



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 02:39 am BST

PDB ID : 3IAS
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

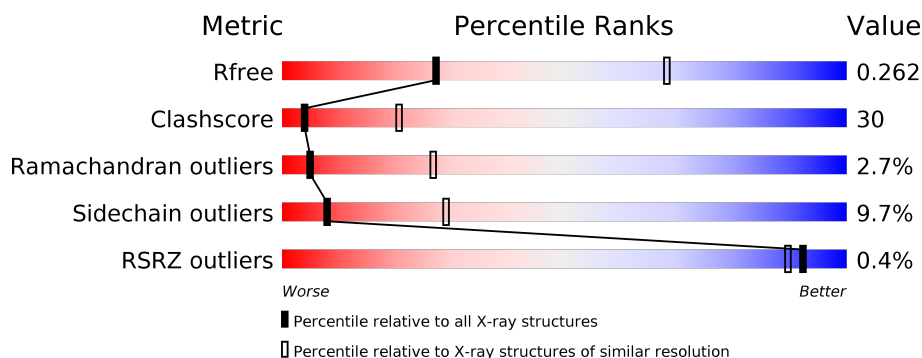
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (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 on 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	<div> <div style="width: 51%;"></div> <div style="width: 42%;"></div> <div style="width: 6%;"></div> </div> <div>51% 42% 6%</div>
1	A	438	<div> <div style="width: 50%;"></div> <div style="width: 43%;"></div> <div style="width: 7%;"></div> </div> <div>50% 43% 7%</div>
1	J	438	<div> <div style="width: 50%;"></div> <div style="width: 43%;"></div> <div style="width: 7%;"></div> </div> <div>50% 43% 7%</div>
1	S	438	<div> <div style="width: 51%;"></div> <div style="width: 42%;"></div> <div style="width: 7%;"></div> </div> <div>51% 42% 7%</div>
2	2	181	<div> <div style="width: 54%;"></div> <div style="width: 39%;"></div> <div style="width: 6%;"></div> <div style="width: 1%;"></div> </div> <div>54% 39% 6% .</div>
2	B	181	<div> <div style="width: 57%;"></div> <div style="width: 35%;"></div> <div style="width: 6%;"></div> <div style="width: 2%;"></div> </div> <div>57% 35% 6% .</div>

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Mol	Chain	Length	Quality of chain
2	K	181	% 55% 38% 6% .
2	T	181	55% 38% 6% .
3	3	783	48% 42% 7% .
3	C	783	48% 41% 7% .
3	L	783	% 48% 42% 7% .
3	U	783	48% 41% 7% .
4	4	409	39% 45% 8% 8%
4	D	409	38% 45% 9% 8%
4	M	409	40% 44% 8% 8%
4	V	409	2% 37% 47% 8% 8%
5	5	207	44% 42% 9% 5%
5	E	207	42% 43% 9% 5%
5	N	207	44% 42% 9% 5%
5	W	207	2% 42% 44% 9% 5%
6	6	181	35% 36% 9% 20%
6	F	181	36% 36% 7% 20%
6	O	181	36% 38% 7% 20%
6	X	181	% 34% 38% 8% 20%
7	9	182	48% 34% . 15%
7	G	182	48% 33% . 15%
7	P	182	48% 33% . 15%
7	Y	182	49% 32% . 15%
8	7	129	62% 32% 5% .
8	H	129	% 56% 37% 5% .
8	Q	129	55% 39% 5% .

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Mol	Chain	Length	Quality of chain
8	Z	129	<div> <div>%</div> <div> </div> <div>59%36% . .</div> </div>

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
10	FMN	J	440	-	-	X	-
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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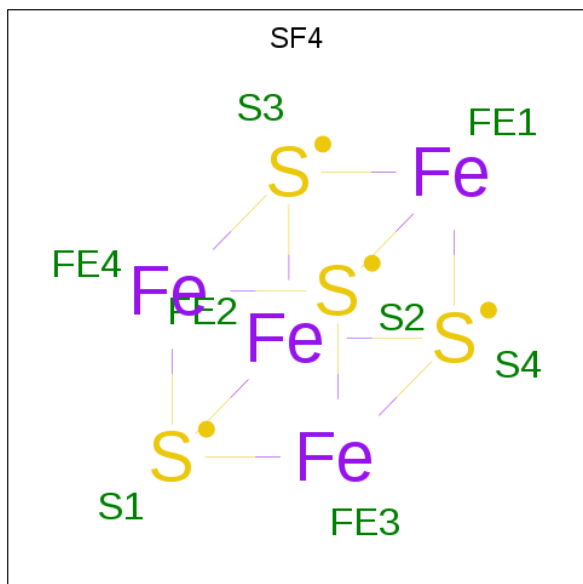
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Y	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			

- 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 (three-letter code: SF4) (formula: Fe₄S₄).



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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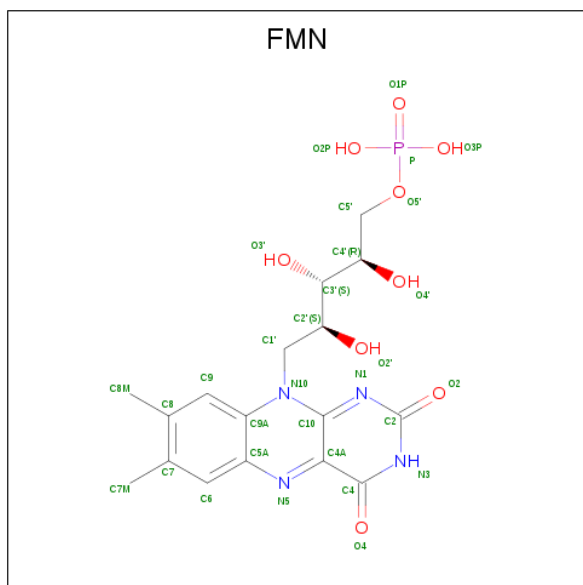
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	6	1	Total 8	Fe 4	S 4	0	0
9	9	1	Total 8	Fe 4	S 4	0	0
9	9	1	Total 8	Fe 4	S 4	0	0
9	A	1	Total 8	Fe 4	S 4	0	0
9	C	1	Total 8	Fe 4	S 4	0	0
9	C	1	Total 8	Fe 4	S 4	0	0
9	C	1	Total 8	Fe 4	S 4	0	0
9	F	1	Total 8	Fe 4	S 4	0	0
9	G	1	Total 8	Fe 4	S 4	0	0
9	G	1	Total 8	Fe 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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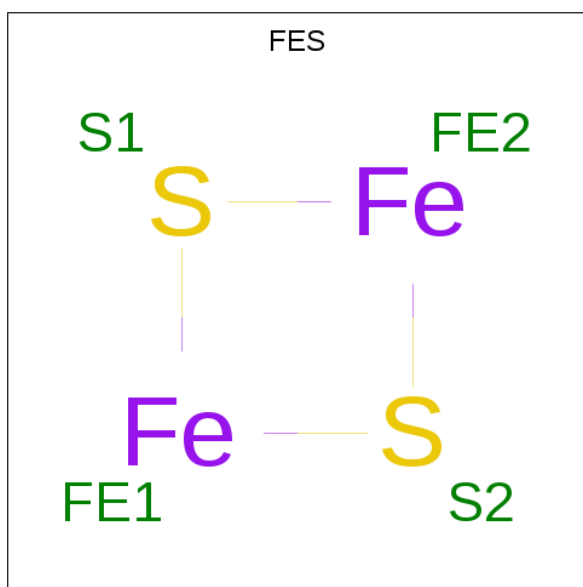
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	X	1	Total	Fe	S	0	0
			8	4	4		
9	Y	1	Total	Fe	S	0	0
			8	4	4		
9	Y	1	Total	Fe	S	0	0
			8	4	4		

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



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

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: 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 (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	P	1	Total	Ca	0	0
			1	1		
12	G	1	Total	Ca	0	0
			1	1		
12	Y	1	Total	Ca	0	0
			1	1		
12	K	1	Total	Ca	0	0
			1	1		

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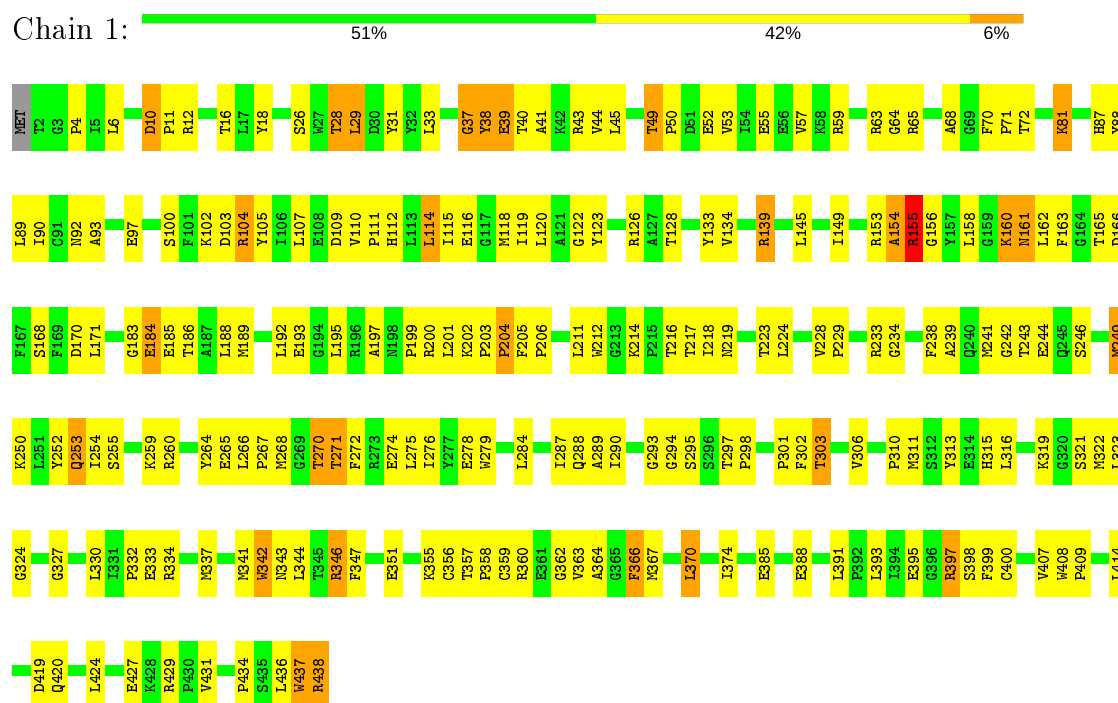
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	H	1	Total 1	Ca 1	0	0
12	B	1	Total 1	Ca 1	0	0
12	C	1	Total 1	Ca 1	0	0
12	Z	1	Total 1	Ca 1	0	0
12	T	1	Total 1	Ca 1	0	0
12	U	1	Total 1	Ca 1	0	0
12	2	1	Total 1	Ca 1	0	0
12	9	1	Total 1	Ca 1	0	0
12	L	2	Total 2	Ca 2	0	0
12	3	2	Total 2	Ca 2	0	0

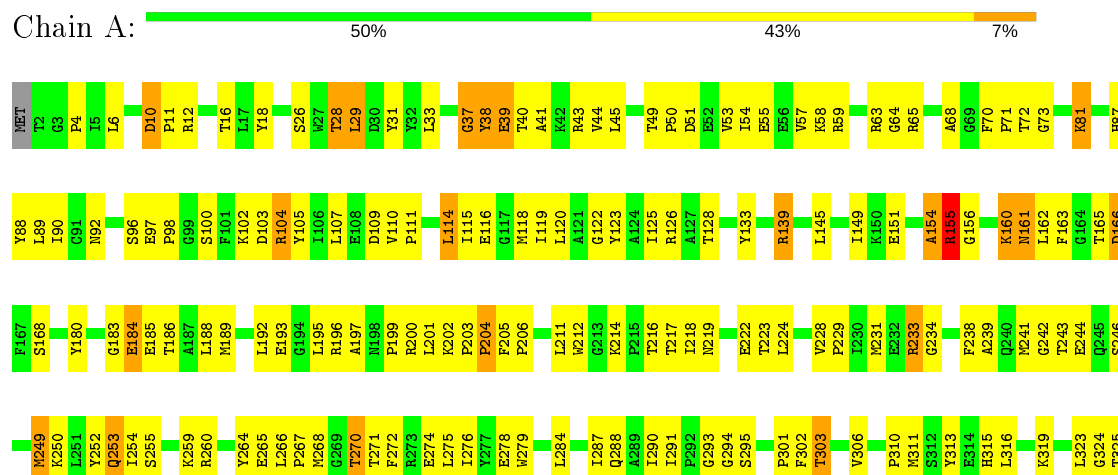
3 Residue-property plots

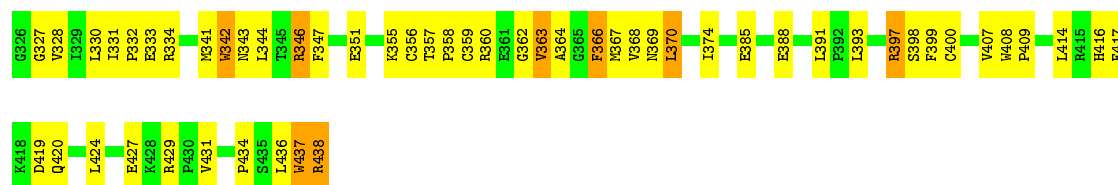
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



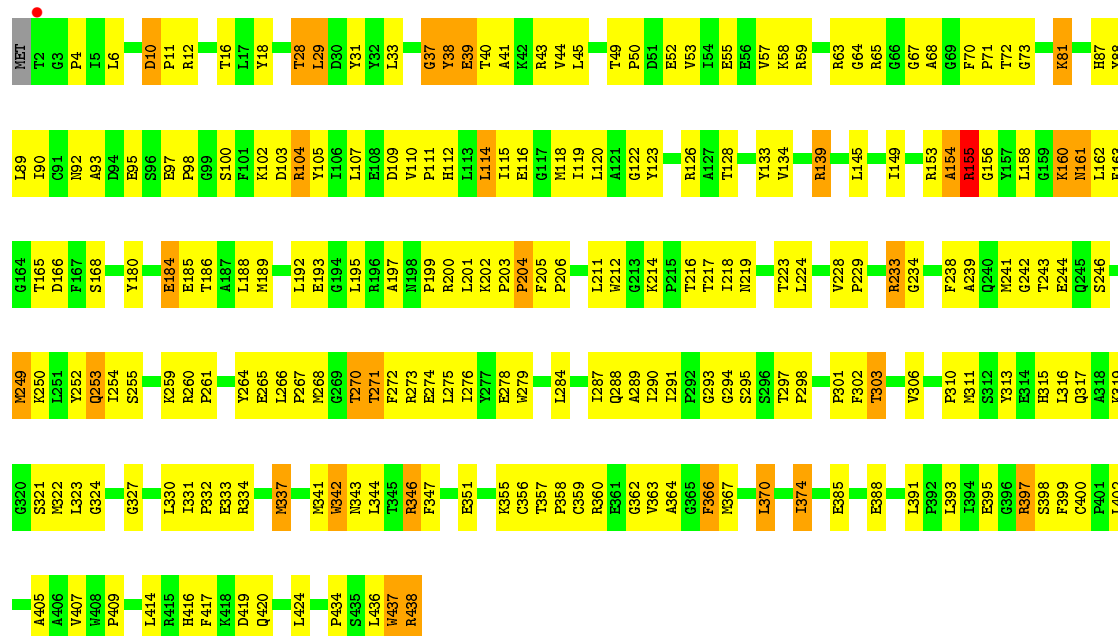
- Molecule 1: NADH-quinone oxidoreductase subunit 1





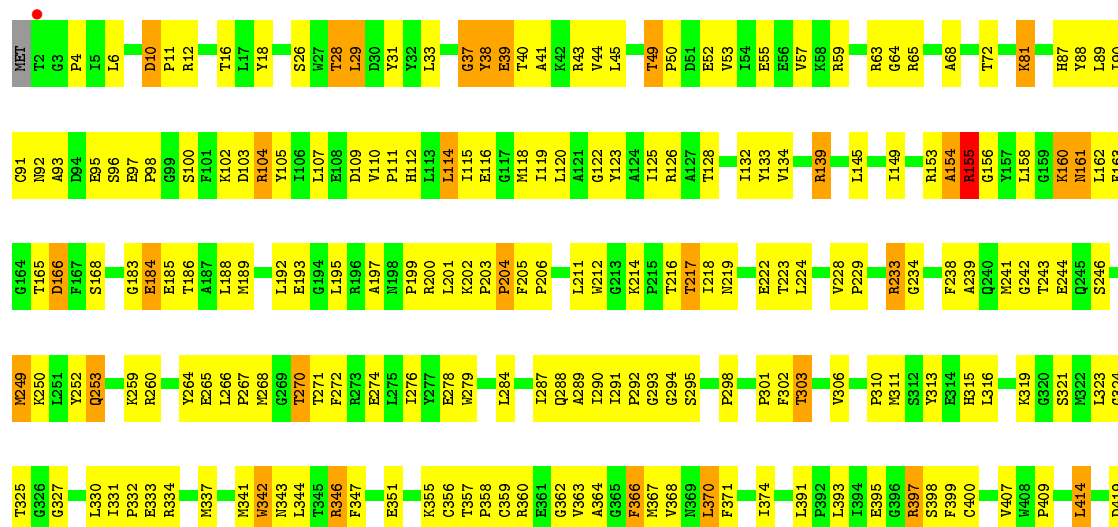
• Molecule 1: NADH-quinone oxidoreductase subunit 1

Chain J: 50% 43% 7%



• Molecule 1: NADH-quinone oxidoreductase subunit 1

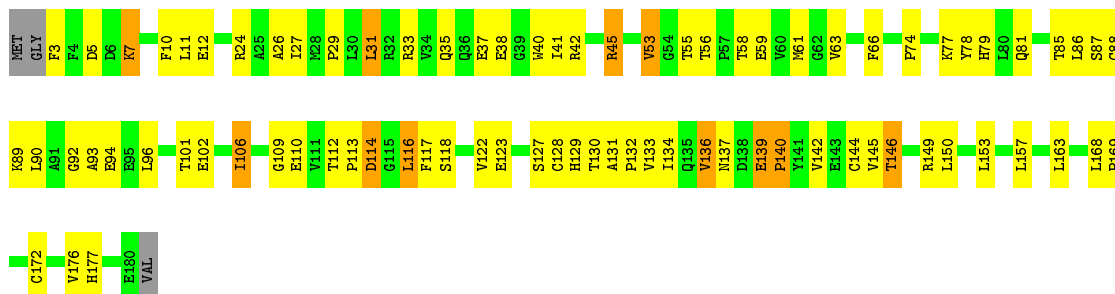
Chain S: 51% 42% 7%





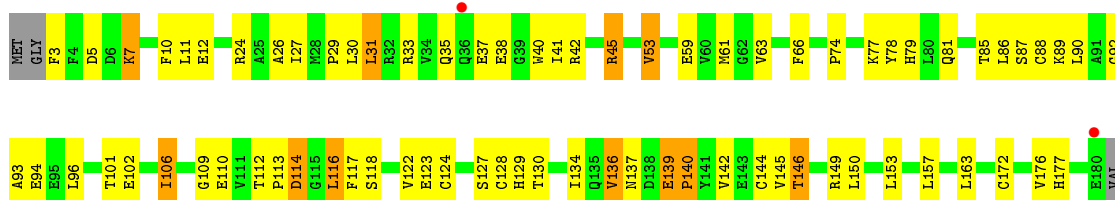
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2: 54% 39% 6%



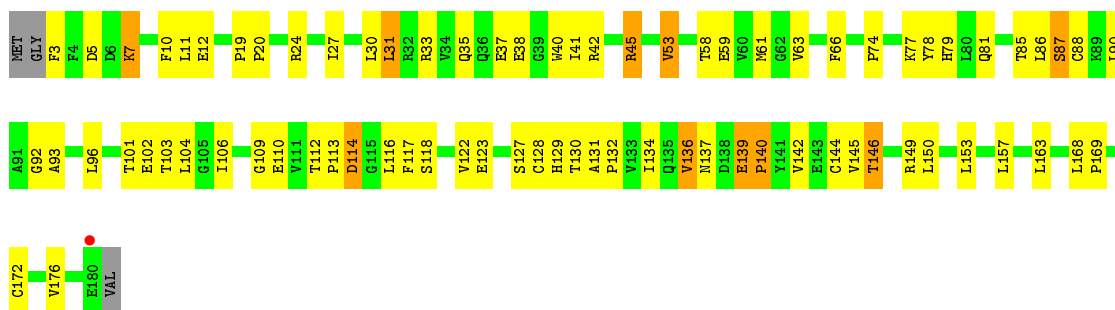
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain B: 57% 35% 6%



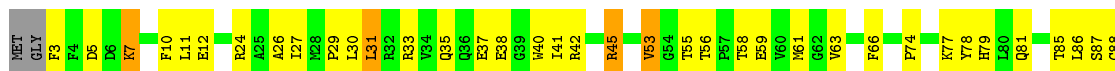
• Molecule 2: NADH-quinone oxidoreductase subunit 2

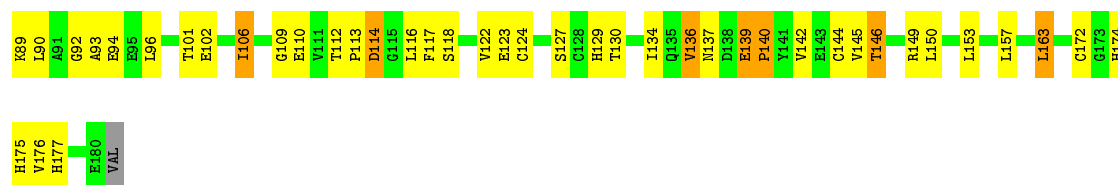
Chain K: 55% 38% 6%



• Molecule 2: NADH-quinone oxidoreductase subunit 2

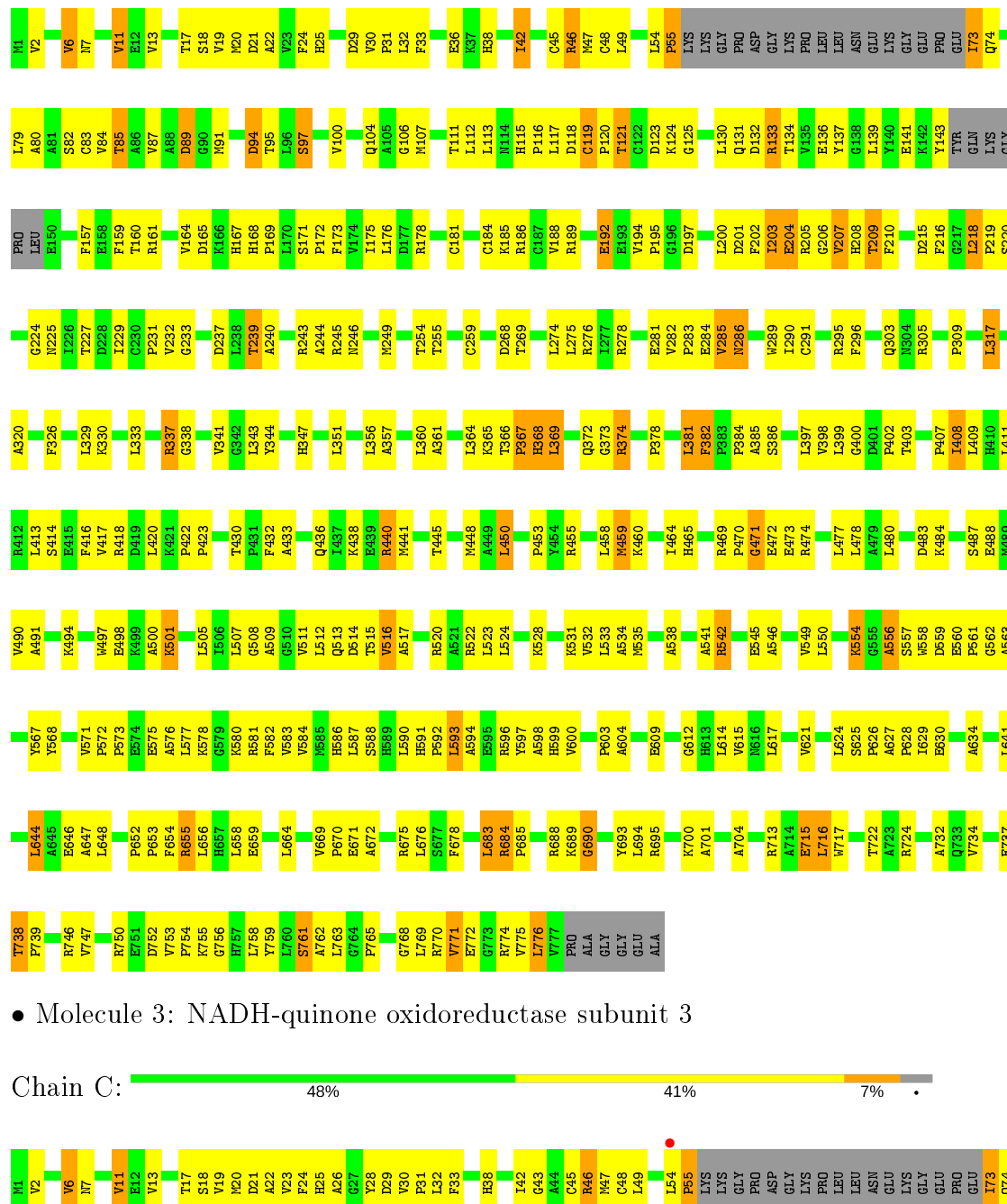
Chain T: 55% 38% 6%





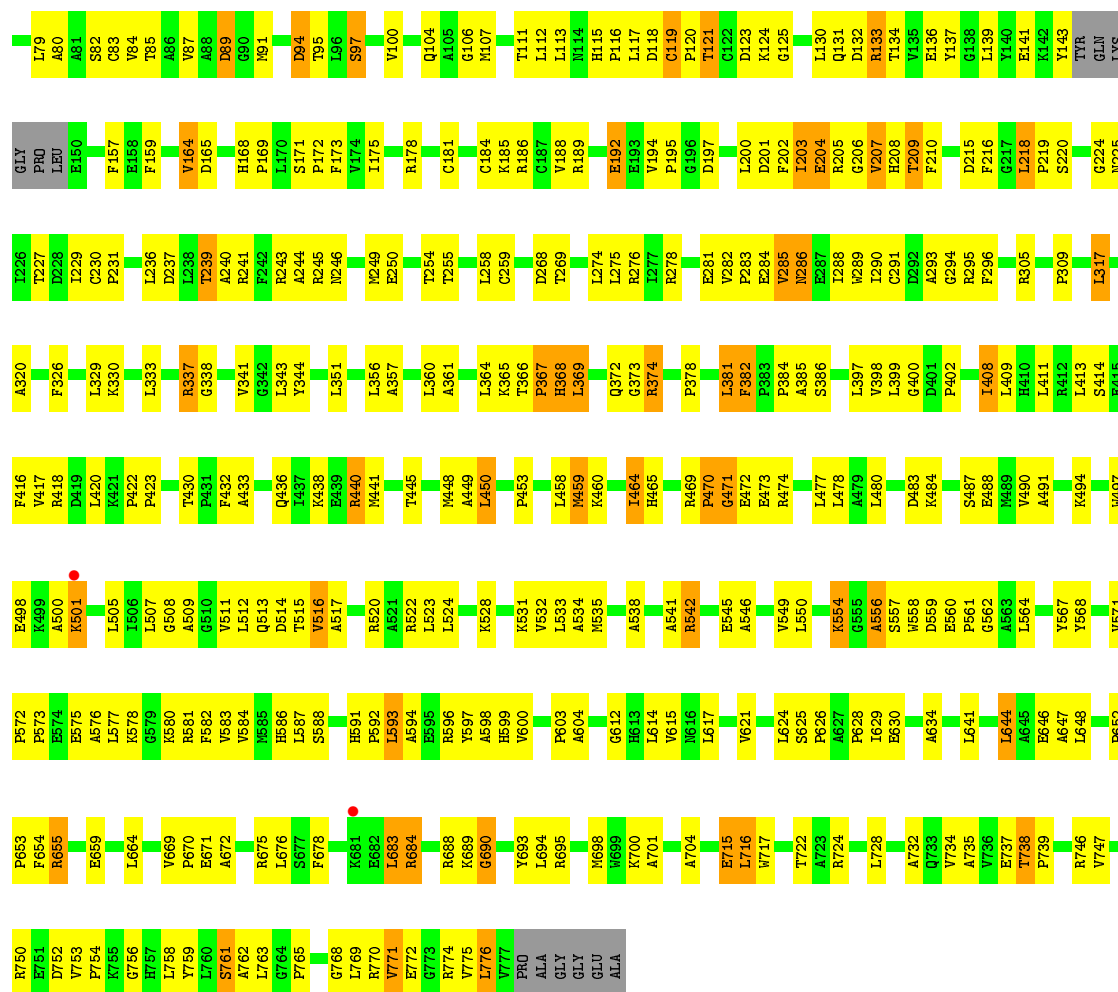
• Molecule 3: NADH-quinone oxidoreductase subunit 3

