



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 06:57 AM BST

PDB ID : 6I0D  
Title : Respiratory complex I from *Thermus thermophilus* with bound Decyl-Ubiquinone  
Authors : Gutierrez-Fernandez, J.; Minhas, G.S.; Sazanov, L.A.  
Deposited on : 2018-10-25  
Resolution : 3.60 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](mailto: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.

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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 : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

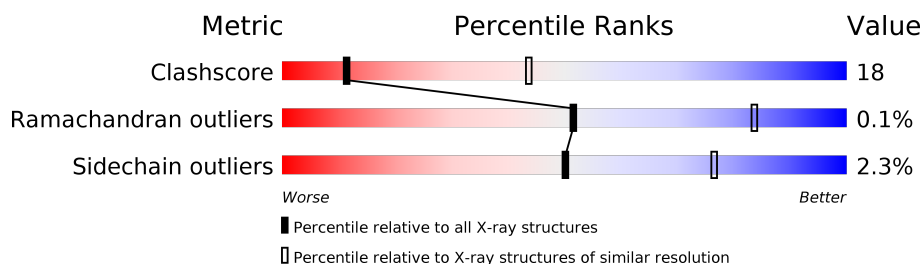
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 Å.





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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
















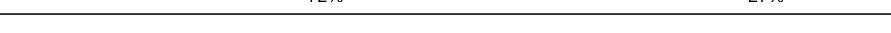

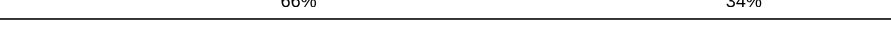
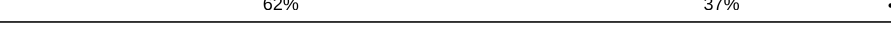
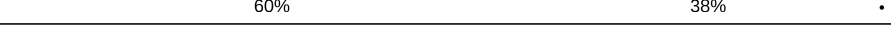




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	438	 61% 39% .
1	B	438	 53% 47% .
2	2	181	 67% 30% ..
2	C	181	 58% 39% ..
3	3	783	 62% 34% ..
3	D	783	 62% 34% ..
4	4	409	 48% 44% . 6%
4	E	409	 54% 40% 6%

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Mol	Chain	Length	Quality of chain
5	5	207	
5	F	207	
6	6	181	
6	G	181	
7	9	182	
7	O	182	
8	7	129	
8	I	129	
9	W	131	
9	X	131	
10	A	119	
10	P	119	
11	J	176	
11	R	176	
12	K	95	
12	S	95	
13	L	606	
13	T	606	
14	M	469	
14	U	469	
15	N	427	
15	V	427	
16	H	365	
16	Q	365	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	SF4	3	803	-	-	X	-
17	SF4	9	201	-	-	X	-
17	SF4	B	501	-	-	X	-
17	SF4	D	803	-	-	X	-
17	SF4	O	201	-	-	X	-
18	FMN	1	502	-	-	X	-
18	FMN	B	502	-	-	X	-
19	FES	D	804	-	-	X	-

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 74132 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	B	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	C	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	756	Total	C	N	O	S	0	0	0
			5895	3754	1057	1053	31			
3	D	756	Total	C	N	O	S	0	0	0
			5895	3754	1057	1053	31			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	384	Total	C	N	O	S	0	0	0
			3067	1975	522	559	11			
4	E	384	Total	C	N	O	S	0	0	0
			3067	1975	522	559	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	F	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	166	Total	C	N	O	S	0	0	0
			1289	815	235	226	13			
6	G	166	Total	C	N	O	S	0	0	0
			1289	815	235	226	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	9	180	Total	C	N	O	S	0	0	0
			1388	890	232	255	11			
7	O	180	Total	C	N	O	S	0	0	0
			1388	890	232	255	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	I	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	W	127	Total	C	N	O	S	0	0	0
			967	623	165	175	4			
9	X	127	Total	C	N	O	S	0	0	0
			967	623	165	175	4			

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	A	117	Total	C	N	O	S	0	0	0
			910	624	138	144	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	P	117	Total	C	N	O	S	0	0	0
			910	624	138	144	4			

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	160	Total	C	N	O	S	0	0	0
			1183	806	183	191	3			
11	R	160	Total	C	N	O	S	0	0	0
			1183	806	183	191	3			

- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	95	Total	C	N	O	S	0	0	0
			703	456	118	126	3			
12	S	95	Total	C	N	O	S	0	0	0
			703	456	118	126	3			

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	605	Total	C	N	O	S	0	0	0
			4604	3089	740	756	19			
13	T	605	Total	C	N	O	S	0	0	0
			4604	3089	740	756	19			

- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	467	Total	C	N	O	S	0	0	0
			3489	2363	546	572	8			
14	U	467	Total	C	N	O	S	0	0	0
			3489	2363	546	572	8			

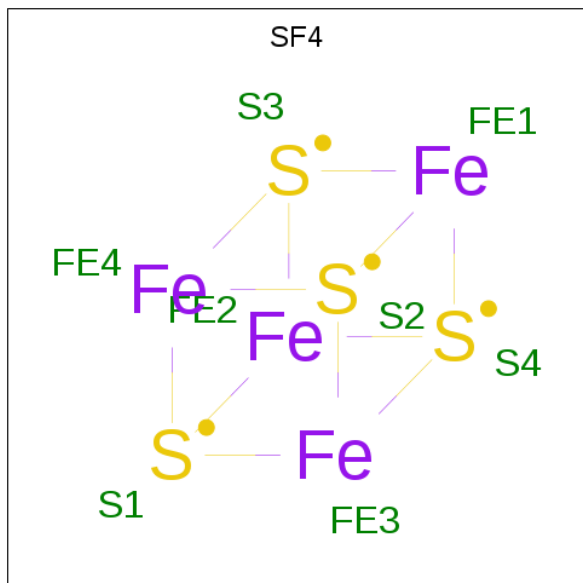
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	427	Total	C	N	O	S	0	0	0
			3154	2125	505	518	6			
15	V	427	Total	C	N	O	S	0	0	0
			3154	2125	505	518	6			

- Molecule 16 is a protein called NADH-quinone oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	H	353	Total	C	N	O	S	0	0	0
			2838	1943	431	457	7			
16	Q	353	Total	C	N	O	S	0	0	0
			2838	1943	431	457	7			

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	1	1	Total	Fe	S	0	0
			8	4	4		
17	3	1	Total	Fe	S	0	0
			8	4	4		
17	3	1	Total	Fe	S	0	0
			8	4	4		
17	3	1	Total	Fe	S	0	0
			8	4	4		
17	6	1	Total	Fe	S	0	0
			8	4	4		
17	9	1	Total	Fe	S	0	0
			8	4	4		
17	9	1	Total	Fe	S	0	0
			8	4	4		
17	B	1	Total	Fe	S	0	0
			8	4	4		
17	D	1	Total	Fe	S	0	0
			8	4	4		

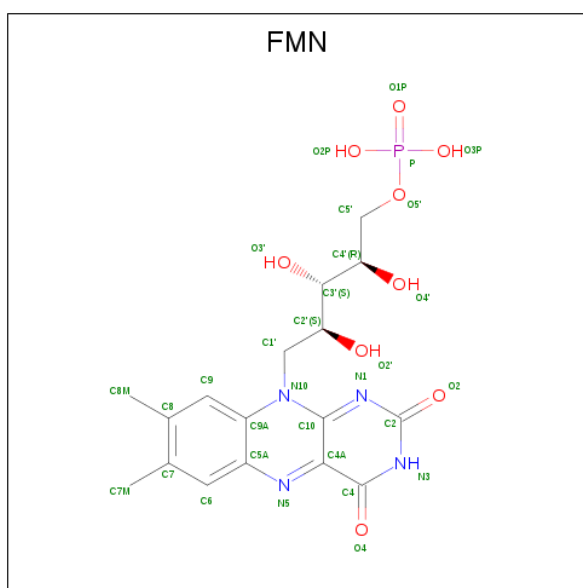
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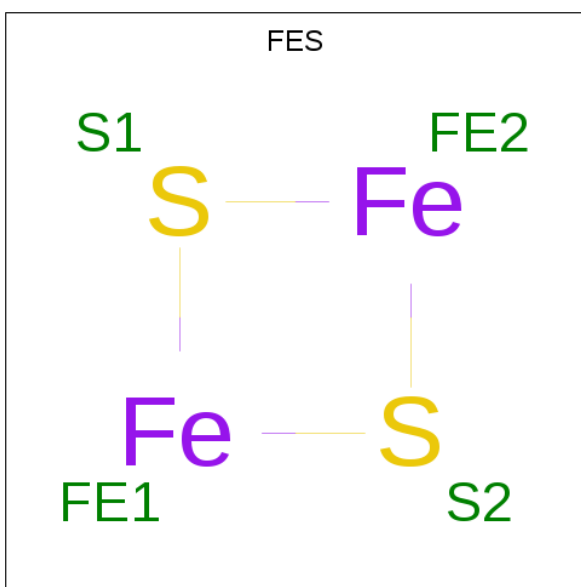
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	D	1	Total	Fe	S	0	0
			8	4	4		
17	D	1	Total	Fe	S	0	0
			8	4	4		
17	G	1	Total	Fe	S	0	0
			8	4	4		
17	O	1	Total	Fe	S	0	0
			8	4	4		
17	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 18 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



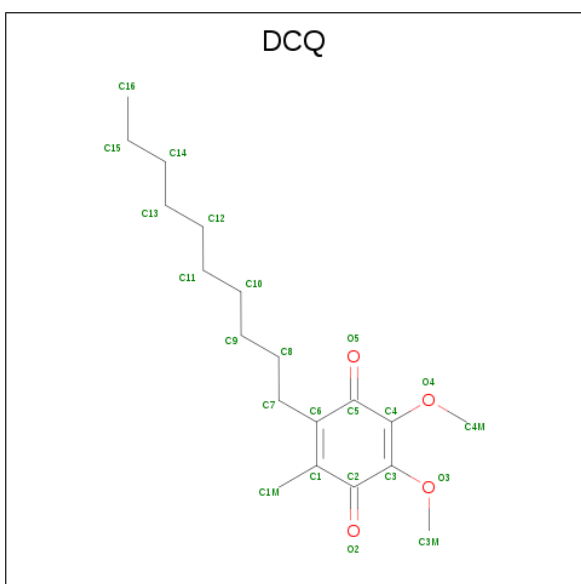
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
18	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	2	1	Total	Fe	S	0	0
			4	2	2		
19	3	1	Total	Fe	S	0	0
			4	2	2		
19	C	1	Total	Fe	S	0	0
			4	2	2		
19	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 20 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (three-letter code: DCQ) (formula: C<sub>19</sub>H<sub>30</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by author).



