139:GLU:HB2	2:K:140:PRO:HD2	1.58	0.84
3:L:360:LEU:O	3:L:364:LEU:HB3	1.77	0.84
1:S:397:ARG:HE	3:U:79:LEU:HD12	1.42	0.84
5:W:193:ARG:HH11	5:W:193:ARG:CG	1.91	0.84
5:N:175:THR:HG23	5:N:178:ASP:HB2	1.59	0.84
4:D:314:ARG:HH11	4:D:314:ARG:HG2	1.41	0.84
6:F:163:TYR:CE1	7:G:152:ARG:HD2	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:33:LEU:HD11	7:P:161:TYR:HB2	1.59	0.84
2:T:139:GLU:HB2	2:T:140:PRO:HD2	1.58	0.84
3:U:694:LEU:HB3	3:U:762:ALA:HB2	1.60	0.84
1:1:16:THR:HG21	1:1:229:PRO:HB3	1.59	0.83
4:D:88:LEU:HD21	6:F:48:ILE:HD13	1.60	0.83
7:9:33:LEU:HD11	7:9:161:TYR:HB2	1.59	0.83
1:J:16:THR:HG21	1:J:229:PRO:HB3	1.58	0.83
3:U:360:LEU:O	3:U:364:LEU:HB3	1.78	0.83
3:3:567:TYR:HA	3:3:584:VAL:HG23	1.60	0.83
5:5:42:LYS:HD3	5:5:107:LEU:HD22	1.58	0.83
1:A:16:THR:HG21	1:A:229:PRO:HB3	1.57	0.83
3:C:567:TYR:HA	3:C:584:VAL:HG23	1.61	0.83
3:C:694:LEU:HB3	3:C:762:ALA:HB2	1.58	0.83
5:W:16:PRO:HD2	5:W:28:VAL:HG13	1.61	0.83
3:L:216:PHE:HZ	8:Q:128:PHE:CD2	1.96	0.83
3:3:216:PHE:HZ	8:7:128:PHE:CD2	1.96	0.83
3:3:285:VAL:HG13	3:3:286:ASN:H	1.43	0.83
3:C:614:LEU:HD11	3:C:624:LEU:HD12	1.60	0.83
4:D:94:ASP:HB3	4:D:173:ILE:HG21	1.60	0.83
5:N:193:ARG:HH11	5:N:193:ARG:CG	1.92	0.83
3:L:567:TYR:HA	3:L:584:VAL:HG23	1.60	0.83
1:1:184:GLU:OE1	1:1:186:THR:HG22	1.79	0.82
3:3:374:ARG:NH2	3:3:684:ARG:HG3	1.94	0.82
4:4:254:TYR:CE2	4:4:346:THR:HA	2.14	0.82
4:D:367:ARG:NH1	4:D:369:LYS:HB2	1.94	0.82
4:M:94:ASP:HB3	4:M:173:ILE:HG21	1.60	0.82
5:5:5:ARG:HG3	5:5:5:ARG:NH1	1.85	0.82
4:V:314:ARG:HG2	4:V:314:ARG:HH11	1.42	0.82
4:D:254:TYR:CE2	4:D:346:THR:HA	2.14	0.82
3:3:694:LEU:HB3	3:3:762:ALA:HB2	1.61	0.82
3:3:360:LEU:O	3:3:364:LEU:HB3	1.80	0.82
1:1:90:ILE:HD11	1:1:211:LEU:HD22	1.61	0.82
5:E:5:ARG:HG3	5:E:5:ARG:NH1	1.90	0.82
5:E:26:TRP:NE1	5:E:91:ARG:HH21	1.76	0.82
3:U:386:SER:HB2	3:U:675:ARG:NH1	1.95	0.82
4:4:367:ARG:HH12	4:4:369:LYS:HB2	1.45	0.82
1:A:33:LEU:HD23	1:A:37:GLY:HA3	1.61	0.82
5:E:42:LYS:HD3	5:E:107:LEU:HD22	1.61	0.82
3:3:614:LEU:HD11	3:3:624:LEU:HD12	1.62	0.81
6:6:163:TYR:HD2	6:6:169:ARG:HA	1.45	0.81
2:B:7:LYS:H	2:B:7:LYS:HD2	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:193:ARG:HG2	5:W:193:ARG:NH1	1.90	0.81
3:C:244:ALA:HB3	3:C:249:MET:HE2	1.63	0.81
5:W:52:ILE:HG23	5:W:114:LEU:HB3	1.62	0.81
3:3:538:ALA:HB3	3:3:541:ALA:HB2	1.60	0.81
4:M:314:ARG:HG2	4:M:314:ARG:HH11	1.45	0.81
4:V:94:ASP:HB3	4:V:173:ILE:HG21	1.61	0.81
6:6:81:ALA:HA	6:6:108:MET:HB3	1.63	0.81
3:U:567:TYR:HA	3:U:584:VAL:HG23	1.62	0.81
5:E:193:ARG:HG2	5:E:193:ARG:NH1	1.90	0.81
2:K:79:HIS:ND1	2:K:118:SER:HB2	1.96	0.81
3:L:115:HIS:CG	3:L:116:PRO:HD2	2.16	0.81
3:C:206:GLY:O	3:C:209:THR:HG23	1.81	0.80
5:5:16:PRO:HD2	5:5:28:VAL:HG13	1.63	0.80
3:3:115:HIS:CG	3:3:116:PRO:HD2	2.16	0.80
1:A:310:PRO:HG2	1:A:315:HIS:CD2	2.16	0.80
4:M:235:THR:HA	4:M:239:LEU:HD12	1.64	0.80
3:U:538:ALA:HB3	3:U:541:ALA:HB2	1.64	0.80
5:W:42:LYS:HD3	5:W:107:LEU:HD22	1.63	0.80
4:4:235:THR:HA	4:4:239:LEU:HD12	1.64	0.80
3:C:538:ALA:HB3	3:C:541:ALA:HB2	1.61	0.80
6:F:163:TYR:HD2	6:F:169:ARG:HA	1.47	0.80
3:3:46:ARG:HH11	3:3:46:ARG:CG	1.89	0.80
5:5:193:ARG:HH11	5:5:193:ARG:CG	1.94	0.80
2:K:7:LYS:H	2:K:7:LYS:HD2	1.46	0.80
3:L:11:VAL:HG11	3:L:25:HIS:CD2	2.16	0.80
3:L:374:ARG:NH2	3:L:684:ARG:HG3	1.97	0.80
1:S:33:LEU:HD23	1:S:37:GLY:HA3	1.63	0.80
5:5:193:ARG:HG2	5:5:193:ARG:NH1	1.94	0.80
6:F:81:ALA:HA	6:F:108:MET:HB3	1.61	0.80
6:O:99:MET:HG2	6:O:100:PRO:HD2	1.61	0.80
4:4:94:ASP:HB3	4:4:173:ILE:HG21	1.62	0.80
5:5:52:ILE:HG23	5:5:114:LEU:HB3	1.64	0.80
5:E:52:ILE:HG23	5:E:114:LEU:HB3	1.64	0.80
5:N:52:ILE:HG23	5:N:114:LEU:HB3	1.63	0.80
3:U:115:HIS:HB3	4:V:321:MET:HE3	1.64	0.80
6:X:163:TYR:HD2	6:X:169:ARG:HA	1.45	0.80
3:3:545:GLU:HA	3:3:550:LEU:HD11	1.63	0.80
3:C:515:THR:HG23	3:C:683:LEU:HD12	1.62	0.80
5:N:193:ARG:HG2	5:N:193:ARG:NH1	1.93	0.80
3:U:374:ARG:NH2	3:U:684:ARG:HG3	1.95	0.80
6:O:163:TYR:HD2	6:O:169:ARG:HA	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:115:HIS:CG	3:U:116:PRO:HD2	2.18	0.79
1:1:33:LEU:HD23	1:1:37:GLY:HA3	1.64	0.79
3:C:474:ARG:HH21	3:C:516:VAL:HG21	1.43	0.79
3:C:545:GLU:HA	3:C:550:LEU:HD11	1.65	0.79
3:L:11:VAL:HG11	3:L:25:HIS:HD2	1.46	0.79
3:L:614:LEU:HD11	3:L:624:LEU:HD12	1.64	0.79
5:N:26:TRP:NE1	5:N:91:ARG:HH21	1.81	0.79
2:T:110:GLU:HA	8:Z:121:ARG:HH12	1.47	0.79
6:F:96:TRP:HA	6:F:99:MET:HE3	1.65	0.79
5:E:80:TRP:HA	5:E:80:TRP:CE3	2.16	0.79
4:M:350:ARG:NE	4:M:403:VAL:HG23	1.96	0.79
6:O:81:ALA:HA	6:O:108:MET:HB3	1.65	0.79
3:U:205:ARG:HA	3:U:209:THR:HG22	1.64	0.79
2:B:79:HIS:ND1	2:B:118:SER:HB2	1.97	0.79
3:C:285:VAL:HG13	3:C:286:ASN:H	1.45	0.79
3:U:285:VAL:HG13	3:U:286:ASN:H	1.48	0.79
2:K:146:THR:HG23	2:K:149:ARG:HB2	1.63	0.79
7:Y:26:TYR:N	7:Y:27:PRO:HD3	1.97	0.79
2:2:7:LYS:H	2:2:7:LYS:HD2	1.48	0.79
7:9:26:TYR:N	7:9:27:PRO:HD3	1.97	0.78
3:C:20:MET:HE3	3:C:432:PHE:HB3	1.65	0.78
3:C:360:LEU:O	3:C:364:LEU:HB3	1.82	0.78
3:C:386:SER:HB2	3:C:675:ARG:NH1	1.97	0.78
4:D:64:THR:HG23	6:F:123:ILE:HD11	1.65	0.78
3:L:205:ARG:HA	3:L:209:THR:HG22	1.65	0.78
6:X:143:ARG:HG2	6:X:145:GLU:OE1	1.83	0.78
5:5:80:TRP:HA	5:5:80:TRP:CE3	2.18	0.78
3:3:11:VAL:HG11	3:3:25:HIS:HD2	1.48	0.78
1:A:184:GLU:OE1	1:A:186:THR:HG22	1.83	0.78
2:B:146:THR:HG23	2:B:149:ARG:HB2	1.65	0.78
5:N:80:TRP:CE3	5:N:80:TRP:HA	2.19	0.78
3:L:515:THR:HG23	3:L:683:LEU:HD12	1.64	0.78
2:T:79:HIS:ND1	2:T:118:SER:HB2	1.99	0.78
3:3:11:VAL:HG11	3:3:25:HIS:CD2	2.19	0.78
6:6:99:MET:HG2	6:6:100:PRO:HD2	1.63	0.78
4:M:61:TYR:HB3	6:O:88:MET:HE2	1.63	0.78
4:V:105:LEU:HB3	4:V:337:PRO:HB3	1.65	0.78
3:L:386:SER:HB2	3:L:675:ARG:NH1	1.98	0.78
5:W:39:ALA:HA	5:W:107:LEU:HD12	1.64	0.78
6:X:99:MET:HG2	6:X:100:PRO:HD2	1.65	0.78
4:4:88:LEU:HD21	6:6:48:ILE:HD13	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:163:TYR:HE1	7:G:152:ARG:HD2	1.47	0.78
1:S:184:GLU:OE1	1:S:186:THR:HG22	1.84	0.78
5:E:16:PRO:HD2	5:E:28:VAL:HG13	1.64	0.78
3:L:206:GLY:O	3:L:209:THR:HG23	1.84	0.78
1:1:243:THR:HG22	1:1:244:GLU:H	1.49	0.78
4:4:371:ARG:HG3	5:5:51:ASP:OD1	1.83	0.77
3:U:11:VAL:HG11	3:U:25:HIS:CD2	2.19	0.77
4:V:350:ARG:NE	4:V:403:VAL:HG23	1.99	0.77
6:X:148:ILE:HG21	7:Y:27:PRO:HG3	1.64	0.77
3:3:205:ARG:HA	3:3:209:THR:HG22	1.66	0.77
5:5:39:ALA:HA	5:5:107:LEU:HD12	1.65	0.77
3:U:409:LEU:HD12	3:U:535:MET:HE2	1.66	0.77
4:4:74:THR:HG22	4:4:76:LEU:H	1.49	0.77
3:L:545:GLU:HA	3:L:550:LEU:HD11	1.65	0.77
4:V:235:THR:HA	4:V:239:LEU:HD12	1.67	0.77
1:J:33:LEU:HD23	1:J:37:GLY:HA3	1.64	0.77
5:5:26:TRP:NE1	5:5:91:ARG:HH21	1.83	0.77
3:L:409:LEU:HD12	3:L:535:MET:HE2	1.67	0.77
4:4:234:LEU:O	4:4:239:LEU:HG	1.84	0.77
3:C:205:ARG:HA	3:C:209:THR:HG22	1.67	0.77
3:C:614:LEU:HD11	3:C:624:LEU:CD1	2.14	0.77
4:M:367:ARG:HH12	4:M:369:LYS:HB2	1.48	0.77
6:X:96:TRP:HA	6:X:99:MET:HE3	1.65	0.77
3:L:117:LEU:H	4:M:321:MET:HE1	1.48	0.77
4:V:222:GLY:HA3	4:V:396:ILE:HD11	1.67	0.77
3:3:440:ARG:HG2	3:3:440:ARG:HH11	1.48	0.77
4:D:167:ARG:HD3	6:F:143:ARG:HH12	1.50	0.77
3:U:545:GLU:HA	3:U:550:LEU:HD11	1.64	0.77
3:U:614:LEU:HD11	3:U:624:LEU:HD12	1.67	0.77
5:W:80:TRP:HA	5:W:80:TRP:CE3	2.17	0.77
4:D:350:ARG:NE	4:D:403:VAL:HG23	1.99	0.77
2:T:7:LYS:H	2:T:7:LYS:HD2	1.50	0.77
4:V:367:ARG:HH12	4:V:369:LYS:HB2	1.47	0.77
3:U:244:ALA:HB3	3:U:249:MET:HE2	1.66	0.77
3:3:614:LEU:HD11	3:3:624:LEU:CD1	2.15	0.76
5:5:175:THR:O	5:5:177:LYS:N	2.18	0.76
5:E:39:ALA:HA	5:E:107:LEU:HD12	1.66	0.76
1:A:139:ARG:HG2	2:B:140:PRO:HD3	1.67	0.76
3:3:206:GLY:O	3:3:209:THR:HG23	1.84	0.76
1:A:16:THR:HG21	1:A:229:PRO:CB	2.15	0.76
1:J:184:GLU:OE1	1:J:186:THR:HG22	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:11:VAL:HG11	3:U:25:HIS:HD2	1.50	0.76
2:T:146:THR:HG23	2:T:149:ARG:HB2	1.67	0.76
3:U:474:ARG:HH21	3:U:516:VAL:HG21	1.50	0.76
4:4:389:GLN:HG3	4:4:391:PRO:HD2	1.68	0.76
3:C:115:HIS:CG	3:C:116:PRO:HD2	2.20	0.76
7:G:26:TYR:N	7:G:27:PRO:HD3	2.00	0.76
4:M:222:GLY:HA3	4:M:396:ILE:HD11	1.67	0.76
4:4:89:HIS:CE1	4:4:92:ALA:HB2	2.20	0.76
3:C:11:VAL:HG11	3:C:25:HIS:HD2	1.51	0.76
1:J:192:LEU:HD22	1:J:211:LEU:HD11	1.67	0.76
1:S:192:LEU:HD22	1:S:211:LEU:HD11	1.68	0.76
1:S:243:THR:HG22	1:S:244:GLU:H	1.50	0.76
3:C:11:VAL:HG11	3:C:25:HIS:CD2	2.20	0.76
6:O:143:ARG:HG2	6:O:145:GLU:OE1	1.84	0.75
4:V:59:ILE:HD11	5:W:135:ILE:HG23	1.66	0.75
1:1:253:GLN:HG2	1:1:327:GLY:HA2	1.69	0.75
2:K:139:GLU:CB	2:K:140:PRO:HD2	2.16	0.75
3:L:244:ALA:HB3	3:L:249:MET:HE2	1.68	0.75
8:Z:121:ARG:HH11	8:Z:121:ARG:HG3	1.50	0.75
3:U:614:LEU:HD11	3:U:624:LEU:CD1	2.17	0.75
6:X:164:ASN:HB2	7:Y:128:ASP:OD2	1.85	0.75
3:C:157:PHE:CE1	3:C:159:PHE:HB2	2.20	0.75
5:E:80:TRP:HA	5:E:80:TRP:HE3	1.50	0.75
3:3:386:SER:HB2	3:3:675:ARG:NH1	2.01	0.75
3:L:474:ARG:HH21	3:L:516:VAL:HG21	1.47	0.75
2:2:139:GLU:CB	2:2:140:PRO:HD2	2.16	0.75
6:6:96:TRP:HA	6:6:99:MET:HE3	1.68	0.75
2:B:139:GLU:CB	2:B:140:PRO:HD2	2.15	0.75
7:G:175:ALA:O	7:G:177:THR:HG23	1.86	0.75
1:J:243:THR:HG22	1:J:244:GLU:H	1.51	0.75
3:L:614:LEU:HD11	3:L:624:LEU:CD1	2.17	0.75
4:D:105:LEU:HB3	4:D:337:PRO:HB3	1.69	0.75
2:T:139:GLU:CB	2:T:140:PRO:HD2	2.16	0.75
3:3:515:THR:HG23	3:3:683:LEU:HD12	1.67	0.75
6:F:148:ILE:HG21	7:G:27:PRO:HG3	1.69	0.75
4:M:341:GLU:HG2	4:M:358:VAL:HG22	1.69	0.75
4:V:252:TYR:HE2	5:W:87:ARG:HH21	1.35	0.75
8:7:121:ARG:HH11	8:7:121:ARG:HG3	1.49	0.75
7:P:26:TYR:N	7:P:27:PRO:HD3	2.01	0.75
6:X:114:SER:HB2	7:Y:97:ARG:HD2	1.69	0.75
4:M:105:LEU:HB3	4:M:337:PRO:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:THR:HG22	1:A:244:GLU:H	1.51	0.74
3:C:115:HIS:HB3	4:D:321:MET:HE3	1.69	0.74
1:J:370:LEU:O	1:J:374:ILE:HG22	1.88	0.74
5:W:175:THR:O	5:W:177:LYS:N	2.20	0.74
4:4:371:ARG:HH22	4:4:376:VAL:HG21	1.52	0.74
4:V:241:ALA:HA	4:V:278:VAL:HG21	1.69	0.74
1:1:107:LEU:O	1:1:111:PRO:HG3	1.86	0.74
4:D:371:ARG:HH22	4:D:376:VAL:HG21	1.53	0.74
4:D:389:GLN:HG3	4:D:391:PRO:HD2	1.70	0.74
6:F:99:MET:HG2	6:F:100:PRO:HD2	1.69	0.74
1:1:397:ARG:HE	3:3:79:LEU:HD12	1.53	0.74
6:6:163:TYR:CE1	7:9:152:ARG:HD2	2.22	0.74
4:4:222:GLY:HA3	4:4:396:ILE:HD11	1.69	0.74
4:M:389:GLN:HG3	4:M:391:PRO:HD2	1.70	0.74
3:3:409:LEU:HD12	3:3:535:MET:HE2	1.70	0.74
5:5:5:ARG:HH11	5:5:5:ARG:CG	1.99	0.74
5:N:66:GLU:CG	5:N:95:PRO:HA	2.17	0.74
4:V:234:LEU:O	4:V:239:LEU:HG	1.88	0.74
4:M:234:LEU:O	4:M:239:LEU:HG	1.87	0.74
3:U:157:PHE:CE1	3:U:159:PHE:HB2	2.23	0.74
4:4:120:LEU:HD13	4:4:160:PHE:HE1	1.53	0.74
8:H:121:ARG:HH11	8:H:121:ARG:HG3	1.52	0.74
4:M:371:ARG:HG3	5:N:51:ASP:OD1	1.87	0.73
5:N:13:LYS:HZ3	5:N:33:ARG:HH21	1.36	0.73
2:2:146:THR:HG23	2:2:149:ARG:HB2	1.69	0.73
5:5:80:TRP:HA	5:5:80:TRP:HE3	1.52	0.73
4:D:235:THR:HA	4:D:239:LEU:HD12	1.69	0.73
3:L:556:ALA:HB2	3:L:562:GLY:HA3	1.69	0.73
3:U:20:MET:HE3	3:U:432:PHE:HB3	1.69	0.73
3:3:115:HIS:HB3	4:4:321:MET:HE3	1.70	0.73
5:W:80:TRP:HA	5:W:80:TRP:HE3	1.52	0.73
3:3:474:ARG:HH21	3:3:516:VAL:HG21	1.51	0.73
4:4:350:ARG:NE	4:4:403:VAL:HG23	2.01	0.73
6:6:148:ILE:HG21	7:9:27:PRO:HG3	1.69	0.73
3:U:46:ARG:HH11	3:U:46:ARG:CG	1.85	0.73
1:1:16:THR:HG21	1:1:229:PRO:CB	2.18	0.73
4:D:89:HIS:CE1	4:D:92:ALA:HB2	2.24	0.73
6:X:112:ALA:O	6:X:127:VAL:HG23	1.89	0.73
6:6:145:GLU:HG2	7:9:31:VAL:CG2	2.19	0.73
3:L:157:PHE:CE1	3:L:159:PHE:HB2	2.23	0.73
4:4:236:GLY:HA2	4:4:351:GLY:HA3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:556:ALA:HB2	3:C:562:GLY:HA3	1.70	0.73
3:L:229:ILE:HD11	3:L:289:TRP:CZ3	2.24	0.73
6:O:163:TYR:CE1	7:P:152:ARG:HD2	2.23	0.73
1:S:246:SER:HB3	1:S:268:MET:HG2	1.71	0.73
1:1:246:SER:HB3	1:1:268:MET:HG2	1.70	0.73
3:3:157:PHE:CE1	3:3:159:PHE:HB2	2.23	0.73
3:C:374:ARG:NH2	3:C:684:ARG:HG3	2.02	0.73
4:D:367:ARG:HH12	4:D:369:LYS:HB2	1.53	0.72
3:L:55:PRO:HG2	3:L:73:ILE:N	2.05	0.72
1:J:253:GLN:HG2	1:J:327:GLY:HA2	1.71	0.72
6:O:96:TRP:HA	6:O:99:MET:HE3	1.69	0.72
1:1:192:LEU:HD22	1:1:211:LEU:HD11	1.71	0.72
5:E:1:MET:SD	8:Z:113:GLU:CD	2.71	0.72
5:E:13:LYS:HZ3	5:E:33:ARG:HH21	1.37	0.72
1:S:16:THR:HG21	1:S:229:PRO:CB	2.19	0.72
3:C:684:ARG:HG2	3:C:684:ARG:HH11	1.54	0.72
3:L:440:ARG:HG2	3:L:440:ARG:HH11	1.53	0.72
1:A:192:LEU:HD22	1:A:211:LEU:HD11	1.70	0.72
5:N:80:TRP:HA	5:N:80:TRP:HE3	1.53	0.72
1:S:6:LEU:HD21	1:S:12:ARG:HG3	1.72	0.72
3:3:629:ILE:HG22	3:3:630:GLU:H	1.54	0.72
6:6:143:ARG:HG2	6:6:145:GLU:OE1	1.88	0.72
4:M:250:LYS:HE2	4:M:262:PHE:HB3	1.70	0.72
3:U:497:TRP:NE1	3:U:524:LEU:HD11	2.04	0.72
2:2:110:GLU:HA	8:7:121:ARG:HH12	1.54	0.72
4:4:61:TYR:HB3	6:6:88:MET:HE2	1.70	0.72
4:M:47:LEU:HD13	4:M:52:VAL:HA	1.70	0.72
5:N:16:PRO:HD2	5:N:28:VAL:HG13	1.72	0.72
5:N:175:THR:O	5:N:177:LYS:N	2.23	0.72
4:V:74:THR:HG22	4:V:76:LEU:H	1.54	0.72
4:V:371:ARG:HH22	4:V:376:VAL:HG21	1.54	0.72
5:W:13:LYS:HZ3	5:W:33:ARG:HH21	1.36	0.72
4:4:224:ILE:HD11	4:4:275:ARG:NH1	2.05	0.72
5:5:66:GLU:CG	5:5:95:PRO:HA	2.19	0.72
5:E:175:THR:O	5:E:177:LYS:N	2.22	0.72
1:J:310:PRO:HG2	1:J:315:HIS:CD2	2.25	0.72
3:L:629:ILE:HG22	3:L:630:GLU:H	1.55	0.72
3:U:515:THR:HG23	3:U:683:LEU:HD12	1.72	0.72
4:D:234:LEU:O	4:D:239:LEU:HG	1.88	0.72
6:F:41:PHE:CE2	6:F:92:MET:HB2	2.24	0.72
1:J:139:ARG:HG2	2:K:140:PRO:HD3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:190:LEU:O	4:M:194:LEU:HB2	1.90	0.72
4:V:389:GLN:HG3	4:V:391:PRO:HD2	1.70	0.72
4:4:105:LEU:HB3	4:4:337:PRO:HB3	1.71	0.71
4:4:314:ARG:HG2	4:4:314:ARG:NH1	2.05	0.71
3:C:629:ILE:HG22	3:C:630:GLU:H	1.53	0.71
4:D:74:THR:HG22	4:D:76:LEU:H	1.54	0.71
4:M:74:THR:HG22	4:M:76:LEU:H	1.54	0.71
5:N:39:ALA:HA	5:N:107:LEU:HD12	1.70	0.71
3:U:55:PRO:HG2	3:U:73:ILE:N	2.04	0.71
3:3:398:VAL:HB	3:3:450:LEU:HD22	1.71	0.71
6:6:163:TYR:HE1	7:9:152:ARG:HD2	1.54	0.71
3:C:229:ILE:HD11	3:C:289:TRP:CZ3	2.26	0.71
2:K:122:VAL:HG12	2:K:123:GLU:H	1.54	0.71
4:M:88:LEU:HD21	6:O:48:ILE:HD13	1.71	0.71
4:V:236:GLY:HA2	4:V:351:GLY:HA3	1.72	0.71
3:3:31:PRO:HB2	3:3:47:MET:HB3	1.72	0.71
1:S:310:PRO:HG2	1:S:315:HIS:CD2	2.24	0.71
3:U:31:PRO:HB2	3:U:47:MET:HB3	1.72	0.71
4:V:88:LEU:HD21	6:X:48:ILE:HD13	1.72	0.71
3:3:55:PRO:HG2	3:3:73:ILE:N	2.06	0.71
3:C:31:PRO:HB2	3:C:47:MET:HB3	1.71	0.71
3:C:55:PRO:HG2	3:C:73:ILE:N	2.04	0.71
3:U:206:GLY:O	3:U:209:THR:HG23	1.90	0.71
3:L:203:ILE:HG22	3:L:204:GLU:N	2.05	0.71
2:T:134:ILE:HG13	2:T:145:VAL:HG21	1.72	0.71
2:2:79:HIS:ND1	2:2:118:SER:HB2	2.05	0.71
4:D:254:TYR:O	4:D:256:GLY:N	2.23	0.71
4:M:241:ALA:HA	4:M:278:VAL:HG21	1.71	0.71
1:J:107:LEU:O	1:J:111:PRO:HG3	1.90	0.71
1:J:246:SER:HB3	1:J:268:MET:HG2	1.71	0.71
2:K:110:GLU:HA	8:Q:121:ARG:HH12	1.55	0.71
3:U:556:ALA:HB2	3:U:562:GLY:HA3	1.73	0.71
3:3:655:ARG:HB2	3:3:655:ARG:NH1	2.05	0.71
4:4:252:TYR:HE2	5:5:87:ARG:HH21	1.37	0.71
2:B:122:VAL:HG12	2:B:123:GLU:H	1.54	0.71
4:M:64:THR:HG23	6:O:123:ILE:HD11	1.72	0.71
4:M:89:HIS:CE1	4:M:92:ALA:HB2	2.26	0.71
3:3:556:ALA:HB2	3:3:562:GLY:HA3	1.71	0.71
3:L:285:VAL:HG13	3:L:286:ASN:H	1.55	0.71
4:M:120:LEU:HD13	4:M:160:PHE:HE1	1.56	0.71
4:M:224:ILE:HD11	4:M:275:ARG:NH1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:40:ARG:HB2	7:P:121:MET:CE	2.19	0.71
5:W:66:GLU:CG	5:W:95:PRO:HA	2.21	0.71
6:X:41:PHE:CE2	6:X:92:MET:HB2	2.26	0.71
2:T:122:VAL:HG12	2:T:123:GLU:H	1.55	0.70
1:A:253:GLN:HG2	1:A:327:GLY:HA2	1.73	0.70
4:D:222:GLY:HA3	4:D:396:ILE:HD11	1.72	0.70
6:O:148:ILE:HG21	7:P:27:PRO:HG3	1.73	0.70
1:A:219:ASN:HD22	1:A:223:THR:HG21	1.56	0.70
4:M:236:GLY:HA2	4:M:351:GLY:HA3	1.73	0.70
3:C:112:LEU:HD12	4:D:322:GLU:HG3	1.71	0.70
5:E:66:GLU:CG	5:E:95:PRO:HA	2.22	0.70
6:F:143:ARG:HG2	6:F:145:GLU:OE1	1.91	0.70
6:F:145:GLU:HG2	7:G:31:VAL:CG2	2.20	0.70
8:Q:121:ARG:HG3	8:Q:121:ARG:HH11	1.54	0.70
7:Y:175:ALA:O	7:Y:177:THR:HG23	1.92	0.70
3:3:216:PHE:HZ	8:7:128:PHE:HD2	1.37	0.70
4:4:341:GLU:HG2	4:4:358:VAL:HG22	1.74	0.70
3:L:46:ARG:HH11	3:L:46:ARG:CG	1.85	0.70
4:V:85:MET:HE3	4:V:409:ARG:HG3	1.71	0.70
3:3:285:VAL:HG13	3:3:286:ASN:N	2.05	0.70
4:4:236:GLY:HA2	4:4:351:GLY:CA	2.22	0.70
6:6:163:TYR:HB3	6:6:168:GLU:O	1.91	0.70
4:V:84:ARG:NE	6:X:117:MET:HE1	2.06	0.70
7:9:40:ARG:HB2	7:9:121:MET:CE	2.21	0.70
4:D:85:MET:HE3	4:D:409:ARG:HG3	1.72	0.70
3:L:20:MET:HE3	3:L:432:PHE:HB3	1.73	0.70
4:4:59:ILE:HD11	5:5:135:ILE:HG23	1.72	0.70
3:C:337:ARG:H	3:C:337:ARG:HD2	1.56	0.70
4:D:64:THR:HG23	6:F:123:ILE:CD1	2.21	0.70
4:M:254:TYR:O	4:M:256:GLY:N	2.22	0.70
1:S:289:ALA:HB3	1:S:337:MET:HE3	1.74	0.70
4:V:238:SER:HB3	4:V:279:ARG:NH2	2.07	0.70
3:3:229:ILE:HD11	3:3:289:TRP:CZ3	2.27	0.70
3:C:508:GLY:O	3:C:512:LEU:HB2	1.92	0.70
3:C:550:LEU:HB3	3:C:684:ARG:HH21	1.57	0.70
3:L:402:PRO:HG3	3:L:535:MET:HE1	1.74	0.70
3:U:337:ARG:H	3:U:337:ARG:HD2	1.55	0.70
1:A:397:ARG:H	1:A:397:ARG:HD2	1.56	0.69
3:L:186:ARG:HD3	3:L:229:ILE:HG22	1.73	0.69
4:4:367:ARG:HH12	4:4:369:LYS:CB	2.05	0.69
7:P:34:LYS:HB3	7:P:35:PRO:HD2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:216:PHE:HZ	8:Z:128:PHE:CD2	2.09	0.69
7:Y:40:ARG:HB2	7:Y:121:MET:CE	2.21	0.69
1:J:397:ARG:HE	3:L:79:LEU:HD12	1.58	0.69
3:L:216:PHE:HZ	8:Q:128:PHE:HD2	1.38	0.69
4:V:47:LEU:HD13	4:V:52:VAL:HA	1.74	0.69
3:3:20:MET:HE3	3:3:432:PHE:HB3	1.73	0.69
1:A:370:LEU:O	1:A:374:ILE:HG22	1.93	0.69
3:L:603:PRO:HB2	3:L:634:ALA:HB2	1.73	0.69
3:L:684:ARG:HG2	3:L:684:ARG:HH11	1.55	0.69
6:O:145:GLU:HG2	7:P:31:VAL:CG2	2.22	0.69
1:S:139:ARG:HG2	2:T:140:PRO:HD3	1.75	0.69
4:4:241:ALA:HA	4:4:278:VAL:HG21	1.73	0.69
2:B:110:GLU:HA	8:H:121:ARG:HH12	1.58	0.69
4:D:120:LEU:HD13	4:D:160:PHE:HE1	1.57	0.69
3:L:229:ILE:HD11	3:L:289:TRP:HZ3	1.57	0.69
3:L:534:ALA:HB3	3:L:542:ARG:HH12	1.56	0.69
4:M:239:LEU:HD22	4:M:244:VAL:HB	1.74	0.69
6:O:163:TYR:HB3	6:O:168:GLU:O	1.93	0.69
3:U:229:ILE:HD11	3:U:289:TRP:CZ3	2.27	0.69
3:3:684:ARG:HG2	3:3:684:ARG:HH11	1.56	0.69
4:4:85:MET:HE3	4:4:409:ARG:HG3	1.74	0.69
1:J:65:ARG:CZ	1:J:268:MET:HE1	2.21	0.69
4:M:129:HIS:HE1	4:M:349:ALA:HB1	1.57	0.69
1:S:393:LEU:HD22	3:U:106:GLY:HA3	1.75	0.69
4:V:213:ILE:HG21	4:V:217:ARG:HH11	1.58	0.69
1:1:397:ARG:H	1:1:397:ARG:HD2	1.57	0.69
3:3:171:SER:HB2	3:3:172:PRO:HD2	1.75	0.69
3:3:337:ARG:H	3:3:337:ARG:HD2	1.55	0.69
7:9:34:LYS:HB3	7:9:35:PRO:HD2	1.74	0.69
3:C:440:ARG:HG2	3:C:440:ARG:HH11	1.58	0.69
1:J:16:THR:HG21	1:J:229:PRO:CB	2.22	0.69
4:M:85:MET:HE3	4:M:409:ARG:HG3	1.72	0.69
1:1:289:ALA:HB3	1:1:337:MET:HE3	1.75	0.69
4:4:190:LEU:O	4:4:194:LEU:HB2	1.92	0.69
6:6:112:ALA:O	6:6:127:VAL:HG23	1.92	0.69
1:A:246:SER:HB3	1:A:268:MET:HG2	1.74	0.69
3:C:203:ILE:HG22	3:C:204:GLU:N	2.06	0.69
4:D:236:GLY:HA2	4:D:351:GLY:HA3	1.73	0.69
7:G:45:ARG:NH2	7:G:137:LEU:HD23	2.07	0.69
3:L:31:PRO:HB2	3:L:47:MET:HB3	1.75	0.69
4:M:314:ARG:HG2	4:M:314:ARG:NH1	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:66:GLU:HG3	5:N:95:PRO:HA	1.73	0.69
3:U:655:ARG:HB2	3:U:655:ARG:NH1	2.07	0.69
4:4:105:LEU:HD23	4:4:337:PRO:HG3	1.74	0.69
3:L:31:PRO:HG3	3:L:137:TYR:CD1	2.28	0.69
1:S:438:ARG:H	1:S:438:ARG:HD2	1.57	0.69
3:C:285:VAL:HG13	3:C:286:ASN:N	2.08	0.69
3:C:716:LEU:HD21	3:C:758:LEU:HB3	1.74	0.69
1:S:55:GLU:O	1:S:59:ARG:HB2	1.93	0.69
3:U:440:ARG:HH11	3:U:440:ARG:HG2	1.58	0.69
3:C:438:LYS:O	3:C:441:MET:HG3	1.93	0.68
7:G:40:ARG:HB2	7:G:121:MET:CE	2.23	0.68
1:S:370:LEU:O	1:S:374:ILE:HG22	1.92	0.68
3:U:438:LYS:O	3:U:441:MET:HG3	1.92	0.68
6:X:153:GLN:HG3	7:Y:124:TYR:CZ	2.28	0.68
4:D:167:ARG:HD3	6:F:143:ARG:NH1	2.08	0.68
1:J:65:ARG:NH2	1:J:268:MET:HE1	2.08	0.68
1:S:397:ARG:H	1:S:397:ARG:HD2	1.57	0.68
4:4:250:LYS:HE2	4:4:262:PHE:HB3	1.74	0.68
1:A:351:GLU:HA	3:C:205:ARG:HH12	1.58	0.68
4:V:254:TYR:HD1	4:V:255:SER:N	1.87	0.68
4:D:47:LEU:HD13	4:D:52:VAL:HA	1.75	0.68
4:D:190:LEU:O	4:D:194:LEU:HB2	1.94	0.68
7:G:34:LYS:HB3	7:G:35:PRO:HD2	1.74	0.68
3:U:31:PRO:HG3	3:U:137:TYR:CD1	2.29	0.68
3:U:550:LEU:HB3	3:U:684:ARG:HH21	1.58	0.68
1:1:310:PRO:HG2	1:1:315:HIS:CD2	2.29	0.68
2:2:122:VAL:HG12	2:2:123:GLU:H	1.57	0.68
4:4:318:GLU:HB2	8:7:39:ASP:HA	1.74	0.68
7:9:175:ALA:O	7:9:177:THR:HG23	1.92	0.68
3:L:508:GLY:O	3:L:512:LEU:HB2	1.94	0.68
3:U:629:ILE:HG22	3:U:630:GLU:H	1.58	0.68
4:V:254:TYR:O	4:V:256:GLY:N	2.25	0.68
4:D:252:TYR:HE2	5:E:87:ARG:HH21	1.39	0.68
1:J:289:ALA:HB3	1:J:337:MET:HE3	1.76	0.68
3:L:337:ARG:H	3:L:337:ARG:HD2	1.57	0.68
7:P:175:ALA:O	7:P:177:THR:HG23	1.92	0.68
1:1:55:GLU:O	1:1:59:ARG:HB2	1.93	0.68
4:4:254:TYR:O	4:4:256:GLY:N	2.23	0.68
4:M:371:ARG:HH22	4:M:376:VAL:HG21	1.58	0.68
5:N:18:GLU:HB2	5:N:26:TRP:HB2	1.76	0.68
6:O:165:GLU:HG2	7:P:148:ARG:HH11	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:47:LEU:HD13	4:4:52:VAL:HA	1.74	0.68
4:D:237:GLY:HA2	4:D:240:ARG:CZ	2.23	0.68
8:H:108:ILE:HG22	8:H:114:ARG:NH1	2.09	0.68
3:U:186:ARG:HD3	3:U:229:ILE:HG22	1.75	0.68
4:V:367:ARG:HH12	4:V:369:LYS:CB	2.06	0.68
5:5:13:LYS:NZ	5:5:33:ARG:HH21	1.90	0.68
4:V:250:LYS:HE2	4:V:262:PHE:HB3	1.76	0.68
3:3:203:ILE:HG22	3:3:204:GLU:N	2.08	0.68
3:3:550:LEU:HB3	3:3:684:ARG:HH21	1.59	0.68
4:D:236:GLY:HA2	4:D:351:GLY:CA	2.24	0.68
5:E:13:LYS:NZ	5:E:33:ARG:HH21	1.92	0.68
3:L:507:LEU:HD22	3:L:511:VAL:HG11	1.76	0.68
4:M:133:LEU:HD21	4:M:204:TYR:CD2	2.29	0.68
4:M:252:TYR:HE2	5:N:87:ARG:HH21	1.42	0.68
5:N:168:ALA:HA	5:N:171:ARG:NH1	2.09	0.68
1:S:253:GLN:HG2	1:S:327:GLY:HA2	1.75	0.68
4:V:371:ARG:HG3	5:W:51:ASP:OD1	1.93	0.68
3:3:6:VAL:HG12	3:3:7:ASN:N	2.08	0.67
3:3:507:LEU:HD22	3:3:511:VAL:HG11	1.76	0.67
4:4:254:TYR:HD1	4:4:255:SER:N	1.89	0.67
3:C:6:VAL:HG12	3:C:7:ASN:N	2.09	0.67
4:V:190:LEU:O	4:V:194:LEU:HB2	1.94	0.67
4:V:237:GLY:HA2	4:V:240:ARG:CZ	2.24	0.67
5:W:18:GLU:HB2	5:W:26:TRP:HB2	1.76	0.67
1:1:219:ASN:HD22	1:1:223:THR:HG21	1.59	0.67
5:5:66:GLU:HG3	5:5:95:PRO:HA	1.75	0.67
4:V:236:GLY:HA2	4:V:351:GLY:CA	2.24	0.67
3:C:171:SER:HB2	3:C:172:PRO:HD2	1.74	0.67
4:D:142:ALA:HB1	4:D:145:PRO:HG2	1.77	0.67
4:M:236:GLY:HA2	4:M:351:GLY:CA	2.24	0.67
4:V:350:ARG:O	4:V:373:PRO:HB2	1.95	0.67
5:W:66:GLU:HG3	5:W:95:PRO:HA	1.77	0.67
6:X:163:TYR:HB3	6:X:168:GLU:O	1.94	0.67
2:B:87:SER:HB3	11:B:182:FES:S2	2.35	0.67
2:B:134:ILE:HG13	2:B:145:VAL:HG21	1.76	0.67
3:C:655:ARG:HB2	3:C:655:ARG:NH1	2.10	0.67
3:C:229:ILE:HD11	3:C:289:TRP:HZ3	1.60	0.67
1:J:55:GLU:O	1:J:59:ARG:HB2	1.94	0.67
4:V:311:PRO:HD3	4:V:330:HIS:NE2	2.09	0.67
3:3:31:PRO:HG3	3:3:137:TYR:CD1	2.29	0.67
3:C:337:ARG:H	3:C:337:ARG:CD	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:371:ARG:HG3	5:E:51:ASP:OD1	1.94	0.67
1:S:397:ARG:HE	3:U:79:LEU:CD1	2.07	0.67
3:L:550:LEU:HB3	3:L:684:ARG:HH21	1.58	0.67
2:T:87:SER:HB3	11:T:182:FES:S2	2.34	0.67
4:V:213:ILE:HG21	4:V:217:ARG:NH1	2.10	0.67
1:1:139:ARG:HG2	2:2:140:PRO:HD3	1.75	0.67
3:3:716:LEU:HD21	3:3:758:LEU:HB3	1.76	0.67
3:C:216:PHE:HZ	8:H:128:PHE:CD2	2.12	0.67
1:J:267:PRO:HG2	1:J:270:THR:HG22	1.77	0.67
4:M:254:TYR:HD1	4:M:255:SER:N	1.90	0.67
3:U:337:ARG:H	3:U:337:ARG:CD	2.07	0.67
4:V:44:MET:HA	4:V:44:MET:CE	2.25	0.67
1:A:393:LEU:HD22	3:C:106:GLY:HA3	1.77	0.67
1:J:397:ARG:H	1:J:397:ARG:HD2	1.59	0.67
5:N:13:LYS:NZ	5:N:33:ARG:HH21	1.92	0.67
6:O:163:TYR:HE1	7:P:152:ARG:HD2	1.57	0.67
3:U:20:MET:HE3	3:U:432:PHE:CB	2.25	0.67
3:U:125:GLY:HA3	3:U:246:ASN:HD22	1.60	0.67
3:C:507:LEU:HD22	3:C:511:VAL:HG11	1.77	0.67
5:E:66:GLU:HG3	5:E:95:PRO:HA	1.77	0.67
1:J:6:LEU:HD21	1:J:12:ARG:HG3	1.77	0.67
4:V:89:HIS:CE1	4:V:92:ALA:HB2	2.29	0.67
1:1:370:LEU:O	1:1:374:ILE:HG22	1.95	0.66
4:D:224:ILE:HD11	4:D:275:ARG:NH1	2.11	0.66
1:J:438:ARG:H	1:J:438:ARG:HD2	1.60	0.66
3:U:285:VAL:HG13	3:U:286:ASN:N	2.09	0.66
1:1:6:LEU:HD21	1:1:12:ARG:HG3	1.77	0.66
6:F:114:SER:HB2	7:G:97:ARG:HD2	1.77	0.66
3:L:655:ARG:HB2	3:L:655:ARG:NH1	2.09	0.66
4:M:237:GLY:HA2	4:M:240:ARG:CZ	2.25	0.66
3:C:534:ALA:HB3	3:C:542:ARG:HH12	1.59	0.66
4:V:105:LEU:HD23	4:V:337:PRO:HG3	1.77	0.66
1:1:438:ARG:H	1:1:438:ARG:HD2	1.60	0.66
6:6:114:SER:HB2	7:9:97:ARG:HD2	1.77	0.66
1:J:393:LEU:HD22	3:L:106:GLY:HA3	1.77	0.66
1:S:219:ASN:HD22	1:S:223:THR:HG21	1.61	0.66
3:U:684:ARG:HG2	3:U:684:ARG:HH11	1.60	0.66
4:V:120:LEU:HD13	4:V:160:PHE:HE1	1.59	0.66
4:V:133:LEU:HD21	4:V:204:TYR:CD2	2.31	0.66
4:V:341:GLU:HG2	4:V:358:VAL:HG22	1.78	0.66
7:Y:48:ASN:HB2	7:Y:50:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:184:GLU:CD	1:1:186:THR:HG22	2.21	0.66
3:3:337:ARG:H	3:3:337:ARG:CD	2.08	0.66
1:A:6:LEU:HD21	1:A:12:ARG:HG3	1.78	0.66
1:A:107:LEU:O	1:A:111:PRO:HG3	1.96	0.66
3:C:497:TRP:NE1	3:C:524:LEU:HD11	2.11	0.66
4:D:44:MET:CE	4:D:44:MET:HA	2.26	0.66
7:G:153:THR:HG22	7:G:155:LYS:H	1.60	0.66
5:W:13:LYS:NZ	5:W:33:ARG:HH21	1.94	0.66
7:Y:153:THR:HG22	7:Y:155:LYS:H	1.61	0.66
3:3:534:ALA:HB3	3:3:542:ARG:HH12	1.59	0.66
4:4:225:PRO:CG	4:4:228:VAL:HB	2.26	0.66
1:A:184:GLU:CD	1:A:186:THR:HG22	2.21	0.66
4:D:59:ILE:HD11	5:E:135:ILE:HG23	1.78	0.66
1:S:65:ARG:CZ	1:S:268:MET:HE1	2.26	0.66
1:A:50:PRO:O	1:A:53:VAL:HG12	1.95	0.66
4:D:133:LEU:HD21	4:D:204:TYR:CD2	2.31	0.66
4:D:241:ALA:HA	4:D:278:VAL:HG21	1.77	0.66
1:J:110:VAL:N	1:J:111:PRO:HD3	2.11	0.66
4:M:40:VAL:HG22	4:M:40:VAL:O	1.96	0.66
4:V:239:LEU:HD22	4:V:244:VAL:HB	1.77	0.66
6:6:41:PHE:CE2	6:6:92:MET:HB2	2.30	0.66
3:C:398:VAL:HB	3:C:450:LEU:HD22	1.78	0.66
3:C:409:LEU:HD12	3:C:535:MET:HE2	1.77	0.66
4:D:213:ILE:HG21	4:D:217:ARG:HH11	1.61	0.66
4:D:225:PRO:CG	4:D:228:VAL:HB	2.25	0.66
5:E:135:ILE:HG22	5:E:136:LEU:HG	1.78	0.66
3:L:716:LEU:HD21	3:L:758:LEU:HB3	1.77	0.66
4:M:367:ARG:HH12	4:M:369:LYS:CB	2.08	0.66
1:S:184:GLU:CD	1:S:186:THR:HG22	2.21	0.66
1:S:214:LYS:O	1:S:216:THR:HG23	1.96	0.66
1:1:267:PRO:HG2	1:1:270:THR:HG22	1.78	0.66
3:3:87:VAL:HA	3:3:91:MET:CE	2.24	0.66
3:3:205:ARG:CA	3:3:209:THR:HG22	2.26	0.66
4:4:64:THR:HG23	6:6:123:ILE:HD11	1.77	0.66
4:D:250:LYS:HE2	4:D:262:PHE:HB3	1.77	0.66
4:M:44:MET:HA	4:M:44:MET:CE	2.26	0.66
3:U:398:VAL:HB	3:U:450:LEU:HD22	1.77	0.66
1:1:50:PRO:O	1:1:53:VAL:HG12	1.94	0.65
4:4:44:MET:HA	4:4:44:MET:CE	2.26	0.65
1:A:10:ASP:OD1	1:A:11:PRO:HD2	1.96	0.65
4:M:105:LEU:HD23	4:M:337:PRO:HG3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:253:GLN:N	1:S:253:GLN:HE21	1.95	0.65
7:P:48:ASN:HB2	7:P:50:LEU:HD23	1.78	0.65
3:U:507:LEU:HD22	3:U:511:VAL:HG11	1.77	0.65
4:V:249:ARG:HB3	4:V:257:TYR:HD1	1.60	0.65
3:3:186:ARG:HD3	3:3:229:ILE:HG22	1.78	0.65
3:3:402:PRO:HG3	3:3:535:MET:HE1	1.78	0.65
4:D:238:SER:HB3	4:D:279:ARG:NH2	2.11	0.65
6:O:41:PHE:CE2	6:O:92:MET:HB2	2.31	0.65
6:O:117:MET:HB3	7:P:99:ILE:HD13	1.79	0.65
4:V:142:ALA:HB1	4:V:145:PRO:HG2	1.79	0.65
7:Y:34:LYS:HB3	7:Y:35:PRO:HD2	1.78	0.65
3:3:497:TRP:NE1	3:3:524:LEU:HD11	2.12	0.65
6:F:112:ALA:O	6:F:127:VAL:HG23	1.96	0.65
3:L:6:VAL:HG12	3:L:7:ASN:N	2.11	0.65
4:V:213:ILE:HG22	4:V:217:ARG:CG	2.27	0.65
4:4:84:ARG:NE	6:6:117:MET:HE1	2.11	0.65
4:4:237:GLY:HA2	4:4:240:ARG:CZ	2.27	0.65
4:4:311:PRO:HD3	4:4:330:HIS:NE2	2.11	0.65
4:D:239:LEU:HD22	4:D:244:VAL:HB	1.78	0.65
4:M:213:ILE:HG21	4:M:217:ARG:HH11	1.61	0.65
3:3:384:PRO:HG3	3:3:542:ARG:HE	1.62	0.65
3:3:440:ARG:HH11	3:3:440:ARG:CG	2.09	0.65
4:D:105:LEU:HD23	4:D:337:PRO:HG3	1.77	0.65
4:D:254:TYR:HD1	4:D:255:SER:N	1.89	0.65
7:P:45:ARG:NH2	7:P:137:LEU:HD23	2.12	0.65
8:Q:108:ILE:HG22	8:Q:114:ARG:NH1	2.12	0.65
1:S:50:PRO:O	1:S:53:VAL:HG12	1.95	0.65
5:5:18:GLU:HB2	5:5:26:TRP:HB2	1.78	0.65
1:A:214:LYS:O	1:A:216:THR:HG23	1.96	0.65
1:A:267:PRO:HG2	1:A:270:THR:HG22	1.77	0.65
3:C:31:PRO:HG3	3:C:137:TYR:CD1	2.32	0.65
5:E:5:ARG:HH11	5:E:5:ARG:CG	2.04	0.65
6:F:163:TYR:HB3	6:F:168:GLU:O	1.97	0.65
1:S:397:ARG:NE	3:U:79:LEU:HD12	2.12	0.65
6:X:83:ARG:HA	6:X:111:CYS:HB3	1.78	0.65
4:4:133:LEU:HD21	4:4:204:TYR:CD2	2.32	0.65
1:A:366:PHE:CD1	1:A:370:LEU:HD21	2.31	0.65
3:U:229:ILE:HD11	3:U:289:TRP:HZ3	1.61	0.65
3:U:603:PRO:HB2	3:U:634:ALA:HB2	1.78	0.65
1:1:214:LYS:O	1:1:216:THR:HG23	1.96	0.65
1:A:438:ARG:HD2	1:A:438:ARG:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:219:ASN:HD22	1:J:223:THR:HG21	1.61	0.65
1:1:360:ARG:O	3:3:207:VAL:HG13	1.97	0.65
3:3:508:GLY:O	3:3:512:LEU:HB2	1.97	0.65
5:5:135:ILE:HG22	5:5:136:LEU:HG	1.77	0.65
3:U:534:ALA:HB3	3:U:542:ARG:HH12	1.62	0.65
1:1:110:VAL:N	1:1:111:PRO:HD3	2.13	0.64
3:C:20:MET:HE3	3:C:432:PHE:CB	2.26	0.64
7:G:48:ASN:HB2	7:G:50:LEU:HD23	1.79	0.64
7:P:153:THR:HG22	7:P:155:LYS:H	1.62	0.64
7:9:153:THR:HG22	7:9:155:LYS:H	1.62	0.64
4:D:314:ARG:HG2	4:D:314:ARG:NH1	2.05	0.64
3:L:115:HIS:HB3	4:M:321:MET:HE3	1.80	0.64
3:U:173:PHE:HB3	3:U:296:PHE:CE1	2.32	0.64
4:V:84:ARG:CD	6:X:117:MET:HE1	2.27	0.64
4:V:122:GLU:HB2	4:V:290:ILE:HD11	1.79	0.64
4:V:225:PRO:CG	4:V:228:VAL:HB	2.27	0.64
3:U:112:LEU:HD12	4:V:322:GLU:HG3	1.79	0.64
3:U:508:GLY:O	3:U:512:LEU:HB2	1.97	0.64
5:W:5:ARG:HH11	5:W:5:ARG:CG	2.01	0.64
1:1:186:THR:CG2	1:1:200:ARG:H	2.10	0.64
1:1:341:MET:HE1	1:1:409:PRO:HB2	1.78	0.64
3:L:87:VAL:HA	3:L:91:MET:CE	2.24	0.64
1:A:344:LEU:O	1:A:347:PHE:HB3	1.98	0.64
3:C:120:PRO:HG2	8:H:42:TYR:OH	1.97	0.64
4:D:371:ARG:NH2	4:D:376:VAL:HG21	2.12	0.64
1:J:50:PRO:O	1:J:53:VAL:HG12	1.96	0.64
3:L:205:ARG:CA	3:L:209:THR:HG22	2.28	0.64
3:L:337:ARG:H	3:L:337:ARG:CD	2.09	0.64
3:U:6:VAL:HG12	3:U:7:ASN:N	2.12	0.64
4:V:254:TYR:HE2	4:V:346:THR:HA	1.58	0.64
4:4:213:ILE:HG21	4:4:217:ARG:HH11	1.62	0.64
4:4:381:LEU:HD11	4:4:397:ILE:HG12	1.80	0.64
4:M:122:GLU:HB2	4:M:290:ILE:HD11	1.79	0.64
3:U:205:ARG:CA	3:U:209:THR:HG22	2.28	0.64
3:3:438:LYS:O	3:3:441:MET:HG3	1.98	0.64
1:A:364:ALA:HB1	3:C:207:VAL:HG22	1.79	0.64
3:C:603:PRO:HB2	3:C:634:ALA:HB2	1.80	0.64
4:D:40:VAL:O	4:D:40:VAL:HG22	1.98	0.64
3:L:715:GLU:HB3	3:L:746:ARG:CZ	2.27	0.64
4:M:102:GLU:HG2	4:M:175:ILE:O	1.98	0.64
4:M:142:ALA:HB1	4:M:145:PRO:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:104:VAL:HG12	5:N:108:TRP:HE3	1.63	0.64
1:S:316:LEU:HD12	1:S:323:LEU:HB2	1.80	0.64
1:1:393:LEU:HD22	3:3:106:GLY:HA3	1.80	0.64
3:3:300:TRP:CD1	3:3:300:TRP:H	2.16	0.64
4:4:239:LEU:HD22	4:4:244:VAL:HB	1.80	0.64
1:A:55:GLU:O	1:A:59:ARG:HB2	1.97	0.64
1:A:65:ARG:CZ	1:A:268:MET:HE1	2.27	0.64
1:A:253:GLN:N	1:A:253:GLN:HE21	1.96	0.64
4:D:213:ILE:HG21	4:D:217:ARG:NH1	2.13	0.64
4:D:249:ARG:HB3	4:D:257:TYR:HD1	1.63	0.64
6:6:77:VAL:HG22	6:6:104:TRP:HB2	1.79	0.64
1:A:110:VAL:N	1:A:111:PRO:HD3	2.13	0.64
3:C:30:VAL:HG22	3:C:48:CYS:HA	1.80	0.64
5:E:18:GLU:HB2	5:E:26:TRP:HB2	1.80	0.64
7:G:153:THR:HG22	7:G:155:LYS:N	2.11	0.64
4:V:371:ARG:NH2	4:V:376:VAL:HG21	2.12	0.64
4:D:84:ARG:HG2	9:F:182:SF4:S2	2.39	0.64
5:W:26:TRP:HE1	5:W:91:ARG:HH21	1.45	0.64
4:4:238:SER:HB3	4:4:279:ARG:NH2	2.12	0.63
3:C:402:PRO:HG3	3:C:535:MET:HE1	1.80	0.63
1:S:65:ARG:NH2	1:S:268:MET:HE1	2.13	0.63
1:S:115:ILE:O	1:S:119:ILE:HG13	1.98	0.63
3:U:171:SER:HB2	3:U:172:PRO:HD2	1.79	0.63
3:3:285:VAL:HG22	3:3:286:ASN:N	2.14	0.63
4:4:371:ARG:NH2	4:4:376:VAL:HG21	2.12	0.63
4:D:102:GLU:HG2	4:D:175:ILE:O	1.99	0.63
3:L:584:VAL:HG12	3:L:600:VAL:HB	1.80	0.63
7:Y:71:GLU:HB2	7:Y:90:VAL:HB	1.80	0.63
4:4:213:ILE:HD12	4:4:213:ILE:H	1.64	0.63
6:6:153:GLN:HG3	7:9:124:TYR:CZ	2.34	0.63
6:6:165:GLU:HG2	7:9:148:ARG:HH11	1.62	0.63
4:4:40:VAL:O	4:4:40:VAL:HG22	1.98	0.63
4:4:142:ALA:HB1	4:4:145:PRO:HG2	1.80	0.63
8:7:108:ILE:HG22	8:7:114:ARG:NH1	2.14	0.63
4:M:64:THR:HG23	6:O:123:ILE:CD1	2.28	0.63
1:S:344:LEU:O	1:S:347:PHE:HB3	1.99	0.63
4:V:64:THR:HG23	6:X:123:ILE:HD11	1.81	0.63
7:Y:153:THR:HG22	7:Y:155:LYS:N	2.13	0.63
1:A:186:THR:CG2	1:A:200:ARG:H	2.12	0.63
3:C:469:ARG:HB2	3:C:470:PRO:HD2	1.81	0.63
3:L:300:TRP:CD1	3:L:300:TRP:H	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:393:MET:O	4:M:396:ILE:HG22	1.99	0.63
5:N:71:VAL:HG11	5:N:89:PHE:HD2	1.64	0.63
3:U:30:VAL:HG22	3:U:48:CYS:HA	1.79	0.63
4:V:164:THR:OG1	4:V:170:HIS:HB3	1.99	0.63
1:1:65:ARG:CZ	1:1:268:MET:HE1	2.28	0.63
3:3:603:PRO:HB2	3:3:634:ALA:HB2	1.79	0.63
3:C:125:GLY:HA3	3:C:246:ASN:HD22	1.63	0.63
1:J:366:PHE:CD1	1:J:370:LEU:HD21	2.33	0.63
2:K:134:ILE:HG13	2:K:145:VAL:HG21	1.79	0.63
4:V:84:ARG:HD3	6:X:117:MET:HE1	1.80	0.63
8:Z:108:ILE:HG22	8:Z:114:ARG:NH1	2.14	0.63
1:1:332:PRO:HD2	2:2:90:LEU:HD23	1.80	0.63
3:3:317:LEU:HD22	3:3:317:LEU:N	2.13	0.63
3:C:509:ALA:HB1	3:C:768:GLY:CA	2.27	0.63
3:L:285:VAL:HG22	3:L:286:ASN:N	2.14	0.63
4:M:64:THR:HB	4:M:66:PHE:CE1	2.34	0.63
3:U:716:LEU:HD21	3:U:758:LEU:HB3	1.81	0.63
5:W:104:VAL:HG12	5:W:108:TRP:HE3	1.63	0.63
4:M:222:GLY:CA	4:M:396:ILE:HD11	2.28	0.63
3:U:509:ALA:HB1	3:U:768:GLY:CA	2.29	0.63
4:V:155:THR:HB	4:V:193:LEU:HD12	1.80	0.63
1:1:65:ARG:NH2	1:1:268:MET:HE1	2.13	0.63
1:1:364:ALA:HB1	3:3:207:VAL:HG22	1.81	0.63
3:3:30:VAL:HG22	3:3:48:CYS:HA	1.79	0.63
3:3:509:ALA:HB1	3:3:768:GLY:CA	2.27	0.63
5:5:13:LYS:HZ3	5:5:33:ARG:HH21	1.44	0.63
7:9:48:ASN:HB2	7:9:50:LEU:HD23	1.80	0.63
1:A:115:ILE:O	1:A:119:ILE:HG13	1.98	0.63
4:D:140:LEU:O	4:D:140:LEU:HD23	1.98	0.63
5:E:168:ALA:HA	5:E:171:ARG:NH1	2.14	0.63
4:M:64:THR:OG1	6:O:83:ARG:NH1	2.30	0.63
1:S:107:LEU:O	1:S:111:PRO:HG3	1.99	0.63
3:U:216:PHE:HZ	8:Z:128:PHE:HD2	1.46	0.63
3:U:317:LEU:HD22	3:U:317:LEU:N	2.14	0.63
3:U:398:VAL:HG21	3:U:448:MET:HE2	1.81	0.63
4:V:230:ILE:HD11	4:V:244:VAL:HG21	1.80	0.63
5:W:42:LYS:HB2	5:W:108:TRP:CZ2	2.34	0.63
5:5:104:VAL:HG12	5:5:108:TRP:HE3	1.63	0.62
1:A:53:VAL:HG23	1:A:231:MET:HE2	1.81	0.62
4:D:64:THR:OG1	6:F:83:ARG:NH1	2.32	0.62
1:J:115:ILE:O	1:J:119:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:357:ALA:HB2	3:L:641:LEU:HD11	1.81	0.62
3:L:509:ALA:HB1	3:L:768:GLY:CA	2.26	0.62
2:2:61:MET:HE2	3:3:214:MET:HG2	1.81	0.62
3:3:229:ILE:HD11	3:3:289:TRP:HZ3	1.63	0.62
4:4:64:THR:HB	4:4:66:PHE:CE1	2.35	0.62
4:M:230:ILE:HD11	4:M:244:VAL:HG21	1.81	0.62
4:M:311:PRO:HD3	4:M:330:HIS:NE2	2.14	0.62
1:1:436:LEU:HD23	2:2:90:LEU:HA	1.81	0.62
4:D:236:GLY:C	4:D:238:SER:H	2.07	0.62
4:M:238:SER:HB3	4:M:279:ARG:NH2	2.14	0.62
6:O:112:ALA:O	6:O:127:VAL:HG23	1.99	0.62
3:U:373:GLY:HA3	3:U:538:ALA:HB2	1.81	0.62
3:U:571:VAL:HG21	3:U:591:HIS:CD2	2.34	0.62
4:V:236:GLY:C	4:V:238:SER:H	2.08	0.62
2:T:110:GLU:HA	8:Z:121:ARG:NH1	2.14	0.62
1:1:366:PHE:CD1	1:1:370:LEU:HD21	2.34	0.62
4:4:213:ILE:HG22	4:4:217:ARG:CG	2.29	0.62
4:D:212:PRO:CG	4:D:213:ILE:HD12	2.27	0.62
4:D:341:GLU:HG2	4:D:358:VAL:HG22	1.81	0.62
5:E:104:VAL:HG12	5:E:108:TRP:HE3	1.64	0.62
1:J:186:THR:CG2	1:J:200:ARG:H	2.12	0.62
3:L:13:VAL:HG21	3:L:17:THR:HG21	1.82	0.62
3:L:438:LYS:O	3:L:441:MET:HG3	2.00	0.62
3:L:440:ARG:HH11	3:L:440:ARG:CG	2.12	0.62
3:L:469:ARG:HB2	3:L:470:PRO:HD2	1.80	0.62
3:L:546:ALA:HA	3:L:678:PHE:CE2	2.34	0.62
4:M:84:ARG:HG2	9:O:182:SF4:S2	2.39	0.62
4:V:167:ARG:HD3	6:X:143:ARG:HH12	1.64	0.62
4:V:265:PRO:HG2	4:V:282:GLU:HG2	1.80	0.62
4:4:252:TYR:HE2	5:5:87:ARG:NH2	1.98	0.62
2:B:42:ARG:H	2:B:45:ARG:HG3	1.64	0.62
3:C:165:ASP:HB3	3:C:178:ARG:HD2	1.80	0.62
4:D:70:MET:HG2	4:D:78:ASN:OD1	2.00	0.62
4:V:222:GLY:CA	4:V:396:ILE:HD11	2.28	0.62
7:Y:45:ARG:NH2	7:Y:137:LEU:HD23	2.14	0.62
4:4:262:PHE:HD1	4:4:289:ILE:HD11	1.65	0.62
7:9:153:THR:HG22	7:9:155:LYS:N	2.15	0.62
3:C:205:ARG:CA	3:C:209:THR:HG22	2.28	0.62
1:J:184:GLU:CD	1:J:186:THR:HG22	2.24	0.62
6:O:114:SER:HB2	7:P:97:ARG:HD2	1.81	0.62
6:O:153:GLN:HG3	7:P:124:TYR:CZ	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:242:GLY:HA2	1:S:268:MET:O	1.99	0.62
3:U:203:ILE:HG22	3:U:204:GLU:N	2.13	0.62
4:V:43:LEU:HD11	4:V:397:ILE:HD11	1.82	0.62
4:V:64:THR:HB	4:V:66:PHE:CE1	2.35	0.62
3:3:469:ARG:HB2	3:3:470:PRO:HD2	1.81	0.62
1:A:16:THR:CG2	1:A:229:PRO:HB3	2.29	0.62
4:D:238:SER:HB3	4:D:279:ARG:HH22	1.65	0.62
4:M:213:ILE:HG21	4:M:217:ARG:NH1	2.13	0.62
3:U:715:GLU:HB3	3:U:746:ARG:CZ	2.30	0.62
5:W:135:ILE:HG22	5:W:136:LEU:HG	1.79	0.62
6:X:138:PRO:CG	7:Y:121:MET:HG3	2.29	0.62
3:3:20:MET:HE3	3:3:432:PHE:CB	2.30	0.62
1:A:65:ARG:NH2	1:A:268:MET:HE1	2.15	0.62
5:E:42:LYS:HB2	5:E:108:TRP:CZ2	2.34	0.62
1:J:364:ALA:HB1	3:L:207:VAL:HG22	1.81	0.62
7:P:153:THR:HG22	7:P:155:LYS:N	2.15	0.62
1:S:436:LEU:HD23	2:T:90:LEU:HA	1.80	0.62
4:V:314:ARG:HG2	4:V:314:ARG:NH1	2.08	0.62
1:A:289:ALA:HB3	1:A:337:MET:HE3	1.81	0.62
1:A:397:ARG:HE	3:C:79:LEU:HD12	1.63	0.62
1:S:332:PRO:CD	2:T:90:LEU:HD23	2.30	0.62
3:U:591:HIS:ND1	3:U:592:PRO:HD2	2.15	0.62
4:V:381:LEU:HD11	4:V:397:ILE:HG12	1.80	0.62
1:1:332:PRO:CD	2:2:90:LEU:HD23	2.29	0.61
4:4:213:ILE:HG21	4:4:217:ARG:NH1	2.13	0.61
4:4:249:ARG:HB3	4:4:257:TYR:HD1	1.65	0.61
3:C:186:ARG:HD3	3:C:229:ILE:HG22	1.82	0.61
3:C:300:TRP:CD1	3:C:300:TRP:H	2.16	0.61
4:D:213:ILE:HD12	4:D:213:ILE:H	1.64	0.61
3:L:398:VAL:HB	3:L:450:LEU:HD22	1.81	0.61
4:M:140:LEU:O	4:M:140:LEU:HD23	1.99	0.61
1:S:10:ASP:OD1	1:S:11:PRO:HD2	1.99	0.61
2:2:134:ILE:HG13	2:2:145:VAL:HG21	1.82	0.61
1:J:341:MET:HE1	1:J:409:PRO:HB2	1.81	0.61
3:L:282:VAL:HG22	3:L:285:VAL:HG12	1.82	0.61
6:X:43:LEU:HD13	6:X:83:ARG:O	1.99	0.61
4:4:230:ILE:HG22	4:4:230:ILE:O	2.00	0.61
5:5:42:LYS:HB2	5:5:108:TRP:CZ2	2.35	0.61
4:D:213:ILE:HG22	4:D:217:ARG:CG	2.30	0.61
3:L:384:PRO:HG3	3:L:542:ARG:HE	1.66	0.61
4:M:236:GLY:C	4:M:238:SER:H	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:249:ARG:HB3	4:M:257:TYR:HD1	1.65	0.61
4:M:254:TYR:HE2	4:M:346:THR:HA	1.64	0.61
1:S:259:LYS:HA	1:S:284:LEU:HD21	1.83	0.61
1:S:366:PHE:CD1	1:S:370:LEU:HD21	2.35	0.61
3:U:300:TRP:CD1	3:U:300:TRP:H	2.17	0.61
7:Y:33:LEU:CD1	7:Y:161:TYR:HB2	2.28	0.61
3:3:586:HIS:CD2	3:3:604:ALA:HB2	2.36	0.61
3:L:591:HIS:ND1	3:L:592:PRO:HD2	2.16	0.61
4:M:213:ILE:HD12	4:M:213:ILE:H	1.66	0.61
5:N:92:VAL:O	5:N:92:VAL:HG23	2.00	0.61
4:V:215:TYR:O	4:V:219:ARG:HB2	1.99	0.61
3:3:169:PRO:HA	3:3:175:ILE:HA	1.83	0.61
3:3:205:ARG:C	3:3:209:THR:HG22	2.25	0.61
4:4:122:GLU:HB2	4:4:290:ILE:HD11	1.82	0.61
4:4:222:GLY:CA	4:4:396:ILE:HD11	2.29	0.61
3:C:317:LEU:HD22	3:C:317:LEU:N	2.15	0.61
3:C:722:THR:HG21	3:C:756:GLY:N	2.16	0.61
7:G:71:GLU:HB2	7:G:90:VAL:HB	1.82	0.61
5:N:42:LYS:HB2	5:N:108:TRP:CZ2	2.35	0.61
5:W:71:VAL:HG11	5:W:89:PHE:HD2	1.66	0.61
1:1:88:TYR:HB2	1:1:216:THR:HG22	1.82	0.61
3:3:690:GLY:HA3	3:3:770:ARG:NH2	2.16	0.61
3:C:586:HIS:CD2	3:C:604:ALA:HB2	2.35	0.61
5:E:35:LYS:HD3	5:E:102:PRO:HB2	1.83	0.61
3:U:87:VAL:HA	3:U:91:MET:CE	2.28	0.61
5:W:168:ALA:HA	5:W:171:ARG:NH1	2.16	0.61
3:3:120:PRO:HG2	8:7:42:TYR:OH	2.00	0.61
1:A:278:GLU:OE2	6:X:19:ILE:N	2.31	0.61
4:D:96:ALA:HB2	4:D:346:THR:HG21	1.82	0.61
4:D:188:PRO:HB3	3:U:724:ARG:HD3	1.71	0.61
4:D:252:TYR:HE2	5:E:87:ARG:NH2	1.99	0.61
3:U:285:VAL:HG22	3:U:286:ASN:N	2.15	0.61
7:9:46:HIS:CE1	7:9:52:LYS:HG2	2.35	0.61
4:D:262:PHE:HD1	4:D:289:ILE:HD11	1.65	0.61
5:N:34:PHE:HE1	5:N:38:MET:SD	2.23	0.61
6:O:16:ARG:O	6:O:21:PHE:HD2	1.83	0.61
1:S:186:THR:CG2	1:S:200:ARG:H	2.13	0.61
3:U:169:PRO:HA	3:U:175:ILE:HA	1.82	0.61
3:U:584:VAL:HG12	3:U:600:VAL:HB	1.82	0.61
4:V:44:MET:HA	4:V:44:MET:HE2	1.83	0.61
5:W:167:PRO:HB3	7:Y:66:TYR:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:77:VAL:HG22	6:X:104:TRP:HB2	1.83	0.61
1:1:242:GLY:HA2	1:1:268:MET:O	2.01	0.61
3:3:398:VAL:HG21	3:3:448:MET:HE2	1.83	0.61
6:6:153:GLN:HG3	7:9:124:TYR:OH	2.01	0.61
1:A:197:ALA:HB3	2:B:66:PHE:CZ	2.35	0.61
3:C:586:HIS:NE2	3:C:604:ALA:HB2	2.14	0.61
4:D:230:ILE:HD11	4:D:244:VAL:HG21	1.82	0.61
4:D:367:ARG:HH12	4:D:369:LYS:CB	2.14	0.61
2:K:87:SER:HB3	11:K:182:FES:S2	2.41	0.61
4:M:213:ILE:HG22	4:M:217:ARG:CG	2.31	0.61
3:U:398:VAL:C	3:U:399:LEU:HD12	2.26	0.61
3:U:546:ALA:HA	3:U:678:PHE:CE2	2.36	0.61
6:X:153:GLN:HG3	7:Y:124:TYR:OH	1.99	0.61
4:4:393:MET:O	4:4:396:ILE:HG22	2.01	0.61
5:5:168:ALA:HA	5:5:171:ARG:NH1	2.16	0.61
1:A:360:ARG:O	3:C:207:VAL:HG13	2.01	0.61
1:J:253:GLN:HE21	1:J:253:GLN:N	1.98	0.61
2:K:136:VAL:HG12	2:K:137:ASN:N	2.16	0.61
3:L:173:PHE:HB3	3:L:296:PHE:CE1	2.35	0.61
4:M:161:GLU:OE1	7:P:34:LYS:HG2	2.00	0.61
5:N:5:ARG:HH11	5:N:5:ARG:CG	2.01	0.61
4:V:224:ILE:HD11	4:V:275:ARG:NH1	2.15	0.61
1:1:162:LEU:O	1:1:165:THR:HG22	2.01	0.60
3:3:13:VAL:HG21	3:3:17:THR:HG21	1.83	0.60
3:3:254:THR:OG1	3:3:624:LEU:HD23	2.01	0.60
3:3:571:VAL:HG21	3:3:591:HIS:CD2	2.35	0.60
1:J:97:GLU:O	1:J:100:SER:HB3	2.00	0.60
3:U:200:LEU:O	3:U:201:ASP:HB2	2.01	0.60
1:1:92:ASN:ND2	10:1:440:FMN:C2	2.64	0.60
2:2:87:SER:HB3	11:2:182:FES:S2	2.41	0.60
3:3:546:ALA:HA	3:3:678:PHE:CE2	2.36	0.60
4:4:155:THR:HB	4:4:193:LEU:HD12	1.83	0.60
4:4:236:GLY:C	4:4:238:SER:H	2.09	0.60
6:6:117:MET:HB3	7:9:99:ILE:HD13	1.84	0.60
4:D:350:ARG:O	4:D:373:PRO:HB2	2.01	0.60
7:G:33:LEU:CD1	7:G:161:TYR:HB2	2.29	0.60
1:J:92:ASN:ND2	10:J:440:FMN:N1	2.49	0.60
3:L:690:GLY:HA3	3:L:770:ARG:NH2	2.16	0.60
4:V:238:SER:HB3	4:V:279:ARG:HH22	1.63	0.60
3:3:584:VAL:HG12	3:3:600:VAL:HB	1.83	0.60
4:4:153:ARG:HH11	4:4:153:ARG:HG3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:212:PRO:CG	4:4:213:ILE:HD12	2.28	0.60
4:4:350:ARG:O	4:4:373:PRO:HB2	2.01	0.60
6:6:99:MET:CG	6:6:100:PRO:HD2	2.31	0.60
3:C:216:PHE:HZ	8:H:128:PHE:HD2	1.49	0.60
3:C:694:LEU:HB3	3:C:762:ALA:CB	2.31	0.60
4:M:230:ILE:O	4:M:230:ILE:HG22	2.01	0.60
4:M:381:LEU:HD11	4:M:397:ILE:HG12	1.82	0.60
3:U:690:GLY:HA3	3:U:770:ARG:NH2	2.16	0.60
6:X:99:MET:CG	6:X:100:PRO:HD2	2.32	0.60
1:1:253:GLN:N	1:1:253:GLN:HE21	1.98	0.60
1:1:259:LYS:HA	1:1:284:LEU:HD21	1.83	0.60
1:A:242:GLY:HA2	1:A:268:MET:O	2.01	0.60
3:C:584:VAL:HG12	3:C:600:VAL:HB	1.82	0.60
3:L:171:SER:HB2	3:L:172:PRO:HD2	1.83	0.60
4:M:363:SER:HB2	5:N:174:LEU:H	1.66	0.60
5:N:135:ILE:HG22	5:N:136:LEU:HG	1.82	0.60
5:N:174:LEU:HD22	5:N:180:GLY:HA2	1.84	0.60
4:V:61:TYR:HB3	6:X:88:MET:HE2	1.83	0.60
3:3:715:GLU:HB3	3:3:746:ARG:CZ	2.30	0.60
8:7:89:ALA:O	8:7:91:ILE:HG13	2.01	0.60
1:J:160:LYS:HG3	1:J:161:ASN:H	1.66	0.60
4:M:263:ASP:HB2	4:M:285:GLU:CD	2.26	0.60
3:U:185:LYS:HG2	3:U:188:VAL:HG22	1.84	0.60
4:4:230:ILE:HD11	4:4:244:VAL:HG21	1.83	0.60
6:F:16:ARG:O	6:F:21:PHE:HD2	1.85	0.60
6:F:77:VAL:HG22	6:F:104:TRP:HB2	1.83	0.60
6:F:138:PRO:CG	7:G:121:MET:HG3	2.31	0.60
3:L:30:VAL:HG22	3:L:48:CYS:HA	1.83	0.60
6:O:16:ARG:HG2	6:O:21:PHE:CE2	2.37	0.60
6:O:153:GLN:HG3	7:P:124:TYR:OH	2.02	0.60
1:S:88:TYR:HB2	1:S:216:THR:HG22	1.83	0.60
2:T:42:ARG:H	2:T:45:ARG:HG3	1.67	0.60
1:S:160:LYS:HG3	1:S:161:ASN:H	1.67	0.60
4:V:110:PRO:HB3	4:V:301:PRO:HG2	1.83	0.60
4:4:148:TYR:HB3	4:4:200:ARG:NH1	2.17	0.60
4:4:238:SER:HB3	4:4:279:ARG:HH22	1.65	0.60
1:A:341:MET:HE1	1:A:409:PRO:HB2	1.83	0.60
4:D:222:GLY:CA	4:D:396:ILE:HD11	2.32	0.60
5:E:116:ARG:HG3	5:E:129:HIS:CE1	2.36	0.60
5:E:175:THR:CG2	5:E:178:ASP:HB2	2.29	0.60
3:3:112:LEU:HD12	4:4:322:GLU:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:141:GLU:OE2	3:3:143:TYR:HE1	1.85	0.60
4:4:116:ILE:HD11	4:4:182:LEU:HG	1.84	0.60
4:D:64:THR:HB	4:D:66:PHE:CE1	2.36	0.60
3:L:20:MET:HE3	3:L:432:PHE:CB	2.32	0.60
4:V:148:TYR:HB3	4:V:200:ARG:NH1	2.17	0.60
1:1:97:GLU:O	1:1:100:SER:HB3	2.01	0.60
3:C:87:VAL:HA	3:C:91:MET:CE	2.29	0.60
3:C:546:ALA:HA	3:C:678:PHE:CE2	2.36	0.60
3:C:715:GLU:HB3	3:C:746:ARG:CZ	2.31	0.60
4:D:263:ASP:HB2	4:D:285:GLU:CD	2.27	0.60
3:U:240:ALA:CB	3:U:276:ARG:HB2	2.32	0.60
4:V:367:ARG:HE	5:W:122:PHE:HZ	1.50	0.60
1:1:41:ALA:HB2	1:1:116:GLU:HG3	1.84	0.59
1:1:53:VAL:HG23	1:1:231:MET:HE2	1.84	0.59
5:5:174:LEU:HD22	5:5:180:GLY:HA2	1.84	0.59
8:7:33:LYS:HD2	8:7:36:ASP:OD1	2.02	0.59
3:C:169:PRO:HA	3:C:175:ILE:HA	1.84	0.59
4:D:122:GLU:HB2	4:D:290:ILE:HD11	1.83	0.59
1:J:88:TYR:HB2	1:J:216:THR:HG22	1.84	0.59
2:K:40:TRP:CD1	2:K:74:PRO:HA	2.37	0.59
4:M:110:PRO:HB3	4:M:301:PRO:HG2	1.82	0.59
4:M:155:THR:HB	4:M:193:LEU:HD12	1.84	0.59
5:N:42:LYS:CB	5:N:107:LEU:HD13	2.26	0.59
6:O:99:MET:CG	6:O:100:PRO:HD2	2.31	0.59
4:V:252:TYR:HE2	5:W:87:ARG:NH2	1.97	0.59
7:Y:33:LEU:HD11	7:Y:161:TYR:CB	2.29	0.59
2:2:86:LEU:O	2:2:90:LEU:HD12	2.02	0.59
3:3:216:PHE:CZ	8:7:128:PHE:CD2	2.86	0.59
4:4:43:LEU:HD11	4:4:397:ILE:HD11	1.84	0.59
7:9:71:GLU:HB2	7:9:90:VAL:HB	1.84	0.59
3:C:240:ALA:CB	3:C:276:ARG:HB2	2.31	0.59
3:C:384:PRO:HG3	3:C:542:ARG:HE	1.67	0.59
3:C:571:VAL:HG21	3:C:591:HIS:CD2	2.37	0.59
4:D:84:ARG:O	6:F:83:ARG:NH2	2.35	0.59
4:D:393:MET:O	4:D:396:ILE:HG22	2.02	0.59
3:L:317:LEU:HD22	3:L:317:LEU:N	2.16	0.59
3:L:497:TRP:NE1	3:L:524:LEU:HD11	2.17	0.59
3:L:571:VAL:CG2	3:L:587:LEU:HD11	2.31	0.59
4:M:59:ILE:HD11	5:N:135:ILE:HG23	1.83	0.59
3:U:254:THR:OG1	3:U:624:LEU:HD23	2.02	0.59
5:W:116:ARG:HG3	5:W:129:HIS:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:148:ILE:HG22	6:X:149:TYR:N	2.16	0.59
1:1:115:ILE:O	1:1:119:ILE:HG13	2.02	0.59
1:1:437:TRP:CZ3	2:2:96:LEU:HB2	2.37	0.59
1:A:363:VAL:HA	1:A:367:MET:HB2	1.83	0.59
3:C:205:ARG:C	3:C:209:THR:HG22	2.27	0.59
4:D:153:ARG:HH11	4:D:153:ARG:HG3	1.67	0.59
1:J:332:PRO:HD2	2:K:90:LEU:HD23	1.84	0.59
1:J:344:LEU:O	1:J:347:PHE:HB3	2.01	0.59
3:L:240:ALA:CB	3:L:276:ARG:HB2	2.32	0.59
4:M:350:ARG:O	4:M:373:PRO:HB2	2.02	0.59
4:M:371:ARG:NH2	4:M:376:VAL:HG21	2.16	0.59
3:U:330:LYS:HA	3:U:647:ALA:HB1	1.85	0.59
6:X:16:ARG:O	6:X:21:PHE:HD2	1.85	0.59
4:4:96:ALA:HB2	4:4:346:THR:HG21	1.85	0.59
8:7:37:PHE:CD1	8:7:55:MET:HB2	2.37	0.59
2:B:139:GLU:HB2	2:B:140:PRO:CD	2.31	0.59
3:C:173:PHE:HB3	3:C:296:PHE:CE1	2.37	0.59
3:C:477:LEU:HD22	3:C:517:ALA:HB1	1.84	0.59
6:F:83:ARG:HA	6:F:111:CYS:HB3	1.84	0.59
1:J:10:ASP:OD1	1:J:11:PRO:HD2	2.02	0.59
3:L:216:PHE:CZ	8:Q:128:PHE:CD2	2.86	0.59
3:L:285:VAL:HG13	3:L:286:ASN:N	2.16	0.59
3:L:722:THR:HG21	3:L:756:GLY:N	2.18	0.59
4:M:247:ASP:OD1	4:M:249:ARG:HG3	2.02	0.59
6:O:77:VAL:HG22	6:O:104:TRP:HB2	1.83	0.59
6:O:148:ILE:HG22	6:O:149:TYR:N	2.17	0.59
3:U:55:PRO:HG3	3:U:74:GLN:H	1.67	0.59
4:V:213:ILE:CG2	4:V:217:ARG:HH11	2.16	0.59
2:2:81:GLN:HB3	2:2:122:VAL:HG21	1.84	0.59
3:3:165:ASP:HB3	3:3:178:ARG:HD2	1.83	0.59
4:4:254:TYR:HE2	4:4:346:THR:HA	1.66	0.59
4:4:363:SER:HB2	5:5:174:LEU:H	1.67	0.59
4:M:367:ARG:HE	5:N:122:PHE:HZ	1.49	0.59
1:S:16:THR:CG2	1:S:229:PRO:HB3	2.31	0.59
3:U:202:PHE:C	3:U:203:ILE:HD13	2.28	0.59
3:3:586:HIS:NE2	3:3:604:ALA:HB2	2.18	0.59
2:B:106:ILE:HG22	2:B:110:GLU:HB2	1.85	0.59
3:C:192:GLU:OE2	3:C:440:ARG:HA	2.03	0.59
4:D:116:ILE:HD11	4:D:182:LEU:HG	1.85	0.59
5:E:134:LYS:HD3	5:E:137:THR:OG1	2.02	0.59
6:F:77:VAL:O	6:F:77:VAL:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:53:VAL:HG23	1:J:231:MET:HE2	1.85	0.59
2:K:114:ASP:OD2	2:K:116:LEU:HD21	2.03	0.59
4:V:161:GLU:OE1	7:Y:34:LYS:HG2	2.02	0.59
2:2:77:LYS:H	2:2:116:LEU:HA	1.67	0.59
3:C:689:LYS:HE3	3:C:771:VAL:HG13	1.85	0.59
3:L:202:PHE:C	3:L:203:ILE:HD13	2.28	0.59
3:L:689:LYS:HE3	3:L:771:VAL:HG13	1.83	0.59
8:Q:37:PHE:CD1	8:Q:55:MET:HB2	2.38	0.59
2:T:136:VAL:HG12	2:T:137:ASN:N	2.18	0.59
4:V:140:LEU:HD23	4:V:140:LEU:O	2.02	0.59
4:V:240:ARG:HG3	4:V:265:PRO:O	2.02	0.59
6:X:77:VAL:O	6:X:77:VAL:HG12	2.02	0.59
1:1:351:GLU:HA	3:3:205:ARG:HH12	1.67	0.59
4:D:148:TYR:HB3	4:D:200:ARG:NH1	2.17	0.59
4:D:211:SER:HB2	4:D:214:PHE:HB3	1.85	0.59
6:F:16:ARG:HG2	6:F:21:PHE:CE2	2.37	0.59
1:J:332:PRO:CD	2:K:90:LEU:HD23	2.32	0.59
1:J:351:GLU:HA	3:L:205:ARG:HH12	1.67	0.59
5:W:167:PRO:HB3	7:Y:66:TYR:CD2	2.37	0.59
7:Y:128:ASP:O	7:Y:144:LYS:HD3	2.03	0.59
3:L:254:THR:OG1	3:L:624:LEU:HD23	2.03	0.59
7:P:71:GLU:HB2	7:P:90:VAL:HB	1.84	0.59
8:Q:13:TRP:CE2	8:Q:17:LEU:HD11	2.38	0.59
4:V:64:THR:HG23	6:X:123:ILE:CD1	2.33	0.59
4:V:213:ILE:HD12	4:V:213:ILE:H	1.68	0.59
6:6:16:ARG:HG2	6:6:21:PHE:CE2	2.38	0.59
4:D:44:MET:HA	4:D:44:MET:HE2	1.84	0.59
4:D:155:THR:HB	4:D:193:LEU:HD12	1.85	0.59
4:D:164:THR:OG1	4:D:170:HIS:HB3	2.02	0.59
3:L:169:PRO:HA	3:L:175:ILE:HA	1.85	0.59
4:M:225:PRO:CG	4:M:228:VAL:HB	2.27	0.59
4:M:265:PRO:HG2	4:M:282:GLU:HG2	1.84	0.59
1:S:110:VAL:N	1:S:111:PRO:HD3	2.18	0.59
3:U:458:LEU:H	3:U:458:LEU:HD12	1.67	0.59
4:V:102:GLU:HG2	4:V:175:ILE:O	2.03	0.59
3:3:173:PHE:HB3	3:3:296:PHE:CE1	2.37	0.58
3:3:693:TYR:HB3	3:3:759:TYR:CD2	2.39	0.58
1:A:92:ASN:ND2	10:A:440:FMN:C2	2.66	0.58
6:F:115:GLY:HA2	6:F:125:GLN:HA	1.85	0.58
6:F:148:ILE:HG22	6:F:149:TYR:N	2.18	0.58
7:G:33:LEU:HD11	7:G:161:TYR:CB	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:259:LYS:HA	1:J:284:LEU:HD21	1.85	0.58
1:S:332:PRO:HD2	2:T:90:LEU:HD23	1.85	0.58
3:U:227:THR:HG21	3:U:237:ASP:HB2	1.85	0.58
7:Y:123:ASP:HB2	7:Y:129:LEU:HD21	1.85	0.58
3:C:494:LYS:O	3:C:498:GLU:HG2	2.02	0.58
3:U:469:ARG:HB2	3:U:470:PRO:HD2	1.85	0.58
3:U:670:PRO:HD2	3:U:676:LEU:HD23	1.83	0.58
4:V:230:ILE:HG22	4:V:230:ILE:O	2.03	0.58
5:W:35:LYS:HD3	5:W:102:PRO:HB2	1.84	0.58
8:Z:33:LYS:HD2	8:Z:36:ASP:OD1	2.03	0.58
2:B:86:LEU:O	2:B:90:LEU:HD12	2.03	0.58
1:J:342:TRP:HE3	1:J:342:TRP:O	1.86	0.58
3:L:136:GLU:CG	5:N:189:ARG:HG2	2.30	0.58
4:M:238:SER:HB3	4:M:279:ARG:HH22	1.66	0.58
5:W:59:THR:HG22	5:W:59:THR:O	2.03	0.58
1:1:53:VAL:O	1:1:57:VAL:HG23	2.03	0.58
3:3:344:TYR:CD1	3:3:568:TYR:CE1	2.92	0.58
4:4:110:PRO:HB3	4:4:301:PRO:HG2	1.85	0.58
5:5:42:LYS:CB	5:5:107:LEU:HD13	2.28	0.58
4:D:265:PRO:HG2	4:D:282:GLU:HG2	1.83	0.58
6:F:43:LEU:HD13	6:F:83:ARG:O	2.03	0.58
2:K:42:ARG:H	2:K:45:ARG:HG3	1.68	0.58
3:L:165:ASP:HB3	3:L:178:ARG:HD2	1.85	0.58
4:M:148:TYR:HB3	4:M:200:ARG:NH1	2.19	0.58
3:U:402:PRO:CB	3:U:535:MET:HE1	2.33	0.58
4:4:115:THR:CG2	4:4:297:LEU:HD23	2.34	0.58
5:5:71:VAL:HG11	5:5:89:PHE:HD2	1.67	0.58
5:5:175:THR:CG2	5:5:178:ASP:HB2	2.32	0.58
4:D:129:HIS:HE1	4:D:349:ALA:HB1	1.66	0.58
5:E:71:VAL:HG11	5:E:89:PHE:HD2	1.68	0.58
8:H:33:LYS:HD2	8:H:36:ASP:OD1	2.03	0.58
1:J:92:ASN:ND2	10:J:440:FMN:C2	2.67	0.58
3:U:13:VAL:HG21	3:U:17:THR:HG21	1.84	0.58
3:U:112:LEU:HD21	3:U:130:LEU:HD11	1.84	0.58
3:U:402:PRO:HG3	3:U:535:MET:HE1	1.85	0.58
3:U:683:LEU:HD23	3:U:683:LEU:N	2.19	0.58
4:V:263:ASP:HB2	4:V:285:GLU:CD	2.28	0.58
6:X:16:ARG:HG2	6:X:21:PHE:CE2	2.37	0.58
3:3:591:HIS:ND1	3:3:592:PRO:HD2	2.19	0.58
4:4:409:ARG:O	4:4:409:ARG:HG2	2.03	0.58
2:B:81:GLN:HB3	2:B:122:VAL:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:385:ALA:HB2	3:C:531:LYS:HB3	1.85	0.58
4:D:367:ARG:HE	5:E:122:PHE:HZ	1.51	0.58
6:F:115:GLY:HA3	6:F:125:GLN:OE1	2.04	0.58
2:K:58:THR:HG21	3:L:200:LEU:N	2.18	0.58
3:U:586:HIS:NE2	3:U:604:ALA:HB2	2.18	0.58
4:V:287:VAL:O	4:V:291:LYS:HG3	2.03	0.58
3:3:440:ARG:CG	3:3:440:ARG:NH1	2.67	0.58
4:4:64:THR:HG23	6:6:123:ILE:CD1	2.33	0.58
4:4:164:THR:OG1	4:4:170:HIS:HB3	2.02	0.58
4:4:263:ASP:HB2	4:4:285:GLU:CD	2.28	0.58
4:D:409:ARG:O	4:D:409:ARG:HG2	2.03	0.58
1:J:360:ARG:O	3:L:207:VAL:HG13	2.04	0.58
3:U:344:TYR:CD1	3:U:568:TYR:CE1	2.92	0.58
4:V:212:PRO:CG	4:V:213:ILE:HD12	2.29	0.58
2:2:40:TRP:CD1	2:2:74:PRO:HA	2.39	0.58
3:3:202:PHE:C	3:3:203:ILE:HD13	2.29	0.58
4:M:212:PRO:CG	4:M:213:ILE:HD12	2.31	0.58
1:S:437:TRP:CZ3	2:T:96:LEU:HB2	2.39	0.58
2:T:81:GLN:HB3	2:T:122:VAL:HG21	1.85	0.58
3:U:694:LEU:HB3	3:U:762:ALA:CB	2.32	0.58
1:1:303:THR:OG1	1:1:306:VAL:HG23	2.03	0.58
2:2:42:ARG:H	2:2:45:ARG:HG3	1.68	0.58
3:C:684:ARG:HG2	3:C:684:ARG:NH1	2.18	0.58
4:D:43:LEU:HD11	4:D:397:ILE:HD11	1.84	0.58
4:D:110:PRO:HB3	4:D:301:PRO:HG2	1.85	0.58
5:E:42:LYS:CB	5:E:107:LEU:HD13	2.30	0.58
1:J:197:ALA:HB3	2:K:66:PHE:CZ	2.38	0.58
2:K:86:LEU:O	2:K:90:LEU:HD12	2.04	0.58
3:L:494:LYS:O	3:L:498:GLU:HG2	2.03	0.58
3:L:572:PRO:HD2	3:L:577:LEU:HD21	1.84	0.58
3:L:586:HIS:CD2	3:L:604:ALA:HB2	2.39	0.58