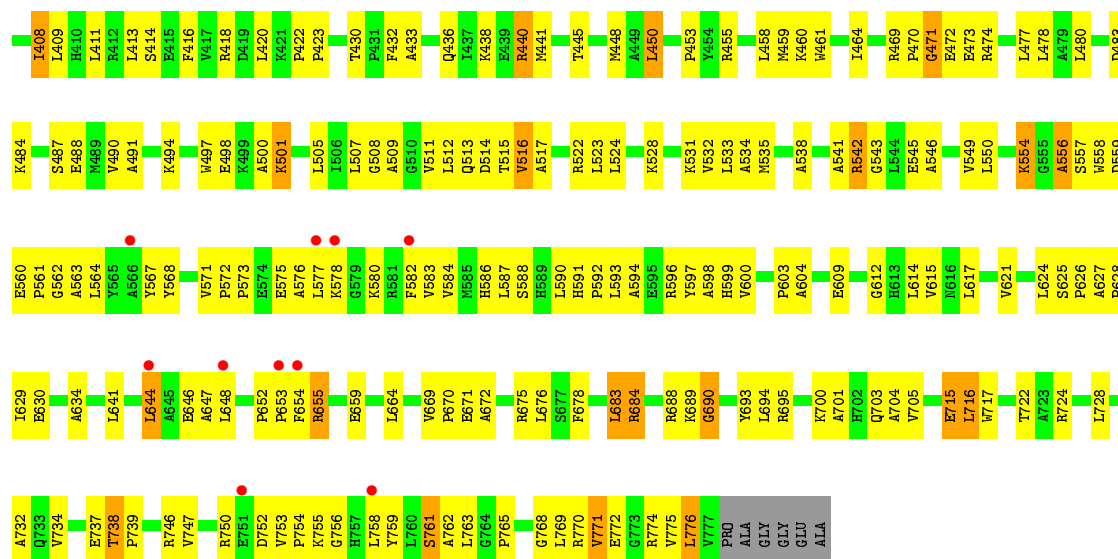
Chain 3: 48% 42% 7%



• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain C: 48% 41% 7%

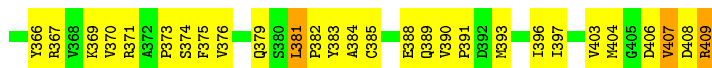
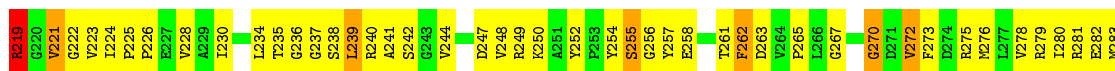
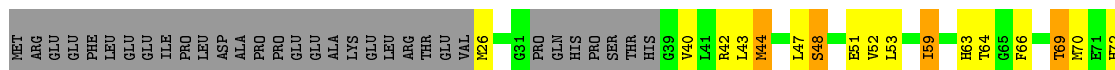






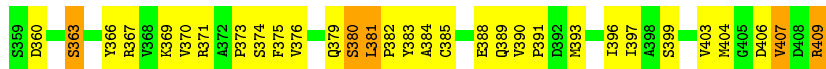
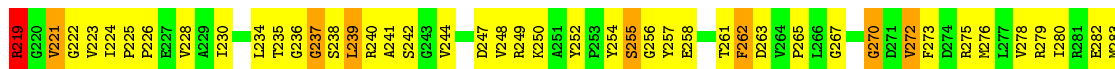
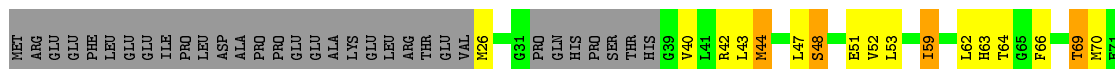
• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain 4: 39% 45% 8% 8%

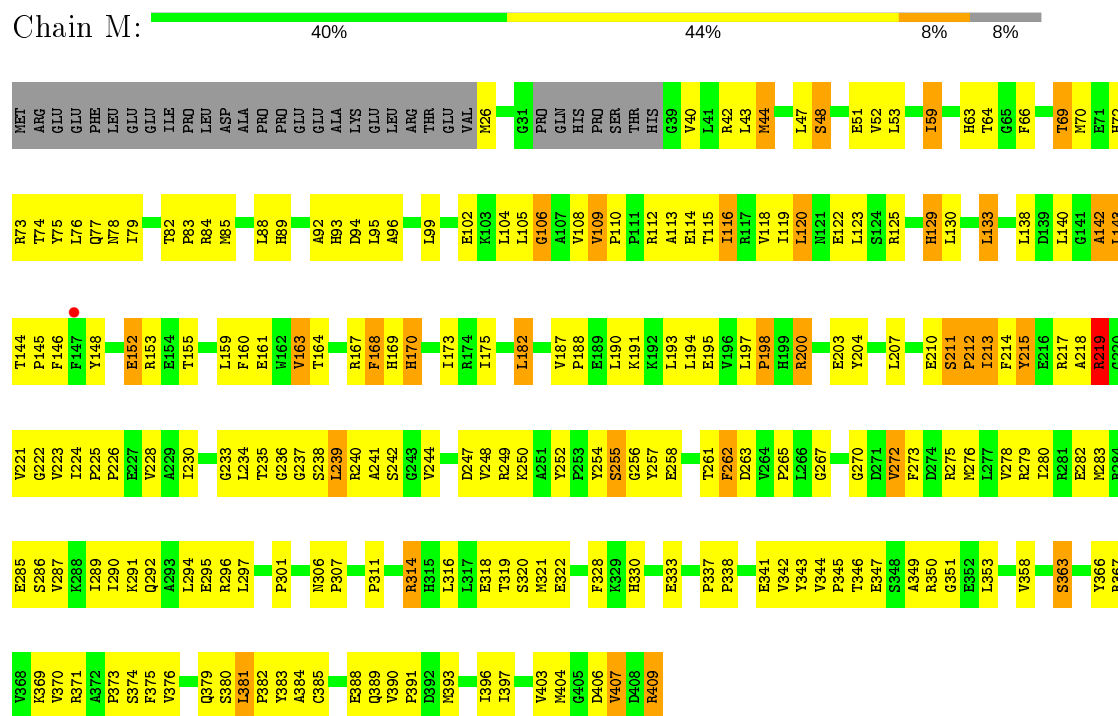


• Molecule 4: NADH-quinone oxidoreductase subunit 4

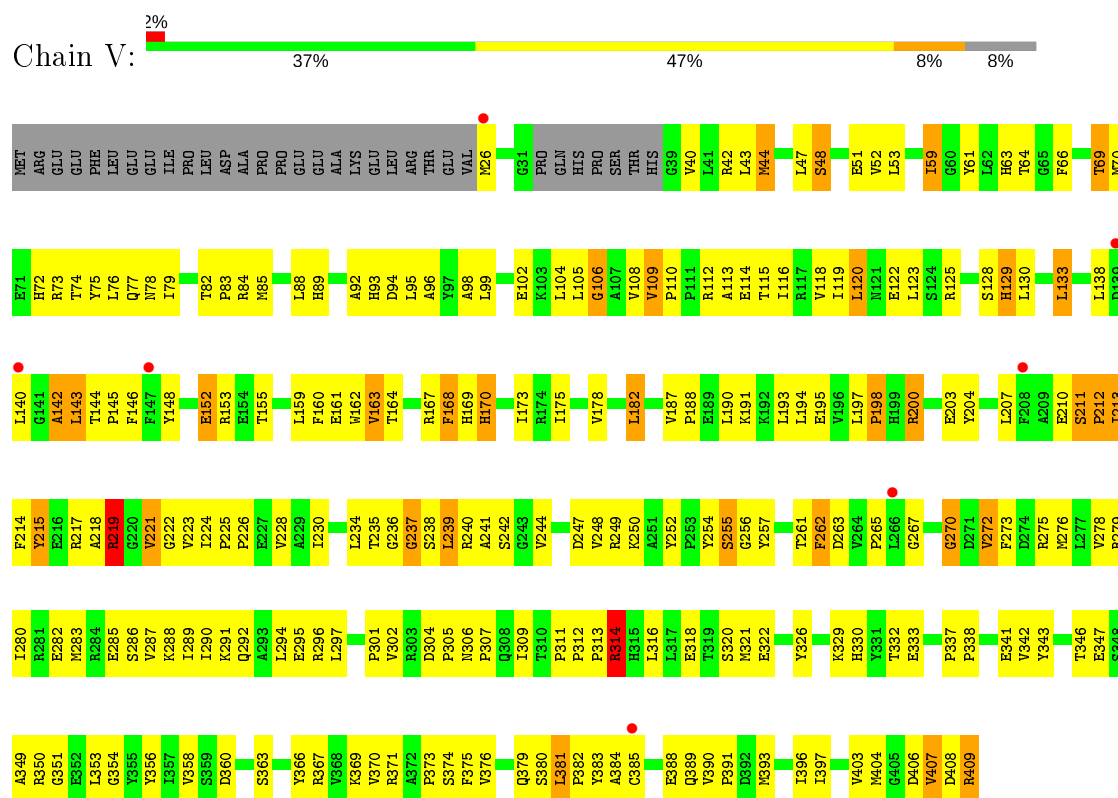
Chain D: 38% 45% 9% 8%



• Molecule 4: NADH-quinone oxidoreductase subunit 4

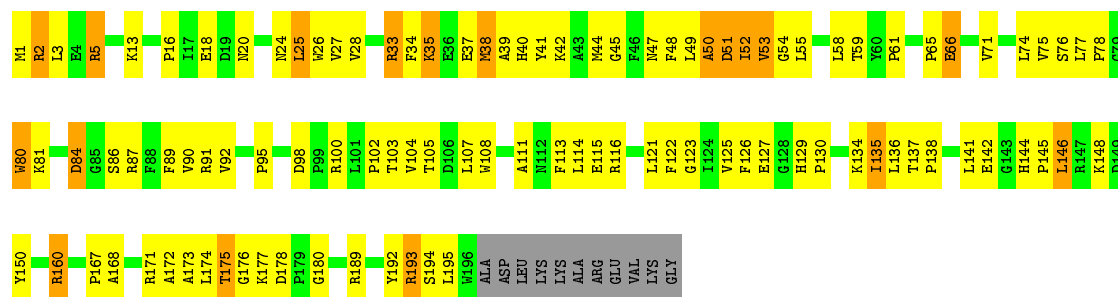


• Molecule 4: NADH-quinone oxidoreductase subunit 4



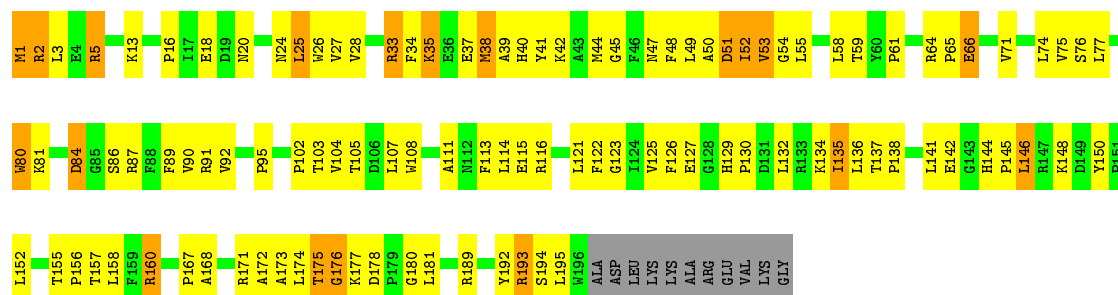
• Molecule 5: NADH-quinone oxidoreductase subunit 5





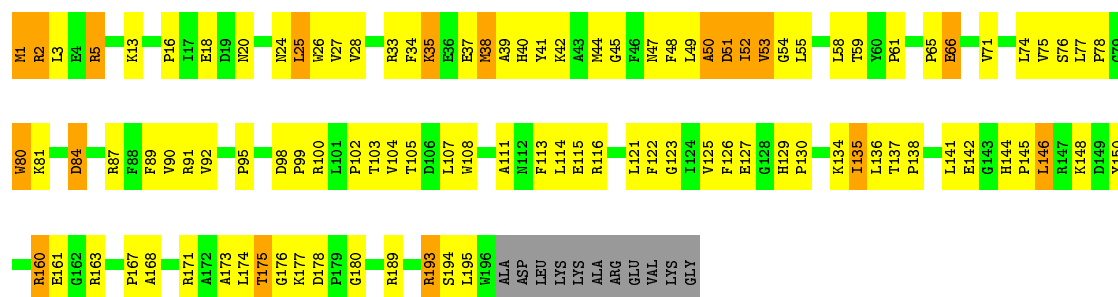
- Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain E: 42% 43% 9% 5%



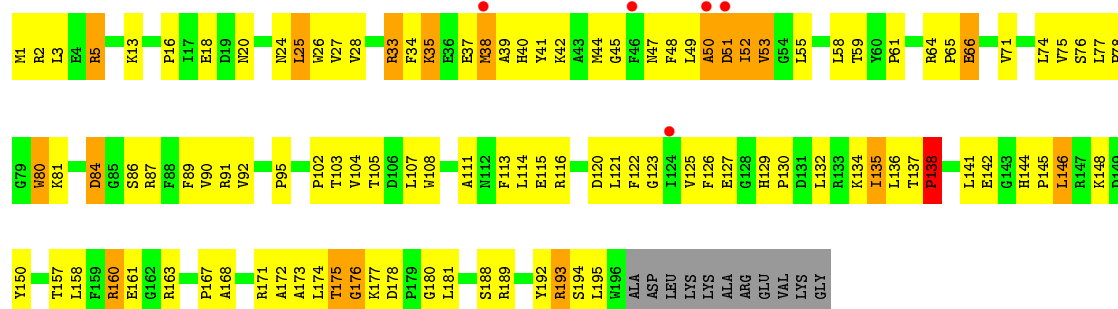
- Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain N: 44% 42% 9% 5%



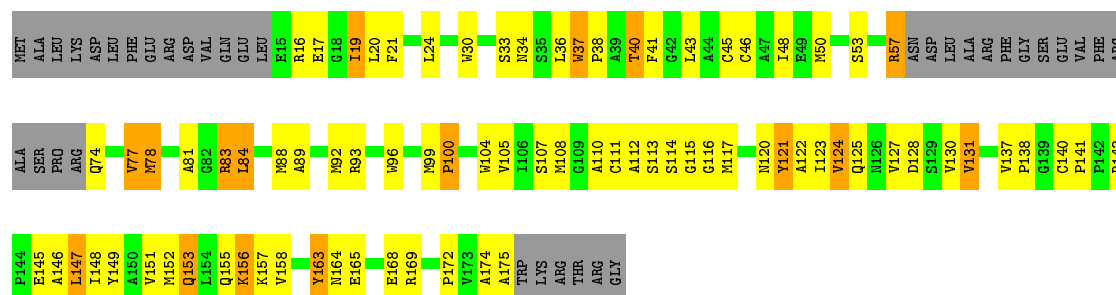
- Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain W: 2% 42% 44% 9% 5%



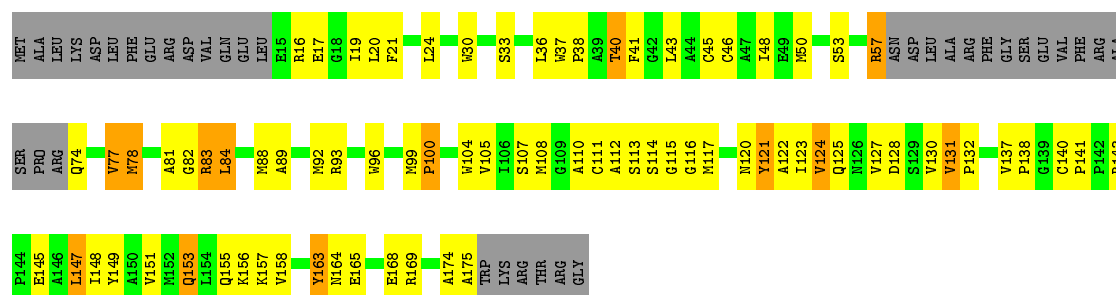
- Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain 6: 



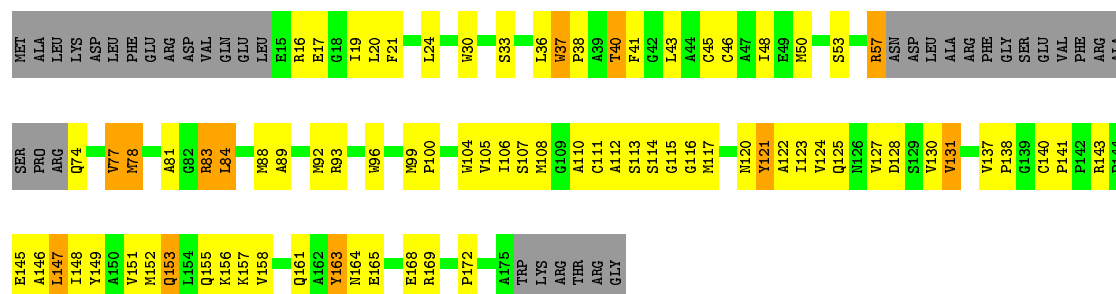
- Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain F: 



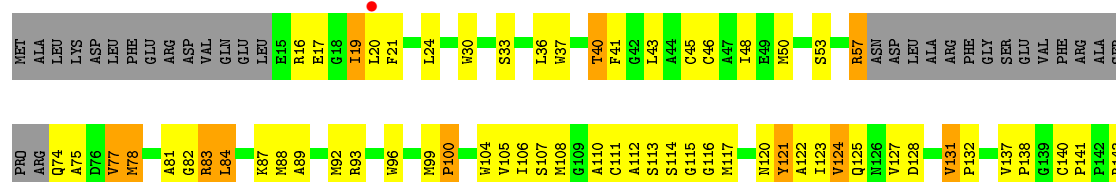
- Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain O: 



- Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain X: 

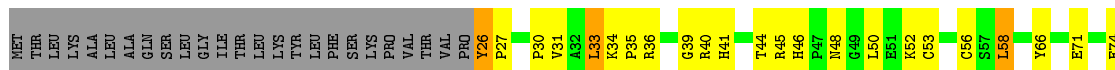




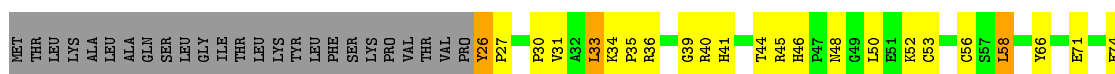
• Molecule 7: NADH-quinone oxidoreductase subunit 9



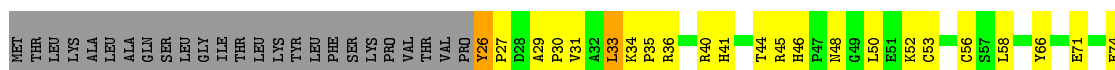
• Molecule 7: NADH-quinone oxidoreductase subunit 9

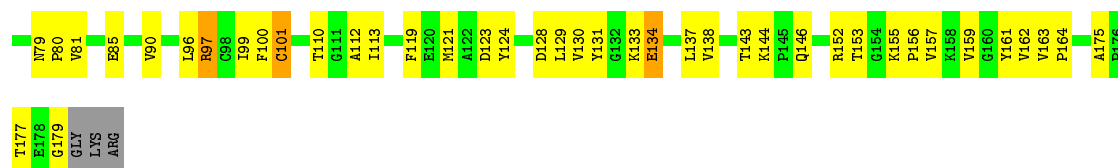


• Molecule 7: NADH-quinone oxidoreductase subunit 9



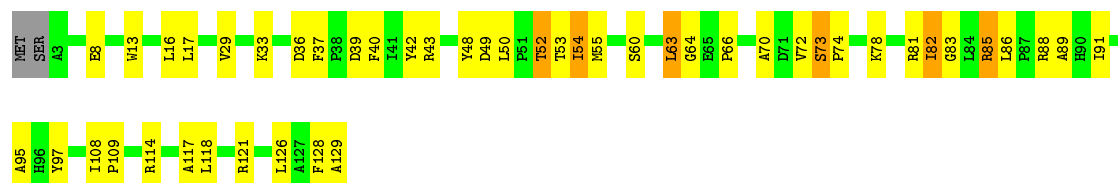
• Molecule 7: NADH-quinone oxidoreductase subunit 9





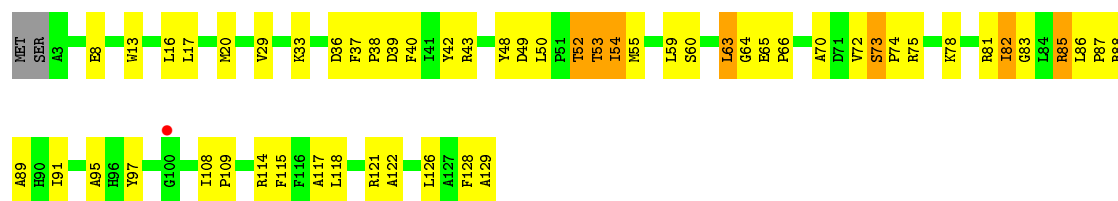
- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7: 62% 32% 5% .



- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain H: 56% 37% 5% .



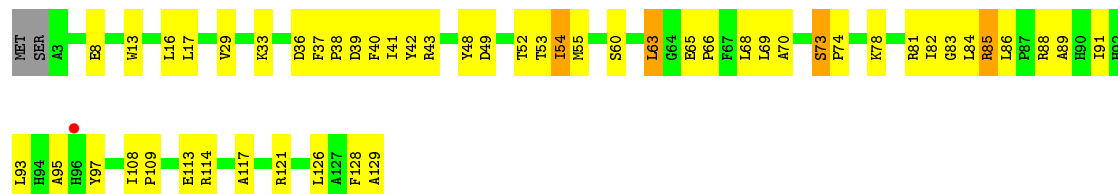
- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain Q: 55% 39% 5% .



- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain Z: 59% 36% 5% .



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 29.99 – 3.15	Depositor EDS
% Data completeness (in resolution range)	82.5 (29.98-3.15) 82.5 (29.99-3.15)	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 0.231 , 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)	0.29 , 15.4	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	0.89	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.43	0/3506	0.61	0/4745
1	A	0.41	0/3506	0.61	0/4745
1	J	0.44	0/3506	0.61	0/4745
1	S	0.40	0/3506	0.61	0/4745
2	2	0.46	0/1439	0.58	0/1953
2	B	0.42	0/1439	0.57	0/1953
2	K	0.46	0/1439	0.58	0/1953
2	T	0.42	0/1439	0.56	0/1953
3	3	0.42	0/6019	0.61	1/8163 (0.0%)
3	C	0.41	0/6019	0.60	1/8163 (0.0%)
3	L	0.41	0/6019	0.61	1/8163 (0.0%)
3	U	0.41	0/6019	0.60	1/8163 (0.0%)
4	4	0.40	0/3089	0.59	0/4197
4	D	0.40	0/3089	0.59	0/4197
4	M	0.42	0/3089	0.59	0/4197
4	V	0.42	0/3089	0.59	0/4197
5	5	0.39	0/1656	0.61	0/2246
5	E	0.39	0/1656	0.61	0/2246
5	N	0.41	0/1656	0.62	0/2246
5	W	0.40	0/1656	0.61	0/2246
6	6	0.45	0/1137	0.60	0/1542
6	F	0.46	0/1137	0.60	0/1542
6	O	0.44	0/1137	0.59	0/1542
6	X	0.47	0/1137	0.59	0/1542
7	9	0.47	0/1224	0.62	0/1663
7	G	0.46	0/1224	0.63	0/1663
7	P	0.43	0/1224	0.62	0/1663
7	Y	0.46	0/1224	0.61	0/1663
8	7	0.41	0/1059	0.58	0/1429
8	H	0.40	0/1059	0.59	0/1429
8	Q	0.42	0/1059	0.59	0/1429
8	Z	0.41	0/1059	0.57	0/1429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.42	0/76516	0.60	4/103752 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	55	PRO	CB-CA-C	-6.57	95.58	112.00
3	C	55	PRO	CB-CA-C	-6.30	96.24	112.00
3	U	55	PRO	CB-CA-C	-6.29	96.28	112.00
3	3	55	PRO	CB-CA-C	-6.29	96.28	112.00

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	201	0
1	A	3417	0	3388	202	0
1	J	3417	0	3388	213	0
1	S	3417	0	3388	198	0
2	2	1406	0	1373	75	0
2	B	1406	0	1373	76	0
2	K	1406	0	1373	76	0
2	T	1406	0	1373	76	0
3	3	5880	0	5911	356	0
3	C	5880	0	5911	347	0
3	L	5880	0	5911	359	0
3	U	5880	0	5911	369	0
4	4	3011	0	3000	258	0
4	D	3011	0	3000	278	0
4	M	3011	0	3000	250	0
4	V	3011	0	3000	277	0
5	5	1607	0	1574	108	0
5	E	1607	0	1574	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	1607	0	1574	107	0
5	W	1607	0	1574	122	0
6	6	1113	0	1121	105	0
6	F	1113	0	1121	100	0
6	O	1113	0	1121	101	0
6	X	1113	0	1121	109	0
7	9	1193	0	1160	72	0
7	G	1193	0	1160	74	0
7	P	1193	0	1160	74	0
7	Y	1193	0	1160	70	0
8	7	1031	0	1029	47	0
8	H	1031	0	1029	58	0
8	Q	1031	0	1029	53	0
8	Z	1031	0	1029	49	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	8	0
10	A	31	0	19	7	0
10	J	31	0	19	10	0
10	S	31	0	19	7	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	4528	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 30.