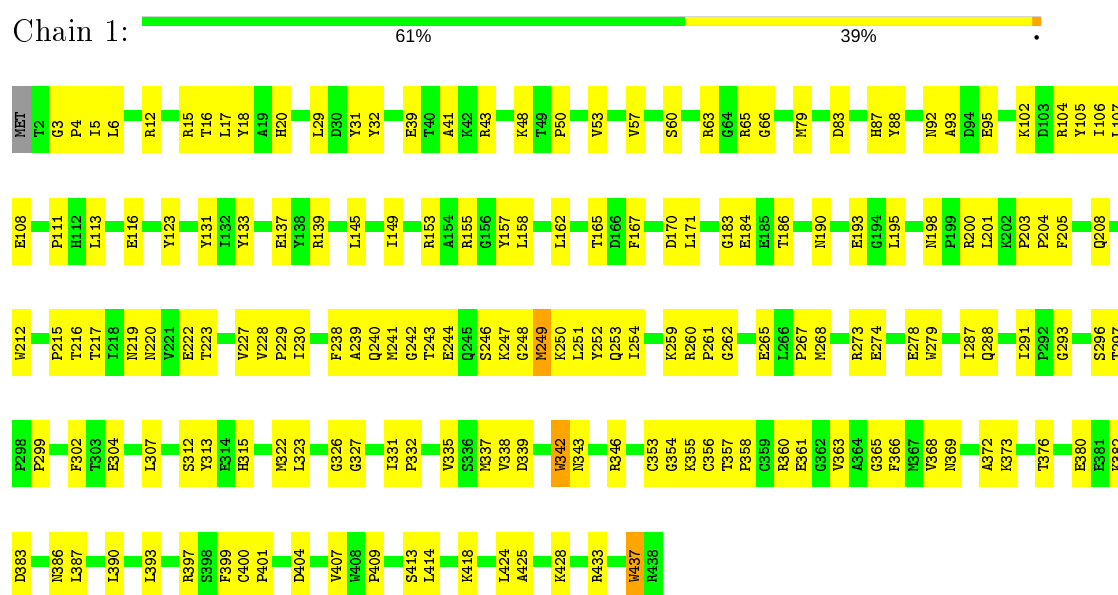
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	4	1	Total	C	O	0	0
			23	19	4		
20	E	1	Total	C	O	0	0
			23	19	4		

### 3 Residue-property plots

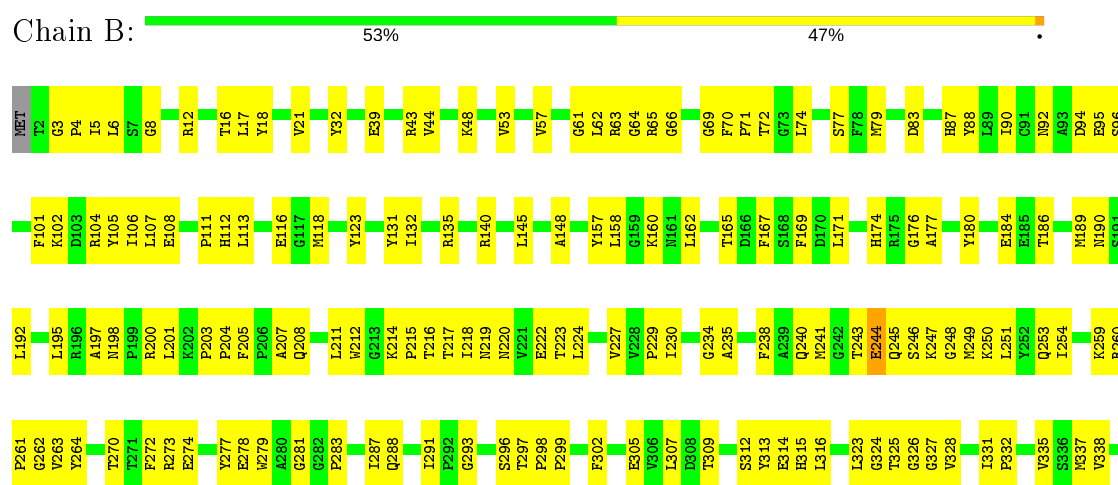
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

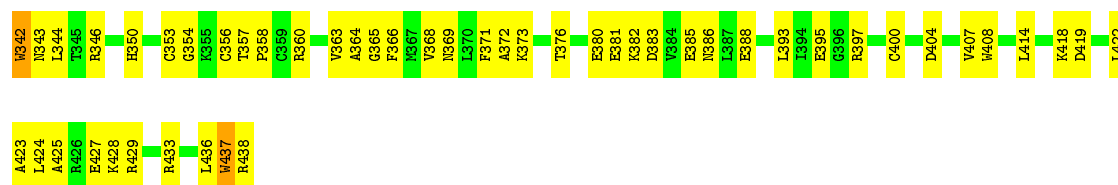
Note EDS failed to run properly.

#### • Molecule 1: NADH-quinone oxidoreductase subunit 1



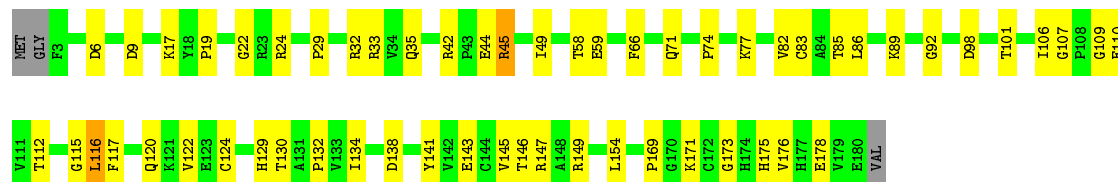
#### • Molecule 1: NADH-quinone oxidoreductase subunit 1





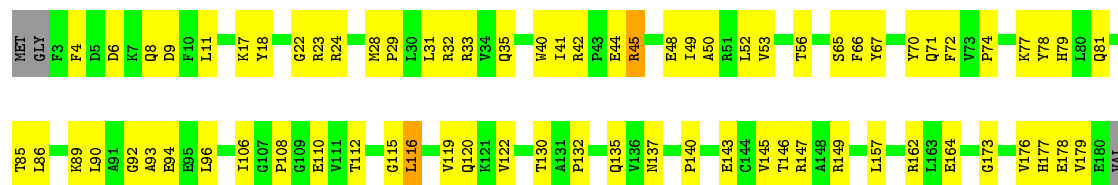
• Molecule 2: NADH-quinone oxidoreductase subunit 2

Chain 2: 67% 30% ..



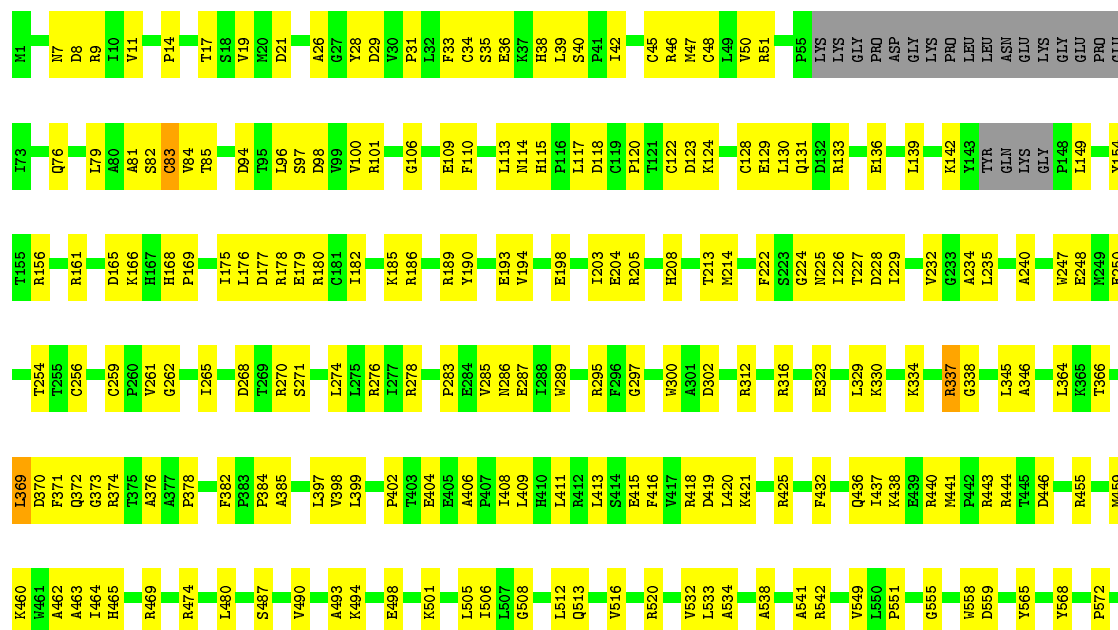
• Molecule 2: NADH-quinone oxidoreductase subunit 2