5:N:33:ARG:O	5:N:37:GLU:HB2	2.03	0.58
3:U:282:VAL:HG22	3:U:285:VAL:HG12	1.84	0.58
4:V:40:VAL:O	4:V:40:VAL:HG22	2.02	0.58
4:V:363:SER:HB2	5:W:174:LEU:H	1.69	0.58
1:1:92:ASN:ND2	10:1:440:FMN:N1	2.52	0.58
3:3:373:GLY:HA3	3:3:538:ALA:HB2	1.84	0.58
4:4:102:GLU:HG2	4:4:175:ILE:O	2.04	0.58
5:5:92:VAL:HG23	5:5:92:VAL:O	2.04	0.58
1:A:197:ALA:HB3	2:B:66:PHE:CE1	2.39	0.58
4:D:311:PRO:HD3	4:D:330:HIS:NE2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:153:GLN:HG3	7:G:124:TYR:CZ	2.39	0.58
1:J:109:ASP:C	1:J:111:PRO:HD3	2.29	0.58
3:L:205:ARG:C	3:L:209:THR:HG22	2.29	0.58
3:U:477:LEU:HD22	3:U:517:ALA:HB1	1.86	0.58
3:U:546:ALA:C	3:U:547:MET:HE2	2.29	0.58
2:2:81:GLN:HB3	2:2:122:VAL:CG2	2.34	0.57
4:4:262:PHE:CD1	4:4:289:ILE:HD11	2.38	0.57
1:A:250:LYS:HB3	1:A:252:TYR:CE2	2.39	0.57
2:B:130:THR:HB	2:B:144:CYS:SG	2.43	0.57
3:C:254:THR:OG1	3:C:624:LEU:HD23	2.03	0.57
4:D:215:TYR:O	4:D:219:ARG:HB2	2.04	0.57
1:J:104:ARG:HH21	2:K:127:SER:CB	2.17	0.57
1:J:301:PRO:O	1:J:306:VAL:HG21	2.04	0.57
3:L:684:ARG:HG2	3:L:684:ARG:NH1	2.18	0.57
5:N:35:LYS:HD3	5:N:102:PRO:HB2	1.85	0.57
1:S:341:MET:HE1	1:S:409:PRO:HB2	1.86	0.57
3:U:586:HIS:CD2	3:U:604:ALA:HB2	2.38	0.57
3:U:689:LYS:HE3	3:U:771:VAL:HG13	1.85	0.57
4:V:254:TYR:CD2	4:V:346:THR:HA	2.38	0.57
6:6:43:LEU:HD13	6:6:83:ARG:O	2.04	0.57
3:C:497:TRP:O	3:C:528:LYS:HE3	2.04	0.57
4:D:230:ILE:HG22	4:D:230:ILE:O	2.03	0.57
4:D:262:PHE:CD1	4:D:289:ILE:HD11	2.38	0.57
3:L:671:GLU:HA	3:L:671:GLU:OE2	2.05	0.57
4:M:215:TYR:CE2	4:M:219:ARG:HG3	2.39	0.57
6:O:77:VAL:HA	6:O:104:TRP:O	2.05	0.57
6:O:78:MET:HG3	6:O:78:MET:O	2.03	0.57
1:S:274:GLU:HG2	1:S:279:TRP:HE1	1.69	0.57
1:1:16:THR:CG2	1:1:229:PRO:HB3	2.30	0.57
3:3:722:THR:HG21	3:3:756:GLY:N	2.19	0.57
5:5:134:LYS:HD3	5:5:137:THR:OG1	2.03	0.57
3:C:13:VAL:HG21	3:C:17:THR:HG21	1.87	0.57
3:C:185:LYS:HG2	3:C:188:VAL:HG22	1.85	0.57
4:D:73:ARG:HG3	4:D:77:GLN:OE1	2.04	0.57
6:F:164:ASN:HB2	7:G:128:ASP:OD2	2.03	0.57
3:L:693:TYR:HB3	3:L:759:TYR:CD2	2.40	0.57
3:L:715:GLU:HB3	3:L:746:ARG:NH1	2.19	0.57
4:M:44:MET:HA	4:M:44:MET:HE2	1.85	0.57
4:V:211:SER:HB2	4:V:214:PHE:HB3	1.85	0.57
1:1:250:LYS:HB3	1:1:252:TYR:CE2	2.39	0.57
1:1:344:LEU:O	1:1:347:PHE:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:140:LEU:O	4:4:140:LEU:HD23	2.03	0.57
7:9:45:ARG:NH2	7:9:137:LEU:HD23	2.20	0.57
8:7:121:ARG:HG3	8:7:121:ARG:NH1	2.19	0.57
1:A:356:CYS:HB3	1:A:358:PRO:HG2	1.84	0.57
3:L:694:LEU:HB3	3:L:762:ALA:CB	2.31	0.57
4:M:262:PHE:HD1	4:M:289:ILE:HD11	1.70	0.57
5:N:58:LEU:O	5:N:58:LEU:HD12	2.05	0.57
3:U:385:ALA:HB2	3:U:531:LYS:HB3	1.86	0.57
4:V:70:MET:HG2	4:V:78:ASN:OD1	2.03	0.57
1:1:186:THR:HG23	1:1:200:ARG:H	1.69	0.57
3:3:185:LYS:HG3	3:3:202:PHE:HE2	1.69	0.57
3:3:671:GLU:HA	3:3:671:GLU:OE2	2.04	0.57
3:3:684:ARG:HG2	3:3:684:ARG:NH1	2.19	0.57
6:6:148:ILE:HG22	6:6:149:TYR:N	2.18	0.57
1:A:238:PHE:HE1	1:A:249:MET:CE	2.16	0.57
3:C:281:GLU:HG2	3:C:283:PRO:HD3	1.87	0.57
1:J:242:GLY:HA2	1:J:268:MET:O	2.04	0.57
5:N:66:GLU:HG2	5:N:95:PRO:HA	1.86	0.57
6:O:138:PRO:CG	7:P:121:MET:HG3	2.35	0.57
3:U:494:LYS:O	3:U:498:GLU:HG2	2.04	0.57
1:1:10:ASP:OD1	1:1:11:PRO:HD2	2.04	0.57
3:3:469:ARG:HA	3:3:754:PRO:HG3	1.86	0.57
1:A:53:VAL:O	1:A:57:VAL:HG23	2.04	0.57
6:F:153:GLN:HG3	7:G:124:TYR:OH	2.05	0.57
7:G:45:ARG:HH21	7:G:137:LEU:HD23	1.70	0.57
2:K:61:MET:HE2	3:L:214:MET:HG2	1.87	0.57
3:L:309:PRO:HG2	3:L:320:ALA:O	2.05	0.57
3:L:670:PRO:HD2	3:L:676:LEU:HD23	1.87	0.57
3:U:194:VAL:HG12	3:U:411:LEU:HD22	1.87	0.57
3:U:326:PHE:CE2	3:U:330:LYS:HE3	2.39	0.57
2:2:106:ILE:HG22	2:2:110:GLU:HB2	1.87	0.57
2:2:139:GLU:HB2	2:2:140:PRO:CD	2.32	0.57
3:3:125:GLY:HA3	3:3:246:ASN:HD22	1.68	0.57
3:3:240:ALA:CB	3:3:276:ARG:HB2	2.35	0.57
3:3:497:TRP:O	3:3:528:LYS:HE3	2.04	0.57
5:5:25:LEU:CD2	5:5:25:LEU:N	2.68	0.57
1:A:41:ALA:HB2	1:A:116:GLU:HG3	1.86	0.57
6:F:165:GLU:HG2	7:G:148:ARG:HH11	1.68	0.57
1:J:356:CYS:HB3	1:J:358:PRO:HG2	1.85	0.57
3:L:402:PRO:CG	3:L:535:MET:HE1	2.35	0.57
4:M:43:LEU:HD11	4:M:397:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:83:ARG:HA	6:O:111:CYS:HB3	1.86	0.57
6:O:107:SER:O	6:O:137:VAL:HG12	2.04	0.57
3:U:384:PRO:HG3	3:U:542:ARG:HE	1.68	0.57
4:V:119:ILE:O	4:V:123:LEU:HB2	2.05	0.57
4:4:64:THR:OG1	6:6:83:ARG:NH1	2.37	0.57
2:B:129:HIS:CD2	2:B:130:THR:HG23	2.40	0.57
3:C:546:ALA:C	3:C:547:MET:HE2	2.29	0.57
3:C:591:HIS:ND1	3:C:592:PRO:HD2	2.19	0.57
4:D:168:PHE:HE1	6:F:141:PRO:HG3	1.69	0.57
2:K:81:GLN:HB3	2:K:122:VAL:HG21	1.85	0.57
3:L:402:PRO:CB	3:L:535:MET:HE1	2.34	0.57
4:M:153:ARG:HH11	4:M:153:ARG:HG3	1.69	0.57
4:M:211:SER:HB2	4:M:214:PHE:HB3	1.87	0.57
7:P:30:PRO:HB2	7:P:162:VAL:HG13	1.86	0.57
4:V:63:HIS:O	6:X:122:ALA:HB1	2.05	0.57
3:3:341:VAL:HG21	3:3:364:LEU:HD11	1.85	0.57
4:4:44:MET:HA	4:4:44:MET:HE2	1.87	0.57
6:6:83:ARG:HA	6:6:111:CYS:HB3	1.85	0.57
2:B:114:ASP:OD2	2:B:116:LEU:HD21	2.05	0.57
3:C:690:GLY:HA3	3:C:770:ARG:NH2	2.19	0.57
6:F:82:GLY:HA2	9:F:182:SF4:S4	2.45	0.57
4:M:164:THR:OG1	4:M:170:HIS:HB3	2.04	0.57
6:O:164:ASN:HB2	7:P:128:ASP:OD2	2.04	0.57
4:V:73:ARG:HG3	4:V:77:GLN:OE1	2.05	0.57
6:X:138:PRO:HG3	7:Y:121:MET:HG3	1.87	0.57
7:Y:48:ASN:CB	7:Y:50:LEU:HD23	2.35	0.57
8:Z:82:ILE:HG23	8:Z:95:ALA:HB3	1.87	0.57
1:A:266:LEU:HB3	1:A:270:THR:HG21	1.87	0.57
1:J:214:LYS:O	1:J:216:THR:HG23	2.04	0.57
1:J:287:ILE:HG22	1:J:302:PHE:CG	2.40	0.57
4:M:215:TYR:O	4:M:219:ARG:HB2	2.03	0.57
5:N:25:LEU:CD2	5:N:25:LEU:N	2.68	0.57
1:S:53:VAL:O	1:S:57:VAL:HG23	2.04	0.57
1:S:162:LEU:O	1:S:165:THR:HG22	2.04	0.57
7:Y:46:HIS:CE1	7:Y:52:LYS:HG2	2.40	0.57
8:Z:121:ARG:HG3	8:Z:121:ARG:NH1	2.20	0.57
3:3:458:LEU:HD12	3:3:458:LEU:H	1.69	0.56
3:3:497:TRP:O	3:3:500:ALA:HB3	2.05	0.56
1:A:160:LYS:HG3	1:A:161:ASN:H	1.70	0.56
3:C:671:GLU:HA	3:C:671:GLU:OE2	2.04	0.56
2:T:101:THR:HG23	2:T:106:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:114:ASP:OD2	2:T:116:LEU:HD21	2.05	0.56
3:U:688:ARG:HB3	3:U:770:ARG:HD3	1.87	0.56
6:6:115:GLY:HA2	6:6:125:GLN:HA	1.87	0.56
1:A:270:THR:O	1:A:311:MET:HG3	2.05	0.56
3:C:497:TRP:O	3:C:500:ALA:HB3	2.05	0.56
8:H:89:ALA:O	8:H:91:ILE:HG13	2.05	0.56
3:L:398:VAL:C	3:L:399:LEU:HD12	2.30	0.56
1:S:97:GLU:O	1:S:100:SER:HB3	2.05	0.56
1:S:287:ILE:HG22	1:S:302:PHE:CG	2.40	0.56
2:2:136:VAL:HG12	2:2:137:ASN:N	2.20	0.56
3:3:494:LYS:O	3:3:498:GLU:HG2	2.05	0.56
3:3:670:PRO:HD2	3:3:676:LEU:HD23	1.87	0.56
4:4:153:ARG:HG3	4:4:153:ARG:NH1	2.20	0.56
1:A:88:TYR:HB2	1:A:216:THR:HG22	1.88	0.56
1:A:303:THR:OG1	1:A:306:VAL:HG23	2.05	0.56
2:B:10:PHE:CZ	2:B:33:ARG:HG3	2.40	0.56
2:B:40:TRP:CD1	2:B:74:PRO:HA	2.40	0.56
2:B:139:GLU:CB	2:B:140:PRO:CD	2.82	0.56
3:C:285:VAL:HG22	3:C:286:ASN:N	2.20	0.56
3:C:398:VAL:C	3:C:399:LEU:HD12	2.30	0.56
3:C:571:VAL:CG2	3:C:587:LEU:HD11	2.36	0.56
4:D:254:TYR:CD1	4:D:255:SER:N	2.70	0.56
5:E:92:VAL:HG23	5:E:92:VAL:O	2.05	0.56
6:F:117:MET:HB3	7:G:99:ILE:HD13	1.86	0.56
1:J:16:THR:CG2	1:J:229:PRO:HB3	2.33	0.56
4:M:84:ARG:NE	6:O:117:MET:HE1	2.21	0.56
5:N:175:THR:CG2	5:N:178:ASP:HB2	2.34	0.56
7:P:134:GLU:H	7:P:134:GLU:CD	2.12	0.56
1:S:53:VAL:HG23	1:S:231:MET:HE2	1.88	0.56
1:S:186:THR:HG23	1:S:200:ARG:H	1.69	0.56
1:S:438:ARG:HD2	1:S:438:ARG:N	2.20	0.56
2:T:106:ILE:HG22	2:T:110:GLU:HB2	1.87	0.56
3:U:701:ALA:HB2	3:U:763:LEU:HB2	1.86	0.56
4:V:43:LEU:HD11	4:V:397:ILE:CD1	2.36	0.56
5:W:25:LEU:N	5:W:25:LEU:CD2	2.68	0.56
6:X:77:VAL:HA	6:X:104:TRP:O	2.06	0.56
7:Y:30:PRO:HB2	7:Y:162:VAL:HG13	1.87	0.56
3:3:402:PRO:CB	3:3:535:MET:HE1	2.35	0.56
3:3:572:PRO:HD2	3:3:577:LEU:HD21	1.87	0.56
4:4:240:ARG:HG3	4:4:265:PRO:O	2.06	0.56
6:6:138:PRO:CG	7:9:121:MET:HG3	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:GLN:HB3	2:B:122:VAL:CG2	2.35	0.56
3:C:373:GLY:HA3	3:C:538:ALA:HB2	1.87	0.56
3:C:693:TYR:HB3	3:C:759:TYR:CD2	2.41	0.56
4:D:363:SER:HB2	5:E:174:LEU:H	1.69	0.56
8:H:37:PHE:HD1	8:H:53:THR:O	1.88	0.56
3:L:473:GLU:O	3:L:477:LEU:HD13	2.04	0.56
4:M:409:ARG:O	4:M:409:ARG:HG2	2.05	0.56
7:P:33:LEU:HD11	7:P:161:TYR:CB	2.33	0.56
3:U:46:ARG:O	3:U:107:MET:HG2	2.05	0.56
3:U:571:VAL:CG2	3:U:587:LEU:HD11	2.35	0.56
5:W:134:LYS:HD3	5:W:137:THR:OG1	2.04	0.56
7:9:30:PRO:HB2	7:9:162:VAL:HG13	1.87	0.56
7:9:96:LEU:HD21	7:9:129:LEU:HD12	1.87	0.56
3:C:94:ASP:OD2	3:C:97:SER:HB2	2.06	0.56
4:D:254:TYR:HE2	4:D:346:THR:HA	1.67	0.56
8:H:8:GLU:HG2	8:H:97:TYR:CZ	2.41	0.56
4:M:40:VAL:HG23	6:O:88:MET:CE	2.36	0.56
1:S:64:GLY:HA3	10:S:440:FMN:O1P	2.05	0.56
1:S:92:ASN:ND2	10:S:440:FMN:O3'	2.38	0.56
3:U:208:HIS:HB3	8:Z:85:ARG:NH2	2.20	0.56
3:U:572:PRO:HD2	3:U:577:LEU:HD21	1.87	0.56
4:V:115:THR:CG2	4:V:297:LEU:HD23	2.36	0.56
8:Z:37:PHE:HD1	8:Z:53:THR:O	1.87	0.56
2:2:114:ASP:OD2	2:2:116:LEU:HD21	2.06	0.56
3:3:281:GLU:HG2	3:3:283:PRO:HD3	1.86	0.56
3:3:701:ALA:HB2	3:3:763:LEU:HB2	1.86	0.56
6:6:107:SER:O	6:6:137:VAL:HG12	2.06	0.56
3:C:688:ARG:HB3	3:C:770:ARG:HD3	1.87	0.56
6:F:16:ARG:HG2	6:F:21:PHE:HE2	1.70	0.56
1:J:104:ARG:HH21	2:K:127:SER:HB2	1.70	0.56
3:L:326:PHE:CE2	3:L:330:LYS:HE3	2.40	0.56
3:L:469:ARG:HA	3:L:754:PRO:HG3	1.87	0.56
4:M:213:ILE:CG2	4:M:217:ARG:HH11	2.18	0.56
4:M:252:TYR:HE2	5:N:87:ARG:NH2	2.04	0.56
6:O:43:LEU:HD13	6:O:83:ARG:O	2.06	0.56
3:U:54:LEU:N	3:U:55:PRO:HD3	2.21	0.56
4:V:167:ARG:HD3	6:X:143:ARG:NH1	2.20	0.56
5:W:33:ARG:O	5:W:37:GLU:HB2	2.05	0.56
5:W:37:GLU:O	5:W:41:TYR:HD1	1.88	0.56
1:1:438:ARG:HD2	1:1:438:ARG:N	2.21	0.56
2:2:10:PHE:CZ	2:2:33:ARG:HG3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:215:TYR:CE2	4:4:219:ARG:HG3	2.41	0.56
6:6:78:MET:O	6:6:78:MET:HG3	2.04	0.56
7:9:33:LEU:CD1	7:9:161:TYR:HB2	2.32	0.56
1:A:259:LYS:HA	1:A:284:LEU:HD21	1.87	0.56
6:F:78:MET:O	6:F:78:MET:HG3	2.05	0.56
1:J:162:LEU:O	1:J:165:THR:HG22	2.06	0.56
1:J:250:LYS:HB3	1:J:252:TYR:CE2	2.41	0.56
3:L:333:LEU:HD22	3:L:648:LEU:HD21	1.88	0.56
5:N:116:ARG:HG3	5:N:129:HIS:CE1	2.39	0.56
5:N:121:LEU:O	5:N:144:HIS:HB3	2.05	0.56
6:O:16:ARG:HG2	6:O:21:PHE:HE2	1.70	0.56
7:P:33:LEU:CD1	7:P:161:TYR:HB2	2.31	0.56
1:S:37:GLY:C	1:S:39:GLU:H	2.14	0.56
3:U:94:ASP:OD2	3:U:97:SER:HB2	2.06	0.56
4:V:254:TYR:CD1	4:V:255:SER:N	2.68	0.56
3:3:571:VAL:CG2	3:3:587:LEU:HD11	2.35	0.56
4:4:76:LEU:HD12	4:4:76:LEU:O	2.06	0.56
1:A:397:ARG:HG2	3:C:49:LEU:HD13	1.87	0.56
3:C:55:PRO:HG3	3:C:74:GLN:H	1.66	0.56
3:C:202:PHE:C	3:C:203:ILE:HD13	2.29	0.56
3:C:282:VAL:HG22	3:C:285:VAL:HG12	1.88	0.56
3:C:629:ILE:HG22	3:C:630:GLU:N	2.21	0.56
4:D:247:ASP:OD1	4:D:249:ARG:HG3	2.05	0.56
4:M:84:ARG:O	6:O:83:ARG:NH2	2.39	0.56
4:M:153:ARG:HG3	4:M:153:ARG:NH1	2.21	0.56
7:P:46:HIS:CE1	7:P:52:LYS:HG2	2.41	0.56
1:S:303:THR:OG1	1:S:306:VAL:HG23	2.06	0.56
4:V:409:ARG:HG2	4:V:409:ARG:O	2.03	0.56
1:1:266:LEU:HB3	1:1:270:THR:HG21	1.88	0.56
2:2:38:GLU:OE2	2:2:45:ARG:NH1	2.39	0.56
4:4:213:ILE:CG2	4:4:217:ARG:HH11	2.19	0.56
8:7:37:PHE:HD1	8:7:53:THR:O	1.88	0.56
3:C:344:TYR:CD1	3:C:568:TYR:CE1	2.93	0.56
3:C:474:ARG:HA	3:C:517:ALA:HB2	1.88	0.56
5:E:58:LEU:HD12	5:E:58:LEU:O	2.05	0.56
3:L:55:PRO:HG3	3:L:74:GLN:H	1.66	0.56
3:L:571:VAL:HG21	3:L:591:HIS:CD2	2.40	0.56
4:M:26:MET:N	4:M:48:SER:HG	2.03	0.56
4:M:64:THR:HB	4:M:66:PHE:HE1	1.71	0.56
1:1:89:LEU:HD23	1:1:118:MET:HE3	1.88	0.56
1:1:287:ILE:HG22	1:1:302:PHE:CG	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:357:ALA:HB2	3:3:641:LEU:HD11	1.88	0.56
4:4:215:TYR:O	4:4:219:ARG:HB2	2.05	0.56
6:6:77:VAL:O	6:6:77:VAL:HG12	2.06	0.56
3:C:357:ALA:HB2	3:C:641:LEU:HD11	1.88	0.56
3:C:469:ARG:HA	3:C:754:PRO:HG3	1.88	0.56
7:G:123:ASP:HB2	7:G:129:LEU:HD21	1.87	0.56
1:J:316:LEU:HD12	1:J:323:LEU:HB2	1.88	0.56
3:L:285:VAL:HG22	3:L:286:ASN:H	1.70	0.56
1:S:238:PHE:HE1	1:S:249:MET:CE	2.19	0.56
2:T:38:GLU:OE2	2:T:45:ARG:NH1	2.38	0.56
3:U:205:ARG:C	3:U:209:THR:HG22	2.31	0.56
4:V:116:ILE:HD11	4:V:182:LEU:HG	1.86	0.56
4:V:332:THR:O	5:W:172:ALA:HB3	2.06	0.56
6:X:78:MET:HG3	6:X:78:MET:O	2.06	0.56
1:1:357:THR:N	1:1:358:PRO:HD2	2.21	0.55
3:3:546:ALA:C	3:3:547:MET:HE2	2.30	0.55
4:4:211:SER:HB2	4:4:214:PHE:HB3	1.89	0.55
5:5:58:LEU:HD12	5:5:58:LEU:O	2.06	0.55
6:6:152:MET:HE2	6:6:156:LYS:HE2	1.88	0.55
3:C:227:THR:HG21	3:C:237:ASP:HB2	1.88	0.55
3:C:398:VAL:HG21	3:C:448:MET:HE2	1.87	0.55
3:C:400:GLY:O	3:C:402:PRO:HD3	2.06	0.55
3:C:695:ARG:NH1	3:C:715:GLU:OE1	2.39	0.55
7:G:30:PRO:HB2	7:G:162:VAL:HG13	1.88	0.55
3:L:54:LEU:N	3:L:55:PRO:HD3	2.20	0.55
3:L:373:GLY:HA3	3:L:538:ALA:HB2	1.87	0.55
4:M:52:VAL:HG23	4:M:388:GLU:O	2.06	0.55
5:N:20:ASN:HD21	5:N:24:ASN:HB2	1.70	0.55
3:U:399:LEU:HD12	3:U:399:LEU:N	2.21	0.55
4:V:262:PHE:HD1	4:V:289:ILE:HD11	1.72	0.55
8:Z:13:TRP:CE2	8:Z:17:LEU:HD11	2.41	0.55
6:6:115:GLY:HA3	6:6:125:GLN:OE1	2.06	0.55
1:A:29:LEU:CD1	1:A:155:ARG:HG3	2.37	0.55
1:A:186:THR:HG23	1:A:200:ARG:H	1.71	0.55
2:B:7:LYS:HD2	2:B:7:LYS:N	2.18	0.55
2:B:61:MET:HE2	3:C:214:MET:HG2	1.87	0.55
5:E:1:MET:C	5:E:3:LEU:H	2.14	0.55
8:H:37:PHE:CD1	8:H:55:MET:HB2	2.42	0.55
3:L:94:ASP:OD2	3:L:97:SER:HB2	2.07	0.55
3:L:583:VAL:CG2	3:L:598:ALA:HA	2.36	0.55
5:N:59:THR:O	5:N:59:THR:HG22	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:125:VAL:HG12	5:N:126:PHE:N	2.21	0.55
1:S:363:VAL:HA	1:S:367:MET:HB2	1.89	0.55
6:X:16:ARG:HG2	6:X:21:PHE:HE2	1.69	0.55
1:1:160:LYS:HG3	1:1:161:ASN:H	1.71	0.55
3:3:227:THR:HG21	3:3:237:ASP:HB2	1.88	0.55
3:3:477:LEU:HD22	3:3:517:ALA:HB1	1.87	0.55
4:4:148:TYR:CB	4:4:200:ARG:HH12	2.18	0.55
4:4:367:ARG:HE	5:5:122:PHE:HZ	1.54	0.55
1:A:265:GLU:O	1:A:266:LEU:HG	2.06	0.55
4:D:85:MET:HE3	4:D:409:ARG:CG	2.36	0.55
4:D:381:LEU:HD11	4:D:397:ILE:HG12	1.87	0.55
1:J:37:GLY:C	1:J:39:GLU:H	2.14	0.55
1:J:41:ALA:HB2	1:J:116:GLU:HG3	1.89	0.55
3:L:330:LYS:HA	3:L:647:ALA:HB1	1.88	0.55
3:L:456:ALA:HB3	3:L:459:MET:HE3	1.89	0.55
1:S:18:TYR:OH	1:S:105:TYR:HB2	2.06	0.55
3:U:112:LEU:CD2	3:U:130:LEU:HD11	2.37	0.55
3:U:185:LYS:HG3	3:U:202:PHE:HE2	1.71	0.55
3:U:341:VAL:HG21	3:U:364:LEU:HD11	1.87	0.55
4:V:252:TYR:CE2	5:W:87:ARG:NH2	2.74	0.55
4:4:74:THR:HB	4:4:77:GLN:H	1.71	0.55
1:A:238:PHE:HE1	1:A:249:MET:HE1	1.72	0.55
3:C:341:VAL:HG21	3:C:364:LEU:HD11	1.87	0.55
7:G:46:HIS:CE1	7:G:52:LYS:HG2	2.41	0.55
3:L:227:THR:HG21	3:L:237:ASP:HB2	1.88	0.55
1:S:63:ARG:HD3	1:S:313:TYR:HD2	1.71	0.55
2:T:139:GLU:CB	2:T:140:PRO:CD	2.83	0.55
3:U:671:GLU:HA	3:U:671:GLU:OE2	2.07	0.55
3:U:722:THR:HG21	3:U:756:GLY:N	2.20	0.55
8:Z:37:PHE:CD1	8:Z:55:MET:HB2	2.41	0.55
1:1:265:GLU:O	1:1:266:LEU:HG	2.07	0.55
6:6:16:ARG:O	6:6:21:PHE:HD2	1.89	0.55
6:6:163:TYR:CD2	6:6:169:ARG:HA	2.34	0.55
1:A:97:GLU:O	1:A:100:SER:HB3	2.06	0.55
1:A:109:ASP:C	1:A:111:PRO:HD3	2.32	0.55
1:A:274:GLU:HG2	1:A:279:TRP:HE1	1.72	0.55
3:C:458:LEU:H	3:C:458:LEU:HD12	1.72	0.55
1:J:239:ALA:C	1:J:241:MET:H	2.15	0.55
3:L:185:LYS:HG2	3:L:188:VAL:HG22	1.88	0.55
3:L:440:ARG:CG	3:L:440:ARG:NH1	2.70	0.55
4:M:96:ALA:HB2	4:M:346:THR:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:266:LEU:HB3	1:S:270:THR:HG21	1.89	0.55
6:X:36:LEU:HD22	6:X:77:VAL:HG21	1.87	0.55
6:X:152:MET:HE2	6:X:156:LYS:HE2	1.88	0.55
6:6:16:ARG:HG2	6:6:21:PHE:HE2	1.70	0.55
6:6:77:VAL:HA	6:6:104:TRP:O	2.06	0.55
2:B:77:LYS:H	2:B:116:LEU:HA	1.72	0.55
6:F:41:PHE:CZ	6:F:92:MET:HB2	2.41	0.55
6:F:138:PRO:HG2	7:G:121:MET:HG3	1.89	0.55
1:J:186:THR:HG23	1:J:200:ARG:H	1.71	0.55
4:M:240:ARG:HG3	4:M:265:PRO:O	2.07	0.55
4:M:318:GLU:HB2	8:Q:39:ASP:HA	1.89	0.55
1:S:356:CYS:HB3	1:S:358:PRO:HG2	1.88	0.55
4:V:64:THR:OG1	6:X:83:ARG:NH1	2.39	0.55
4:V:148:TYR:CB	4:V:200:ARG:HH12	2.19	0.55
4:V:213:ILE:HG22	4:V:217:ARG:HG3	1.89	0.55
7:Y:44:THR:OG1	7:Y:52:LYS:HD2	2.07	0.55
1:1:109:ASP:C	1:1:111:PRO:HD3	2.32	0.55
3:3:216:PHE:CZ	8:7:128:PHE:HD2	2.20	0.55
3:3:413:LEU:HA	3:3:416:PHE:HB3	1.88	0.55
3:C:54:LEU:N	3:C:55:PRO:HD3	2.22	0.55
1:J:357:THR:N	1:J:358:PRO:HD2	2.21	0.55
3:L:398:VAL:HG21	3:L:448:MET:HE2	1.89	0.55
3:L:701:ALA:HB2	3:L:763:LEU:HB2	1.87	0.55
1:S:145:LEU:O	1:S:149:ILE:HG13	2.06	0.55
3:U:309:PRO:HG2	3:U:320:ALA:O	2.07	0.55
3:U:483:ASP:O	3:U:484:LYS:HG2	2.07	0.55
1:1:397:ARG:HE	3:3:79:LEU:CD1	2.19	0.55
5:5:35:LYS:HD3	5:5:102:PRO:HB2	1.87	0.55
5:5:116:ARG:HB3	5:5:135:ILE:HG13	1.87	0.55
6:6:36:LEU:HD22	6:6:77:VAL:HG21	1.89	0.55
7:9:134:GLU:CD	7:9:134:GLU:H	2.14	0.55
1:A:162:LEU:O	1:A:165:THR:HG22	2.06	0.55
3:C:200:LEU:O	3:C:201:ASP:HB2	2.07	0.55
3:C:309:PRO:HG2	3:C:320:ALA:O	2.06	0.55
1:J:265:GLU:O	1:J:266:LEU:HG	2.07	0.55
4:M:70:MET:HG2	4:M:78:ASN:OD1	2.07	0.55
3:U:440:ARG:HH11	3:U:440:ARG:CG	2.19	0.55
5:W:42:LYS:CB	5:W:107:LEU:HD13	2.32	0.55
3:3:326:PHE:CE2	3:3:330:LYS:HE3	2.41	0.55
3:3:689:LYS:HE3	3:3:771:VAL:HG13	1.88	0.55
4:D:148:TYR:CB	4:D:200:ARG:HH12	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:10:PHE:CZ	2:K:33:ARG:HG3	2.42	0.55
3:L:141:GLU:OE2	3:L:143:TYR:HE1	1.90	0.55
3:L:305:ARG:HG2	3:L:588:SER:O	2.07	0.55
4:M:250:LYS:CE	4:M:262:PHE:HB3	2.37	0.55
6:O:57:ARG:C	6:O:57:ARG:NE	2.65	0.55
6:O:115:GLY:HA3	6:O:125:GLN:OE1	2.07	0.55
1:S:397:ARG:HG2	3:U:49:LEU:HD13	1.89	0.55
3:U:141:GLU:OE2	3:U:143:TYR:HE1	1.90	0.55
3:U:497:TRP:O	3:U:528:LYS:HE3	2.06	0.55
3:U:497:TRP:O	3:U:500:ALA:HB3	2.06	0.55
5:5:20:ASN:HD21	5:5:24:ASN:HB2	1.72	0.55
5:5:66:GLU:HG2	5:5:95:PRO:HA	1.88	0.55
8:7:60:SER:HA	8:7:66:PRO:HA	1.89	0.55
1:A:189:MET:O	1:A:193:GLU:HB2	2.07	0.55
5:E:20:ASN:HD21	5:E:24:ASN:HB2	1.72	0.55
8:H:121:ARG:HG3	8:H:121:ARG:NH1	2.22	0.55
2:K:38:GLU:OE2	2:K:45:ARG:NH1	2.40	0.55
2:K:139:GLU:HB2	2:K:140:PRO:CD	2.35	0.55
3:L:112:LEU:HD12	4:M:322:GLU:HG3	1.88	0.55
3:L:497:TRP:O	3:L:528:LYS:HE3	2.06	0.55
4:M:85:MET:HE3	4:M:409:ARG:CG	2.37	0.55
4:M:115:THR:CG2	4:M:297:LEU:HD23	2.37	0.55
4:4:70:MET:HG2	4:4:78:ASN:OD1	2.08	0.54
5:5:59:THR:O	5:5:59:THR:HG22	2.06	0.54
4:D:153:ARG:HG3	4:D:153:ARG:NH1	2.21	0.54
4:D:213:ILE:CG2	4:D:217:ARG:HH11	2.19	0.54
6:F:57:ARG:C	6:F:57:ARG:NE	2.65	0.54
3:L:281:GLU:HG2	3:L:283:PRO:HD3	1.88	0.54
3:L:413:LEU:HA	3:L:416:PHE:HB3	1.87	0.54
4:M:381:LEU:H	4:M:382:PRO:HD2	1.72	0.54
3:U:115:HIS:CD2	3:U:116:PRO:HD2	2.41	0.54
3:U:501:LYS:H	3:U:501:LYS:CD	2.03	0.54
5:W:92:VAL:HG23	5:W:92:VAL:O	2.07	0.54
2:2:110:GLU:HA	8:7:121:ARG:NH1	2.21	0.54
3:3:54:LEU:N	3:3:55:PRO:HD3	2.22	0.54
1:A:104:ARG:HH21	2:B:127:SER:HB2	1.71	0.54
1:A:438:ARG:HD2	1:A:438:ARG:N	2.22	0.54
3:C:399:LEU:HD12	3:C:399:LEU:N	2.23	0.54
3:C:572:PRO:HD2	3:C:577:LEU:HD21	1.89	0.54
4:D:248:VAL:HB	4:D:347:GLU:HB2	1.89	0.54
7:G:134:GLU:H	7:G:134:GLU:CD	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:72:THR:HG21	1:J:223:THR:HG21	1.90	0.54
1:J:438:ARG:HD2	1:J:438:ARG:N	2.23	0.54
3:L:18:SER:HB2	3:L:433:ALA:O	2.06	0.54
3:L:125:GLY:HA3	3:L:246:ASN:HD22	1.72	0.54
3:L:329:LEU:HD21	3:L:644:LEU:HA	1.89	0.54
3:L:477:LEU:HD22	3:L:517:ALA:HB1	1.87	0.54
4:M:85:MET:HE1	4:M:370:VAL:HG11	1.89	0.54
5:N:1:MET:C	5:N:3:LEU:H	2.14	0.54
1:S:238:PHE:HE1	1:S:249:MET:HE1	1.72	0.54
1:S:391:LEU:HD22	1:S:407:VAL:HB	1.90	0.54
3:U:117:LEU:H	4:V:321:MET:CE	2.16	0.54
3:U:469:ARG:HA	3:U:754:PRO:HG3	1.88	0.54
3:U:715:GLU:HB3	3:U:746:ARG:NH1	2.22	0.54
3:3:282:VAL:HG22	3:3:285:VAL:HG12	1.90	0.54
4:4:84:ARG:O	6:6:83:ARG:NH2	2.40	0.54
4:4:363:SER:CB	5:5:174:LEU:H	2.19	0.54
1:A:196:ARG:NH2	3:C:204:GLU:O	2.41	0.54
3:C:20:MET:HE2	3:C:433:ALA:HB2	1.90	0.54
3:C:402:PRO:CB	3:C:535:MET:HE1	2.37	0.54
1:J:53:VAL:O	1:J:57:VAL:HG23	2.06	0.54
1:J:197:ALA:HB3	2:K:66:PHE:CE1	2.43	0.54
3:L:184:CYS:O	9:L:785:SF4:S4	2.66	0.54
3:L:344:TYR:CD1	3:L:568:TYR:CE1	2.96	0.54
6:O:115:GLY:HA2	6:O:125:GLN:HA	1.89	0.54
8:Q:89:ALA:O	8:Q:91:ILE:HG13	2.08	0.54
2:T:10:PHE:CZ	2:T:33:ARG:HG3	2.42	0.54
1:1:341:MET:HE2	1:1:409:PRO:O	2.08	0.54
4:4:43:LEU:HD11	4:4:397:ILE:CD1	2.38	0.54
4:4:83:PRO:HB2	4:4:169:HIS:HA	1.89	0.54
4:4:119:ILE:O	4:4:123:LEU:HB2	2.07	0.54
4:4:240:ARG:NH2	4:4:347:GLU:OE2	2.39	0.54
4:4:287:VAL:O	4:4:291:LYS:HG3	2.07	0.54
1:A:287:ILE:HG22	1:A:302:PHE:CG	2.42	0.54
5:E:25:LEU:N	5:E:25:LEU:CD2	2.71	0.54
4:M:404:MET:HA	4:M:407:VAL:CG1	2.38	0.54
1:S:41:ALA:HB2	1:S:116:GLU:HG3	1.90	0.54
4:V:74:THR:HB	4:V:77:GLN:HG3	1.88	0.54
4:V:241:ALA:CA	4:V:278:VAL:HG21	2.37	0.54
5:W:1:MET:C	5:W:3:LEU:H	2.15	0.54
1:1:63:ARG:HD3	1:1:313:TYR:HD2	1.73	0.54
2:2:139:GLU:CB	2:2:140:PRO:CD	2.84	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:683:LEU:N	3:3:683:LEU:HD23	2.23	0.54
4:4:161:GLU:OE1	7:9:34:LYS:HG2	2.07	0.54
5:5:84:ASP:OD1	5:5:84:ASP:N	2.39	0.54
6:6:57:ARG:C	6:6:57:ARG:NE	2.66	0.54
1:A:342:TRP:O	1:A:342:TRP:HE3	1.90	0.54
3:C:282:VAL:HG22	3:C:282:VAL:O	2.06	0.54
3:C:330:LYS:HA	3:C:647:ALA:HB1	1.90	0.54
3:C:440:ARG:HH11	3:C:440:ARG:CG	2.19	0.54
1:J:186:THR:HA	1:J:189:MET:HE2	1.89	0.54
1:J:303:THR:OG1	1:J:306:VAL:HG23	2.07	0.54
3:L:112:LEU:HD21	3:L:130:LEU:HD11	1.88	0.54
3:L:515:THR:HG23	3:L:683:LEU:CD1	2.35	0.54
3:L:688:ARG:HB3	3:L:770:ARG:HD3	1.89	0.54
4:M:342:VAL:HG22	4:M:343:TYR:H	1.73	0.54
3:U:414:SER:O	3:U:418:ARG:HG3	2.08	0.54
4:V:249:ARG:HD2	4:V:257:TYR:CE1	2.43	0.54
5:W:20:ASN:HD21	5:W:24:ASN:HB2	1.73	0.54
5:W:174:LEU:HD22	5:W:180:GLY:HA2	1.90	0.54
1:1:92:ASN:ND2	10:1:440:FMN:O3'	2.41	0.54
3:3:94:ASP:OD2	3:3:97:SER:HB2	2.08	0.54
3:3:694:LEU:HB3	3:3:762:ALA:CB	2.34	0.54
1:A:360:ARG:O	1:A:364:ALA:HB3	2.07	0.54
3:C:241:ARG:HH11	7:G:74:GLU:CD	2.15	0.54
4:D:74:THR:HB	4:D:77:GLN:HG3	1.90	0.54
5:E:1:MET:SD	8:Z:113:GLU:OE2	2.65	0.54
7:G:128:ASP:O	7:G:144:LYS:HD3	2.07	0.54
2:K:77:LYS:H	2:K:116:LEU:HA	1.72	0.54
2:K:81:GLN:HB3	2:K:122:VAL:CG2	2.37	0.54
4:M:59:ILE:HD13	4:M:59:ILE:H	1.71	0.54
3:U:333:LEU:HD22	3:U:648:LEU:HD21	1.90	0.54
3:U:402:PRO:HD2	3:U:458:LEU:HD13	1.89	0.54
3:U:409:LEU:HD12	3:U:535:MET:CE	2.37	0.54
4:V:215:TYR:CE2	4:V:219:ARG:HG3	2.43	0.54
5:W:116:ARG:HB3	5:W:135:ILE:HG13	1.88	0.54
5:W:175:THR:CG2	5:W:178:ASP:HB2	2.32	0.54
6:X:115:GLY:HA2	6:X:125:GLN:HA	1.88	0.54
1:1:274:GLU:HG2	1:1:279:TRP:HE1	1.72	0.54
1:1:363:VAL:HA	1:1:367:MET:HB2	1.89	0.54
3:3:400:GLY:O	3:3:402:PRO:HD3	2.07	0.54
3:3:688:ARG:HB3	3:3:770:ARG:HD3	1.88	0.54
4:4:84:ARG:HG2	9:6:182:SF4:S2	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:167:ARG:HD3	6:6:143:ARG:HH12	1.73	0.54
4:4:252:TYR:CE2	5:5:87:ARG:NH2	2.75	0.54
4:4:265:PRO:HG2	4:4:282:GLU:HG2	1.89	0.54
4:D:119:ILE:O	4:D:123:LEU:HB2	2.08	0.54
3:L:341:VAL:HG21	3:L:364:LEU:HD11	1.88	0.54
3:L:586:HIS:NE2	3:L:604:ALA:HB2	2.23	0.54
6:O:155:GLN:O	6:O:158:VAL:HG22	2.08	0.54
3:U:192:GLU:OE2	3:U:440:ARG:HA	2.08	0.54
3:U:281:GLU:HG2	3:U:283:PRO:HD3	1.88	0.54
4:V:69:THR:HG21	6:X:120:ASN:HD22	1.71	0.54
4:V:85:MET:HE3	4:V:409:ARG:CG	2.37	0.54
4:V:283:MET:O	4:V:287:VAL:HG23	2.08	0.54
6:X:117:MET:HB3	7:Y:99:ILE:HD13	1.89	0.54
8:Z:8:GLU:HG2	8:Z:97:TYR:CZ	2.43	0.54
1:1:274:GLU:HA	1:1:278:GLU:HG2	1.90	0.54
5:5:33:ARG:O	5:5:37:GLU:HB2	2.07	0.54
7:9:33:LEU:HD11	7:9:161:TYR:CB	2.34	0.54
3:C:414:SER:O	3:C:418:ARG:HG3	2.08	0.54
3:C:701:ALA:HB2	3:C:763:LEU:HB2	1.90	0.54
3:C:734:VAL:CG1	3:C:775:VAL:HG13	2.37	0.54
4:D:59:ILE:H	4:D:59:ILE:HD13	1.71	0.54
1:J:341:MET:HE2	1:J:409:PRO:O	2.08	0.54
3:L:216:PHE:CZ	8:Q:128:PHE:HD2	2.20	0.54
7:P:48:ASN:CB	7:P:50:LEU:HD23	2.36	0.54
8:Q:13:TRP:CZ2	8:Q:17:LEU:HD11	2.42	0.54
6:X:43:LEU:HD11	6:X:84:LEU:HD23	1.89	0.54
1:A:201:LEU:HG	1:A:203:PRO:HD2	1.90	0.54
1:A:366:PHE:HD1	1:A:370:LEU:HD21	1.72	0.54
1:A:436:LEU:HD23	2:B:90:LEU:HA	1.90	0.54
4:D:84:ARG:NE	6:F:117:MET:HE1	2.22	0.54
4:D:112:ARG:HH21	4:D:297:LEU:HD11	1.72	0.54
4:D:162:TRP:CE2	7:G:34:LYS:HD2	2.41	0.54
5:E:33:ARG:O	5:E:37:GLU:HB2	2.08	0.54
6:F:93:ARG:NH1	6:F:96:TRP:CZ3	2.76	0.54
1:J:397:ARG:HE	3:L:79:LEU:CD1	2.19	0.54
2:K:7:LYS:HD2	2:K:7:LYS:N	2.20	0.54
3:L:400:GLY:O	3:L:402:PRO:HD3	2.08	0.54
3:U:478:LEU:CD2	3:U:483:ASP:HB2	2.38	0.54
4:V:106:GLY:O	5:W:194:SER:HB3	2.08	0.54
4:V:363:SER:CB	5:W:174:LEU:H	2.21	0.54
6:X:57:ARG:C	6:X:57:ARG:NE	2.65	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:145:GLU:CG	7:Y:31:VAL:HG21	2.20	0.54
3:3:185:LYS:HG2	3:3:188:VAL:HG22	1.89	0.54
3:3:341:VAL:HG11	3:3:364:LEU:HD21	1.89	0.54
4:4:247:ASP:OD1	4:4:249:ARG:HG3	2.07	0.54
1:A:274:GLU:HG3	1:A:278:GLU:HG3	1.90	0.54
1:A:332:PRO:CD	2:B:90:LEU:HD23	2.38	0.54
2:K:139:GLU:CB	2:K:140:PRO:CD	2.85	0.54
3:L:269:THR:HG22	3:L:274:LEU:HA	1.90	0.54
4:M:241:ALA:CA	4:M:278:VAL:HG21	2.38	0.54
3:U:357:ALA:HB2	3:U:641:LEU:HD11	1.90	0.54
4:V:74:THR:HB	4:V:77:GLN:H	1.73	0.54
4:V:84:ARG:HG2	9:X:182:SF4:S2	2.48	0.54
4:V:393:MET:O	4:V:396:ILE:HG22	2.07	0.54
6:X:107:SER:O	6:X:137:VAL:HG12	2.07	0.54
1:1:356:CYS:HB3	1:1:358:PRO:HG2	1.89	0.53
3:3:192:GLU:OE2	3:3:440:ARG:HA	2.08	0.53
4:4:74:THR:HB	4:4:77:GLN:HG3	1.88	0.53
4:4:85:MET:HE3	4:4:409:ARG:CG	2.38	0.53
4:M:116:ILE:HD11	4:M:182:LEU:HG	1.90	0.53
4:M:148:TYR:CB	4:M:200:ARG:HH12	2.21	0.53
4:M:254:TYR:CD2	4:M:346:THR:HA	2.42	0.53
5:N:84:ASP:OD1	5:N:84:ASP:N	2.40	0.53
5:N:116:ARG:HB3	5:N:135:ILE:HG13	1.89	0.53
8:Q:86:LEU:HD12	8:Q:91:ILE:HD12	1.90	0.53
1:S:301:PRO:O	1:S:306:VAL:HG21	2.08	0.53
2:T:61:MET:HE2	3:U:214:MET:HG2	1.89	0.53
3:U:473:GLU:O	3:U:477:LEU:HD13	2.08	0.53
6:X:138:PRO:HG2	7:Y:121:MET:HG3	1.89	0.53
3:3:402:PRO:HD2	3:3:458:LEU:HD13	1.90	0.53
3:3:583:VAL:CG2	3:3:598:ALA:HA	2.38	0.53
4:4:123:LEU:HD21	4:4:159:LEU:HD12	1.90	0.53
4:4:404:MET:HA	4:4:407:VAL:CG1	2.38	0.53
5:5:37:GLU:O	5:5:41:TYR:HD1	1.90	0.53
5:E:26:TRP:HE1	5:E:91:ARG:HH21	1.53	0.53
1:J:266:LEU:HB3	1:J:270:THR:HG21	1.90	0.53
3:L:46:ARG:O	3:L:107:MET:HG2	2.08	0.53
4:M:342:VAL:HG22	4:M:343:TYR:N	2.24	0.53
8:Q:37:PHE:CE2	8:Q:74:PRO:HA	2.43	0.53
3:U:24:PHE:CE1	3:U:29:ASP:HA	2.42	0.53
3:U:501:LYS:HD2	3:U:501:LYS:N	2.08	0.53
8:Z:117:ALA:O	8:Z:121:ARG:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:185:LYS:HG3	3:3:202:PHE:CE2	2.43	0.53
3:3:473:GLU:O	3:3:477:LEU:HD13	2.08	0.53
4:4:254:TYR:CD1	4:4:255:SER:N	2.70	0.53
3:C:413:LEU:HA	3:C:416:PHE:HB3	1.89	0.53
3:C:670:PRO:HD2	3:C:676:LEU:HD23	1.90	0.53
5:E:37:GLU:O	5:E:41:TYR:HD1	1.91	0.53
3:L:474:ARG:HA	3:L:517:ALA:HB2	1.91	0.53
3:L:583:VAL:HG23	3:L:599:HIS:H	1.73	0.53
4:M:119:ILE:O	4:M:123:LEU:HB2	2.08	0.53
4:M:374:SER:HB2	4:M:406:ASP:HB3	1.90	0.53
5:N:71:VAL:CG1	5:N:89:PHE:HD2	2.21	0.53
1:S:398:SER:HA	3:U:46:ARG:HD2	1.89	0.53
3:U:173:PHE:HB3	3:U:296:PHE:CZ	2.43	0.53
3:U:341:VAL:HG11	3:U:364:LEU:HD21	1.90	0.53
4:V:187:VAL:N	4:V:188:PRO:HD2	2.24	0.53
5:W:121:LEU:O	5:W:144:HIS:HB3	2.08	0.53
3:3:402:PRO:CG	3:3:535:MET:HE1	2.39	0.53
4:4:342:VAL:HG22	4:4:343:TYR:H	1.73	0.53
5:5:1:MET:C	5:5:3:LEU:H	2.15	0.53
1:A:37:GLY:C	1:A:39:GLU:H	2.17	0.53
3:C:24:PHE:CE1	3:C:29:ASP:HA	2.43	0.53
4:D:404:MET:HA	4:D:407:VAL:CG1	2.39	0.53
1:J:270:THR:O	1:J:311:MET:HG3	2.08	0.53
1:J:437:TRP:CZ3	2:K:96:LEU:HB2	2.44	0.53
3:L:192:GLU:OE2	3:L:440:ARG:HA	2.09	0.53
4:M:123:LEU:HD21	4:M:159:LEU:HD12	1.91	0.53
4:M:187:VAL:N	4:M:188:PRO:HD2	2.23	0.53
3:U:750:ARG:HB3	3:U:752:ASP:OD1	2.07	0.53
4:V:254:TYR:CE2	4:V:346:THR:CA	2.87	0.53
1:1:341:MET:CE	1:1:409:PRO:HB2	2.38	0.53
3:3:305:ARG:HG2	3:3:588:SER:O	2.08	0.53
3:3:557:SER:H	3:3:560:GLU:HB2	1.74	0.53
4:4:73:ARG:HG3	4:4:77:GLN:OE1	2.08	0.53
8:7:82:ILE:HG23	8:7:95:ALA:HB3	1.90	0.53
1:A:92:ASN:ND2	10:A:440:FMN:N1	2.57	0.53
3:C:456:ALA:HB3	3:C:459:MET:HE3	1.90	0.53
3:C:515:THR:HG23	3:C:683:LEU:CD1	2.35	0.53
4:D:84:ARG:HD3	6:F:117:MET:HE1	1.90	0.53
6:F:36:LEU:HD22	6:F:77:VAL:HG21	1.89	0.53
6:F:155:GLN:O	6:F:158:VAL:HG22	2.09	0.53
2:K:101:THR:HG23	2:K:106:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:694:LEU:CB	3:L:762:ALA:HB2	2.35	0.53
6:O:163:TYR:CD2	6:O:169:ARG:HA	2.36	0.53
5:W:66:GLU:HG2	5:W:95:PRO:HA	1.91	0.53
6:X:41:PHE:CZ	6:X:92:MET:HB2	2.43	0.53
1:1:49:THR:OG1	1:1:52:GLU:HG3	2.09	0.53
3:3:161:ARG:HG2	3:3:161:ARG:HH11	1.74	0.53
3:3:474:ARG:HA	3:3:517:ALA:HB2	1.91	0.53
4:4:120:LEU:HD13	4:4:160:PHE:CE1	2.39	0.53
5:5:167:PRO:HB3	7:9:66:TYR:CE2	2.44	0.53
3:C:268:ASP:OD2	3:C:278:ARG:NH1	2.41	0.53
3:C:341:VAL:HG11	3:C:364:LEU:HD21	1.91	0.53
5:E:157:THR:C	5:E:158:LEU:HD23	2.34	0.53
6:F:99:MET:CG	6:F:100:PRO:HD2	2.36	0.53
2:K:106:ILE:HG22	2:K:110:GLU:HB2	1.91	0.53
3:L:194:VAL:HG12	3:L:411:LEU:HD22	1.90	0.53
3:L:341:VAL:HG11	3:L:364:LEU:HD21	1.89	0.53
3:L:683:LEU:N	3:L:683:LEU:HD23	2.24	0.53
5:N:134:LYS:HD3	5:N:137:THR:OG1	2.07	0.53
8:Q:37:PHE:HD1	8:Q:53:THR:O	1.90	0.53
8:Q:60:SER:HA	8:Q:66:PRO:HA	1.90	0.53
1:S:342:TRP:O	1:S:342:TRP:HE3	1.92	0.53
2:T:86:LEU:O	2:T:90:LEU:HD12	2.08	0.53
4:V:248:VAL:HB	4:V:347:GLU:HB2	1.91	0.53
8:Z:70:ALA:HA	8:Z:83:GLY:O	2.09	0.53
4:4:187:VAL:N	4:4:188:PRO:HD2	2.23	0.53
5:5:141:LEU:HD11	5:5:150:TYR:OH	2.09	0.53
4:D:338:PRO:HG3	5:E:192:TYR:O	2.09	0.53
4:M:219:ARG:NH1	4:M:273:PHE:CD2	2.77	0.53
2:T:130:THR:HB	2:T:144:CYS:SG	2.49	0.53
3:U:684:ARG:HG2	3:U:684:ARG:NH1	2.22	0.53
3:3:55:PRO:HG3	3:3:74:GLN:H	1.68	0.53
3:3:372:GLN:O	3:3:558:TRP:CE2	2.62	0.53
6:6:93:ARG:NH1	6:6:96:TRP:CZ3	2.76	0.53
1:A:357:THR:N	1:A:358:PRO:HD2	2.24	0.53
3:C:583:VAL:HG23	3:C:599:HIS:H	1.73	0.53
3:C:612:GLY:O	3:C:624:LEU:HB2	2.09	0.53
4:D:74:THR:HB	4:D:77:GLN:H	1.73	0.53
6:F:77:VAL:HA	6:F:104:TRP:O	2.08	0.53
3:L:497:TRP:O	3:L:500:ALA:HB3	2.09	0.53
6:O:117:MET:HE2	7:P:99:ILE:HG12	1.91	0.53
1:S:270:THR:O	1:S:311:MET:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:120:PRO:HG2	8:Z:42:TYR:OH	2.09	0.53
4:V:61:TYR:CZ	6:X:87:LYS:HE2	2.44	0.53
3:3:330:LYS:HA	3:3:647:ALA:HB1	1.89	0.53
3:3:333:LEU:HD22	3:3:648:LEU:HD21	1.91	0.53
1:A:81:LYS:HA	1:A:81:LYS:CE	2.39	0.53
1:J:145:LEU:O	1:J:149:ILE:HG13	2.09	0.53
3:U:413:LEU:HA	3:U:416:PHE:HB3	1.89	0.53
3:U:693:TYR:HB3	3:U:759:TYR:CD2	2.44	0.53
3:3:282:VAL:HG22	3:3:282:VAL:O	2.10	0.53
3:3:382:PHE:CD1	3:3:382:PHE:N	2.76	0.53
5:5:116:ARG:HG3	5:5:129:HIS:CE1	2.43	0.53
1:A:145:LEU:O	1:A:149:ILE:HG13	2.09	0.53
3:C:18:SER:HB3	3:C:21:ASP:OD1	2.08	0.53
3:C:45:CYS:O	3:C:46:ARG:HB2	2.07	0.53
3:C:333:LEU:HD22	3:C:648:LEU:HD21	1.91	0.53
3:L:18:SER:HB3	3:L:21:ASP:OD1	2.08	0.53
3:L:399:LEU:HD12	3:L:399:LEU:N	2.24	0.53
3:L:458:LEU:H	3:L:458:LEU:HD12	1.73	0.53
8:Q:121:ARG:HG3	8:Q:121:ARG:NH1	2.24	0.53
2:T:40:TRP:CD1	2:T:74:PRO:HA	2.43	0.53
3:U:550:LEU:HD23	3:U:684:ARG:NH2	2.24	0.53
3:U:583:VAL:CG2	3:U:598:ALA:HA	2.39	0.53
3:U:695:ARG:NH1	3:U:715:GLU:OE1	2.40	0.53
4:V:52:VAL:HG23	4:V:388:GLU:O	2.08	0.53
1:1:29:LEU:CD1	1:1:155:ARG:HG3	2.38	0.52
1:1:189:MET:O	1:1:193:GLU:HB2	2.08	0.52
3:3:112:LEU:HD21	3:3:130:LEU:HD11	1.89	0.52
3:3:269:THR:HG22	3:3:274:LEU:HA	1.92	0.52
3:3:693:TYR:HB3	3:3:759:TYR:HD2	1.73	0.52
4:4:64:THR:HB	4:4:66:PHE:HE1	1.74	0.52
4:4:168:PHE:HE1	6:6:141:PRO:HG3	1.74	0.52
1:A:89:LEU:HD23	1:A:118:MET:HE3	1.90	0.52
1:A:301:PRO:O	1:A:306:VAL:HG21	2.08	0.52
1:A:437:TRP:CZ3	2:B:96:LEU:HB2	2.44	0.52
3:C:269:THR:HG22	3:C:274:LEU:HA	1.91	0.52
3:C:326:PHE:CE2	3:C:330:LYS:HE3	2.43	0.52
4:D:254:TYR:CD2	4:D:346:THR:HA	2.44	0.52
4:D:363:SER:CB	5:E:174:LEU:H	2.22	0.52
6:O:84:LEU:O	6:O:124:VAL:HG23	2.09	0.52
6:O:93:ARG:NH1	6:O:96:TRP:CZ3	2.76	0.52
6:O:108:MET:HA	6:O:137:VAL:CG1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:189:MET:O	1:S:193:GLU:HB2	2.09	0.52
3:U:245:ARG:NH1	7:Y:56:CYS:O	2.41	0.52
2:2:129:HIS:CD2	2:2:130:THR:HG23	2.43	0.52
1:A:274:GLU:HA	1:A:278:GLU:HG2	1.90	0.52
5:E:167:PRO:HB3	7:G:66:TYR:CE2	2.44	0.52
1:J:274:GLU:HG2	1:J:279:TRP:HE1	1.73	0.52
1:J:366:PHE:CE1	1:J:370:LEU:HD21	2.44	0.52
4:M:74:THR:HB	4:M:77:GLN:H	1.73	0.52
7:P:128:ASP:O	7:P:144:LYS:HD3	2.10	0.52
3:U:18:SER:HB3	3:U:21:ASP:OD1	2.08	0.52
4:V:247:ASP:OD1	4:V:249:ARG:HG3	2.08	0.52
1:1:40:THR:O	1:1:44:VAL:HG23	2.09	0.52
3:3:546:ALA:O	3:3:547:MET:HE2	2.09	0.52
4:4:367:ARG:HH12	4:4:369:LYS:CA	2.21	0.52
7:9:128:ASP:O	7:9:144:LYS:HD3	2.10	0.52
1:A:40:THR:O	1:A:44:VAL:HG23	2.09	0.52
2:B:136:VAL:HG12	2:B:137:ASN:N	2.23	0.52
3:C:185:LYS:HG3	3:C:202:PHE:HE2	1.74	0.52
8:H:82:ILE:HG23	8:H:95:ALA:HB3	1.91	0.52
3:L:506:ILE:CG2	3:L:535:MET:HE3	2.39	0.52
1:S:186:THR:HG23	1:S:199:PRO:HA	1.92	0.52
1:S:267:PRO:HG2	1:S:270:THR:HG22	1.90	0.52
1:S:274:GLU:HA	1:S:278:GLU:HG2	1.91	0.52
3:U:165:ASP:HB3	3:U:178:ARG:HD2	1.89	0.52
3:U:305:ARG:HG2	3:U:588:SER:O	2.08	0.52
4:4:144:THR:N	4:4:145:PRO:CD	2.72	0.52
5:5:26:TRP:HE1	5:5:91:ARG:HH21	1.55	0.52
3:C:46:ARG:HH11	3:C:46:ARG:CG	1.96	0.52
4:D:187:VAL:N	4:D:188:PRO:HD2	2.24	0.52
8:H:60:SER:HA	8:H:66:PRO:HA	1.90	0.52
1:J:358:PRO:O	1:J:362:GLY:HA3	2.10	0.52
3:L:115:HIS:CD2	3:L:116:PRO:HD2	2.45	0.52
3:L:120:PRO:HG2	8:Q:42:TYR:OH	2.09	0.52
3:L:372:GLN:O	3:L:558:TRP:CE2	2.62	0.52
6:O:77:VAL:O	6:O:77:VAL:HG12	2.09	0.52
8:Q:29:VAL:HG22	8:Q:60:SER:O	2.08	0.52
4:V:219:ARG:NH1	4:V:273:PHE:CD2	2.78	0.52
4:V:376:VAL:O	4:V:379:GLN:HG3	2.09	0.52
5:W:71:VAL:CG1	5:W:89:PHE:HD2	2.22	0.52
1:1:37:GLY:C	1:1:39:GLU:H	2.18	0.52
1:1:197:ALA:HB3	2:2:66:PHE:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:734:VAL:CG1	3:3:775:VAL:HG13	2.38	0.52
3:3:750:ARG:HB3	3:3:752:ASP:OD1	2.10	0.52
4:4:316:LEU:C	4:4:318:GLU:H	2.17	0.52
1:A:139:ARG:CG	2:B:140:PRO:HD3	2.38	0.52
2:B:33:ARG:HH21	2:B:37:GLU:CG	2.22	0.52
3:C:683:LEU:N	3:C:683:LEU:HD23	2.24	0.52
4:D:123:LEU:HD21	4:D:159:LEU:HD12	1.90	0.52
1:J:274:GLU:HA	1:J:278:GLU:HG2	1.92	0.52
5:N:26:TRP:HE1	5:N:91:ARG:HH21	1.55	0.52
6:O:152:MET:HE2	6:O:156:LYS:HE2	1.91	0.52
1:S:293:GLY:HA3	1:S:324:GLY:N	2.08	0.52
4:V:96:ALA:HB2	4:V:346:THR:HG21	1.91	0.52
6:X:146:ALA:HB2	7:Y:119:PHE:HD1	1.74	0.52
2:2:7:LYS:HD2	2:2:7:LYS:N	2.22	0.52
2:B:38:GLU:OE2	2:B:45:ARG:NH1	2.43	0.52
4:D:249:ARG:HD2	4:D:257:TYR:CE1	2.45	0.52
3:L:186:ARG:HD2	3:L:231:PRO:HD3	1.91	0.52
1:S:250:LYS:HB3	1:S:252:TYR:CE2	2.45	0.52
1:S:265:GLU:O	1:S:266:LEU:HG	2.09	0.52
3:U:186:ARG:HD2	3:U:231:PRO:HD3	1.91	0.52
4:V:168:PHE:N	4:V:168:PHE:CD1	2.78	0.52
3:3:232:VAL:HB	9:3:784:SF4:S2	2.50	0.52
3:3:385:ALA:HB2	3:3:531:LYS:HB3	1.90	0.52
3:3:488:GLU:O	3:3:491:ALA:HB3	2.10	0.52
3:3:513:GLN:HG2	3:3:769:LEU:HD23	1.91	0.52
3:3:715:GLU:HB3	3:3:746:ARG:NH1	2.24	0.52
4:4:385:CYS:HB3	4:4:396:ILE:HG12	1.90	0.52
1:A:211:LEU:H	1:A:216:THR:HG21	1.73	0.52
2:B:42:ARG:HB2	2:B:45:ARG:HG2	1.91	0.52
3:L:385:ALA:HB3	3:L:533:LEU:CD2	2.40	0.52
3:L:501:LYS:HD2	3:L:501:LYS:N	2.10	0.52
1:S:274:GLU:HG3	1:S:278:GLU:HG3	1.91	0.52
1:S:357:THR:N	1:S:358:PRO:HD2	2.25	0.52
3:U:2:VAL:HG13	3:U:89:ASP:HA	1.90	0.52
3:U:185:LYS:HG3	3:U:202:PHE:CE2	2.44	0.52
5:W:141:LEU:HD11	5:W:150:TYR:OH	2.10	0.52
6:X:163:TYR:CD2	6:X:169:ARG:HA	2.35	0.52
8:Z:37:PHE:CE2	8:Z:74:PRO:HA	2.45	0.52
1:1:104:ARG:HH21	2:2:127:SER:HB2	1.74	0.52
1:1:118:MET:HG2	1:1:224:LEU:HD13	1.91	0.52
1:1:239:ALA:C	1:1:241:MET:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:409:LEU:HD12	3:3:535:MET:CE	2.39	0.52
8:7:16:LEU:HG	8:7:82:ILE:HD11	1.92	0.52
1:A:63:ARG:HD3	1:A:313:TYR:HD2	1.75	0.52
3:C:141:GLU:OE2	3:C:143:TYR:HE1	1.92	0.52
5:E:53:VAL:HG22	5:E:55:LEU:CD1	2.40	0.52
5:E:174:LEU:HD22	5:E:180:GLY:HA2	1.91	0.52
2:K:33:ARG:HH21	2:K:37:GLU:CG	2.23	0.52
4:M:240:ARG:NH2	4:M:347:GLU:OE2	2.40	0.52
4:M:254:TYR:CE2	4:M:346:THR:CA	2.91	0.52
4:M:363:SER:HB3	5:N:173:ALA:HB1	1.91	0.52
5:N:53:VAL:HG22	5:N:55:LEU:CD1	2.40	0.52
1:S:110:VAL:HG23	1:S:110:VAL:O	2.10	0.52
2:T:7:LYS:HD2	2:T:7:LYS:N	2.23	0.52
8:Z:20:MET:HE3	8:Z:59:LEU:HG	1.91	0.52
5:5:2:ARG:NH1	5:5:45:GLY:HA3	2.25	0.52
2:B:33:ARG:HH21	2:B:37:GLU:HG3	1.75	0.52
1:J:49:THR:OG1	1:J:52:GLU:HG3	2.10	0.52
4:M:144:THR:N	4:M:145:PRO:CD	2.73	0.52
6:O:165:GLU:HG2	7:P:148:ARG:NH1	2.25	0.52
8:Q:8:GLU:HG2	8:Q:97:TYR:CZ	2.45	0.52
1:S:109:ASP:C	1:S:111:PRO:HD3	2.34	0.52
3:3:83:CYS:SG	3:3:84:VAL:HG13	2.50	0.52
4:4:241:ALA:CA	4:4:278:VAL:HG21	2.40	0.52
5:5:121:LEU:O	5:5:144:HIS:HB3	2.09	0.52
7:9:48:ASN:CB	7:9:50:LEU:HD23	2.39	0.52
1:A:41:ALA:HA	1:A:120:LEU:HD21	1.92	0.52
1:A:183:GLY:O	10:A:440:FMN:H2'	2.10	0.52
4:D:43:LEU:HD11	4:D:397:ILE:CD1	2.40	0.52
5:E:125:VAL:HG12	5:E:126:PHE:N	2.24	0.52
6:F:93:ARG:NH1	6:F:96:TRP:CE3	2.78	0.52
4:M:393:MET:C	4:M:396:ILE:HG22	2.35	0.52
1:S:29:LEU:CD1	1:S:155:ARG:HG3	2.39	0.52
1:S:89:LEU:HD23	1:S:118:MET:HE3	1.91	0.52
1:S:116:GLU:HG2	1:S:228:VAL:HG22	1.92	0.52
1:S:118:MET:HG2	1:S:224:LEU:HD13	1.91	0.52
3:U:125:GLY:HA3	3:U:246:ASN:ND2	2.23	0.52
6:X:20:LEU:O	6:X:24:LEU:HD13	2.10	0.52
1:1:397:ARG:NE	3:3:79:LEU:HD12	2.23	0.51
6:6:40:THR:HB	6:6:50:MET:SD	2.50	0.51
3:C:194:VAL:HG12	3:C:411:LEU:HD22	1.91	0.51
3:C:372:GLN:O	3:C:558:TRP:CE2	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:215:TYR:CE2	4:D:219:ARG:HG3	2.45	0.51
5:E:66:GLU:HG2	5:E:95:PRO:HA	1.92	0.51
1:J:341:MET:CE	1:J:409:PRO:HB2	2.39	0.51
3:L:478:LEU:CD2	3:L:483:ASP:HB2	2.40	0.51
3:U:734:VAL:CG1	3:U:775:VAL:HG13	2.39	0.51
1:1:110:VAL:O	1:1:110:VAL:HG23	2.10	0.51
3:3:24:PHE:CE1	3:3:29:ASP:HA	2.45	0.51
4:4:248:VAL:HB	4:4:347:GLU:HB2	1.92	0.51
4:4:249:ARG:HD2	4:4:257:TYR:CE1	2.45	0.51
4:4:250:LYS:CE	4:4:262:PHE:HB3	2.41	0.51
2:B:102:GLU:HA	8:H:108:ILE:HD11	1.93	0.51
4:D:168:PHE:N	4:D:168:PHE:CD1	2.77	0.51
5:E:59:THR:HG22	5:E:59:THR:O	2.09	0.51
5:E:141:LEU:HD11	5:E:150:TYR:OH	2.10	0.51
1:J:436:LEU:HD23	2:K:90:LEU:HA	1.90	0.51
3:L:385:ALA:HB2	3:L:531:LYS:HB3	1.91	0.51
3:L:734:VAL:CG1	3:L:775:VAL:HG13	2.39	0.51
4:M:262:PHE:CD1	4:M:289:ILE:HD11	2.45	0.51
1:S:239:ALA:C	1:S:241:MET:H	2.18	0.51
1:1:366:PHE:HD1	1:1:370:LEU:HD21	1.76	0.51
5:5:160:ARG:HG3	7:9:130:VAL:HG11	1.92	0.51
6:6:84:LEU:O	6:6:124:VAL:HG23	2.10	0.51
7:9:44:THR:HA	7:9:138:VAL:HG13	1.91	0.51
8:7:13:TRP:CE2	8:7:17:LEU:HD11	2.45	0.51
2:B:101:THR:HG23	2:B:106:ILE:O	2.10	0.51
6:F:138:PRO:HG3	7:G:121:MET:HG3	1.91	0.51
5:N:174:LEU:CD2	5:N:180:GLY:HA2	2.39	0.51
7:P:163:VAL:HB	7:P:164:PRO:HD2	1.92	0.51
8:Q:16:LEU:O	8:Q:16:LEU:HD13	2.09	0.51
1:S:355:LYS:HD3	1:S:399:PHE:CD2	2.45	0.51
3:U:456:ALA:HB3	3:U:459:MET:HE3	1.93	0.51
3:U:474:ARG:HA	3:U:517:ALA:HB2	1.92	0.51
3:U:497:TRP:CD1	3:U:524:LEU:HD11	2.46	0.51
3:U:583:VAL:HG23	3:U:599:HIS:H	1.75	0.51
4:V:211:SER:HB2	4:V:215:TYR:N	2.26	0.51
4:V:294:LEU:O	4:V:294:LEU:HD23	2.11	0.51
8:Z:16:LEU:HG	8:Z:82:ILE:HD11	1.92	0.51
1:1:355:LYS:HD3	1:1:399:PHE:CD2	2.45	0.51
3:3:115:HIS:CD2	3:3:116:PRO:HD2	2.45	0.51
3:3:385:ALA:HB3	3:3:533:LEU:CD2	2.41	0.51
3:3:398:VAL:C	3:3:399:LEU:HD12	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:629:ILE:HG22	3:3:630:GLU:N	2.22	0.51
4:4:219:ARG:NH1	4:4:273:PHE:CD2	2.79	0.51
8:7:121:ARG:NH1	8:7:121:ARG:CG	2.74	0.51
3:C:402:PRO:CG	3:C:535:MET:HE1	2.40	0.51
3:C:715:GLU:HB3	3:C:746:ARG:NH1	2.26	0.51
5:E:34:PHE:HE1	5:E:38:MET:SD	2.33	0.51
5:E:84:ASP:OD1	5:E:84:ASP:N	2.42	0.51
5:E:103:THR:HG23	5:E:127:GLU:O	2.10	0.51
7:G:163:VAL:HB	7:G:164:PRO:HD2	1.92	0.51
1:J:366:PHE:HD1	1:J:370:LEU:HD21	1.76	0.51
3:L:185:LYS:HG3	3:L:202:PHE:HE2	1.76	0.51
3:L:188:VAL:CG2	3:L:189:ARG:N	2.74	0.51
3:L:513:GLN:HG2	3:L:769:LEU:HD23	1.91	0.51
4:M:74:THR:HB	4:M:77:GLN:HG3	1.90	0.51
6:O:138:PRO:HG2	7:P:121:MET:HG3	1.93	0.51
1:S:201:LEU:HG	1:S:203:PRO:HD2	1.92	0.51
3:U:750:ARG:HB2	3:U:753:VAL:HG23	1.91	0.51
4:V:85:MET:HE1	4:V:370:VAL:HG11	1.92	0.51
4:V:379:GLN:HG2	5:W:113:PHE:CD1	2.46	0.51
6:X:115:GLY:HA3	6:X:125:GLN:OE1	2.09	0.51
6:X:155:GLN:O	6:X:158:VAL:HG22	2.11	0.51
1:1:272:PHE:CE2	1:1:311:MET:HE3	2.45	0.51
3:3:285:VAL:HG22	3:3:286:ASN:H	1.74	0.51
3:3:309:PRO:HG2	3:3:320:ALA:O	2.11	0.51
3:3:695:ARG:NH1	3:3:715:GLU:OE1	2.42	0.51
4:4:363:SER:HB3	5:5:173:ALA:HB1	1.91	0.51
1:A:316:LEU:HD12	1:A:323:LEU:HB2	1.91	0.51
3:C:382:PHE:CD1	3:C:382:PHE:N	2.79	0.51
3:C:750:ARG:HB2	3:C:753:VAL:HG23	1.93	0.51
4:D:219:ARG:NH1	4:D:273:PHE:CD2	2.79	0.51
5:E:121:LEU:O	5:E:144:HIS:HB3	2.10	0.51
6:F:84:LEU:O	6:F:124:VAL:HG23	2.11	0.51
8:H:121:ARG:HH11	8:H:121:ARG:CG	2.21	0.51
1:J:363:VAL:HA	1:J:367:MET:HB2	1.90	0.51
3:L:173:PHE:HB3	3:L:296:PHE:CZ	2.46	0.51
3:L:695:ARG:NH1	3:L:715:GLU:OE1	2.42	0.51
3:L:750:ARG:HB3	3:L:752:ASP:OD1	2.11	0.51
5:N:37:GLU:O	5:N:41:TYR:HD1	1.93	0.51
7:P:44:THR:HA	7:P:138:VAL:HG13	1.93	0.51
8:Q:33:LYS:HD2	8:Q:36:ASP:OD1	2.11	0.51
8:Q:82:ILE:HG23	8:Q:95:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:33:ARG:HH21	2:T:37:GLU:HG3	1.75	0.51
2:T:42:ARG:HB2	2:T:45:ARG:HG2	1.92	0.51
3:U:478:LEU:HD21	3:U:483:ASP:HB2	1.92	0.51
3:U:513:GLN:HG2	3:U:769:LEU:HD23	1.93	0.51
4:V:98:ALA:O	4:V:102:GLU:HG3	2.11	0.51
1:1:274:GLU:HG3	1:1:278:GLU:HG3	1.92	0.51
4:4:115:THR:HG21	4:4:297:LEU:HD23	1.93	0.51
4:4:148:TYR:HB3	4:4:200:ARG:HH12	1.75	0.51
4:4:254:TYR:CD2	4:4:346:THR:HA	2.44	0.51
4:4:381:LEU:H	4:4:382:PRO:HD2	1.75	0.51
6:6:114:SER:HB2	7:9:97:ARG:CD	2.39	0.51
8:7:37:PHE:CE2	8:7:74:PRO:HA	2.46	0.51
1:A:366:PHE:CE1	1:A:370:LEU:HD21	2.45	0.51
8:H:40:PHE:HB2	8:H:48:TYR:CE2	2.45	0.51
3:L:693:TYR:HB3	3:L:759:TYR:HD2	1.75	0.51
4:M:112:ARG:HH21	4:M:297:LEU:HD11	1.76	0.51
6:O:93:ARG:NH1	6:O:96:TRP:CE3	2.78	0.51
2:T:33:ARG:HH21	2:T:37:GLU:CG	2.23	0.51
3:U:116:PRO:O	3:U:117:LEU:HB2	2.11	0.51
4:V:153:ARG:HG3	4:V:153:ARG:HH11	1.75	0.51
5:W:53:VAL:HG22	5:W:55:LEU:CD1	2.40	0.51
8:Z:60:SER:HA	8:Z:66:PRO:HA	1.92	0.51
4:4:118:VAL:HB	4:4:257:TYR:HE2	1.75	0.51
3:C:2:VAL:HG13	3:C:89:ASP:HA	1.93	0.51
3:C:18:SER:HB2	3:C:433:ALA:O	2.11	0.51
3:C:173:PHE:HB3	3:C:296:PHE:CZ	2.45	0.51
6:F:20:LEU:O	6:F:24:LEU:HD13	2.10	0.51
2:K:110:GLU:HA	8:Q:121:ARG:NH1	2.25	0.51
3:L:202:PHE:HA	3:L:210:PHE:O	2.11	0.51
6:O:113:SER:HB3	7:P:96:LEU:HD13	1.93	0.51
7:P:45:ARG:HH21	7:P:137:LEU:HD23	1.75	0.51
4:V:93:HIS:HA	4:V:353:LEU:HD21	1.92	0.51
4:V:120:LEU:HD13	4:V:160:PHE:CE1	2.43	0.51
5:W:58:LEU:HD12	5:W:58:LEU:O	2.11	0.51
6:X:82:GLY:HA2	9:X:182:SF4:S4	2.51	0.51
7:Y:44:THR:HA	7:Y:138:VAL:HG13	1.93	0.51
1:1:359:CYS:O	1:1:363:VAL:HG22	2.11	0.51
2:2:101:THR:HG23	2:2:106:ILE:O	2.10	0.51
3:3:515:THR:HG23	3:3:683:LEU:CD1	2.39	0.51
3:3:750:ARG:HB2	3:3:753:VAL:HG23	1.91	0.51
4:4:213:ILE:HG22	4:4:217:ARG:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:PRO:HD2	2:B:90:LEU:HD23	1.92	0.51
3:C:546:ALA:O	3:C:547:MET:HE2	2.10	0.51
3:C:557:SER:H	3:C:560:GLU:HB2	1.76	0.51
1:S:364:ALA:HB1	3:U:207:VAL:HG22	1.92	0.51
4:V:198:PRO:HG3	4:V:291:LYS:NZ	2.26	0.51
4:4:261:THR:HB	4:4:292:GLN:OE1	2.11	0.51
4:4:332:THR:O	5:5:172:ALA:HB3	2.11	0.51
5:5:103:THR:HG23	5:5:127:GLU:O	2.11	0.51
8:7:8:GLU:HG2	8:7:97:TYR:CZ	2.46	0.51
4:D:252:TYR:CE2	5:E:87:ARG:NH2	2.77	0.51
6:F:84:LEU:HD11	6:F:89:ALA:HA	1.92	0.51
5:N:2:ARG:NH1	5:N:45:GLY:HA3	2.26	0.51
6:O:36:LEU:HD22	6:O:77:VAL:HG21	1.92	0.51
8:Q:37:PHE:HE2	8:Q:74:PRO:HA	1.76	0.51
8:Q:40:PHE:HB2	8:Q:48:TYR:CE2	2.46	0.51
1:S:186:THR:HA	1:S:189:MET:HE2	1.93	0.51
2:T:81:GLN:HB3	2:T:122:VAL:CG2	2.40	0.51
3:U:372:GLN:O	3:U:558:TRP:CE2	2.63	0.51
4:V:218:ALA:HB1	4:V:272:VAL:HG22	1.93	0.51
6:X:93:ARG:NH1	6:X:96:TRP:CZ3	2.79	0.51
2:2:42:ARG:HB2	2:2:45:ARG:HG2	1.92	0.51
4:4:129:HIS:HE1	4:4:349:ALA:HB1	1.66	0.51
4:4:379:GLN:HG2	5:5:113:PHE:CD1	2.46	0.51
3:C:55:PRO:CG	3:C:74:GLN:N	2.70	0.51
3:C:116:PRO:O	3:C:117:LEU:HB2	2.10	0.51
3:C:125:GLY:HA3	3:C:246:ASN:ND2	2.26	0.51
6:F:107:SER:O	6:F:137:VAL:HG12	2.11	0.51
1:J:298:PRO:HD2	1:J:321:SER:OG	2.11	0.51
4:M:93:HIS:HA	4:M:353:LEU:HD21	1.93	0.51
4:M:210:GLU:O	4:M:212:PRO:HD3	2.11	0.51
4:M:287:VAL:O	4:M:291:LYS:HG3	2.11	0.51
5:N:141:LEU:HD11	5:N:150:TYR:OH	2.11	0.51
6:O:155:GLN:C	6:O:157:LYS:H	2.19	0.51
4:V:64:THR:HB	4:V:66:PHE:HE1	1.74	0.51
4:V:168:PHE:HE1	6:X:141:PRO:HG3	1.75	0.51
7:Y:53:CYS:HB2	7:Y:112:ALA:HB1	1.93	0.51
3:3:200:LEU:O	3:3:201:ASP:HB2	2.09	0.50
3:3:268:ASP:OD2	3:3:278:ARG:NH1	2.44	0.50
3:3:329:LEU:HD21	3:3:644:LEU:HA	1.93	0.50
3:C:112:LEU:HD21	3:C:130:LEU:HD11	1.93	0.50
3:C:368:HIS:CD2	3:C:556:ALA:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:750:ARG:HB3	3:C:752:ASP:OD1	2.11	0.50
4:D:79:ILE:O	4:D:79:ILE:HG22	2.11	0.50
1:J:110:VAL:HG23	1:J:110:VAL:O	2.11	0.50
4:M:249:ARG:HD2	4:M:257:TYR:CE1	2.46	0.50
6:O:114:SER:HB2	7:P:97:ARG:CD	2.41	0.50
4:V:346:THR:HG22	4:V:353:LEU:O	2.11	0.50
7:Y:134:GLU:CD	7:Y:134:GLU:H	2.18	0.50
3:3:505:LEU:HB3	3:3:532:VAL:HG22	1.93	0.50
4:4:85:MET:HE1	4:4:370:VAL:HG11	1.93	0.50
4:4:218:ALA:HB1	4:4:272:VAL:HG22	1.94	0.50
1:A:288:GLN:HB3	1:A:333:GLU:HG2	1.93	0.50
2:B:110:GLU:HA	8:H:121:ARG:NH1	2.23	0.50
3:C:185:LYS:HG3	3:C:202:PHE:CE2	2.47	0.50
8:H:13:TRP:CE2	8:H:17:LEU:HD11	2.45	0.50
2:K:33:ARG:HH21	2:K:37:GLU:HG3	1.75	0.50
3:U:18:SER:HB2	3:U:433:ALA:O	2.11	0.50
4:V:153:ARG:HG3	4:V:153:ARG:NH1	2.27	0.50
4:V:385:CYS:HB3	4:V:396:ILE:HG12	1.93	0.50
6:X:117:MET:HE3	6:X:118:PHE:CZ	2.46	0.50
1:1:186:THR:HG23	1:1:199:PRO:HA	1.93	0.50
1:1:366:PHE:CE1	1:1:370:LEU:HD21	2.46	0.50
3:3:132:ASP:O	3:3:136:GLU:HG3	2.11	0.50
1:A:64:GLY:HA3	10:A:440:FMN:O1P	2.12	0.50
3:C:583:VAL:CG2	3:C:598:ALA:HA	2.41	0.50
7:G:41:HIS:ND1	7:G:95:MET:HE1	2.27	0.50
1:J:189:MET:O	1:J:193:GLU:HB2	2.10	0.50
1:J:238:PHE:HE1	1:J:249:MET:CE	2.25	0.50
4:M:120:LEU:HD13	4:M:160:PHE:CE1	2.42	0.50
1:S:366:PHE:CE1	1:S:370:LEU:HD21	2.47	0.50
2:T:77:LYS:H	2:T:116:LEU:HA	1.75	0.50
4:V:83:PRO:HB2	4:V:169:HIS:HA	1.94	0.50
4:V:144:THR:N	4:V:145:PRO:CD	2.74	0.50
4:V:367:ARG:HH12	4:V:369:LYS:CA	2.25	0.50
6:X:84:LEU:O	6:X:124:VAL:HG23	2.11	0.50
8:Z:121:ARG:HH11	8:Z:121:ARG:CG	2.20	0.50
1:1:288:GLN:HB3	1:1:333:GLU:HG2	1.93	0.50
3:3:173:PHE:HB3	3:3:296:PHE:CZ	2.47	0.50
3:3:456:ALA:HB3	3:3:459:MET:HE3	1.94	0.50
3:3:501:LYS:HD2	3:3:501:LYS:N	2.11	0.50
4:4:79:ILE:O	4:4:79:ILE:HG22	2.12	0.50
1:A:92:ASN:HD21	10:A:440:FMN:C2	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:VAL:O	1:A:110:VAL:HG23	2.11	0.50
3:C:329:LEU:HD21	3:C:644:LEU:HA	1.92	0.50
3:C:478:LEU:CD2	3:C:483:ASP:HB2	2.41	0.50
6:F:152:MET:HE2	6:F:156:LYS:HE2	1.93	0.50
1:J:391:LEU:HD22	1:J:407:VAL:HB	1.92	0.50
3:L:414:SER:O	3:L:418:ARG:HG3	2.12	0.50
2:T:112:THR:HG22	2:T:116:LEU:H	1.77	0.50
1:1:39:GLU:O	1:1:43:ARG:HG3	2.12	0.50
1:1:290:ILE:HG22	1:1:330:LEU:HD22	1.93	0.50
1:1:360:ARG:O	1:1:364:ALA:HB3	2.11	0.50
6:6:117:MET:HE2	7:9:99:ILE:HG12	1.94	0.50
1:A:180:TYR:CE2	10:A:440:FMN:H6	2.47	0.50
3:C:305:ARG:HG2	3:C:588:SER:O	2.11	0.50
4:D:211:SER:HB2	4:D:215:TYR:N	2.26	0.50
3:L:402:PRO:HD2	3:L:458:LEU:HD13	1.94	0.50
3:L:409:LEU:HD12	3:L:535:MET:CE	2.39	0.50
3:L:505:LEU:HD21	3:L:507:LEU:HD23	1.94	0.50
3:L:750:ARG:HB2	3:L:753:VAL:HG23	1.91	0.50
4:M:381:LEU:H	4:M:382:PRO:CD	2.24	0.50
1:S:87:HIS:HB2	1:S:126:ARG:O	2.11	0.50
1:S:183:GLY:O	10:S:440:FMN:H2'	2.11	0.50
3:U:368:HIS:CD2	3:U:556:ALA:HB3	2.47	0.50
3:3:487:SER:OG	3:3:490:VAL:HG23	2.12	0.50
3:3:670:PRO:CD	3:3:676:LEU:HD23	2.42	0.50
4:4:59:ILE:H	4:4:59:ILE:HD13	1.75	0.50
4:4:200:ARG:O	4:4:204:TYR:HD1	1.94	0.50
3:C:473:GLU:O	3:C:477:LEU:HD13	2.11	0.50
3:C:694:LEU:CB	3:C:762:ALA:HB2	2.37	0.50
4:D:210:GLU:O	4:D:212:PRO:HD3	2.11	0.50
4:D:213:ILE:HG22	4:D:217:ARG:HG3	1.92	0.50
5:E:116:ARG:HB3	5:E:135:ILE:HG13	1.92	0.50
3:L:112:LEU:CD2	3:L:130:LEU:HD11	2.41	0.50
4:M:76:LEU:O	4:M:76:LEU:HD12	2.12	0.50
4:M:294:LEU:HD23	4:M:294:LEU:O	2.12	0.50
1:S:39:GLU:O	1:S:43:ARG:HG3	2.11	0.50
1:S:395:GLU:HB2	1:S:407:VAL:HG21	1.92	0.50
3:U:185:LYS:HG2	3:U:188:VAL:CG2	2.41	0.50
6:X:141:PRO:HB3	9:X:182:SF4:S1	2.52	0.50
1:1:238:PHE:HE1	1:1:249:MET:CE	2.25	0.50
3:3:112:LEU:CD2	3:3:130:LEU:HD11	2.41	0.50
3:3:414:SER:O	3:3:418:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:583:VAL:HG23	3:3:599:HIS:H	1.75	0.50
4:4:168:PHE:N	4:4:168:PHE:CD1	2.77	0.50
5:5:71:VAL:CG1	5:5:89:PHE:HD2	2.24	0.50
3:C:250:GLU:CD	3:C:628:PRO:HG2	2.36	0.50
4:D:93:HIS:HA	4:D:353:LEU:HD21	1.94	0.50
5:E:167:PRO:HB3	7:G:66:TYR:CD2	2.47	0.50
7:G:39:GLY:O	7:G:40:ARG:C	2.55	0.50
2:K:129:HIS:CD2	2:K:130:THR:HG23	2.45	0.50
3:L:737:GLU:HB2	3:L:776:LEU:HD21	1.93	0.50
4:M:263:ASP:HB2	4:M:285:GLU:OE1	2.12	0.50
7:P:93:ILE:HG13	7:P:136:MET:HE1	1.93	0.50
7:P:123:ASP:HB2	7:P:129:LEU:HD21	1.93	0.50
2:T:129:HIS:CD2	2:T:130:THR:HG23	2.47	0.50
3:U:224:GLY:HA3	3:U:295:ARG:HD2	1.93	0.50
4:V:210:GLU:O	4:V:212:PRO:HD3	2.12	0.50
4:V:381:LEU:H	4:V:382:PRO:HD2	1.77	0.50
7:Y:45:ARG:HH21	7:Y:137:LEU:HD23	1.75	0.50
1:1:133:TYR:HB2	1:1:188:LEU:HD21	1.93	0.50
1:1:270:THR:O	1:1:311:MET:HG3	2.12	0.50
1:1:391:LEU:HD22	1:1:407:VAL:HB	1.94	0.50
2:2:130:THR:HB	2:2:144:CYS:SG	2.52	0.50
6:6:93:ARG:NH1	6:6:96:TRP:CE3	2.79	0.50
7:9:99:ILE:HG22	7:9:101:CYS:SG	2.51	0.50
8:7:86:LEU:HD12	8:7:91:ILE:HD12	1.94	0.50
1:A:98:PRO:HA	2:B:124:CYS:SG	2.52	0.50
3:C:46:ARG:O	3:C:107:MET:HG2	2.11	0.50
4:D:69:THR:HG21	6:F:120:ASN:ND2	2.27	0.50
4:D:240:ARG:HG3	4:D:265:PRO:O	2.12	0.50
4:M:350:ARG:NE	4:M:403:VAL:CG2	2.71	0.50
4:M:363:SER:CB	5:N:174:LEU:H	2.23	0.50
3:U:670:PRO:CD	3:U:676:LEU:HD23	2.40	0.50
4:V:114:GLU:O	4:V:118:VAL:HG13	2.11	0.50
4:V:226:PRO:HG3	4:V:242:SER:O	2.11	0.50
6:X:93:ARG:NH1	6:X:96:TRP:CE3	2.80	0.50
1:1:301:PRO:O	1:1:306:VAL:HG21	2.11	0.50
4:4:112:ARG:HH21	4:4:297:LEU:HD11	1.77	0.50
5:5:53:VAL:HG22	5:5:55:LEU:CD1	2.42	0.50
1:A:239:ALA:C	1:A:241:MET:H	2.20	0.50
3:C:188:VAL:CG2	3:C:189:ARG:N	2.74	0.50
4:D:168:PHE:CE1	6:F:141:PRO:HG3	2.45	0.50
4:D:385:CYS:HB3	4:D:396:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:44:THR:HA	7:G:138:VAL:HG13	1.93	0.50
7:G:48:ASN:CB	7:G:50:LEU:HD23	2.41	0.50
1:J:29:LEU:CD1	1:J:155:ARG:HG3	2.41	0.50
1:J:397:ARG:HG2	3:L:49:LEU:HD13	1.92	0.50
3:L:119:CYS:O	3:L:120:PRO:C	2.53	0.50
3:L:488:GLU:O	3:L:491:ALA:HB3	2.12	0.50
3:U:385:ALA:HB2	3:U:531:LYS:CB	2.42	0.50
4:V:148:TYR:HB3	4:V:200:ARG:HH12	1.75	0.50
4:V:262:PHE:CD1	4:V:289:ILE:HD11	2.47	0.50
6:X:105:VAL:HG11	6:X:131:VAL:CG2	2.41	0.50
1:1:293:GLY:HA3	1:1:324:GLY:N	2.10	0.49
1:1:398:SER:HA	3:3:46:ARG:HD2	1.93	0.49
3:3:131:GLN:O	3:3:134:THR:HB	2.12	0.49
4:4:346:THR:HG22	4:4:353:LEU:O	2.12	0.49
6:6:20:LEU:O	6:6:24:LEU:HD13	2.12	0.49
6:6:117:MET:CE	7:9:99:ILE:HG12	2.42	0.49
3:C:269:THR:HG23	3:C:274:LEU:HD13	1.94	0.49
3:C:732:ALA:H	3:C:747:VAL:CG1	2.25	0.49
4:D:52:VAL:HG23	4:D:388:GLU:O	2.12	0.49
4:D:118:VAL:HB	4:D:257:TYR:HE2	1.77	0.49
1:J:398:SER:HA	3:L:46:ARG:HD2	1.93	0.49
3:L:24:PHE:CE1	3:L:29:ASP:HA	2.47	0.49
3:L:550:LEU:HD23	3:L:684:ARG:NH2	2.27	0.49
4:M:254:TYR:CD1	4:M:255:SER:N	2.71	0.49
6:O:105:VAL:HG11	6:O:131:VAL:CG2	2.41	0.49
1:S:397:ARG:HD2	1:S:397:ARG:N	2.26	0.49
3:U:20:MET:HE2	3:U:433:ALA:HB2	1.93	0.49
3:U:689:LYS:HB2	3:U:772:GLU:HG2	1.93	0.49
3:U:694:LEU:CB	3:U:762:ALA:HB2	2.37	0.49
4:V:338:PRO:HG3	5:W:192:TYR:O	2.11	0.49
6:X:84:LEU:HD11	6:X:89:ALA:HA	1.93	0.49
2:2:102:GLU:HA	8:7:108:ILE:HD11	1.94	0.49
3:3:202:PHE:HA	3:3:210:PHE:O	2.12	0.49
4:4:342:VAL:HG22	4:4:343:TYR:N	2.27	0.49
7:9:26:TYR:N	7:9:27:PRO:CD	2.72	0.49
2:B:106:ILE:CG2	2:B:110:GLU:HB2	2.41	0.49
3:C:474:ARG:CZ	3:C:516:VAL:HG21	2.36	0.49
4:D:84:ARG:CD	6:F:117:MET:HE1	2.42	0.49