All (4528) 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:HH11	3:3:46:ARG:HG2	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:HH11	3:L:46:ARG:HG2	0.94	1.05
3:3:474:ARG:NH2	3:3:516:VAL:HG21	1.71	1.04
5:N:5:ARG:HH11	5:N:5:ARG:HG3	1.19	1.03
5:5:121:LEU:HB3	5:5:146:LEU:HB2	1.39	1.02
5:E:5:ARG:HG3	5:E:5:ARG:HH11	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:HH11	3:U:46:ARG:HG2	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: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
1:A:293:GLY:HA3	1:A:324:GLY:H	1.27	0.98
3:L:501:LYS:HD2	3:L:501:LYS:H	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:NH1	3:U:46:ARG:HG2	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
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:212:PRO:HG2	4:D:213:ILE:HD12	1.50	0.93
4:D:188:PRO:HB3	3:U:724:ARG:HD2	0.95	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:4:254:TYR:HD1	4:4:255:SER:H	1.14	0.92
5:N:193:ARG:HH11	5:N:193:ARG:HG2	1.31	0.92
5:5:193:ARG:HH11	5:5:193:ARG:HG2	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
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:L:46:ARG:NH1	3:L:46:ARG:HG2	1.73	0.90
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:655:ARG:HB2	3:U:655:ARG:HH11	1.37	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
3:L:655:ARG:HH11	3:L:655:ARG:HB2	1.38	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
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
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
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:NH1	3:C:46:ARG:HG2	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:HH11	4:4:314:ARG:HG2	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
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:NH1	5:W:5:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:55:PRO:HG3	3:3:74:GLN:N	1.92	0.85
5:E:193:ARG:CG	5:E:193:ARG:HH11	1.90	0.84
7:G:33:LEU:HD11	7:G:161:TYR:HB2	1.58	0.84
5:N:5:ARG:NH1	5:N:5:ARG:HG3	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
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:I:16:THR:HG21	1:I: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
3:3:285:VAL:HG13	3:3:286:ASN:H	1.43	0.83
3:3:216:PHE:HZ	8:7:128:PHE:CD2	1.96	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:I:184:GLU:OE1	1:I: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:5:ARG:NH1	5:5:5:ARG:HG3	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
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
5:W:193:ARG:NH1	5:W:193:ARG:HG2	1.90	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:HH11	4:M:314:ARG:HG2	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:HD2	2:K:7:LYS:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:NH1	5:N:193:ARG:HG2	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
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
2:T:110:GLU:HA	8:Z:121:ARG:HH12	1.47	0.79
5:E:80:TRP:CE3	5:E:80:TRP:HA	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: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:CE3	5:5:80:TRP:HA	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:HA	5:N:80:TRP:CE3	2.19	0.78
3:L:515:THR:HG23	3:L:683:LEU:HD12	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
6:X:96:TRP:HA	6:X:99:MET:HE3	1.65	0.78
4:4:88:LEU:HD21	6:6:48:ILE:HD13	1.64	0.78
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:117:LEU:H	4:V:321:MET:HE1	1.50	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
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
4:V:222:GLY:HA3	4:V:396:ILE:HD11	1.67	0.77
3:3:440:ARG:HH11	3:3:440:ARG:HG2	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:HD2	2:T:7:LYS:H	1.50	0.77
4:V:367:ARG:HH12	4:V:369:LYS:HB2	1.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:3:117:LEU:H	4:4:321:MET:HE1	1.50	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
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:HE3	5:E:80:TRP:HA	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
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
3:3:87:VAL:HA	3:3:91:MET:HE1	1.67	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
3:U:117:LEU:N	4:V:321:MET:HE1	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:243:THR:HG22	1:A:244:GLU:H	1.51	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
5:5:5:ARG:CG	5:5:5:ARG:HH11	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
3:U:87:VAL:HA	3:U:91:MET:HE1	1.69	0.74
4:M:371:ARG:HG3	5:N:51:ASP:OD1	1.87	0.73
2:2:146:THR:HG23	2:2:149:ARG:HB2	1.69	0.73
5:5:80:TRP:HE3	5:5:80:TRP:HA	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
5:W:80:TRP:HE3	5:W:80:TRP:HA	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:L:87:VAL:HA	3:L:91:MET:HE1	1.70	0.73
3:U:46:ARG:CG	3:U:46:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:1:192:LEU:HD22	1:1:211:LEU:HD11	1.71	0.72
3:3:117:LEU:N	4:4:321:MET:HE1	2.03	0.72
6:F:96:TRP:HA	6:F:99:MET:HE3	1.70	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:HH11	3:L:440:ARG:HG2	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
3:C:87:VAL:HA	3:C:91:MET:HE1	1.72	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:M:47:LEU:HD13	4:M:52:VAL:HA	1.70	0.72
5:N:175:THR:O	5:N:177:LYS:N	2.23	0.72
5:N:16:PRO:HD2	5:N:28:VAL:HG13	1.72	0.72
4:V:371:ARG:HH22	4:V:376:VAL:HG21	1.54	0.72
4:V:74:THR:HG22	4:V:76:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:139:ARG:HG2	2:K:140:PRO:HD3	1.70	0.72
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
4:4:314:ARG:NH1	4:4:314:ARG:HG2	2.05	0.71
4:4:105:LEU:HB3	4:4:337:PRO:HB3	1.71	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
3:L:117:LEU:N	4:M:321:MET:HE1	2.06	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
3:L:402:PRO:HG3	3:L:535:MET:HE1	1.70	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
7:P:40:ARG:HB2	7:P:121:MET:CE	2.19	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:89:HIS:CE1	4:M:92:ALA:HB2	2.26	0.71
4:M:64:THR:HG23	6:O:123:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:556:ALA:HB2	3:3:562:GLY:HA3	1.71	0.71
7:9:40:ARG:HB2	7:9:121:MET:CE	2.21	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
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:HH11	8:Q:121:ARG:HG3	1.54	0.70
7:Y:175:ALA:O	7:Y:177:THR:HG23	1.92	0.70
4:4:341:GLU:HG2	4:4:358:VAL:HG22	1.74	0.70
3:3:216:PHE:HZ	8:7:128:PHE:HD2	1.37	0.70
3:L:46:ARG:CG	3:L:46:ARG:HH11	1.85	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
7:Y:40:ARG:HB2	7:Y:121:MET:CE	2.21	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
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: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
3:U:216:PHE:HZ	8:Z:128:PHE:CD2	2.09	0.69
3:L:216:PHE:HZ	8:Q:128:PHE:HD2	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:397:ARG:HE	3:L:79:LEU:HD12	1.58	0.69
4:V:47:LEU:HD13	4:V:52:VAL:HA	1.74	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
4:D:120:LEU:HD13	4:D:160:PHE:HE1	1.57	0.69
2:B:110:GLU:HA	8:H:121:ARG:HH12	1.58	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
7:9:40:ARG:HB2	7:9:121:MET:HE2	1.72	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
4:4:190: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:L:31:PRO:HB2	3:L:47:MET:HB3	1.75	0.69
4:M:314:ARG:NH1	4:M:314:ARG:HG2	2.07	0.69
5:N:66:GLU:HG3	5:N:95:PRO:HA	1.73	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:117:LEU:H	4:M:321:MET:HE1	1.57	0.69
3:U:655:ARG:NH1	3:U:655:ARG:HB2	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:HD2	1:S:438:ARG:H	1.57	0.69
3:3:402:PRO:HG3	3:3:535:MET:HE1	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:P:40:ARG:HB2	7:P:121:MET:HE2	1.74	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: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:190:LEU:O	4:D:194:LEU:HB2	1.94	0.68
4:D:47:LEU:HD13	4:D:52:VAL:HA	1.75	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
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
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:E:1:MET:SD	8:Z:113:GLU:CD	2.71	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:507:LEU:HD22	3:3:511:VAL:HG11	1.76	0.67
3:3:6:VAL:HG12	3:3:7:ASN:N	2.08	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:134:ILE:HG13	2:B:145:VAL:HG21	1.76	0.67
2:B:87:SER:HB3	11:B:182:FES:S2	2.35	0.67
3:C:655:ARG:NH1	3:C:655:ARG:HB2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD2	1:J:438:ARG:H	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:NH1	3:L:655:ARG:HB2	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:HD2	1:1:438:ARG:H	1.60	0.66
3:3:87:VAL:HA	3:3:91:MET:CE	2.24	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
3:L:87:VAL:HA	3:L:91:MET:CE	2.24	0.66
1:S:219:ASN:HD22	1:S:223:THR:HG21	1.61	0.66
3:U:684:ARG:HH11	3:U:684:ARG:HG2	1.60	0.66
4:V:133:LEU:HD21	4:V:204:TYR:CD2	2.31	0.66
4:V:120:LEU:HD13	4:V:160:PHE:HE1	1.59	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
3:3:337:ARG:H	3:3:337:ARG:CD	2.08	0.66
1:A:107:LEU:O	1:A:111:PRO:HG3	1.96	0.66
1:A:6:LEU:HD21	1:A:12:ARG:HG3	1.78	0.66
3:C:497:TRP:NE1	3:C:524:LEU:HD11	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:44:MET:HA	4:D:44:MET:CE	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
4:D:59:ILE:HD11	5:E:135:ILE:HG23	1.78	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
3:U:20:MET:HE3	3:U:432:PHE:HB3	1.78	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
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: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
3:3:205: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:CE	4:4:44:MET:HA	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
1:S:253:GLN:HE21	1:S:253:GLN:N	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:402:PRO:HG3	3:C:535:MET:HE1	1.78	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
4:4:237: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:L:117:LEU:HG	4:M:321:MET:HE2	1.79	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:254:TYR:HD1	4:D:255:SER:N	1.89	0.65
4:D:105:LEU:HD23	4:D:337:PRO:HG3	1.77	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:CG	5:E:5:ARG:HH11	2.04	0.65
6:F:163:TYR:HB3	6:F:168:GLU:O	1.97	0.65
1:S:184:GLU:HG2	10:S:440:FMN:HM82	1.79	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:C:117:LEU:H	4:D:321:MET:HE1	1.60	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:H	1:A:438:ARG:HD2	1.61	0.65
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
7:G:48:ASN:HB2	7:G:50:LEU:HD23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	4:D:314:ARG:HG2	2.05	0.64
3:U:173:PHE:HB3	3:U:296:PHE:CE1	2.32	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:508:GLY:O	3:U:512:LEU:HB2	1.97	0.64
3:U:112:LEU:HD12	4:V:322:GLU:HG3	1.79	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:A:344:LEU:O	1:A:347:PHE:HB3	1.98	0.64
4:D:371:ARG:NH2	4:D:376:VAL:HG21	2.12	0.64
3:C:120:PRO:HG2	8:H:42:TYR:OH	1.97	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:CD	3:L:337:ARG:H	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
1:J:184:GLU:HG2	10:J:440:FMN:HM82	1.79	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:HG22	4:D:40:VAL:O	1.98	0.64
3:L:715:GLU:HB3	3:L:746:ARG:CZ	2.27	0.64
4:M:142:ALA:HB1	4:M:145:PRO:HG2	1.80	0.64
4:M:102:GLU:HG2	4:M:175:ILE:O	1.98	0.64
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
3:U:87:VAL:HA	3:U:91:MET:CE	2.28	0.64
1:1:393:LEU:HD22	3:3:106:GLY:HA3	1.80	0.64
4:4:239:LEU:HD22	4:4:244:VAL:HB	1.80	0.64
1:A:253:GLN:HE21	1:A:253:GLN:N	1.96	0.64
1:A:55:GLU:O	1:A:59:ARG:HB2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:40:ARG:HB2	7:Y:121:MET:HE1	1.79	0.63
7:Y:71:GLU:HB2	7:Y:90:VAL:HB	1.80	0.63
4:4:213:ILE:H	4:4:213:ILE:HD12	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
4:4:142:ALA:HB1	4:4:145:PRO:HG2	1.80	0.63
4:4:40:VAL:O	4:4:40:VAL:HG22	1.98	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
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
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
8:Z:108:ILE:HG22	8:Z:114:ARG:NH1	2.14	0.63
1:1:184:GLU:HG2	10:1:440:FMN:HM82	1.81	0.63
1:1:332:PRO:HD2	2:2:90:LEU:HD23	1.80	0.63
3:3:317:LEU:N	3:3:317:LEU:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:364: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:317:LEU:N	3:U:317:LEU:HD22	2.14	0.63
3:U:409:LEU:HD12	3:U:535:MET:HE3	1.80	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
3:U:216:PHE:HZ	8:Z:128:PHE:HD2	1.46	0.63
5:5:104:VAL:HG12	5:5:108:TRP:HE3	1.63	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
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
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: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
3:U:402:PRO:HG3	3:U:535:MET:HE1	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:440:ARG:HH11	3:L:440:ARG:CG	2.12	0.62
3:L:438:LYS:O	3:L:441:MET:HG3	2.00	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:265:PRO:HG2	4:V:282:GLU:HG2	1.80	0.62
4:V:167:ARG:HD3	6:X:143:ARG:HH12	1.64	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
5:N:13:LYS:HZ3	5:N:33:ARG:HH21	1.45	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
7:G:40:ARG:HB2	7:G:121:MET:HE2	1.82	0.62
6:O:153:GLN:HG3	7:P:124:TYR:CZ	2.35	0.62
6:O:114:SER:HB2	7:P:97:ARG:HD2	1.81	0.62
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
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:NH1	4:V:314:ARG:HG2	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HD23	4:M:140:LEU:O	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
3:C:87:VAL:HA	3:C:91:MET:CE	2.29	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
1:1:89:LEU:HD23	1:1:118:MET:HE3	1.82	0.61
4:4:230:ILE:O	4:4:230:ILE:HG22	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:254:TYR:HE2	4:M:346:THR:HA	1.64	0.61
4:M:249:ARG:HB3	4:M:257:TYR:HD1	1.65	0.61
5:N:92:VAL:HG23	5:N:92:VAL:O	2.00	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
7:Y:33:LEU:CD1	7:Y:161:TYR:HB2	2.28	0.61
1:1:184:GLU:CD	1:1:186:THR:HG22	2.21	0.61
3:3:586:HIS:CD2	3:3:604:ALA:HB2	2.36	0.61
3:C:409:LEU:HD12	3:C:535:MET:HE3	1.83	0.61
3:L:591:HIS:ND1	3:L:592:PRO:HD2	2.16	0.61
4:M:213:ILE:H	4:M:213:ILE:HD12	1.66	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
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
1:A:184:GLU:CD	1:A:186:THR:HG22	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
4:D:96:ALA:HB2	4:D:346:THR:HG21	1.82	0.61
1:S:184:GLU:CD	1:S:186:THR:HG22	2.21	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
6:X:77:VAL:HG22	6:X:104:TRP:HB2	1.83	0.61
5:W:167:PRO:HB3	7:Y:66:TYR:CE2	2.36	0.61
1:1:242:GLY:HA2	1:1:268:MET:O	2.01	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: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:N	1:J:253:GLN:HE21	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
5:N:5:ARG:HH11	5:N:5:ARG:CG	2.01	0.61
4:M:161:GLU:OE1	7:P:34:LYS:HG2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:HG22	4:M:230:ILE:O	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
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:M:363:SER:HB2	5:N:174:LEU:H	1.66	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:30:VAL:HG22	3:L:48:CYS:HA	1.83	0.60
6:O:153:GLN:HG3	7:P:124:TYR:OH	2.02	0.60
6:O:16:ARG:HG2	6:O:21:PHE:CE2	2.37	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
3:C:20:MET:HE3	3:C:432:PHE:HB3	1.82	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
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
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
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: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
3:C:117:LEU:N	4:D:321:MET:HE1	2.17	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
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:155:THR:HB	4:M:193:LEU:HD12	1.84	0.59
4:M:110:PRO:HB3	4:M:301:PRO:HG2	1.82	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
4:4:43:LEU:HD11	4:4:397:ILE:HD11	1.84	0.59
3:3:216:PHE:CZ	8:7:128:PHE:CD2	2.86	0.59
7:9:71:GLU:HB2	7:9:90:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:393:MET:O	4:D:396:ILE:HG22	2.02	0.59
4:D:84:ARG:O	6:F:83:ARG:NH2	2.35	0.59
3:L:317:LEU:N	3:L:317:LEU:HD22	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
6:X:148:ILE:HG22	6:X:149:TYR:N	2.16	0.59
1:I:115:ILE:O	1:I:119:ILE:HG13	2.02	0.59
1:I: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
4:D:153:ARG:HH11	4:D:153:ARG:HG3	1.67	0.59
1:J:344:LEU:O	1:J:347:PHE:HB3	2.01	0.59
1:J:332:PRO:HD2	2:K:90:LEU:HD23	1.84	0.59
3:L:240:ALA:CB	3:L:276:ARG:HB2	2.32	0.59
4:M:371:ARG:NH2	4:M:376:VAL:HG21	2.16	0.59
4:M:350:ARG:O	4:M:373:PRO:HB2	2.02	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
6:6:96:TRP:HA	6:6:99:MET:HE1	1.84	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: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:L:216:PHE:CZ	8:Q:128:PHE:CD2	2.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:586:HIS:NE2	3:3:604:ALA:HB2	2.18	0.59
1:A:341:MET:HE1	1:A:409:PRO:HB2	1.83	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
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: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:351:GLU:HA	3:L:205:ARG:HH12	1.67	0.59
1:J:332:PRO:CD	2:K:90:LEU:HD23	2.32	0.59
1:S:89:LEU:HD23	1:S:118:MET:HE3	1.83	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:213:ILE:H	4:V:213:ILE:HD12	1.68	0.59
4:V:64:THR:HG23	6:X:123:ILE:CD1	2.33	0.59
6:6:16:ARG:HG2	6:6:21:PHE:CE2	2.38	0.59
4:D:164:THR:OG1	4:D:170:HIS:HB3	2.02	0.59
4:D:155:THR:HB	4:D:193:LEU:HD12	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:110:VAL:N	1:S:111:PRO:HD3	2.18	0.59
3:U:458:LEU:HD12	3:U:458:LEU:H	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
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
1:S:355:LYS:HZ1	3:U:42:ILE:HG21	1.68	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:O	4:V:230:ILE:HG22	2.03	0.58
5:W:35:LYS:HD3	5:W:102:PRO:HB2	1.84	0.58
5:W:59:THR:HG22	5:W:59:THR:O	2.03	0.58
8:Z:33:LYS:HD2	8:Z:36:ASP:OD1	2.03	0.58
1:1:341:MET:HE1	1:1:409:PRO:HB2	1.85	0.58
2:B:86:LEU:O	2:B:90:LEU:HD12	2.03	0.58
3:C:117:LEU:H	4:D:321:MET:CE	2.16	0.58
3:C:117:LEU:N	4:D:321:MET:CE	2.66	0.58
1:J:342:TRP:O	1:J:342:TRP:HE3	1.86	0.58
4:M:238:SER:HB3	4:M:279:ARG:HH22	1.66	0.58
3:L:136:GLU:CG	5:N:189:ARG:HG2	2.30	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
4:4:115:THR:CG2	4:4:297:LEU:HD23	2.34	0.58
4:4:409:ARG:HG2	4:4:409:ARG:O	2.03	0.58
5:5:175:THR:CG2	5:5:178:ASP:HB2	2.32	0.58
5:5:71:VAL:HG11	5:5:89:PHE:HD2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:236:GLY:C	4:D:238:SER:H	2.07	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:112:LEU:HD21	3:U:130:LEU:HD11	1.84	0.58
3:U:13:VAL:HG21	3:U:17:THR:HG21	1.84	0.58
3:U:683:LEU:N	3:U:683:LEU:HD23	2.19	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
5:5:92:VAL:O	5:5:92:VAL:HG23	2.04	0.58
2:B:81:GLN:HB3	2:B:122:VAL:HG21	1.84	0.58
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:L:409:LEU:HD12	3:L:535:MET:HE3	1.86	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
4:4:164:THR:OG1	4:4:170:HIS:HB3	2.02	0.58
4:4:64:THR:HG23	6:6:123:ILE:CD1	2.33	0.58
1:A:238:PHE:HE1	1:A:249:MET:HE2	1.69	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
4:M:212:PRO:CG	4:M:213:ILE:HD12	2.31	0.58
2:T:81:GLN:HB3	2:T:122:VAL:HG21	1.85	0.58
1:S:437:TRP:CZ3	2:T:96:LEU:HB2	2.39	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:NH1	3:C:684:ARG:HG2	2.18	0.58
4:D:110:PRO:HB3	4:D:301:PRO:HG2	1.85	0.58
4:D:43:LEU:HD11	4:D:397:ILE:HD11	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:117:LEU:N	4:V:321:MET:CE	2.67	0.58
3:U:282:VAL:HG22	3:U:285:VAL:HG12	1.84	0.58
4:V:40:VAL:HG22	4:V:40:VAL:O	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
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
6:F:153:GLN:HG3	7:G:124:TYR:CZ	2.39	0.58
3:U:477:LEU:HD22	3:U:517:ALA:HB1	1.86	0.58
4:V:236:GLY:C	4:V:238:SER:H	2.08	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
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:OE2	3:L:671:GLU:HA	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:O	6:O:78:MET:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:715:GLU:HB3	3:L:746:ARG:NH1	2.19	0.57
3:L:693:TYR:HB3	3:L:759:TYR:CD2	2.40	0.57
4:V:211:SER:HB2	4:V:214:PHE:HB3	1.85	0.57
1:I:250:LYS:HB3	1:I:252:TYR:CE2	2.39	0.57
1:I:344:LEU:O	1:I:347:PHE:HB3	2.04	0.57
4:4:140:LEU:O	4:4:140:LEU:HD23	2.03	0.57
8:7:121:ARG:NH1	8:7:121:ARG:HG3	2.19	0.57
7:9:45:ARG:NH2	7:9:137:LEU:HD23	2.20	0.57
1:A:356:CYS:HB3	1:A:358:PRO:HG2	1.84	0.57
1:J:184:GLU:CD	1:J:186:THR:HG22	2.24	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:HD12	5:N:58:LEU:O	2.05	0.57
3:U:385:ALA:HB2	3:U:531:LYS:HB3	1.86	0.57
4:V:409:ARG:O	4:V:409:ARG:HG2	2.03	0.57
4:V:70:MET:HG2	4:V:78:ASN:OD1	2.03	0.57
1:I:186:THR:HG23	1:I: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:I:10:ASP:OD1	1:I: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
3:L:20:MET:HE3	3:L:432:PHE:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:139:GLU:HB2	2:2:140:PRO:CD	2.32	0.57
3:3:240:ALA:CB	3:3:276:ARG:HB2	2.35	0.57
3:3:125:GLY:HA3	3:3:246:ASN:HD22	1.68	0.57
3:3:497:TRP:O	3:3:528:LYS:HE3	2.04	0.57
5:5:25:LEU:N	5:5:25:LEU:CD2	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
4:M:43:LEU:HD11	4:M:397:ILE:HD11	1.87	0.57
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:591:HIS:ND1	3:C:592:PRO:HD2	2.19	0.57
5:E:13:LYS:HZ3	5:E:33:ARG:HH21	1.51	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
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
3:U:117:LEU:H	4:V:321:MET:CE	2.16	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
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
5:E:92:VAL:O	5:E:92:VAL:HG23	2.05	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
4:M:236:GLY:C	4:M:238:SER:H	2.09	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:26:MET:N	4:M:48:SER:HG	2.02	0.57
5:N:25:LEU:CD2	5:N:25:LEU:N	2.68	0.57
1:S:162:LEU:O	1:S:165:THR:HG22	2.04	0.57
1:S:53:VAL:O	1:S:57:VAL:HG23	2.04	0.57
6:X:108:MET:CE	6:X:147:LEU:HG	2.35	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:H	3:3:458:LEU:HD12	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:OE2	3:C:671:GLU:HA	2.04	0.56
2:T:101:THR:HG23	2:T:106:ILE:O	2.05	0.56
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
3:3:205:ARG:C	3:3:209:THR:HG22	2.25	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
1:S:287:ILE:HG22	1:S:302:PHE:CG	2.40	0.56
1:S:97:GLU:O	1:S:100:SER:HB3	2.05	0.56
2:2:136:VAL:HG12	2:2:137:ASN:N	2.20	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:303:THR:OG1	1:A:306:VAL:HG23	2.05	0.56
2:B:40:TRP:CD1	2:B:74:PRO:HA	2.40	0.56
3:C:285:VAL:HG22	3:C:286:ASN:N	2.20	0.56
6:F:117:MET:HB3	7:G:99:ILE:HD13	1.86	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
4:V:43:LEU:HD11	4:V:397:ILE:CD1	2.36	0.56
5:W:25:LEU:CD2	5:W:25:LEU:N	2.68	0.56
4:V:84:ARG:HD3	6:X:117:MET:HE3	1.87	0.56
3:3:494:LYS:O	3:3:498:GLU:HG2	2.05	0.56
1:A:88:TYR:HB2	1:A:216:THR:HG22	1.88	0.56
2:B:10:PHE:CZ	2:B:33:ARG:HG3	2.40	0.56
2:B:139:GLU:CB	2:B:140:PRO:CD	2.82	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
1:J:16:THR:CG2	1:J:229:PRO:HB3	2.33	0.56
5:N:175:THR:CG2	5:N:178:ASP:HB2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:3:572: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
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:HG2	4:M:409:ARG:O	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
3:3:117:LEU:N	4:4:321:MET:CE	2.68	0.56
7:9:96:LEU:HD21	7:9:129:LEU:HD12	1.87	0.56
7:9:30:PRO:HB2	7:9:162:VAL:HG13	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:92:ASN:ND2	10:S:440:FMN:O3'	2.38	0.56
1:S:64:GLY:HA3	10:S:440:FMN:O1P	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:398:VAL:C	3:U:399:LEU:HD12	2.26	0.56
3:U:54:LEU:N	3:U:55:PRO:HD3	2.21	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
4:V:167:ARG:HD3	6:X:143:ARG:NH1	2.20	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
4:4:215:TYR:CE2	4:4:219:ARG:HG3	2.41	0.56
6:6:78:MET:HG3	6:6:78:MET:O	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
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
4:4:236:GLY:C	4:4:238:SER:H	2.09	0.56
4:4:76:LEU:O	4:4:76:LEU:HD12	2.06	0.56
1:A:397:ARG:HG2	3:C:49:LEU:HD13	1.87	0.56
3:C:282:VAL:HG22	3:C:285:VAL:HG12	1.88	0.56
3:C:55:PRO:HG3	3:C:74:GLN:H	1.66	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
1:J:341:MET:HE1	1:J:409:PRO:HB2	1.85	0.56
1:J:355:LYS:HZ1	3:L:42:ILE:HG21	1.71	0.56
4:M:153:ARG:NH1	4:M:153:ARG:HG3	2.21	0.56
4:M:84:ARG:O	6:O:83:ARG:NH2	2.39	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
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
4:4:44:MET:HE3	4:4:44:MET:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:37:PHE:HD1	8:7:53:THR:O	1.88	0.56
3:C:474:ARG:HA	3:C:517:ALA:HB2	1.88	0.56
3:C:344:TYR:CD1	3:C:568:TYR:CE1	2.93	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:64:THR:HB	4:M:66:PHE:HE1	1.71	0.56
6:O:96:TRP:HA	6:O:99:MET:HE1	1.87	0.56
1:1:287:ILE:HG22	1:1:302:PHE:CG	2.41	0.56
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
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
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
3:C:227:THR:HG21	3:C:237:ASP:HB2	1.88	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:373:GLY:HA3	3:L:538:ALA:HB2	1.87	0.55
3:L:54:LEU:N	3:L:55:PRO:HD3	2.20	0.55
4:M:263:ASP:HB2	4:M:285:GLU:CD	2.26	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
1:S:341:MET:HE1	1:S:409:PRO:HB2	1.88	0.55
3:U:399:LEU:N	3:U:399:LEU:HD12	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:186:THR:HG23	1:A:200:ARG:H	1.71	0.55
1:A:29:LEU:CD1	1:A:155:ARG:HG3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:LYS:N	2:B:7:LYS:HD2	2.18	0.55
8:H:37:PHE:CD1	8:H:55:MET:HB2	2.42	0.55
3:L:583:VAL:CG2	3:L:598:ALA:HA	2.36	0.55
3:L:94:ASP:OD2	3:L:97:SER:HB2	2.07	0.55
5:N:125:VAL:HG12	5:N:126:PHE:N	2.21	0.55
5:N:59:THR:O	5:N:59:THR:HG22	2.05	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
3:3:409:LEU:HD12	3:3:535:MET:HE3	1.88	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:381:LEU:HD11	4:D:397:ILE:HG12	1.87	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
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
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
6:6:163:TYR:CD2	6:6:169:ARG:HA	2.34	0.55
6:6:16:ARG:O	6:6:21:PHE:HD2	1.89	0.55
1:A:274:GLU:HG2	1:A:279:TRP:HE1	1.72	0.55
1:A:97:GLU:O	1:A:100:SER:HB3	2.06	0.55
3:C:458:LEU:H	3:C:458:LEU:HD12	1.72	0.55
4:D:263:ASP:HB2	4:D:285:GLU:CD	2.27	0.55
3:L:185:LYS:HG2	3:L:188:VAL:HG22	1.88	0.55
3:L:440:ARG:NH1	3:L:440:ARG:CG	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:96:ALA:HB2	4:M:346:THR:HG21	1.89	0.55
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
6:6:16: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:138:PRO:HG2	7:G:121:MET:HG3	1.89	0.55
6:F:41:PHE:CZ	6:F:92:MET:HB2	2.41	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: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
4:V:64:THR:OG1	6:X:83:ARG:NH1	2.39	0.55
7:Y:44:THR:OG1	7:Y:52:LYS:HD2	2.07	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: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
5:5:116:ARG:HB3	5:5:135:ILE:HG13	1.87	0.55
5:5:35:LYS:HD3	5:5:102:PRO:HB2	1.87	0.55
6:6:36:LEU:HD22	6:6:77:VAL:HG21	1.89	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
7:Y:40:ARG:HB2	7:Y:121:MET:HE2	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:C:205:ARG:C	3:C:209:THR:HG22	2.27	0.55
5:E:20:ASN:HD21	5:E:24:ASN:HB2	1.72	0.55
8:H:121:ARG:NH1	8:H:121:ARG:HG3	2.22	0.55
2:K:139:GLU:HB2	2:K:140:PRO:CD	2.35	0.55
2:K:38:GLU:OE2	2:K:45:ARG:NH1	2.40	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: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:HG22	5:5:59:THR:O	2.06	0.54
4:D:153:ARG:NH1	4:D:153:ARG:HG3	2.21	0.54
4:D:213:ILE:CG2	4:D:217:ARG:HH11	2.19	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
3:3:54:LEU:N	3:3:55:PRO:HD3	2.22	0.54
2:2:110:GLU:HA	8:7:121:ARG:NH1	2.21	0.54
1:A:104:ARG:HH21	2:B:127:SER:HB2	1.71	0.54
1:A:438:ARG:N	1:A:438:ARG:HD2	2.22	0.54
3:C:399:LEU:N	3:C:399:LEU:HD12	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
1:J:438:ARG:N	1:J:438:ARG:HD2	2.23	0.54
1:J:72:THR:HG21	1:J:223:THR:HG21	1.90	0.54
3:L:125:GLY:HA3	3:L:246:ASN:HD22	1.72	0.54
3:L:18:SER:HB2	3:L:433:ALA:O	2.06	0.54
3:L:477:LEU:HD22	3:L:517:ALA:HB1	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:329:LEU:HD21	3:L:644:LEU:HA	1.89	0.54
1:S:391:LEU:HD22	1:S:407:VAL:HB	1.90	0.54
3:U:202:PHE:C	3:U:203:ILE:HD13	2.28	0.54
3:U:715:GLU:HB3	3:U:746:ARG:NH1	2.22	0.54
3:U:469:ARG:HA	3:U:754:PRO:HG3	1.88	0.54
3:3:282:VAL:HG22	3:3:285:VAL:HG12	1.90	0.54
4:4:363:SER:CB	5:5:174:LEU:H	2.19	0.54
4:4:84:ARG:O	6:6:83:ARG:NH2	2.40	0.54
1:A:196:ARG:NH2	3:C:204:GLU:O	2.41	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:202:PHE:C	3:L:203:ILE:HD13	2.28	0.54
3:L:344:TYR:CD1	3:L:568:TYR:CE1	2.96	0.54
3:L:184:CYS:O	9:L:785:SF4:S4	2.66	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
4:4:119:ILE:O	4:4:123:LEU:HB2	2.07	0.54
4:4:287:VAL:O	4:4:291:LYS:HG3	2.07	0.54
4:4:240:ARG:NH2	4:4:347:GLU:OE2	2.39	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
1:A:287:ILE:HG22	1:A:302:PHE:CG	2.42	0.54
5:E:25:LEU:CD2	5:E:25:LEU:N	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:241:ALA:CA	4:V:278:VAL:HG21	2.37	0.54
4:V:74:THR:HB	4:V:77:GLN:HG3	1.88	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
3:3:683:LEU:HD23	3:3:683:LEU:N	2.23	0.54
3:3:117:LEU:H	4:4:321:MET:CE	2.19	0.54
5:5:84:ASP:OD1	5:5:84:ASP:N	2.39	0.54
4:4:161:GLU:OE1	7:9:34:LYS:HG2	2.07	0.54
1:A:342:TRP:HE3	1:A:342:TRP:O	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:174:LEU:HD22	5:W:180:GLY:HA2	1.90	0.54
5:W:20:ASN:HD21	5:W:24:ASN:HB2	1.73	0.54
1:1:92:ASN:ND2	10:1:440:FMN:O3'	2.41	0.54
3:3:694:LEU:HB3	3:3:762:ALA:CB	2.34	0.54
3:3:94:ASP:OD2	3:3:97:SER:HB2	2.08	0.54
1:A:360:ARG:O	1:A:364:ALA:HB3	2.07	0.54
4:D:74:THR:HB	4:D:77:GLN:HG3	1.90	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:409:LEU:HD12	3:U:535:MET:CE	2.37	0.54
3:U:402:PRO:HD2	3:U:458:LEU:HD13	1.89	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
5:E:1:MET:SD	8:Z:113:GLU:OE2	2.65	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
4:4:265:PRO:HG2	4:4:282:GLU:HG2	1.89	0.54
4:4:84:ARG:HG2	9:6:182:SF4:S2	2.47	0.54
4:4:252:TYR:CE2	5:5:87:ARG:NH2	2.75	0.54
4:4:167:ARG:HD3	6:6:143:ARG:HH12	1.73	0.54
1:A:184:GLU:HG2	10:A:440:FMN:HM82	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: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
4:V:69:THR:HG21	6:X:120:ASN:HD22	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	4:D:59:ILE:H	1.71	0.54
1:J:238:PHE:HE1	1:J:249:MET:HE2	1.72	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:162:TRP:CE2	7:G:34:LYS:HD2	2.41	0.54
4:D:112:ARG:HH21	4:D:297:LEU:HD11	1.72	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:363:SER:CB	5:W:174:LEU:H	2.21	0.54
4:V:106:GLY:O	5:W:194:SER:HB3	2.08	0.54
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:393:MET:O	4:V:396:ILE:HG22	2.07	0.54
4:V:74:THR:HB	4:V:77:GLN:H	1.73	0.54
6:X:107:SER:O	6:X:137:VAL:HG12	2.07	0.54
4:V:84:ARG:HG2	9:X:182:SF4:S2	2.48	0.54
1:1:356:CYS:HB3	1:1:358:PRO:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:192:GLU:OE2	3:3:440:ARG:HA	2.08	0.53
4:4:263:ASP:HB2	4:4:285:GLU:CD	2.28	0.53
4:4:74:THR:HB	4:4:77:GLN:HG3	1.88	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:116:ARG:HB3	5:N:135:ILE:HG13	1.89	0.53
5:N:84:ASP:N	5:N:84:ASP:OD1	2.40	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
3:U:473:GLU:O	3:U:477:LEU:HD13	2.08	0.53
4:V:263:ASP:HB2	4:V:285:GLU:CD	2.28	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
3:C:117:LEU:HG	4:D:321:MET:HE2	1.89	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
1:S:238:PHE:HE1	1:S:249:MET:HE2	1.72	0.53
3:U:24:PHE:CE1	3:U:29:ASP:HA	2.42	0.53
3:U:501:LYS:N	3:U:501:LYS:HD2	2.08	0.53
8:Z:117:ALA:O	8:Z:121:ARG:HG2	2.08	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:202:PHE:C	3:3:203:ILE:HD13	2.29	0.53
4:4:342:VAL:HG22	4:4:343:TYR:H	1.73	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
4:M:44:MET:HA	4:M:44:MET:HE3	1.90	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
1:1:238:PHE:HE1	1:1:249:MET:HE2	1.74	0.53
1:1:341:MET:CE	1:1:409:PRO:HB2	2.38	0.53
3:3:557:SER:H	3:3:560:GLU:HB2	1.74	0.53
3:3:305:ARG:HG2	3:3:588:SER:O	2.08	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:515:THR:HG23	3:C:683:LEU:CD1	2.35	0.53
4:D:26:MET:N	4:D:48:SER:HG	2.06	0.53
6:F:155:GLN:O	6:F:158:VAL:HG22	2.09	0.53
6:F:36:LEU:HD22	6:F:77:VAL:HG21	1.89	0.53
1:J:109:ASP:C	1:J:111:PRO:HD3	2.29	0.53
2:K:101:THR:HG23	2:K:106:ILE:O	2.08	0.53
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:108:MET:HE3	6:X:147:LEU:HG	1.90	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
6:F:99:MET:CG	6:F:100:PRO:HD2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:205:ARG:C	3:L:209:THR:HG22	2.29	0.53