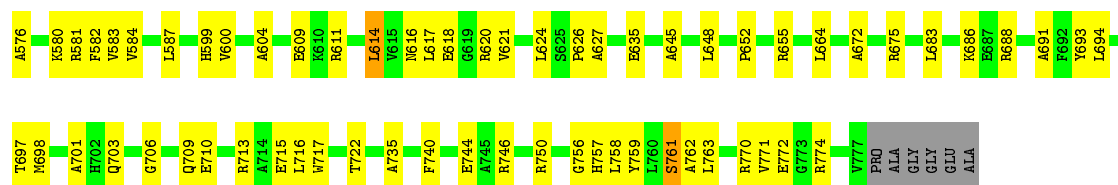
Chain C: 58% 39% ..



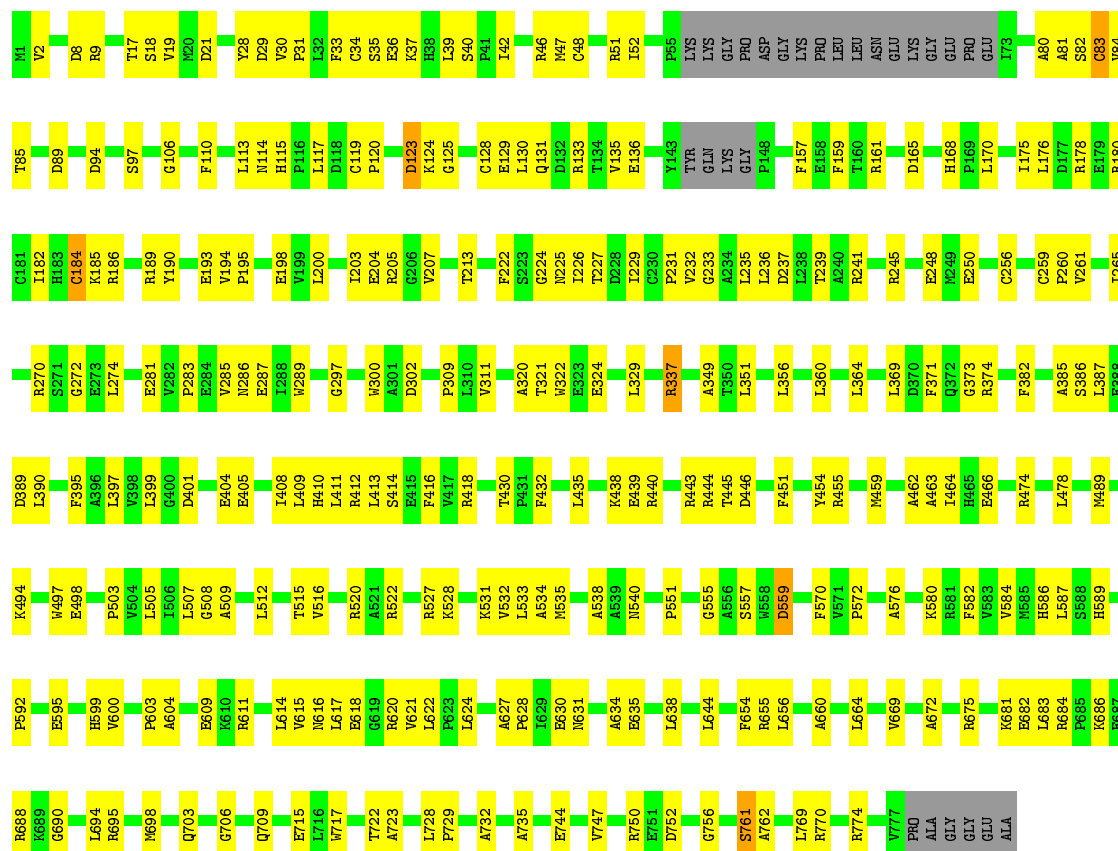
• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain 3: 62% 34% ..

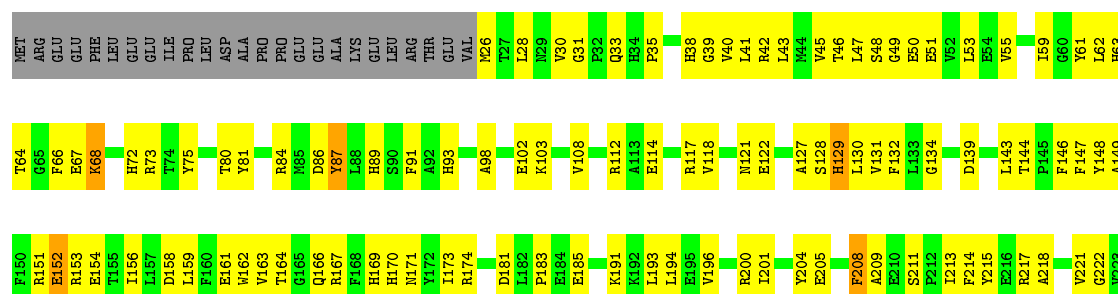


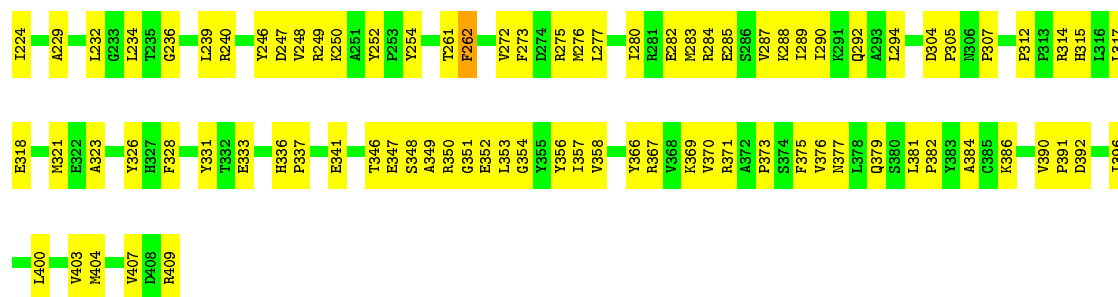


• Molecule 3: NADH-quinone oxidoreductase subunit 3



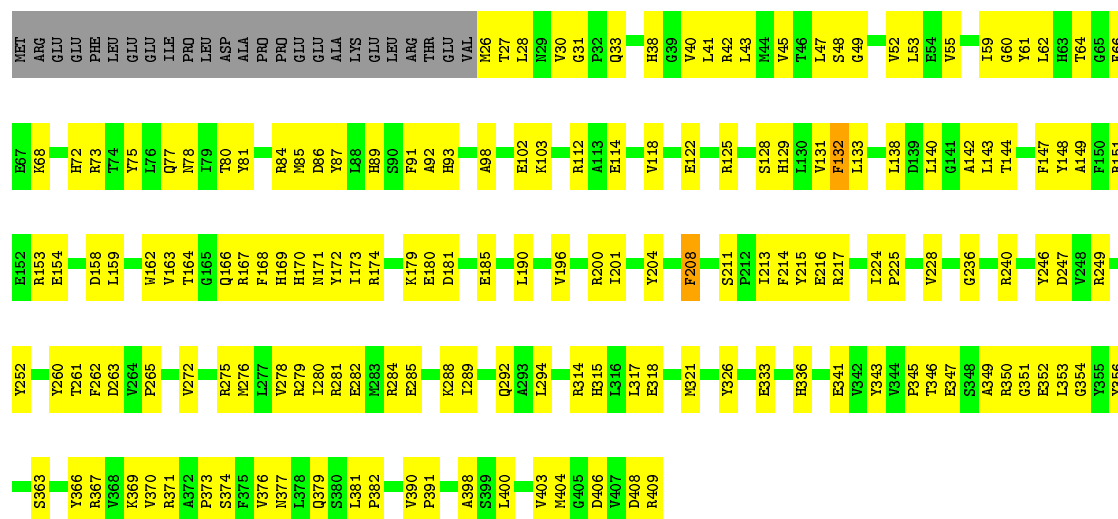
• Molecule 4: NADH-quinone oxidoreductase subunit 4





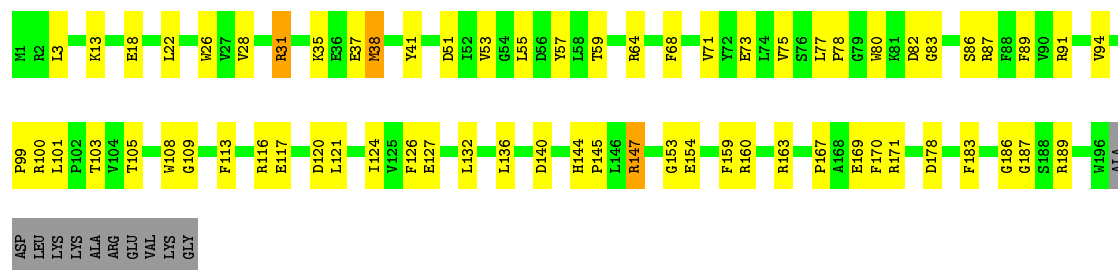
• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain E: 54% 40% 6%