7:G:26:TYR:N	7:G:27:PRO:CD	2.73	0.49
8:H:29:VAL:HG22	8:H:60:SER:O	2.13	0.49
1:J:18:TYR:OH	1:J:105:TYR:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:38:TYR:OH	1:J:112:HIS:ND1	2.37	0.49
1:J:118:MET:HG2	1:J:224:LEU:HD13	1.94	0.49
2:K:116:LEU:N	2:K:116:LEU:HD23	2.28	0.49
3:L:629:ILE:HG22	3:L:630:GLU:N	2.23	0.49
6:O:43:LEU:HD11	6:O:84:LEU:HD23	1.92	0.49
3:U:382:PHE:CD1	3:U:382:PHE:N	2.79	0.49
3:U:400:GLY:O	3:U:402:PRO:HD3	2.13	0.49
3:U:488:GLU:O	3:U:491:ALA:HB3	2.12	0.49
5:W:2:ARG:NH1	5:W:45:GLY:HA3	2.26	0.49
1:1:92:ASN:HD21	10:1:440:FMN:C2	2.25	0.49
1:1:316:LEU:HD12	1:1:323:LEU:HB2	1.95	0.49
3:3:483:ASP:O	3:3:484:LYS:HG2	2.11	0.49
3:C:402:PRO:HD2	3:C:458:LEU:HD13	1.93	0.49
3:C:478:LEU:HD21	3:C:483:ASP:HB2	1.94	0.49
4:D:200:ARG:O	4:D:204:TYR:HD1	1.95	0.49
6:F:105:VAL:HG11	6:F:131:VAL:CG2	2.43	0.49
6:F:163:TYR:CD2	6:F:169:ARG:HA	2.36	0.49
1:J:116:GLU:HG2	1:J:228:VAL:HG22	1.94	0.49
2:K:109:GLY:HA2	8:Q:91:ILE:HD13	1.93	0.49
4:M:133:LEU:HD21	4:M:204:TYR:CE2	2.47	0.49
4:M:248:VAL:HB	4:M:347:GLU:HB2	1.94	0.49
8:Q:70:ALA:HA	8:Q:83:GLY:O	2.13	0.49
1:S:88:TYR:HB2	1:S:216:THR:CG2	2.42	0.49
1:S:203:PRO:HB2	1:S:204:PRO:HD3	1.93	0.49
1:S:351:GLU:HA	3:U:205:ARG:HH12	1.77	0.49
1:S:366:PHE:HD1	1:S:370:LEU:HD21	1.77	0.49
3:U:131:GLN:O	3:U:134:THR:HB	2.12	0.49
3:U:402:PRO:CG	3:U:535:MET:HE1	2.43	0.49
3:U:694:LEU:C	3:U:762:ALA:HB2	2.38	0.49
4:V:188:PRO:O	4:V:191:LYS:HB2	2.13	0.49
1:1:41:ALA:HA	1:1:120:LEU:HD21	1.95	0.49
2:2:33:ARG:HH21	2:2:37:GLU:CG	2.26	0.49
2:2:153:LEU:C	2:2:153:LEU:HD13	2.37	0.49
3:3:194:VAL:HG12	3:3:411:LEU:HD22	1.94	0.49
3:3:337:ARG:HD2	3:3:337:ARG:N	2.27	0.49
4:4:338:PRO:HG3	5:5:192:TYR:O	2.12	0.49
6:6:155:GLN:C	6:6:157:LYS:H	2.20	0.49
8:7:117:ALA:O	8:7:121:ARG:HG2	2.12	0.49
3:C:333:LEU:HD13	3:C:648:LEU:HD21	1.94	0.49
3:C:385:ALA:HB2	3:C:531:LYS:CB	2.42	0.49
3:C:513:GLN:HG2	3:C:769:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:115:THR:CG2	4:D:297:LEU:HD23	2.42	0.49
5:E:13:LYS:HG2	5:E:13:LYS:O	2.13	0.49
1:J:88:TYR:HB2	1:J:216:THR:CG2	2.42	0.49
3:L:2:VAL:HG13	3:L:89:ASP:HA	1.94	0.49
3:L:185:LYS:HG3	3:L:202:PHE:CE2	2.48	0.49
4:M:43:LEU:HD11	4:M:397:ILE:CD1	2.42	0.49
4:M:118:VAL:HB	4:M:257:TYR:HE2	1.77	0.49
4:M:200:ARG:O	4:M:204:TYR:HD1	1.94	0.49
1:S:288:GLN:HB3	1:S:333:GLU:HG2	1.93	0.49
1:S:341:MET:HE2	1:S:409:PRO:O	2.12	0.49
3:U:2:VAL:CG1	3:U:89:ASP:HA	2.42	0.49
4:V:200:ARG:O	4:V:204:TYR:HD1	1.95	0.49
1:1:88:TYR:HB2	1:1:216:THR:CG2	2.42	0.49
1:1:211:LEU:H	1:1:216:THR:HG21	1.77	0.49
2:2:40:TRP:CH2	2:2:42:ARG:HG2	2.47	0.49
3:3:118:ASP:O	3:3:119:CYS:C	2.55	0.49
3:3:188:VAL:CG2	3:3:189:ARG:N	2.76	0.49
3:3:550:LEU:HD23	3:3:684:ARG:NH2	2.27	0.49
3:C:361:ALA:HB1	3:C:366:THR:CG2	2.42	0.49
4:D:144:THR:N	4:D:145:PRO:CD	2.75	0.49
4:D:316:LEU:C	4:D:316:LEU:HD12	2.36	0.49
1:J:63:ARG:HD3	1:J:313:TYR:HD2	1.78	0.49
4:M:168:PHE:N	4:M:168:PHE:CD1	2.78	0.49
5:N:25:LEU:CD2	5:N:25:LEU:H	2.26	0.49
3:U:282:VAL:HG22	3:U:282:VAL:O	2.12	0.49
3:U:671:GLU:HG3	3:U:672:ALA:H	1.77	0.49
4:V:59:ILE:HD13	4:V:59:ILE:H	1.77	0.49
4:V:342:VAL:HG22	4:V:343:TYR:H	1.78	0.49
1:1:342:TRP:O	1:1:342:TRP:HE3	1.96	0.49
4:4:52:VAL:HG23	4:4:388:GLU:O	2.13	0.49
4:4:393:MET:C	4:4:396:ILE:HG22	2.38	0.49
7:9:163:VAL:HB	7:9:164:PRO:HD2	1.93	0.49
1:A:118:MET:HG2	1:A:224:LEU:HD13	1.95	0.49
1:A:391:LEU:HD22	1:A:407:VAL:HB	1.94	0.49
3:C:49:LEU:HA	3:C:80:ALA:O	2.12	0.49
3:C:498:GLU:C	3:C:500:ALA:H	2.19	0.49
3:C:693:TYR:HB3	3:C:759:TYR:HD2	1.76	0.49
4:D:64:THR:HB	4:D:66:PHE:HE1	1.75	0.49
4:D:342:VAL:HG22	4:D:343:TYR:H	1.78	0.49
1:J:186:THR:HG23	1:J:199:PRO:HA	1.94	0.49
1:J:274:GLU:HG3	1:J:278:GLU:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:130:THR:HB	2:K:144:CYS:SG	2.52	0.49
3:L:381:LEU:HD12	3:L:522:ARG:HD3	1.94	0.49
3:L:557:SER:H	3:L:560:GLU:HB2	1.78	0.49
3:L:670:PRO:CD	3:L:676:LEU:HD23	2.43	0.49
1:S:272:PHE:CE2	1:S:311:MET:HE3	2.48	0.49
1:S:358:PRO:O	1:S:362:GLY:HA3	2.13	0.49
2:T:102:GLU:HA	8:Z:108:ILE:HD11	1.95	0.49
4:V:84:ARG:O	6:X:83:ARG:NH2	2.46	0.49
7:Y:163:VAL:HB	7:Y:164:PRO:HD2	1.95	0.49
8:Z:40:PHE:HB2	8:Z:48:TYR:CE2	2.47	0.49
1:I:163:PHE:C	1:I:165:THR:H	2.20	0.49
3:3:497:TRP:CD1	3:3:524:LEU:HD11	2.47	0.49
8:7:37:PHE:CE1	8:7:55:MET:HB2	2.47	0.49
1:A:398:SER:HA	3:C:46:ARG:HD2	1.95	0.49
4:D:122:GLU:OE2	4:D:249:ARG:NH1	2.42	0.49
4:D:294:LEU:O	4:D:294:LEU:HD23	2.13	0.49
1:J:355:LYS:HD3	1:J:399:PHE:CD2	2.48	0.49
3:L:268:ASP:OD2	3:L:278:ARG:NH1	2.45	0.49
3:L:326:PHE:CZ	3:L:330:LYS:HE3	2.48	0.49
3:L:333:LEU:HD13	3:L:648:LEU:HD21	1.93	0.49
3:L:470:PRO:O	3:L:471:GLY:C	2.55	0.49
4:M:115:THR:HG22	4:M:297:LEU:HD23	1.94	0.49
6:O:138:PRO:HG3	7:P:121:MET:HG3	1.94	0.49
1:S:298:PRO:HD2	1:S:321:SER:OG	2.13	0.49
3:U:689:LYS:HD2	3:U:772:GLU:H	1.77	0.49
4:V:363:SER:HB3	5:W:173:ALA:HB1	1.94	0.49
8:Z:13:TRP:CZ2	8:Z:17:LEU:HD11	2.46	0.49
4:4:74:THR:HG22	4:4:75:TYR:N	2.27	0.49
6:6:138:PRO:HG2	7:9:121:MET:HG3	1.93	0.49
1:A:186:THR:HA	1:A:189:MET:HE2	1.95	0.49
1:A:272:PHE:O	1:A:276:ILE:HG13	2.13	0.49
3:C:237:ASP:OD1	3:C:239:THR:HG22	2.13	0.49
4:D:125:ARG:HD2	4:D:286:SER:OG	2.13	0.49
4:D:363:SER:HB3	5:E:173:ALA:HB1	1.95	0.49
4:D:374:SER:HB2	4:D:406:ASP:HB3	1.94	0.49
5:E:71:VAL:CG1	5:E:89:PHE:HD2	2.25	0.49
1:J:288:GLN:HB3	1:J:333:GLU:HG2	1.95	0.49
3:L:200:LEU:O	3:L:201:ASP:HB2	2.12	0.49
4:M:74:THR:HG22	4:M:75:TYR:N	2.27	0.49
4:M:224:ILE:HD11	4:M:275:ARG:CZ	2.43	0.49
5:N:107:LEU:HD23	5:N:107:LEU:HA	1.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:41:ALA:HA	1:S:120:LEU:HD21	1.94	0.49
2:T:116:LEU:N	2:T:116:LEU:HD23	2.27	0.49
3:U:19:VAL:HG12	3:U:82:SER:HB2	1.95	0.49
4:V:123:LEU:HD21	4:V:159:LEU:HD12	1.95	0.49
4:V:125:ARG:HD2	4:V:286:SER:OG	2.13	0.49
4:V:261:THR:HB	4:V:292:GLN:OE1	2.13	0.49
6:X:128:ASP:HA	6:X:131:VAL:O	2.12	0.49
1:1:18:TYR:OH	1:1:105:TYR:HB2	2.12	0.49
1:1:358:PRO:O	1:1:362:GLY:HA3	2.13	0.49
2:2:85:THR:HG22	2:2:86:LEU:N	2.28	0.49
4:4:40:VAL:HG23	6:6:88:MET:CE	2.43	0.49
5:5:123:GLY:HA2	5:5:144:HIS:CD2	2.48	0.49
3:C:112:LEU:CD2	3:C:130:LEU:HD11	2.43	0.49
4:D:69:THR:HG21	6:F:120:ASN:HD22	1.78	0.49
4:D:197:LEU:N	4:D:198:PRO:HD2	2.28	0.49
1:J:238:PHE:HE1	1:J:249:MET:HE1	1.78	0.49
3:L:55:PRO:CG	3:L:74:GLN:N	2.72	0.49
6:O:16:ARG:HA	6:O:21:PHE:CD2	2.47	0.49
6:O:41:PHE:CZ	6:O:92:MET:HB2	2.48	0.49
3:U:385:ALA:HB3	3:U:533:LEU:CD2	2.43	0.49
5:W:123:GLY:HA2	5:W:144:HIS:CD2	2.48	0.49
5:W:125:VAL:HG12	5:W:126:PHE:N	2.28	0.49
8:Z:86:LEU:HD12	8:Z:91:ILE:HD12	1.94	0.49
3:3:237:ASP:OD1	3:3:239:THR:HG22	2.13	0.49
4:4:210:GLU:O	4:4:212:PRO:HD3	2.13	0.49
1:A:397:ARG:HD2	1:A:397:ARG:N	2.25	0.49
2:B:116:LEU:HD23	2:B:116:LEU:N	2.28	0.49
4:D:85:MET:HE3	4:D:409:ARG:CB	2.43	0.49
4:D:212:PRO:HG2	4:D:213:ILE:H	1.78	0.49
8:H:49:ASP:OD1	8:H:49:ASP:N	2.46	0.49
3:L:655:ARG:HH12	3:L:659:GLU:CB	2.26	0.49
4:M:79:ILE:O	4:M:79:ILE:HG22	2.13	0.49
2:T:139:GLU:HB2	2:T:140:PRO:CD	2.33	0.49
3:U:329:LEU:HD21	3:U:644:LEU:HA	1.94	0.49
4:V:69:THR:HG21	6:X:120:ASN:ND2	2.27	0.49
4:V:118:VAL:HB	4:V:257:TYR:HE2	1.77	0.49
4:V:230:ILE:HD11	4:V:244:VAL:CG2	2.43	0.49
8:Z:89:ALA:O	8:Z:91:ILE:HG13	2.13	0.49
1:1:72:THR:HG21	1:1:223:THR:HG21	1.95	0.48
3:3:478:LEU:CD2	3:3:483:ASP:HB2	2.43	0.48
3:3:646:GLU:C	3:3:648:LEU:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:41:PHE:CZ	6:6:92:MET:HB2	2.48	0.48
1:A:341:MET:CE	1:A:409:PRO:HB2	2.42	0.48
3:C:440:ARG:CG	3:C:440:ARG:NH1	2.75	0.48
4:D:104:LEU:HD22	4:D:338:PRO:HD2	1.95	0.48
8:H:108:ILE:N	8:H:108:ILE:HD12	2.28	0.48
1:J:40:THR:O	1:J:44:VAL:HG23	2.13	0.48
1:J:211:LEU:H	1:J:216:THR:HG21	1.77	0.48
4:M:84:ARG:HD3	6:O:117:MET:HE1	1.94	0.48
4:M:198:PRO:HG3	4:M:291:LYS:NZ	2.28	0.48
4:M:393:MET:HA	4:M:396:ILE:CG2	2.43	0.48
8:Q:108:ILE:HD12	8:Q:108:ILE:N	2.27	0.48
3:U:232:VAL:HB	9:U:784:SF4:S2	2.53	0.48
3:U:629:ILE:HG22	3:U:630:GLU:N	2.25	0.48
5:W:160:ARG:HG3	7:Y:130:VAL:HG11	1.95	0.48
7:Y:96:LEU:HD21	7:Y:129:LEU:HD12	1.95	0.48
8:Z:49:ASP:N	8:Z:49:ASP:OD1	2.46	0.48
3:3:20:MET:HE2	3:3:433:ALA:HB2	1.95	0.48
3:3:117:LEU:H	4:4:321:MET:CE	2.19	0.48
3:3:381:LEU:HD12	3:3:522:ARG:HD3	1.94	0.48
6:6:108:MET:HA	6:6:137:VAL:CG1	2.43	0.48
8:7:40:PHE:HB2	8:7:48:TYR:CE2	2.49	0.48
1:A:133:TYR:HB2	1:A:188:LEU:HD21	1.94	0.48
2:B:85:THR:HG22	2:B:86:LEU:N	2.27	0.48
6:F:114:SER:HB2	7:G:97:ARG:CD	2.42	0.48
1:J:334:ARG:O	1:J:434:PRO:HG3	2.13	0.48
2:K:85:THR:HG22	2:K:86:LEU:N	2.28	0.48
3:L:118:ASP:O	3:L:119:CYS:C	2.56	0.48
4:M:366:TYR:CE1	5:N:148:LYS:HE3	2.48	0.48
5:N:25:LEU:H	5:N:25:LEU:HD23	1.78	0.48
8:Q:16:LEU:HG	8:Q:82:ILE:HD11	1.95	0.48
1:S:197:ALA:HB3	2:T:66:PHE:CZ	2.48	0.48
4:V:404:MET:HA	4:V:407:VAL:CG1	2.43	0.48
3:3:498:GLU:C	3:3:500:ALA:H	2.21	0.48
4:4:198:PRO:HG3	4:4:291:LYS:NZ	2.28	0.48
6:6:164:ASN:HB2	7:9:128:ASP:OD2	2.12	0.48
6:6:165:GLU:HG2	7:9:148:ARG:NH1	2.28	0.48
8:7:29:VAL:HG22	8:7:60:SER:O	2.12	0.48
1:A:358:PRO:O	1:A:362:GLY:HA3	2.13	0.48
3:C:115:HIS:CD2	3:C:116:PRO:HD2	2.48	0.48
3:C:184:CYS:O	9:C:785:SF4:S4	2.72	0.48
3:C:497:TRP:CD1	3:C:524:LEU:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:VAL:HG23	6:F:88:MET:CE	2.43	0.48
4:D:83:PRO:HB2	4:D:169:HIS:HA	1.94	0.48
5:E:2:ARG:NH1	5:E:45:GLY:HA3	2.28	0.48
6:F:163:TYR:CD1	7:G:152:ARG:HD2	2.48	0.48
1:J:133:TYR:HB2	1:J:188:LEU:HD21	1.93	0.48
3:L:361:ALA:HB1	3:L:366:THR:CG2	2.43	0.48
3:L:583:VAL:HG23	3:L:598:ALA:HA	1.95	0.48
4:M:316:LEU:C	4:M:318:GLU:H	2.22	0.48
8:Q:68:LEU:HD13	8:Q:69:LEU:N	2.28	0.48
4:V:250:LYS:CE	4:V:262:PHE:HB3	2.43	0.48
5:W:34:PHE:HE1	5:W:38:MET:SD	2.35	0.48
6:X:83:ARG:HD3	6:X:111:CYS:SG	2.53	0.48
2:2:58:THR:HG21	3:3:200:LEU:N	2.27	0.48
3:3:2:VAL:HG13	3:3:89:ASP:HA	1.94	0.48
3:3:31:PRO:HD2	3:3:104:GLN:NE2	2.27	0.48
3:3:671:GLU:HG3	3:3:672:ALA:H	1.79	0.48
3:3:694:LEU:CB	3:3:762:ALA:HB2	2.39	0.48
4:4:222:GLY:HA2	4:4:384:ALA:O	2.14	0.48
4:4:224:ILE:HD11	4:4:275:ARG:CZ	2.43	0.48
5:5:107:LEU:HA	5:5:107:LEU:HD23	1.74	0.48
5:5:125:VAL:HG12	5:5:126:PHE:N	2.28	0.48
6:6:155:GLN:O	6:6:158:VAL:HG22	2.14	0.48
2:B:66:PHE:CE1	3:C:205:ARG:HD3	2.48	0.48
4:D:237:GLY:HA2	4:D:240:ARG:NH2	2.28	0.48
1:J:139:ARG:CG	2:K:140:PRO:HD3	2.39	0.48
4:M:104:LEU:HD22	4:M:338:PRO:HD2	1.95	0.48
6:O:128:ASP:HA	6:O:131:VAL:O	2.13	0.48
7:P:41:HIS:ND1	7:P:95:MET:HE1	2.29	0.48
1:S:260:ARG:HA	2:T:177:HIS:O	2.12	0.48
3:U:269:THR:HG23	3:U:274:LEU:HD13	1.95	0.48
3:U:487:SER:OG	3:U:490:VAL:HG23	2.12	0.48
3:U:557:SER:H	3:U:560:GLU:HB2	1.78	0.48
4:V:168:PHE:HA	4:V:170:HIS:CD2	2.48	0.48
5:W:103:THR:HG23	5:W:127:GLU:O	2.13	0.48
7:Y:41:HIS:ND1	7:Y:95:MET:HE1	2.27	0.48
1:1:201:LEU:HG	1:1:203:PRO:HD2	1.94	0.48
3:3:361:ALA:HB1	3:3:366:THR:CG2	2.44	0.48
3:3:399:LEU:HD12	3:3:399:LEU:N	2.28	0.48
4:4:93:HIS:HA	4:4:353:LEU:HD21	1.96	0.48
5:5:25:LEU:CD2	5:5:25:LEU:H	2.27	0.48
5:5:25:LEU:H	5:5:25:LEU:HD23	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:16:ARG:HA	6:6:21:PHE:CD2	2.48	0.48
8:7:16:LEU:HD13	8:7:16:LEU:O	2.13	0.48
1:A:186:THR:HG23	1:A:199:PRO:HA	1.94	0.48
4:D:218:ALA:HB1	4:D:272:VAL:HG22	1.95	0.48
5:E:123:GLY:HA2	5:E:144:HIS:CD2	2.48	0.48
1:J:397:ARG:NE	3:L:79:LEU:HD12	2.25	0.48
3:L:688:ARG:HD3	3:L:688:ARG:HA	1.53	0.48
4:M:367:ARG:HH12	4:M:369:LYS:CA	2.25	0.48
1:S:332:PRO:HD2	2:T:90:LEU:CD2	2.43	0.48
2:T:11:LEU:O	2:T:12:GLU:C	2.56	0.48
3:U:188:VAL:CG2	3:U:189:ARG:N	2.76	0.48
3:U:546:ALA:O	3:U:547:MET:HE2	2.13	0.48
8:Z:121:ARG:NH1	8:Z:121:ARG:CG	2.75	0.48
1:1:87:HIS:HB2	1:1:126:ARG:O	2.13	0.48
1:1:104:ARG:HH21	2:2:127:SER:CB	2.26	0.48
4:4:188:PRO:O	4:4:191:LYS:HB2	2.14	0.48
5:5:167:PRO:HB3	7:9:66:TYR:CD2	2.48	0.48
5:E:160:ARG:HD2	7:G:92:GLU:OE2	2.14	0.48
4:M:261:THR:HB	4:M:292:GLN:OE1	2.13	0.48
3:U:285:VAL:HG22	3:U:286:ASN:H	1.75	0.48
3:U:594:ALA:C	3:U:596:ARG:H	2.22	0.48
4:V:311:PRO:HD3	4:V:330:HIS:CE1	2.49	0.48
5:W:16:PRO:HB2	5:W:28:VAL:CG1	2.44	0.48
5:W:52:ILE:CG2	5:W:114:LEU:HB3	2.40	0.48
3:3:186:ARG:HD2	3:3:231:PRO:HD3	1.95	0.48
1:A:315:HIS:O	1:A:319:LYS:HB2	2.14	0.48
5:E:44:MET:HB2	5:E:44:MET:HE3	1.63	0.48
6:F:113:SER:HB3	7:G:96:LEU:HD13	1.95	0.48
1:J:65:ARG:NH2	1:J:268:MET:CE	2.75	0.48
1:J:211:LEU:HB2	1:J:216:THR:HG21	1.95	0.48
3:L:385:ALA:HB2	3:L:531:LYS:CB	2.44	0.48
4:M:230:ILE:HD11	4:M:244:VAL:CG2	2.44	0.48
5:N:16:PRO:HB2	5:N:28:VAL:CG1	2.44	0.48
7:P:96:LEU:HD21	7:P:129:LEU:HD12	1.96	0.48
1:S:195:LEU:HA	2:T:24:ARG:HH21	1.78	0.48
1:S:359:CYS:O	1:S:363:VAL:HG22	2.13	0.48
4:V:237:GLY:HA2	4:V:240:ARG:NH2	2.28	0.48
5:W:141:LEU:HD21	5:W:145:PRO:HD3	1.96	0.48
1:1:116:GLU:HG2	1:1:228:VAL:HG22	1.95	0.48
1:1:397:ARG:HD2	1:1:397:ARG:N	2.27	0.48
3:3:46:ARG:O	3:3:107:MET:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:738:THR:HG22	3:C:739:PRO:CD	2.37	0.48
4:D:85:MET:HE1	4:D:370:VAL:HG11	1.95	0.48
4:D:161:GLU:OE1	7:G:34:LYS:HG2	2.13	0.48
4:D:197:LEU:N	4:D:198:PRO:CD	2.76	0.48
4:D:390:VAL:N	4:D:391:PRO:CD	2.77	0.48
8:H:17:LEU:HD13	8:H:54:ILE:HD13	1.96	0.48
1:J:385:GLU:O	1:J:388:GLU:HB3	2.13	0.48
2:K:112:THR:HG22	2:K:116:LEU:H	1.79	0.48
3:L:19:VAL:HG23	3:L:85:THR:O	2.14	0.48
3:L:282:VAL:HG22	3:L:282:VAL:O	2.14	0.48
3:L:546:ALA:C	3:L:547:MET:HE2	2.38	0.48
4:M:83:PRO:HB2	4:M:169:HIS:HA	1.96	0.48
4:M:168:PHE:HE1	6:O:141:PRO:HG3	1.79	0.48
1:S:360:ARG:O	1:S:364:ALA:HB3	2.14	0.48
3:U:614:LEU:O	3:U:621:VAL:HA	2.14	0.48
4:V:112:ARG:HH21	4:V:297:LEU:HD11	1.79	0.48
5:W:84:ASP:OD1	5:W:84:ASP:N	2.43	0.48
6:X:37:TRP:HA	6:X:37:TRP:CE3	2.49	0.48
6:X:114:SER:HB2	7:Y:97:ARG:CD	2.39	0.48
2:2:106:ILE:CG2	2:2:110:GLU:HB2	2.44	0.48
3:3:583:VAL:HG23	3:3:598:ALA:HA	1.95	0.48
3:3:737:GLU:HB2	3:3:776:LEU:HD21	1.96	0.48
4:4:350:ARG:HG3	4:4:350:ARG:NH1	2.29	0.48
1:A:72:THR:HG21	1:A:223:THR:HG21	1.96	0.48
1:A:264:TYR:CD2	1:A:279:TRP:HB3	2.49	0.48
3:C:664:LEU:O	3:C:669:VAL:HG12	2.13	0.48
3:C:671:GLU:HG3	3:C:672:ALA:H	1.79	0.48
6:F:96:TRP:HA	6:F:99:MET:CE	2.40	0.48
6:F:155:GLN:C	6:F:157:LYS:H	2.22	0.48
4:M:241:ALA:CB	4:M:278:VAL:HG21	2.44	0.48
6:O:84:LEU:HD11	6:O:89:ALA:HA	1.95	0.48
3:U:55:PRO:HG3	3:U:73:ILE:C	2.37	0.48
3:U:241:ARG:HH11	7:Y:74:GLU:CD	2.20	0.48
3:U:646:GLU:C	3:U:648:LEU:H	2.22	0.48
4:V:133:LEU:HD21	4:V:204:TYR:CE2	2.48	0.48
4:V:223:VAL:O	4:V:383:TYR:HE1	1.97	0.48
7:Y:26:TYR:N	7:Y:27:PRO:CD	2.71	0.48
3:3:18:SER:HB2	3:3:433:ALA:O	2.12	0.48
3:3:119:CYS:O	3:3:120:PRO:C	2.55	0.48
3:3:326:PHE:CZ	3:3:330:LYS:HE3	2.49	0.48
3:3:398:VAL:CB	3:3:450:LEU:HD22	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:211:SER:HB2	4:4:215:TYR:N	2.28	0.48
1:A:39:GLU:O	1:A:43:ARG:HG3	2.14	0.48
1:A:97:GLU:OE2	1:A:294:GLY:HA3	2.14	0.48
1:A:184:GLU:OE1	1:A:186:THR:N	2.47	0.48
1:A:334:ARG:O	1:A:434:PRO:HG3	2.14	0.48
1:A:385:GLU:O	1:A:388:GLU:HB3	2.13	0.48
3:C:33:PHE:HE2	3:C:111:THR:HG21	1.79	0.48
3:C:409:LEU:HD12	3:C:535:MET:CE	2.42	0.48
3:C:488:GLU:O	3:C:491:ALA:HB3	2.14	0.48
4:D:148:TYR:HB3	4:D:200:ARG:HH12	1.77	0.48
4:D:161:GLU:OE2	6:F:143:ARG:NH1	2.47	0.48
4:D:236:GLY:C	4:D:238:SER:N	2.71	0.48
8:H:63:LEU:HD13	8:H:129:ALA:HB3	1.96	0.48
1:J:29:LEU:HD22	1:J:33:LEU:CD1	2.44	0.48
3:L:237:ASP:OD1	3:L:239:THR:HG22	2.14	0.48
6:O:140:CYS:SG	7:P:99:ILE:HG13	2.54	0.48
1:S:290:ILE:HG22	1:S:330:LEU:HD22	1.96	0.48
3:U:470:PRO:O	3:U:471:GLY:C	2.57	0.48
3:3:19:VAL:HG23	3:3:85:THR:O	2.14	0.47
3:3:55:PRO:CG	3:3:74:GLN:N	2.73	0.47
3:3:184:CYS:O	9:3:785:SF4:S4	2.71	0.47
4:4:85:MET:HE3	4:4:409:ARG:CB	2.44	0.47
6:6:138:PRO:HG3	7:9:121:MET:HG3	1.96	0.47
2:B:27:ILE:HG13	2:B:53:VAL:HG21	1.96	0.47
3:C:185:LYS:HG2	3:C:188:VAL:CG2	2.44	0.47
3:L:168:HIS:HA	3:L:169:PRO:HD2	1.74	0.47
3:L:382:PHE:CD1	3:L:382:PHE:N	2.81	0.47
4:M:252:TYR:CE2	5:N:87:ARG:NH2	2.82	0.47
6:O:121:TYR:HD1	6:O:121:TYR:H	1.62	0.47
7:P:39:GLY:O	7:P:40:ARG:C	2.55	0.47
1:S:341:MET:CE	1:S:409:PRO:HB2	2.43	0.47
1:S:360:ARG:O	3:U:207:VAL:HG13	2.14	0.47
4:V:203:GLU:O	4:V:207:LEU:HG	2.14	0.47
1:1:195:LEU:HA	2:2:24:ARG:HH21	1.79	0.47
6:6:128:ASP:HA	6:6:131:VAL:O	2.14	0.47
1:A:424:LEU:HD21	1:A:431:VAL:HG12	1.97	0.47
4:D:168:PHE:HA	4:D:170:HIS:CD2	2.49	0.47
4:D:197:LEU:HA	4:D:200:ARG:HB3	1.96	0.47
4:D:393:MET:C	4:D:396:ILE:HG22	2.39	0.47
6:F:130:VAL:HG23	6:F:131:VAL:HG13	1.96	0.47
1:J:92:ASN:HD21	10:J:440:FMN:C2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:84:ARG:CD	6:O:117:MET:HE1	2.44	0.47
4:M:148:TYR:HB3	4:M:200:ARG:HH12	1.77	0.47
5:N:98:ASP:C	5:N:100:ARG:H	2.23	0.47
3:U:269:THR:HG22	3:U:274:LEU:HA	1.95	0.47
3:U:591:HIS:ND1	3:U:592:PRO:CD	2.76	0.47
1:1:183:GLY:O	10:1:440:FMN:H2'	2.14	0.47
3:3:583:VAL:HG21	3:3:597:TYR:O	2.14	0.47
4:4:133:LEU:HD21	4:4:204:TYR:CE2	2.49	0.47
4:4:263:ASP:HB2	4:4:285:GLU:OE1	2.14	0.47
4:4:381:LEU:H	4:4:382:PRO:CD	2.27	0.47
5:5:16:PRO:HB2	5:5:28:VAL:CG1	2.44	0.47
6:6:84:LEU:HD11	6:6:89:ALA:HA	1.96	0.47
2:B:87:SER:OG	2:B:128:CYS:HB3	2.13	0.47
3:C:550:LEU:HD23	3:C:684:ARG:NH2	2.29	0.47
4:D:254:TYR:CE2	4:D:346:THR:CA	2.94	0.47
1:J:360:ARG:O	1:J:364:ALA:HB3	2.13	0.47
3:L:337:ARG:HD2	3:L:337:ARG:N	2.29	0.47
3:L:368:HIS:CD2	3:L:556:ALA:HB3	2.48	0.47
4:M:213:ILE:HG22	4:M:217:ARG:HG3	1.95	0.47
5:N:104:VAL:CG1	5:N:108:TRP:HE3	2.27	0.47
8:Q:117:ALA:O	8:Q:121:ARG:HG2	2.14	0.47
1:S:104:ARG:HH21	2:T:127:SER:HB2	1.79	0.47
3:U:337:ARG:HD2	3:U:337:ARG:N	2.27	0.47
3:U:612:GLY:O	3:U:624:LEU:HB2	2.14	0.47
4:V:393:MET:HA	4:V:396:ILE:CG2	2.43	0.47
6:X:165:GLU:HG3	7:Y:144:LYS:HE2	1.97	0.47
1:1:272:PHE:CE1	1:1:311:MET:HG2	2.49	0.47
4:4:115:THR:HG22	4:4:297:LEU:HD23	1.97	0.47
4:4:263:ASP:O	4:4:285:GLU:HG3	2.14	0.47
6:6:96:TRP:HA	6:6:99:MET:CE	2.41	0.47
3:C:2:VAL:CG1	3:C:89:ASP:HA	2.44	0.47
3:C:470:PRO:O	3:C:471:GLY:C	2.58	0.47
6:F:48:ILE:O	6:F:48:ILE:HG22	2.13	0.47
1:J:205:PHE:HD1	1:J:206:PRO:HD2	1.80	0.47
2:K:3:PHE:C	2:K:3:PHE:CD1	2.92	0.47
2:K:88:CYS:HB3	2:K:93:ALA:HB2	1.97	0.47
2:K:102:GLU:HA	8:Q:108:ILE:HD11	1.96	0.47
3:L:20:MET:HE2	3:L:433:ALA:HB2	1.96	0.47
4:M:197:LEU:N	4:M:198:PRO:CD	2.78	0.47
4:M:211:SER:HB2	4:M:215:TYR:N	2.29	0.47
4:M:226:PRO:HG3	4:M:242:SER:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:263:ASP:O	4:M:285:GLU:HG3	2.14	0.47
6:O:110:ALA:HB1	6:O:116:GLY:HA2	1.96	0.47
2:T:109:GLY:HA2	8:Z:91:ILE:HD13	1.97	0.47
4:V:316:LEU:C	4:V:318:GLU:H	2.21	0.47
1:1:332:PRO:HD2	2:2:90:LEU:CD2	2.42	0.47
1:1:420:GLN:O	1:1:424:LEU:HD13	2.14	0.47
3:3:732:ALA:H	3:3:747:VAL:CG1	2.28	0.47
6:6:105:VAL:HG11	6:6:131:VAL:CG2	2.44	0.47
6:6:121:TYR:HD1	6:6:121:TYR:H	1.63	0.47
8:7:108:ILE:HD12	8:7:108:ILE:N	2.29	0.47
1:A:260:ARG:HA	2:B:177:HIS:O	2.15	0.47
1:A:341:MET:HE2	1:A:409:PRO:O	2.14	0.47
3:C:186:ARG:HD2	3:C:231:PRO:HD3	1.95	0.47
4:D:376:VAL:O	4:D:379:GLN:HG3	2.15	0.47
6:F:43:LEU:HD11	6:F:84:LEU:HD23	1.96	0.47
1:J:184:GLU:HG2	10:J:440:FMN:C8M	2.45	0.47
3:L:506:ILE:HG21	3:L:535:MET:HE3	1.95	0.47
1:S:40:THR:O	1:S:44:VAL:HG23	2.15	0.47
1:S:267:PRO:O	1:S:268:MET:C	2.56	0.47
3:U:378:PRO:O	3:U:381:LEU:HB2	2.15	0.47
3:U:498:GLU:C	3:U:500:ALA:H	2.21	0.47
4:V:350:ARG:HD3	4:V:374:SER:OG	2.15	0.47
2:2:3:PHE:CD1	2:2:3:PHE:C	2.92	0.47
4:4:116:ILE:HD11	4:4:182:LEU:CD2	2.44	0.47
6:6:130:VAL:HG23	6:6:131:VAL:HG13	1.97	0.47
8:7:37:PHE:HE2	8:7:74:PRO:HA	1.80	0.47
3:C:55:PRO:HG3	3:C:73:ILE:C	2.39	0.47
4:D:343:TYR:C	4:D:343:TYR:CD1	2.92	0.47
8:H:37:PHE:CE2	8:H:74:PRO:HA	2.49	0.47
1:J:161:ASN:OD1	1:J:166:ASP:HA	2.14	0.47
3:L:241:ARG:HH11	7:P:74:GLU:CD	2.22	0.47
3:L:385:ALA:HB3	3:L:533:LEU:HD23	1.96	0.47
3:L:732:ALA:H	3:L:747:VAL:CG1	2.28	0.47
5:N:141:LEU:HD21	5:N:145:PRO:HD3	1.96	0.47
2:T:3:PHE:CD1	2:T:3:PHE:C	2.92	0.47
3:U:693:TYR:HB3	3:U:759:TYR:HD2	1.78	0.47
3:U:724:ARG:O	3:U:724:ARG:HG2	2.14	0.47
1:1:102:LYS:HG3	1:1:103:ASP:N	2.30	0.47
1:1:205:PHE:HD1	1:1:206:PRO:HD2	1.80	0.47
2:2:116:LEU:HD23	2:2:116:LEU:N	2.30	0.47
3:3:197:ASP:OD2	3:3:220:SER:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:688:ARG:HD3	3:3:688:ARG:HA	1.52	0.47
4:4:106:GLY:O	5:5:194:SER:HB3	2.15	0.47
4:4:226:PRO:HG3	4:4:242:SER:O	2.15	0.47
4:4:256:GLY:C	4:4:258:GLU:N	2.71	0.47
4:4:376:VAL:O	4:4:379:GLN:HG3	2.15	0.47
6:6:37:TRP:CE3	6:6:37:TRP:HA	2.48	0.47
6:6:110:ALA:HB1	6:6:116:GLY:HA2	1.97	0.47
1:A:399:PHE:HB3	9:A:439:SF4:S2	2.55	0.47
4:D:106:GLY:O	5:E:194:SER:HB3	2.14	0.47
4:D:188:PRO:O	4:D:191:LYS:HB2	2.14	0.47
4:D:314:ARG:NH1	4:D:314:ARG:CG	2.75	0.47
4:D:346:THR:HG22	4:D:353:LEU:O	2.14	0.47
6:F:16:ARG:HA	6:F:21:PHE:CD2	2.50	0.47
6:F:108:MET:HA	6:F:137:VAL:CG1	2.44	0.47
8:H:8:GLU:HG2	8:H:97:TYR:OH	2.14	0.47
8:H:88:ARG:HE	8:H:126:LEU:CD2	2.28	0.47
1:J:272:PHE:CE2	1:J:311:MET:HE3	2.50	0.47
2:K:11:LEU:O	2:K:12:GLU:C	2.57	0.47
2:K:42:ARG:HB2	2:K:45:ARG:HG2	1.96	0.47
3:L:224:GLY:HA3	3:L:295:ARG:HD2	1.97	0.47
3:L:508:GLY:HA2	3:L:535:MET:HB2	1.97	0.47
3:L:689:LYS:HB2	3:L:772:GLU:HG2	1.96	0.47
6:O:149:TYR:CZ	6:O:153:GLN:NE2	2.82	0.47
8:Q:63:LEU:HD13	8:Q:129:ALA:HB3	1.97	0.47
8:Q:121:ARG:NH1	8:Q:121:ARG:CG	2.78	0.47
1:S:162:LEU:HB3	1:S:163:PHE:CD1	2.49	0.47
1:S:163:PHE:C	1:S:165:THR:H	2.23	0.47
2:T:106:ILE:CG2	2:T:110:GLU:HB2	2.44	0.47
3:U:381:LEU:HD12	3:U:522:ARG:HD3	1.96	0.47
3:U:505:LEU:HD21	3:U:507:LEU:HD23	1.97	0.47
3:U:506:ILE:CG2	3:U:535:MET:HE3	2.45	0.47
4:V:79:ILE:HG22	4:V:79:ILE:O	2.14	0.47
6:X:108:MET:HA	6:X:137:VAL:CG1	2.45	0.47
3:3:385:ALA:HB2	3:3:531:LYS:CB	2.45	0.47
4:4:138:LEU:HD11	4:4:146:PHE:CD2	2.50	0.47
4:4:311:PRO:HD3	4:4:330:HIS:CE1	2.49	0.47
5:5:174:LEU:CD2	5:5:180:GLY:HA2	2.44	0.47
7:9:53:CYS:HB2	7:9:112:ALA:HB1	1.95	0.47
3:C:19:VAL:HG12	3:C:82:SER:HB2	1.97	0.47
3:C:381:LEU:HD12	3:C:522:ARG:HD3	1.97	0.47
4:D:99:LEU:HD13	4:D:99:LEU:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:211:SER:CB	4:D:214:PHE:HB3	2.45	0.47
4:D:358:VAL:O	4:D:366:TYR:HB3	2.15	0.47
5:E:168:ALA:HA	5:E:171:ARG:HH12	1.80	0.47
8:H:20:MET:HE3	8:H:59:LEU:HG	1.97	0.47
1:J:41:ALA:HA	1:J:120:LEU:HD21	1.97	0.47
3:L:478:LEU:HD21	3:L:483:ASP:HB2	1.96	0.47
3:L:671:GLU:HG3	3:L:672:ALA:H	1.80	0.47
4:M:85:MET:HE3	4:M:409:ARG:CB	2.45	0.47
4:V:211:SER:HB2	4:V:215:TYR:H	1.79	0.47
5:W:25:LEU:CD2	5:W:25:LEU:H	2.28	0.47
5:5:34:PHE:HE1	5:5:38:MET:SD	2.37	0.47
5:5:77:LEU:HA	5:5:78:PRO:HD3	1.59	0.47
6:6:17:GLU:O	1:J:273:ARG:HD3	2.15	0.47
8:7:86:LEU:HD11	8:7:118:LEU:HD11	1.97	0.47
4:D:198:PRO:HG3	4:D:291:LYS:NZ	2.30	0.47
4:D:287:VAL:O	4:D:291:LYS:HG3	2.15	0.47
4:D:342:VAL:HG22	4:D:343:TYR:N	2.29	0.47
1:J:195:LEU:HA	2:K:24:ARG:HH21	1.80	0.47
1:J:267:PRO:O	1:J:268:MET:C	2.57	0.47
1:J:293:GLY:HA3	1:J:324:GLY:N	2.10	0.47
4:M:73:ARG:HG3	4:M:77:GLN:OE1	2.14	0.47
3:U:361:ALA:HB1	3:U:366:THR:CG2	2.44	0.47
3:U:655:ARG:HH12	3:U:659:GLU:CB	2.27	0.47
3:U:664:LEU:O	3:U:669:VAL:HG12	2.15	0.47
5:W:25:LEU:H	5:W:25:LEU:HD23	1.80	0.47
6:X:33:SER:HA	6:X:158:VAL:HG21	1.96	0.47
7:Y:40:ARG:CB	7:Y:121:MET:HE1	2.35	0.47
1:1:38:TYR:OH	1:1:112:HIS:ND1	2.40	0.47
3:3:254:THR:HG23	3:3:255:THR:N	2.28	0.47
6:6:146:ALA:HB2	7:9:119:PHE:HD1	1.79	0.47
8:7:13:TRP:CZ2	8:7:17:LEU:HD11	2.49	0.47
4:D:261:THR:HB	4:D:292:GLN:OE1	2.15	0.47
5:E:141:LEU:HD21	5:E:145:PRO:HD3	1.97	0.47
1:J:89:LEU:HD23	1:J:118:MET:HE3	1.97	0.47
1:J:264:TYR:CD2	1:J:279:TRP:HB3	2.50	0.47
3:L:513:GLN:HG2	3:L:769:LEU:CD2	2.45	0.47
4:M:188:PRO:O	4:M:191:LYS:HB2	2.15	0.47
5:N:168:ALA:HA	5:N:171:ARG:HH12	1.79	0.47
6:O:117:MET:HE3	6:O:118:PHE:CZ	2.50	0.47
1:S:291:ILE:HD11	1:S:331:ILE:HD11	1.97	0.47
2:T:58:THR:HG21	3:U:200:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:100:VAL:O	3:U:104:GLN:HG3	2.14	0.47
3:U:440:ARG:CG	3:U:440:ARG:NH1	2.76	0.47
3:U:591:HIS:ND1	3:U:592:PRO:N	2.63	0.47
8:Z:29:VAL:HG22	8:Z:60:SER:O	2.15	0.47
1:1:162:LEU:HB3	1:1:163:PHE:CD1	2.51	0.46
1:A:98:PRO:HB3	2:B:85:THR:HG21	1.97	0.46
3:C:409:LEU:HD23	3:C:409:LEU:HA	1.76	0.46
3:C:483:ASP:O	3:C:484:LYS:HG2	2.15	0.46
3:C:670:PRO:CD	3:C:676:LEU:HD23	2.44	0.46
4:D:76:LEU:HD12	4:D:76:LEU:O	2.15	0.46
1:J:81:LYS:CE	1:J:81:LYS:HA	2.46	0.46
2:K:142:VAL:HG11	2:K:153:LEU:HG	1.96	0.46
4:M:122:GLU:OE2	4:M:249:ARG:NH1	2.47	0.46
1:S:6:LEU:HD21	1:S:12:ARG:CG	2.44	0.46
1:S:29:LEU:HD22	1:S:33:LEU:CD1	2.46	0.46
2:T:85:THR:HG22	2:T:86:LEU:N	2.30	0.46
3:U:45:CYS:O	3:U:46:ARG:HB2	2.15	0.46
4:V:173:ILE:HG23	4:V:173:ILE:O	2.14	0.46
2:2:33:ARG:HH21	2:2:37:GLU:HG3	1.79	0.46
2:2:89:LYS:HE3	2:2:94:GLU:OE1	2.15	0.46
5:5:13:LYS:HG2	5:5:13:LYS:O	2.15	0.46
5:5:195:LEU:HD22	5:5:195:LEU:N	2.31	0.46
1:A:211:LEU:HG	1:A:212:TRP:CE3	2.49	0.46
1:A:211:LEU:HG	1:A:212:TRP:CZ3	2.49	0.46
3:C:225:ASN:O	3:C:229:ILE:HG13	2.15	0.46
3:C:285:VAL:HG22	3:C:286:ASN:H	1.80	0.46
4:D:133:LEU:HD21	4:D:204:TYR:CE2	2.50	0.46
4:D:369:LYS:HD3	4:D:370:VAL:N	2.30	0.46
6:F:128:ASP:HA	6:F:131:VAL:O	2.15	0.46
8:H:13:TRP:CZ2	8:H:17:LEU:HD11	2.51	0.46
8:H:117:ALA:O	8:H:121:ARG:HG2	2.15	0.46
1:J:202:LYS:N	1:J:203:PRO:HD2	2.31	0.46
3:L:45:CYS:O	3:L:46:ARG:HB2	2.15	0.46
3:L:378:PRO:O	3:L:381:LEU:HB2	2.14	0.46
4:M:197:LEU:N	4:M:198:PRO:HD2	2.30	0.46
4:M:256:GLY:C	4:M:258:GLU:N	2.71	0.46
1:S:92:ASN:ND2	10:S:440:FMN:N1	2.63	0.46
3:U:326:PHE:CZ	3:U:330:LYS:HE3	2.50	0.46
3:U:497:TRP:NE1	3:U:524:LEU:CD1	2.75	0.46
3:U:583:VAL:HG23	3:U:598:ALA:HA	1.96	0.46
4:V:393:MET:C	4:V:396:ILE:HG22	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:37:PHE:HE2	8:Z:74:PRO:HA	1.79	0.46
3:3:116:PRO:O	3:3:117:LEU:HB2	2.14	0.46
4:4:212:PRO:HG2	4:4:213:ILE:H	1.80	0.46
4:4:283:MET:O	4:4:287:VAL:HG23	2.15	0.46
2:B:142:VAL:HG11	2:B:153:LEU:HG	1.98	0.46
3:C:385:ALA:HB3	3:C:533:LEU:CD2	2.45	0.46
5:E:1:MET:SD	8:Z:113:GLU:OE1	2.73	0.46
6:F:121:TYR:HD1	6:F:121:TYR:H	1.63	0.46
1:J:356:CYS:HB3	1:J:358:PRO:HD2	1.98	0.46
3:L:33:PHE:HB2	3:L:45:CYS:SG	2.55	0.46
3:L:732:ALA:O	3:L:747:VAL:HG12	2.15	0.46
4:M:125:ARG:HD2	4:M:286:SER:OG	2.16	0.46
1:S:420:GLN:O	1:S:424:LEU:HD13	2.15	0.46
3:U:160:THR:OG1	8:Z:73:SER:HB3	2.15	0.46
3:U:237:ASP:OD1	3:U:239:THR:HG22	2.15	0.46
4:V:115:THR:HG22	4:V:297:LEU:HD23	1.96	0.46
4:V:338:PRO:HG3	5:W:193:ARG:HB2	1.96	0.46
5:W:13:LYS:O	5:W:13:LYS:HG2	2.15	0.46
7:Y:29:ALA:HA	7:Y:30:PRO:HD2	1.79	0.46
2:2:11:LEU:O	2:2:12:GLU:C	2.57	0.46
3:3:506:ILE:CG2	3:3:535:MET:HE3	2.45	0.46
4:4:254:TYR:CE2	4:4:346:THR:CA	2.93	0.46
8:7:63:LEU:HD13	8:7:129:ALA:HB3	1.97	0.46
8:7:70:ALA:HA	8:7:83:GLY:O	2.16	0.46
1:A:154:ALA:O	1:A:156:GLY:N	2.48	0.46
3:C:583:VAL:HG21	3:C:597:TYR:O	2.16	0.46
5:E:195:LEU:HD22	5:E:195:LEU:N	2.31	0.46
3:L:290:ILE:HG22	3:L:291:CYS:O	2.16	0.46
3:L:497:TRP:CD1	3:L:524:LEU:HD11	2.49	0.46
3:L:591:HIS:ND1	3:L:592:PRO:CD	2.78	0.46
3:L:664:LEU:O	3:L:669:VAL:HG12	2.16	0.46
5:N:13:LYS:O	5:N:13:LYS:HG2	2.15	0.46
5:N:37:GLU:O	5:N:40:HIS:HB3	2.16	0.46
8:Q:86:LEU:HD11	8:Q:118:LEU:HD11	1.98	0.46
1:S:107:LEU:HD23	1:S:114:LEU:HD12	1.97	0.46
2:T:24:ARG:O	2:T:27:ILE:HD12	2.15	0.46
4:V:197:LEU:N	4:V:198:PRO:HD2	2.31	0.46
6:X:96:TRP:HA	6:X:99:MET:CE	2.41	0.46
1:1:334:ARG:O	1:1:434:PRO:HG3	2.16	0.46
3:3:700:LYS:HA	3:3:763:LEU:O	2.16	0.46
1:A:116:GLU:HG2	1:A:228:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ARG:NE	3:C:79:LEU:HD12	2.31	0.46
2:B:112:THR:HG22	2:B:116:LEU:H	1.81	0.46
3:C:243:ARG:HB3	3:C:275:LEU:HD12	1.98	0.46
3:C:478:LEU:HD12	3:C:520:ARG:NH1	2.30	0.46
4:D:211:SER:HB2	4:D:215:TYR:H	1.80	0.46
4:D:230:ILE:HD11	4:D:244:VAL:CG2	2.46	0.46
5:E:104:VAL:CG1	5:E:108:TRP:HE3	2.29	0.46
1:J:249:MET:HE2	1:J:249:MET:H	1.80	0.46
3:L:689:LYS:HD2	3:L:772:GLU:H	1.81	0.46
4:M:379:GLN:HG2	5:N:113:PHE:CD1	2.50	0.46
8:Q:49:ASP:N	8:Q:49:ASP:OD1	2.49	0.46
1:S:49:THR:OG1	1:S:52:GLU:HG3	2.15	0.46
1:S:72:THR:HG21	1:S:223:THR:HG21	1.96	0.46
3:U:268:ASP:OD2	3:U:278:ARG:NH1	2.48	0.46
4:V:211:SER:OG	4:V:215:TYR:HB2	2.16	0.46
4:V:381:LEU:H	4:V:382:PRO:CD	2.28	0.46
6:X:40:THR:HB	6:X:50:MET:SD	2.55	0.46
1:1:211:LEU:HG	1:1:212:TRP:CE3	2.50	0.46
3:3:732:ALA:O	3:3:747:VAL:HG12	2.15	0.46
4:4:159:LEU:O	4:4:163:VAL:HG12	2.15	0.46
4:4:294:LEU:O	4:4:294:LEU:HD23	2.16	0.46
5:5:54:GLY:C	5:5:55:LEU:HD12	2.41	0.46
6:6:30:TRP:O	6:6:33:SER:HB3	2.15	0.46
1:A:162:LEU:HB3	1:A:163:PHE:CD1	2.50	0.46
1:A:366:PHE:O	1:A:370:LEU:HD23	2.14	0.46
3:C:700:LYS:HA	3:C:763:LEU:O	2.15	0.46
6:F:149:TYR:CZ	6:F:153:GLN:NE2	2.83	0.46
2:K:85:THR:HG22	2:K:86:LEU:H	1.81	0.46
4:M:254:TYR:C	4:M:256:GLY:H	2.19	0.46
6:O:117:MET:CE	7:P:99:ILE:HG12	2.45	0.46
4:V:240:ARG:NH2	4:V:347:GLU:OE2	2.45	0.46
4:V:369:LYS:HD3	4:V:370:VAL:N	2.31	0.46
1:1:298:PRO:HD2	1:1:321:SER:OG	2.16	0.46
3:3:18:SER:HB3	3:3:21:ASP:OD1	2.15	0.46
3:3:290:ILE:HG22	3:3:291:CYS:O	2.16	0.46
4:4:236:GLY:C	4:4:238:SER:N	2.73	0.46
4:4:393:MET:HA	4:4:396:ILE:CG2	2.46	0.46
7:9:33:LEU:HD22	7:9:37:PHE:CD2	2.50	0.46
7:9:44:THR:OG1	7:9:52:LYS:HD2	2.15	0.46
1:A:163:PHE:C	1:A:165:THR:H	2.23	0.46
2:B:3:PHE:CD1	2:B:3:PHE:C	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:732:ALA:H	3:C:747:VAL:HG12	1.80	0.46
4:D:173:ILE:HG23	4:D:173:ILE:O	2.16	0.46
6:F:78:MET:HE2	6:F:99:MET:HE1	1.98	0.46
8:H:38:PRO:C	8:H:40:PHE:H	2.24	0.46
8:H:88:ARG:HE	8:H:126:LEU:HD22	1.81	0.46
3:L:31:PRO:HD2	3:L:104:GLN:NE2	2.30	0.46
5:N:194:SER:O	5:N:195:LEU:HD13	2.15	0.46
7:P:134:GLU:CD	7:P:134:GLU:N	2.73	0.46
3:U:19:VAL:HG23	3:U:85:THR:O	2.16	0.46
3:U:732:ALA:H	3:U:747:VAL:CG1	2.29	0.46
4:V:104:LEU:HD22	4:V:338:PRO:HD2	1.97	0.46
1:1:264:TYR:CD2	1:1:279:TRP:HB3	2.51	0.46
3:3:641:LEU:HD23	3:3:641:LEU:HA	1.77	0.46
1:A:211:LEU:HB2	1:A:216:THR:HG21	1.96	0.46
3:C:337:ARG:HD2	3:C:337:ARG:N	2.27	0.46
3:C:646:GLU:C	3:C:648:LEU:H	2.24	0.46
4:D:62:LEU:HD21	6:F:43:LEU:HB3	1.97	0.46
4:D:256:GLY:C	4:D:258:GLU:N	2.70	0.46
6:F:141:PRO:HB3	9:F:182:SF4:S1	2.56	0.46
1:J:87:HIS:HB2	1:J:126:ARG:O	2.16	0.46
1:J:107:LEU:CD2	1:J:114:LEU:HD12	2.46	0.46
1:J:323:LEU:HD23	1:J:323:LEU:C	2.40	0.46
1:J:397:ARG:HD2	1:J:397:ARG:N	2.29	0.46
3:L:161:ARG:HG2	3:L:161:ARG:HH11	1.81	0.46
4:M:385:CYS:HB3	4:M:396:ILE:HG12	1.96	0.46
1:S:201:LEU:O	1:S:204:PRO:HD2	2.16	0.46
1:S:264:TYR:CD2	1:S:279:TRP:HB3	2.50	0.46
4:V:138:LEU:HD11	4:V:146:PHE:CD2	2.51	0.46
4:V:263:ASP:O	4:V:285:GLU:HG3	2.15	0.46
4:V:276:MET:O	4:V:280:ILE:HG13	2.15	0.46
1:1:341:MET:HE2	1:1:409:PRO:C	2.41	0.46
2:2:59:GLU:O	2:2:63:VAL:HG23	2.16	0.46
3:3:385:ALA:HB3	3:3:533:LEU:HD23	1.97	0.46
5:5:98:ASP:C	5:5:100:ARG:H	2.24	0.46
6:6:34:ASN:C	6:6:36:LEU:H	2.24	0.46
2:B:11:LEU:O	2:B:12:GLU:C	2.58	0.46
2:B:85:THR:HG22	2:B:86:LEU:H	1.80	0.46
2:B:88:CYS:HB3	2:B:93:ALA:HB2	1.98	0.46
3:C:197:ASP:CB	3:C:220:SER:HB3	2.46	0.46
3:C:559:ASP:HB2	3:C:573:PRO:HG3	1.96	0.46
1:J:272:PHE:CE1	1:J:311:MET:HG2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:2:VAL:CG1	3:L:89:ASP:HA	2.46	0.46
3:L:132:ASP:O	3:L:136:GLU:HG3	2.15	0.46
3:L:250:GLU:CD	3:L:628:PRO:HG2	2.40	0.46
3:L:559:ASP:HB2	3:L:573:PRO:HG3	1.97	0.46
4:M:249:ARG:HB2	4:M:262:PHE:HE2	1.81	0.46
5:N:123:GLY:HA2	5:N:144:HIS:CD2	2.50	0.46
7:P:26:TYR:N	7:P:27:PRO:CD	2.76	0.46
3:U:690:GLY:HA3	3:U:770:ARG:HH21	1.81	0.46
5:W:132:LEU:HD23	5:W:132:LEU:HA	1.68	0.46
6:X:16:ARG:HA	6:X:21:PHE:CD2	2.50	0.46
6:X:106:ILE:CD1	6:X:151:VAL:HG12	2.46	0.46
4:4:125:ARG:HD2	4:4:286:SER:OG	2.16	0.46
4:4:173:ILE:O	4:4:173:ILE:HG23	2.15	0.46
4:4:223:VAL:O	4:4:383:TYR:HE1	1.99	0.46
6:6:19:ILE:HD11	1:J:271:THR:HG23	1.96	0.46
1:A:29:LEU:HD22	1:A:33:LEU:CD1	2.45	0.46
1:A:290:ILE:HG22	1:A:330:LEU:HD22	1.98	0.46
3:C:216:PHE:CZ	8:H:128:PHE:CD2	3.00	0.46
3:C:420:LEU:HD22	3:C:436:GLN:HG2	1.98	0.46
3:C:689:LYS:HD2	3:C:772:GLU:H	1.81	0.46
5:E:52:ILE:CG2	5:E:114:LEU:HB3	2.42	0.46
5:E:132:LEU:HD23	5:E:132:LEU:HA	1.65	0.46
8:H:16:LEU:O	8:H:16:LEU:HD13	2.16	0.46
2:K:24:ARG:O	2:K:27:ILE:HD12	2.15	0.46
3:L:218:LEU:N	3:L:219:PRO:HD3	2.31	0.46
3:L:225:ASN:O	3:L:229:ILE:HG13	2.16	0.46
3:L:367:PRO:CB	3:L:554:LYS:HB2	2.46	0.46
3:L:641:LEU:HD23	3:L:641:LEU:HA	1.79	0.46
4:M:276:MET:O	4:M:280:ILE:HG13	2.16	0.46
6:O:106:ILE:CD1	6:O:151:VAL:HG12	2.46	0.46
8:Q:37:PHE:CE1	8:Q:55:MET:HB2	2.50	0.46
1:S:315:HIS:O	1:S:319:LYS:HB2	2.17	0.46
4:V:168:PHE:CE1	6:X:141:PRO:HG3	2.51	0.46
6:X:149:TYR:CZ	6:X:153:GLN:NE2	2.84	0.46
7:Y:123:ASP:CB	7:Y:129:LEU:HD21	2.46	0.46
1:1:107:LEU:CD2	1:1:114:LEU:HD12	2.47	0.45
1:1:254:ILE:HB	1:1:275:LEU:HD21	1.98	0.45
4:4:241:ALA:CB	4:4:278:VAL:HG21	2.46	0.45
4:4:374:SER:HB2	4:4:406:ASP:HB3	1.97	0.45
1:A:104:ARG:HH21	2:B:127:SER:CB	2.28	0.45
1:A:202:LYS:N	1:A:203:PRO:HD2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:H	1:A:233:ARG:HG2	1.57	0.45
1:A:249:MET:H	1:A:249:MET:HE2	1.82	0.45
1:A:420:GLN:O	1:A:424:LEU:HD13	2.16	0.45
3:C:30:VAL:CG2	3:C:31:PRO:HD2	2.46	0.45
3:C:397:LEU:HD21	3:C:480:LEU:HD13	1.98	0.45
4:D:263:ASP:HB2	4:D:285:GLU:OE1	2.15	0.45
4:D:371:ARG:NH2	4:D:376:VAL:CG2	2.79	0.45
4:D:381:LEU:H	4:D:382:PRO:HD2	1.80	0.45
6:F:37:TRP:CE3	6:F:37:TRP:HA	2.51	0.45
3:L:116:PRO:O	3:L:117:LEU:HB2	2.16	0.45
3:L:583:VAL:HG21	3:L:597:TYR:O	2.15	0.45
4:M:241:ALA:O	4:M:267:GLY:HA3	2.15	0.45
3:U:118:ASP:O	3:U:121:THR:N	2.49	0.45
3:U:583:VAL:HG21	3:U:597:TYR:O	2.16	0.45
4:V:221:VAL:O	4:V:272:VAL:HG12	2.16	0.45
4:V:241:ALA:O	4:V:267:GLY:HA3	2.16	0.45
6:X:48:ILE:O	6:X:48:ILE:HG22	2.15	0.45
6:X:114:SER:CB	7:Y:97:ARG:HD2	2.43	0.45
8:Z:8:GLU:HG2	8:Z:97:TYR:OH	2.15	0.45
1:1:385:GLU:O	1:1:388:GLU:HB3	2.16	0.45
3:3:655:ARG:HH12	3:3:659:GLU:CB	2.29	0.45
3:3:689:LYS:HB2	3:3:772:GLU:HG2	1.97	0.45
4:4:224:ILE:HA	4:4:225:PRO:HD2	1.76	0.45
5:5:194:SER:C	5:5:195:LEU:HD22	2.42	0.45
6:6:46:CYS:HB3	6:6:81:ALA:HB1	1.98	0.45
1:A:267:PRO:O	1:A:270:THR:HG23	2.16	0.45
2:B:40:TRP:CH2	2:B:42:ARG:HG2	2.51	0.45
3:C:513:GLN:HG2	3:C:769:LEU:CD2	2.46	0.45
1:J:39:GLU:O	1:J:43:ARG:HG3	2.16	0.45
1:J:64:GLY:HA3	10:J:440:FMN:O1P	2.16	0.45
3:L:180:ARG:O	3:L:181:CYS:C	2.60	0.45
3:L:455:ARG:HG3	3:L:455:ARG:O	2.17	0.45
5:N:34:PHE:O	5:N:35:LYS:C	2.60	0.45
6:O:37:TRP:HA	6:O:37:TRP:CE3	2.50	0.45
3:U:19:VAL:O	3:U:22:ALA:HB3	2.16	0.45
3:U:83:CYS:SG	3:U:84:VAL:HG13	2.57	0.45
3:U:515:THR:HG23	3:U:683:LEU:CD1	2.43	0.45
4:V:197:LEU:N	4:V:198:PRO:CD	2.79	0.45
5:W:157:THR:C	5:W:158:LEU:HD23	2.41	0.45
6:X:110:ALA:HB1	6:X:116:GLY:HA2	1.98	0.45
1:1:145:LEU:O	1:1:149:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:211:LEU:HG	1:1:212:TRP:CZ3	2.50	0.45
3:3:45:CYS:O	3:3:46:ARG:HB2	2.16	0.45
3:3:55:PRO:HG3	3:3:73:ILE:C	2.40	0.45
3:3:508:GLY:HA2	3:3:535:MET:HB2	1.99	0.45
3:3:513:GLN:HG2	3:3:769:LEU:CD2	2.45	0.45
4:4:254:TYR:C	4:4:256:GLY:H	2.20	0.45
5:5:1:MET:C	5:5:3:LEU:N	2.75	0.45
6:6:43:LEU:HD11	6:6:84:LEU:HD23	1.97	0.45
6:6:152:MET:HE2	6:6:152:MET:HB3	1.50	0.45
7:9:39:GLY:O	7:9:40:ARG:C	2.59	0.45
8:7:49:ASP:N	8:7:49:ASP:OD1	2.50	0.45
1:A:145:LEU:HA	1:A:145:LEU:HD23	1.70	0.45
1:A:359:CYS:O	1:A:363:VAL:HG22	2.16	0.45
3:C:118:ASP:O	3:C:119:CYS:C	2.59	0.45
4:D:249:ARG:HB2	4:D:262:PHE:HE2	1.81	0.45
4:D:367:ARG:HH12	4:D:369:LYS:CA	2.30	0.45
5:E:194:SER:O	5:E:195:LEU:HD13	2.16	0.45
7:G:45:ARG:NH2	7:G:137:LEU:CD2	2.77	0.45
3:L:232:VAL:HB	9:L:784:SF4:S2	2.56	0.45
4:M:82:THR:N	4:M:83:PRO:HD2	2.31	0.45
4:M:328:PHE:CD2	4:M:328:PHE:C	2.95	0.45
5:N:1:MET:C	5:N:3:LEU:N	2.75	0.45
1:S:184:GLU:OE1	1:S:186:THR:N	2.49	0.45
3:U:184:CYS:O	9:U:785:SF4:S4	2.75	0.45
3:U:243:ARG:HB3	3:U:275:LEU:HD12	1.98	0.45
3:U:397:LEU:HD21	3:U:480:LEU:HD13	1.98	0.45
3:U:513:GLN:HG2	3:U:769:LEU:CD2	2.45	0.45
4:V:122:GLU:HB2	4:V:290:ILE:CD1	2.44	0.45
6:X:155:GLN:C	6:X:157:LYS:H	2.23	0.45
7:Y:93:ILE:HG13	7:Y:136:MET:HE1	1.98	0.45
7:Y:129:LEU:HD23	7:Y:129:LEU:HA	1.72	0.45
1:1:149:ILE:O	1:1:153:ARG:HB2	2.17	0.45
3:3:197:ASP:CB	3:3:220:SER:HB3	2.46	0.45
3:3:470:PRO:O	3:3:471:GLY:C	2.59	0.45
4:4:197:LEU:HA	4:4:200:ARG:HB3	1.98	0.45
6:6:123:ILE:HG22	6:6:124:VAL:N	2.32	0.45
7:9:134:GLU:CD	7:9:134:GLU:N	2.74	0.45
3:C:184:CYS:SG	3:C:186:ARG:HB2	2.57	0.45
3:C:487:SER:OG	3:C:490:VAL:HG23	2.16	0.45
3:C:737:GLU:HB2	3:C:776:LEU:HD21	1.97	0.45
5:E:54:GLY:C	5:E:55:LEU:HD12	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:181:LEU:HD12	5:E:181:LEU:HA	1.80	0.45
1:J:264:TYR:CE2	1:J:279:TRP:HB3	2.51	0.45
3:L:131:GLN:O	3:L:134:THR:HB	2.17	0.45
3:L:269:THR:HG23	3:L:274:LEU:HD13	1.98	0.45
3:L:646:GLU:C	3:L:648:LEU:H	2.25	0.45
4:M:122:GLU:HB2	4:M:290:ILE:CD1	2.47	0.45
4:M:376:VAL:O	4:M:379:GLN:HG3	2.16	0.45
5:N:48:PHE:CE2	5:N:50:ALA:HB2	2.51	0.45
1:S:202:LYS:N	1:S:203:PRO:HD2	2.31	0.45
3:U:250:GLU:CD	3:U:628:PRO:HG2	2.40	0.45
3:U:732:ALA:O	3:U:747:VAL:HG12	2.16	0.45
7:Y:99:ILE:HG22	7:Y:101:CYS:SG	2.56	0.45
1:1:238:PHE:HE1	1:1:249:MET:HE1	1.81	0.45
1:1:297:THR:HG22	1:1:322:MET:HG3	1.99	0.45
3:3:351:LEU:HD12	3:3:351:LEU:HA	1.79	0.45
3:3:594:ALA:C	3:3:596:ARG:H	2.24	0.45
4:4:84:ARG:CD	6:6:117:MET:HE1	2.45	0.45
4:4:197:LEU:N	4:4:198:PRO:CD	2.80	0.45
5:5:37:GLU:O	5:5:40:HIS:HB3	2.17	0.45
3:C:83:CYS:SG	3:C:84:VAL:HG13	2.56	0.45
3:C:117:LEU:H	4:D:321:MET:CE	2.16	0.45
3:C:216:PHE:CZ	8:H:128:PHE:HD2	2.31	0.45
3:C:459:MET:HG3	3:C:465:HIS:HB2	1.99	0.45
3:C:505:LEU:HB3	3:C:532:VAL:HG22	1.98	0.45
3:C:583:VAL:HG23	3:C:598:ALA:HA	1.98	0.45
1:J:118:MET:O	1:J:122:GLY:N	2.47	0.45
4:M:222:GLY:HA2	4:M:384:ALA:O	2.16	0.45
5:N:195:LEU:HD22	5:N:195:LEU:N	2.32	0.45
6:O:16:ARG:NH1	6:O:17:GLU:OE2	2.50	0.45
1:S:211:LEU:HG	1:S:212:TRP:CE3	2.52	0.45
2:T:88:CYS:HB3	2:T:93:ALA:HB2	1.99	0.45
3:U:6:VAL:HG21	3:U:26:ALA:CB	2.47	0.45
3:U:197:ASP:CB	3:U:220:SER:HB3	2.46	0.45
3:U:245:ARG:HA	3:U:245:ARG:HD2	1.74	0.45
4:V:263:ASP:HB2	4:V:285:GLU:OE1	2.17	0.45
5:W:104:VAL:CG1	5:W:108:TRP:HE3	2.29	0.45
8:Z:108:ILE:HD12	8:Z:108:ILE:N	2.31	0.45
1:1:202:LYS:N	1:1:203:PRO:HD2	2.32	0.45
3:3:368:HIS:CD2	3:3:556:ALA:HB3	2.51	0.45
8:H:16:LEU:HG	8:H:82:ILE:HD11	1.97	0.45
1:J:107:LEU:HD23	1:J:114:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:110:VAL:N	1:J:111:PRO:CD	2.79	0.45
1:J:317:GLN:C	1:J:319:LYS:H	2.25	0.45
1:J:332:PRO:HD2	2:K:90:LEU:CD2	2.44	0.45
3:L:109:GLU:OE1	3:L:156:ARG:NH1	2.50	0.45
3:L:343:LEU:O	3:L:369:LEU:HA	2.16	0.45
1:S:334:ARG:O	1:S:434:PRO:HG3	2.17	0.45
4:V:360:ASP:OD2	5:W:176:GLY:HA3	2.17	0.45
1:1:272:PHE:CD1	1:1:311:MET:HG2	2.52	0.45
1:1:356:CYS:HB3	1:1:358:PRO:HD2	1.99	0.45
3:3:305:ARG:NH2	3:3:609:GLU:OE1	2.47	0.45
3:3:403:THR:O	3:3:403:THR:HG22	2.16	0.45
4:4:316:LEU:C	4:4:318:GLU:N	2.74	0.45
5:5:129:HIS:CD2	5:5:130:PRO:HD2	2.51	0.45
6:6:48:ILE:HG22	6:6:48:ILE:O	2.15	0.45
1:A:18:TYR:OH	1:A:105:TYR:HB2	2.17	0.45
1:A:366:PHE:HD1	1:A:370:LEU:CD2	2.29	0.45
2:B:89:LYS:HE3	2:B:94:GLU:OE1	2.16	0.45
3:C:132:ASP:O	3:C:136:GLU:HG3	2.17	0.45
7:G:177:THR:O	7:G:179:GLY:N	2.49	0.45
3:L:286:ASN:ND2	3:L:286:ASN:C	2.74	0.45
3:L:724:ARG:HG2	3:L:724:ARG:O	2.16	0.45
4:M:237:GLY:HA2	4:M:240:ARG:NH2	2.31	0.45
4:M:350:ARG:HG3	4:M:350:ARG:NH1	2.32	0.45
7:P:108:CYS:HA	9:P:184:SF4:S3	2.56	0.45
1:S:104:ARG:HH21	2:T:127:SER:CB	2.29	0.45
1:S:205:PHE:HD1	1:S:206:PRO:HD2	1.80	0.45
2:T:142:VAL:HG11	2:T:153:LEU:HG	1.99	0.45
3:U:55:PRO:CG	3:U:74:GLN:N	2.72	0.45
3:U:113:LEU:HD12	3:U:157:PHE:CG	2.51	0.45
3:U:119:CYS:O	3:U:120:PRO:C	2.60	0.45
3:U:132:ASP:O	3:U:136:GLU:HG3	2.16	0.45
2:2:78:TYR:CE1	2:2:157:LEU:HD22	2.52	0.45
2:2:85:THR:HG22	2:2:86:LEU:H	1.82	0.45
3:3:218:LEU:N	3:3:219:PRO:HD3	2.31	0.45
3:3:559:ASP:HB2	3:3:573:PRO:HG3	1.98	0.45
1:A:88:TYR:HB2	1:A:216:THR:CG2	2.46	0.45
2:B:59:GLU:O	2:B:63:VAL:HG23	2.16	0.45
3:C:689:LYS:HB2	3:C:772:GLU:HG2	1.98	0.45
4:D:26:MET:N	4:D:48:SER:HG	2.15	0.45
4:D:138:LEU:HD11	4:D:146:PHE:CD2	2.51	0.45
4:D:188:PRO:CB	3:U:724:ARG:CD	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:254:TYR:C	4:D:256:GLY:H	2.20	0.45
4:D:306:ASN:HA	4:D:307:PRO:HD3	1.77	0.45
4:D:321:MET:HE2	4:D:321:MET:HB2	1.65	0.45
4:D:375:PHE:HD1	4:D:407:VAL:HG23	1.82	0.45
5:E:37:GLU:O	5:E:40:HIS:HB3	2.17	0.45
5:E:111:ALA:HB1	5:E:115:GLU:HG3	1.98	0.45
1:J:315:HIS:O	1:J:319:LYS:HB2	2.17	0.45
2:K:131:ALA:HB1	2:K:132:PRO:HA	1.99	0.45
3:L:594:ALA:C	3:L:596:ARG:H	2.25	0.45
5:N:54:GLY:C	5:N:55:LEU:HD12	2.42	0.45
1:S:92:ASN:ND2	10:S:440:FMN:C2	2.80	0.45
1:S:197:ALA:HB3	2:T:66:PHE:CE1	2.52	0.45
3:U:218:LEU:N	3:U:219:PRO:HD3	2.32	0.45
4:V:178:VAL:CG2	4:V:302:VAL:HB	2.47	0.45
4:V:321:MET:HE2	4:V:321:MET:HB2	1.74	0.45
5:W:1:MET:C	5:W:3:LEU:N	2.75	0.45
5:W:35:LYS:HD3	5:W:102:PRO:CB	2.47	0.45
1:1:203:PRO:HB2	1:1:204:PRO:HD3	1.98	0.45
2:2:88:CYS:HB3	2:2:93:ALA:HB2	1.99	0.45
2:2:112:THR:HG22	2:2:116:LEU:H	1.82	0.45
3:3:19:VAL:HG12	3:3:82:SER:HB2	1.98	0.45
3:3:168:HIS:HA	3:3:169:PRO:HD2	1.73	0.45
4:4:211:SER:HB2	4:4:215:TYR:H	1.82	0.45
5:5:54:GLY:O	5:5:55:LEU:HD12	2.17	0.45
5:5:141:LEU:HD21	5:5:145:PRO:HD3	1.98	0.45
6:6:16:ARG:NH1	6:6:17:GLU:OE2	2.50	0.45
8:7:60:SER:HB3	8:7:64:GLY:O	2.16	0.45
1:A:205:PHE:HD1	1:A:206:PRO:HD2	1.82	0.45
1:A:291:ILE:O	1:A:328:VAL:HA	2.17	0.45
1:A:424:LEU:CD2	1:A:431:VAL:HG12	2.47	0.45
3:C:19:VAL:O	3:C:22:ALA:HB3	2.17	0.45
3:C:351:LEU:HD12	3:C:351:LEU:HA	1.78	0.45
3:C:732:ALA:O	3:C:747:VAL:HG12	2.16	0.45
4:D:242:SER:HB2	4:D:270:GLY:HA3	1.99	0.45
4:D:350:ARG:NE	4:D:403:VAL:CG2	2.75	0.45
8:H:37:PHE:CE1	8:H:55:MET:HB2	2.52	0.45
1:J:163:PHE:C	1:J:165:THR:H	2.24	0.45
2:K:11:LEU:HD22	2:K:30:LEU:HD21	1.98	0.45
3:L:498:GLU:C	3:L:500:ALA:H	2.24	0.45
4:M:63:HIS:O	6:O:122:ALA:HB1	2.17	0.45
4:M:211:SER:HB2	4:M:215:TYR:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:264:TYR:CE2	1:S:279:TRP:HB3	2.52	0.45
4:V:241:ALA:CB	4:V:278:VAL:HG21	2.46	0.45
8:Z:38:PRO:C	8:Z:40:PHE:H	2.24	0.45
3:3:38:HIS:CE1	3:3:430:THR:HG21	2.52	0.45
3:3:612:GLY:O	3:3:624:LEU:HB2	2.17	0.45
4:4:249:ARG:HB2	4:4:262:PHE:HE2	1.82	0.45
1:A:264:TYR:CE2	1:A:279:TRP:HB3	2.52	0.45
1:A:267:PRO:O	1:A:268:MET:C	2.60	0.45
2:B:86:LEU:CD1	2:B:90:LEU:HD11	2.47	0.45
4:D:306:ASN:C	4:D:306:ASN:OD1	2.60	0.45
5:E:1:MET:C	5:E:3:LEU:N	2.74	0.45
5:E:192:TYR:CG	5:E:193:ARG:N	2.85	0.45
1:J:93:ALA:O	1:J:134:VAL:HA	2.17	0.45
1:J:417:PHE:O	1:J:418:LYS:C	2.60	0.45
4:M:218:ALA:HB1	4:M:272:VAL:HG22	1.99	0.45
5:N:77:LEU:HA	5:N:78:PRO:HD3	1.57	0.45
6:O:96:TRP:HA	6:O:99:MET:CE	2.44	0.45
1:S:211:LEU:HG	1:S:212:TRP:CZ3	2.52	0.45
4:V:122:GLU:OE2	4:V:249:ARG:NH1	2.49	0.45
4:V:212:PRO:HG2	4:V:213:ILE:H	1.81	0.45
8:Z:68:LEU:HD13	8:Z:69:LEU:N	2.32	0.45
1:1:154:ALA:O	1:1:156:GLY:N	2.50	0.44
1:1:211:LEU:HD12	1:1:211:LEU:HA	1.80	0.44
1:1:316:LEU:HD23	1:1:316:LEU:HA	1.83	0.44
1:1:397:ARG:HG2	3:3:49:LEU:HD13	1.97	0.44
3:3:33:PHE:HE2	3:3:111:THR:HG21	1.81	0.44
3:3:378:PRO:O	3:3:381:LEU:HB2	2.16	0.44
4:4:104:LEU:HD22	4:4:338:PRO:HD2	1.99	0.44
1:A:81:LYS:HA	1:A:81:LYS:HE3	1.99	0.44
2:B:144:CYS:O	2:B:149:ARG:HD3	2.16	0.44
3:C:168:HIS:HA	3:C:169:PRO:HD2	1.72	0.44
3:C:326:PHE:CZ	3:C:330:LYS:HE3	2.52	0.44
3:C:655:ARG:HH12	3:C:659:GLU:CB	2.29	0.44
4:D:109:VAL:HG12	4:D:113:ALA:HB3	1.98	0.44
5:E:194:SER:C	5:E:195:LEU:HD22	2.42	0.44
7:G:134:GLU:CD	7:G:134:GLU:N	2.74	0.44
8:H:37:PHE:HE2	8:H:74:PRO:HA	1.82	0.44
1:J:233:ARG:H	1:J:233:ARG:HG2	1.57	0.44
1:J:420:GLN:O	1:J:424:LEU:HD13	2.16	0.44
2:K:106:ILE:CG2	2:K:110:GLU:HB2	2.47	0.44
3:L:281:GLU:HG3	3:L:288:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:487:SER:OG	3:L:490:VAL:HG23	2.17	0.44
4:M:235:THR:O	4:M:235:THR:HG22	2.17	0.44
1:S:38:TYR:OH	1:S:112:HIS:ND1	2.42	0.44
2:T:27:ILE:HG13	2:T:53:VAL:HG21	1.99	0.44
3:U:30:VAL:CG2	3:U:31:PRO:HD2	2.47	0.44
3:U:290:ILE:HD13	3:U:290:ILE:HA	1.76	0.44
3:U:470:PRO:HG3	3:U:759:TYR:HE2	1.82	0.44
4:V:85:MET:HE3	4:V:409:ARG:CB	2.47	0.44
4:V:115:THR:HG21	4:V:297:LEU:HD23	1.97	0.44
4:V:224:ILE:HA	4:V:225:PRO:HD2	1.77	0.44
4:V:236:GLY:C	4:V:238:SER:N	2.72	0.44
4:V:278:VAL:O	4:V:282:GLU:HG3	2.17	0.44
4:V:375:PHE:HD1	4:V:407:VAL:HG23	1.81	0.44
6:X:105:VAL:HG11	6:X:131:VAL:HG21	1.98	0.44
7:Y:100:PHE:N	7:Y:100:PHE:CD1	2.85	0.44
1:1:197:ALA:HB3	2:2:66:PHE:CE1	2.52	0.44
2:2:27:ILE:HG13	2:2:53:VAL:HG21	1.98	0.44
3:3:478:LEU:HD21	3:3:483:ASP:HB2	1.98	0.44
3:3:664:LEU:O	3:3:669:VAL:HG12	2.18	0.44
3:3:689:LYS:HD2	3:3:772:GLU:H	1.83	0.44
4:4:95:LEU:HA	4:4:173:ILE:CD1	2.47	0.44
1:A:355:LYS:HD3	1:A:399:PHE:CD2	2.52	0.44
3:C:31:PRO:HD2	3:C:104:GLN:NE2	2.33	0.44
3:C:594:ALA:C	3:C:596:ARG:H	2.24	0.44
3:C:724:ARG:O	3:C:724:ARG:HG2	2.17	0.44
6:F:110:ALA:HB1	6:F:116:GLY:HA2	1.99	0.44
1:J:162:LEU:HB3	1:J:163:PHE:CD1	2.52	0.44
2:K:86:LEU:CD1	2:K:90:LEU:HD11	2.47	0.44
2:K:90:LEU:HD12	2:K:90:LEU:H	1.82	0.44
3:L:33:PHE:HE2	3:L:111:THR:HG21	1.82	0.44
3:L:203:ILE:HD13	3:L:203:ILE:N	2.32	0.44
3:L:505:LEU:HB3	3:L:532:VAL:HG22	1.99	0.44
3:L:583:VAL:HG21	3:L:598:ALA:HA	1.99	0.44
4:M:63:HIS:HA	4:M:409:ARG:OXT	2.16	0.44
4:M:224:ILE:HA	4:M:225:PRO:HD2	1.79	0.44
8:Q:88:ARG:HE	8:Q:126:LEU:HD22	1.82	0.44
1:S:139:ARG:CG	2:T:140:PRO:HD3	2.45	0.44
1:S:162:LEU:HB3	1:S:163:PHE:HD1	1.83	0.44
3:U:118:ASP:O	3:U:119:CYS:C	2.60	0.44
3:U:202:PHE:HA	3:U:210:PHE:O	2.17	0.44
3:U:700:LYS:HA	3:U:763:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:758:LEU:HD12	3:U:758:LEU:N	2.32	0.44
4:V:358:VAL:O	4:V:366:TYR:HB3	2.17	0.44
6:X:108:MET:CE	6:X:147:LEU:HG	2.35	0.44
2:2:45:ARG:HG2	2:2:45:ARG:H	1.66	0.44
4:4:241:ALA:O	4:4:267:GLY:HA3	2.16	0.44
5:5:157:THR:C	5:5:158:LEU:HD23	2.42	0.44
3:C:38:HIS:CE1	3:C:430:THR:HG21	2.52	0.44
4:D:237:GLY:HA2	4:D:240:ARG:NE	2.31	0.44
4:D:241:ALA:CA	4:D:278:VAL:HG21	2.45	0.44
4:D:283:MET:O	4:D:287:VAL:HG23	2.17	0.44
8:H:70:ALA:HA	8:H:83:GLY:O	2.17	0.44
8:H:86:LEU:HD12	8:H:91:ILE:HD12	1.98	0.44
3:L:483:ASP:O	3:L:484:LYS:HG2	2.17	0.44
3:L:694:LEU:C	3:L:762:ALA:HB2	2.42	0.44
4:M:369:LYS:HD3	4:M:370:VAL:N	2.32	0.44
7:P:99:ILE:HG22	7:P:101:CYS:SG	2.57	0.44
3:U:31:PRO:HD2	3:U:104:GLN:NE2	2.31	0.44
3:U:367:PRO:CB	3:U:554:LYS:HB2	2.47	0.44
3:U:408:ILE:HD12	3:U:408:ILE:HA	1.77	0.44
3:U:508:GLY:HA2	3:U:535:MET:HB2	1.99	0.44
4:V:211:SER:CB	4:V:214:PHE:HB3	2.47	0.44
4:V:342:VAL:HG22	4:V:343:TYR:N	2.31	0.44
1:1:192:LEU:HD23	1:1:192:LEU:C	2.42	0.44
2:2:109:GLY:HA2	8:7:91:ILE:HD13	1.99	0.44
2:2:168:LEU:HA	2:2:169:PRO:HD2	1.81	0.44
4:4:168:PHE:HA	4:4:170:HIS:CD2	2.53	0.44
3:C:202:PHE:HA	3:C:210:PHE:O	2.18	0.44
3:C:422:PRO:HA	3:C:423:PRO:HD2	1.81	0.44
2:K:27:ILE:HG13	2:K:53:VAL:HG21	1.97	0.44
3:L:208:HIS:HB3	8:Q:85:ARG:NH2	2.32	0.44
4:M:195:GLU:C	4:M:198:PRO:HD2	2.42	0.44
2:T:59:GLU:O	2:T:63:VAL:HG23	2.16	0.44
3:U:33:PHE:HB2	3:U:45:CYS:SG	2.57	0.44
3:U:478:LEU:HD12	3:U:520:ARG:NH1	2.32	0.44
3:U:559:ASP:HB2	3:U:573:PRO:HG3	1.99	0.44
4:V:159:LEU:O	4:V:163:VAL:HG12	2.17	0.44
4:V:249:ARG:HB2	4:V:262:PHE:HE2	1.82	0.44
4:V:343:TYR:CD1	4:V:343:TYR:C	2.94	0.44
1:1:267:PRO:O	1:1:268:MET:C	2.60	0.44
1:1:315:HIS:O	1:1:319:LYS:HB2	2.18	0.44
1:1:363:VAL:CG2	1:1:364:ALA:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:30:VAL:CG2	3:3:31:PRO:HD2	2.47	0.44
3:3:30:VAL:CG2	3:3:48:CYS:HA	2.45	0.44
3:3:356:LEU:HD13	3:3:654:PHE:HD1	1.83	0.44
4:4:82:THR:N	4:4:83:PRO:HD2	2.32	0.44
4:4:350:ARG:HG3	4:4:350:ARG:HH11	1.82	0.44
1:A:6:LEU:HD21	1:A:12:ARG:CG	2.47	0.44
2:B:153:LEU:C	2:B:153:LEU:HD13	2.43	0.44
4:D:236:GLY:O	4:D:238:SER:N	2.51	0.44
4:D:350:ARG:HG3	4:D:350:ARG:NH1	2.33	0.44
4:D:380:SER:O	4:D:384:ALA:HB2	2.18	0.44
7:G:123:ASP:CB	7:G:129:LEU:HD21	2.48	0.44
2:K:78:TYR:CE1	2:K:157:LEU:HD22	2.53	0.44
3:L:55:PRO:HG3	3:L:73:ILE:C	2.40	0.44
3:L:469:ARG:HB2	3:L:470:PRO:CD	2.46	0.44
6:O:40:THR:HB	6:O:50:MET:SD	2.58	0.44
7:P:40:ARG:CB	7:P:121:MET:HE1	2.34	0.44
3:U:225:ASN:O	3:U:229:ILE:HG13	2.17	0.44
4:V:379:GLN:CD	5:W:113:PHE:HB2	2.43	0.44
5:W:104:VAL:HG12	5:W:108:TRP:CE3	2.49	0.44
6:X:16:ARG:NH1	6:X:17:GLU:OE2	2.51	0.44
6:X:157:LYS:O	6:X:157:LYS:HG2	2.17	0.44
8:Z:84:LEU:HB2	8:Z:93:LEU:HB2	2.00	0.44
1:1:28:THR:HB	1:1:31:TYR:H	1.83	0.44
3:3:125:GLY:HA3	3:3:246:ASN:ND2	2.31	0.44
3:3:224:GLY:HA3	3:3:295:ARG:HD2	1.99	0.44
3:3:582:PHE:HA	3:3:599:HIS:ND1	2.32	0.44
3:3:591:HIS:ND1	3:3:592:PRO:CD	2.81	0.44
4:4:306:ASN:HA	4:4:307:PRO:HD3	1.78	0.44
4:4:390:VAL:N	4:4:391:PRO:CD	2.80	0.44
7:9:40:ARG:CB	7:9:121:MET:HE1	2.35	0.44
4:D:211:SER:OG	4:D:215:TYR:HB2	2.18	0.44
4:D:226:PRO:HG3	4:D:242:SER:O	2.17	0.44
4:D:240:ARG:NH2	4:D:347:GLU:OE2	2.46	0.44
4:D:250:LYS:CE	4:D:262:PHE:HB3	2.44	0.44
4:D:379:GLN:HG2	5:E:113:PHE:CD1	2.52	0.44
5:E:107:LEU:HA	5:E:107:LEU:HD23	1.72	0.44
2:K:59:GLU:O	2:K:63:VAL:HG23	2.17	0.44
3:L:738:THR:HG22	3:L:739:PRO:CD	2.38	0.44
4:M:108:VAL:HG23	4:M:108:VAL:O	2.17	0.44
6:O:105:VAL:HG11	6:O:131:VAL:HG21	2.00	0.44
7:P:100:PHE:HA	9:P:183:SF4:S4	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:20:MET:HE3	8:Q:59:LEU:HG	1.98	0.44
1:S:81:LYS:HA	1:S:81:LYS:CE	2.47	0.44
4:V:198:PRO:HG3	4:V:291:LYS:HZ3	1.81	0.44
4:V:285:GLU:O	4:V:289:ILE:HG12	2.17	0.44
1:1:272:PHE:O	1:1:276:ILE:HG13	2.17	0.44
3:3:422:PRO:HA	3:3:423:PRO:HD2	1.79	0.44
3:3:469:ARG:HB2	3:3:470:PRO:CD	2.47	0.44
4:4:230:ILE:HD11	4:4:244:VAL:CG2	2.48	0.44
4:4:235:THR:O	4:4:235:THR:HG22	2.17	0.44
1:A:53:VAL:HG23	1:A:231:MET:CE	2.46	0.44
1:A:408:TRP:N	1:A:409:PRO:HD2	2.32	0.44
3:C:185:LYS:HB3	3:C:189:ARG:HH11	1.83	0.44
3:C:575:GLU:OE1	3:C:575:GLU:HA	2.17	0.44
5:E:16:PRO:HB2	5:E:28:VAL:CG1	2.48	0.44
6:F:33:SER:HA	6:F:158:VAL:HG21	1.98	0.44
6:F:117:MET:HE3	6:F:118:PHE:CZ	2.52	0.44
8:H:73:SER:HA	8:H:74:PRO:HD2	1.81	0.44
1:J:145:LEU:HA	1:J:145:LEU:HD23	1.75	0.44
1:J:201:LEU:HG	1:J:203:PRO:HD2	1.98	0.44
3:L:30:VAL:CG2	3:L:31:PRO:HD2	2.48	0.44
3:L:243:ARG:HB3	3:L:275:LEU:HD12	1.99	0.44
3:L:690:GLY:HA3	3:L:770:ARG:HH21	1.82	0.44
4:M:138:LEU:HD11	4:M:146:PHE:CD2	2.52	0.44
7:P:53:CYS:HB2	7:P:112:ALA:HB1	1.99	0.44
2:T:89:LYS:HE3	2:T:94:GLU:OE1	2.16	0.44
3:U:30:VAL:CG2	3:U:48:CYS:HA	2.46	0.44
3:U:115:HIS:C	4:V:321:MET:HE3	2.43	0.44
3:U:417:VAL:O	3:U:417:VAL:HG12	2.18	0.44
4:V:222:GLY:HA2	4:V:384:ALA:O	2.18	0.44
4:V:304:ASP:HA	4:V:305:PRO:HD2	1.85	0.44
6:X:34:ASN:C	6:X:36:LEU:H	2.25	0.44
1:1:161:ASN:OD1	1:1:166:ASP:HA	2.17	0.44
2:2:24:ARG:O	2:2:27:ILE:HD12	2.17	0.44
3:3:194:VAL:HB	3:3:195:PRO:CD	2.48	0.44
3:3:690:GLY:HA3	3:3:770:ARG:HH21	1.82	0.44
4:4:63:HIS:O	6:6:122:ALA:HB1	2.18	0.44
3:C:230:CYS:HA	3:C:231:PRO:HD2	1.72	0.44
3:C:368:HIS:CG	3:C:556:ALA:HB3	2.53	0.44
4:D:116:ILE:O	4:D:120:LEU:HB2	2.18	0.44
5:E:25:LEU:CD2	5:E:25:LEU:H	2.31	0.44
7:G:53:CYS:HB2	7:G:112:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:38:TYR:HA	1:J:116:GLU:OE1	2.18	0.44
4:M:106:GLY:O	5:N:194:SER:HB3	2.18	0.44
5:N:157:THR:C	5:N:158:LEU:HD23	2.42	0.44
6:O:34:ASN:C	6:O:36:LEU:H	2.26	0.44
6:O:146:ALA:HB2	7:P:119:PHE:HD1	1.82	0.44
3:U:333:LEU:HD13	3:U:648:LEU:HD21	1.99	0.44
4:V:76:LEU:HD12	4:V:76:LEU:O	2.18	0.44
4:V:235:THR:HG22	4:V:235:THR:O	2.18	0.44
5:W:48:PHE:CE2	5:W:50:ALA:HB2	2.53	0.44
5:W:48:PHE:CD2	5:W:77:LEU:HD21	2.52	0.44
6:X:146:ALA:HB2	7:Y:119:PHE:CD1	2.52	0.44
1:1:162:LEU:HB3	1:1:163:PHE:HD1	1.83	0.44