3:L:341:VAL:HG11	3:L:364:LEU:HD21	1.89	0.53
3:L:683:LEU:HD23	3:L:683:LEU:N	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
4:V:44:MET:HE2	4:V:44:MET:HA	1.90	0.53
8:Z:70:ALA:HA	8:Z:83:GLY:O	2.09	0.53
1:1:355:LYS:HZ1	3:3:42:ILE:HG21	1.74	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
6:6:108:MET:CE	6:6:147:LEU:HG	2.39	0.53
3:C:45:CYS:O	3:C:46:ARG:HB2	2.07	0.53
4:D:338:PRO:HG3	5:E:192:TYR:O	2.09	0.53
3:L:409:LEU:HD12	3:L:535:MET:CE	2.39	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:NH1	3:U:684:ARG:HG2	2.22	0.53
3:3:372:GLN:O	3:3:558:TRP:CE2	2.62	0.53
3:3:55:PRO:HG3	3:3:74:GLN:H	1.68	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
1:J:184:GLU:CG	10:J:440:FMN:HM82	2.39	0.53
3:L:497:TRP:O	3:L:500:ALA:HB3	2.09	0.53
1:S:270:THR:O	1:S:311:MET:HG3	2.09	0.53
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:CE	1:A:81:LYS:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:693:TYR:HB3	3:U:759:TYR:CD2	2.44	0.53
3:U:115:HIS:HB3	4:V:321:MET:HE3	1.91	0.53
3:3:282:VAL:O	3:3:282:VAL:HG22	2.10	0.53
3:3:382:PHE:N	3:3:382:PHE:CD1	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: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:N	3:L:399:LEU:HD12	2.24	0.53
3:L:458:LEU:HD12	3:L:458:LEU:H	1.73	0.53
8:Q:121:ARG:NH1	8:Q:121:ARG:HG3	2.24	0.53
2:T:40:TRP:CD1	2:T:74:PRO:HA	2.43	0.53
3:U:583:VAL:CG2	3:U:598:ALA:HA	2.39	0.53
3:U:550:LEU:HD23	3:U:684:ARG:NH2	2.24	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
1:1:189:MET:O	1:1:193:GLU:HB2	2.08	0.52
1:1:29:LEU:CD1	1:1:155:ARG:HG3	2.38	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: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:108:MET:HA	6:O:137:VAL:CG1	2.39	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:F:96:TRP:HA	6:F:99:MET:CE	2.40	0.52
8:H:82:ILE:HG23	8:H:95:ALA:HB3	1.91	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:CG	3:C:46:ARG:HH11	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: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
3:L:120:PRO:HG2	8:Q:42:TYR:OH	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
1:1:197:ALA:HB3	2:2:66:PHE:CZ	2.44	0.52
3:3:750:ARG:HB3	3:3:752:ASP:OD1	2.10	0.52
3:3:734:VAL:CG1	3:3:775:VAL:HG13	2.38	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:108:MET:CE	6:O:147:LEU:HG	2.40	0.52
1:S:293:GLY:HA3	1:S:324:GLY:N	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:413:LEU:HD13	3:3:448:MET:CE	2.39	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:CD1	4:V:168:PHE:N	2.78	0.52
3:3:232:VAL:HB	9:3:784:SF4:S2	2.50	0.52
3:3:488:GLU:O	3:3:491:ALA:HB3	2.10	0.52
3:3:385:ALA:HB2	3:3:531:LYS:HB3	1.90	0.52
3:3:715:GLU:HB3	3:3:746:ARG:NH1	2.24	0.52
3:3:513:GLN:HG2	3:3:769:LEU:HD23	1.91	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:C:202:PHE:C	3:C:203:ILE:HD13	2.29	0.52
4:D:84:ARG:HD3	6:F:117:MET:HE3	1.92	0.52
3:L:385:ALA:HB3	3:L:533:LEU:CD2	2.40	0.52
3:L:501:LYS:N	3:L:501:LYS:HD2	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:117:LEU:HG	4:V:321:MET:HE2	1.91	0.52
3:U:185:LYS:HG3	3:U:202:PHE:CE2	2.44	0.52
3:U:2:VAL:HG13	3:U:89:ASP:HA	1.90	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
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:174:LEU:HD22	5:E:180:GLY:HA2	1.91	0.52
5:E:53:VAL:HG22	5:E:55:LEU:CD1	2.40	0.52
7:G:40:ARG:HB2	7:G:121:MET:HE1	1.90	0.52
2:K:33:ARG:HH21	2:K:37:GLU:CG	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:398:VAL:C	3:L:399:LEU:HD12	2.30	0.52
4:M:254:TYR:CE2	4:M:346:THR:CA	2.91	0.52
4:M:240:ARG:NH2	4:M:347:GLU:OE2	2.40	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:O	1:S:110:VAL:HG23	2.10	0.52
2:T:7:LYS:HD2	2:T:7:LYS:N	2.23	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
3:C:398:VAL:C	3:C:399:LEU:HD12	2.30	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
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
7:P:134:GLU:H	7:P:134:GLU:CD	2.12	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
1:S:29:LEU:CD1	1:S:155:ARG:HG3	2.39	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
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
4:4:249:ARG:HD2	4:4:257:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:250:LYS:CE	4:4:262:PHE:HB3	2.41	0.51
4:4:248:VAL:HB	4:4:347:GLU:HB2	1.92	0.51
2:B:102:GLU:HA	8:H:108:ILE:HD11	1.93	0.51
4:D:168:PHE:CD1	4:D:168:PHE:N	2.77	0.51
5:E:141:LEU:HD11	5:E:150:TYR:OH	2.10	0.51
5:E:59:THR:O	5:E:59:THR:HG22	2.09	0.51
6:F:108:MET:CE	6:F:147:LEU:HG	2.40	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
1:1:366: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
8:7:13:TRP:CE2	8:7:17:LEU:HD11	2.45	0.51
7:9:44:THR:HA	7:9:138:VAL:HG13	1.91	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:497:TRP:CD1	3:U:524:LEU:HD11	2.46	0.51
3:U:474:ARG:HA	3:U:517:ALA:HB2	1.92	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:HD23	4:V:294:LEU:O	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
3:3:629: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:CG	8:7:121:ARG:NH1	2.74	0.51
3:C:715:GLU:HB3	3:C:746:ARG:NH1	2.26	0.51
5:E:103:THR:HG23	5:E:127:GLU:O	2.10	0.51
5:E:34:PHE:HE1	5:E:38:MET:SD	2.33	0.51
5:E:84:ASP:N	5:E:84:ASP:OD1	2.42	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:188:VAL:CG2	3:L:189:ARG:N	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:185:LYS:HG3	3:L:202:PHE:HE2	1.76	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
1:S:37:GLY:C	1:S:39:GLU:H	2.14	0.51
3:U:750:ARG:HB2	3:U:753:VAL:HG23	1.91	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
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
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
4:4:148: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
4:4:115:THR:HG21	4:4:297:LEU:HD23	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	4:V:153:ARG:HG3	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:173:PHE:HB3	3:C:296:PHE:CZ	2.45	0.51
3:C:18:SER:HB2	3:C:433:ALA:O	2.11	0.51
3:C:2:VAL:HG13	3:C:89:ASP:HA	1.93	0.51
6:F:20:LEU:O	6:F:24:LEU:HD13	2.10	0.51
3:L:202:PHE:HA	3:L:210:PHE:O	2.11	0.51
7:P:45:ARG:HH21	7:P:137:LEU:HD23	1.75	0.51
6:O:113:SER:HB3	7:P:96:LEU:HD13	1.93	0.51
2:K:110:GLU:HA	8:Q:121:ARG:NH1	2.25	0.51
3:U:205:ARG:C	3:U:209:THR:HG22	2.31	0.51
4:V:120:LEU:HD13	4:V:160:PHE:CE1	2.43	0.51
4:V:93:HIS:HA	4:V:353:LEU:HD21	1.92	0.51
5:W:58:LEU:O	5:W:58:LEU:HD12	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
1:A:332:PRO:HD2	2:B:90:LEU:HD23	1.92	0.51
3:C:557:SER:H	3:C:560:GLU:HB2	1.76	0.51
5:E:1:MET:C	5:E:3:LEU:H	2.14	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
5:5:103:THR:HG23	5:5:127:GLU:O	2.11	0.51
4:4:332:THR:O	5:5:172:ALA:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:2:ARG:NH1	5:N:45:GLY:HA3	2.26	0.51
4:M:84:ARG:HD3	6:O:117:MET:HE3	1.92	0.51
6:O:36:LEU:HD22	6:O:77:VAL:HG21	1.92	0.51
8:Q:40:PHE:HB2	8:Q:48:TYR:CE2	2.46	0.51
8:Q:37:PHE:HE2	8:Q:74:PRO:HA	1.76	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
1:A:89:LEU:HD23	1:A:118:MET:HE3	1.92	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
3:C:55:PRO:CG	3:C:74:GLN:N	2.70	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: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
4:M:93:HIS:HA	4:M:353:LEU:HD21	1.93	0.51
5:N:141:LEU:HD11	5:N:150:TYR:OH	2.11	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
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
1:J:37:GLY:C	1:J:39:GLU:H	2.14	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
3:3:505:LEU:HB3	3:3:532:VAL:HG22	1.93	0.50
4:4:218:ALA:HB1	4:4:272:VAL:HG22	1.94	0.50
1:A:109:ASP:C	1:A:111:PRO:HD3	2.32	0.50
1:A:288:GLN:HB3	1:A:333:GLU:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:185:LYS:HG3	3:C:202:PHE:CE2	2.47	0.50
2:B:110:GLU:HA	8:H:121:ARG:NH1	2.23	0.50
8:H:13:TRP:CE2	8:H:17:LEU:HD11	2.45	0.50
1:J:239:ALA:C	1:J:241:MET:H	2.15	0.50
1:J:65:ARG:NH2	1:J:268:MET:CE	2.75	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:NH1	4:V:153:ARG:HG3	2.27	0.50
4:V:385:CYS:HB3	4:V:396:ILE:HG12	1.93	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
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
3:L:413:LEU:HD13	3:L:448:MET:CE	2.41	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: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
4:V:83:PRO:HB2	4:V:169:HIS:HA	1.94	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
1:1:109:ASP:C	1:1:111:PRO:HD3	2.32	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
3:3:501:LYS:N	3:3:501:LYS:HD2	2.11	0.50
4:4:79:ILE:HG22	4:4:79:ILE:O	2.12	0.50
1:A:110:VAL:HG23	1:A:110:VAL:O	2.11	0.50
1:A:92:ASN:HD21	10:A:440:FMN:C2	2.23	0.50
3:C:478:LEU:CD2	3:C:483:ASP:HB2	2.41	0.50
3:C:329:LEU:HD21	3:C:644:LEU:HA	1.92	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
7:P:40:ARG:HB2	7:P:121:MET:HE1	1.92	0.50
2:T:112:THR:HG22	2:T:116:LEU:H	1.77	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
1:1:39:GLU:O	1:1:43:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:134:GLU:CD	7:9:134:GLU:H	2.14	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: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
4:4:200:ARG:O	4:4:204:TYR:HD1	1.94	0.50
4:4:59:ILE:H	4:4:59:ILE:HD13	1.75	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
4:D:44:MET:HE3	4:D:44:MET:HA	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:294:LEU:HD23	4:M:294:LEU:O	2.12	0.50
4:M:76:LEU:O	4:M:76:LEU:HD12	2.12	0.50
6:O:57:ARG:C	6:O:57:ARG:NE	2.65	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
3:3:583:VAL:HG23	3:3:599:HIS:H	1.75	0.50
4:4:168:PHE:CD1	4:4:168:PHE:N	2.77	0.50
5:5:71:VAL:CG1	5:5:89:PHE:HD2	2.24	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
2:K:129:HIS:CD2	2:K:130:THR:HG23	2.45	0.50
3:L:117:LEU:N	4:M:321:MET:CE	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:7:86:LEU:HD12	8:7:91:ILE:HD12	1.94	0.50
7:9:99:ILE:HG22	7:9:101:CYS:SG	2.51	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:240:ARG:HG3	4:D:265:PRO:O	2.12	0.50
4:D:69:THR:HG21	6:F:120:ASN:ND2	2.27	0.50
6:F:57:ARG:NE	6:F:57:ARG:C	2.65	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
3:C:188:VAL:CG2	3:C:189:ARG:N	2.74	0.50
4:D:385:CYS:HB3	4:D:396:ILE:HG12	1.93	0.50
4:D:168:PHE:CE1	6:F:141:PRO:HG3	2.45	0.50
7:G:134:GLU:CD	7:G:134:GLU:H	2.14	0.50
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:488:GLU:O	3:L:491:ALA:HB3	2.12	0.50
5:N:1:MET:C	5:N:3:LEU:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:118:VAL:HB	4:D:257:TYR:HE2	1.77	0.49
4:D:52:VAL:HG23	4:D:388:GLU:O	2.12	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:694:LEU:CB	3:U:762:ALA:HB2	2.37	0.49
3:U:689:LYS:HB2	3:U:772:GLU:HG2	1.93	0.49
4:V:338:PRO:HG3	5:W:192:TYR:O	2.11	0.49
5:W:1:MET:C	5:W:3:LEU:H	2.15	0.49
4:V:84:ARG:NE	6:X:117:MET:HE1	2.27	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
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
1:J:118:MET:HG2	1:J:224:LEU:HD13	1.94	0.49
1:J:38:TYR:OH	1:J:112:HIS:ND1	2.37	0.49
2:K:116:LEU:HD23	2:K:116:LEU:N	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
1:1:316:LEU:HD12	1:1:323:LEU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:92:ASN:HD21	10:1:440:FMN:C2	2.25	0.49
3:3:483:ASP:O	3:3:484:LYS:HG2	2.11	0.49
6:6:57:ARG:NE	6:6:57:ARG:C	2.66	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
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
2:K:109:GLY:HA2	8:Q:91:ILE:HD13	1.93	0.49
1:S:203:PRO:HB2	1:S:204:PRO:HD3	1.93	0.49
1:S:366:PHE:HD1	1:S:370:LEU:HD21	1.77	0.49
1:S:88:TYR:HB2	1:S:216:THR:CG2	2.42	0.49
3:U:131:GLN:O	3:U:134:THR:HB	2.12	0.49
1:S:351:GLU:HA	3:U:205:ARG:HH12	1.77	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
3:3:337:ARG:HD2	3:3:337:ARG:N	2.27	0.49
3:3:194:VAL:HG12	3:3:411:LEU:HD22	1.94	0.49
4:4:338:PRO:HG3	5:5:192:TYR:O	2.12	0.49
8:7:117:ALA:O	8:7:121:ARG:HG2	2.12	0.49
3:C:241:ARG:HH11	7:G:74:GLU:CD	2.15	0.49
3:C:385:ALA:HB2	3:C:531:LYS:CB	2.42	0.49
3:C:333:LEU:HD13	3:C:648:LEU:HD21	1.94	0.49
3:C:513:GLN:HG2	3:C:769:LEU:HD23	1.93	0.49
4:D:115:THR:CG2	4:D:297:LEU:HD23	2.42	0.49
5:E:13:LYS:O	5:E:13:LYS:HG2	2.13	0.49
1:J:88:TYR:HB2	1:J:216:THR:CG2	2.42	0.49
3:L:185:LYS:HG3	3:L:202:PHE:CE2	2.48	0.49
3:L:2:VAL:HG13	3:L:89:ASP:HA	1.94	0.49
4:M:200:ARG:O	4:M:204:TYR:HD1	1.94	0.49
4:M:118:VAL:HB	4:M:257:TYR:HE2	1.77	0.49
4:M:43:LEU:HD11	4:M:397:ILE:CD1	2.42	0.49
1:S:288:GLN:HB3	1:S:333:GLU:HG2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:188: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
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:342:VAL:HG22	4:V:343:TYR:H	1.78	0.49
4:V:59:ILE:H	4:V:59:ILE:HD13	1.77	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
6:6:96:TRP:HA	6:6:99:MET:CE	2.41	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:693:TYR:HB3	3:C:759:TYR:HD2	1.76	0.49
4:D:342:VAL:HG22	4:D:343:TYR:H	1.78	0.49
4:D:64:THR:HB	4:D:66:PHE:HE1	1.75	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
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:358:PRO:O	1:S:362:GLY:HA3	2.13	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
2:T:102:GLU:HA	8:Z:108:ILE:HD11	1.95	0.49
8:Z:40:PHE:HB2	8:Z:48:TYR:CE2	2.47	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:HD23	4:D:294:LEU:O	2.13	0.49
4:D:85:MET:HE2	4:D:370:VAL:HG11	1.94	0.49
1:J:355:LYS:HD3	1:J:399:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:M:115:THR:HG22	4:M:297:LEU:HD23	1.94	0.49
5:N:41:TYR:HA	5:N:44:MET:HE3	1.95	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
5:W:41:TYR:HA	5:W:44:MET:HE3	1.94	0.49
6:X:57:ARG:C	6:X:57:ARG:NE	2.65	0.49
8:Z:13:TRP:CZ2	8:Z:17:LEU:HD11	2.46	0.49
3:3:117:LEU:HG	4:4:321:MET:HE2	1.95	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: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:224:ILE:HD11	4:M:275:ARG:CZ	2.43	0.49
4:M:74:THR:HG22	4:M:75:TYR:N	2.27	0.49
5:N:107:LEU:HD23	5:N:107:LEU:HA	1.70	0.49
1:S:289:ALA:HB3	1:S:337:MET:HE3	1.95	0.49
1:S:41:ALA:HA	1:S:120:LEU:HD21	1.94	0.49
2:T:116:LEU:HD23	2:T:116:LEU:N	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:261:THR:HB	4:V:292:GLN:OE1	2.13	0.49
4:V:125:ARG:HD2	4:V:286:SER:OG	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
3:3:20:MET:HE3	3:3:432:PHE:HB3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:197:LEU:N	4:D:198:PRO:HD2	2.28	0.49
4:D:69:THR:HG21	6:F:120:ASN:HD22	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
5:W:40:HIS:NE2	5:W:44:MET:HE1	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:N	1:A:397:ARG:HD2	2.25	0.49
2:B:116:LEU:HD23	2:B:116:LEU:N	2.28	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: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
4:V:69:THR:HG21	6:X:120:ASN:ND2	2.27	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
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:409:LEU:HD12	3:C:535:MET:CE	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
5:E:157:THR:C	5:E:158:LEU:HD23	2.34	0.48
8:H:108:ILE:N	8:H:108:ILE:HD12	2.28	0.48
8:H:20:MET:HE3	8:H:59:LEU:HG	1.95	0.48
1:J:211:LEU:H	1:J:216:THR:HG21	1.77	0.48
1:J:40:THR:O	1:J:44:VAL:HG23	2.13	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:N	8:Q:108:ILE:HD12	2.27	0.48
3:U:629:ILE:HG22	3:U:630:GLU:N	2.25	0.48
3:U:232:VAL:HB	9:U:784:SF4:S2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:96:LEU:HD21	7:Y:129:LEU:HD12	1.95	0.48
5:W:160:ARG:HG3	7:Y:130:VAL:HG11	1.95	0.48
8:Z:49:ASP:OD1	8:Z:49:ASP:N	2.46	0.48
3:3:254:THR:HG23	3:3:255:THR:N	2.28	0.48
3:3:381:LEU:HD12	3:3:522:ARG:HD3	1.94	0.48
5:5:1:MET:C	5:5:3:LEU:H	2.15	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
1:A:37:GLY:C	1:A:39:GLU:H	2.17	0.48
2:B:85:THR:HG22	2:B:86:LEU:N	2.27	0.48
3:C:413:LEU:HD13	3:C:448:MET:HE3	1.95	0.48
3:C:20:MET:HE1	3:C:433:ALA:HB2	1.95	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
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
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:497:TRP:CD1	3:C:524:LEU:HD11	2.49	0.48
3:C:184:CYS:O	9:C:785:SF4:S4	2.72	0.48
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:244:ALA:HB3	3:3:249:MET:CE	2.43	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
3:3:2:VAL:HG13	3:3:89:ASP:HA	1.94	0.48
4:4:224:ILE:HD11	4:4:275:ARG:CZ	2.43	0.48
4:4:222:GLY:HA2	4:4:384:ALA:O	2.14	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
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
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:N	3:3:399:LEU:HD12	2.28	0.48
4:4:93:HIS:HA	4:4:353:LEU:HD21	1.96	0.48
5:5:25:LEU:H	5:5:25:LEU:CD2	2.27	0.48
5:5:25:LEU:HD23	5:5:25:LEU:H	1.78	0.48
6:6:16:ARG:HA	6:6:21:PHE:CD2	2.48	0.48
8:7:16:LEU:O	8:7:16:LEU:HD13	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
3:L:688:ARG:HD3	3:L:688:ARG:HA	1.53	0.48
1:J:397:ARG:NE	3:L:79:LEU:HD12	2.25	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
3:U:188:VAL:CG2	3:U:189:ARG:N	2.76	0.48
8:Z:121:ARG:CG	8:Z:121:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:167:PRO:HB3	7:9:66:TYR:CD2	2.48	0.48
3:C:244:ALA:HB3	3:C:249:MET:CE	2.44	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
4:V:311:PRO:HD3	4:V:330:HIS:CE1	2.49	0.48
5:W:52:ILE:CG2	5:W:114:LEU:HB3	2.40	0.48
5:W:16:PRO:HB2	5:W:28:VAL:CG1	2.44	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
6:F:113:SER:HB3	7:G:96:LEU:HD13	1.95	0.48
1:J:211:LEU:HB2	1:J:216:THR:HG21	1.95	0.48
3:L:413:LEU:HD13	3:L:448:MET:HE3	1.94	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:359:CYS:O	1:S:363:VAL:HG22	2.13	0.48
1:S:195:LEU:HA	2:T:24:ARG:HH21	1.78	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:N	1:1:397:ARG:HD2	2.27	0.48
3:3:46:ARG:O	3:3:107:MET:HG2	2.13	0.48
3:C:738:THR:HG22	3:C:739:PRO:CD	2.37	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
5:E:41:TYR:HA	5:E:44:MET:HE3	1.96	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
4:M:168:PHE:HE1	6:O:141:PRO:HG3	1.79	0.48
4:M:83:PRO:HB2	4:M:169:HIS:HA	1.96	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:114:SER:HB2	7:Y:97:ARG:CD	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:37:TRP:CE3	6:X:37:TRP:HA	2.49	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:NH1	4:4:350:ARG:HG3	2.29	0.48
5:5:41:TYR:HA	5:5:44:MET:HE3	1.96	0.48
1:A:264:TYR:CD2	1:A:279:TRP:HB3	2.49	0.48
1:A:72:THR:HG21	1:A:223:THR:HG21	1.96	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
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
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
3:3:326: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
4:4:211:SER:HB2	4:4:215:TYR:N	2.28	0.48
1:A:184:GLU:OE1	1:A:186:THR:N	2.47	0.48
1:A:97:GLU:OE2	1:A:294:GLY:HA3	2.14	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
1:A:39:GLU:O	1:A:43:ARG:HG3	2.14	0.48
3:C:33:PHE:HE2	3:C:111:THR:HG21	1.79	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
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
6:X:96:TRP:HA	6:X:99:MET:CE	2.41	0.48
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
3:3:19:VAL:HG23	3:3:85:THR:O	2.14	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
4:D:44:MET:HA	4:D:44:MET:HE2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	6:O:121:TYR:HD1	1.62	0.47
1:S:360:ARG:O	3:U:207:VAL:HG13	2.14	0.47
1:S:341:MET:CE	1:S:409:PRO:HB2	2.43	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
4:4:316:LEU:C	4:4:318:GLU:H	2.17	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
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
4:M:148:TYR:HB3	4:M:200:ARG:HH12	1.77	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
1:1:37:GLY:C	1:1:39:GLU:H	2.18	0.47
1:1:183:GLY:O	10:1:440:FMN:H2'	2.14	0.47
3:3:116:PRO:O	3:3:117:LEU:HB2	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:N	3:L:337:ARG:HD2	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:N	3:U:337:ARG:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:272:PHE:CE1	1:1:311:MET:HG2	2.49	0.47
4:4:263:ASP:O	4:4:285:GLU:HG3	2.14	0.47
4:4:115:THR:HG22	4:4:297:LEU:HD23	1.97	0.47
3:C:2:VAL:CG1	3:C:89:ASP:HA	2.44	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:102:GLU:HA	8:Q:108:ILE:HD11	1.96	0.47
2:K:88:CYS:HB3	2:K:93:ALA:HB2	1.97	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
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
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:H	6:6:121:TYR:HD1	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
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
6:O:96:TRP:HA	6:O:99:MET:CE	2.44	0.47
1:S:40:THR:O	1:S:44:VAL:HG23	2.15	0.47
3:U:378:PRO:O	3:U:381:LEU:HB2	2.15	0.47
4:V:350:ARG:HD3	4:V:374:SER:OG	2.15	0.47
1:1:239:ALA:C	1:1:241:MET:H	2.18	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
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: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
3:U:724:ARG:O	3:U:724:ARG:HG2	2.14	0.47
3:U:693:TYR:HB3	3:U:759:TYR:HD2	1.78	0.47
1:1:205:PHE:HD1	1:1:206:PRO:HD2	1.80	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)
4:4:376:VAL:O	4:4:379:GLN:HG3	2.15	0.47
4:D:188:PRO:O	4:D:191:LYS:HB2	2.14	0.47
4:D:314:ARG:CG	4:D:314:ARG:NH1	2.75	0.47
6:F:108:MET:HA	6:F:137:VAL:CG1	2.44	0.47
3:L:508:GLY:HA2	3:L:535:MET:HB2	1.97	0.47
6:O:149:TYR:CZ	6:O:153:GLN:NE2	2.82	0.47
8:Q:121:ARG:NH1	8:Q:121:ARG:CG	2.78	0.47
8:Q:63:LEU:HD13	8:Q:129:ALA:HB3	1.97	0.47
1:S:109:ASP:C	1:S:111:PRO:HD3	2.34	0.47
1:S:162:LEU:HB3	1:S:163:PHE:CD1	2.49	0.47
3:U:381:LEU:HD12	3:U:522:ARG:HD3	1.96	0.47
4:V:79:ILE:O	4:V:79:ILE:HG22	2.14	0.47
6:X:108:MET:HA	6:X:137:VAL:CG1	2.45	0.47
1:1:102:LYS:HG3	1:1:103:ASP:N	2.30	0.47
2:2:116:LEU:N	2:2:116:LEU:HD23	2.30	0.47
3:3:688:ARG:HA	3:3:688:ARG:HD3	1.52	0.47
4:4:226:PRO:HG3	4:4:242:SER:O	2.15	0.47
4:4:106:GLY:O	5:5:194:SER:HB3	2.15	0.47
6:6:110:ALA:HB1	6:6:116:GLY:HA2	1.97	0.47
4:4:84:ARG:HD3	6:6:117:MET:HE3	1.95	0.47
6:6:37:TRP:CE3	6:6:37:TRP:HA	2.48	0.47
1:A:399:PHE:HB3	9:A:439:SF4:S2	2.55	0.47
4:D:346:THR:HG22	4:D:353:LEU:O	2.14	0.47
4:D:106:GLY:O	5:E:194:SER:HB3	2.14	0.47
6:F:16:ARG:HA	6:F:21:PHE:CD2	2.50	0.47
8:H:88:ARG:HE	8:H:126:LEU:CD2	2.28	0.47
8:H:8:GLU:HG2	8:H:97:TYR:OH	2.14	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:689:LYS:HB2	3:L:772:GLU:HG2	1.96	0.47
4:M:393:MET:C	4:M:396:ILE:HG22	2.35	0.47
2:T:106:ILE:CG2	2:T:110:GLU:HB2	2.44	0.47
3:U:505:LEU:HD21	3:U:507:LEU:HD23	1.97	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:211:SER:CB	4:D:214:PHE:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:358:VAL:O	4:D:366:TYR:HB3	2.15	0.47
4:D:99:LEU:HD13	4:D:99:LEU:HA	1.80	0.47
5:E:168:ALA:HA	5:E:171:ARG:HH12	1.80	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: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
4:4:84:ARG:NE	6:6:117:MET:HE1	2.30	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
6:6:17:GLU:O	1:J:273:ARG:HD3	2.15	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
1:S:239:ALA:C	1:S:241:MET:H	2.18	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:HD23	5:W:25:LEU:H	1.80	0.47
6:X:33:SER:HA	6:X:158:VAL:HG21	1.96	0.47
3:3:398:VAL:C	3:3:399:LEU:HD12	2.34	0.47
4:4:26:MET:N	4:4:48:SER:HG	2.12	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: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
4:M:44:MET:HE2	4:M:44:MET:HA	1.97	0.47
5:N:168:ALA:HA	5:N:171:ARG:HH12	1.79	0.47
1:S:291:ILE:HD11	1:S:331:ILE:HD11	1.97	0.47
3:U:100:VAL:O	3:U:104:GLN:HG3	2.14	0.47
2:T:58:THR:HG21	3:U:200:LEU:N	2.29	0.47
3:U:440:ARG:NH1	3:U:440:ARG:CG	2.76	0.47
3:U:591:HIS:ND1	3:U:592:PRO:N	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:9:40:ARG:HB2	7:9:121:MET:HE1	1.95	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:O	4:D:76:LEU:HD12	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:29:LEU:HD22	1:S:33:LEU:CD1	2.46	0.46
1:S:6:LEU:HD21	1:S:12:ARG:CG	2.44	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:O	4:V:173:ILE:HG23	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:N	5:5:195:LEU:HD22	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:117:ALA:O	8:H:121:ARG:HG2	2.15	0.46
8:H:13:TRP:CZ2	8:H:17:LEU:HD11	2.51	0.46
1:J:202:LYS:N	1:J:203:PRO:HD2	2.31	0.46
3:L:378:PRO:O	3:L:381:LEU:HB2	2.14	0.46
3:L:45:CYS:O	3:L:46:ARG:HB2	2.15	0.46
4:M:197:LEU:N	4:M:198:PRO:HD2	2.30	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
8:Z:37:PHE:HE2	8:Z:74:PRO:HA	1.79	0.46
4:4:173:ILE:HG23	4:4:173:ILE:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:289:ALA:HB3	1:J:337:MET:HE3	1.97	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
5:W:13:LYS:HG2	5:W:13:LYS:O	2.15	0.46
4:V:338:PRO:HG3	5:W:193:ARG:HB2	1.96	0.46
7:Y:29:ALA:HA	7:Y:30:PRO:HD2	1.79	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
4:M:85:MET:HE2	4:M:370:VAL:HG11	1.98	0.46
5:N:13:LYS:HG2	5:N:13:LYS:O	2.15	0.46
5:N:37:GLU:O	5:N:40:HIS:HB3	2.16	0.46
6:O:117:MET:CE	7:P:99:ILE:HG12	2.45	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
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
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
1:A:397:ARG:NE	3:C:79:LEU:HD12	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:OD1	8:Q:49:ASP:N	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
3:U:413:LEU:HD13	3:U:448:MET:CE	2.45	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:HD23	4:4:294:LEU:O	2.16	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: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
1:1:289:ALA:HB3	1:1:337:MET:HE3	1.98	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
4:4:393: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
3:C:250:GLU:CD	3:C:628:PRO:HG2	2.36	0.46
3:C:732:ALA:H	3:C:747:VAL:HG12	1.80	0.46
4:D:173:ILE:O	4:D:173:ILE:HG23	2.16	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
6:O:155:GLN:C	6:O:157:LYS:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:62:LEU:HD21	6:F:43:LEU:HB3	1.97	0.46
6:F:141:PRO:HB3	9:F:182:SF4:S1	2.56	0.46
1:J:107:LEU:CD2	1:J:114:LEU:HD12	2.46	0.46
1:J:87:HIS:HB2	1:J:126:ARG:O	2.16	0.46
1:J:397:ARG:N	1:J:397:ARG:HD2	2.29	0.46
3:L:117:LEU:H	4:M:321:MET:CE	2.28	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:276:MET:O	4:V:280:ILE:HG13	2.15	0.46
4:V:263:ASP:O	4:V:285:GLU:HG3	2.15	0.46
7:Y:134:GLU:CD	7:Y:134:GLU:H	2.18	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
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
3:L:132:ASP:O	3:L:136:GLU:HG3	2.15	0.46
3:L:559:ASP:HB2	3:L:573:PRO:HG3	1.97	0.46
3:L:2:VAL:CG1	3:L:89:ASP:HA	2.46	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:106:ILE:CD1	6:X:151:VAL:HG12	2.46	0.46
6:X:16:ARG:HA	6:X:21:PHE:CD2	2.50	0.46
4:4:125:ARG:HD2	4:4:286:SER:OG	2.16	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:290:ILE:HG22	1:A:330:LEU:HD22	1.98	0.46
1:A:29:LEU:HD22	1:A:33:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	5:E:132:LEU:HD23	1.65	0.46
3:C:216:PHE:CZ	8:H:128:PHE:CD2	3.00	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:65:ARG:NH2	1:S:268:MET:CE	2.79	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:202:LYS:N	1:A:203:PRO:HD2	2.30	0.45
1:A:233:ARG:HG2	1:A:233:ARG:H	1.57	0.45
1:A:420:GLN:O	1:A:424:LEU:HD13	2.16	0.45
1:A:104:ARG:HH21	2:B:127:SER:CB	2.28	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:HA	6:F:37:TRP:CE3	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
6:O:157:LYS:O	6:O:157:LYS:HG2	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:48:ILE:HG22	6:X:48:ILE:O	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
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
6:F:157:LYS:HG2	6:F:157:LYS:O	2.16	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:455:ARG:HG3	3:L:455:ARG:O	2.17	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:515:THR:HG23	3:U:683:LEU:CD1	2.43	0.45
3:U:83:CYS:SG	3:U:84:VAL:HG13	2.57	0.45
4:V:197:LEU:N	4:V:198:PRO:CD	2.79	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
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
3:3:508: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
6:6:43:LEU:HD11	6:6:84:LEU:HD23	1.97	0.45
8:7:49:ASP:OD1	8:7:49:ASP:N	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:413:LEU:HD13	3:C:448:MET:CE	2.45	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
1:J:89:LEU:HD23	1:J:118:MET:HE3	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:V:44:MET:HA	4:V:44:MET:HE3	1.95	0.45
7:Y:129:LEU:HA	7:Y:129:LEU:HD23	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
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
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:181:LEU:HA	5:E:181:LEU:HD12	1.80	0.45
7:G:39:GLY:O	7:G:40:ARG:C	2.55	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
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: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
1:1:297: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
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: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
3:C:83:CYS:SG	3:C:84:VAL:HG13	2.56	0.45
3:C:216:PHE:CZ	8:H:128:PHE:HD2	2.31	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:N	5:N:195:LEU:HD22	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:197:ASP:CB	3:U:220:SER:HB3	2.46	0.45
3:U:245:ARG:HD2	3:U:245:ARG:HA	1.74	0.45
3:U:6:VAL:HG21	3:U:26:ALA:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:263:ASP:HB2	4:V:285:GLU:OE1	2.17	0.45
4:V:84:ARG:HD3	6:X:117:MET:CE	2.47	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
1:1:38:TYR:OH	1:1:112:HIS:ND1	2.40	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
1:A:239:ALA:C	1:A:241:MET:H	2.20	0.45
8:H:16:LEU:HG	8:H:82:ILE:HD11	1.97	0.45
1:J:110:VAL:N	1:J:111:PRO:CD	2.79	0.45
1:J:107:LEU:HD23	1:J:114:LEU:HD12	1.98	0.45
1:J:332:PRO:HD2	2:K:90:LEU:CD2	2.44	0.45
3:L:119:CYS:O	3:L:120:PRO:C	2.53	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
3:3:403:THR:HG22	3:3:403:THR:O	2.16	0.45
3:3:20:MET:HE1	3:3:433:ALA:HB2	1.97	0.45
3:3:305:ARG:NH2	3:3:609:GLU:OE1	2.47	0.45
5:5:129:HIS:CD2	5:5:130:PRO:HD2	2.51	0.45
6:6:48:ILE:O	6:6:48:ILE:HG22	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: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:205:PHE:HD1	1:S:206:PRO:HD2	1.80	0.45
1:S:104:ARG:HH21	2:T:127:SER:CB	2.29	0.45
2:T:142:VAL:HG11	2:T:153:LEU:HG	1.99	0.45
3:U:113:LEU:HD12	3:U:157:PHE:CG	2.51	0.45
3:U:132:ASP:O	3:U:136:GLU:HG3	2.16	0.45
3:U:55:PRO:CG	3:U:74:GLN:N	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:218:LEU:N	3:3:219:PRO:HD3	2.31	0.45
3:3:413:LEU:HD13	3:3:448:MET:HE1	1.99	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:138:LEU:HD11	4:D:146:PHE:CD2	2.51	0.45
4:D:306:ASN:HA	4:D:307:PRO:HD3	1.77	0.45
4:D:316:LEU:C	4:D:316:LEU:HD12	2.36	0.45
4:D:375:PHE:HD1	4:D:407:VAL:HG23	1.82	0.45
5:E:111:ALA:HB1	5:E:115:GLU:HG3	1.98	0.45
5:E:37:GLU:O	5:E:40:HIS:HB3	2.17	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
1:S:197:ALA:HB3	2:T:66:PHE:CE1	2.52	0.45
1:S:92:ASN:ND2	10:S:440:FMN:C2	2.80	0.45
3:U:218:LEU:N	3:U:219:PRO:HD3	2.32	0.45
4:D:188:PRO:CB	3:U:724:ARG:CD	2.59	0.45
4:V:178:VAL:CG2	4:V:302:VAL:HB	2.47	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
1:1:184:GLU:CG	10:1:440:FMN:HM82	2.45	0.45
1:1:65:ARG:NH2	1:1:268:MET:CE	2.80	0.45
2:2:112:THR:HG22	2:2:116:LEU:H	1.82	0.45
2:2:88:CYS:HB3	2:2:93:ALA:HB2	1.99	0.45
3:3:168:HIS:HA	3:3:169:PRO:HD2	1.73	0.45
3:3:19:VAL:HG12	3:3:82:SER:HB2	1.98	0.45
4:4:211:SER:HB2	4:4:215:TYR:H	1.82	0.45
5:5:141:LEU:HD21	5:5:145:PRO:HD3	1.98	0.45
5:5:54:GLY:O	5:5:55:LEU:HD12	2.17	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:HA	3:C:351:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:11:LEU:HD22	2:K:30:LEU:HD21	1.98	0.45
4:M:211:SER:HB2	4:M:215:TYR:H	1.82	0.45
4:M:63:HIS:O	6:O:122:ALA:HB1	2.17	0.45
1:S:264:TYR:CE2	1:S:279:TRP:HB3	2.52	0.45
3:U:115:HIS:HB3	4:V:321:MET:CE	2.46	0.45
3:U:694:LEU:C	3:U:762:ALA:HB2	2.38	0.45
4:V:241:ALA:CB	4:V:278:VAL:HG21	2.46	0.45
2:2:153:LEU:C	2:2:153:LEU:HD13	2.37	0.45
3:3:119:CYS:O	3:3:120:PRO:C	2.55	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
6:6:155:GLN:C	6:6:157:LYS:H	2.20	0.45
1:A:264:TYR:CE2	1:A:279:TRP:HB3	2.52	0.45
2:B:86:LEU:CD1	2:B:90:LEU:HD11	2.47	0.45
3:C:498:GLU:C	3:C:500:ALA:H	2.19	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
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
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
3:3:33:PHE:HE2	3:3:111:THR:HG21	1.81	0.44
3:3:118:ASP:O	3:3:119:CYS:C	2.55	0.44
3:3:378:PRO:O	3:3:381:LEU:HB2	2.16	0.44
1:1:397:ARG:HG2	3:3:49:LEU:HD13	1.97	0.44
4:4:104:LEU:HD22	4:4:338:PRO:HD2	1.99	0.44
1:A:53:VAL:HG23	1:A:231:MET:CE	2.46	0.44
1:A:81:LYS:HE3	1:A:81:LYS:HA	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:40:HIS:NE2	5:E:44:MET:HE1	2.32	0.44
8:H:37:PHE:HE2	8:H:74:PRO:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:233:ARG:HG2	1:J:233:ARG:H	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
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:290:ILE:HD13	3:U:290:ILE:HA	1.76	0.44
3:U:30:VAL:CG2	3:U:31:PRO:HD2	2.47	0.44
3:U:470:PRO:HG3	3:U:759:TYR:HE2	1.82	0.44