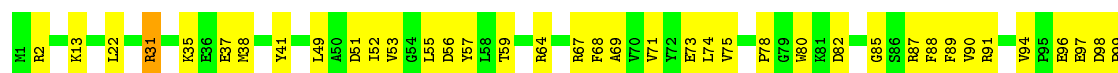
• Molecule 5: NADH-quinone oxidoreductase subunit 5

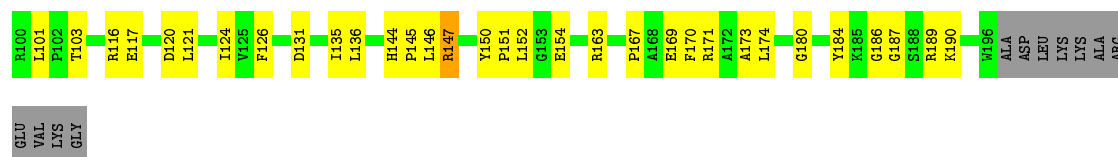
Chain 5: 63% 30% 5%



• Molecule 5: NADH-quinone oxidoreductase subunit 5

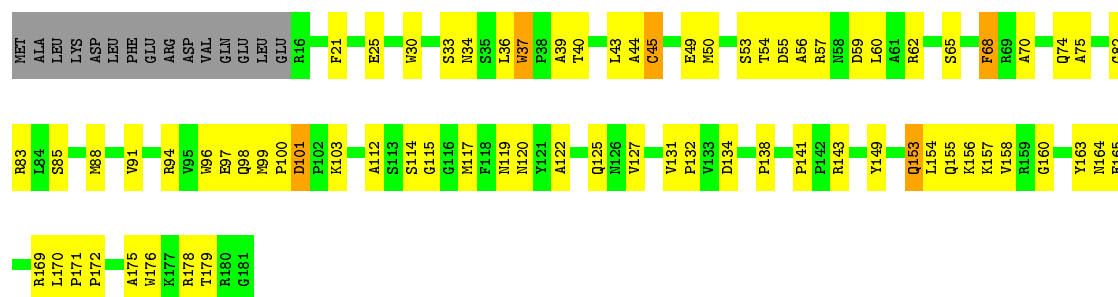
Chain F: 61% 33% 5%





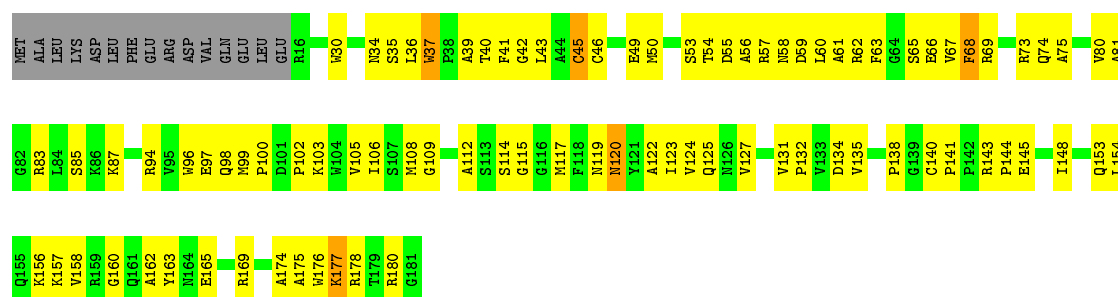
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain 6: 51% 38% 8%



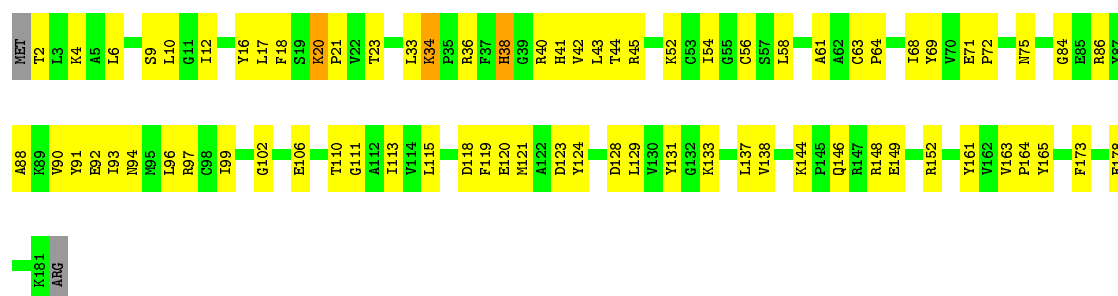
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain G: 43% 46% 8%



• Molecule 7: NADH-quinone oxidoreductase subunit 9

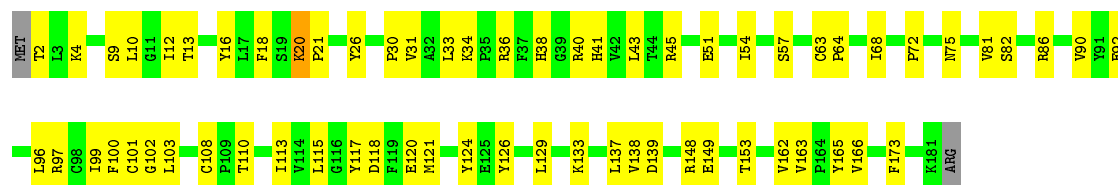
Chain 9: 58% 39% 2%



• Molecule 7: NADH-quinone oxidoreductase subunit 9

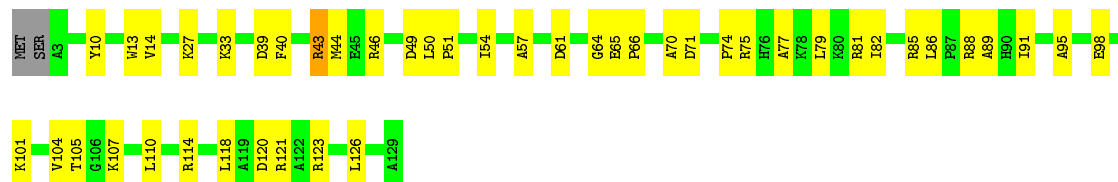
Chain O: 64% 35% 1%





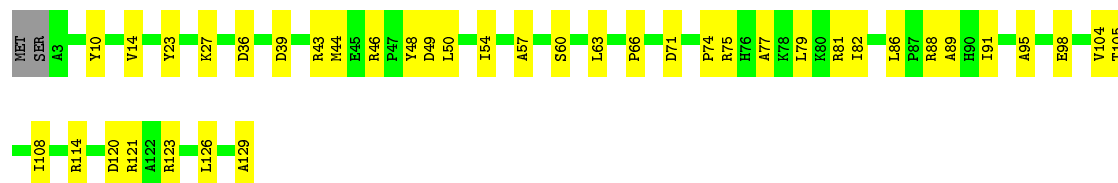
- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7: 64% 34% ..



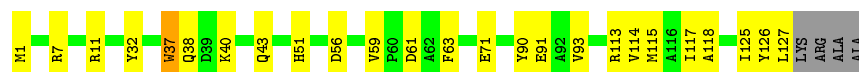
- Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain I: 68% 30% .



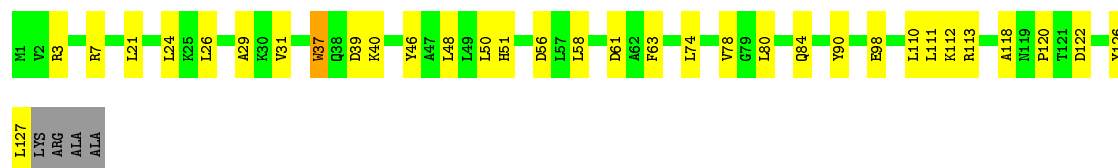
- Molecule 9: NADH-quinone oxidoreductase subunit 16

Chain W: 78% 18% ..



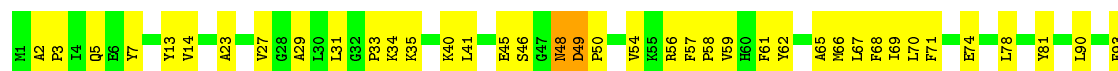
- Molecule 9: NADH-quinone oxidoreductase subunit 16

Chain X: 72% 24% ..



- Molecule 10: NADH-quinone oxidoreductase subunit 7

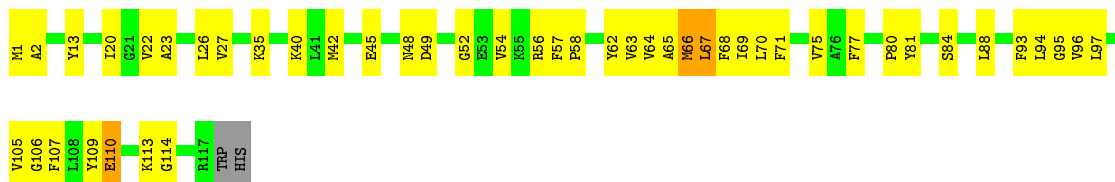
Chain A: 55% 41% ..