1:1:211:LEU:HB2	1:1:216:THR:HG21	1.99	0.44
1:1:264:TYR:CE2	1:1:279:TRP:HB3	2.52	0.44
3:3:243:ARG:HB3	3:3:275:LEU:HD12	1.99	0.44
3:3:555:GLY:O	3:3:556:ALA:C	2.61	0.44
3:3:694:LEU:C	3:3:762:ALA:HB2	2.43	0.44
7:9:100:PHE:HA	9:9:183:SF4:S4	2.58	0.44
1:A:195:LEU:HA	2:B:24:ARG:HH21	1.83	0.44
1:A:291:ILE:HD11	1:A:331:ILE:HD11	1.99	0.44
3:C:164:VAL:HB	3:C:165:ASP:H	1.56	0.44
4:D:82:THR:N	4:D:83:PRO:HD2	2.32	0.44
4:D:116:ILE:HD11	4:D:182:LEU:CD2	2.47	0.44
4:D:223:VAL:O	4:D:383:TYR:HE1	2.00	0.44
4:D:278:VAL:O	4:D:282:GLU:HG3	2.18	0.44
6:F:157:LYS:O	6:F:157:LYS:HG2	2.16	0.44
7:G:115:LEU:HD23	7:G:115:LEU:HA	1.66	0.44
3:L:49:LEU:HA	3:L:80:ALA:O	2.18	0.44
3:L:372:GLN:O	3:L:558:TRP:CD2	2.71	0.44
5:N:104:VAL:CG1	5:N:108:TRP:CE3	3.01	0.44
8:Q:38:PRO:C	8:Q:40:PHE:H	2.26	0.44
2:T:144:CYS:O	2:T:149:ARG:HD3	2.18	0.44
3:U:560:GLU:HA	3:U:561:PRO:HD2	1.93	0.44
4:V:82:THR:N	4:V:83:PRO:HD2	2.33	0.44
5:W:121:LEU:HB3	5:W:146:LEU:CB	2.26	0.44
6:X:140:CYS:HA	6:X:141:PRO:HA	1.69	0.44
1:1:107:LEU:HD23	1:1:114:LEU:HD12	1.99	0.43
1:1:323:LEU:HD23	1:1:323:LEU:C	2.43	0.43
3:3:229:ILE:HD11	3:3:289:TRP:CH2	2.53	0.43
3:3:614:LEU:O	3:3:621:VAL:HA	2.18	0.43
3:3:734:VAL:HG13	3:3:775:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:168:PHE:CE1	6:6:141:PRO:HG3	2.53	0.43
7:9:123:ASP:CG	7:9:148:ARG:HH22	2.24	0.43
1:A:107:LEU:HD23	1:A:114:LEU:HD12	2.00	0.43
1:A:323:LEU:HD23	1:A:323:LEU:C	2.42	0.43
1:A:356:CYS:HB3	1:A:358:PRO:CG	2.48	0.43
1:A:356:CYS:HB3	1:A:358:PRO:HD2	2.00	0.43
3:C:6:VAL:HG21	3:C:26:ALA:CB	2.47	0.43
3:C:245:ARG:NH1	7:G:56:CYS:O	2.50	0.43
7:G:44:THR:OG1	7:G:52:LYS:HD2	2.17	0.43
8:H:72:VAL:HG22	8:H:73:SER:N	2.33	0.43
1:J:272:PHE:CD1	1:J:311:MET:HG2	2.53	0.43
1:J:341:MET:HE2	1:J:409:PRO:C	2.43	0.43
3:L:403:THR:O	3:L:403:THR:HG22	2.18	0.43
3:L:612:GLY:O	3:L:624:LEU:HB2	2.17	0.43
4:M:316:LEU:C	4:M:316:LEU:HD12	2.42	0.43
4:M:321:MET:HE2	4:M:321:MET:HB2	1.70	0.43
5:N:167:PRO:HB3	7:P:66:TYR:CD2	2.53	0.43
6:O:117:MET:HB3	7:P:99:ILE:CD1	2.47	0.43
3:U:168:HIS:HA	3:U:169:PRO:HD2	1.71	0.43
3:U:290:ILE:HG22	3:U:291:CYS:O	2.17	0.43
3:U:641:LEU:HD23	3:U:641:LEU:HA	1.77	0.43
4:V:108:VAL:O	4:V:108:VAL:HG23	2.18	0.43
4:V:129:HIS:HE1	4:V:349:ALA:HB1	1.76	0.43
4:V:354:GLY:H	4:V:371:ARG:HB3	1.83	0.43
5:W:161:GLU:HG2	5:W:163:ARG:NH2	2.33	0.43
6:X:137:VAL:HA	6:X:138:PRO:HD2	1.79	0.43
7:Y:39:GLY:O	7:Y:40:ARG:C	2.61	0.43
1:1:81:LYS:HA	1:1:81:LYS:CE	2.46	0.43
1:1:267:PRO:O	1:1:270:THR:HG23	2.18	0.43
2:2:131:ALA:HB1	2:2:132:PRO:HA	2.00	0.43
3:3:2:VAL:CG1	3:3:89:ASP:HA	2.48	0.43
3:3:241:ARG:HH11	7:9:74:GLU:CD	2.26	0.43
3:3:269:THR:HG23	3:3:274:LEU:HD13	1.99	0.43
3:3:333:LEU:HD13	3:3:648:LEU:HD21	1.99	0.43
3:3:497:TRP:NE1	3:3:524:LEU:CD1	2.80	0.43
3:3:724:ARG:O	3:3:724:ARG:HG2	2.18	0.43
4:4:63:HIS:HA	4:4:409:ARG:OXT	2.18	0.43
4:4:122:GLU:OE2	4:4:249:ARG:NH1	2.50	0.43
4:4:369:LYS:HD3	4:4:370:VAL:N	2.33	0.43
5:5:41:TYR:HA	5:5:44:MET:HE3	2.01	0.43
6:6:141:PRO:HB3	9:6:182:SF4:S1	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HD23	1:A:123:TYR:CG	2.53	0.43
3:C:119:CYS:O	3:C:120:PRO:C	2.58	0.43
3:C:290:ILE:HG22	3:C:291:CYS:O	2.18	0.43
4:D:143:LEU:HD23	4:D:143:LEU:O	2.18	0.43
4:D:393:MET:HA	4:D:396:ILE:CG2	2.47	0.43
1:J:102:LYS:HG3	1:J:103:ASP:N	2.33	0.43
1:J:149:ILE:O	1:J:153:ARG:HB2	2.18	0.43
1:J:254:ILE:HB	1:J:275:LEU:HD21	2.00	0.43
3:L:343:LEU:HD12	3:L:361:ALA:HB2	1.99	0.43
3:L:722:THR:HG23	3:L:755:LYS:HD2	2.00	0.43
4:M:159:LEU:O	4:M:163:VAL:HG12	2.18	0.43
6:O:140:CYS:HA	6:O:141:PRO:HA	1.70	0.43
1:S:102:LYS:HG3	1:S:103:ASP:N	2.33	0.43
1:S:243:THR:HG22	1:S:244:GLU:N	2.27	0.43
3:U:505:LEU:HB3	3:U:532:VAL:HG22	2.00	0.43
3:U:737:GLU:HB2	3:U:776:LEU:HD21	2.00	0.43
5:W:38:MET:O	5:W:41:TYR:HB2	2.18	0.43
1:1:45:LEU:HD23	1:1:123:TYR:CG	2.53	0.43
1:1:65:ARG:NH2	1:1:268:MET:CE	2.80	0.43
1:1:366:PHE:O	1:1:370:LEU:HD23	2.17	0.43
3:3:161:ARG:HG2	3:3:161:ARG:NH1	2.32	0.43
3:3:225:ASN:O	3:3:229:ILE:HG13	2.18	0.43
3:3:372:GLN:O	3:3:558:TRP:CD2	2.72	0.43
3:3:532:VAL:HG12	3:3:533:LEU:N	2.34	0.43
4:4:84:ARG:HD3	6:6:117:MET:HE1	2.00	0.43
4:4:130:LEU:HD23	4:4:283:MET:HE1	2.00	0.43
6:6:149:TYR:CZ	6:6:153:GLN:NE2	2.86	0.43
6:6:158:VAL:HA	6:6:172:PRO:HB3	2.01	0.43
8:7:17:LEU:HD13	8:7:54:ILE:HD13	1.99	0.43
1:A:416:HIS:HB2	1:A:417:PHE:CE1	2.52	0.43
3:C:596:ARG:C	3:C:597:TYR:HD1	2.27	0.43
3:C:739:PRO:HD2	3:C:771:VAL:HG11	2.00	0.43
4:D:275:ARG:HD2	4:D:399:SER:O	2.18	0.43
1:J:290:ILE:HG22	1:J:330:LEU:HD22	2.00	0.43
1:J:356:CYS:HB3	1:J:358:PRO:CG	2.47	0.43
1:J:366:PHE:O	1:J:370:LEU:HD23	2.18	0.43
4:M:346:THR:HG22	4:M:353:LEU:O	2.18	0.43
5:N:103:THR:HB	5:N:115:GLU:OE1	2.18	0.43
5:N:161:GLU:HG2	5:N:163:ARG:NH2	2.32	0.43
6:O:48:ILE:HG22	6:O:48:ILE:O	2.17	0.43
6:O:163:TYR:CD1	7:P:152:ARG:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:177:THR:O	7:P:179:GLY:N	2.51	0.43
1:S:366:PHE:O	1:S:370:LEU:HD23	2.18	0.43
1:S:427:GLU:HB2	1:S:429:ARG:HD3	2.00	0.43
3:U:23:VAL:HG13	3:U:28:TYR:HB2	2.00	0.43
3:U:356:LEU:HD13	3:U:654:PHE:HD1	1.83	0.43
4:V:109:VAL:HG12	4:V:113:ALA:HB3	2.00	0.43
4:V:234:LEU:O	4:V:239:LEU:CG	2.64	0.43
4:V:291:LYS:O	4:V:295:GLU:HG3	2.18	0.43
5:W:77:LEU:HA	5:W:78:PRO:HD3	1.60	0.43
5:W:129:HIS:CD2	5:W:130:PRO:HD2	2.53	0.43
6:X:117:MET:HB3	7:Y:99:ILE:CD1	2.48	0.43
6:X:158:VAL:HA	6:X:172:PRO:HB3	2.00	0.43
7:Y:125:GLU:O	7:Y:126:TYR:C	2.61	0.43
8:Z:108:ILE:HA	8:Z:109:PRO:HD3	1.90	0.43
1:1:145:LEU:HD23	1:1:145:LEU:HA	1.69	0.43
3:3:49:LEU:HA	3:3:80:ALA:O	2.19	0.43
3:3:185:LYS:HG2	3:3:188:VAL:CG2	2.47	0.43
5:5:111:ALA:HB1	5:5:115:GLU:HG3	2.01	0.43
7:9:123:ASP:HB2	7:9:129:LEU:HD21	1.99	0.43
2:B:116:LEU:HG	2:B:117:PHE:CD2	2.53	0.43
3:C:478:LEU:HD12	3:C:520:ARG:CZ	2.48	0.43
3:C:555:GLY:O	3:C:556:ALA:C	2.61	0.43
4:D:108:VAL:HG23	4:D:108:VAL:O	2.18	0.43
6:F:34:ASN:C	6:F:36:LEU:H	2.26	0.43
6:F:40:THR:HB	6:F:50:MET:SD	2.58	0.43
6:F:43:LEU:HA	6:F:43:LEU:HD23	1.75	0.43
8:H:16:LEU:HD21	8:H:115:PHE:CE1	2.54	0.43
3:L:203:ILE:HG22	3:L:204:GLU:HG3	2.00	0.43
3:L:582:PHE:HA	3:L:599:HIS:ND1	2.34	0.43
5:N:42:LYS:HB3	5:N:107:LEU:CD1	2.33	0.43
6:O:141:PRO:HB3	9:O:182:SF4:S1	2.59	0.43
3:U:286:ASN:ND2	3:U:286:ASN:C	2.76	0.43
3:U:688:ARG:HD3	3:U:688:ARG:HA	1.51	0.43
4:V:242:SER:HB2	4:V:270:GLY:HA3	2.00	0.43
4:V:374:SER:HB2	4:V:406:ASP:HB3	2.00	0.43
5:W:195:LEU:HD22	5:W:195:LEU:N	2.33	0.43
1:1:38:TYR:HA	1:1:116:GLU:OE1	2.19	0.43
2:2:87:SER:OG	2:2:128:CYS:HB3	2.18	0.43
2:2:116:LEU:HG	2:2:117:PHE:CD2	2.53	0.43
3:3:197:ASP:HB2	3:3:220:SER:HB3	2.00	0.43
3:3:286:ASN:ND2	3:3:286:ASN:C	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:455:ARG:O	3:3:455:ARG:HG3	2.19	0.43
4:4:44:MET:HA	4:4:44:MET:HE3	2.01	0.43
4:4:76:LEU:HD12	4:4:76:LEU:C	2.43	0.43
4:4:167:ARG:HD3	6:6:143:ARG:NH1	2.32	0.43
4:4:350:ARG:NE	4:4:403:VAL:CG2	2.77	0.43
5:5:194:SER:O	5:5:195:LEU:HD13	2.18	0.43
7:9:177:THR:O	7:9:179:GLY:N	2.50	0.43
1:A:118:MET:O	1:A:122:GLY:N	2.44	0.43
3:C:366:THR:OG1	3:C:367:PRO:HD2	2.17	0.43
3:C:497:TRP:NE1	3:C:524:LEU:CD1	2.79	0.43
4:D:159:LEU:O	4:D:163:VAL:HG12	2.18	0.43
4:D:235:THR:O	4:D:235:THR:HG22	2.18	0.43
4:D:319:THR:HG22	4:D:320:SER:N	2.32	0.43
5:E:38:MET:O	5:E:41:TYR:HB2	2.18	0.43
8:H:121:ARG:NH1	8:H:121:ARG:CG	2.76	0.43
1:J:272:PHE:O	1:J:276:ILE:HG13	2.17	0.43
1:J:297:THR:HG22	1:J:322:MET:HG3	2.01	0.43
4:M:173:ILE:O	4:M:173:ILE:HG23	2.18	0.43
5:N:104:VAL:HG12	5:N:108:TRP:CE3	2.48	0.43
5:N:111:ALA:HB1	5:N:115:GLU:HG3	2.01	0.43
3:U:197:ASP:OD2	3:U:220:SER:CB	2.67	0.43
3:3:180:ARG:O	3:3:181:CYS:C	2.61	0.43
3:3:367:PRO:CB	3:3:554:LYS:HB2	2.49	0.43
3:3:397:LEU:HD21	3:3:480:LEU:HD13	2.00	0.43
3:3:408:ILE:HD12	3:3:408:ILE:HA	1.78	0.43
3:3:469:ARG:O	3:3:472:GLU:HB3	2.19	0.43
4:4:122:GLU:HB2	4:4:290:ILE:CD1	2.49	0.43
4:4:276:MET:O	4:4:280:ILE:HG13	2.18	0.43
4:4:343:TYR:C	4:4:343:TYR:CD1	2.97	0.43
6:6:117:MET:HB3	7:9:99:ILE:CD1	2.48	0.43
7:9:105:GLU:HG3	7:9:114:VAL:HA	1.99	0.43
3:C:398:VAL:CB	3:C:450:LEU:HD22	2.48	0.43
3:C:591:HIS:ND1	3:C:592:PRO:CD	2.80	0.43
5:E:152:LEU:O	5:E:152:LEU:HG	2.19	0.43
6:F:108:MET:CE	6:F:147:LEU:HG	2.40	0.43
6:F:137:VAL:HA	6:F:138:PRO:HD2	1.79	0.43
1:J:211:LEU:HG	1:J:212:TRP:CE3	2.53	0.43
1:J:267:PRO:O	1:J:270:THR:HG23	2.19	0.43
1:J:343:ASN:O	1:J:346:ARG:HG2	2.18	0.43
3:L:469:ARG:O	3:L:472:GLU:HB3	2.18	0.43
3:L:695:ARG:NH1	3:L:717:TRP:CZ2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:168:PHE:HA	4:M:170:HIS:CD2	2.53	0.43
4:M:390:VAL:N	4:M:391:PRO:CD	2.81	0.43
5:N:129:HIS:CD2	5:N:130:PRO:HD2	2.53	0.43
6:O:36:LEU:O	6:O:38:PRO:HD3	2.18	0.43
8:Q:16:LEU:HD21	8:Q:115:PHE:CE1	2.53	0.43
1:S:65:ARG:NH2	1:S:268:MET:CE	2.79	0.43
1:S:161:ASN:OD1	1:S:166:ASP:HA	2.17	0.43
2:T:116:LEU:HG	2:T:117:PHE:CD2	2.53	0.43
3:U:184:CYS:SG	3:U:186:ARG:HB2	2.58	0.43
3:U:203:ILE:HD13	3:U:203:ILE:N	2.34	0.43
3:U:398:VAL:CB	3:U:450:LEU:HD22	2.45	0.43
3:U:509:ALA:O	3:U:510:GLY:C	2.62	0.43
4:V:109:VAL:HG12	4:V:113:ALA:CB	2.49	0.43
6:X:46:CYS:HB3	6:X:81:ALA:HB1	2.00	0.43
1:1:139:ARG:CG	2:2:140:PRO:HD3	2.45	0.43
1:1:184:GLU:OE1	1:1:186:THR:N	2.52	0.43
6:6:33:SER:HA	6:6:158:VAL:HG21	2.01	0.43
1:A:58:LYS:HA	1:A:73:GLY:HA3	2.01	0.43
1:A:102:LYS:HG3	1:A:103:ASP:N	2.33	0.43
1:A:434:PRO:HG2	1:A:436:LEU:CD1	2.49	0.43
2:B:112:THR:OG1	2:B:113:PRO:HD2	2.19	0.43
3:C:317:LEU:N	3:C:317:LEU:CD2	2.82	0.43
3:C:505:LEU:HD21	3:C:507:LEU:HD23	2.00	0.43
4:D:224:ILE:HA	4:D:225:PRO:HD2	1.79	0.43
4:D:276:MET:O	4:D:280:ILE:HG13	2.19	0.43
6:F:117:MET:HE2	7:G:99:ILE:HG12	1.99	0.43
1:J:276:ILE:HG23	1:J:330:LEU:HD11	2.01	0.43
1:J:363:VAL:CG2	1:J:364:ALA:N	2.81	0.43
4:M:197:LEU:HA	4:M:200:ARG:HB3	2.00	0.43
4:M:211:SER:CB	4:M:214:PHE:HB3	2.47	0.43
4:M:311:PRO:HD3	4:M:330:HIS:CE1	2.53	0.43
6:O:108:MET:CE	6:O:147:LEU:HG	2.40	0.43
6:O:123:ILE:HG22	6:O:124:VAL:N	2.34	0.43
1:S:107:LEU:CD2	1:S:114:LEU:HD12	2.48	0.43
1:S:133:TYR:HB2	1:S:188:LEU:HD21	2.01	0.43
1:S:249:MET:H	1:S:249:MET:HE2	1.83	0.43
1:S:343:ASN:O	1:S:346:ARG:HG2	2.19	0.43
3:U:230:CYS:HA	3:U:231:PRO:HD2	1.69	0.43
3:U:368:HIS:CG	3:U:556:ALA:HB3	2.53	0.43
4:V:254:TYR:C	4:V:256:GLY:H	2.23	0.43
4:V:306:ASN:HA	4:V:307:PRO:HD3	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:49:LEU:HD13	5:W:74:LEU:HD23	2.00	0.43
5:W:116:ARG:HG3	5:W:129:HIS:HE1	1.83	0.43
7:Y:110:THR:HG22	8:Z:41:ILE:O	2.19	0.43
3:3:160:THR:CG2	8:7:73:SER:HB3	2.48	0.43
5:5:75:VAL:HG12	5:5:76:SER:N	2.34	0.43
7:9:113:ILE:HG23	7:9:113:ILE:O	2.18	0.43
3:C:469:ARG:O	3:C:472:GLU:HB3	2.19	0.43
3:C:509:ALA:O	3:C:510:GLY:C	2.61	0.43
5:E:48:PHE:CD2	5:E:77:LEU:HD21	2.54	0.43
1:J:184:GLU:OE1	1:J:186:THR:N	2.52	0.43
2:K:31:LEU:HD13	2:K:31:LEU:HA	1.90	0.43
3:L:474:ARG:CZ	3:L:516:VAL:HG21	2.42	0.43
3:L:583:VAL:HG23	3:L:583:VAL:O	2.19	0.43
5:N:41:TYR:HA	5:N:44:MET:HE3	2.01	0.43
8:Q:16:LEU:HD13	8:Q:16:LEU:C	2.44	0.43
1:S:93:ALA:O	1:S:134:VAL:HA	2.19	0.43
1:S:95:GLU:HA	10:S:440:FMN:HN3	1.84	0.43
1:S:323:LEU:C	1:S:323:LEU:HD23	2.43	0.43
3:U:385:ALA:HB3	3:U:533:LEU:HD23	2.01	0.43
3:U:398:VAL:CG2	3:U:448:MET:HE2	2.48	0.43
3:U:403:THR:OG1	3:U:458:LEU:HD11	2.19	0.43
3:U:469:ARG:O	3:U:472:GLU:HB3	2.19	0.43
3:U:575:GLU:HA	3:U:575:GLU:OE1	2.18	0.43
4:V:366:TYR:CE1	5:W:148:LYS:HE3	2.54	0.43
5:W:3:LEU:HB2	5:W:86:SER:HB2	2.00	0.43
5:W:54:GLY:C	5:W:55:LEU:HD12	2.44	0.43
6:X:30:TRP:CD1	6:X:30:TRP:C	2.97	0.43
6:X:121:TYR:H	6:X:121:TYR:HD1	1.67	0.43
8:Z:88:ARG:HE	8:Z:126:LEU:CD2	2.32	0.43
1:1:317:GLN:C	1:1:319:LYS:H	2.27	0.43
3:3:474:ARG:H	3:3:474:ARG:HG2	1.65	0.43
3:3:505:LEU:HD21	3:3:507:LEU:HD23	2.01	0.43
4:4:338:PRO:HG3	5:5:193:ARG:HB2	2.00	0.43
1:A:38:TYR:HA	1:A:116:GLU:OE1	2.18	0.43
1:A:161:ASN:OD1	1:A:166:ASP:HA	2.19	0.43
1:A:162:LEU:HB3	1:A:163:PHE:HD1	1.84	0.43
1:A:203:PRO:HB2	1:A:204:PRO:HD3	2.00	0.43
3:C:614:LEU:O	3:C:621:VAL:HA	2.18	0.43
4:D:74:THR:HG22	4:D:75:TYR:N	2.34	0.43
4:D:109:VAL:HG12	4:D:113:ALA:CB	2.48	0.43
4:D:112:ARG:HH21	4:D:297:LEU:CD1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:30:TRP:O	6:F:33:SER:HB3	2.18	0.43
3:L:546:ALA:O	3:L:547:MET:HE2	2.18	0.43
3:L:575:GLU:OE1	3:L:575:GLU:HA	2.18	0.43
3:L:652:PRO:HA	3:L:653:PRO:HD3	1.87	0.43
4:M:167:ARG:HD3	6:O:143:ARG:HH12	1.84	0.43
4:M:306:ASN:HA	4:M:307:PRO:HD3	1.80	0.43
5:N:160:ARG:HD2	7:P:92:GLU:OE2	2.19	0.43
1:S:154:ALA:O	1:S:156:GLY:N	2.52	0.43
1:S:211:LEU:H	1:S:216:THR:HG21	1.83	0.43
1:S:276:ILE:HG23	1:S:330:LEU:HD11	2.00	0.43
2:T:11:LEU:HD22	2:T:30:LEU:HD21	2.00	0.43
3:U:343:LEU:O	3:U:369:LEU:HA	2.19	0.43
3:U:695:ARG:NH1	3:U:717:TRP:CZ2	2.87	0.43
4:V:40:VAL:HG23	6:X:88:MET:CE	2.49	0.43
4:V:329:LYS:HD2	4:V:329:LYS:HA	1.94	0.43
5:W:107:LEU:HA	5:W:107:LEU:HD23	1.74	0.43
5:W:174:LEU:CD2	5:W:180:GLY:HA2	2.48	0.43
5:W:187:GLY:C	5:W:189:ARG:H	2.27	0.43
6:X:171:PRO:HA	6:X:172:PRO:HD3	1.89	0.43
1:1:219:ASN:ND2	1:1:223:THR:HG21	2.31	0.43
1:1:253:GLN:HG2	1:1:327:GLY:CA	2.46	0.43
3:3:290:ILE:HD13	3:3:290:ILE:HA	1.78	0.43
3:3:591:HIS:CE1	3:3:593:LEU:HB2	2.54	0.43
3:3:652:PRO:HA	3:3:653:PRO:HD3	1.86	0.43
4:4:197:LEU:N	4:4:198:PRO:HD2	2.34	0.43
4:4:358:VAL:O	4:4:366:TYR:HB3	2.18	0.43
1:A:45:LEU:HB3	1:A:165:THR:HG21	2.01	0.43
3:C:258:LEU:HD12	3:C:294:GLY:HA2	2.01	0.43
3:C:417:VAL:O	3:C:417:VAL:HG12	2.18	0.43
3:C:564:LEU:HD12	3:C:564:LEU:HA	1.82	0.43
3:C:591:HIS:ND1	3:C:592:PRO:N	2.66	0.43
4:D:63:HIS:O	6:F:122:ALA:HB1	2.18	0.43
4:D:98:ALA:O	4:D:102:GLU:HG3	2.18	0.43
4:D:197:LEU:O	4:D:198:PRO:C	2.60	0.43
5:E:126:PHE:H	5:E:132:LEU:HD11	1.84	0.43
6:F:123:ILE:HG22	6:F:124:VAL:N	2.34	0.43
7:G:40:ARG:CB	7:G:121:MET:HE1	2.38	0.43
1:J:6:LEU:HD21	1:J:12:ARG:CG	2.47	0.43
1:J:70:PHE:HA	1:J:71:PRO:HD3	1.92	0.43
3:L:397:LEU:HD21	3:L:480:LEU:HD13	2.00	0.43
3:L:420:LEU:HD22	3:L:436:GLN:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:591:HIS:ND1	3:L:592:PRO:N	2.67	0.43
5:N:103:THR:HG23	5:N:127:GLU:O	2.19	0.43
6:O:161:GLN:HG2	6:O:161:GLN:O	2.19	0.43
1:S:98:PRO:HB3	2:T:85:THR:HG21	1.99	0.43
3:U:239:THR:HG21	3:U:298:HIS:NE2	2.34	0.43
5:W:160:ARG:HH21	7:Y:144:LYS:NZ	2.16	0.43
1:1:29:LEU:HD22	1:1:33:LEU:CD1	2.48	0.42
3:3:118:ASP:O	3:3:121:THR:N	2.51	0.42
3:3:298:HIS:ND1	3:3:298:HIS:C	2.77	0.42
3:3:317:LEU:N	3:3:317:LEU:CD2	2.80	0.42
3:3:575:GLU:OE1	3:3:575:GLU:HA	2.18	0.42
4:4:114:GLU:O	4:4:118:VAL:HG13	2.19	0.42
4:4:203:GLU:O	4:4:207:LEU:HG	2.19	0.42
5:5:187:GLY:C	5:5:189:ARG:H	2.27	0.42
8:7:88:ARG:HE	8:7:126:LEU:HD22	1.83	0.42
1:A:295:SER:C	1:A:297:THR:H	2.26	0.42
3:C:117:LEU:HD23	4:D:321:MET:HA	2.01	0.42
3:C:582:PHE:HA	3:C:599:HIS:ND1	2.33	0.42
6:F:117:MET:CE	7:G:99:ILE:HG12	2.49	0.42
1:J:95:GLU:HA	10:J:440:FMN:HN3	1.83	0.42
1:J:180:TYR:CE2	10:J:440:FMN:H6	2.54	0.42
2:K:40:TRP:CH2	2:K:42:ARG:HG2	2.54	0.42
3:L:329:LEU:CD1	3:L:584:VAL:HG11	2.49	0.42
3:L:351:LEU:HD12	3:L:351:LEU:HA	1.77	0.42
3:L:700:LYS:HA	3:L:763:LEU:O	2.18	0.42
4:M:109:VAL:HG12	4:M:113:ALA:HB3	2.01	0.42
4:M:115:THR:HG21	4:M:297:LEU:HD23	2.01	0.42
1:S:291:ILE:HA	1:S:292:PRO:HD2	1.86	0.42
3:U:317:LEU:N	3:U:317:LEU:CD2	2.81	0.42
3:U:372:GLN:O	3:U:558:TRP:CD2	2.72	0.42
4:V:312:PRO:HA	4:V:313:PRO:HD2	1.90	0.42
4:V:404:MET:O	4:V:408:ASP:HB2	2.19	0.42
5:W:52:ILE:HG23	5:W:114:LEU:CB	2.42	0.42
6:X:30:TRP:O	6:X:33:SER:HB3	2.19	0.42
2:2:142:VAL:HG11	2:2:153:LEU:HG	2.00	0.42
3:3:19:VAL:O	3:3:22:ALA:HB3	2.18	0.42
3:3:208:HIS:HB3	8:7:85:ARG:NH2	2.34	0.42
3:3:669:VAL:HA	3:3:670:PRO:HD2	1.83	0.42
6:6:105:VAL:HG11	6:6:131:VAL:HG21	2.02	0.42
6:6:140:CYS:HA	6:6:141:PRO:HA	1.71	0.42
1:A:192:LEU:HD23	1:A:192:LEU:C	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:HB	1:A:275:LEU:HD21	2.01	0.42
3:C:298:HIS:ND1	3:C:298:HIS:C	2.77	0.42
3:C:378:PRO:O	3:C:381:LEU:HB2	2.19	0.42
4:D:222:GLY:HA2	4:D:384:ALA:O	2.18	0.42
4:D:381:LEU:H	4:D:382:PRO:CD	2.32	0.42
5:E:160:ARG:HG3	7:G:130:VAL:HG11	2.01	0.42
5:E:175:THR:O	5:E:175:THR:OG1	2.28	0.42
3:L:347:HIS:N	3:L:372:GLN:HB3	2.35	0.42
5:N:35:LYS:HD3	5:N:102:PRO:CB	2.49	0.42
5:N:75:VAL:HG12	5:N:76:SER:N	2.34	0.42
6:O:43:LEU:HD23	6:O:43:LEU:HA	1.80	0.42
6:O:130:VAL:HG23	6:O:131:VAL:HG13	2.01	0.42
7:P:45:ARG:NH2	7:P:137:LEU:CD2	2.82	0.42
1:S:26:SER:HA	1:S:31:TYR:CD2	2.54	0.42
1:S:98:PRO:HA	2:T:124:CYS:SG	2.59	0.42
4:V:236:GLY:O	4:V:238:SER:N	2.52	0.42
6:X:83:ARG:H	6:X:83:ARG:HG2	1.60	0.42
8:Z:88:ARG:HE	8:Z:126:LEU:HD22	1.84	0.42
2:2:86:LEU:CD1	2:2:90:LEU:HD11	2.49	0.42
3:3:684:ARG:HA	3:3:685:PRO:HD2	1.85	0.42
6:6:36:LEU:O	6:6:38:PRO:HD3	2.18	0.42
8:7:8:GLU:HG2	8:7:97:TYR:OH	2.19	0.42
8:7:20:MET:HE3	8:7:59:LEU:HG	2.00	0.42
1:A:417:PHE:O	1:A:418:LYS:C	2.61	0.42
2:B:109:GLY:HA2	8:H:91:ILE:HD13	2.01	0.42
3:C:136:GLU:CG	5:E:189:ARG:HG2	2.39	0.42
3:C:208:HIS:HB3	8:H:85:ARG:NH2	2.34	0.42
3:C:517:ALA:O	3:C:518:ALA:C	2.62	0.42
3:C:591:HIS:CE1	3:C:593:LEU:HB2	2.54	0.42
4:D:285:GLU:O	4:D:289:ILE:HG12	2.19	0.42
5:E:35:LYS:HD3	5:E:102:PRO:CB	2.47	0.42
5:E:64:ARG:HA	5:E:64:ARG:HD3	1.75	0.42
1:J:97:GLU:OE2	1:J:294:GLY:HA3	2.20	0.42
1:J:203:PRO:HB2	1:J:204:PRO:HD3	2.00	0.42
1:J:359:CYS:O	1:J:363:VAL:HG22	2.19	0.42
2:K:87:SER:OG	2:K:128:CYS:HB3	2.18	0.42
3:L:356:LEU:HA	3:L:654:PHE:CE1	2.55	0.42
3:L:356:LEU:HD13	3:L:654:PHE:HD1	1.84	0.42
4:M:236:GLY:C	4:M:238:SER:N	2.72	0.42
4:M:343:TYR:CD1	4:M:343:TYR:C	2.98	0.42
4:M:358:VAL:O	4:M:366:TYR:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:46:CYS:HB3	6:O:81:ALA:HB1	2.00	0.42
7:P:129:LEU:HD23	7:P:129:LEU:HA	1.62	0.42
2:T:153:LEU:HD13	2:T:153:LEU:C	2.43	0.42
3:U:449:ALA:HA	3:U:464:ILE:O	2.19	0.42
4:V:143:LEU:HD23	4:V:143:LEU:O	2.19	0.42
1:1:64:GLY:HA3	10:1:440:FMN:O1P	2.18	0.42
1:1:243:THR:HG22	1:1:244:GLU:N	2.26	0.42
1:1:271:THR:H	1:1:271:THR:HG23	1.51	0.42
3:3:133:ARG:HA	3:3:136:GLU:HB2	2.00	0.42
3:3:571:VAL:HG23	3:3:587:LEU:HD11	2.01	0.42
3:3:758:LEU:HD12	3:3:758:LEU:N	2.34	0.42
4:4:304:ASP:HA	4:4:305:PRO:HD2	1.86	0.42
5:5:48:PHE:CE2	5:5:50:ALA:HB2	2.54	0.42
5:5:104:VAL:HG12	5:5:108:TRP:CE3	2.49	0.42
8:7:38:PRO:C	8:7:40:PHE:H	2.28	0.42
1:A:202:LYS:N	1:A:203:PRO:CD	2.83	0.42
1:A:391:LEU:HA	1:A:391:LEU:HD23	1.88	0.42
3:C:408:ILE:HD12	3:C:408:ILE:HA	1.77	0.42
4:D:120:LEU:HD13	4:D:160:PHE:CE1	2.45	0.42
4:D:224:ILE:HD11	4:D:275:ARG:CZ	2.48	0.42
4:D:366:TYR:CE1	5:E:148:LYS:HE3	2.54	0.42
6:F:148:ILE:O	6:F:151:VAL:HG22	2.19	0.42
7:G:96:LEU:HD23	7:G:96:LEU:HA	1.69	0.42
8:H:60:SER:HB3	8:H:64:GLY:O	2.19	0.42
1:J:253:GLN:HG2	1:J:327:GLY:CA	2.46	0.42
3:L:509:ALA:O	3:L:510:GLY:C	2.63	0.42
5:N:66:GLU:HG2	5:N:95:PRO:CA	2.48	0.42
5:N:194:SER:C	5:N:195:LEU:HD22	2.45	0.42
6:O:33:SER:HA	6:O:158:VAL:HG21	2.01	0.42
6:O:114:SER:CB	7:P:97:ARG:HD2	2.50	0.42
8:Q:17:LEU:HD13	8:Q:54:ILE:HD13	2.00	0.42
2:T:7:LYS:H	2:T:7:LYS:CD	2.27	0.42
3:U:37:LYS:O	3:U:38:HIS:HB2	2.19	0.42
3:U:139:LEU:HD12	4:V:326:TYR:CE2	2.54	0.42
3:U:351:LEU:HD12	3:U:351:LEU:HA	1.82	0.42
3:U:403:THR:O	3:U:403:THR:HG22	2.18	0.42
4:V:316:LEU:C	4:V:316:LEU:HD12	2.44	0.42
5:W:98:ASP:C	5:W:100:ARG:H	2.26	0.42
5:W:111:ALA:HB1	5:W:115:GLU:HG3	2.02	0.42
8:Z:63:LEU:HD13	8:Z:129:ALA:HB3	2.01	0.42
1:1:6:LEU:HD21	1:1:12:ARG:CG	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:117:LEU:HD23	4:4:321:MET:HA	2.02	0.42
3:3:197:ASP:OD2	3:3:220:SER:CB	2.68	0.42
3:3:732:ALA:H	3:3:747:VAL:HG12	1.83	0.42
4:4:69:THR:HG21	6:6:120:ASN:ND2	2.35	0.42
4:4:140:LEU:HD11	4:4:214:PHE:HB2	2.01	0.42
1:A:100:SER:HB2	1:A:325:THR:OG1	2.19	0.42
1:A:107:LEU:CD2	1:A:114:LEU:HD12	2.49	0.42
1:A:110:VAL:N	1:A:111:PRO:CD	2.81	0.42
3:C:508:GLY:HA2	3:C:535:MET:HB2	2.02	0.42
4:D:195:GLU:C	4:D:198:PRO:HD2	2.45	0.42
7:G:100:PHE:N	7:G:100:PHE:CD1	2.87	0.42
1:J:211:LEU:HD12	1:J:211:LEU:HA	1.85	0.42
3:L:37:LYS:O	3:L:38:HIS:HB2	2.18	0.42
3:L:584:VAL:HG21	3:L:644:LEU:CD1	2.49	0.42
3:L:695:ARG:CZ	3:L:717:TRP:CH2	3.02	0.42
4:M:44:MET:HA	4:M:44:MET:HE3	2.02	0.42
4:M:95:LEU:HA	4:M:173:ILE:CD1	2.50	0.42
4:M:130:LEU:HD11	4:M:152:GLU:HB3	2.01	0.42
4:M:195:GLU:O	4:M:198:PRO:HD2	2.19	0.42
4:M:212:PRO:HG2	4:M:213:ILE:H	1.84	0.42
5:N:129:HIS:O	5:N:130:PRO:C	2.63	0.42
7:P:96:LEU:HA	7:P:96:LEU:HD23	1.74	0.42
3:U:366:THR:OG1	3:U:367:PRO:HD2	2.19	0.42
3:U:582:PHE:HA	3:U:599:HIS:ND1	2.35	0.42
4:V:328:PHE:CD2	4:V:328:PHE:C	2.96	0.42
7:Y:113:ILE:HG23	7:Y:113:ILE:O	2.19	0.42
3:3:366:THR:OG1	3:3:367:PRO:HD2	2.20	0.42
3:3:478:LEU:HD12	3:3:520:ARG:NH1	2.35	0.42
4:4:350:ARG:HD3	4:4:374:SER:OG	2.19	0.42
6:6:174:ALA:O	6:6:175:ALA:HB2	2.20	0.42
8:7:16:LEU:HD13	8:7:16:LEU:C	2.45	0.42
1:A:4:PRO:C	1:A:12:ARG:HH22	2.28	0.42
1:A:343:ASN:O	1:A:346:ARG:HG2	2.18	0.42
3:C:113:LEU:HD12	3:C:157:PHE:CG	2.55	0.42
3:C:694:LEU:C	3:C:762:ALA:HB2	2.44	0.42
4:D:168:PHE:HE1	6:F:141:PRO:CG	2.32	0.42
4:D:316:LEU:C	4:D:318:GLU:H	2.27	0.42
6:F:131:VAL:HA	6:F:132:PRO:HD3	1.89	0.42
6:F:163:TYR:HD1	7:G:152:ARG:NH1	2.17	0.42
1:J:267:PRO:O	1:J:270:THR:CG2	2.68	0.42
2:K:116:LEU:HG	2:K:117:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:47:LEU:HD11	4:M:51:GLU:C	2.44	0.42
4:M:383:TYR:O	4:M:384:ALA:C	2.62	0.42
5:N:52:ILE:CG2	5:N:114:LEU:HB3	2.42	0.42
6:O:104:TRP:NE1	6:O:172:PRO:O	2.47	0.42
1:S:45:LEU:HD23	1:S:123:TYR:CG	2.54	0.42
1:S:135:ARG:C	1:S:137:GLU:H	2.28	0.42
2:T:24:ARG:HE	2:T:24:ARG:HB3	1.76	0.42
2:T:112:THR:HG22	2:T:117:PHE:H	1.84	0.42
2:T:114:ASP:HB2	2:T:116:LEU:CD2	2.50	0.42
3:U:543:GLY:HA2	3:U:615:VAL:HG21	2.02	0.42
3:U:738:THR:HG22	3:U:739:PRO:CD	2.36	0.42
3:U:753:VAL:HA	3:U:754:PRO:HD2	1.93	0.42
5:W:37:GLU:O	5:W:40:HIS:HB3	2.19	0.42
8:Z:37:PHE:CE1	8:Z:55:MET:HB2	2.54	0.42
1:1:110:VAL:N	1:1:111:PRO:CD	2.81	0.42
3:3:343:LEU:O	3:3:369:LEU:HA	2.20	0.42
5:5:52:ILE:CG2	5:5:114:LEU:HB3	2.41	0.42
1:A:29:LEU:HB2	1:A:151:GLU:OE1	2.20	0.42
1:A:276:ILE:HG23	1:A:330:LEU:HD11	2.00	0.42
1:A:351:GLU:HA	3:C:205:ARG:NH1	2.30	0.42
2:B:45:ARG:HG2	2:B:45:ARG:H	1.65	0.42
3:C:171:SER:CB	3:C:172:PRO:HD2	2.48	0.42
3:C:449:ALA:HA	3:C:464:ILE:O	2.20	0.42
3:C:690:GLY:HA3	3:C:770:ARG:HH21	1.84	0.42
8:H:50:LEU:HD12	8:H:50:LEU:HA	1.81	0.42
1:J:155:ARG:H	1:J:155:ARG:HG2	1.64	0.42
2:K:114:ASP:HB2	2:K:116:LEU:CD2	2.50	0.42
3:L:115:HIS:CG	3:L:116:PRO:CD	2.97	0.42
3:L:739:PRO:HG2	3:L:771:VAL:HG12	2.01	0.42
8:Q:84:LEU:HB2	8:Q:93:LEU:HB2	2.01	0.42
2:T:55:THR:HG23	2:T:56:THR:N	2.34	0.42
3:U:564:LEU:HD12	3:U:564:LEU:HA	1.83	0.42
5:W:5:ARG:NH1	5:W:5:ARG:CG	2.67	0.42
5:W:120:ASP:OD1	5:W:134:LYS:HG3	2.20	0.42
6:X:113:SER:HB3	7:Y:96:LEU:HD13	2.02	0.42
6:X:132:PRO:HB2	6:X:174:ALA:HB1	2.01	0.42
1:1:363:VAL:HG23	1:1:364:ALA:N	2.35	0.42
1:1:395:GLU:HB2	1:1:407:VAL:HG21	2.02	0.42
3:3:581:ARG:O	3:3:599:HIS:HE1	2.03	0.42
4:4:103:LYS:HE2	4:4:344:VAL:HG11	2.02	0.42
4:4:108:VAL:HG23	4:4:108:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:130:LEU:HD11	4:4:152:GLU:HB3	2.02	0.42
4:4:366:TYR:CE1	5:5:148:LYS:HE3	2.55	0.42
7:9:43:LEU:CD2	7:9:113:ILE:HD13	2.50	0.42
1:A:65:ARG:HB2	1:A:222:GLU:HB3	2.02	0.42
1:A:186:THR:HG21	1:A:200:ARG:H	1.84	0.42
7:G:108:CYS:HA	9:G:184:SF4:S3	2.60	0.42
7:G:113:ILE:O	7:G:113:ILE:HG23	2.20	0.42
8:H:86:LEU:HD11	8:H:118:LEU:HD11	2.01	0.42
1:J:45:LEU:HD23	1:J:123:TYR:CG	2.55	0.42
1:J:81:LYS:HA	1:J:81:LYS:HE3	2.02	0.42
1:J:104:ARG:NH2	2:K:127:SER:CB	2.82	0.42
1:J:356:CYS:HB3	1:J:358:PRO:CD	2.50	0.42
2:K:168:LEU:HA	2:K:169:PRO:HD2	1.81	0.42
3:L:550:LEU:HD12	3:L:550:LEU:N	2.35	0.42
3:L:564:LEU:HD12	3:L:564:LEU:HA	1.81	0.42
3:L:596:ARG:C	3:L:597:TYR:HD1	2.28	0.42
4:M:223:VAL:O	4:M:383:TYR:HE1	2.02	0.42
3:U:101:ARG:NH1	3:U:140:TYR:CD1	2.88	0.42
3:U:200:LEU:HD12	3:U:200:LEU:HA	1.93	0.42
3:U:402:PRO:CA	3:U:535:MET:HE1	2.49	0.42
3:U:695:ARG:CZ	3:U:717:TRP:CH2	3.02	0.42
4:V:256:GLY:C	4:V:258:GLU:N	2.75	0.42
4:V:316:LEU:C	4:V:318:GLU:N	2.77	0.42
5:W:104:VAL:CG1	5:W:108:TRP:CE3	3.03	0.42
6:X:104:TRP:NE1	6:X:172:PRO:O	2.50	0.42
1:1:276:ILE:HG23	1:1:330:LEU:HD11	2.02	0.42
1:1:434:PRO:HG2	1:1:436:LEU:CD1	2.50	0.42
3:3:100:VAL:O	3:3:104:GLN:HG3	2.20	0.42
3:3:517:ALA:O	3:3:518:ALA:C	2.62	0.42
3:3:658:LEU:O	3:3:658:LEU:HD23	2.20	0.42
4:4:375:PHE:HD1	4:4:407:VAL:HG23	1.85	0.42
1:A:87:HIS:HB2	1:A:126:ARG:O	2.19	0.42
1:A:125:ILE:O	1:A:126:ARG:HB2	2.20	0.42
1:A:267:PRO:O	1:A:270:THR:CG2	2.68	0.42
2:B:101:THR:HG22	8:H:108:ILE:CD1	2.50	0.42
3:C:224:GLY:HA3	3:C:295:ARG:HD2	2.02	0.42
7:G:129:LEU:HD23	7:G:129:LEU:HA	1.68	0.42
1:J:192:LEU:HD23	1:J:192:LEU:C	2.45	0.42
1:J:202:LYS:N	1:J:203:PRO:CD	2.83	0.42
2:K:19:PRO:HB3	2:K:20:PRO:HD2	2.02	0.42
3:L:18:SER:OG	3:L:433:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:184:CYS:SG	3:L:186:ARG:HB2	2.60	0.42
3:L:555:GLY:O	3:L:556:ALA:C	2.63	0.42
6:O:30:TRP:O	6:O:33:SER:HB3	2.19	0.42
6:O:137:VAL:HG13	6:O:137:VAL:O	2.20	0.42
8:Q:112:LYS:O	8:Q:116:PHE:HD1	2.02	0.42
1:S:45:LEU:HB3	1:S:165:THR:HG21	2.01	0.42
1:S:63:ARG:CD	1:S:313:TYR:HD2	2.32	0.42
1:S:211:LEU:HB2	1:S:216:THR:HG21	2.02	0.42
2:T:76:GLY:H	2:T:118:SER:HG	1.65	0.42
3:U:417:VAL:HG12	3:U:443:ARG:HB3	2.01	0.42
3:U:471:GLY:HA2	3:U:473:GLU:OE2	2.20	0.42
8:Z:65:GLU:HA	8:Z:66:PRO:HD3	1.85	0.42
1:1:290:ILE:CG2	1:1:330:LEU:HD22	2.49	0.42
3:3:113:LEU:HD12	3:3:157:PHE:CG	2.55	0.42
3:3:232:VAL:HB	3:3:233:GLY:H	1.70	0.42
4:4:47:LEU:HD11	4:4:51:GLU:O	2.19	0.42
4:4:109:VAL:HG12	4:4:113:ALA:CB	2.50	0.42
4:4:221:VAL:O	4:4:272:VAL:HG12	2.20	0.42
4:4:236:GLY:O	4:4:238:SER:N	2.53	0.42
5:5:34:PHE:O	5:5:35:LYS:C	2.63	0.42
5:5:104:VAL:CG1	5:5:108:TRP:CE3	3.03	0.42
7:9:45:ARG:HH21	7:9:137:LEU:HD23	1.85	0.42
1:A:155:ARG:H	1:A:155:ARG:HG2	1.60	0.42
1:A:397:ARG:HG2	3:C:49:LEU:CD1	2.50	0.42
3:C:356:LEU:HD13	3:C:654:PHE:HD1	1.85	0.42
5:E:75:VAL:HG12	5:E:76:SER:N	2.35	0.42
1:J:92:ASN:ND2	10:J:440:FMN:O3'	2.52	0.42
3:L:185:LYS:HB3	3:L:189:ARG:HH11	1.85	0.42
4:M:69:THR:HG21	6:O:120:ASN:ND2	2.34	0.42
4:M:285:GLU:O	4:M:289:ILE:HG12	2.20	0.42
1:S:202:LYS:N	1:S:203:PRO:CD	2.82	0.42
2:T:26:ALA:O	2:T:29:PRO:HG2	2.20	0.42
3:U:506:ILE:HG21	3:U:535:MET:HE3	2.01	0.42
3:U:655:ARG:NH1	3:U:659:GLU:HG3	2.35	0.42
4:V:84:ARG:HG3	4:V:169:HIS:CE1	2.54	0.42
5:W:194:SER:O	5:W:195:LEU:HD13	2.20	0.42
3:3:184:CYS:SG	3:3:186:ARG:HB2	2.60	0.41
3:3:583:VAL:HG21	3:3:598:ALA:HA	2.02	0.41
3:3:627:ALA:HA	3:3:628:PRO:HD3	1.91	0.41
3:3:722:THR:HG23	3:3:755:LYS:HD2	2.02	0.41
4:4:195:GLU:C	4:4:198:PRO:HD2	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:404:MET:SD	4:4:407:VAL:HG11	2.59	0.41
1:A:26:SER:HA	1:A:31:TYR:CD2	2.55	0.41
1:A:51:ASP:O	1:A:54:ILE:HB	2.20	0.41
1:A:317:GLN:C	1:A:319:LYS:H	2.27	0.41
2:B:24:ARG:HE	2:B:24:ARG:HB3	1.76	0.41
3:C:43:GLY:HA2	11:C:787:FES:S1	2.60	0.41
3:C:229:ILE:HD11	3:C:289:TRP:CH2	2.55	0.41
3:C:329:LEU:CD1	3:C:584:VAL:HG11	2.50	0.41
3:C:372:GLN:O	3:C:558:TRP:CD2	2.73	0.41
3:C:652:PRO:HA	3:C:653:PRO:HD3	1.87	0.41
4:D:130:LEU:HD11	4:D:152:GLU:HB3	2.02	0.41
4:D:338:PRO:HG3	5:E:193:ARG:HB2	2.01	0.41
6:F:174:ALA:O	6:F:175:ALA:HB2	2.20	0.41
7:G:58:LEU:HA	7:G:58:LEU:HD12	1.79	0.41
1:J:434:PRO:HG2	1:J:436:LEU:CD1	2.50	0.41
3:L:83:CYS:SG	3:L:84:VAL:HG13	2.60	0.41
3:L:197:ASP:CB	3:L:220:SER:HB3	2.50	0.41
3:L:368:HIS:CG	3:L:556:ALA:HB3	2.55	0.41
3:L:408:ILE:HD12	3:L:408:ILE:HA	1.78	0.41
3:L:422:PRO:HA	3:L:423:PRO:HD2	1.77	0.41
3:L:627:ALA:HA	3:L:628:PRO:HD3	1.91	0.41
3:L:689:LYS:HE3	3:L:771:VAL:CG1	2.49	0.41
3:L:739:PRO:HD2	3:L:771:VAL:HG11	2.02	0.41
4:M:40:VAL:O	4:M:40:VAL:CG2	2.67	0.41
5:N:167:PRO:HB3	7:P:66:TYR:CE2	2.55	0.41
6:O:152:MET:O	6:O:156:LYS:HG3	2.21	0.41
7:P:123:ASP:CG	7:P:148:ARG:HH22	2.27	0.41
1:S:149:ILE:O	1:S:153:ARG:HB2	2.20	0.41
3:U:313:LYS:HB3	3:U:314:GLU:H	1.72	0.41
3:U:394:ASP:CB	3:U:501:LYS:HD3	2.50	0.41
3:U:422:PRO:HA	3:U:423:PRO:HD2	1.79	0.41
4:V:343:TYR:HB2	4:V:356:TYR:HD1	1.85	0.41
5:W:168:ALA:HA	5:W:171:ARG:HH12	1.85	0.41
6:X:174:ALA:O	6:X:175:ALA:HB2	2.20	0.41
3:3:509:ALA:O	3:3:510:GLY:C	2.64	0.41
4:4:219:ARG:NH1	4:4:273:PHE:HD2	2.18	0.41
4:4:242:SER:HB2	4:4:270:GLY:HA3	2.01	0.41
4:4:306:ASN:C	4:4:306:ASN:OD1	2.62	0.41
4:4:328:PHE:CD2	4:4:328:PHE:C	2.97	0.41
5:5:192:TYR:CG	5:5:193:ARG:N	2.88	0.41
6:6:145:GLU:CG	7:9:31:VAL:HG21	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:108:CYS:HA	9:9:184:SF4:S3	2.60	0.41
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.83	0.41
3:C:218:LEU:N	3:C:219:PRO:HD3	2.34	0.41
3:C:293:ALA:HB2	3:C:698:MET:HG2	2.02	0.41
3:C:498:GLU:C	3:C:500:ALA:N	2.77	0.41
3:C:501:LYS:HD2	3:C:501:LYS:N	2.13	0.41
3:C:695:ARG:NH1	3:C:717:TRP:CZ2	2.89	0.41
4:D:95:LEU:HA	4:D:173:ILE:CD1	2.50	0.41
7:G:96:LEU:HD21	7:G:129:LEU:HD12	2.01	0.41
8:H:65:GLU:HA	8:H:66:PRO:HD3	1.83	0.41
2:K:112:THR:OG1	2:K:113:PRO:HD2	2.20	0.41
3:L:245:ARG:HA	3:L:245:ARG:HD2	1.81	0.41
3:L:473:GLU:O	3:L:477:LEU:CD1	2.68	0.41
4:M:143:LEU:O	4:M:143:LEU:HD23	2.19	0.41
4:M:404:MET:SD	4:M:407:VAL:HG11	2.59	0.41
8:Q:72:VAL:HG22	8:Q:73:SER:N	2.35	0.41
1:S:192:LEU:HD23	1:S:192:LEU:C	2.44	0.41
3:U:478:LEU:HD12	3:U:520:ARG:CZ	2.50	0.41
4:V:161:GLU:OE2	6:X:143:ARG:NH1	2.52	0.41
4:V:197:LEU:HA	4:V:200:ARG:HB3	2.02	0.41
1:1:408:TRP:N	1:1:409:PRO:HD2	2.34	0.41
3:3:115:HIS:CG	3:3:116:PRO:CD	2.98	0.41
3:3:591:HIS:ND1	3:3:592:PRO:N	2.68	0.41
3:3:615:VAL:HG22	3:3:621:VAL:HG12	2.02	0.41
4:4:321:MET:HB2	4:4:321:MET:HE2	1.82	0.41
5:5:38:MET:O	5:5:41:TYR:HB2	2.21	0.41
5:5:137:THR:O	5:5:138:PRO:C	2.63	0.41
7:9:93:ILE:HG13	7:9:136:MET:HE1	2.00	0.41
8:7:52:THR:CG2	8:7:54:ILE:HG22	2.50	0.41
1:A:341:MET:HE2	1:A:409:PRO:C	2.45	0.41
3:C:30:VAL:CG2	3:C:48:CYS:HA	2.46	0.41
3:C:100:VAL:O	3:C:104:GLN:HG3	2.21	0.41
3:C:118:ASP:O	3:C:121:THR:N	2.51	0.41
3:C:203:ILE:HG22	3:C:204:GLU:HG3	2.02	0.41
3:C:317:LEU:HD22	3:C:317:LEU:H	1.84	0.41
3:C:689:LYS:HE3	3:C:771:VAL:CG1	2.50	0.41
4:D:116:ILE:HD11	4:D:182:LEU:CG	2.49	0.41
4:D:263:ASP:O	4:D:285:GLU:HG3	2.20	0.41
5:E:3:LEU:HB2	5:E:86:SER:HB2	2.02	0.41
5:E:104:VAL:CG1	5:E:108:TRP:CE3	3.03	0.41
1:J:366:PHE:HD1	1:J:370:LEU:CD2	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:395:GLU:HB2	1:J:407:VAL:HG21	2.02	0.41
3:L:38:HIS:CE1	3:L:430:THR:HG21	2.55	0.41
3:L:571:VAL:HG23	3:L:587:LEU:HD11	2.01	0.41
3:L:577:LEU:HD13	3:L:577:LEU:HA	1.92	0.41
5:N:38:MET:O	5:N:41:TYR:HB2	2.21	0.41
7:P:44:THR:OG1	7:P:52:LYS:HD2	2.19	0.41
1:S:434:PRO:HG2	1:S:436:LEU:CD1	2.51	0.41
2:T:45:ARG:HG2	2:T:45:ARG:H	1.64	0.41
3:U:155:THR:CG2	4:V:320:SER:HB2	2.50	0.41
3:U:356:LEU:HA	3:U:654:PHE:CE1	2.55	0.41
3:U:517:ALA:O	3:U:518:ALA:C	2.63	0.41
4:V:95:LEU:HA	4:V:173:ILE:CD1	2.49	0.41
4:V:162:TRP:CE2	7:Y:34:LYS:HD2	2.55	0.41
4:V:219:ARG:NH1	4:V:273:PHE:HD2	2.18	0.41
5:W:91:ARG:HE	5:W:91:ARG:HB2	1.57	0.41
1:1:260:ARG:HA	2:2:177:HIS:O	2.20	0.41
3:3:115:HIS:ND1	3:3:116:PRO:HD2	2.36	0.41
4:4:109:VAL:HG12	4:4:113:ALA:HB3	2.02	0.41
1:A:63:ARG:CD	1:A:313:TYR:HD2	2.33	0.41
1:A:70:PHE:HA	1:A:71:PRO:HD3	1.92	0.41
3:C:197:ASP:HB2	3:C:220:SER:HB3	2.02	0.41
3:C:367:PRO:CB	3:C:554:LYS:HB2	2.50	0.41
3:C:506:ILE:CG2	3:C:535:MET:HE3	2.49	0.41
4:D:328:PHE:CD2	4:D:328:PHE:C	2.98	0.41
5:E:187:GLY:C	5:E:189:ARG:H	2.28	0.41
1:J:28:THR:HB	1:J:31:TYR:H	1.86	0.41
1:J:45:LEU:HB3	1:J:165:THR:HG21	2.03	0.41
3:L:95:THR:C	3:L:96:LEU:HD12	2.45	0.41
3:L:229:ILE:HD11	3:L:289:TRP:CH2	2.56	0.41
3:L:615:VAL:HG22	3:L:621:VAL:HG12	2.02	0.41
3:L:669:VAL:HA	3:L:670:PRO:HD2	1.82	0.41
4:M:236:GLY:O	4:M:238:SER:N	2.54	0.41
4:M:375:PHE:HD1	4:M:407:VAL:HG23	1.85	0.41
8:Q:8:GLU:HG2	8:Q:97:TYR:OH	2.20	0.41
8:Q:52:THR:CG2	8:Q:54:ILE:HG22	2.50	0.41
1:S:4:PRO:C	1:S:5:ILE:HG13	2.45	0.41
1:S:97:GLU:OE2	1:S:294:GLY:HA3	2.20	0.41
1:S:233:ARG:H	1:S:233:ARG:HG2	1.57	0.41
1:S:414:LEU:HD12	1:S:414:LEU:HA	1.83	0.41
3:U:402:PRO:HB3	3:U:535:MET:HE1	2.02	0.41
4:V:84:ARG:HD3	6:X:117:MET:CE	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:110:PRO:HD2	4:V:113:ALA:CB	2.51	0.41
4:V:237:GLY:HA2	4:V:240:ARG:NE	2.34	0.41
5:W:38:MET:HA	5:W:41:TYR:CD1	2.55	0.41
5:W:40:HIS:CE1	5:W:44:MET:HE2	2.55	0.41
5:W:64:ARG:HA	5:W:64:ARG:HD3	1.74	0.41
6:X:37:TRP:CD1	6:X:75:ALA:HB2	2.56	0.41
7:Y:131:TYR:CZ	7:Y:144:LYS:HB2	2.56	0.41
8:Z:17:LEU:HD13	8:Z:54:ILE:HD13	2.02	0.41
1:1:93:ALA:O	1:1:134:VAL:HA	2.20	0.41
1:1:267:PRO:O	1:1:270:THR:CG2	2.69	0.41
3:3:46:ARG:NH1	3:3:46:ARG:CG	2.59	0.41
3:3:176:LEU:HD21	3:3:178:ARG:HG3	2.02	0.41
3:3:185:LYS:HB3	3:3:189:ARG:HH11	1.85	0.41
3:3:203:ILE:HD13	3:3:203:ILE:N	2.35	0.41
3:3:347:HIS:N	3:3:372:GLN:HB3	2.36	0.41
4:4:101:VAL:HG12	4:4:175:ILE:HG23	2.02	0.41
4:4:116:ILE:HD11	4:4:182:LEU:CG	2.48	0.41
4:4:404:MET:O	4:4:408:ASP:HB2	2.20	0.41
5:5:3:LEU:HB2	5:5:86:SER:HB2	2.01	0.41
5:5:40:HIS:CE1	5:5:44:MET:HE2	2.55	0.41
7:9:32:ALA:HA	7:9:162:VAL:O	2.20	0.41
8:7:72:VAL:HG22	8:7:73:SER:N	2.36	0.41
1:A:293:GLY:HA3	1:A:324:GLY:N	2.11	0.41
2:B:11:LEU:HD22	2:B:30:LEU:HD21	2.00	0.41
7:G:99:ILE:HG22	7:G:101:CYS:SG	2.60	0.41
1:J:260:ARG:HA	1:J:261:PRO:HD2	1.90	0.41
1:J:344:LEU:HD23	1:J:344:LEU:HA	1.80	0.41
1:J:351:GLU:HA	3:L:205:ARG:NH1	2.35	0.41
1:J:416:HIS:HB2	1:J:417:PHE:CE1	2.55	0.41
2:K:86:LEU:HD11	2:K:90:LEU:HD11	2.03	0.41
3:L:133:ARG:HA	3:L:136:GLU:HB2	2.02	0.41
3:L:197:ASP:OD2	3:L:220:SER:HB2	2.21	0.41
3:L:236:LEU:HD23	3:L:236:LEU:HA	1.82	0.41
3:L:614:LEU:O	3:L:621:VAL:HA	2.20	0.41
3:L:728:LEU:HB3	3:L:747:VAL:HG21	2.03	0.41
3:L:732:ALA:H	3:L:747:VAL:HG12	1.86	0.41
4:M:278:VAL:O	4:M:282:GLU:HG3	2.20	0.41
6:O:152:MET:HE2	6:O:152:MET:HB3	1.47	0.41
1:S:366:PHE:HD1	1:S:370:LEU:CD2	2.34	0.41
1:S:424:LEU:CD2	1:S:431:VAL:HG12	2.51	0.41
2:T:174:HIS:HB3	2:T:175:HIS:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:264:GLY:C	3:U:280:ARG:HB3	2.45	0.41
3:U:317:LEU:HD22	3:U:317:LEU:H	1.83	0.41
4:V:74:THR:HG22	4:V:75:TYR:N	2.34	0.41
4:V:130:LEU:HD11	4:V:152:GLU:HB3	2.03	0.41
4:V:195:GLU:C	4:V:198:PRO:HD2	2.45	0.41
4:V:366:TYR:CZ	5:W:148:LYS:HE3	2.55	0.41
5:W:34:PHE:O	5:W:35:LYS:C	2.63	0.41
5:W:175:THR:O	5:W:175:THR:OG1	2.31	0.41
7:Y:133:LYS:O	7:Y:137:LEU:HD13	2.21	0.41
7:Y:177:THR:O	7:Y:179:GLY:N	2.53	0.41
1:1:427:GLU:HB2	1:1:429:ARG:HD3	2.02	0.41
2:2:114:ASP:HB2	2:2:116:LEU:CD2	2.51	0.41
3:3:329:LEU:CD1	3:3:584:VAL:HG11	2.51	0.41
3:3:417:VAL:O	3:3:417:VAL:HG12	2.21	0.41
4:4:211:SER:CB	4:4:214:PHE:HB3	2.49	0.41
4:4:281:ARG:HG3	4:4:281:ARG:HH11	1.86	0.41
5:5:66:GLU:HG2	5:5:95:PRO:CA	2.50	0.41
5:5:160:ARG:HH21	7:9:144:LYS:NZ	2.18	0.41
7:9:56:CYS:SG	7:9:58:LEU:HB2	2.61	0.41
3:C:203:ILE:O	3:C:204:GLU:O	2.38	0.41
3:C:586:HIS:CE1	3:C:604:ALA:HB2	2.55	0.41
4:D:47:LEU:HD11	4:D:51:GLU:O	2.20	0.41
4:D:230:ILE:HD13	5:E:77:LEU:HD12	2.03	0.41
4:D:390:VAL:H	4:D:391:PRO:CD	2.34	0.41
5:E:155:THR:HG22	5:E:156:PRO:O	2.21	0.41
7:G:143:THR:HG23	7:G:146:GLN:OE1	2.21	0.41
8:H:39:ASP:OD2	8:H:75:ARG:HG2	2.20	0.41
1:J:291:ILE:HD11	1:J:331:ILE:HD11	2.03	0.41
3:L:100:VAL:O	3:L:104:GLN:HG3	2.21	0.41
3:L:160:THR:CG2	8:Q:73:SER:HB3	2.50	0.41
3:L:202:PHE:CE1	3:L:211:ILE:HD11	2.55	0.41
3:L:364:LEU:O	3:L:364:LEU:HG	2.19	0.41
3:L:532:VAL:HG12	3:L:533:LEU:N	2.35	0.41
4:M:76:LEU:HD12	4:M:76:LEU:C	2.46	0.41
4:M:291:LYS:O	4:M:295:GLU:HG3	2.21	0.41
4:M:319:THR:HG22	4:M:320:SER:N	2.35	0.41
6:O:151:VAL:O	6:O:155:GLN:HB2	2.20	0.41
6:O:157:LYS:O	6:O:157:LYS:HG2	2.16	0.41
6:O:158:VAL:HA	6:O:172:PRO:HB3	2.02	0.41
8:Q:60:SER:HB3	8:Q:64:GLY:O	2.19	0.41
1:S:118:MET:O	1:S:122:GLY:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:272:PHE:O	1:S:276:ILE:HG13	2.21	0.41
2:T:78:TYR:CE1	2:T:157:LEU:HD22	2.55	0.41
3:U:49:LEU:HA	3:U:80:ALA:O	2.21	0.41
4:V:63:HIS:HA	4:V:409:ARG:OXT	2.20	0.41
5:W:25:LEU:N	5:W:25:LEU:HD22	2.35	0.41
5:W:126:PHE:H	5:W:132:LEU:HD11	1.86	0.41
1:1:40:THR:HB	1:1:116:GLU:OE2	2.21	0.41
1:1:63:ARG:CD	1:1:313:TYR:HD2	2.33	0.41
1:1:118:MET:O	1:1:122:GLY:N	2.50	0.41
1:1:417:PHE:O	1:1:418:LYS:C	2.63	0.41
3:3:245:ARG:NH1	7:9:56:CYS:O	2.53	0.41
6:6:30:TRP:CD1	6:6:30:TRP:C	2.99	0.41
1:A:211:LEU:H	1:A:216:THR:CG2	2.33	0.41
1:A:427:GLU:HB2	1:A:429:ARG:HD3	2.03	0.41
2:B:6:ASP:OD1	2:B:6:ASP:C	2.63	0.41
2:B:78:TYR:CE1	2:B:157:LEU:HD22	2.56	0.41
3:C:23:VAL:HG13	3:C:28:TYR:HB2	2.01	0.41
3:C:47:MET:HE1	3:C:108:VAL:HA	2.03	0.41
3:C:254:THR:HG23	3:C:255:THR:N	2.35	0.41
3:C:264:GLY:C	3:C:280:ARG:HB3	2.46	0.41
3:C:470:PRO:HG3	3:C:759:TYR:HE2	1.85	0.41
3:C:615:VAL:HG22	3:C:621:VAL:HG12	2.03	0.41
4:D:87:TYR:CD1	6:F:48:ILE:HD12	2.56	0.41
4:D:194:LEU:HD12	4:D:194:LEU:HA	1.90	0.41
4:D:360:ASP:OD2	5:E:176:GLY:HA3	2.21	0.41
5:E:129:HIS:CD2	5:E:130:PRO:HD2	2.55	0.41
5:E:174:LEU:CD2	5:E:180:GLY:HA2	2.50	0.41
1:J:98:PRO:HB3	2:K:85:THR:HG21	2.02	0.41
3:L:113:LEU:HD12	3:L:157:PHE:CG	2.56	0.41
3:L:366:THR:OG1	3:L:367:PRO:HD2	2.20	0.41
3:L:734:VAL:HG13	3:L:775:VAL:HG13	2.03	0.41
4:M:343:TYR:CE1	4:M:345:PRO:HD3	2.56	0.41
7:P:131:TYR:CZ	7:P:144:LYS:HB2	2.55	0.41
1:S:107:LEU:HD22	1:S:145:LEU:CD1	2.50	0.41
3:U:20:MET:HE3	3:U:432:PHE:HB2	2.00	0.41
3:U:197:ASP:OD2	3:U:220:SER:HB2	2.20	0.41
4:V:371:ARG:NH2	4:V:376:VAL:CG2	2.81	0.41
5:W:44:MET:HE3	5:W:44:MET:HB2	1.62	0.41
6:X:43:LEU:HD23	6:X:43:LEU:HA	1.87	0.41
2:2:26:ALA:O	2:2:29:PRO:HG2	2.21	0.41
4:4:47:LEU:HD11	4:4:51:GLU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:88:LEU:HD21	6:6:48:ILE:CD1	2.42	0.41
1:A:28:THR:HB	1:A:31:TYR:H	1.86	0.41
1:A:272:PHE:CE2	1:A:311:MET:HE3	2.55	0.41
1:A:369:ASN:HB3	3:C:159:PHE:CD2	2.56	0.41
2:B:31:LEU:HD13	2:B:31:LEU:HA	1.92	0.41
3:C:194:VAL:HB	3:C:195:PRO:CD	2.51	0.41
4:D:115:THR:HG21	4:D:297:LEU:HD23	2.03	0.41
4:D:178:VAL:CG2	4:D:302:VAL:HB	2.50	0.41
4:D:241:ALA:O	4:D:267:GLY:HA3	2.21	0.41
5:E:25:LEU:H	5:E:25:LEU:HD23	1.85	0.41
6:F:36:LEU:O	6:F:38:PRO:HD3	2.20	0.41
6:F:46:CYS:HB3	6:F:81:ALA:HB1	2.02	0.41
7:G:105:GLU:HG3	7:G:114:VAL:HA	2.03	0.41
3:L:397:LEU:O	3:L:505:LEU:HD12	2.21	0.41
4:M:350:ARG:HG3	4:M:350:ARG:HH11	1.85	0.41
6:O:137:VAL:HA	6:O:138:PRO:HD2	1.76	0.41
1:S:91:CYS:HB3	1:S:132:ILE:HG23	2.03	0.41
1:S:158:LEU:CA	1:S:162:LEU:HD21	2.50	0.41
3:U:180:ARG:O	3:U:181:CYS:C	2.63	0.41
3:U:397:LEU:O	3:U:505:LEU:HD12	2.21	0.41
3:U:571:VAL:HG23	3:U:587:LEU:HD11	2.03	0.41
3:U:669:VAL:HA	3:U:670:PRO:HD2	1.83	0.41
3:U:680:LEU:CD2	3:U:682:GLU:HG2	2.51	0.41
4:V:89:HIS:HB2	4:V:128:SER:CB	2.51	0.41
4:V:383:TYR:O	4:V:384:ALA:C	2.64	0.41
5:W:181:LEU:HA	5:W:181:LEU:HD12	1.80	0.41
1:1:97:GLU:OE2	1:1:294:GLY:HA3	2.21	0.41
1:1:158:LEU:CA	1:1:162:LEU:HD21	2.51	0.41
1:1:184:GLU:HG2	10:1:440:FMN:C8M	2.51	0.41
1:1:344:LEU:HD23	1:1:344:LEU:HA	1.82	0.41
1:1:351:GLU:HA	3:3:205:ARG:NH1	2.35	0.41
1:1:424:LEU:CD2	1:1:431:VAL:HG12	2.50	0.41
2:2:55:THR:HG23	2:2:56:THR:N	2.35	0.41
3:3:420:LEU:HD22	3:3:436:GLN:HG2	2.03	0.41
3:3:577:LEU:O	3:3:578:LYS:C	2.63	0.41
4:4:40:VAL:HG13	4:4:404:MET:HG3	2.03	0.41
4:4:99:LEU:HD13	4:4:99:LEU:HA	1.80	0.41
4:4:237:GLY:HA2	4:4:240:ARG:NH2	2.34	0.41
5:5:35:LYS:HD3	5:5:102:PRO:CB	2.51	0.41
7:9:115:LEU:HA	7:9:115:LEU:HD23	1.68	0.41
7:9:130:VAL:O	7:9:130:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:50:LEU:HD12	8:7:50:LEU:HA	1.83	0.41
3:C:18:SER:OG	3:C:433:ALA:HB3	2.21	0.41
3:C:571:VAL:HG23	3:C:587:LEU:HD11	2.02	0.41
3:C:734:VAL:HG13	3:C:775:VAL:HG13	2.02	0.41
4:D:62:LEU:HD23	4:D:62:LEU:HA	1.87	0.41
4:D:300:GLY:HA3	4:D:301:PRO:HD2	1.94	0.41
4:D:350:ARG:HD3	4:D:374:SER:OG	2.20	0.41
4:D:390:VAL:HB	4:D:391:PRO:HD3	2.03	0.41
5:E:34:PHE:O	5:E:35:LYS:C	2.63	0.41
5:E:49:LEU:HD13	5:E:74:LEU:HD23	2.02	0.41
5:E:129:HIS:O	5:E:130:PRO:C	2.63	0.41
6:F:16:ARG:NH1	6:F:17:GLU:OE2	2.54	0.41
8:H:86:LEU:HA	8:H:87:PRO:HD2	1.83	0.41
3:L:232:VAL:HB	3:L:233:GLY:H	1.73	0.41
3:L:264:GLY:C	3:L:280:ARG:HB3	2.45	0.41
3:L:474:ARG:H	3:L:474:ARG:HG2	1.65	0.41
3:L:543:GLY:HA2	3:L:615:VAL:HG21	2.03	0.41
3:L:590:LEU:HD12	3:L:590:LEU:HA	1.87	0.41
3:L:750:ARG:HB2	3:L:753:VAL:CG2	2.51	0.41
4:M:109:VAL:HG12	4:M:113:ALA:CB	2.50	0.41
4:M:237:GLY:HA2	4:M:240:ARG:NE	2.36	0.41
4:M:338:PRO:HG3	5:N:193:ARG:HB2	2.02	0.41
5:N:49:LEU:HD13	5:N:74:LEU:HD23	2.03	0.41
6:O:20:LEU:O	6:O:24:LEU:HD13	2.21	0.41
7:P:56:CYS:SG	7:P:58:LEU:HB2	2.61	0.41
7:P:105:GLU:HG3	7:P:114:VAL:HA	2.01	0.41
7:P:143:THR:H	7:P:146:GLN:HB2	1.86	0.41
8:Q:88:ARG:HE	8:Q:126:LEU:CD2	2.34	0.41
1:S:28:THR:HB	1:S:31:TYR:H	1.86	0.41
1:S:100:SER:HB2	1:S:325:THR:OG1	2.21	0.41
1:S:424:LEU:HD21	1:S:431:VAL:HG12	2.02	0.41
3:U:197:ASP:HB2	3:U:220:SER:HB3	2.02	0.41
4:V:47:LEU:HD11	4:V:51:GLU:O	2.21	0.41
4:V:116:ILE:HD11	4:V:182:LEU:CD2	2.51	0.41
4:V:140:LEU:HD11	4:V:214:PHE:HB2	2.03	0.41
4:V:249:ARG:HD2	4:V:257:TYR:HE1	1.84	0.41
5:W:75:VAL:HG12	5:W:76:SER:N	2.36	0.41
3:3:200:LEU:HD12	3:3:200:LEU:HA	1.93	0.41
3:3:409:LEU:HD23	3:3:409:LEU:HA	1.80	0.41
3:3:459:MET:HG2	3:3:465:HIS:CD2	2.56	0.41
3:3:590:LEU:HD12	3:3:590:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:291:LYS:O	4:4:295:GLU:HG3	2.21	0.41
3:C:243:ARG:HB3	3:C:275:LEU:CD1	2.51	0.41
3:C:343:LEU:O	3:C:369:LEU:HA	2.20	0.41
3:C:564:LEU:HG	3:C:581:ARG:HG3	2.03	0.41
4:D:140:LEU:HD11	4:D:214:PHE:HB2	2.03	0.41
7:G:100:PHE:HA	9:G:183:SF4:S4	2.61	0.41
1:J:394:ILE:O	1:J:395:GLU:C	2.63	0.41
4:M:219:ARG:NH1	4:M:273:PHE:HD2	2.17	0.41
8:Q:108:ILE:HA	8:Q:109:PRO:HD3	1.93	0.41
1:S:363:VAL:CG2	1:S:364:ALA:N	2.84	0.41
3:U:136:GLU:CG	5:W:189:ARG:HG2	2.41	0.41
3:U:432:PHE:N	3:U:432:PHE:CD1	2.88	0.41
3:U:701:ALA:N	3:U:763:LEU:HB3	2.36	0.41
4:V:396:ILE:HA	4:V:396:ILE:HD12	1.83	0.41
5:W:192:TYR:CG	5:W:193:ARG:N	2.88	0.41
7:Y:143:THR:H	7:Y:146:GLN:HB2	1.86	0.41
1:1:70:PHE:HA	1:1:71:PRO:HD3	1.96	0.40
3:3:167:HIS:O	3:3:167:HIS:ND1	2.53	0.40
3:3:343:LEU:HD12	3:3:361:ALA:HB2	2.02	0.40
4:4:178:VAL:CG2	4:4:302:VAL:HB	2.51	0.40
4:4:371:ARG:NH2	4:4:376:VAL:CG2	2.80	0.40
6:6:114:SER:CB	7:9:97:ARG:HD2	2.47	0.40
7:9:41:HIS:ND1	7:9:95:MET:HE1	2.36	0.40
1:A:356:CYS:HB3	1:A:358:PRO:CD	2.52	0.40
1:A:367:MET:HE1	1:A:410:VAL:HG21	2.02	0.40
3:C:728:LEU:HB3	3:C:747:VAL:HG21	2.02	0.40
4:D:311:PRO:HD3	4:D:330:HIS:CE1	2.56	0.40
5:E:41:TYR:HA	5:E:44:MET:HE3	2.03	0.40
6:F:140:CYS:SG	7:G:99:ILE:HG13	2.61	0.40
8:H:52:THR:CG2	8:H:54:ILE:HG22	2.51	0.40
1:J:316:LEU:HA	1:J:316:LEU:HD23	1.85	0.40
2:K:103:THR:HG22	2:K:104:LEU:N	2.36	0.40
3:L:290:ILE:HG23	9:L:786:SF4:S4	2.61	0.40
3:L:497:TRP:NE1	3:L:524:LEU:CD1	2.83	0.40
4:M:47:LEU:HD11	4:M:51:GLU:O	2.20	0.40
4:M:193:LEU:O	4:M:193:LEU:HD23	2.22	0.40
4:M:197:LEU:O	4:M:198:PRO:C	2.63	0.40
3:U:185:LYS:HB3	3:U:189:ARG:HH11	1.87	0.40
3:U:399:LEU:HD22	3:U:477:LEU:HD11	2.03	0.40
3:U:555:GLY:O	3:U:556:ALA:C	2.63	0.40
3:U:669:VAL:O	3:U:669:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:47:LEU:HD11	4:V:51:GLU:C	2.46	0.40
4:V:116:ILE:O	4:V:120:LEU:HB2	2.21	0.40
4:V:168:PHE:HE1	6:X:141:PRO:CG	2.35	0.40
5:W:137:THR:HA	5:W:138:PRO:HD2	1.87	0.40
6:X:151:VAL:O	6:X:155:GLN:HB2	2.21	0.40
7:Y:79:ASN:HA	7:Y:80:PRO:HD2	1.95	0.40
1:1:26:SER:HA	1:1:31:TYR:CD2	2.56	0.40
1:1:170:ASP:O	1:1:171:LEU:HD12	2.21	0.40
3:3:407:PRO:HB2	9:3:786:SF4:S1	2.61	0.40
4:4:197:LEU:O	4:4:198:PRO:C	2.63	0.40
6:6:151:VAL:O	6:6:155:GLN:HB2	2.21	0.40
6:6:152:MET:O	6:6:156:LYS:HG3	2.22	0.40
6:6:157:LYS:O	6:6:157:LYS:HG2	2.18	0.40
7:9:63:CYS:HA	7:9:64:PRO:HD2	1.89	0.40
3:C:133:ARG:HA	3:C:136:GLU:HB2	2.03	0.40
3:C:402:PRO:CA	3:C:535:MET:HE1	2.52	0.40
3:C:688:ARG:HA	3:C:688:ARG:HD3	1.50	0.40
4:D:221:VAL:O	4:D:272:VAL:HG12	2.22	0.40
4:D:241:ALA:CB	4:D:278:VAL:HG21	2.51	0.40
4:D:249:ARG:CZ	4:D:262:PHE:HZ	2.34	0.40
4:D:332:THR:O	5:E:172:ALA:HB3	2.21	0.40
6:F:78:MET:HE3	6:F:96:TRP:HB2	2.04	0.40
8:H:122:ALA:O	8:H:126:LEU:HB2	2.21	0.40
1:J:133:TYR:CB	1:J:188:LEU:HD21	2.51	0.40
1:J:158:LEU:CA	1:J:162:LEU:HD21	2.51	0.40
1:J:402:LEU:O	1:J:405:ALA:HB3	2.21	0.40
3:L:305:ARG:NH2	3:L:609:GLU:OE1	2.52	0.40
3:L:382:PHE:CE1	3:L:512:LEU:HD11	2.56	0.40
4:M:283:MET:O	4:M:287:VAL:HG23	2.21	0.40
1:S:65:ARG:HB2	1:S:222:GLU:HB3	2.02	0.40
1:S:89:LEU:HD12	1:S:217:THR:HG22	2.03	0.40
1:S:290:ILE:CG2	1:S:330:LEU:HD22	2.51	0.40
1:S:317:GLN:C	1:S:319:LYS:H	2.30	0.40
3:U:203:ILE:O	3:U:204:GLU:O	2.39	0.40
3:U:498:GLU:C	3:U:500:ALA:N	2.79	0.40
4:V:290:ILE:O	4:V:294:LEU:HB2	2.22	0.40
1:1:186:THR:HA	1:1:189:MET:HE2	2.02	0.40
1:1:343:ASN:O	1:1:346:ARG:HG2	2.21	0.40
3:3:317:LEU:HD22	3:3:317:LEU:H	1.82	0.40
1:A:65:ARG:NH2	1:A:268:MET:CE	2.83	0.40
2:B:112:THR:HG22	2:B:117:PHE:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:GLN:O	3:C:134:THR:HB	2.22	0.40
3:C:236:LEU:HD23	3:C:236:LEU:HA	1.84	0.40
3:C:286:ASN:ND2	3:C:286:ASN:C	2.76	0.40
3:C:577:LEU:O	3:C:578:LYS:C	2.64	0.40
4:D:40:VAL:HG13	4:D:404:MET:HG3	2.02	0.40
4:D:63:HIS:HA	4:D:409:ARG:OXT	2.20	0.40
4:D:239:LEU:HD22	4:D:244:VAL:CB	2.50	0.40
4:D:298:GLU:CG	4:D:299:PRO:HD2	2.51	0.40
6:F:165:GLU:HG2	7:G:148:ARG:NH1	2.35	0.40
7:G:125:GLU:O	7:G:126:TYR:C	2.63	0.40
1:J:67:GLY:HA2	1:J:324:GLY:O	2.20	0.40
3:L:130:LEU:HD12	3:L:130:LEU:O	2.20	0.40
3:L:243:ARG:HB3	3:L:275:LEU:CD1	2.52	0.40
3:L:317:LEU:N	3:L:317:LEU:CD2	2.83	0.40
3:L:414:SER:HA	3:L:461:TRP:CZ3	2.57	0.40
4:M:233:GLY:O	4:M:235:THR:N	2.54	0.40
4:M:286:SER:O	4:M:290:ILE:HG12	2.22	0.40
5:N:25:LEU:N	5:N:25:LEU:HD22	2.36	0.40
7:P:130:VAL:O	7:P:130:VAL:HG13	2.21	0.40
1:S:160:LYS:HG3	1:S:161:ASN:N	2.35	0.40
1:S:341:MET:HB2	1:S:371:PHE:CE1	2.57	0.40
1:S:344:LEU:HD23	1:S:344:LEU:HA	1.80	0.40
3:U:532:VAL:HG12	3:U:533:LEU:N	2.35	0.40
3:U:750:ARG:HB2	3:U:753:VAL:CG2	2.52	0.40
4:V:72:HIS:O	4:V:73:ARG:CD	2.49	0.40
4:V:215:TYR:CD2	4:V:215:TYR:C	3.00	0.40
1:1:154:ALA:C	1:1:156:GLY:H	2.29	0.40
1:1:312:SER:C	1:1:314:GLU:H	2.28	0.40
2:2:112:THR:OG1	2:2:113:PRO:HD2	2.21	0.40
3:3:36:GLU:OE2	3:3:229:ILE:HG23	2.21	0.40
3:3:474:ARG:CZ	3:3:516:VAL:HG21	2.46	0.40
3:3:596:ARG:C	3:3:597:TYR:HD1	2.29	0.40
3:3:713:ARG:HE	3:3:713:ARG:HB2	1.72	0.40
4:4:234:LEU:O	4:4:239:LEU:CG	2.61	0.40
5:5:48:PHE:CD2	5:5:77:LEU:HD21	2.56	0.40
6:6:113:SER:HB3	7:9:96:LEU:HD13	2.04	0.40
1:A:363:VAL:CG2	1:A:364:ALA:N	2.85	0.40
2:B:26:ALA:O	2:B:29:PRO:HG2	2.21	0.40
2:B:86:LEU:HD11	2:B:90:LEU:HD11	2.02	0.40
3:C:55:PRO:CG	3:C:73:ILE:C	2.95	0.40
3:C:244:ALA:HB3	3:C:249:MET:CE	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:281:GLU:HG3	3:C:288:ILE:HG22	2.04	0.40
4:D:354:GLY:H	4:D:371:ARG:HB3	1.86	0.40
5:E:40:HIS:CE1	5:E:44:MET:HE2	2.57	0.40
6:F:152:MET:HE2	6:F:152:MET:HB3	1.51	0.40
7:G:143:THR:H	7:G:146:GLN:HB2	1.87	0.40
8:H:87:PRO:O	8:H:88:ARG:CB	2.69	0.40
1:J:58:LYS:HA	1:J:73:GLY:HA3	2.02	0.40
1:J:154:ALA:O	1:J:156:GLY:N	2.55	0.40
1:J:158:LEU:HA	1:J:162:LEU:HD21	2.02	0.40
1:J:271:THR:HG23	1:J:271:THR:H	1.50	0.40
4:M:114:GLU:O	4:M:118:VAL:HG13	2.21	0.40
4:M:163:VAL:HG13	4:M:164:THR:HG23	2.03	0.40
6:O:114:SER:C	6:O:116:GLY:H	2.30	0.40
8:Q:65:GLU:HA	8:Q:66:PRO:HD3	1.83	0.40
1:S:125:ILE:O	1:S:126:ARG:HB2	2.20	0.40
2:T:112:THR:OG1	2:T:113:PRO:HD2	2.21	0.40
3:U:123:ASP:HB3	3:U:236:LEU:HD13	2.02	0.40
3:U:164:VAL:HB	3:U:165:ASP:H	1.61	0.40
3:U:258:LEU:HD12	3:U:294:GLY:HA2	2.03	0.40
3:U:329:LEU:CD1	3:U:584:VAL:HG11	2.51	0.40
3:U:469:ARG:HB2	3:U:470:PRO:CD	2.50	0.40
3:U:577:LEU:O	3:U:578:LYS:C	2.65	0.40
3:U:654:PHE:HE2	3:U:663:ALA:HB3	1.86	0.40
4:V:215:TYR:C	4:V:215:TYR:HD2	2.30	0.40
4:V:390:VAL:N	4:V:391:PRO:CD	2.84	0.40
1:1:158:LEU:HA	1:1:162:LEU:HD21	2.03	0.40
1:1:202:LYS:N	1:1:203:PRO:CD	2.85	0.40
1:1:424:LEU:HD21	1:1:431:VAL:HG12	2.02	0.40
3:3:695:ARG:NH1	3:3:717:TRP:CZ2	2.90	0.40
5:5:49:LEU:HD13	5:5:74:LEU:HD23	2.04	0.40
6:6:104:TRP:NE1	6:6:172:PRO:O	2.50	0.40
6:6:163:TYR:CD1	7:9:152:ARG:HD2	2.56	0.40
8:7:108:ILE:HA	8:7:109:PRO:HD3	1.94	0.40
1:A:107:LEU:HD22	1:A:145:LEU:CD1	2.51	0.40
3:C:180:ARG:O	3:C:181:CYS:C	2.64	0.40
3:C:343:LEU:HD12	3:C:361:ALA:HB2	2.03	0.40
3:C:368:HIS:CB	3:C:556:ALA:HB3	2.52	0.40
3:C:734:VAL:HG12	3:C:735:ALA:N	2.36	0.40
4:D:115:THR:HG22	4:D:297:LEU:HD23	2.02	0.40
8:H:108:ILE:HA	8:H:109:PRO:HD3	1.92	0.40
1:J:211:LEU:HG	1:J:212:TRP:CZ3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:115:HIS:ND1	3:L:116:PRO:HD2	2.37	0.40
3:L:254:THR:HG23	3:L:255:THR:N	2.36	0.40
3:L:703:GLN:O	3:L:705:VAL:N	2.54	0.40
4:M:140:LEU:HD11	4:M:214:PHE:HB2	2.03	0.40
4:M:203:GLU:O	4:M:207:LEU:HG	2.22	0.40
4:M:344:VAL:HG23	4:M:344:VAL:O	2.21	0.40
4:M:344:VAL:HA	4:M:345:PRO:HD2	1.96	0.40
7:P:58:LEU:HD12	7:P:58:LEU:HA	1.76	0.40
7:P:125:GLU:O	7:P:126:TYR:C	2.64	0.40
7:P:150:ALA:HA	7:P:153:THR:HB	2.04	0.40
1:S:158:LEU:HA	1:S:162:LEU:HD21	2.03	0.40
1:S:267:PRO:O	1:S:270:THR:HG23	2.21	0.40
2:T:136:VAL:HG21	2:T:163:LEU:HD13	2.04	0.40
3:U:133:ARG:HA	3:U:136:GLU:HB2	2.04	0.40
3:U:334:LYS:NZ	3:U:334:LYS:HB3	2.37	0.40
3:U:459:MET:HG3	3:U:465:HIS:HB2	2.03	0.40
3:U:583:VAL:HG23	3:U:583:VAL:O	2.21	0.40
3:U:695:ARG:HA	3:U:696:PRO:HD2	1.92	0.40
4:V:195:GLU:O	4:V:198:PRO:HD2	2.22	0.40
4:V:285:GLU:OE1	4:V:288:LYS:HD3	2.21	0.40
5:W:41:TYR:HA	5:W:44:MET:HE3	2.03	0.40
5:W:137:THR:O	5:W:138:PRO:C	2.64	0.40
6:X:145:GLU:H	6:X:145:GLU:CD	2.29	0.40
7:Y:134:GLU:CD	7:Y:134:GLU:N	2.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	435/438 (99%)	366 (84%)	59 (14%)	10 (2%)	5 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/438 (99%)	359 (82%)	65 (15%)	11 (2%)	4	22
1	J	435/438 (99%)	363 (83%)	62 (14%)	10 (2%)	5	24
1	S	435/438 (99%)	362 (83%)	62 (14%)	11 (2%)	4	22
2	2	176/181 (97%)	147 (84%)	26 (15%)	3 (2%)	7	30
2	B	176/181 (97%)	145 (82%)	28 (16%)	3 (2%)	7	30
2	K	176/181 (97%)	145 (82%)	29 (16%)	2 (1%)	11	39
2	T	176/181 (97%)	147 (84%)	27 (15%)	2 (1%)	11	39
3	3	748/783 (96%)	628 (84%)	96 (13%)	24 (3%)	3	17
3	C	748/783 (96%)	632 (84%)	93 (12%)	23 (3%)	3	18
3	L	748/783 (96%)	630 (84%)	93 (12%)	25 (3%)	3	17
3	U	748/783 (96%)	633 (85%)	93 (12%)	22 (3%)	3	20
4	4	373/409 (91%)	319 (86%)	44 (12%)	10 (3%)	4	21
4	D	373/409 (91%)	320 (86%)	41 (11%)	12 (3%)	3	17
4	M	373/409 (91%)	319 (86%)	44 (12%)	10 (3%)	4	21
4	V	373/409 (91%)	319 (86%)	42 (11%)	12 (3%)	3	17
5	5	194/207 (94%)	162 (84%)	21 (11%)	11 (6%)	1	9
5	E	194/207 (94%)	160 (82%)	23 (12%)	11 (6%)	1	9
5	N	194/207 (94%)	160 (82%)	23 (12%)	11 (6%)	1	9
5	W	194/207 (94%)	157 (81%)	26 (13%)	11 (6%)	1	9
6	6	141/181 (78%)	121 (86%)	17 (12%)	3 (2%)	5	26
6	F	141/181 (78%)	120 (85%)	18 (13%)	3 (2%)	5	26
6	O	141/181 (78%)	119 (84%)	21 (15%)	1 (1%)	18	49
6	X	141/181 (78%)	120 (85%)	18 (13%)	3 (2%)	5	26
7	9	152/182 (84%)	127 (84%)	23 (15%)	2 (1%)	9	36
7	G	152/182 (84%)	128 (84%)	22 (14%)	2 (1%)	9	36
7	P	152/182 (84%)	128 (84%)	22 (14%)	2 (1%)	9	36
7	Y	152/182 (84%)	130 (86%)	20 (13%)	2 (1%)	9	36
8	7	125/129 (97%)	114 (91%)	11 (9%)	0	100	100
8	H	125/129 (97%)	115 (92%)	10 (8%)	0	100	100
8	Q	125/129 (97%)	115 (92%)	10 (8%)	0	100	100
8	Z	125/129 (97%)	114 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	9376/10040 (93%)	7924 (84%)	1200 (13%)	252 (3%)	4	21