4:V:224:ILE:HA	4:V:225:PRO:HD2	1.77	0.44
4:V:278:VAL:O	4:V:282:GLU:HG3	2.17	0.44
4:V:115:THR:HG21	4:V:297:LEU:HD23	1.97	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:CD1	7:Y:100:PHE:N	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:724:ARG:HG2	3:C:724:ARG:O	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:N	3:L:203:ILE:HD13	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:224:ILE:HA	4:M:225:PRO:HD2	1.79	0.44
4:M:63:HIS:HA	4:M:409:ARG:OXT	2.16	0.44
8:Q:88:ARG:HE	8:Q:126:LEU:HD22	1.82	0.44
1:S:162:LEU:HB3	1:S:163:PHE:HD1	1.83	0.44
1:S:139:ARG:CG	2:T:140:PRO:HD3	2.45	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
1:1:163:PHE:C	1:1:165:THR:H	2.20	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
4:4:393:MET:C	4:4:396:ILE:HG22	2.38	0.44
4:4:44:MET:HE2	4:4:44:MET:HA	1.99	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:470:PRO:O	3:L:471:GLY:C	2.55	0.44
3:L:483:ASP:O	3:L:484:LYS:HG2	2.17	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:408:ILE:HA	3:U:408:ILE:HD12	1.77	0.44
3:U:508:GLY:HA2	3:U:535:MET:HB2	1.99	0.44
3:U:367:PRO:CB	3:U:554:LYS:HB2	2.47	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
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
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:26:MET:N	4:V:48:SER:HG	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:356:LEU:HD13	3:3:654:PHE:HD1	1.83	0.44
4:4:350:ARG:HG3	4:4:350:ARG:HH11	1.82	0.44
4:4:82:THR:N	4:4:83:PRO:HD2	2.32	0.44
1:A:6:LEU:HD21	1:A:12:ARG:CG	2.47	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
1:J:184:GLU:HG2	10:J:440:FMN:C8M	2.45	0.44
2:K:78:TYR:CE1	2:K:157:LEU:HD22	2.53	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
3:U:225:ASN:O	3:U:229:ILE:HG13	2.17	0.44
5:W:104:VAL:HG12	5:W:108:TRP:CE3	2.49	0.44
6:X:157:LYS:HG2	6:X:157:LYS:O	2.17	0.44
6:X:16:ARG:NH1	6:X:17:GLU:OE2	2.51	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
3:3:591:HIS:ND1	3:3:592:PRO:CD	2.81	0.44
3:3:582:PHE:HA	3:3:599:HIS:ND1	2.32	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
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:250:LYS:CE	4:D:262:PHE:HB3	2.44	0.44
4:D:240:ARG:NH2	4:D:347:GLU:OE2	2.46	0.44
5:E:107:LEU:HD23	5:E:107:LEU:HA	1.72	0.44
4:D:379:GLN:HG2	5:E:113:PHE:CD1	2.52	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
1:S:81:LYS:CE	1:S:81:LYS:HA	2.47	0.44
4:V:285:GLU:O	4:V:289:ILE:HG12	2.17	0.44
4:V:198:PRO:HG3	4:V:291:LYS:HZ3	1.81	0.44
1:1:272:PHE:O	1:1:276:ILE:HG13	2.17	0.44
1:1:289:ALA:HB3	1:1:337:MET:CE	2.48	0.44
3:3:422:PRO:HA	3:3:423:PRO:HD2	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:469:ARG:HB2	3:3:470:PRO:CD	2.47	0.44
3:3:646:GLU:C	3:3:648:LEU:H	2.21	0.44
4:4:235:THR:O	4:4:235:THR:HG22	2.17	0.44
4:4:230:ILE:HD11	4:4:244:VAL:CG2	2.48	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:HA	3:C:575:GLU:OE1	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
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:243:ARG:HB3	3:L:275:LEU:HD12	1.99	0.44
3:L:30:VAL:CG2	3:L:31:PRO:HD2	2.48	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
4:M:173:ILE:O	4:M:173:ILE:HG23	2.18	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:417:VAL:O	3:U:417:VAL:HG12	2.18	0.44
3:U:30:VAL:CG2	3:U:48:CYS:HA	2.46	0.44
4:V:304:ASP:HA	4:V:305:PRO:HD2	1.85	0.44
4:V:222:GLY:HA2	4:V:384:ALA:O	2.18	0.44
1:1:161:ASN:OD1	1:1:166:ASP:HA	2.17	0.44
1:1:65:ARG:NH2	1:1:268:MET:HE3	2.33	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
3:C:115:HIS:C	4:D:321:MET:HE1	2.38	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
1:J:38:TYR:HA	1:J:116:GLU:OE1	2.18	0.44
3:L:118:ASP:O	3:L:119:CYS:C	2.56	0.44
4:M:106:GLY:O	5:N:194:SER:HB3	2.18	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:235:THR:O	4:V:235:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:76:LEU:HD12	4:V:76:LEU: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
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:116:ILE:HD11	4:D:182:LEU:CD2	2.47	0.44
4:D:278:VAL:O	4:D:282:GLU:HG3	2.18	0.44
4:D:223:VAL:O	4:D:383:TYR:HE1	2.00	0.44
4:D:82:THR:N	4:D:83:PRO:HD2	2.32	0.44
7:G:115:LEU:HA	7:G:115:LEU:HD23	1.66	0.44
3:L:372:GLN:O	3:L:558:TRP:CD2	2.71	0.44
3:L:49:LEU:HA	3:L:80:ALA:O	2.18	0.44
4:M:316:LEU:C	4:M:318:GLU:H	2.22	0.44
5:N:104:VAL:CG1	5:N:108:TRP:CE3	3.01	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
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
4:4:168:PHE:CE1	6:6:141:PRO:HG3	2.53	0.43
1:A:107:LEU:HD23	1:A:114:LEU:HD12	2.00	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
4:D:236:GLY:C	4:D:238:SER:N	2.71	0.43
7:G:44:THR:OG1	7:G:52:LYS:HD2	2.17	0.43
3:C:245:ARG:NH1	7:G:56:CYS:O	2.50	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
3:L:37:LYS:O	3:L:38:HIS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:403:THR:HG22	3:L:403:THR:O	2.18	0.43
3:L:612:GLY:O	3:L:624:LEU:HB2	2.17	0.43
6:O:117:MET:HB3	7:P:99:ILE:CD1	2.47	0.43
5:N:167:PRO:HB3	7:P:66:TYR:CD2	2.53	0.43
3:U:168:HIS:HA	3:U:169:PRO:HD2	1.71	0.43
3:U:244:ALA:HB3	3:U:249:MET:CE	2.48	0.43
3:U:290:ILE:HG22	3:U:291:CYS:O	2.17	0.43
3:U:641:LEU:HA	3:U:641:LEU:HD23	1.77	0.43
4:V:108:VAL:HG23	4:V:108:VAL:O	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
1:1:267:PRO:O	1:1:270:THR:HG23	2.18	0.43
1:1:81:LYS:CE	1:1:81:LYS:HA	2.46	0.43
2:2:131:ALA:HB1	2:2:132:PRO:HA	2.00	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
3:3:2:VAL:CG1	3:3:89:ASP:HA	2.48	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
4:4:63:HIS:HA	4:4:409:ARG:OXT	2.18	0.43
5:5:40:HIS:NE2	5:5:44:MET:HE1	2.33	0.43
6:6:141:PRO:HB3	9:6:182:SF4:S1	2.58	0.43
1:A:45:LEU:HD23	1:A:123:TYR:CG	2.53	0.43
3:C:290:ILE:HG22	3:C:291:CYS:O	2.18	0.43
4:D:143:LEU:O	4:D:143:LEU:HD23	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
2:T:11:LEU:O	2:T:12:GLU:C	2.56	0.43
3:U:505:LEU:HB3	3:U:532:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:366:PHE:O	1:1:370:LEU:HD23	2.17	0.43
3:3:161:ARG:NH1	3:3:161:ARG:HG2	2.32	0.43
3:3:225:ASN:O	3:3:229:ILE:HG13	2.18	0.43
3:3:532:VAL:HG12	3:3:533:LEU:N	2.34	0.43
3:3:372:GLN:O	3:3:558:TRP:CD2	2.72	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:249:MET:H	1:A:249:MET:HE2	1.83	0.43
1:A:416:HIS:HB2	1:A:417:PHE:CE1	2.52	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
7:G:119:PHE:HA	7:G:121:MET:HE3	2.01	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
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:594:ALA:C	3:U:596:ARG:H	2.22	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:129:HIS:CD2	5:W:130:PRO:HD2	2.53	0.43
5:W:77:LEU:HA	5:W:78:PRO:HD3	1.60	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
8:Z:108:ILE:HA	8:Z:109:PRO:HD3	1.90	0.43
1:1:145:LEU:HA	1:1:145:LEU:HD23	1.69	0.43
3:3:185:LYS:HG2	3:3:188:VAL:CG2	2.47	0.43
3:3:49:LEU:HA	3:3:80:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:108:VAL:HG23	4:D:108:VAL:O	2.18	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:688:ARG:HA	3:U:688:ARG:HD3	1.51	0.43
4:V:242:SER:HB2	4:V:270:GLY:HA3	2.00	0.43
4:V:316:LEU:C	4:V:318:GLU:H	2.21	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
2:2:116:LEU:HG	2:2:117:PHE:CD2	2.53	0.43
2:2:87:SER:OG	2:2:128:CYS:HB3	2.18	0.43
3:3:197:ASP:HB2	3:3:220:SER:HB3	2.00	0.43
3:3:455:ARG:O	3:3:455:ARG:HG3	2.19	0.43
4:4:350:ARG:NE	4:4:403:VAL:CG2	2.77	0.43
4:4:85:MET:HE2	4:4:370:VAL:HG11	2.01	0.43
5:5:194:SER:O	5:5:195:LEU:HD13	2.18	0.43
4:4:167:ARG:HD3	6:6:143:ARG:NH1	2.32	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
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:U:241:ARG:HH11	7:Y:74:GLU:CD	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:367:PRO:CB	3:3:554:LYS:HB2	2.49	0.43
3:3:408:ILE:HA	3:3:408:ILE:HD12	1.78	0.43
3:3:469:ARG:O	3:3:472:GLU:HB3	2.19	0.43
3:3:397:LEU:HD21	3:3:480:LEU:HD13	2.00	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
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:20:MET:CE	3:C:432:PHE:HB3	2.47	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:HG	5:E:152:LEU:O	2.19	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
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: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:470:PRO:O	3:U:471:GLY:C	2.57	0.43
3:U:646:GLU:C	3:U:648:LEU:H	2.22	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
1:1:184:GLU:OE1	1:1:186:THR:N	2.52	0.43
1:1:139:ARG:CG	2:2:140:PRO:HD3	2.45	0.43
3:3:413:LEU:HD13	3:3:448:MET:HE3	2.01	0.43
6:6:157:LYS:O	6:6:157:LYS:HG2	2.18	0.43
6:6:33:SER:HA	6:6:158:VAL:HG21	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
1:A:58:LYS:HA	1:A:73:GLY:HA3	2.01	0.43
2:B:112:THR:OG1	2:B:113:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:L:244:ALA:HB3	3:L:249:MET:CE	2.49	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: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: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
3:U:55:PRO:HG3	3:U:73:ILE:C	2.37	0.43
4:V:306:ASN:HA	4:V:307:PRO:HD3	1.79	0.43
5:W:116:ARG:HG3	5:W:129:HIS:HE1	1.83	0.43
5:W:49:LEU:HD13	5:W:74:LEU:HD23	2.00	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:O	7:9:113:ILE:HG23	2.18	0.43
3:C:469:ARG:O	3:C:472:GLU:HB3	2.19	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
1:J:249:MET:H	1:J:249:MET:HE2	1.83	0.43
2:K:31:LEU:HA	2:K:31:LEU:HD13	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
7:P:39:GLY:O	7:P:40:ARG:C	2.55	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
3:U:20:MET:CE	3:U:432:PHE:HB3	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:385:ALA:HB3	3:U:533:LEU:HD23	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:121:TYR:HD1	6:X:121:TYR:H	1.67	0.43
8:Z:88:ARG:HE	8:Z:126:LEU:CD2	2.32	0.43
3:3:474:ARG:HG2	3:3:474:ARG:H	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:162:LEU:HB3	1:A:163:PHE:HD1	1.84	0.43
1:A:161:ASN:OD1	1:A:166:ASP:HA	2.19	0.43
1:A:203:PRO:HB2	1:A:204:PRO:HD3	2.00	0.43
1:A:38:TYR:HA	1:A:116:GLU:OE1	2.18	0.43
3:C:614:LEU:O	3:C:621:VAL:HA	2.18	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
4:D:393:MET:C	4:D:396:ILE:HG22	2.39	0.43
4:D:74:THR:HG22	4:D:75:TYR:N	2.34	0.43
6:F:123:ILE:HG22	6:F:124:VAL:N	2.34	0.43
6:F:30:TRP:O	6:F:33:SER:HB3	2.18	0.43
3:L:575:GLU:HA	3:L:575:GLU:OE1	2.18	0.43
3:L:652:PRO:HA	3:L:653:PRO:HD3	1.87	0.43
4:M:306:ASN:HA	4:M:307:PRO:HD3	1.80	0.43
5:N:98:ASP:C	5:N:100:ARG:H	2.23	0.43
5:N:160:ARG:HD2	7:P:92:GLU:OE2	2.19	0.43
4:M:167:ARG:HD3	6:O:143:ARG:HH12	1.84	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:329:LYS:HD2	4:V:329:LYS:HA	1.94	0.43
4:V:40:VAL:HG23	6:X:88:MET:CE	2.49	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
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:HA	3:3:290:ILE:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:98:ALA:O	4:D:102:GLU:HG3	2.18	0.43
4:D:63:HIS:O	6:F:122:ALA:HB1	2.18	0.43
5:E:126:PHE:H	5:E:132:LEU:HD11	1.84	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:420:LEU:HD22	3:L:436:GLN:HG2	2.01	0.43
3:L:397:LEU:HD21	3:L:480:LEU:HD13	2.00	0.43
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
5:N:44:MET:HB2	5:N:44:MET:HE3	1.77	0.43
6:O:161:GLN:O	6:O:161:GLN:HG2	2.19	0.43
1:S:65:ARG:NH2	1:S:268:MET:HE1	2.34	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
3:U:498:GLU:C	3:U:500:ALA:H	2.21	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
3:3:317:LEU:CD2	3:3:317:LEU:N	2.80	0.42
3:3:575:GLU:HA	3:3:575:GLU:OE1	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
5:5:44:MET:HE3	5:5:44:MET:HB2	1.79	0.42
8:7:88:ARG:HE	8:7:126:LEU:HD22	1.83	0.42
3:C:117:LEU:HD23	4:D:321:MET:HA	2.01	0.42
3:C:470:PRO:O	3:C:471:GLY:C	2.58	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:180:TYR:CE2	10:J:440:FMN:H6	2.54	0.42
1:J:95:GLU:HA	10:J:440:FMN:HN3	1.83	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:HA	3:L:351:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:317:LEU:CD2	3:U:317:LEU:N	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
3:3:498:GLU:C	3:3:500:ALA:H	2.21	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:254:ILE:HB	1:A:275:LEU:HD21	2.01	0.42
3:C:378:PRO:O	3:C:381:LEU:HB2	2.19	0.42
4:D:381:LEU:H	4:D:382:PRO:CD	2.32	0.42
4:D:222:GLY:HA2	4:D:384:ALA:O	2.18	0.42
5:E:175:THR:O	5:E:175:THR:OG1	2.28	0.42
6:F:155:GLN:C	6:F:157:LYS:H	2.22	0.42
5:E:160:ARG:HG3	7:G:130:VAL:HG11	2.01	0.42
2:K:3:PHE:CD1	2:K:3:PHE:C	2.92	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:130:VAL:HG23	6:O:131:VAL:HG13	2.01	0.42
6:O:43:LEU:HA	6:O:43:LEU:HD23	1.80	0.42
7:P:45:ARG:NH2	7:P:137:LEU:CD2	2.82	0.42
1:S:267:PRO:O	1:S:268:MET:C	2.56	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
2:2:3:PHE:C	2:2:3:PHE:CD1	2.92	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
4:4:256:GLY:C	4:4:258:GLU:N	2.71	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:343:TYR:C	4:D:343:TYR:CD1	2.92	0.42
3:C:136:GLU:CG	5:E:189:ARG:HG2	2.39	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
3:C:208:HIS:HB3	8:H:85:ARG:NH2	2.34	0.42
2:B:109:GLY:HA2	8:H:91:ILE:HD13	2.01	0.42
1:J:203:PRO:HB2	1:J:204:PRO:HD3	2.00	0.42
1:J:97:GLU:OE2	1:J:294:GLY:HA3	2.20	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:241:ARG:HH11	7:P:74:GLU:CD	2.22	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:358:VAL:O	4:M:366:TYR:HB3	2.18	0.42
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:3:PHE:CD1	2:T:3:PHE:C	2.92	0.42
3:U:403:THR:HG22	3:U:403:THR:O	2.18	0.42
3:U:449:ALA:HA	3:U:464:ILE:O	2.19	0.42
4:V:143:LEU:O	4:V:143:LEU:HD23	2.19	0.42
1:1:243:THR:HG22	1:1:244:GLU:N	2.26	0.42
1:1:271:THR:HG23	1:1:271:THR:H	1.51	0.42
1:1:64:GLY:HA3	10:1:440:FMN:O1P	2.18	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:N	3:3:758:LEU:HD12	2.34	0.42
4:4:304:ASP:HA	4:4:305:PRO:HD2	1.86	0.42
5:5:104:VAL:HG12	5:5:108:TRP:CE3	2.49	0.42
5:5:48:PHE:CE2	5:5:50:ALA:HB2	2.54	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:HA	7:G:96:LEU:HD23	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:532:VAL:HG12	3:L:533:LEU:N	2.35	0.42
5:N:66:GLU:HG2	5:N:95:PRO:CA	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD	2:T:7:LYS:H	2.27	0.42
3:U:351:LEU:HD12	3:U:351:LEU:HA	1.82	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
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
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
4:4:140:LEU:HD11	4:4:214:PHE:HB2	2.01	0.42
3:3:117:LEU:HD23	4:4:321:MET:HA	2.02	0.42
4:4:69:THR:HG21	6:6:120:ASN:ND2	2.35	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
1:A:100:SER:HB2	1:A:325:THR:OG1	2.19	0.42
3:C:508:GLY:HA2	3:C:535:MET:HB2	2.02	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
2:K:11:LEU:O	2:K:12:GLU:C	2.57	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: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
4:M:95:LEU:HA	4:M:173:ILE:CD1	2.50	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
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
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
4:D:168:PHE:HE1	6:F:141:PRO:CG	2.32	0.42
6:F:131:VAL:HA	6:F:132:PRO:HD3	1.89	0.42
7:G:113:ILE:HG23	7:G:113:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:P:119:PHE:HA	7:P:121:MET:HE3	2.01	0.42
1:S:163:PHE:C	1:S:165:THR:H	2.23	0.42
1:S:45:LEU:HD23	1:S:123:TYR:CG	2.54	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
2:T:24:ARG:HE	2:T:24:ARG:HB3	1.76	0.42
3:U:413:LEU:HD13	3:U:448:MET:HE3	2.02	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
4:V:236:GLY:C	4:V:238:SER:N	2.72	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:I:110:VAL:N	1:I: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:HA	8:H:50:LEU:HD12	1.81	0.42
1:J:155:ARG:HG2	1:J:155:ARG:H	1.64	0.42
1:J:267:PRO:O	1:J:268:MET:C	2.57	0.42
1:J:65:ARG:NH2	1:J:268:MET:HE3	2.35	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:120:ASP:OD1	5:W:134:LYS:HG3	2.20	0.42
5:W:5:ARG:CG	5:W:5:ARG:NH1	2.67	0.42
6:X:132:PRO:HB2	6:X:174:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:113:SER:HB3	7:Y:96:LEU:HD13	2.02	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
4:4:108:VAL:O	4:4:108:VAL:HG23	2.20	0.42
4:4:130:LEU:HD11	4:4:152:GLU:HB3	2.02	0.42
4:4:103:LYS:HE2	4:4:344:VAL:HG11	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:186:THR:HG21	1:A:200:ARG:H	1.84	0.42
1:A:65:ARG:HB2	1:A:222:GLU:HB3	2.02	0.42
7:G:108:CYS:HA	9:G:184:SF4:S3	2.60	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:356:CYS:HB3	1:J:358:PRO:CD	2.50	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
2:K:168:LEU:HA	2:K:169:PRO:HD2	1.81	0.42
3:L:550:LEU:N	3:L:550:LEU:HD12	2.35	0.42
3:L:564:LEU:HA	3:L:564:LEU:HD12	1.81	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:695:ARG:CZ	3:U:717:TRP:CH2	3.02	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
3:3:658:LEU:O	3:3:658:LEU:HD23	2.20	0.42
3:3:115:HIS:HB3	4:4:321:MET:HE3	2.01	0.42
4:4:375:PHE:HD1	4:4:407:VAL:HG23	1.85	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
1:A:87:HIS:HB2	1:A:126:ARG:O	2.19	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: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:184:CYS:SG	3:L:186:ARG:HB2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:18:SER:OG	3:L:433:ALA:HB3	2.19	0.42
6:O:137:VAL:HG13	6:O:137:VAL:O	2.20	0.42
6:O:30:TRP:O	6:O:33:SER:HB3	2.19	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:211:LEU:HB2	1:S:216:THR:HG21	2.02	0.42
1:S:63:ARG:CD	1:S:313:TYR:HD2	2.32	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
4:4:109:VAL:HG12	4:4:113:ALA:CB	2.50	0.42
4:4:236:GLY:O	4:4:238:SER:N	2.53	0.42
4:4:221:VAL:O	4:4:272:VAL:HG12	2.20	0.42
4:4:47:LEU:HD11	4:4:51:GLU:O	2.19	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:285:GLU:O	4:M:289:ILE:HG12	2.20	0.42
4:M:69:THR:HG21	6:O:120:ASN:ND2	2.34	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: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
4:4:404: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
2:B:24:ARG:HB3	2:B:24:ARG:HE	1.76	0.41
3:C:229:ILE:HD11	3:C:289:TRP:CH2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:329:LEU:CD1	3:C:584:VAL:HG11	2.50	0.41
3:C:43:GLY:HA2	11:C:787:FES:S1	2.60	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:197:ASP:CB	3:L:220:SER:HB3	2.50	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:368:HIS:CG	3:L:556:ALA:HB3	2.55	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
3:L:83:CYS:SG	3:L:84:VAL:HG13	2.60	0.41
4:M:40:VAL:O	4:M:40:VAL:CG2	2.67	0.41
6:O:152:MET:O	6:O:156:LYS:HG3	2.21	0.41
5:N:167:PRO:HB3	7:P:66:TYR:CE2	2.55	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:422:PRO:HA	3:U:423:PRO:HD2	1.79	0.41
3:U:394:ASP:CB	3:U:501:LYS:HD3	2.50	0.41
3:U:532:VAL:HG12	3:U:533:LEU:N	2.35	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
2:2:11:LEU:O	2:2:12:GLU:C	2.57	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
5:5:192:TYR:CG	5:5:193:ARG:N	2.88	0.41
7:9:108:CYS:HA	9:9:184:SF4:S3	2.60	0.41
6:6:145:GLU:CG	7:9:31:VAL:HG21	2.34	0.41
1:A:316:LEU:HA	1:A:316:LEU:HD23	1.83	0.41
3:C:218:LEU:N	3:C:219:PRO:HD3	2.34	0.41
3:C:501:LYS:HD2	3:C:501:LYS:N	2.13	0.41
3:C:293:ALA:HB2	3:C:698:MET:HG2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD2	3:L:245:ARG:HA	1.81	0.41
3:L:364:LEU:HG	3:L:364:LEU:O	2.19	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:249:MET:H	1:S:249:MET:HE2	1.85	0.41
3:U:478:LEU:HD12	3:U:520:ARG:CZ	2.50	0.41
4:V:197:LEU:HA	4:V:200:ARG:HB3	2.02	0.41
4:V:85:MET:HE2	4:V:370:VAL:HG11	2.00	0.41
4:V:161:GLU:OE2	6:X:143:ARG:NH1	2.52	0.41
1:I:408:TRP:N	1:I: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
5:5:38:MET:O	5:5:41:TYR:HB2	2.21	0.41
8:7:52:THR:CG2	8:7:54:ILE:HG22	2.50	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:30:VAL:CG2	3:C:48:CYS:HA	2.46	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:104:VAL:CG1	5:E:108:TRP:CE3	3.03	0.41
5:E:3:LEU:HB2	5:E:86:SER:HB2	2.02	0.41
1:J:366:PHE:HD1	1:J:370:LEU:CD2	2.32	0.41
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:577:LEU:HD13	3:L:577:LEU:HA	1.92	0.41
3:L:571:VAL:HG23	3:L:587:LEU:HD11	2.01	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:115:HIS:C	4:V:321:MET:HE1	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:95:LEU:HA	4:V:173:ILE:CD1	2.49	0.41
4:V:219:ARG:NH1	4:V:273:PHE:HD2	2.18	0.41
4:V:393:MET:C	4:V:396:ILE:HG22	2.40	0.41
5:W:91:ARG:HE	5:W:91:ARG:HB2	1.57	0.41
4:V:162:TRP:CE2	7:Y:34:LYS:HD2	2.55	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
1:J:163:PHE:C	1:J:165:THR:H	2.24	0.41
1:J:45:LEU:HB3	1:J:165:THR:HG21	2.03	0.41
1:J:28:THR:HB	1:J:31:TYR:H	1.86	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:52:THR:CG2	8:Q:54:ILE:HG22	2.50	0.41
8:Q:8:GLU:HG2	8:Q:97:TYR:OH	2.20	0.41
1:S:233:ARG:H	1:S:233:ARG:HG2	1.57	0.41
1:S:97:GLU:OE2	1:S:294:GLY:HA3	2.20	0.41
1:S:414:LEU:HD12	1:S:414:LEU:HA	1.83	0.41
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: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
1:1:267:PRO:O	1:1:270:THR:CG2	2.69	0.41
1:1:93:ALA:O	1:1:134:VAL:HA	2.20	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:N	3:3:203:ILE:HD13	2.35	0.41
3:3:347:HIS:N	3:3:372:GLN:HB3	2.36	0.41
3:3:46:ARG:NH1	3:3:46:ARG:CG	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:5:54:GLY:C	5:5:55:LEU:HD12	2.41	0.41
8:7:72:VAL:HG22	8:7:73:SER:N	2.36	0.41
7:9:32:ALA:HA	7:9:162:VAL:O	2.20	0.41
1:A:293:GLY:HA3	1:A:324:GLY:N	2.11	0.41
1:A:65:ARG:NH2	1:A:268:MET:CE	2.83	0.41
2:B:11:LEU:HD22	2:B:30:LEU:HD21	2.00	0.41
2:B:3:PHE:CD1	2:B:3:PHE:C	2.94	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:HA	1:J:344:LEU:HD23	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:HA	3:L:236:LEU:HD23	1.82	0.41
3:L:614:LEU:O	3:L:621:VAL:HA	2.20	0.41
3:L:250:GLU:CD	3:L:628:PRO:HG2	2.40	0.41
3:L:732:ALA:H	3:L:747:VAL:HG12	1.86	0.41
3:L:728:LEU:HB3	3:L:747:VAL:HG21	2.03	0.41
4:M:278:VAL:O	4:M:282:GLU:HG3	2.20	0.41
7:P:134:GLU:N	7:P:134:GLU:CD	2.73	0.41
6:O:117:MET:HE1	7:P:99:ILE:HG12	2.02	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
3:U:317:LEU:H	3:U:317:LEU:HD22	1.83	0.41
4:V:130:LEU:HD11	4:V:152:GLU:HB3	2.03	0.41
4:V:366:TYR:CZ	5:W:148:LYS:HE3	2.55	0.41
4:V:74:THR:HG22	4:V:75:TYR:N	2.34	0.41
5:W:175:THR:OG1	5:W:175:THR:O	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
3:3:417:VAL:O	3:3:417:VAL:HG12	2.21	0.41
3:3:329:LEU:CD1	3:3:584:VAL:HG11	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:163:PHE:C	1:A:165:THR:H	2.23	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:256:GLY:C	4:D:258:GLU:N	2.70	0.41
4:D:390:VAL:H	4:D:391:PRO:CD	2.34	0.41
4:D:47:LEU:HD11	4:D:51:GLU:O	2.20	0.41
5:E:155:THR:HG22	5:E:156:PRO:O	2.21	0.41
4:D:230:ILE:HD13	5:E:77:LEU:HD12	2.03	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:323:LEU:HD23	1:J:323:LEU:C	2.40	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:498:GLU:C	3:L:500:ALA:H	2.24	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: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
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:126:PHE:H	5:W:132:LEU:HD11	1.86	0.41
5:W:25:LEU:HD22	5:W:25:LEU:N	2.35	0.41
1:1:40:THR:HB	1:1:116:GLU:OE2	2.21	0.41
1:1:118:MET:O	1:1:122:GLY:N	2.50	0.41
1:1:63:ARG:CD	1:1:313:TYR:HD2	2.33	0.41
3:3:245:ARG:NH1	7:9:56:CYS:O	2.53	0.41
5:5:98:ASP:C	5:5:100:ARG:H	2.24	0.41
6:6:34:ASN:C	6:6:36:LEU:H	2.24	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:11:LEU:O	2:B:12:GLU:C	2.58	0.41
2:B:78:TYR:CE1	2:B:157:LEU:HD22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:254:THR:HG23	3:C:255:THR:N	2.35	0.41
3:C:23:VAL:HG13	3:C:28:TYR:HB2	2.01	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:194:LEU:HA	4:D:194:LEU:HD12	1.90	0.41
4:D:87:TYR:CD1	6:F:48:ILE:HD12	2.56	0.41
5:E:129:HIS:CD2	5:E:130:PRO:HD2	2.55	0.41
4:D:360:ASP:OD2	5:E:176:GLY:HA3	2.21	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
1:S:289:ALA:HB3	1:S:337:MET:CE	2.49	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
6:X:43:LEU:HA	6:X:43:LEU:HD23	1.87	0.41
2:2:26:ALA:O	2:2:29:PRO:HG2	2.21	0.41
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: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:241:ALA:O	4:D:267:GLY:HA3	2.21	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
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:20:MET:HE1	3:U:433:ALA:HB2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:W:157:THR:C	5:W:158:LEU:HD23	2.41	0.41
5:W:181:LEU:HD12	5:W:181:LEU:HA	1.80	0.41
1:1:158:LEU:CA	1:1:162:LEU:HD21	2.51	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
4:4:237:GLY:HA2	4:4:240:ARG:NH2	2.34	0.41
4:4:99:LEU:HA	4:4:99:LEU:HD13	1.80	0.41
7:9:115:LEU:HA	7:9:115:LEU:HD23	1.68	0.41
7:9:130:VAL:HG13	7:9:130:VAL:O	2.21	0.41
3:C:18:SER:OG	3:C:433:ALA:HB3	2.21	0.41
3:C:734:VAL:HG13	3:C:775:VAL:HG13	2.02	0.41
4:D:300:GLY:HA3	4:D:301:PRO:HD2	1.94	0.41
4:D:390:VAL:HB	4:D:391:PRO:HD3	2.03	0.41
4:D:62:LEU:HD23	4:D:62:LEU:HA	1.87	0.41
5:E:13:LYS:HZ1	5:E:33:ARG:HH21	1.67	0.41
3:L:590:LEU:HA	3:L:590:LEU:HD12	1.87	0.41
3:L:543:GLY:HA2	3:L:615:VAL:HG21	2.03	0.41
3:L:750:ARG:HB2	3:L:753:VAL:CG2	2.51	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
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:250:GLU:CD	3:U:628:PRO:HG2	2.40	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
1:1:97:GLU:OE2	1:1:294:GLY:HA3	2.21	0.41
1:1:344:LEU:HA	1:1:344:LEU:HD23	1.82	0.41
3:3:420:LEU:HD22	3:3:436:GLN:HG2	2.03	0.41
4:4:40:VAL:HG13	4:4:404:MET:HG3	2.03	0.41
5:5:35:LYS:HD3	5:5:102:PRO:CB	2.51	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:571:VAL:HG23	3:C:587:LEU:HD11	2.02	0.41
4:D:350:ARG:HD3	4:D:374:SER:OG	2.20	0.41
5:E:1:MET:C	5:E:3:LEU:N	2.74	0.41
5:E:49:LEU:HD13	5:E:74:LEU:HD23	2.02	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:180:ARG:O	3:L:181:CYS:C	2.60	0.41
3:L:20:MET:HE1	3:L:433:ALA:HB2	2.03	0.41
3:L:232:VAL:HB	3:L:233:GLY:H	1.73	0.41
3:L:474:ARG:HG2	3:L:474:ARG:H	1.65	0.41
4:M:109:VAL:HG12	4:M:113:ALA:CB	2.50	0.41
4:M:256:GLY:C	4:M:258:GLU:N	2.71	0.41
5:N:34:PHE:O	5:N:35:LYS:C	2.60	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
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
6:X:155:GLN:C	6:X:157:LYS:H	2.23	0.41
3:3:200:LEU:HA	3:3:200:LEU:HD12	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
3:3:55:PRO:HG3	3:3:73:ILE:C	2.40	0.41
3:3:590:LEU:HA	3:3:590:LEU:HD12	1.91	0.41
4:4:291:LYS:O	4:4:295:GLU:HG3	2.21	0.41
5:5:1:MET:C	5:5:3:LEU:N	2.75	0.41
7:9:39:GLY:O	7:9:40:ARG:C	2.59	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
3:C:594:ALA:C	3:C:596:ARG:H	2.24	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
8:H:38:PRO:C	8:H:40:PHE:H	2.24	0.41
4:M:219:ARG:NH1	4:M:273:PHE:HD2	2.17	0.41
5:N:1:MET:C	5:N:3:LEU:N	2.75	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:432:PHE:N	3:U:432:PHE:CD1	2.88	0.41
3:U:672:ALA:O	3:U:673:MET:HB2	2.21	0.41
3:U:701:ALA:N	3:U:763:LEU:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:396:ILE:HD12	4:V:396:ILE:HA	1.83	0.41
3:U:136:GLU:CG	5:W:189:ARG:HG2	2.41	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:ND1	3:3:167:HIS:O	2.53	0.40
3:3:343:LEU:HD12	3:3:361:ALA:HB2	2.02	0.40
3:3:470:PRO:O	3:3:471:GLY:C	2.59	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
7:9:134:GLU:N	7:9:134:GLU:CD	2.74	0.40
6:6:114:SER:CB	7:9:97:ARG:HD2	2.47	0.40
1:A:356:CYS:HB3	1:A:358:PRO:CD	2.52	0.40
3:C:118:ASP:O	3:C:119:CYS:C	2.59	0.40
3:C:646:GLU:C	3:C:648:LEU:H	2.24	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
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
1:J:289:ALA:HB3	1:J:337:MET:CE	2.51	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:193:LEU:O	4:M:193:LEU:HD23	2.22	0.40
4:M:328:PHE:CD2	4:M:328:PHE:C	2.95	0.40
4:M:47:LEU:HD11	4:M:51:GLU:O	2.20	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:669:VAL:O	3:U:669:VAL:HG13	2.21	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:119:PHE:HA	7:Y:121:MET:HE3	2.02	0.40
7:Y:79:ASN:HA	7:Y:80:PRO:HD2	1.95	0.40
1:1:170:ASP:O	1:1:171:LEU:HD12	2.21	0.40
1:1:26:SER:HA	1:1:31:TYR:CD2	2.56	0.40
3:3:407:PRO:HB2	9:3:786:SF4:S1	2.61	0.40
3:3:594:ALA:C	3:3:596:ARG:H	2.24	0.40
6:6:152:MET:O	6:6:156:LYS:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:151:VAL:O	6:6:155:GLN:HB2	2.21	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:688:ARG:HD3	3:C:688:ARG:HA	1.50	0.40
4:D:249:ARG:CZ	4:D:262:PHE:HZ	2.34	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:332:THR:O	5:E:172:ALA:HB3	2.21	0.40
5:E:54:GLY:C	5:E:55:LEU:HD12	2.41	0.40
8:H:122:ALA:O	8:H:126:LEU:HB2	2.21	0.40
1:J:158:LEU:CA	1:J:162:LEU:HD21	2.51	0.40
1:J:133:TYR:CB	1:J:188:LEU:HD21	2.51	0.40
1:J:402:LEU:O	1:J:405:ALA:HB3	2.21	0.40
3:L:382:PHE:CE1	3:L:512:LEU:HD11	2.56	0.40
3:L:305:ARG:NH2	3:L:609:GLU:OE1	2.52	0.40
4:M:236:GLY:C	4:M:238:SER:N	2.72	0.40
4:M:283:MET:O	4:M:287:VAL:HG23	2.21	0.40
1:S:89:LEU:HD12	1:S:217:THR:HG22	2.03	0.40
1:S:65:ARG:HB2	1:S:222:GLU:HB3	2.02	0.40
1:S:290:ILE:CG2	1:S:330:LEU:HD22	2.51	0.40
3:U:203:ILE:O	3:U:204:GLU:O	2.39	0.40
4:V:290:ILE:O	4:V:294:LEU:HB2	2.22	0.40
8:Z:38:PRO:C	8:Z:40:PHE:H	2.24	0.40
1:1:343:ASN:O	1:1:346:ARG:HG2	2.21	0.40
3:3:317:LEU:H	3:3:317:LEU:HD22	1.82	0.40
4:4:316:LEU:C	4:4:318:GLU:N	2.74	0.40
2:B:112:THR:HG22	2:B:117:PHE:H	1.86	0.40
3:C:131:GLN:O	3:C:134:THR:HB	2.22	0.40
3:C:236:LEU:HA	3:C:236:LEU:HD23	1.84	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
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
6:F:165:GLU:HG2	7:G:148:ARG:NH1	2.35	0.40
1:J:317:GLN:C	1:J:319:LYS:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:286:SER:O	4:M:290:ILE:HG12	2.22	0.40
5:N:25:LEU:HD22	5:N:25:LEU:N	2.36	0.40
7:P:130:VAL:HG13	7:P:130:VAL:O	2.21	0.40
1:S:160:LYS:HG3	1:S:161:ASN:N	2.35	0.40
1:S:344:LEU:HA	1:S:344:LEU:HD23	1.80	0.40
1:S:341:MET:HB2	1:S:371:PHE:CE1	2.57	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
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
3:3:669:VAL:HG13	3:3:669:VAL:O	2.22	0.40
3:3:713:ARG:HB2	3:3:713:ARG:HE	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: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
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: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
1:J:58:LYS:HA	1:J:73:GLY:HA3	2.02	0.40
3:L:286:ASN:C	3:L:286:ASN:ND2	2.74	0.40
3:L:594:ALA:C	3:L:596:ARG:H	2.25	0.40
3:L:646:GLU:C	3:L:648:LEU:H	2.25	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
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:119:CYS:O	3:U:120:PRO:C	2.60	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:469:ARG:HB2	3:U:470:PRO:CD	2.50	0.40
3:U:329:LEU:CD1	3:U:584:VAL:HG11	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:654:PHE:HE2	3:U:663:ALA:HB3	1.86	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
2:2:127:SER:HG	2:2:133:VAL:HG21	1.87	0.40
3:3:695:ARG:NH1	3:3:717:TRP:CZ2	2.90	0.40
5:5:194:SER:C	5:5:195:LEU:HD22	2.42	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
8:7:108:ILE:HA	8:7:109:PRO:HD3	1.94	0.40
6:6:163:TYR:CD1	7:9:152:ARG:HD2	2.56	0.40
1:A:107:LEU:HD22	1:A:145:LEU:CD1	2.51	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
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
5:N:54:GLY:C	5:N:55:LEU:HD12	2.42	0.40
7:P:150:ALA:HA	7:P:153:THR:HB	2.04	0.40
7:P:58:LEU:HD12	7:P:58:LEU:HA	1.76	0.40
8:Q:20:MET:HE3	8:Q:59:LEU:HG	2.02	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:HB3	3:U:334:LYS:NZ	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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	435/438 (99%)	366 (84%)	59 (14%)	10 (2%)	6	31
1	A	435/438 (99%)	359 (82%)	65 (15%)	11 (2%)	5	29
1	J	435/438 (99%)	363 (83%)	62 (14%)	10 (2%)	6	31
1	S	435/438 (99%)	362 (83%)	62 (14%)	11 (2%)	5	29
2	2	176/181 (97%)	147 (84%)	26 (15%)	3 (2%)	9	38
2	B	176/181 (97%)	145 (82%)	28 (16%)	3 (2%)	9	38
2	K	176/181 (97%)	145 (82%)	29 (16%)	2 (1%)	14	48
2	T	176/181 (97%)	147 (84%)	27 (15%)	2 (1%)	14	48
3	3	748/783 (96%)	628 (84%)	96 (13%)	24 (3%)	4	22
3	C	748/783 (96%)	632 (84%)	93 (12%)	23 (3%)	4	23
3	L	748/783 (96%)	630 (84%)	93 (12%)	25 (3%)	4	22
3	U	748/783 (96%)	633 (85%)	93 (12%)	22 (3%)	4	25
4	4	373/409 (91%)	319 (86%)	44 (12%)	10 (3%)	5	27
4	D	373/409 (91%)	320 (86%)	41 (11%)	12 (3%)	4	22
4	M	373/409 (91%)	319 (86%)	44 (12%)	10 (3%)	5	27
4	V	373/409 (91%)	319 (86%)	42 (11%)	12 (3%)	4	22
5	5	194/207 (94%)	162 (84%)	21 (11%)	11 (6%)	1	12
5	E	194/207 (94%)	160 (82%)	23 (12%)	11 (6%)	1	12
5	N	194/207 (94%)	160 (82%)	23 (12%)	11 (6%)	1	12
5	W	194/207 (94%)	157 (81%)	26 (13%)	11 (6%)	1	12
6	6	141/181 (78%)	121 (86%)	17 (12%)	3 (2%)	7	33
6	F	141/181 (78%)	120 (85%)	18 (13%)	3 (2%)	7	33
6	O	141/181 (78%)	119 (84%)	21 (15%)	1 (1%)	22	59
6	X	141/181 (78%)	120 (85%)	18 (13%)	3 (2%)	7	33
7	9	152/182 (84%)	127 (84%)	23 (15%)	2 (1%)	12	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	152/182 (84%)	128 (84%)	22 (14%)	2 (1%)	12	44
7	P	152/182 (84%)	128 (84%)	22 (14%)	2 (1%)	12	44
7	Y	152/182 (84%)	130 (86%)	20 (13%)	2 (1%)	12	44
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
All	All	9376/10040 (93%)	7924 (84%)	1200 (13%)	252 (3%)	5	27