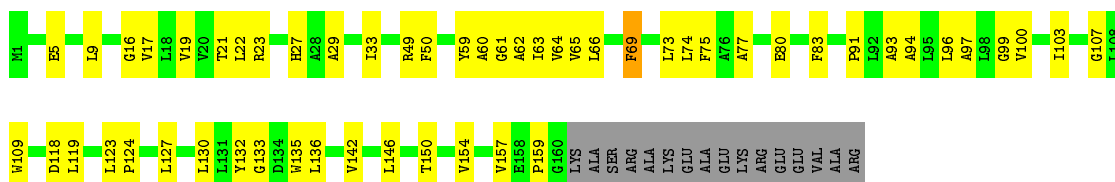
• Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P: 59% 37%



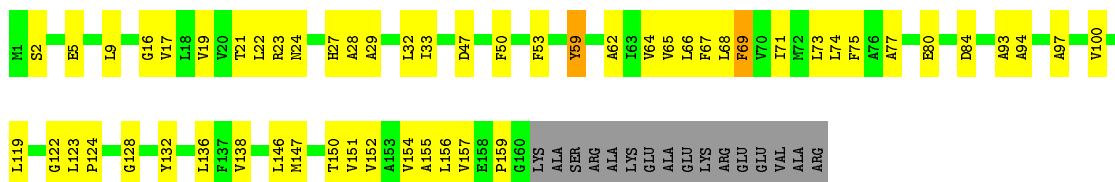
• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J: 60% 30% 9%



• Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R: 60% 30% 9%



• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K: 72% 27%



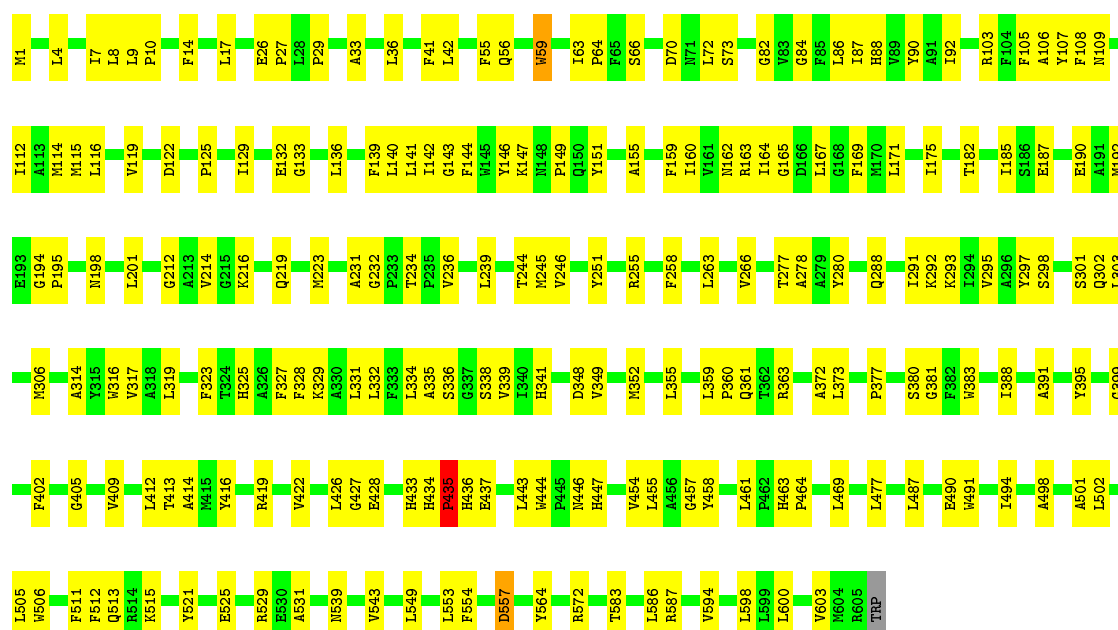
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain S: 77% 22%



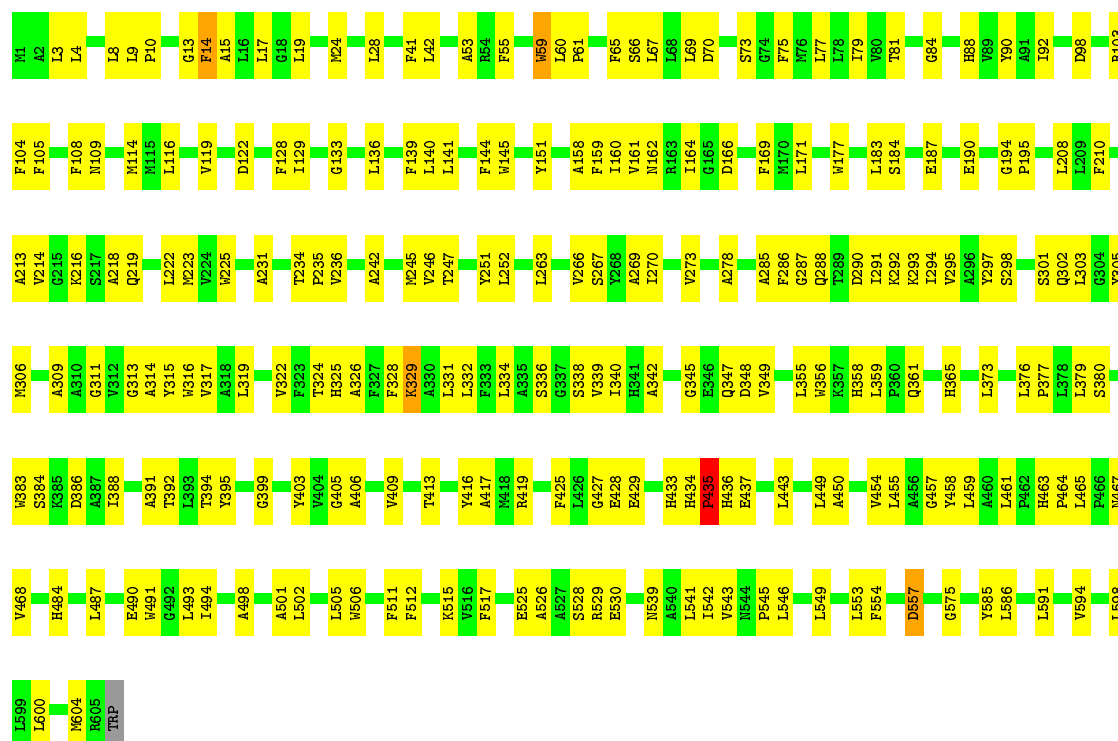
• Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain L:  66% 34%



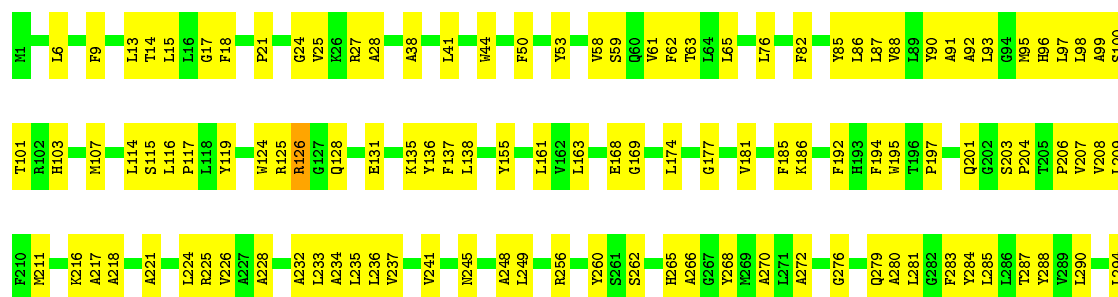
• Molecule 13: NADH-quinone oxidoreductase subunit 12