All (252) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	4	PRO
1	1	68	ALA
1	1	81	LYS
1	1	160	LYS
1	1	234	GLY
4	4	212	PRO
5	5	160	ARG
5	5	176	GLY
1	A	4	PRO
1	A	68	ALA
1	A	81	LYS
1	A	160	LYS
1	A	234	GLY
4	D	212	PRO
4	D	255	SER
5	E	160	ARG
5	E	176	GLY
1	J	4	PRO
1	J	68	ALA
1	J	81	LYS
1	J	160	LYS
1	J	234	GLY
4	M	212	PRO
5	N	160	ARG
5	N	176	GLY
1	S	4	PRO
1	S	81	LYS
1	S	160	LYS
1	S	234	GLY
4	V	212	PRO
5	W	160	ARG
5	W	176	GLY
1	1	37	GLY
1	1	155	ARG
2	2	136	VAL
3	3	6	VAL
3	3	204	GLU

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Mol	Chain	Res	Type
3	3	338	GLY
3	3	365	LYS
3	3	580	LYS
3	3	690	GLY
4	4	53	LEU
4	4	219	ARG
4	4	255	SER
7	9	156	PRO
1	A	37	GLY
1	A	155	ARG
3	C	181	CYS
3	C	204	GLU
3	C	365	LYS
3	C	516	VAL
3	C	580	LYS
3	C	690	GLY
4	D	53	LEU
4	D	219	ARG
5	E	27	VAL
5	E	50	ALA
1	J	37	GLY
1	J	155	ARG
2	K	136	VAL
3	L	204	GLU
3	L	365	LYS
3	L	516	VAL
3	L	556	ALA
3	L	580	LYS
3	L	690	GLY
4	M	53	LEU
4	M	219	ARG
4	M	255	SER
5	N	27	VAL
1	S	37	GLY
1	S	68	ALA
1	S	155	ARG
2	T	136	VAL
3	U	181	CYS
3	U	204	GLU
3	U	338	GLY
3	U	365	LYS
3	U	556	ALA