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	323 (91%)	32 (9%)	9	32
1	A	355/356 (100%)	320 (90%)	35 (10%)	8	28
1	J	355/356 (100%)	322 (91%)	33 (9%)	9	31
1	S	355/356 (100%)	322 (91%)	33 (9%)	9	31
2	2	150/152 (99%)	135 (90%)	15 (10%)	7	28
2	B	150/152 (99%)	135 (90%)	15 (10%)	7	28
2	K	150/152 (99%)	135 (90%)	15 (10%)	7	28
2	T	150/152 (99%)	135 (90%)	15 (10%)	7	28
3	3	607/628 (97%)	550 (91%)	57 (9%)	8	30
3	C	607/628 (97%)	551 (91%)	56 (9%)	9	31
3	L	607/628 (97%)	549 (90%)	58 (10%)	8	29
3	U	607/628 (97%)	550 (91%)	57 (9%)	8	30
4	4	325/355 (92%)	295 (91%)	30 (9%)	9	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	325/355 (92%)	292 (90%)	33 (10%)	7	27
4	M	325/355 (92%)	293 (90%)	32 (10%)	8	28
4	V	325/355 (92%)	294 (90%)	31 (10%)	8	30
5	5	167/175 (95%)	150 (90%)	17 (10%)	7	27
5	E	167/175 (95%)	149 (89%)	18 (11%)	6	25
5	N	167/175 (95%)	149 (89%)	18 (11%)	6	25
5	W	167/175 (95%)	149 (89%)	18 (11%)	6	25
6	6	118/149 (79%)	102 (86%)	16 (14%)	3	16
6	F	118/149 (79%)	103 (87%)	15 (13%)	4	19
6	O	118/149 (79%)	103 (87%)	15 (13%)	4	19
6	X	118/149 (79%)	103 (87%)	15 (13%)	4	19
7	9	126/150 (84%)	115 (91%)	11 (9%)	10	34
7	G	126/150 (84%)	115 (91%)	11 (9%)	10	34
7	P	126/150 (84%)	116 (92%)	10 (8%)	12	40
7	Y	126/150 (84%)	116 (92%)	10 (8%)	12	40
8	7	104/106 (98%)	95 (91%)	9 (9%)	10	34
8	H	104/106 (98%)	94 (90%)	10 (10%)	8	29
8	Q	104/106 (98%)	95 (91%)	9 (9%)	10	34
8	Z	104/106 (98%)	96 (92%)	8 (8%)	13	41
All	All	7808/8284 (94%)	7051 (90%)	757 (10%)	8	29