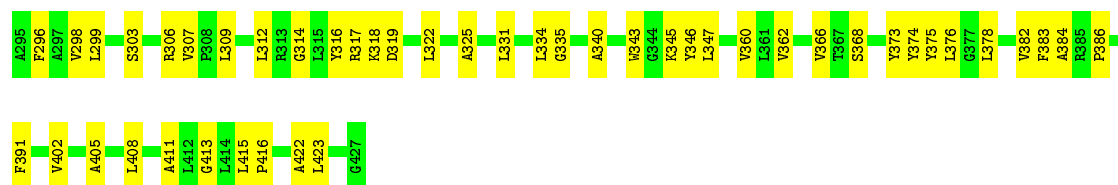
Chain T:  62% 37%



• Molecule 14: NADH-quinone oxidoreductase subunit 13

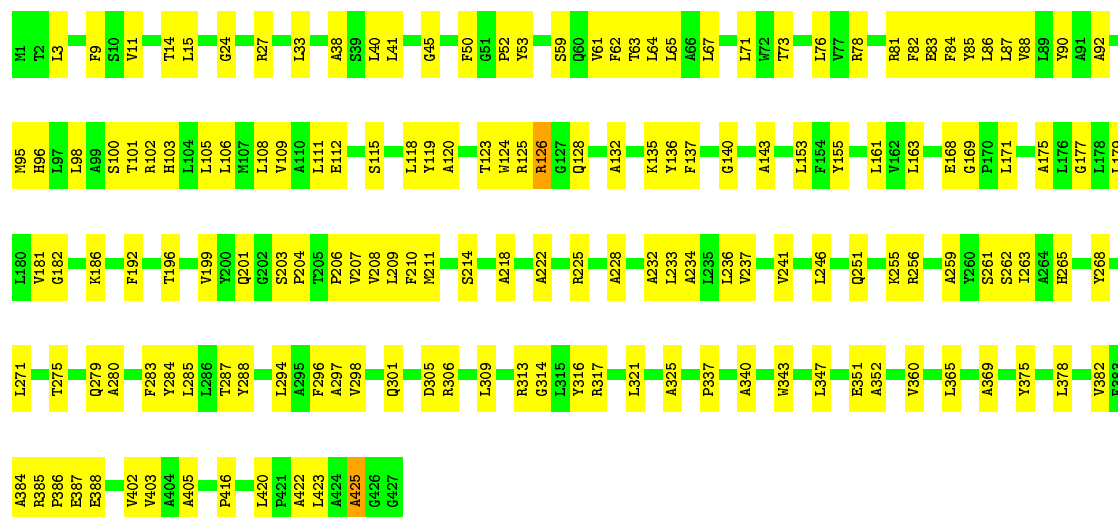
Chain M:  60% 38%





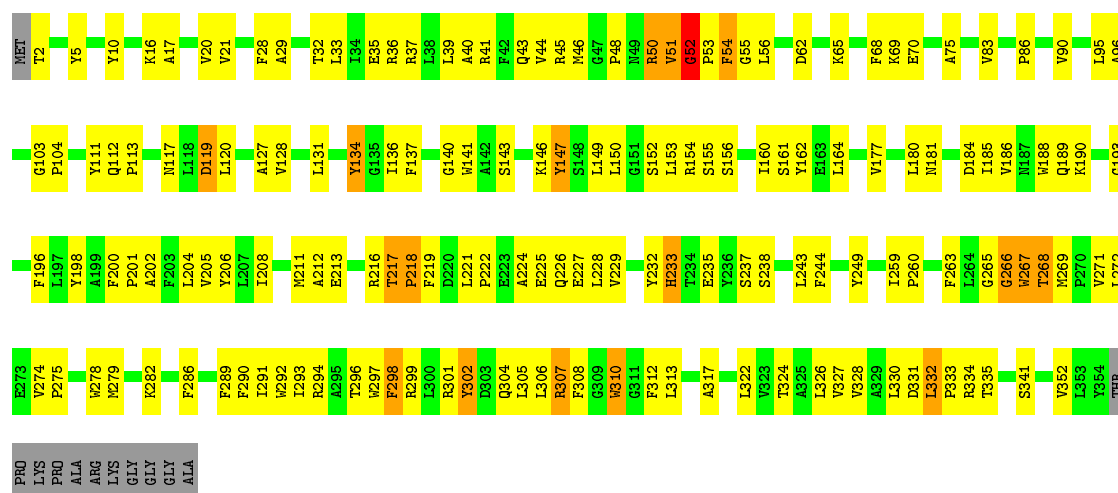
• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain V: 63% 37%



• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain H: 52% 39% 5%



• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q: 51% 43% 2%

L332	P333	T261	Q189	S107	MET
	P334	L262	K190		T2
	T335	L263		Y111	Y5
	Y336	G265	G193	P113	D8
		G266	H194	W114	
	S341	W267	F196		M12
	L348	T268		L119	
		M269	F200	D120	K16
	Y354	T270	P201	G121	A17
	THR	L271		I122	
PRO	L272	L204	L123	V21	
LYS	E273	V205	L125		
PRO	T274			F28	
ALA	T275	L208			
ARG	Y276		V128	K31	
LYS	F280	M211	L131	T32	
GLY	L281	A212		L33	
GLY	K282	E213	Y134	L34	
GLY		A214		E35	
ALA		F286	A215	W141	R36
		L287	R216	A142	R37
		F288	T217	L149	L38
		F289	P218	S143	L39
		T290	F219		A40
		L291	D220	K146	R41
		W292	L221	Y147	F42
		L293	P222	S148	O43
		R294	E223	L149	Y44
		A295	A224	L150	R45
	T296	E225		M46	
	W297	Q226	L153	G47	
	F298	E227	R154	P48	
	R299	L228	S155	N49	
	L300	V229	S156	R50	
	R301	G230	A157	W51	
	D302	G231	S158	G52	
	G303	Y232	L159	P53	
	Q304	H233	T160	F54	
	L305	T234	S161	G55	
	L306	E235	Y162	L56	
	R307	Y236	L163		
		S237	E164	L60	
	W310	S238	G165		
		L239	L166	L64	
	F314	K240	G167	K65	
	P315		L168		
	L316	F244	A169	K69	
	A317		L170		
		Y249		L72	
	W320	L250	V174		
		E251		P86	
	T324	A255	V177	L95	
	A325	S256	S179	A96	
	L326	G257	L180		
	V327	A257	L180	L99	
	V328	L258	L185	L100	
		L259	V195	R101	
	T321	D260			

## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.70 Å 328.00 Å 260.90 Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	29.87 – 3.60	Depositor
% Data completeness (in resolution range)	76.5 (29.87-3.60)	Depositor
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 3.56 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.214 , 0.225	Depositor
Wilson B-factor (Å <sup>2</sup> )	81.1	Xtriage
Anisotropy	0.034	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	0.337 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.490 for -H,-K,H+L	Depositor
Outliers	0 of 137833 reflections	Xtriage
Total number of atoms	74132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, FES, DCQ

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	0.27	0/3506	0.47	1/4745 (0.0%)
1	B	0.26	0/3506	0.48	1/4745 (0.0%)
2	2	0.28	0/1439	0.45	0/1953
2	C	0.27	0/1439	0.47	0/1953
3	3	0.28	0/6035	0.52	2/8185 (0.0%)
3	D	0.28	0/6035	0.50	1/8185 (0.0%)
4	4	0.28	0/3150	0.48	0/4284
4	E	0.28	0/3150	0.48	0/4284
5	5	0.28	0/1656	0.49	0/2246
5	F	0.28	0/1656	0.48	0/2246
6	6	0.30	0/1319	0.53	0/1786
6	G	0.30	0/1319	0.54	0/1786
7	9	0.31	0/1423	0.52	0/1933
7	O	0.31	0/1423	0.51	0/1933
8	7	0.27	0/1059	0.49	0/1429
8	I	0.26	0/1059	0.48	0/1429
9	W	0.27	0/985	0.49	0/1335
9	X	0.26	0/985	0.46	0/1335
10	A	0.29	0/940	0.49	0/1280
10	P	0.30	0/940	0.53	1/1280 (0.1%)
11	J	0.28	0/1206	0.45	0/1649
11	R	0.27	0/1206	0.45	0/1649
12	K	0.28	0/710	0.45	0/962
12	S	0.28	0/710	0.46	0/962
13	L	0.26	0/4741	0.45	0/6460
13	T	0.26	0/4741	0.44	0/6460
14	M	0.27	0/3591	0.47	0/4896
14	U	0.27	0/3591	0.47	0/4896
15	N	0.27	0/3238	0.43	0/4434
15	V	0.27	0/3238	0.42	0/4434
16	H	0.29	0/2935	0.52	0/4014
16	Q	0.29	0/2935	0.51	0/4014



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.28	0/75866	0.48	6/103182 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	9	0	2
7	O	0	2
12	K	0	1
12	S	0	1
13	L	0	1
13	T	0	1
16	H	0	4
16	Q	0	3
All	All	0	15

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	559	ASP	C-N-CA	-6.26	106.06	121.70
10	P	67	LEU	CA-CB-CG	6.00	129.09	115.30
1	1	296	SER	C-N-CA	-5.78	107.25	121.70
3	3	614	LEU	CA-CB-CG	5.54	128.04	115.30
1	B	296	SER	C-N-CA	-5.27	108.53	121.70
3	3	626	PRO	C-N-CA	-5.25	108.58	121.70

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	9	20	LYS	Peptide
7	9	21	PRO	Peptide
16	H	217	THR	Peptide
16	H	266	GLY	Peptide
16	H	267	TRP	Peptide
16	H	52	GLY	Peptide
12	K	50	GLY	Peptide
13	L	435	PRO	Peptide

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Mol	Chain	Res	Type	Group
7	O	20	LYS	Peptide
7	O	21	PRO	Peptide
16	Q	217	THR	Peptide
16	Q	266	GLY	Peptide
16	Q	332	LEU	Peptide
12	S	50	GLY	Peptide
13	T	435	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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	127	0
1	B	3417	0	3389	162	0
2	2	1406	0	1373	49	0
2	C	1406	0	1373	62	0
3	3	5895	0	5931	192	0
3	D	5895	0	5931	193	0
4	4	3067	0	3049	181	0
4	E	3067	0	3049	172	0
5	5	1607	0	1574	66	0
5	F	1607	0	1574	61	0
6	6	1289	0	1298	75	0
6	G	1289	0	1298	88	0
7	9	1388	0	1383	74	0
7	O	1388	0	1383	57	0
8	7	1031	0	1029	38	0
8	I	1031	0	1029	30	0
9	W	967	0	1010	21	0
9	X	967	0	1010	26	0
10	A	910	0	939	59	0
10	P	910	0	939	59	0
11	J	1183	0	1286	61	0
11	R	1183	0	1286	52	0
12	K	703	0	747	26	0
12	S	703	0	747	23	0
13	L	4604	0	4734	153	0
13	T	4604	0	4734	157	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	M	3489	0	3606	136	0
14	U	3489	0	3606	126	0
15	N	3154	0	3343	111	0
15	V	3154	0	3343	114	0
16	H	2838	0	2903	157	0
16	Q	2838	0	2903	165	0
17	1	8	0	0	0	0
17	3	24	0	0	3	0
17	6	8	0	0	1	0
17	9	16	0	0	3	0
17	B	8	0	0	3	0
17	D	24	0	0	2	0
17	G	8	0	0	0	0
17	O	16	0	0	3	0
18	1	31	0	19	9	0
18	B	31	0	19	9	0
19	2	4	0	0	0	0
19	3	4	0	0	1	0
19	C	4	0	0	0	0
19	D	4	0	0	2	0
20	4	23	0	30	4	0
20	E	23	0	30	4	0
All	All	74132	0	75285	2642	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 18.