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Mol	Chain	Res	Type
3	U	580	LYS
3	U	690	GLY
4	V	53	LEU
4	V	219	ARG
4	V	255	SER
5	W	27	VAL
5	W	50	ALA
1	1	38	TYR
2	2	140	PRO
3	3	119	CYS
3	3	181	CYS
3	3	516	VAL
3	3	554	LYS
3	3	556	ALA
4	4	142	ALA
5	5	50	ALA
1	A	38	TYR
1	A	154	ALA
2	B	136	VAL
2	B	140	PRO
3	C	139	LEU
3	C	338	GLY
3	C	554	LYS
3	C	556	ALA
4	D	142	ALA
7	G	156	PRO
1	J	38	TYR
2	K	140	PRO
3	L	6	VAL
3	L	119	CYS
3	L	139	LEU
3	L	181	CYS
3	L	338	GLY
3	L	554	LYS
4	M	142	ALA
5	N	50	ALA
7	P	156	PRO
1	S	38	TYR
1	S	154	ALA
2	T	140	PRO
3	U	554	LYS
4	V	142	ALA

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Mol	Chain	Res	Type
7	Y	156	PRO
1	1	154	ALA
3	3	139	LEU
3	3	367	PRO
5	5	27	VAL
5	5	33	ARG
5	5	138	PRO
6	6	156	LYS
3	C	6	VAL
3	C	119	CYS
3	C	367	PRO
4	D	198	PRO
5	E	2	ARG
5	E	47	ASN
5	E	61	PRO
5	E	138	PRO
3	L	367	PRO
3	L	704	ALA
5	N	138	PRO
3	U	6	VAL
3	U	119	CYS
3	U	139	LEU
3	U	367	PRO
3	U	704	ALA
4	V	198	PRO
5	W	47	ASN
5	W	61	PRO
5	W	138	PRO
2	2	116	LEU
3	3	164	VAL
3	3	704	ALA
4	4	198	PRO
4	4	381	LEU
5	5	2	ARG
5	5	47	ASN
5	5	61	PRO
5	5	65	PRO
3	C	164	VAL
3	C	704	ALA
4	D	381	LEU
5	E	33	ARG
5	E	35	LYS