All (757) 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	139	ARG
1	1	155	ARG
1	1	161	ASN

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Mol	Chain	Res	Type
1	1	168	SER
1	1	184	GLU
1	1	217	THR
1	1	233	ARG
1	1	249	MET
1	1	253	GLN
1	1	255	SER
1	1	270	THR
1	1	271	THR
1	1	295	SER
1	1	303	THR
1	1	342	TRP
1	1	346	ARG
1	1	366	PHE
1	1	370	LEU
1	1	397	ARG
1	1	400	CYS
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	53	VAL
2	2	61	MET
2	2	106	ILE
2	2	114	ASP
2	2	139	GLU
2	2	146	THR
2	2	150	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

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Mol	Chain	Res	Type
3	3	89	ASP
3	3	94	ASP
3	3	95	THR
3	3	97	SER
3	3	121	THR
3	3	123	ASP
3	3	124	LYS
3	3	133	ARG
3	3	192	GLU
3	3	207	VAL
3	3	209	THR
3	3	215	ASP
3	3	218	LEU
3	3	239	THR
3	3	259	CYS
3	3	284	GLU
3	3	286	ASN
3	3	317	LEU
3	3	337	ARG
3	3	368	HIS
3	3	369	LEU
3	3	374	ARG
3	3	381	LEU
3	3	382	PHE
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	501	LYS
3	3	514	ASP
3	3	523	LEU
3	3	542	ARG
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	656	LEU

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Mol	Chain	Res	Type
3	3	683	LEU
3	3	684	ARG
3	3	715	GLU
3	3	716	LEU
3	3	738	THR
3	3	761	SER
3	3	771	VAL
3	3	774	ARG
3	3	776	LEU
4	4	42	ARG
4	4	44	MET
4	4	48	SER
4	4	59	ILE
4	4	69	THR
4	4	99	LEU
4	4	109	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	213	ILE
4	4	215	TYR
4	4	219	ARG
4	4	221	VAL
4	4	239	LEU
4	4	262	PHE
4	4	272	VAL
4	4	296	ARG
4	4	310	THR
4	4	314	ARG
4	4	333	GLU
4	4	407	VAL
4	4	409	ARG
5	5	5	ARG
5	5	25	LEU
5	5	38	MET

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Mol	Chain	Res	Type
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	135	ILE
5	5	142	GLU
5	5	146	LEU
5	5	175	THR
5	5	193	ARG
6	6	19	ILE
6	6	37	TRP
6	6	40	THR
6	6	45	CYS
6	6	53	SER
6	6	57	ARG
6	6	74	GLN
6	6	78	MET
6	6	83	ARG
6	6	84	LEU
6	6	121	TYR
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	58	LEU
7	9	85	GLU
7	9	97	ARG
7	9	101	CYS
7	9	134	GLU
7	9	140	VAL
7	9	157	VAL
7	9	159	VAL
8	7	43	ARG

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Mol	Chain	Res	Type
8	7	52	THR
8	7	54	ILE
8	7	63	LEU
8	7	73	SER
8	7	78	LYS
8	7	81	ARG
8	7	82	ILE
8	7	85	ARG
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	139	ARG
1	A	155	ARG
1	A	161	ASN
1	A	168	SER
1	A	184	GLU
1	A	217	THR
1	A	233	ARG
1	A	249	MET
1	A	253	GLN
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	366	PHE
1	A	368	VAL
1	A	370	LEU
1	A	397	ARG
1	A	400	CYS
1	A	414	LEU
1	A	419	ASP
1	A	437	TRP

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Mol	Chain	Res	Type
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	53	VAL
2	B	61	MET
2	B	106	ILE
2	B	114	ASP
2	B	139	GLU
2	B	146	THR
2	B	150	LEU
2	B	163	LEU
2	B	172	CYS
2	B	176	VAL
3	C	11	VAL
3	C	32	LEU
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	121	THR
3	C	123	ASP
3	C	124	LYS
3	C	133	ARG
3	C	192	GLU
3	C	207	VAL
3	C	209	THR
3	C	215	ASP
3	C	218	LEU
3	C	239	THR
3	C	259	CYS
3	C	284	GLU
3	C	286	ASN
3	C	317	LEU
3	C	337	ARG
3	C	368	HIS

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Mol	Chain	Res	Type
3	C	369	LEU
3	C	374	ARG
3	C	381	LEU
3	C	382	PHE
3	C	408	ILE
3	C	440	ARG
3	C	445	THR
3	C	450	LEU
3	C	459	MET
3	C	460	LYS
3	C	464	ILE
3	C	501	LYS
3	C	514	ASP
3	C	523	LEU
3	C	542	ARG
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	683	LEU
3	C	684	ARG
3	C	715	GLU
3	C	716	LEU
3	C	738	THR
3	C	761	SER
3	C	771	VAL
3	C	774	ARG
3	C	776	LEU
4	D	42	ARG
4	D	44	MET
4	D	48	SER
4	D	59	ILE
4	D	69	THR
4	D	99	LEU
4	D	109	VAL
4	D	120	LEU
4	D	129	HIS
4	D	133	LEU
4	D	143	LEU
4	D	152	GLU

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Mol	Chain	Res	Type
4	D	163	VAL
4	D	168	PHE
4	D	170	HIS
4	D	182	LEU
4	D	200	ARG
4	D	213	ILE
4	D	215	TYR
4	D	219	ARG
4	D	221	VAL
4	D	239	LEU
4	D	262	PHE
4	D	272	VAL
4	D	296	ARG
4	D	309	ILE
4	D	310	THR
4	D	314	ARG
4	D	333	GLU
4	D	363	SER
4	D	380	SER
4	D	407	VAL
4	D	409	ARG
5	E	1	MET
5	E	5	ARG
5	E	25	LEU
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	135	ILE
5	E	142	GLU
5	E	146	LEU
5	E	175	THR
5	E	193	ARG
6	F	19	ILE
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	58	LEU
7	G	85	GLU
7	G	97	ARG
7	G	101	CYS
7	G	134	GLU
7	G	140	VAL
7	G	157	VAL
7	G	159	VAL
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	78	LYS
8	H	81	ARG
8	H	82	ILE
8	H	85	ARG
1	J	10	ASP
1	J	28	THR
1	J	29	LEU
1	J	39	GLU
1	J	104	ARG
1	J	114	LEU
1	J	128	THR
1	J	139	ARG
1	J	155	ARG

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Mol	Chain	Res	Type
1	J	161	ASN
1	J	168	SER
1	J	184	GLU
1	J	217	THR
1	J	233	ARG
1	J	249	MET
1	J	253	GLN
1	J	255	SER
1	J	270	THR
1	J	271	THR
1	J	295	SER
1	J	303	THR
1	J	337	MET
1	J	342	TRP
1	J	346	ARG
1	J	366	PHE
1	J	370	LEU
1	J	374	ILE
1	J	397	ARG
1	J	400	CYS
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	53	VAL
2	K	61	MET
2	K	87	SER
2	K	114	ASP
2	K	139	GLU
2	K	146	THR
2	K	150	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

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Mol	Chain	Res	Type
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	121	THR
3	L	123	ASP
3	L	124	LYS
3	L	128	CYS
3	L	133	ARG
3	L	192	GLU
3	L	207	VAL
3	L	209	THR
3	L	215	ASP
3	L	218	LEU
3	L	239	THR
3	L	259	CYS
3	L	284	GLU
3	L	286	ASN
3	L	317	LEU
3	L	321	THR
3	L	337	ARG
3	L	368	HIS
3	L	369	LEU
3	L	374	ARG
3	L	381	LEU
3	L	382	PHE
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	501	LYS
3	L	514	ASP
3	L	523	LEU
3	L	542	ARG
3	L	578	LYS
3	L	593	LEU

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Mol	Chain	Res	Type
3	L	617	LEU
3	L	625	SER
3	L	644	LEU
3	L	655	ARG
3	L	683	LEU
3	L	684	ARG
3	L	715	GLU
3	L	716	LEU
3	L	738	THR
3	L	761	SER
3	L	771	VAL
3	L	774	ARG
3	L	776	LEU
4	M	42	ARG
4	M	44	MET
4	M	48	SER
4	M	59	ILE
4	M	69	THR
4	M	99	LEU
4	M	109	VAL
4	M	116	ILE
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	213	ILE
4	M	215	TYR
4	M	219	ARG
4	M	221	VAL
4	M	239	LEU
4	M	262	PHE
4	M	272	VAL
4	M	296	ARG
4	M	314	ARG
4	M	333	GLU
4	M	363	SER

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Mol	Chain	Res	Type
4	M	380	SER
4	M	407	VAL
4	M	409	ARG
5	N	1	MET
5	N	5	ARG
5	N	25	LEU
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
5	N	90	VAL
5	N	105	THR
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	37	TRP
6	O	40	THR
6	O	45	CYS
6	O	53	SER
6	O	57	ARG
6	O	74	GLN
6	O	78	MET
6	O	83	ARG
6	O	84	LEU
6	O	121	TYR
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	58	LEU
7	P	85	GLU
7	P	97	ARG

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Mol	Chain	Res	Type
7	P	101	CYS
7	P	134	GLU
7	P	157	VAL
7	P	159	VAL
8	Q	43	ARG
8	Q	52	THR
8	Q	54	ILE
8	Q	63	LEU
8	Q	73	SER
8	Q	78	LYS
8	Q	81	ARG
8	Q	82	ILE
8	Q	85	ARG
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	114	LEU
1	S	128	THR
1	S	139	ARG
1	S	155	ARG
1	S	161	ASN
1	S	168	SER
1	S	184	GLU
1	S	217	THR
1	S	233	ARG
1	S	249	MET
1	S	253	GLN
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	366	PHE
1	S	368	VAL
1	S	370	LEU
1	S	397	ARG
1	S	400	CYS

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Mol	Chain	Res	Type
1	S	414	LEU
1	S	419	ASP
1	S	437	TRP
1	S	438	ARG
2	T	5	ASP
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	139	GLU
2	T	146	THR
2	T	150	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	121	THR
3	U	123	ASP
3	U	124	LYS
3	U	133	ARG
3	U	192	GLU
3	U	207	VAL
3	U	209	THR
3	U	215	ASP
3	U	218	LEU
3	U	239	THR
3	U	259	CYS
3	U	284	GLU
3	U	286	ASN

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Mol	Chain	Res	Type
3	U	317	LEU
3	U	337	ARG
3	U	368	HIS
3	U	369	LEU
3	U	374	ARG
3	U	381	LEU
3	U	382	PHE
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	501	LYS
3	U	514	ASP
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	656	LEU
3	U	683	LEU
3	U	684	ARG
3	U	715	GLU
3	U	716	LEU
3	U	738	THR
3	U	761	SER
3	U	771	VAL
3	U	774	ARG
3	U	776	LEU
4	V	42	ARG
4	V	44	MET
4	V	48	SER
4	V	59	ILE
4	V	69	THR
4	V	99	LEU
4	V	109	VAL
4	V	120	LEU

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Mol	Chain	Res	Type
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	213	ILE
4	V	215	TYR
4	V	219	ARG
4	V	221	VAL
4	V	239	LEU
4	V	262	PHE
4	V	272	VAL
4	V	296	ARG
4	V	309	ILE
4	V	314	ARG
4	V	333	GLU
4	V	380	SER
4	V	407	VAL
4	V	409	ARG
5	W	5	ARG
5	W	25	LEU
5	W	38	MET
5	W	51	ASP
5	W	52	ILE
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	135	ILE
5	W	138	PRO
5	W	142	GLU
5	W	146	LEU
5	W	175	THR
5	W	193	ARG
6	X	19	ILE

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Mol	Chain	Res	Type
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	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	58	LEU
7	Y	85	GLU
7	Y	97	ARG
7	Y	101	CYS
7	Y	134	GLU
7	Y	157	VAL
7	Y	159	VAL
8	Z	43	ARG
8	Z	52	THR
8	Z	54	ILE
8	Z	63	LEU
8	Z	73	SER
8	Z	78	LYS
8	Z	81	ARG
8	Z	85	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	92	ASN
1	1	219	ASN
3	3	104	GLN
3	3	246	ASN
6	6	153	GLN
1	A	92	ASN

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Mol	Chain	Res	Type
1	A	219	ASN
3	C	104	GLN
3	C	246	ASN
6	F	153	GLN
8	H	94	HIS
1	J	92	ASN
1	J	198	ASN
1	J	219	ASN
3	L	104	GLN
3	L	246	ASN
6	O	153	GLN
1	S	92	ASN
1	S	198	ASN
1	S	219	ASN
3	U	104	GLN
3	U	246	ASN
6	X	153	GLN

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 carbohydrates 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
9	SF4	C	786	3	0,12,12	0.00	-	-		
9	SF4	L	786	3	0,12,12	0.00	-	-		
9	SF4	S	439	1	0,12,12	0.00	-	-		
9	SF4	9	184	7	0,12,12	0.00	-	-		
9	SF4	J	439	1	0,12,12	0.00	-	-		
11	FES	L	787	3	0,4,4	0.00	-	-		
11	FES	3	787	3	0,4,4	0.00	-	-		
9	SF4	L	784	3	0,12,12	0.00	-	-		
9	SF4	U	784	3	0,12,12	0.00	-	-		
9	SF4	P	184	7	0,12,12	0.00	-	-		
10	FMN	J	440	-	31,33,33	1.44	4 (12%)	40,50,50	2.15	10 (25%)
9	SF4	Y	183	7	0,12,12	0.00	-	-		
9	SF4	U	785	3	0,12,12	0.00	-	-		
9	SF4	P	183	7	0,12,12	0.00	-	-		
9	SF4	6	182	6	0,12,12	0.00	-	-		
9	SF4	3	786	3	0,12,12	0.00	-	-		
9	SF4	U	786	3	0,12,12	0.00	-	-		
9	SF4	F	182	6	0,12,12	0.00	-	-		
9	SF4	X	182	6	0,12,12	0.00	-	-		
11	FES	T	182	2	0,4,4	0.00	-	-		
9	SF4	9	183	7	0,12,12	0.00	-	-		
11	FES	C	787	3	0,4,4	0.00	-	-		
9	SF4	1	439	1	0,12,12	0.00	-	-		
9	SF4	C	784	3	0,12,12	0.00	-	-		
9	SF4	L	785	3	0,12,12	0.00	-	-		
9	SF4	G	184	7	0,12,12	0.00	-	-		
11	FES	K	182	2	0,4,4	0.00	-	-		
11	FES	U	787	3	0,4,4	0.00	-	-		
11	FES	2	182	2	0,4,4	0.00	-	-		
10	FMN	S	440	-	31,33,33	1.44	3 (9%)	40,50,50	2.31	13 (32%)
9	SF4	G	183	7	0,12,12	0.00	-	-		
9	SF4	3	785	3	0,12,12	0.00	-	-		
9	SF4	O	182	6	0,12,12	0.00	-	-		
10	FMN	A	440	-	31,33,33	1.57	3 (9%)	40,50,50	2.42	10 (25%)
10	FMN	1	440	-	31,33,33	1.42	4 (12%)	40,50,50	2.40	13 (32%)
11	FES	B	182	2	0,4,4	0.00	-	-		
9	SF4	Y	184	7	0,12,12	0.00	-	-		
9	SF4	A	439	1	0,12,12	0.00	-	-		
9	SF4	3	784	3	0,12,12	0.00	-	-		
9	SF4	C	785	3	0,12,12	0.00	-	-		

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	C	785	3	-	-	0/6/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	440	FMN	C4A-N5	4.47	1.39	1.33
10	A	440	FMN	C10-N1	4.27	1.38	1.33
10	1	440	FMN	C4A-N5	4.17	1.39	1.33
10	J	440	FMN	C10-N1	4.13	1.38	1.33
10	S	440	FMN	C10-N1	4.05	1.38	1.33
10	1	440	FMN	C10-N1	4.02	1.38	1.33
10	S	440	FMN	C4A-N5	4.00	1.39	1.33
10	A	440	FMN	C4-N3	3.90	1.39	1.33
10	J	440	FMN	C4A-N5	3.77	1.38	1.33
10	S	440	FMN	C4-N3	3.28	1.38	1.33
10	J	440	FMN	C4-N3	3.18	1.38	1.33
10	1	440	FMN	C4-N3	2.98	1.38	1.33
10	1	440	FMN	C6-C5A	-2.08	1.38	1.41
10	J	440	FMN	C6-C5A	-2.06	1.38	1.41

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	440	FMN	C4-N3-C2	8.22	122.08	115.14
10	1	440	FMN	C5'-C4'-C3'	-8.12	96.52	112.20
10	S	440	FMN	C4-N3-C2	6.78	120.87	115.14
10	S	440	FMN	C5'-C4'-C3'	-6.61	99.44	112.20
10	J	440	FMN	C4-N3-C2	6.37	120.52	115.14
10	A	440	FMN	C1'-C2'-C3'	-6.13	92.66	109.79
10	1	440	FMN	C4-N3-C2	6.09	120.28	115.14
10	J	440	FMN	C1'-C2'-C3'	-5.77	93.67	109.79
10	A	440	FMN	C5'-C4'-C3'	-5.12	102.32	112.20
10	1	440	FMN	C1'-C2'-C3'	-4.98	95.86	109.79
10	S	440	FMN	C1'-C2'-C3'	-4.51	97.17	109.79
10	J	440	FMN	C4A-N5-C5A	4.19	120.96	116.77
10	1	440	FMN	C4A-N5-C5A	4.16	120.93	116.77
10	A	440	FMN	C4A-C4-N3	-3.89	118.11	123.43
10	A	440	FMN	C4A-N5-C5A	3.88	120.65	116.77
10	J	440	FMN	C1'-N10-C9A	3.78	121.27	118.29
10	S	440	FMN	C4A-N5-C5A	3.65	120.41	116.77
10	A	440	FMN	C10-C4A-N5	-3.54	118.81	121.26
10	1	440	FMN	C5A-C9A-N10	3.52	120.26	117.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	440	FMN	C5'-C4'-C3'	-3.36	105.70	112.20
10	J	440	FMN	C4A-C4-N3	-3.26	118.97	123.43
10	S	440	FMN	C4'-C3'-C2'	3.21	120.05	113.36
10	J	440	FMN	O4'-C4'-C5'	3.21	117.14	109.92
10	S	440	FMN	C5A-C9A-N10	3.10	119.96	117.72
10	S	440	FMN	C4A-C4-N3	-3.00	119.33	123.43
10	A	440	FMN	C1'-N10-C9A	2.98	120.64	118.29
10	J	440	FMN	C5A-C9A-N10	2.89	119.81	117.72
10	J	440	FMN	C10-C4A-N5	-2.88	119.26	121.26
10	A	440	FMN	C5A-C9A-N10	2.86	119.79	117.72
10	A	440	FMN	C4-C4A-N5	2.85	121.86	118.60
10	1	440	FMN	C4'-C3'-C2'	2.84	119.26	113.36
10	1	440	FMN	C10-C4A-N5	-2.81	119.31	121.26
10	S	440	FMN	O5'-C5'-C4'	2.81	116.86	109.36
10	S	440	FMN	C1'-N10-C9A	2.75	120.46	118.29
10	S	440	FMN	C10-C4A-N5	-2.72	119.38	121.26
10	1	440	FMN	C4A-C4-N3	-2.69	119.76	123.43
10	1	440	FMN	C1'-N10-C9A	2.46	120.23	118.29
10	1	440	FMN	C4-C4A-N5	2.44	121.39	118.60
10	1	440	FMN	P-O5'-C5'	-2.28	112.01	118.30
10	S	440	FMN	C4-C4A-N5	2.22	121.14	118.60
10	S	440	FMN	O2'-C2'-C3'	2.20	114.45	109.10
10	1	440	FMN	C9A-C5A-N5	-2.15	118.99	122.36
10	1	440	FMN	O2'-C2'-C3'	2.07	114.12	109.10
10	A	440	FMN	O3P-P-O5'	2.04	112.17	106.73
10	S	440	FMN	C7-C6-C5A	-2.02	118.35	121.22
10	J	440	FMN	C4-C4A-N5	2.00	120.89	118.60

There are no chirality outliers.

All (20) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
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	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	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 63 short contacts:

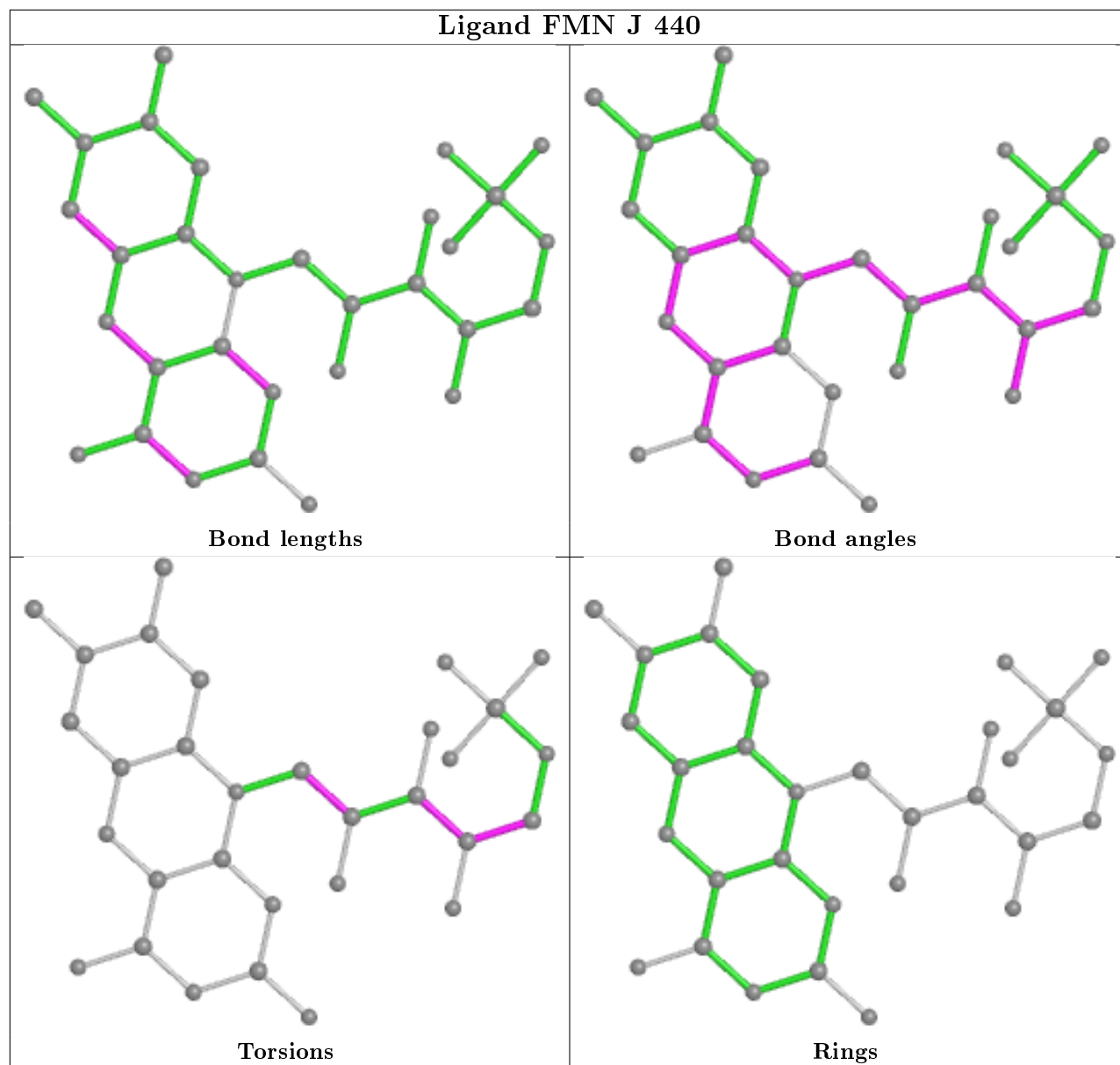
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	786	SF4	1	0
9	9	184	SF4	1	0
9	L	784	SF4	1	0
9	U	784	SF4	1	0
9	P	184	SF4	1	0
10	J	440	FMN	10	0
9	U	785	SF4	1	0
9	P	183	SF4	1	0
9	6	182	SF4	2	0
9	3	786	SF4	1	0
9	F	182	SF4	3	0
9	X	182	SF4	3	0
11	T	182	FES	1	0
9	9	183	SF4	1	0
11	C	787	FES	1	0
9	L	785	SF4	1	0
9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