All (2642) 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)
4:4:162:TRP:CE2	7:9:34:LYS:HD2	1.87	1.09
12:S:28:PHE:CZ	12:S:68:VAL:HA	1.91	1.05
12:S:28:PHE:HZ	12:S:68:VAL:HA	1.16	1.04
4:E:138:LEU:CD1	4:E:143:LEU:HD23	1.89	1.02
7:9:41:HIS:HB3	7:9:113:ILE:HD11	1.45	0.97
4:E:143:LEU:HD21	16:Q:226:GLN:NE2	1.81	0.94
16:H:274:VAL:HG12	16:H:278:TRP:CD1	2.02	0.94
14:M:41:LEU:O	14:M:42:THR:HG22	1.69	0.91
3:3:259:CYS:HG	17:3:803:SF4:FE4	0.88	0.88
1:1:222:GLU:HG3	1:1:251:LEU:HD22	1.52	0.88
3:3:193:GLU:O	3:3:443:ARG:NH2	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:146:LYS:HA	16:Q:149:LEU:HB2	1.54	0.87
4:4:162:TRP:CD2	7:9:34:LYS:HD2	2.11	0.86
4:4:162:TRP:HA	7:9:34:LYS:HG3	1.58	0.85
14:M:69:GLY:O	14:M:73:LEU:HD23	1.76	0.85
6:G:56:ALA:HA	16:Q:45:ARG:HB2	1.59	0.84
13:L:557:ASP:OD1	14:M:211:HIS:NE2	2.10	0.84
16:H:302:TYR:HA	16:H:305:LEU:HB3	1.59	0.84
4:E:138:LEU:HD11	4:E:143:LEU:HD23	1.58	0.84
15:N:294:LEU:HD11	15:N:325:ALA:HB1	1.60	0.84
4:E:138:LEU:HD11	4:E:143:LEU:CD2	2.08	0.83
1:1:288:GLN:NE2	1:1:335:VAL:O	2.12	0.83
16:H:146:LYS:HA	16:H:149:LEU:HB2	1.61	0.83
3:D:259:CYS:HG	17:D:803:SF4:FE4	0.90	0.82
3:D:611:ARG:HA	3:D:624:LEU:O	1.79	0.82
4:E:85:MET:HE1	4:E:370:VAL:HG11	1.61	0.82
4:E:409:ARG:NH2	5:F:117:GLU:OE2	2.13	0.81
14:U:89:ALA:HB1	14:U:91:VAL:HG22	1.61	0.81
15:N:14:THR:HG1	15:N:90:TYR:HH	1.29	0.81
6:6:45:CYS:SG	6:6:83:ARG:NH2	2.55	0.80
14:U:115:LEU:HD13	14:U:163:VAL:HG23	1.63	0.80
14:U:217:PHE:O	14:U:221:ASN:ND2	2.14	0.80
3:3:286:ASN:ND2	3:3:289:TRP:O	2.14	0.80
4:4:341:GLU:OE1	5:5:91:ARG:NH2	2.15	0.80
1:1:92:ASN:ND2	18:1:502:FMN:O3'	2.15	0.79
4:4:128:SER:OG	4:4:350:ARG:NH2	2.15	0.79
6:6:149:TYR:O	6:6:153:GLN:NE2	2.15	0.79
15:N:280:ALA:HB1	15:N:347:LEU:HB3	1.64	0.79
15:V:73:THR:HG21	15:V:210:PHE:HB2	1.64	0.79
5:5:13:LYS:NZ	5:5:37:GLU:OE2	2.16	0.79
1:B:395:GLU:OE2	1:B:408:TRP:NE1	2.16	0.79
14:M:89:ALA:HB1	14:M:91:VAL:HG22	1.63	0.79
3:D:455:ARG:HH21	3:D:750:ARG:HH21	1.31	0.79
13:T:3:LEU:HD23	13:T:55:PHE:HB2	1.64	0.79
3:3:614:LEU:O	3:3:621:VAL:HA	1.82	0.78
13:L:278:ALA:HA	13:L:301:SER:HA	1.65	0.78
14:U:109:LEU:HD21	14:U:236:VAL:HG21	1.65	0.78
1:1:190:ASN:ND2	1:1:198:ASN:O	2.17	0.78
3:3:559:ASP:OD2	3:3:686:LYS:NZ	2.16	0.78
4:4:68:LYS:NZ	5:5:145:PRO:O	2.15	0.78
16:Q:327:VAL:O	16:Q:331:ASP:N	2.17	0.78
6:G:114:SER:HB2	7:O:97:ARG:HE	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ILE:HA	1:B:332:PRO:HA	1.66	0.78
4:E:200:ARG:NH1	7:O:16:TYR:OH	2.16	0.78
16:H:177:VAL:HG21	16:H:185:ILE:HG23	1.66	0.78
16:Q:189:GLN:NE2	16:Q:264:LEU:O	2.16	0.78
1:1:16:THR:HG21	1:1:229:PRO:HB3	1.66	0.77
16:Q:158:SER:HA	16:Q:306:LEU:HD21	1.66	0.77
14:U:124:ALA:HB2	15:V:337:PRO:HB2	1.66	0.77
3:D:614:LEU:O	3:D:621:VAL:HA	1.85	0.77
4:4:222:GLY:HA3	4:4:275:ARG:HH22	1.48	0.77
4:E:144:THR:HG22	4:E:148:TYR:HE1	1.47	0.77
6:G:62:ARG:HD2	16:Q:50:ARG:HH21	1.49	0.77
11:R:23:ARG:HG2	11:R:80:GLU:HG2	1.66	0.77
16:Q:292:TRP:O	16:Q:296:THR:OG1	2.03	0.76
1:B:63:ARG:H	1:B:65:ARG:HH21	1.32	0.76
6:G:160:GLY:O	6:G:169:ARG:NH1	2.17	0.76
14:M:208:PHE:O	14:M:211:HIS:ND1	2.16	0.76
14:M:217:PHE:O	14:M:221:ASN:ND2	2.18	0.76
4:E:166:GLN:NE2	7:O:100:PHE:O	2.18	0.76
15:V:280:ALA:HB1	15:V:347:LEU:HB3	1.67	0.76
3:3:538:ALA:HB3	3:3:541:ALA:HB2	1.68	0.76
13:T:340:ILE:O	13:T:345:GLY:N	2.19	0.76
1:1:220:ASN:ND2	18:1:502:FMN:O2	2.18	0.76
4:E:185:GLU:OE2	7:O:165:TYR:OH	2.03	0.76
1:1:287:ILE:HA	1:1:332:PRO:HA	1.67	0.76
2:2:132:PRO:HG2	2:2:145:VAL:HB	1.67	0.76
1:B:92:ASN:ND2	18:B:502:FMN:O3'	2.19	0.76
16:Q:291:ILE:HA	16:Q:294:ARG:HG3	1.66	0.76
4:4:26:MET:N	4:4:47:LEU:O	2.18	0.76
4:E:201:ILE:HG21	4:E:284:ARG:HG3	1.67	0.76
4:E:281:ARG:HD3	4:E:284:ARG:HH12	1.51	0.76
3:D:401:ASP:OD2	3:D:454:TYR:OH	2.04	0.75
16:H:216:ARG:HD2	16:H:294:ARG:HA	1.68	0.75
14:U:348:ALA:HB2	14:U:414:PHE:HB3	1.68	0.75
4:4:162:TRP:CA	7:9:34:LYS:HG3	2.16	0.75
16:H:265:GLY:O	16:H:282:LYS:NZ	2.18	0.75
16:Q:215:ALA:O	16:Q:294:ARG:NH1	2.16	0.75
14:U:22:ARG:HD2	14:U:23:ALA:N	2.02	0.75
1:B:88:TYR:HB2	1:B:216:THR:HG22	1.67	0.75
6:G:102:PRO:O	16:Q:69:LYS:NZ	2.19	0.75
12:S:64:ALA:O	12:S:68:VAL:HG23	1.86	0.75
16:H:219:PHE:HB3	16:H:299:ARG:HG2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:62:ARG:HB3	16:Q:50:ARG:HB2	1.68	0.75
14:U:268:ALA:HA	14:U:291:SER:HA	1.69	0.75
5:5:35:LYS:NZ	5:5:103:THR:O	2.20	0.75
9:X:37:TRP:HD1	9:X:40:LYS:HB2	1.51	0.75
5:5:144:HIS:HB2	5:5:147:ARG:HD3	1.69	0.74
3:D:297:GLY:O	3:D:300:TRP:NE1	2.16	0.74
1:1:437:TRP:HB3	2:2:92:GLY:HA3	1.67	0.74
7:O:45:ARG:NH2	7:O:139:ASP:OD2	2.17	0.74
16:Q:302:TYR:HA	16:Q:305:LEU:HB3	1.68	0.74
1:1:131:TYR:OH	2:2:17:LYS:O	2.04	0.74
3:D:286:ASN:ND2	3:D:289:TRP:O	2.20	0.74
9:X:51:HIS:ND1	9:X:56:ASP:OD1	2.21	0.74