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Mol	Chain	Res	Type
5	E	65	PRO
1	J	154	ALA
3	L	285	VAL
3	L	453	PRO
3	L	563	ALA
4	M	198	PRO
4	M	381	LEU
5	N	2	ARG
5	N	35	LYS
5	N	47	ASN
5	N	61	PRO
5	N	65	PRO
3	U	164	VAL
3	U	285	VAL
3	U	516	VAL
4	V	314	ARG
4	V	381	LEU
5	W	33	ARG
5	W	188	SER
6	X	156	LYS
3	3	285	VAL
3	3	303	GLN
3	3	453	PRO
3	3	563	ALA
4	4	211	SER
5	5	35	LYS
1	A	166	ASP
2	B	116	LEU
3	C	203	ILE
3	C	285	VAL
3	C	453	PRO
3	C	471	GLY
4	D	211	SER
6	F	156	LYS
3	L	164	VAL
3	L	203	ILE
3	L	303	GLN
4	M	106	GLY
1	S	166	ASP
3	U	453	PRO
4	V	237	GLY
5	W	35	LYS

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Mol	Chain	Res	Type
5	W	65	PRO
1	1	204	PRO
3	3	203	ILE
4	4	270	GLY
6	6	77	VAL
3	C	549	VAL
3	C	765	PRO
6	F	77	VAL
6	O	77	VAL
1	S	204	PRO
3	U	203	ILE
3	U	471	GLY
6	X	77	VAL
3	3	471	GLY
3	3	549	VAL
4	4	106	GLY
1	A	204	PRO
4	D	237	GLY
4	D	270	GLY
6	F	100	PRO
3	L	471	GLY
3	L	549	VAL
4	M	211	SER
4	M	270	GLY
3	U	549	VAL
3	U	765	PRO
4	V	211	SER
4	V	270	GLY
3	3	626	PRO
3	3	765	PRO
7	9	81	VAL
3	C	470	PRO
1	J	204	PRO
3	L	219	PRO
3	L	765	PRO
5	N	99	PRO
6	6	100	PRO
3	C	626	PRO
4	D	106	GLY
3	L	626	PRO
4	V	106	GLY
7	Y	81	VAL

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Mol	Chain	Res	Type
4	D	177	GLY
7	G	81	VAL
7	P	81	VAL
3	U	219	PRO
6	X	100	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	355/356 (100%)	318 (90%)	37 (10%)	7	24
1	A	355/356 (100%)	320 (90%)	35 (10%)	7	27
1	J	355/356 (100%)	316 (89%)	39 (11%)	6	23
1	S	355/356 (100%)	318 (90%)	37 (10%)	7	24
2	2	150/152 (99%)	131 (87%)	19 (13%)	4	18
2	B	150/152 (99%)	131 (87%)	19 (13%)	4	18
2	K	150/152 (99%)	131 (87%)	19 (13%)	4	18
2	T	150/152 (99%)	133 (89%)	17 (11%)	5	21
3	3	607/628 (97%)	541 (89%)	66 (11%)	6	23
3	C	607/628 (97%)	541 (89%)	66 (11%)	6	23
3	L	607/628 (97%)	538 (89%)	69 (11%)	5	21
3	U	607/628 (97%)	541 (89%)	66 (11%)	6	23
4	4	325/355 (92%)	288 (89%)	37 (11%)	5	21
4	D	325/355 (92%)	288 (89%)	37 (11%)	5	21
4	M	325/355 (92%)	288 (89%)	37 (11%)	5	21
4	V	325/355 (92%)	288 (89%)	37 (11%)	5	21
5	5	167/175 (95%)	147 (88%)	20 (12%)	5	20
5	E	167/175 (95%)	146 (87%)	21 (13%)	4	18
5	N	167/175 (95%)	147 (88%)	20 (12%)	5	20
5	W	167/175 (95%)	147 (88%)	20 (12%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	6	118/149 (79%)	103 (87%)	15 (13%)	4	18
6	F	118/149 (79%)	102 (86%)	16 (14%)	3	16
6	O	118/149 (79%)	103 (87%)	15 (13%)	4	18
6	X	118/149 (79%)	101 (86%)	17 (14%)	3	14
7	9	126/150 (84%)	111 (88%)	15 (12%)	5	20
7	G	126/150 (84%)	112 (89%)	14 (11%)	6	22
7	P	126/150 (84%)	111 (88%)	15 (12%)	5	20
7	Y	126/150 (84%)	112 (89%)	14 (11%)	6	22
8	7	104/106 (98%)	96 (92%)	8 (8%)	12	37
8	H	104/106 (98%)	96 (92%)	8 (8%)	12	37
8	Q	104/106 (98%)	96 (92%)	8 (8%)	12	37
8	Z	104/106 (98%)	97 (93%)	7 (7%)	15	42
All	All	7808/8284 (94%)	6938 (89%)	870 (11%)	6	22

All (870) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	10	ASP
1	1	28	THR
1	1	29	LEU
1	1	39	GLU
1	1	49	THR
1	1	104	ARG
1	1	114	LEU
1	1	128	THR
1	1	129	VAL
1	1	155	ARG
1	1	161	ASN
1	1	168	SER
1	1	184	GLU
1	1	186	THR
1	1	217	THR
1	1	228	VAL
1	1	243	THR
1	1	249	MET
1	1	253	GLN
1	1	254	ILE
1	1	255	SER

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Mol	Chain	Res	Type
1	1	270	THR
1	1	271	THR
1	1	284	LEU
1	1	295	SER
1	1	303	THR
1	1	342	TRP
1	1	346	ARG
1	1	363	VAL
1	1	368	VAL
1	1	370	LEU
1	1	374	ILE
1	1	397	ARG
1	1	414	LEU
1	1	419	ASP
1	1	437	TRP
1	1	438	ARG
2	2	5	ASP
2	2	7	LYS
2	2	31	LEU
2	2	35	GLN
2	2	45	ARG
2	2	46	ILE
2	2	53	VAL
2	2	61	MET
2	2	106	ILE
2	2	114	ASP
2	2	122	VAL
2	2	139	GLU
2	2	140	PRO
2	2	146	THR
2	2	150	LEU
2	2	153	LEU
2	2	163	LEU
2	2	172	CYS
2	2	176	VAL
3	3	11	VAL
3	3	32	LEU
3	3	42	ILE
3	3	46	ARG
3	3	73	ILE
3	3	85	THR
3	3	89	ASP

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Mol	Chain	Res	Type
3	3	94	ASP
3	3	95	THR
3	3	97	SER
3	3	99	VAL
3	3	109	GLU
3	3	121	THR
3	3	124	LYS
3	3	133	ARG
3	3	135	VAL
3	3	188	VAL
3	3	192	GLU
3	3	207	VAL
3	3	209	THR
3	3	218	LEU
3	3	239	THR
3	3	269	THR
3	3	284	GLU
3	3	286	ASN
3	3	317	LEU
3	3	321	THR
3	3	334	LYS
3	3	337	ARG
3	3	368	HIS
3	3	369	LEU
3	3	381	LEU
3	3	382	PHE
3	3	387	LEU
3	3	408	ILE
3	3	440	ARG
3	3	445	THR
3	3	450	LEU
3	3	459	MET
3	3	460	LYS
3	3	464	ILE
3	3	473	GLU
3	3	501	LYS
3	3	507	LEU
3	3	512	LEU
3	3	514	ASP
3	3	515	THR
3	3	523	LEU
3	3	542	ARG

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Mol	Chain	Res	Type
3	3	577	LEU
3	3	578	LYS
3	3	593	LEU
3	3	617	LEU
3	3	625	SER
3	3	644	LEU
3	3	655	ARG
3	3	676	LEU
3	3	683	LEU
3	3	684	ARG
3	3	705	VAL
3	3	715	GLU
3	3	716	LEU
3	3	738	THR
3	3	761	SER
3	3	771	VAL
3	3	776	LEU
4	4	40	VAL
4	4	44	MET
4	4	48	SER
4	4	59	ILE
4	4	69	THR
4	4	99	LEU
4	4	101	VAL
4	4	109	VAL
4	4	116	ILE
4	4	118	VAL
4	4	120	LEU
4	4	129	HIS
4	4	133	LEU
4	4	143	LEU
4	4	152	GLU
4	4	163	VAL
4	4	168	PHE
4	4	170	HIS
4	4	182	LEU
4	4	200	ARG
4	4	201	ILE
4	4	213	ILE
4	4	221	VAL
4	4	234	LEU
4	4	239	LEU

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Mol	Chain	Res	Type
4	4	262	PHE
4	4	272	VAL
4	4	296	ARG
4	4	303	ARG
4	4	309	ILE
4	4	310	THR
4	4	314	ARG
4	4	319	THR
4	4	333	GLU
4	4	371	ARG
4	4	380	SER
4	4	407	VAL
5	5	1	MET
5	5	5	ARG
5	5	25	LEU
5	5	27	VAL
5	5	38	MET
5	5	51	ASP
5	5	52	ILE
5	5	53	VAL
5	5	66	GLU
5	5	80	TRP
5	5	81	LYS
5	5	84	ASP
5	5	90	VAL
5	5	105	THR
5	5	124	ILE
5	5	135	ILE
5	5	142	GLU
5	5	146	LEU
5	5	175	THR
5	5	193	ARG
6	6	19	ILE
6	6	27	LEU
6	6	40	THR
6	6	45	CYS
6	6	53	SER
6	6	57	ARG
6	6	74	GLN
6	6	83	ARG
6	6	84	LEU
6	6	121	TYR

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Mol	Chain	Res	Type
6	6	124	VAL
6	6	131	VAL
6	6	147	LEU
6	6	153	GLN
6	6	163	TYR
7	9	26	TYR
7	9	33	LEU
7	9	36	ARG
7	9	42	VAL
7	9	58	LEU
7	9	85	GLU
7	9	97	ARG
7	9	99	ILE
7	9	101	CYS
7	9	134	GLU
7	9	137	LEU
7	9	140	VAL
7	9	153	THR
7	9	157	VAL
7	9	159	VAL
8	7	34	GLU
8	7	43	ARG
8	7	52	THR
8	7	53	THR
8	7	54	ILE
8	7	63	LEU
8	7	73	SER
8	7	82	ILE
1	A	10	ASP
1	A	28	THR
1	A	29	LEU
1	A	39	GLU
1	A	49	THR
1	A	96	SER
1	A	104	ARG
1	A	114	LEU
1	A	128	THR
1	A	129	VAL
1	A	155	ARG
1	A	161	ASN
1	A	168	SER
1	A	184	GLU

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Mol	Chain	Res	Type
1	A	211	LEU
1	A	217	THR
1	A	243	THR
1	A	249	MET
1	A	253	GLN
1	A	254	ILE
1	A	255	SER
1	A	270	THR
1	A	271	THR
1	A	295	SER
1	A	303	THR
1	A	342	TRP
1	A	346	ARG
1	A	363	VAL
1	A	368	VAL
1	A	374	ILE
1	A	397	ARG
1	A	414	LEU
1	A	419	ASP
1	A	437	TRP
1	A	438	ARG
2	B	5	ASP
2	B	7	LYS
2	B	31	LEU
2	B	35	GLN
2	B	45	ARG
2	B	46	ILE
2	B	53	VAL
2	B	61	MET
2	B	106	ILE
2	B	114	ASP
2	B	122	VAL
2	B	139	GLU
2	B	140	PRO
2	B	146	THR
2	B	150	LEU
2	B	153	LEU
2	B	163	LEU
2	B	172	CYS
2	B	176	VAL
3	C	11	VAL
3	C	32	LEU

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Mol	Chain	Res	Type
3	C	42	ILE
3	C	46	ARG
3	C	73	ILE
3	C	85	THR
3	C	89	ASP
3	C	94	ASP
3	C	95	THR
3	C	97	SER
3	C	99	VAL
3	C	109	GLU
3	C	121	THR
3	C	124	LYS
3	C	133	ARG
3	C	135	VAL
3	C	188	VAL
3	C	192	GLU
3	C	203	ILE
3	C	207	VAL
3	C	209	THR
3	C	218	LEU
3	C	239	THR
3	C	269	THR
3	C	274	LEU
3	C	284	GLU
3	C	286	ASN
3	C	317	LEU
3	C	321	THR
3	C	334	LYS
3	C	337	ARG
3	C	368	HIS
3	C	369	LEU
3	C	381	LEU
3	C	382	PHE
3	C	387	LEU
3	C	408	ILE
3	C	440	ARG
3	C	445	THR
3	C	450	LEU
3	C	459	MET
3	C	464	ILE
3	C	473	GLU
3	C	501	LYS

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Mol	Chain	Res	Type
3	C	512	LEU
3	C	514	ASP
3	C	523	LEU
3	C	542	ARG
3	C	577	LEU
3	C	578	LYS
3	C	593	LEU
3	C	617	LEU
3	C	625	SER
3	C	644	LEU
3	C	655	ARG
3	C	671	GLU
3	C	676	LEU
3	C	683	LEU
3	C	684	ARG
3	C	705	VAL
3	C	715	GLU
3	C	716	LEU
3	C	738	THR
3	C	761	SER
3	C	771	VAL
3	C	776	LEU
4	D	40	VAL
4	D	44	MET
4	D	48	SER
4	D	59	ILE
4	D	69	THR
4	D	99	LEU
4	D	101	VAL
4	D	109	VAL
4	D	116	ILE
4	D	118	VAL
4	D	120	LEU
4	D	129	HIS
4	D	133	LEU
4	D	143	LEU
4	D	152	GLU
4	D	163	VAL
4	D	168	PHE
4	D	170	HIS
4	D	182	LEU
4	D	200	ARG