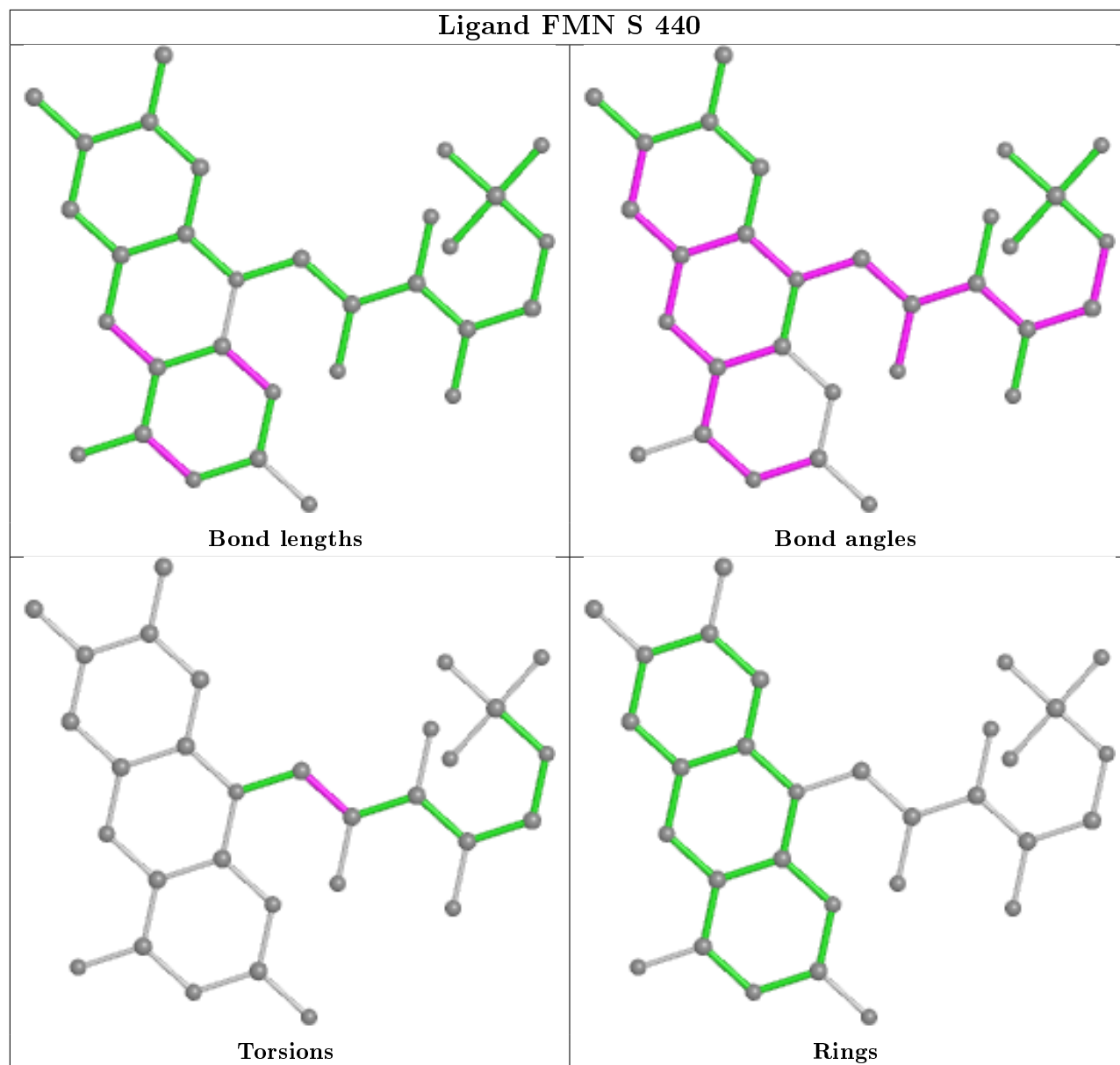
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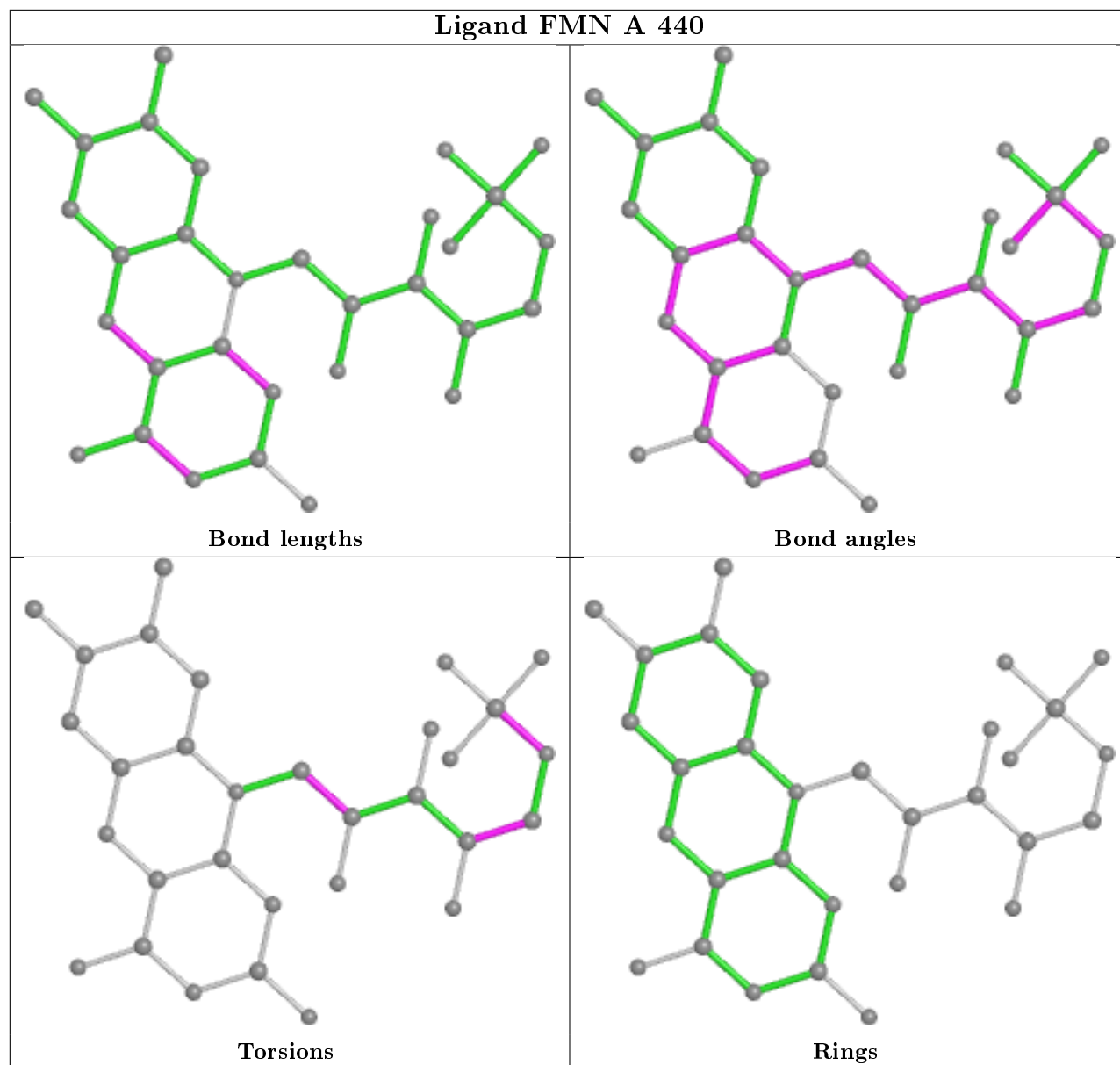
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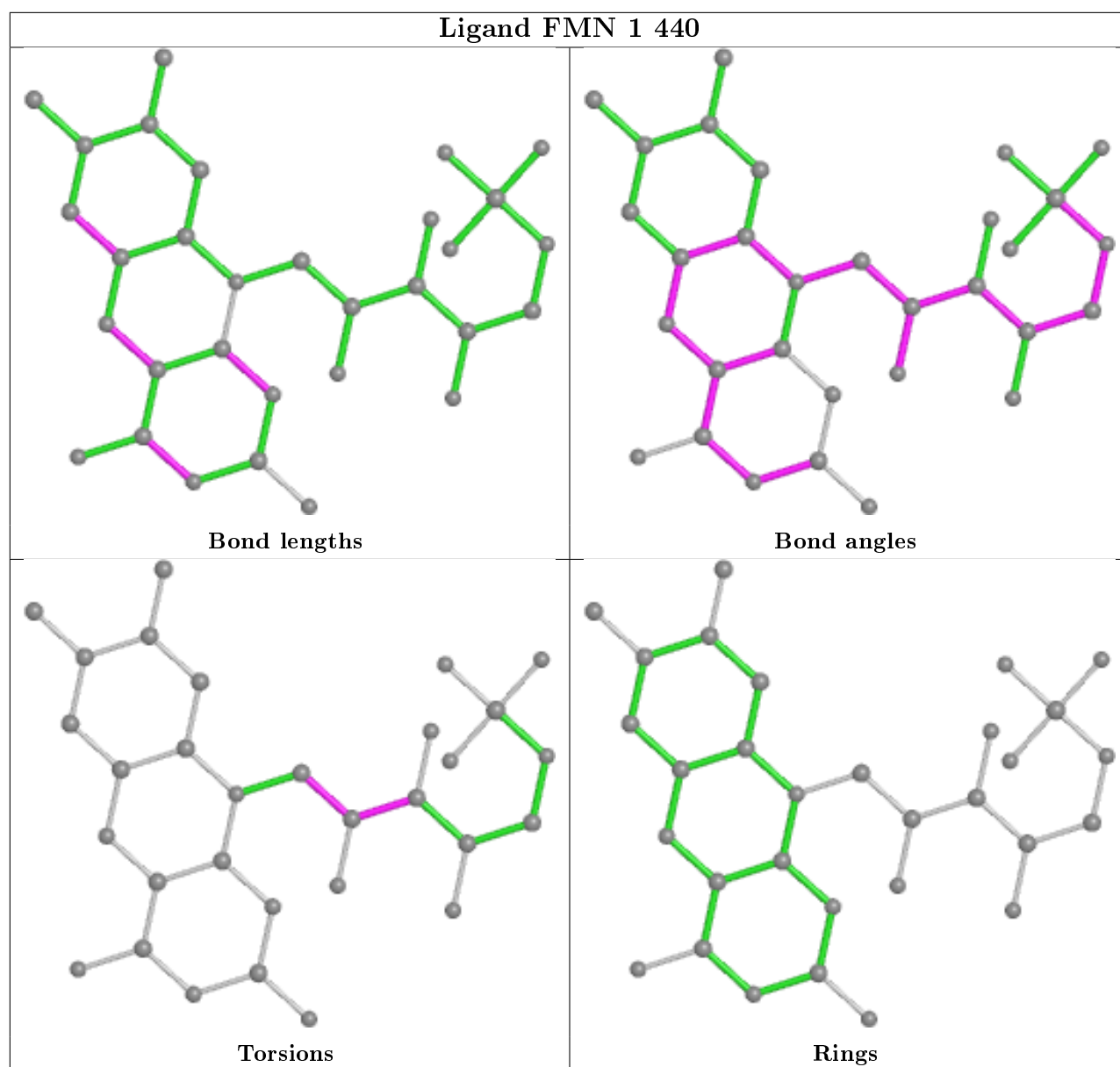
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	3	784	SF4	1	0
9	C	785	SF4	1	0

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%)	-0.25	0 100 100	38, 59, 83, 110	0
1	A	437/438 (99%)	-0.28	0 100 100	40, 60, 84, 110	0
1	J	437/438 (99%)	-0.24	1 (0%) 95 94	39, 59, 83, 110	0
1	S	437/438 (99%)	-0.32	1 (0%) 95 94	39, 60, 83, 111	0
2	2	178/181 (98%)	-0.22	0 100 100	43, 63, 93, 135	0
2	B	178/181 (98%)	-0.21	2 (1%) 80 70	43, 64, 94, 134	0
2	K	178/181 (98%)	-0.18	1 (0%) 89 84	43, 63, 93, 136	0
2	T	178/181 (98%)	-0.28	0 100 100	43, 64, 94, 134	0
3	3	754/783 (96%)	-0.11	0 100 100	36, 74, 112, 133	0
3	C	754/783 (96%)	-0.11	3 (0%) 92 89	36, 75, 113, 134	0
3	L	754/783 (96%)	-0.04	10 (1%) 77 66	37, 75, 114, 133	0
3	U	754/783 (96%)	-0.14	3 (0%) 92 89	36, 75, 113, 134	0
4	4	377/409 (92%)	-0.06	0 100 100	38, 78, 112, 129	0
4	D	377/409 (92%)	-0.10	0 100 100	38, 77, 112, 129	0
4	M	377/409 (92%)	-0.06	1 (0%) 94 92	38, 78, 112, 129	0
4	V	377/409 (92%)	0.04	7 (1%) 66 53	39, 78, 112, 130	0
5	5	196/207 (94%)	-0.10	0 100 100	50, 83, 120, 132	0
5	E	196/207 (94%)	-0.10	0 100 100	51, 83, 120, 132	0
5	N	196/207 (94%)	-0.07	0 100 100	50, 83, 120, 132	0
5	W	196/207 (94%)	0.01	5 (2%) 56 40	52, 84, 120, 133	0
6	6	145/181 (80%)	-0.17	0 100 100	51, 71, 104, 125	0
6	F	145/181 (80%)	-0.10	0 100 100	49, 71, 105, 125	0
6	O	145/181 (80%)	-0.13	0 100 100	50, 71, 105, 125	0
6	X	145/181 (80%)	-0.06	1 (0%) 87 81	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%)	-0.18	0 100 100	37, 59, 96, 136	0
7	G	154/182 (84%)	-0.21	0 100 100	37, 58, 95, 135	0
7	P	154/182 (84%)	-0.22	0 100 100	37, 59, 95, 136	0
7	Y	154/182 (84%)	-0.25	0 100 100	37, 60, 96, 136	0
8	7	127/129 (98%)	-0.21	0 100 100	49, 66, 101, 119	0
8	H	127/129 (98%)	-0.19	1 (0%) 86 78	48, 66, 101, 120	0
8	Q	127/129 (98%)	-0.15	0 100 100	48, 66, 102, 120	0
8	Z	127/129 (98%)	-0.22	1 (0%) 86 78	48, 67, 101, 119	0
All	All	9472/10040 (94%)	-0.14	37 (0%) 92 89	36, 69, 111, 136	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	V	385	CYS	4.4
5	W	50	ALA	3.9
3	L	582	PHE	3.6
1	J	2	THR	3.5
3	L	654	PHE	3.3
2	K	180	GLU	3.1
4	V	26	MET	3.0
4	V	139	ASP	3.0
3	L	577	LEU	3.0
3	U	654	PHE	2.8
1	S	2	THR	2.8
8	H	100	GLY	2.8
3	C	501	LYS	2.7
3	L	758	LEU	2.6
3	L	653	PRO	2.5
6	X	20	LEU	2.5
2	B	180	GLU	2.4
3	C	681	LYS	2.4
4	M	147	PHE	2.3
5	W	46	PHE	2.3
3	L	578	LYS	2.3
3	L	648	LEU	2.3
3	L	566	ALA	2.3
5	W	38	MET	2.2
3	U	682	GLU	2.2
3	C	54	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
8	Z	96	HIS	2.1
5	W	124	ILE	2.1
4	V	140	LEU	2.1
4	V	147	PHE	2.1
3	L	751	GLU	2.0
5	W	51	ASP	2.0
4	V	266	LEU	2.0
4	V	208	PHE	2.0
3	L	644	LEU	2.0
2	B	36	GLN	2.0
3	U	143	TYR	2.0

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 carbohydrates 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	0.81	0.16	100,100,100,100	0
12	CA	B	202	1/1	0.84	0.15	108,108,108,108	0
12	CA	2	202	1/1	0.94	0.13	58,58,58,58	0
10	FMN	A	440	31/31	0.95	0.21	48,60,64,66	0
10	FMN	S	440	31/31	0.96	0.22	53,60,65,66	0
10	FMN	J	440	31/31	0.96	0.24	42,53,60,63	0
10	FMN	1	440	31/31	0.96	0.20	48,54,62,68	0
12	CA	3	789	1/1	0.97	0.16	50,50,50,50	0
12	CA	H	203	1/1	0.97	0.21	55,55,55,55	0
12	CA	U	788	1/1	0.98	0.17	50,50,50,50	0
12	CA	K	202	1/1	0.98	0.12	66,66,66,66	0
12	CA	Z	203	1/1	0.98	0.17	60,60,60,60	0

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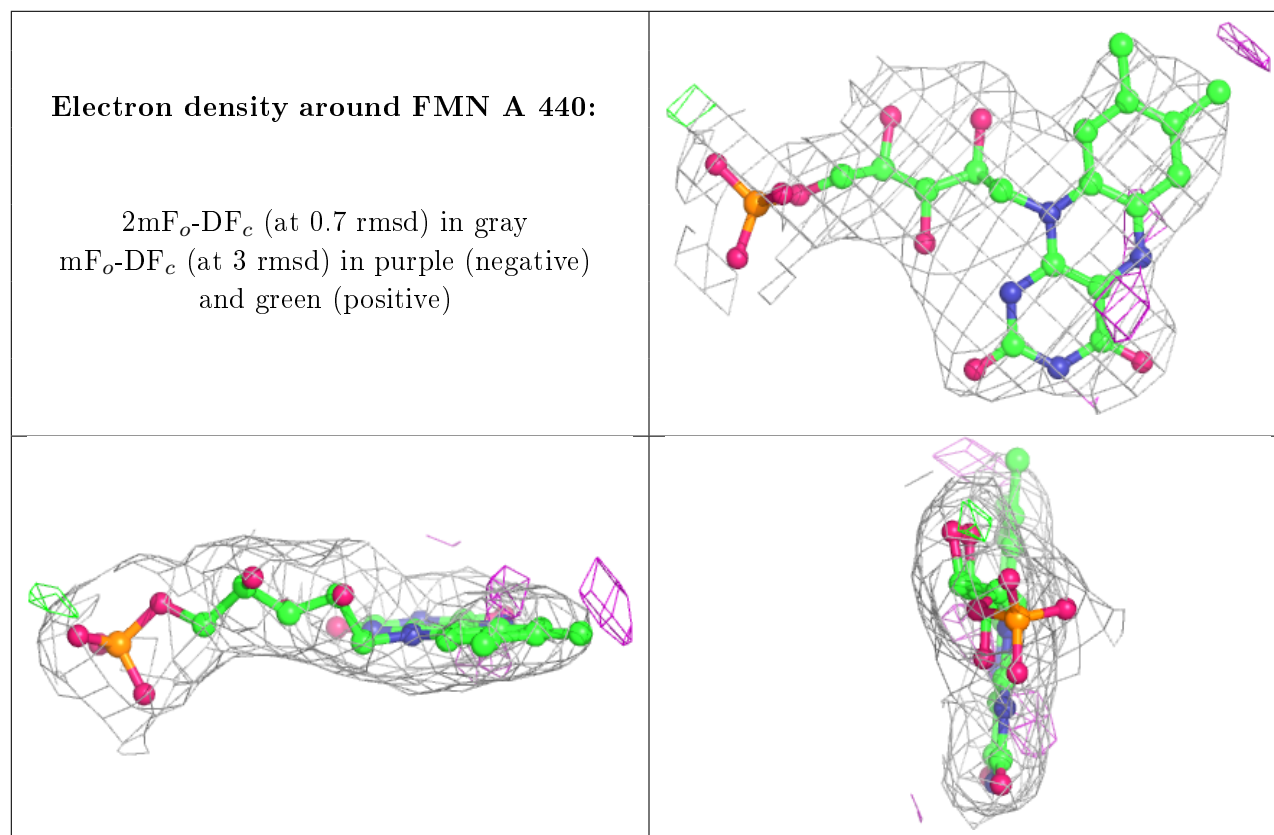
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	CA	L	789	1/1	0.98	0.13	62,62,62,62	0
12	CA	3	788	1/1	0.99	0.15	43,43,43,43	0
12	CA	P	201	1/1	0.99	0.26	40,40,40,40	0
11	FES	U	787	4/4	0.99	0.17	22,28,34,45	0
9	SF4	L	786	8/8	0.99	0.17	30,39,61,62	0
12	CA	Y	201	1/1	0.99	0.20	41,41,41,41	0
12	CA	9	201	1/1	0.99	0.25	37,37,37,37	0
9	SF4	X	182	8/8	0.99	0.17	39,56,81,89	0
12	CA	L	788	1/1	0.99	0.13	50,50,50,50	0
12	CA	G	201	1/1	0.99	0.19	43,43,43,43	0
9	SF4	C	786	8/8	0.99	0.20	21,34,56,59	0
9	SF4	U	786	8/8	1.00	0.18	21,33,51,58	0
11	FES	L	787	4/4	1.00	0.18	16,17,33,41	0
9	SF4	F	182	8/8	1.00	0.19	18,31,51,62	0
11	FES	3	787	4/4	1.00	0.19	17,20,34,47	0
9	SF4	L	784	8/8	1.00	0.20	11,17,34,42	0
11	FES	T	182	4/4	1.00	0.16	18,26,47,47	0
9	SF4	9	183	8/8	1.00	0.19	12,19,45,48	0
11	FES	C	787	4/4	1.00	0.16	22,23,31,43	0
9	SF4	1	439	8/8	1.00	0.20	13,24,43,45	0
9	SF4	C	784	8/8	1.00	0.19	13,18,40,40	0
9	SF4	S	439	8/8	1.00	0.19	19,27,49,51	0
12	CA	C	788	1/1	1.00	0.17	46,46,46,46	0
9	SF4	L	785	8/8	1.00	0.21	11,18,39,39	0
9	SF4	G	184	8/8	1.00	0.19	12,15,39,39	0
11	FES	K	182	4/4	1.00	0.16	14,22,42,44	0
9	SF4	U	784	8/8	1.00	0.19	15,26,43,43	0
9	SF4	P	184	8/8	1.00	0.20	1,19,41,41	0
9	SF4	9	184	8/8	1.00	0.19	7,27,44,48	0
11	FES	2	182	4/4	1.00	0.17	11,18,41,42	0
9	SF4	Y	183	8/8	1.00	0.18	17,35,53,57	0
9	SF4	G	183	8/8	1.00	0.20	11,18,42,46	0
9	SF4	U	785	8/8	1.00	0.20	19,27,43,43	0
9	SF4	3	785	8/8	1.00	0.21	8,18,36,38	0
9	SF4	O	182	8/8	1.00	0.19	18,27,54,59	0
9	SF4	P	183	8/8	1.00	0.19	10,16,42,46	0
9	SF4	J	439	8/8	1.00	0.20	8,25,43,44	0
11	FES	B	182	4/4	1.00	0.15	15,29,43,48	0
9	SF4	Y	184	8/8	1.00	0.17	19,29,51,57	0
9	SF4	6	182	8/8	1.00	0.19	24,37,69,69	0
9	SF4	A	439	8/8	1.00	0.19	13,26,49,50	0
9	SF4	3	784	8/8	1.00	0.19	12,16,36,38	0

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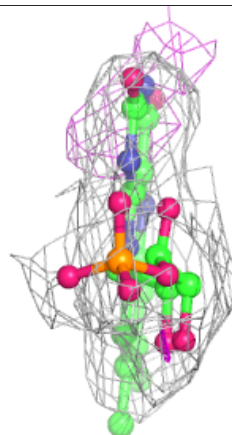
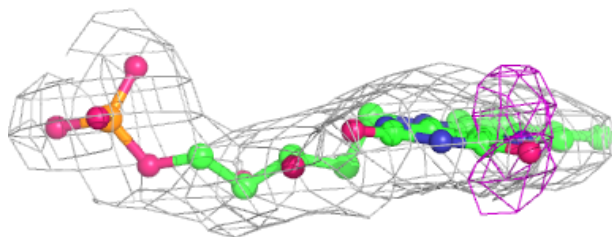
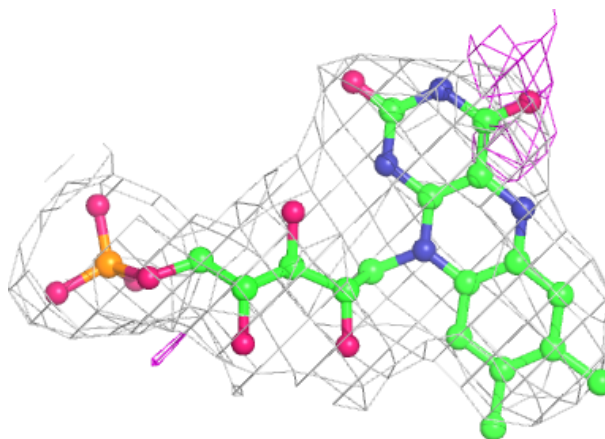
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	SF4	3	786	8/8	1.00	0.19	16,27,50,50	0
9	SF4	C	785	8/8	1.00	0.20	12,22,39,40	0

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.

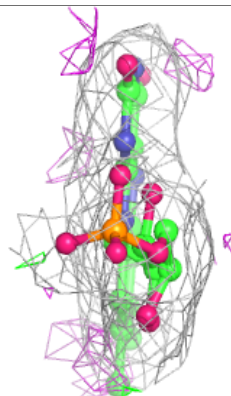
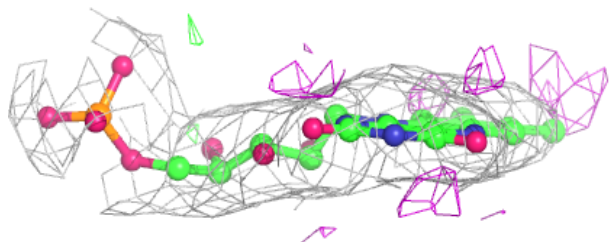
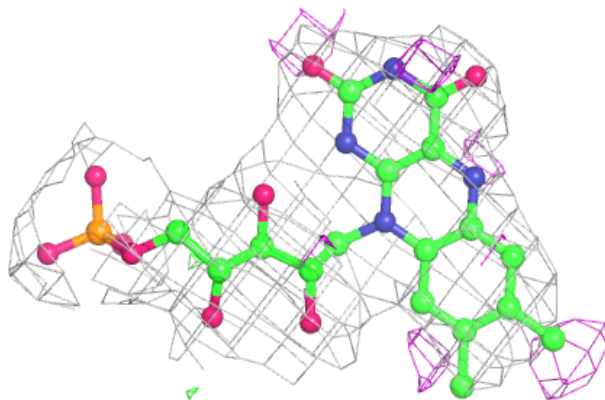


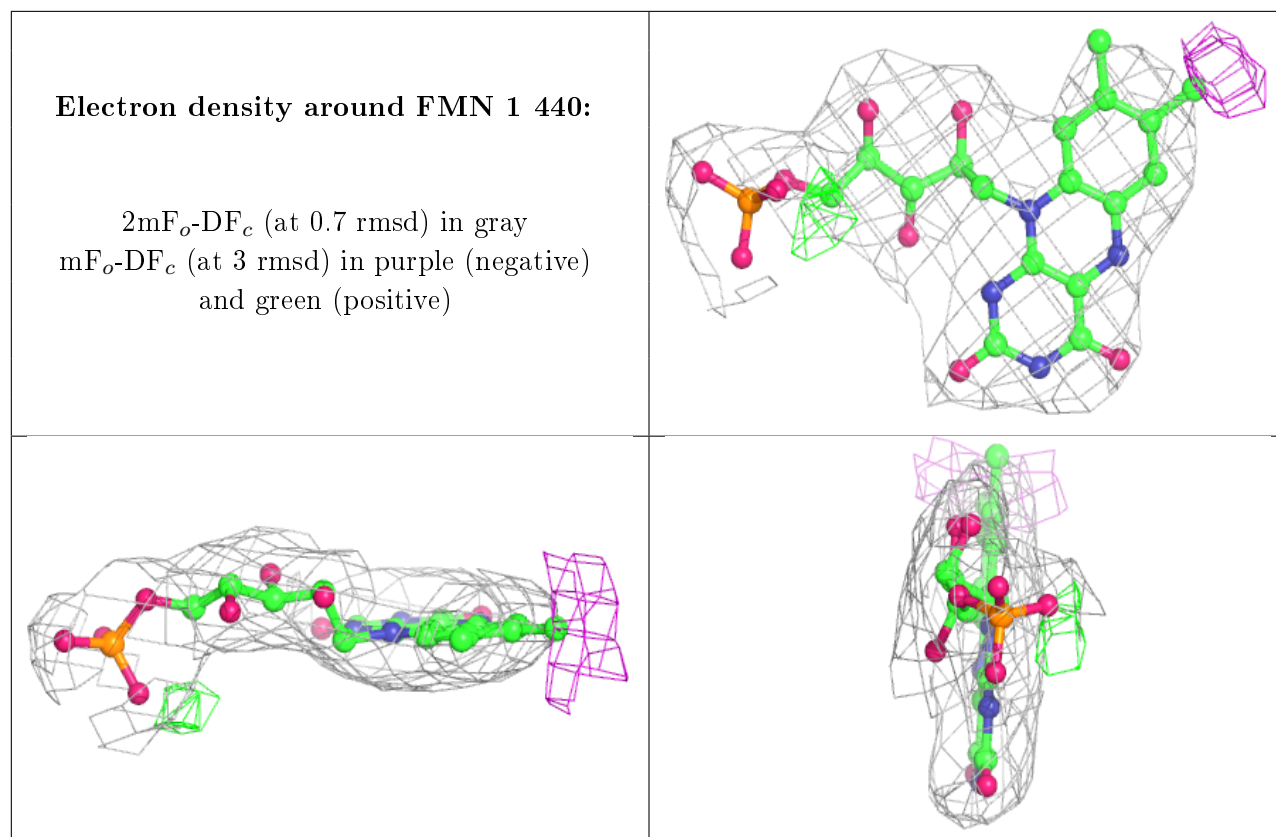
Electron density around FMN S 440:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.