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Mol	Chain	Res	Type
4	D	201	ILE
4	D	213	ILE
4	D	221	VAL
4	D	234	LEU
4	D	239	LEU
4	D	262	PHE
4	D	272	VAL
4	D	296	ARG
4	D	303	ARG
4	D	309	ILE
4	D	310	THR
4	D	314	ARG
4	D	319	THR
4	D	333	GLU
4	D	371	ARG
4	D	380	SER
4	D	407	VAL
5	E	1	MET
5	E	5	ARG
5	E	25	LEU
5	E	27	VAL
5	E	38	MET
5	E	51	ASP
5	E	52	ILE
5	E	53	VAL
5	E	66	GLU
5	E	80	TRP
5	E	81	LYS
5	E	84	ASP
5	E	90	VAL
5	E	105	THR
5	E	124	ILE
5	E	135	ILE
5	E	142	GLU
5	E	146	LEU
5	E	161	GLU
5	E	175	THR
5	E	193	ARG
6	F	19	ILE
6	F	27	LEU
6	F	40	THR
6	F	45	CYS

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Mol	Chain	Res	Type
6	F	53	SER
6	F	57	ARG
6	F	74	GLN
6	F	78	MET
6	F	83	ARG
6	F	84	LEU
6	F	121	TYR
6	F	124	VAL
6	F	131	VAL
6	F	147	LEU
6	F	153	GLN
6	F	163	TYR
7	G	26	TYR
7	G	33	LEU
7	G	36	ARG
7	G	42	VAL
7	G	58	LEU
7	G	85	GLU
7	G	97	ARG
7	G	99	ILE
7	G	101	CYS
7	G	134	GLU
7	G	140	VAL
7	G	153	THR
7	G	157	VAL
7	G	159	VAL
8	H	34	GLU
8	H	43	ARG
8	H	52	THR
8	H	53	THR
8	H	54	ILE
8	H	63	LEU
8	H	73	SER
8	H	82	ILE
1	J	10	ASP
1	J	28	THR
1	J	29	LEU
1	J	39	GLU
1	J	49	THR
1	J	104	ARG
1	J	106	ILE
1	J	114	LEU

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Mol	Chain	Res	Type
1	J	128	THR
1	J	129	VAL
1	J	155	ARG
1	J	161	ASN
1	J	168	SER
1	J	184	GLU
1	J	203	PRO
1	J	211	LEU
1	J	217	THR
1	J	233	ARG
1	J	243	THR
1	J	249	MET
1	J	253	GLN
1	J	254	ILE
1	J	255	SER
1	J	270	THR
1	J	271	THR
1	J	291	ILE
1	J	295	SER
1	J	303	THR
1	J	342	TRP
1	J	346	ARG
1	J	363	VAL
1	J	368	VAL
1	J	370	LEU
1	J	374	ILE
1	J	397	ARG
1	J	414	LEU
1	J	419	ASP
1	J	437	TRP
1	J	438	ARG
2	K	5	ASP
2	K	7	LYS
2	K	31	LEU
2	K	35	GLN
2	K	45	ARG
2	K	46	ILE
2	K	53	VAL
2	K	61	MET
2	K	106	ILE
2	K	114	ASP
2	K	122	VAL

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Mol	Chain	Res	Type
2	K	139	GLU
2	K	140	PRO
2	K	146	THR
2	K	150	LEU
2	K	153	LEU
2	K	163	LEU
2	K	172	CYS
2	K	176	VAL
3	L	11	VAL
3	L	32	LEU
3	L	42	ILE
3	L	46	ARG
3	L	73	ILE
3	L	85	THR
3	L	89	ASP
3	L	94	ASP
3	L	95	THR
3	L	97	SER
3	L	99	VAL
3	L	109	GLU
3	L	121	THR
3	L	124	LYS
3	L	133	ARG
3	L	135	VAL
3	L	188	VAL
3	L	192	GLU
3	L	203	ILE
3	L	207	VAL
3	L	209	THR
3	L	218	LEU
3	L	229	ILE
3	L	239	THR
3	L	269	THR
3	L	274	LEU
3	L	284	GLU
3	L	286	ASN
3	L	317	LEU
3	L	321	THR
3	L	334	LYS
3	L	337	ARG
3	L	368	HIS
3	L	369	LEU

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Mol	Chain	Res	Type
3	L	381	LEU
3	L	382	PHE
3	L	387	LEU
3	L	408	ILE
3	L	440	ARG
3	L	445	THR
3	L	450	LEU
3	L	459	MET
3	L	460	LYS
3	L	464	ILE
3	L	473	GLU
3	L	501	LYS
3	L	512	LEU
3	L	514	ASP
3	L	515	THR
3	L	523	LEU
3	L	542	ARG
3	L	577	LEU
3	L	578	LYS
3	L	593	LEU
3	L	617	LEU
3	L	625	SER
3	L	644	LEU
3	L	655	ARG
3	L	671	GLU
3	L	676	LEU
3	L	683	LEU
3	L	684	ARG
3	L	705	VAL
3	L	715	GLU
3	L	716	LEU
3	L	738	THR
3	L	761	SER
3	L	771	VAL
3	L	776	LEU
4	M	40	VAL
4	M	44	MET
4	M	48	SER
4	M	59	ILE
4	M	69	THR
4	M	99	LEU
4	M	101	VAL

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Mol	Chain	Res	Type
4	M	109	VAL
4	M	116	ILE
4	M	118	VAL
4	M	120	LEU
4	M	129	HIS
4	M	133	LEU
4	M	143	LEU
4	M	152	GLU
4	M	163	VAL
4	M	168	PHE
4	M	170	HIS
4	M	182	LEU
4	M	200	ARG
4	M	201	ILE
4	M	213	ILE
4	M	221	VAL
4	M	234	LEU
4	M	239	LEU
4	M	262	PHE
4	M	272	VAL
4	M	296	ARG
4	M	303	ARG
4	M	309	ILE
4	M	310	THR
4	M	314	ARG
4	M	319	THR
4	M	333	GLU
4	M	371	ARG
4	M	380	SER
4	M	407	VAL
5	N	1	MET
5	N	5	ARG
5	N	25	LEU
5	N	27	VAL
5	N	38	MET
5	N	51	ASP
5	N	52	ILE
5	N	53	VAL
5	N	66	GLU
5	N	80	TRP
5	N	81	LYS
5	N	84	ASP

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Mol	Chain	Res	Type
5	N	90	VAL
5	N	105	THR
5	N	124	ILE
5	N	135	ILE
5	N	142	GLU
5	N	146	LEU
5	N	175	THR
5	N	193	ARG
6	O	19	ILE
6	O	27	LEU
6	O	40	THR
6	O	45	CYS
6	O	53	SER
6	O	57	ARG
6	O	74	GLN
6	O	83	ARG
6	O	84	LEU
6	O	121	TYR
6	O	124	VAL
6	O	131	VAL
6	O	147	LEU
6	O	153	GLN
6	O	163	TYR
7	P	26	TYR
7	P	33	LEU
7	P	36	ARG
7	P	42	VAL
7	P	58	LEU
7	P	85	GLU
7	P	97	ARG
7	P	99	ILE
7	P	101	CYS
7	P	134	GLU
7	P	137	LEU
7	P	140	VAL
7	P	153	THR
7	P	157	VAL
7	P	159	VAL
8	Q	34	GLU
8	Q	43	ARG
8	Q	52	THR
8	Q	53	THR

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Mol	Chain	Res	Type
8	Q	54	ILE
8	Q	63	LEU
8	Q	73	SER
8	Q	82	ILE
1	S	10	ASP
1	S	28	THR
1	S	29	LEU
1	S	39	GLU
1	S	49	THR
1	S	96	SER
1	S	104	ARG
1	S	106	ILE
1	S	114	LEU
1	S	128	THR
1	S	129	VAL
1	S	155	ARG
1	S	161	ASN
1	S	168	SER
1	S	184	GLU
1	S	186	THR
1	S	203	PRO
1	S	211	LEU
1	S	217	THR
1	S	249	MET
1	S	253	GLN
1	S	254	ILE
1	S	255	SER
1	S	270	THR
1	S	271	THR
1	S	295	SER
1	S	303	THR
1	S	342	TRP
1	S	346	ARG
1	S	363	VAL
1	S	368	VAL
1	S	370	LEU
1	S	374	ILE
1	S	397	ARG
1	S	414	LEU
1	S	419	ASP
1	S	438	ARG
2	T	5	ASP

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Mol	Chain	Res	Type
2	T	7	LYS
2	T	31	LEU
2	T	35	GLN
2	T	45	ARG
2	T	53	VAL
2	T	61	MET
2	T	106	ILE
2	T	114	ASP
2	T	122	VAL
2	T	139	GLU
2	T	146	THR
2	T	150	LEU
2	T	153	LEU
2	T	163	LEU
2	T	172	CYS
2	T	176	VAL
3	U	11	VAL
3	U	32	LEU
3	U	42	ILE
3	U	46	ARG
3	U	73	ILE
3	U	85	THR
3	U	89	ASP
3	U	94	ASP
3	U	95	THR
3	U	97	SER
3	U	99	VAL
3	U	109	GLU
3	U	121	THR
3	U	124	LYS
3	U	133	ARG
3	U	135	VAL
3	U	188	VAL
3	U	192	GLU
3	U	207	VAL
3	U	209	THR
3	U	218	LEU
3	U	239	THR
3	U	269	THR
3	U	274	LEU
3	U	284	GLU
3	U	286	ASN

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Mol	Chain	Res	Type
3	U	317	LEU
3	U	321	THR
3	U	334	LYS
3	U	337	ARG
3	U	368	HIS
3	U	369	LEU
3	U	381	LEU
3	U	382	PHE
3	U	387	LEU
3	U	408	ILE
3	U	440	ARG
3	U	445	THR
3	U	450	LEU
3	U	459	MET
3	U	460	LYS
3	U	464	ILE
3	U	473	GLU
3	U	501	LYS
3	U	512	LEU
3	U	514	ASP
3	U	515	THR
3	U	523	LEU
3	U	542	ARG
3	U	578	LYS
3	U	593	LEU
3	U	617	LEU
3	U	625	SER
3	U	644	LEU
3	U	655	ARG
3	U	676	LEU
3	U	683	LEU
3	U	684	ARG
3	U	705	VAL
3	U	715	GLU
3	U	716	LEU
3	U	738	THR
3	U	743	VAL
3	U	761	SER
3	U	771	VAL
3	U	776	LEU
4	V	40	VAL
4	V	44	MET

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Mol	Chain	Res	Type
4	V	48	SER
4	V	59	ILE
4	V	69	THR
4	V	99	LEU
4	V	101	VAL
4	V	109	VAL
4	V	116	ILE
4	V	118	VAL
4	V	120	LEU
4	V	129	HIS
4	V	133	LEU
4	V	143	LEU
4	V	152	GLU
4	V	163	VAL
4	V	168	PHE
4	V	170	HIS
4	V	182	LEU
4	V	200	ARG
4	V	201	ILE
4	V	213	ILE
4	V	221	VAL
4	V	234	LEU
4	V	239	LEU
4	V	262	PHE
4	V	272	VAL
4	V	296	ARG
4	V	303	ARG
4	V	309	ILE
4	V	310	THR
4	V	314	ARG
4	V	319	THR
4	V	333	GLU
4	V	371	ARG
4	V	380	SER
4	V	407	VAL
5	W	1	MET
5	W	5	ARG
5	W	25	LEU
5	W	27	VAL
5	W	38	MET
5	W	51	ASP
5	W	52	ILE

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Mol	Chain	Res	Type
5	W	53	VAL
5	W	66	GLU
5	W	80	TRP
5	W	81	LYS
5	W	84	ASP
5	W	90	VAL
5	W	105	THR
5	W	124	ILE
5	W	135	ILE
5	W	142	GLU
5	W	146	LEU
5	W	175	THR
5	W	193	ARG
6	X	19	ILE
6	X	27	LEU
6	X	40	THR
6	X	45	CYS
6	X	53	SER
6	X	57	ARG
6	X	74	GLN
6	X	78	MET
6	X	83	ARG
6	X	84	LEU
6	X	121	TYR
6	X	123	ILE
6	X	124	VAL
6	X	131	VAL
6	X	147	LEU
6	X	153	GLN
6	X	163	TYR
7	Y	26	TYR
7	Y	33	LEU
7	Y	36	ARG
7	Y	42	VAL
7	Y	58	LEU
7	Y	85	GLU
7	Y	97	ARG
7	Y	99	ILE
7	Y	101	CYS
7	Y	134	GLU
7	Y	137	LEU
7	Y	153	THR

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Mol	Chain	Res	Type
7	Y	157	VAL
7	Y	159	VAL
8	Z	34	GLU
8	Z	43	ARG
8	Z	52	THR
8	Z	54	ILE
8	Z	63	LEU
8	Z	73	SER
8	Z	82	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	86	GLN
1	1	92	ASN
1	1	198	ASN
1	1	288	GLN
3	3	104	GLN
3	3	428	HIS
3	3	613	HIS
3	3	661	GLN
3	3	733	GLN
4	4	72	HIS
4	4	166	GLN
4	4	199	HIS
5	5	129	HIS
5	5	144	HIS
6	6	34	ASN
6	6	153	GLN
8	7	94	HIS
1	A	86	GLN
1	A	92	ASN
1	A	174	HIS
1	A	198	ASN
1	A	219	ASN
3	C	38	HIS
3	C	104	GLN
3	C	246	ASN
3	C	428	HIS
3	C	468	HIS
3	C	613	HIS
3	C	661	GLN

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Mol	Chain	Res	Type
3	C	733	GLN
4	D	72	HIS
4	D	166	GLN
4	D	199	HIS
5	E	129	HIS
6	F	34	ASN
6	F	153	GLN
8	H	94	HIS
1	J	86	GLN
1	J	92	ASN
1	J	198	ASN
1	J	219	ASN
3	L	104	GLN
3	L	183	HIS
3	L	368	HIS
3	L	424	HIS
3	L	468	HIS
3	L	613	HIS
3	L	661	GLN
3	L	733	GLN
4	M	72	HIS
4	M	166	GLN
4	M	169	HIS
4	M	245	ASN
4	M	377	ASN
5	N	129	HIS
6	O	34	ASN
6	O	153	GLN
6	O	155	GLN
8	Q	94	HIS
1	S	86	GLN
1	S	92	ASN
1	S	198	ASN
1	S	219	ASN
3	U	104	GLN
3	U	246	ASN
3	U	428	HIS
3	U	613	HIS
3	U	661	GLN
3	U	733	GLN
4	V	72	HIS
4	V	166	GLN

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Mol	Chain	Res	Type
4	V	169	HIS
4	V	170	HIS
4	V	199	HIS
4	V	377	ASN
5	W	129	HIS
6	X	34	ASN
6	X	153	GLN
8	Z	94	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 16 are monoatomic - leaving 40 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	$\# Z > 2$
11	FES	K	182	2	0,4,4	-	-	-		
9	SF4	9	183	7	0,12,12	-	-	-		
9	SF4	9	184	7	0,12,12	-	-	-		
10	FMN	S	440	-	33,33,33	1.19	3 (9%)	48,50,50	1.94	14 (29%)
11	FES	2	182	2	0,4,4	-	-	-		
9	SF4	F	182	6	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SF4	L	786	3	0,12,12	-	-	-		
11	FES	C	787	3	0,4,4	-	-	-		
9	SF4	J	439	1	0,12,12	-	-	-		
11	FES	U	787	3	0,4,4	-	-	-		
9	SF4	L	784	3	0,12,12	-	-	-		
9	SF4	U	785	3	0,12,12	-	-	-		
9	SF4	U	786	3	0,12,12	-	-	-		
9	SF4	P	183	7	0,12,12	-	-	-		
9	SF4	P	184	7	0,12,12	-	-	-		
9	SF4	3	785	3	0,12,12	-	-	-		
9	SF4	A	439	1	0,12,12	-	-	-		
9	SF4	L	785	3	0,12,12	-	-	-		
9	SF4	3	784	3	0,12,12	-	-	-		
11	FES	B	182	2	0,4,4	-	-	-		
11	FES	3	787	3	0,4,4	-	-	-		
11	FES	L	787	3	0,4,4	-	-	-		
9	SF4	X	182	6	0,12,12	-	-	-		
9	SF4	6	182	6	0,12,12	-	-	-		
9	SF4	U	784	3	0,12,12	-	-	-		
9	SF4	C	786	3	0,12,12	-	-	-		
9	SF4	G	183	7	0,12,12	-	-	-		
9	SF4	C	784	3	0,12,12	-	-	-		
10	FMN	1	440	-	33,33,33	1.23	3 (9%)	48,50,50	2.07	13 (27%)
9	SF4	3	786	3	0,12,12	-	-	-		
9	SF4	O	182	6	0,12,12	-	-	-		
9	SF4	G	184	7	0,12,12	-	-	-		
9	SF4	Y	184	7	0,12,12	-	-	-		
10	FMN	A	440	-	33,33,33	1.25	4 (12%)	48,50,50	1.81	11 (22%)
9	SF4	C	785	3	0,12,12	-	-	-		
9	SF4	1	439	1	0,12,12	-	-	-		
9	SF4	S	439	1	0,12,12	-	-	-		
11	FES	T	182	2	0,4,4	-	-	-		
10	FMN	J	440	-	33,33,33	1.24	3 (9%)	48,50,50	1.73	11 (22%)
9	SF4	Y	183	7	0,12,12	-	-	-		

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
11	FES	K	182	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	9	183	7	-	-	0/6/5/5
9	SF4	9	184	7	-	-	0/6/5/5
10	FMN	S	440	-	-	2/18/18/18	0/3/3/3
11	FES	2	182	2	-	-	0/1/1/1
9	SF4	F	182	6	-	-	0/6/5/5
9	SF4	L	786	3	-	-	0/6/5/5
11	FES	C	787	3	-	-	0/1/1/1
9	SF4	J	439	1	-	-	0/6/5/5
11	FES	U	787	3	-	-	0/1/1/1
9	SF4	L	784	3	-	-	0/6/5/5
9	SF4	U	785	3	-	-	0/6/5/5
9	SF4	U	786	3	-	-	0/6/5/5
9	SF4	P	183	7	-	-	0/6/5/5
9	SF4	P	184	7	-	-	0/6/5/5
9	SF4	3	785	3	-	-	0/6/5/5
9	SF4	A	439	1	-	-	0/6/5/5
9	SF4	3	784	3	-	-	0/6/5/5
9	SF4	L	785	3	-	-	0/6/5/5
11	FES	B	182	2	-	-	0/1/1/1
11	FES	3	787	3	-	-	0/1/1/1
11	FES	L	787	3	-	-	0/1/1/1
9	SF4	X	182	6	-	-	0/6/5/5
9	SF4	6	182	6	-	-	0/6/5/5
9	SF4	U	784	3	-	-	0/6/5/5
9	SF4	C	786	3	-	-	0/6/5/5
9	SF4	G	183	7	-	-	0/6/5/5
9	SF4	C	784	3	-	-	0/6/5/5
10	FMN	1	440	-	-	6/18/18/18	0/3/3/3
9	SF4	3	786	3	-	-	0/6/5/5
9	SF4	O	182	6	-	-	0/6/5/5
9	SF4	G	184	7	-	-	0/6/5/5
10	FMN	A	440	-	-	7/18/18/18	0/3/3/3
9	SF4	Y	184	7	-	-	0/6/5/5
9	SF4	C	785	3	-	-	0/6/5/5
9	SF4	1	439	1	-	-	0/6/5/5
9	SF4	S	439	1	-	-	0/6/5/5
11	FES	T	182	2	-	-	0/1/1/1
10	FMN	J	440	-	-	5/18/18/18	0/3/3/3
9	SF4	Y	183	7	-	-	0/6/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	440	FMN	C4A-N5	4.15	1.39	1.30
10	1	440	FMN	C4A-N5	3.95	1.39	1.30
10	S	440	FMN	C4A-N5	3.84	1.39	1.30
10	J	440	FMN	C4A-N5	3.69	1.38	1.30
10	A	440	FMN	C10-N1	2.73	1.38	1.33
10	J	440	FMN	C10-N1	2.64	1.38	1.33
10	S	440	FMN	C10-N1	2.60	1.38	1.33
10	1	440	FMN	C10-N1	2.57	1.38	1.33
10	A	440	FMN	C1'-C2'	-2.42	1.49	1.52
10	1	440	FMN	C9A-N10	-2.34	1.37	1.41
10	S	440	FMN	C9A-N10	-2.30	1.37	1.41
10	A	440	FMN	C9A-N10	-2.18	1.37	1.41
10	J	440	FMN	C9A-N10	-2.04	1.37	1.41

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	1	440	FMN	C5'-C4'-C3'	-8.32	96.52	112.22
10	S	440	FMN	C5'-C4'-C3'	-6.77	99.44	112.22
10	A	440	FMN	C1'-C2'-C3'	-6.27	92.66	109.66
10	J	440	FMN	C1'-C2'-C3'	-5.90	93.67	109.66
10	A	440	FMN	C5'-C4'-C3'	-5.25	102.32	112.22
10	1	440	FMN	C1'-C2'-C3'	-5.09	95.86	109.66
10	S	440	FMN	C1'-C2'-C3'	-4.61	97.17	109.66
10	S	440	FMN	C4'-C3'-C2'	3.89	120.05	113.57
10	J	440	FMN	C5'-C4'-C3'	-3.45	105.70	112.22
10	1	440	FMN	C4'-C3'-C2'	3.42	119.26	113.57
10	1	440	FMN	C9A-C5A-N5	-3.26	118.99	122.45
10	J	440	FMN	O4'-C4'-C5'	3.24	117.14	109.99
10	1	440	FMN	C4-N3-C2	-3.02	120.28	125.64
10	A	440	FMN	C10-C4A-N5	-2.94	118.81	124.81
10	J	440	FMN	C4-N3-C2	-2.88	120.52	125.64
10	S	440	FMN	O5'-C5'-C4'	2.81	116.86	109.36
10	S	440	FMN	C9A-C5A-N5	-2.79	119.49	122.45
10	J	440	FMN	C9A-C5A-N5	-2.76	119.53	122.45
10	J	440	FMN	C10-C4A-N5	-2.72	119.26	124.81
10	1	440	FMN	C10-C4A-N5	-2.69	119.31	124.81
10	S	440	FMN	C4-N3-C2	-2.69	120.87	125.64
10	S	440	FMN	C10-C4A-N5	-2.66	119.38	124.81
10	A	440	FMN	C9A-C5A-N5	-2.64	119.65	122.45
10	A	440	FMN	C4-C4A-N5	2.64	121.86	118.21
10	S	440	FMN	O4-C4-C4A	-2.59	119.70	126.53
10	1	440	FMN	C4A-C4-N3	2.56	119.76	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	1	440	FMN	C5A-C9A-N10	2.54	120.26	117.97
10	A	440	FMN	C4A-C10-N10	2.43	119.96	116.48
10	1	440	FMN	C9-C9A-N10	-2.43	118.59	121.85
10	1	440	FMN	O4-C4-C4A	-2.39	120.22	126.53
10	J	440	FMN	O4-C4-C4A	-2.39	120.23	126.53
10	S	440	FMN	C4A-C4-N3	2.39	119.33	113.25
10	S	440	FMN	C4A-C10-N10	2.38	119.88	116.48
10	1	440	FMN	C4-C4A-N5	2.30	121.39	118.21
10	J	440	FMN	C4A-C4-N3	2.25	118.97	113.25
10	S	440	FMN	C9-C9A-N10	-2.24	118.84	121.85
10	S	440	FMN	O2'-C2'-C3'	2.22	114.45	109.25
10	S	440	FMN	C5A-C9A-N10	2.21	119.96	117.97
10	A	440	FMN	C9-C9A-N10	-2.21	118.89	121.85
10	J	440	FMN	C2'-C1'-N10	2.21	120.62	110.20
10	A	440	FMN	O4-C4-C4A	-2.14	120.88	126.53
10	S	440	FMN	C4-C4A-N5	2.12	121.14	118.21
10	A	440	FMN	O3P-P-O5'	2.11	112.17	106.67
10	1	440	FMN	O2'-C2'-C3'	2.08	114.12	109.25
10	J	440	FMN	C5A-C9A-N10	2.04	119.81	117.97
10	J	440	FMN	C4A-C10-N10	2.03	119.38	116.48
10	A	440	FMN	C5A-C9A-N10	2.01	119.79	117.97
10	1	440	FMN	C4A-C10-N10	2.01	119.36	116.48
10	A	440	FMN	C4-N3-C2	-2.01	122.08	125.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	1	440	FMN	N10-C1'-C2'-O2'
10	1	440	FMN	N10-C1'-C2'-C3'
10	1	440	FMN	C1'-C2'-C3'-O3'
10	1	440	FMN	C1'-C2'-C3'-C4'
10	A	440	FMN	N10-C1'-C2'-O2'
10	A	440	FMN	N10-C1'-C2'-C3'
10	A	440	FMN	C3'-C4'-C5'-O5'
10	A	440	FMN	O4'-C4'-C5'-O5'
10	A	440	FMN	C5'-O5'-P-O1P
10	A	440	FMN	C5'-O5'-P-O2P
10	A	440	FMN	C5'-O5'-P-O3P
10	J	440	FMN	N10-C1'-C2'-O2'
10	J	440	FMN	N10-C1'-C2'-C3'
10	J	440	FMN	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
10	J	440	FMN	O4'-C4'-C5'-O5'
10	S	440	FMN	N10-C1'-C2'-O2'
10	S	440	FMN	N10-C1'-C2'-C3'
10	1	440	FMN	O2'-C2'-C3'-C4'
10	1	440	FMN	O2'-C2'-C3'-O3'
10	J	440	FMN	O3'-C3'-C4'-C5'

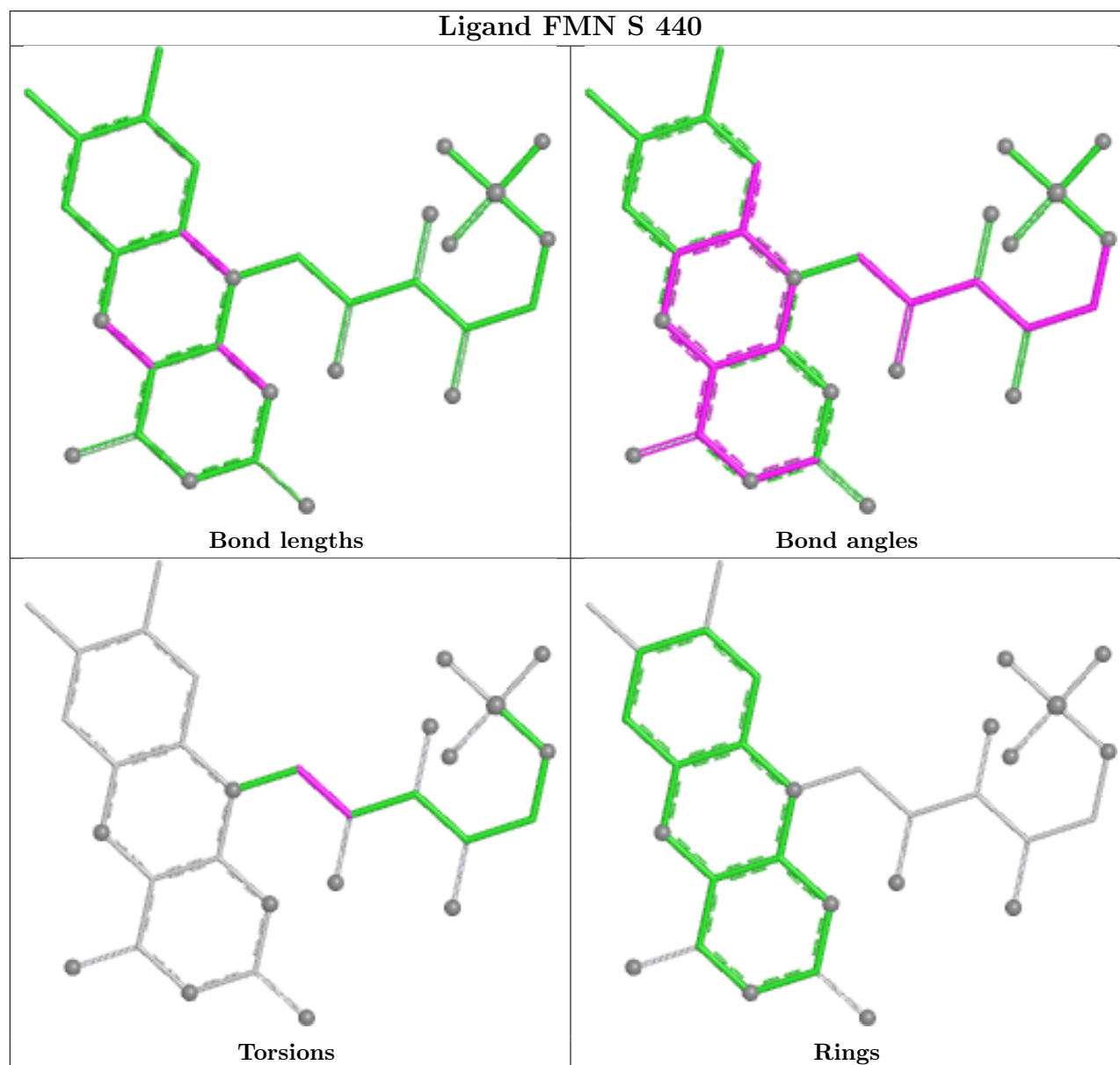
There are no ring outliers.

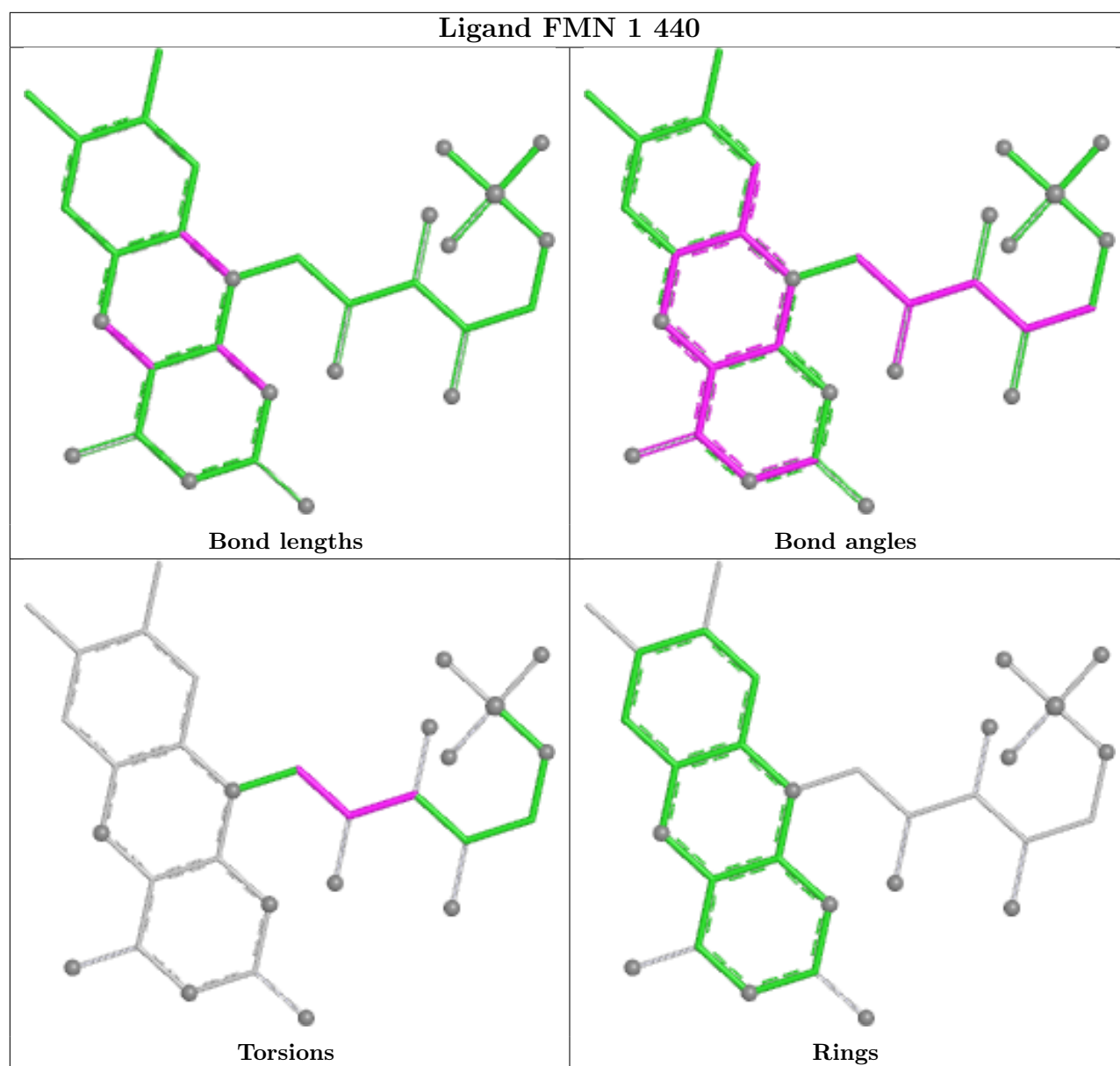
29 monomers are involved in 58 short contacts:

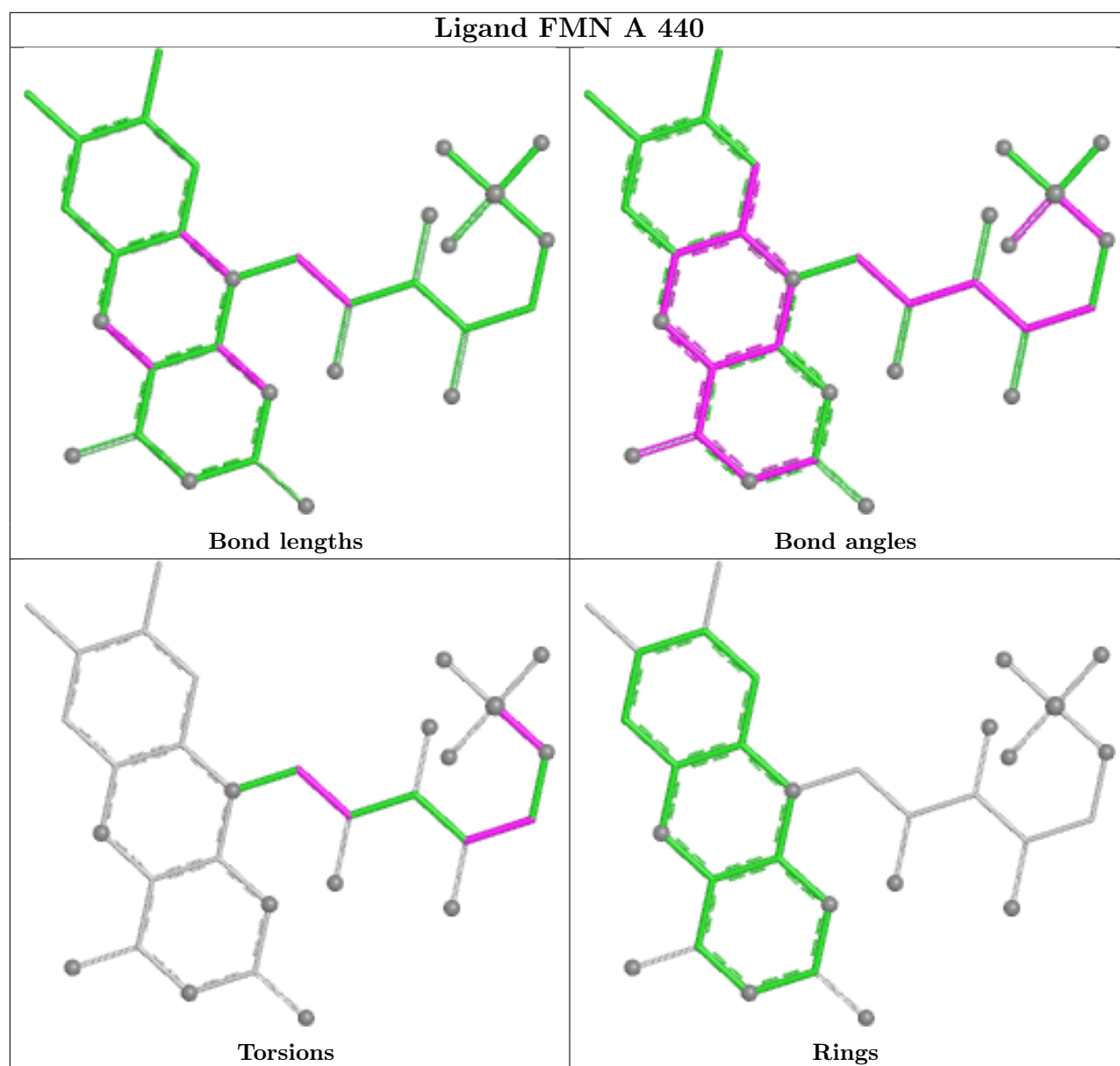
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	182	FES	1	0
9	9	183	SF4	1	0
9	9	184	SF4	1	0
10	S	440	FMN	6	0
11	2	182	FES	1	0
9	F	182	SF4	3	0
9	L	786	SF4	1	0
11	C	787	FES	1	0
9	L	784	SF4	1	0
9	U	785	SF4	1	0
9	P	183	SF4	1	0
9	P	184	SF4	1	0
9	3	785	SF4	1	0
9	A	439	SF4	1	0
9	L	785	SF4	1	0
9	3	784	SF4	1	0
11	B	182	FES	1	0
9	X	182	SF4	3	0
9	6	182	SF4	2	0
9	U	784	SF4	1	0
9	G	183	SF4	1	0
10	1	440	FMN	7	0
9	3	786	SF4	1	0
9	O	182	SF4	2	0
9	G	184	SF4	1	0
10	A	440	FMN	6	0
9	C	785	SF4	1	0
11	T	182	FES	1	0
10	J	440	FMN	8	0

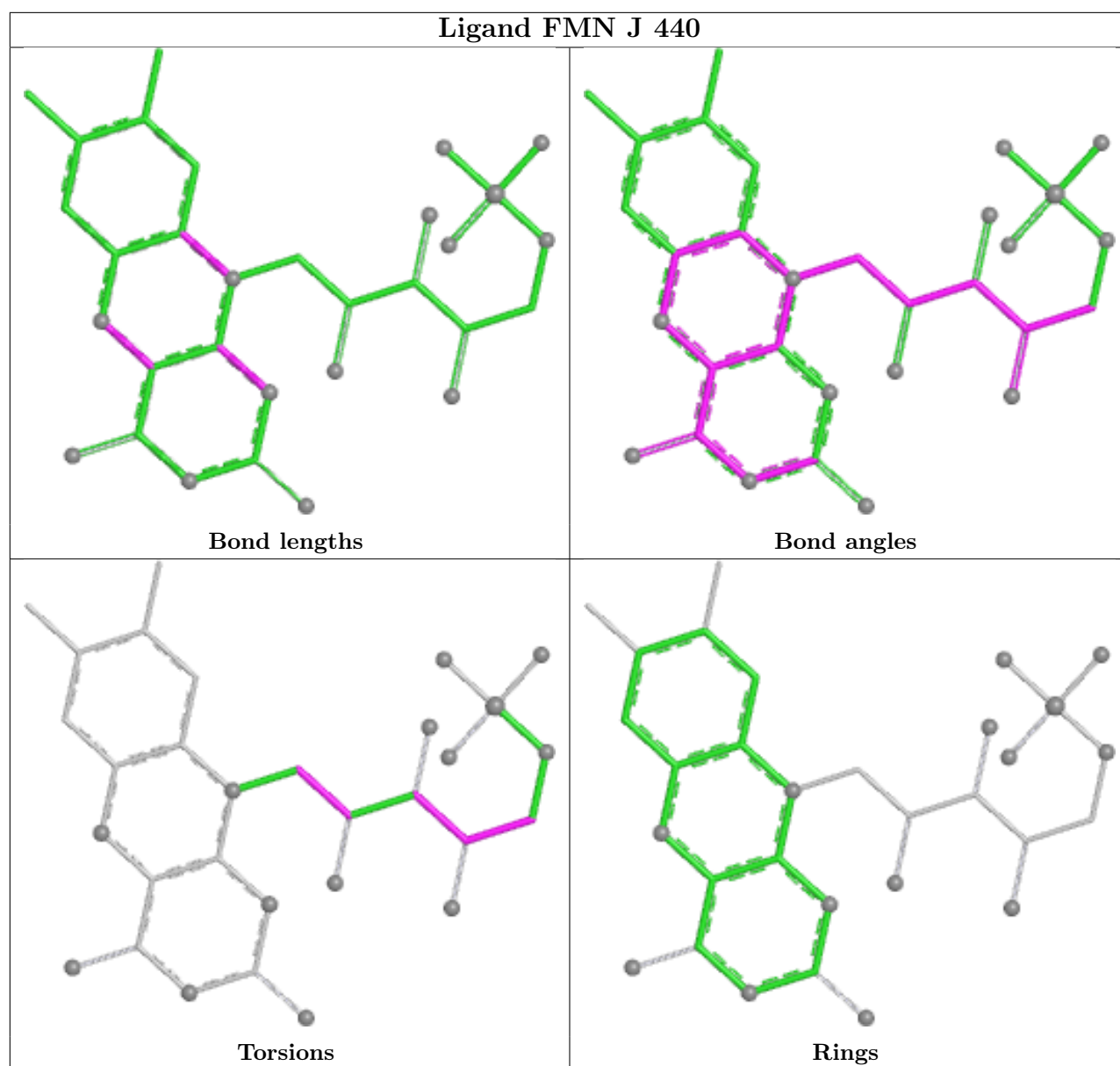
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	437/438 (99%)	-1.75	0 100 100	38, 59, 83, 110	0
1	A	437/438 (99%)	-1.73	0 100 100	40, 60, 84, 110	0
1	J	437/438 (99%)	-1.73	0 100 100	39, 59, 83, 110	0
1	S	437/438 (99%)	-1.77	0 100 100	39, 60, 83, 111	0
2	2	178/181 (98%)	-1.74	0 100 100	43, 63, 93, 135	0
2	B	178/181 (98%)	-1.70	0 100 100	43, 64, 94, 134	0
2	K	178/181 (98%)	-1.73	0 100 100	43, 63, 93, 136	0
2	T	178/181 (98%)	-1.75	0 100 100	43, 64, 94, 134	0
3	3	754/783 (96%)	-1.71	0 100 100	36, 74, 112, 133	0
3	C	754/783 (96%)	-1.72	0 100 100	36, 75, 113, 134	0
3	L	754/783 (96%)	-1.69	0 100 100	37, 75, 114, 133	0
3	U	754/783 (96%)	-1.72	0 100 100	36, 75, 113, 134	0
4	4	377/409 (92%)	-1.68	0 100 100	38, 78, 112, 129	0
4	D	377/409 (92%)	-1.72	0 100 100	38, 77, 112, 129	0
4	M	377/409 (92%)	-1.68	0 100 100	38, 78, 112, 129	0
4	V	377/409 (92%)	-1.67	0 100 100	39, 78, 112, 130	0
5	5	196/207 (94%)	-1.66	0 100 100	50, 83, 120, 132	0
5	E	196/207 (94%)	-1.67	0 100 100	51, 83, 120, 132	0
5	N	196/207 (94%)	-1.68	0 100 100	50, 83, 120, 132	0
5	W	196/207 (94%)	-1.61	0 100 100	52, 84, 120, 133	0
6	6	145/181 (80%)	-1.69	0 100 100	51, 71, 104, 125	0
6	F	145/181 (80%)	-1.64	0 100 100	49, 71, 105, 125	0
6	O	145/181 (80%)	-1.62	0 100 100	50, 71, 105, 125	0
6	X	145/181 (80%)	-1.61	0 100 100	51, 72, 105, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9		
7	9	154/182 (84%)	-1.78	0	100	100	37, 59, 96, 136	0
7	G	154/182 (84%)	-1.74	0	100	100	37, 58, 95, 135	0
7	P	154/182 (84%)	-1.79	0	100	100	37, 59, 95, 136	0
7	Y	154/182 (84%)	-1.72	0	100	100	37, 60, 96, 136	0
8	7	127/129 (98%)	-1.79	0	100	100	49, 66, 101, 119	0
8	H	127/129 (98%)	-1.78	0	100	100	48, 66, 101, 120	0
8	Q	127/129 (98%)	-1.76	0	100	100	48, 66, 102, 120	0
8	Z	127/129 (98%)	-1.77	0	100	100	48, 67, 101, 119	0
All	All	9472/10040 (94%)	-1.71	0	100	100	36, 69, 111, 136	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	CA	T	202	1/1	0.97	0.03	100,100,100,100	0
12	CA	B	202	1/1	0.98	0.02	108,108,108,108	0
10	FMN	A	440	31/31	0.99	0.04	48,60,64,66	0
10	FMN	J	440	31/31	0.99	0.04	42,53,60,63	0
9	SF4	6	182	8/8	1.00	0.01	24,37,69,69	0
9	SF4	9	183	8/8	1.00	0.01	12,19,45,48	0
9	SF4	9	184	8/8	1.00	0.01	7,27,44,48	0
9	SF4	A	439	8/8	1.00	0.01	13,26,49,50	0
9	SF4	C	784	8/8	1.00	0.01	13,18,40,40	0

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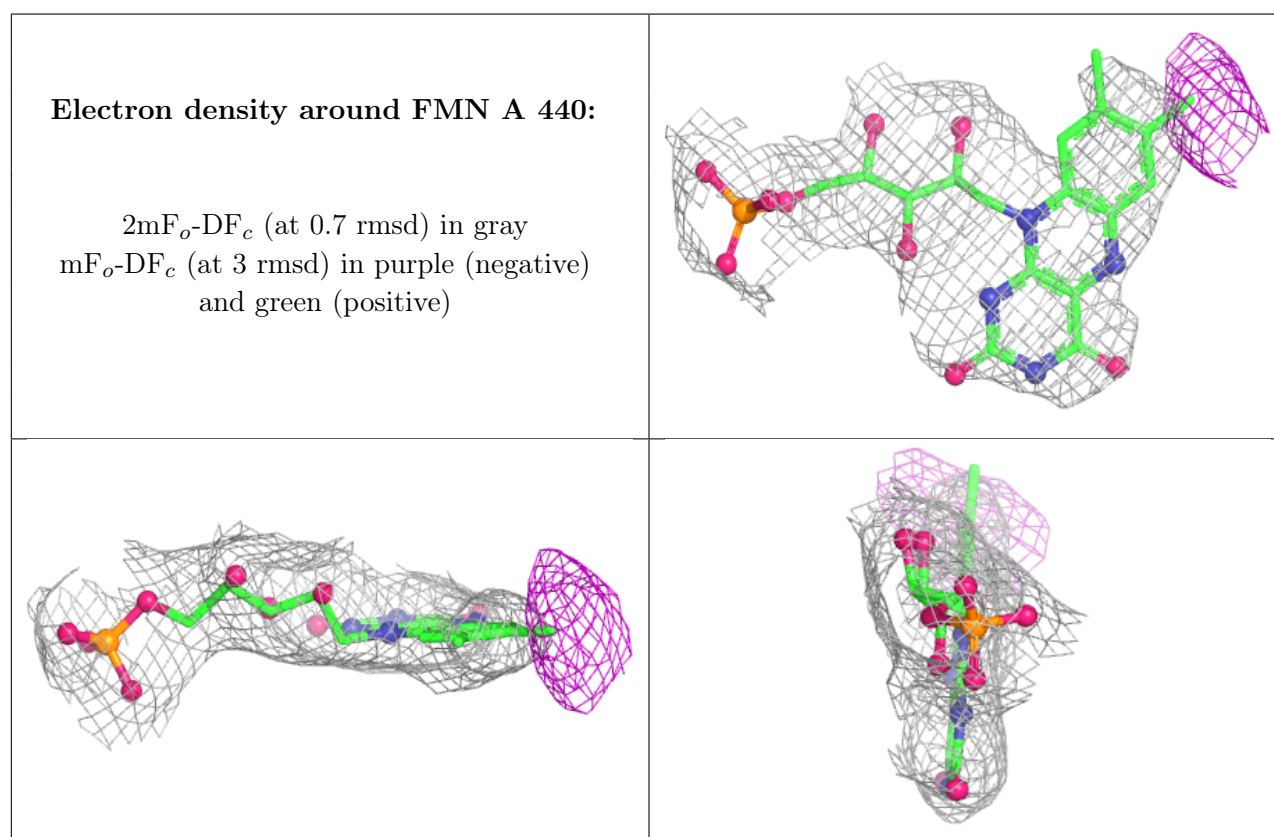
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SF4	C	785	8/8	1.00	0.01	12,22,39,40	0
9	SF4	C	786	8/8	1.00	0.01	21,34,56,59	0
9	SF4	F	182	8/8	1.00	0.01	18,31,51,62	0
9	SF4	G	183	8/8	1.00	0.01	11,18,42,46	0
9	SF4	G	184	8/8	1.00	0.01	12,15,39,39	0
9	SF4	J	439	8/8	1.00	0.01	8,25,43,44	0
9	SF4	L	784	8/8	1.00	0.01	11,17,34,42	0
9	SF4	L	785	8/8	1.00	0.02	11,18,39,39	0
9	SF4	L	786	8/8	1.00	0.01	30,39,61,62	0
9	SF4	O	182	8/8	1.00	0.01	18,27,54,59	0
9	SF4	P	183	8/8	1.00	0.01	10,16,42,46	0
9	SF4	P	184	8/8	1.00	0.02	1,19,41,41	0
9	SF4	S	439	8/8	1.00	0.01	19,27,49,51	0
9	SF4	U	784	8/8	1.00	0.01	15,26,43,43	0
9	SF4	U	785	8/8	1.00	0.02	19,27,43,43	0
9	SF4	U	786	8/8	1.00	0.01	21,33,51,58	0
9	SF4	X	182	8/8	1.00	0.01	39,56,81,89	0
9	SF4	Y	183	8/8	1.00	0.01	17,35,53,57	0
9	SF4	Y	184	8/8	1.00	0.01	19,29,51,57	0
10	FMN	1	440	31/31	1.00	0.03	48,54,62,68	0
9	SF4	1	439	8/8	1.00	0.01	13,24,43,45	0
9	SF4	3	784	8/8	1.00	0.01	12,16,36,38	0
10	FMN	S	440	31/31	1.00	0.02	53,60,65,66	0
11	FES	2	182	4/4	1.00	0.01	11,18,41,42	0
11	FES	3	787	4/4	1.00	0.01	17,20,34,47	0
11	FES	B	182	4/4	1.00	0.01	15,29,43,48	0
11	FES	C	787	4/4	1.00	0.01	22,23,31,43	0
11	FES	K	182	4/4	1.00	0.01	14,22,42,44	0
11	FES	L	787	4/4	1.00	0.01	16,17,33,41	0
11	FES	T	182	4/4	1.00	0.02	18,26,47,47	0
11	FES	U	787	4/4	1.00	0.01	22,28,34,45	0
12	CA	2	202	1/1	1.00	0.03	58,58,58,58	0
12	CA	3	788	1/1	1.00	0.01	43,43,43,43	0
12	CA	3	789	1/1	1.00	0.01	50,50,50,50	0
12	CA	9	201	1/1	1.00	0.05	37,37,37,37	0
9	SF4	3	785	8/8	1.00	0.01	8,18,36,38	0
12	CA	C	788	1/1	1.00	0.01	46,46,46,46	0
12	CA	G	201	1/1	1.00	0.02	43,43,43,43	0
12	CA	H	203	1/1	1.00	0.03	55,55,55,55	0
12	CA	K	202	1/1	1.00	0.03	66,66,66,66	0
12	CA	L	788	1/1	1.00	0.01	50,50,50,50	0
12	CA	L	789	1/1	1.00	0.01	62,62,62,62	0

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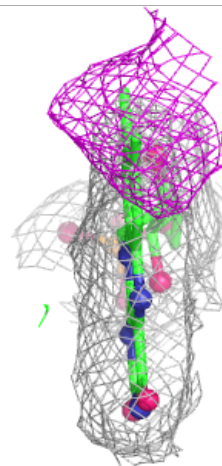
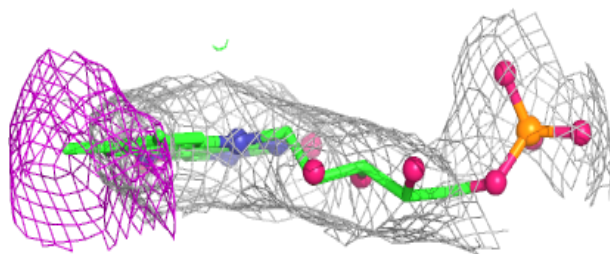
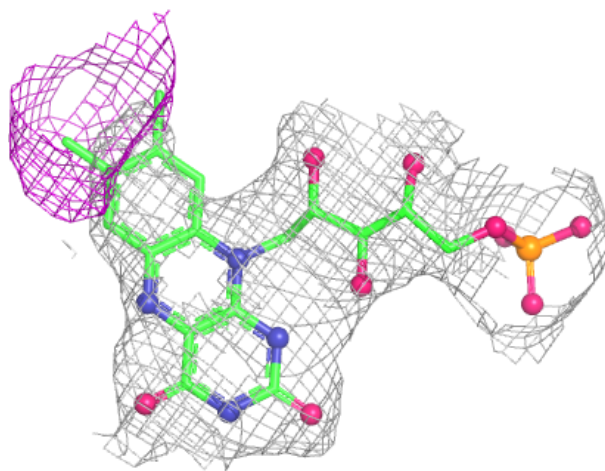
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	CA	P	201	1/1	1.00	0.04	40,40,40,40	0
9	SF4	3	786	8/8	1.00	0.01	16,27,50,50	0
12	CA	U	788	1/1	1.00	0.01	50,50,50,50	0
12	CA	Y	201	1/1	1.00	0.03	41,41,41,41	0
12	CA	Z	203	1/1	1.00	0.03	60,60,60,60	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



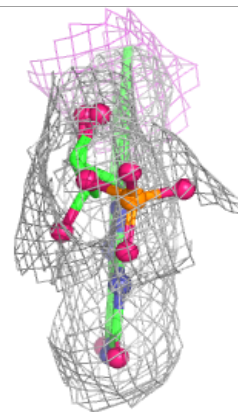
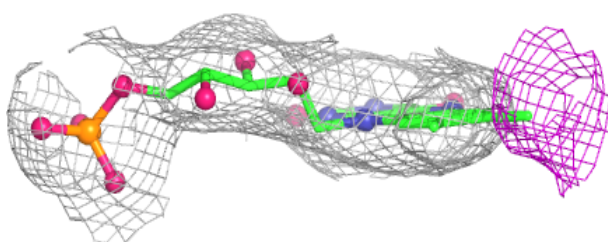
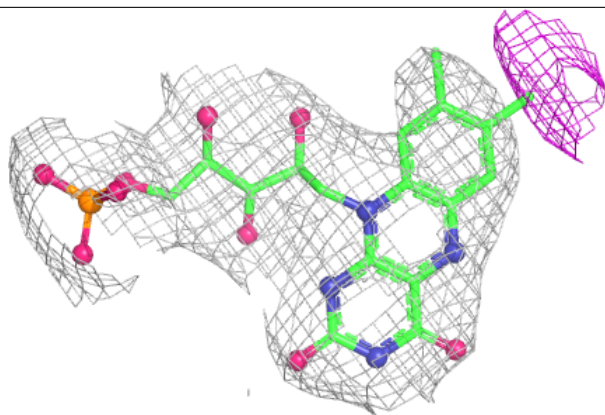
Electron density around FMN J 440:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

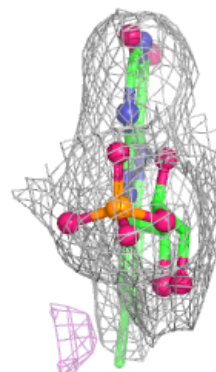
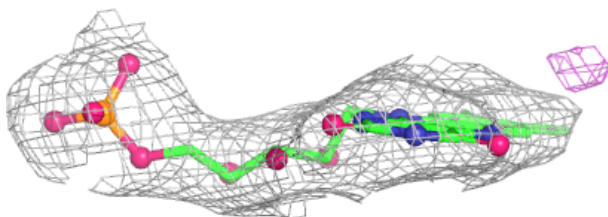
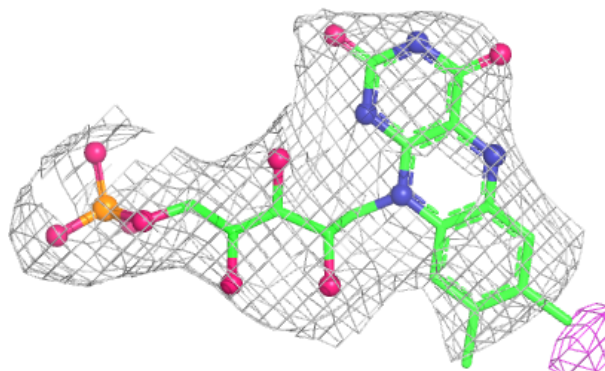


Electron density around FMN 1 440:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FMN S 440:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.