1:B:354:GLY:O	1:B:360:ARG:NH1	2.20	0.74
16:Q:219:PHE:HB3	16:Q:299:ARG:HG2	1.69	0.74
15:N:228:ALA:HB1	15:N:233:LEU:HD11	1.69	0.74
14:M:12:PHE:HB3	14:M:100:LEU:HD13	1.70	0.74
4:4:169:HIS:HD2	6:6:141:PRO:HD3	1.52	0.74
16:H:332:LEU:HB2	16:H:333:PRO:HD3	1.68	0.73
14:M:52:GLN:HE22	14:M:176:LEU:HD11	1.53	0.73
14:M:22:ARG:HD2	14:M:23:ALA:N	2.02	0.73
4:4:144:THR:HG22	4:4:148:TYR:HE1	1.54	0.73
1:B:353:CYS:HG	17:B:501:SF4:FE4	1.04	0.73
4:E:240:ARG:NH1	4:E:282:GLU:OE2	2.20	0.73
8:I:63:LEU:HD13	8:I:129:ALA:HB3	1.69	0.73
4:E:314:ARG:NH2	8:I:44:MET:SD	2.62	0.73
4:4:240:ARG:NH1	4:4:282:GLU:OE2	2.22	0.73
1:B:343:ASN:HB2	2:C:89:LYS:HZ2	1.51	0.73
4:E:45:VAL:HG13	4:E:55:VAL:HG22	1.69	0.73
13:L:458:TYR:HB3	13:L:461:LEU:HD11	1.69	0.73
14:M:363:LEU:HD22	14:M:368:LEU:HD13	1.71	0.73
14:M:348:ALA:HB2	14:M:414:PHE:HB3	1.69	0.73
6:G:74:GLN:HE22	16:Q:233:HIS:HB2	1.54	0.73
13:T:458:TYR:HB3	13:T:461:LEU:HD11	1.71	0.73
14:M:122:PHE:O	14:M:234:TYR:OH	2.04	0.73
8:7:120:ASP:OD1	8:7:123:ARG:NH1	2.22	0.73
2:C:132:PRO:HG2	2:C:145:VAL:HB	1.71	0.73
6:G:30:TRP:O	6:G:34:ASN:ND2	2.22	0.73
7:O:75:ASN:ND2	7:O:82:SER:OG	2.22	0.73
1:1:79:MET:SD	1:1:217:THR:OG1	2.46	0.73
3:D:722:THR:HG21	3:D:756:GLY:H	1.54	0.72
10:P:70:LEU:HD13	11:R:150:THR:HG22	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:26:TYR:OH	7:O:120:GLU:OE2	2.05	0.72
4:4:409:ARG:NH2	5:5:117:GLU:OE2	2.22	0.72
3:D:180:ARG:NH1	3:D:233:GLY:O	2.23	0.72
3:3:259:CYS:SG	17:3:803:SF4:FE4	1.81	0.72
14:U:346:GLY:HA3	14:U:418:GLY:HA2	1.70	0.72
2:2:110:GLU:HA	8:7:121:ARG:HH12	1.53	0.72
13:L:298:SER:OG	13:L:329:LYS:NZ	2.16	0.72
4:E:143:LEU:CD2	16:Q:226:GLN:NE2	2.53	0.72
4:E:143:LEU:HD21	16:Q:226:GLN:HE22	1.55	0.72
6:G:163:TYR:O	7:O:148:ARG:NH2	2.22	0.72
8:I:120:ASP:OD1	8:I:123:ARG:NH1	2.23	0.72
16:H:292:TRP:O	16:H:296:THR:OG1	2.06	0.72
13:L:182:THR:HB	13:L:187:GLU:HG3	1.70	0.72
2:2:109:GLY:O	8:7:121:ARG:NH2	2.21	0.71
16:H:43:GLN:O	16:H:45:ARG:N	2.23	0.71
11:R:50:PHE:HB2	11:R:124:PRO:HD3	1.71	0.71
16:H:52:GLY:HA3	16:H:55:GLY:H	1.53	0.71
15:V:14:THR:HA	15:V:86:LEU:HD21	1.71	0.71
4:4:236:GLY:HA2	4:4:351:GLY:HA3	1.72	0.71
6:G:119:ASN:HA	6:G:125:GLN:HE22	1.54	0.71
11:R:47:ASP:O	11:R:122:GLY:N	2.23	0.71
15:N:314:GLY:HA3	15:N:386:PRO:HG3	1.72	0.71
10:P:109:TYR:OH	10:P:113:LYS:NZ	2.20	0.71
12:S:28:PHE:CE1	12:S:68:VAL:HG22	2.26	0.71
1:B:16:THR:HG21	1:B:229:PRO:HB3	1.71	0.71
4:E:341:GLU:OE2	5:F:57:TYR:OH	2.08	0.71
16:H:226:GLN:HB2	16:H:299:ARG:HH22	1.54	0.71
14:U:54:PRO:HA	14:U:62:TYR:HD1	1.54	0.71
3:3:98:ASP:OD1	3:3:101:ARG:NH2	2.24	0.71
6:6:57:ARG:HA	7:9:23:THR:HA	1.72	0.71
4:E:240:ARG:NH2	4:E:347:GLU:OE2	2.23	0.71
11:J:49:ARG:NH1	16:H:119:ASP:OD2	2.23	0.71
10:A:35:LYS:O	10:A:40:LYS:NZ	2.23	0.71
6:G:175:ALA:O	6:G:180:ARG:NH2	2.22	0.71
12:K:94:ARG:NH1	13:L:583:THR:O	2.23	0.71
1:B:17:LEU:HD12	1:B:251:LEU:HD11	1.72	0.71
1:1:92:ASN:O	1:1:220:ASN:ND2	2.25	0.70
6:6:62:ARG:HB3	16:H:50:ARG:HB2	1.74	0.70
3:D:259:CYS:SG	17:D:803:SF4:FE4	1.84	0.70
4:E:154:GLU:HB3	6:G:57:ARG:HH11	1.56	0.70
8:7:54:ILE:HD11	8:7:57:ALA:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:327:VAL:O	16:H:331:ASP:N	2.18	0.70
3:3:40:SER:O	3:3:189:ARG:NE	2.22	0.70
3:D:193:GLU:O	3:D:443:ARG:NH2	2.22	0.70
14:M:203:ILE:HG13	14:M:210:LEU:HB3	1.73	0.70
11:R:157:VAL:HG12	11:R:159:PRO:HD3	1.74	0.70
3:3:701:ALA:N	3:3:763:LEU:O	2.21	0.70
13:T:328:PHE:O	13:T:332:LEU:HD12	1.92	0.70
3:3:117:LEU:H	4:4:321:MET:HE3	1.57	0.70
13:T:340:ILE:HB	13:T:345:GLY:HA2	1.73	0.70
8:I:54:ILE:HD11	8:I:57:ALA:HB2	1.71	0.70
13:L:426:LEU:HD23	13:L:513:GLN:HE21	1.56	0.70
15:V:317:ARG:NH1	15:V:384:ALA:O	2.25	0.70
3:3:203:ILE:HG22	3:3:204:GLU:HG3	1.74	0.70
4:4:240:ARG:NH2	4:4:347:GLU:OE2	2.22	0.70
16:Q:43:GLN:O	16:Q:45:ARG:N	2.24	0.70
3:3:584:VAL:HG12	3:3:600:VAL:HB	1.73	0.70
15:V:314:GLY:HA3	15:V:386:PRO:HG3	1.74	0.70
3:D:194:VAL:HG12	3:D:411:LEU:HD22	1.74	0.69
13:L:167:LEU:HD21	14:M:396:PHE:HB3	1.74	0.69
15:V:136:TYR:OH	15:V:186:LYS:NZ	2.25	0.69
3:3:48:CYS:SG	3:3:83:CYS:N	2.65	0.69
1:B:192:LEU:HD22	1:B:211:LEU:HD21	1.74	0.69
3:3:31:PRO:HB2	3:3:47:MET:HB3	1.75	0.69
3:3:609:GLU:HA	3:3:627:ALA:H	1.57	0.69
1:1:425:ALA:O	1:1:428:LYS:NZ	2.22	0.69
13:T:278:ALA:HA	13:T:301:SER:HA	1.73	0.69
3:3:261:VAL:HG21	3:3:408:ILE:HG12	1.75	0.69
1:B:220:ASN:ND2	18:B:502:FMN:O2	2.25	0.69
4:E:26:MET:N	4:E:47:LEU:O	2.25	0.69
5:F:144:HIS:HB2	5:F:147:ARG:HD3	1.74	0.69
3:3:373:GLY:HA3	3:3:538:ALA:HB2	1.75	0.69
3:D:584:VAL:HG12	3:D:600:VAL:HB	1.75	0.69
14:M:2:VAL:HB	14:M:67:LEU:HD11	1.75	0.69
10:A:65:ALA:HB3	11:J:66:LEU:HD13	1.75	0.69
1:B:131:TYR:OH	2:C:17:LYS:O	2.10	0.68
4:E:143:LEU:CD2	16:Q:226:GLN:HE22	2.05	0.68
12:S:28:PHE:HE1	12:S:68:VAL:HG22	1.56	0.68
3:D:117:LEU:HD23	4:E:321:MET:HE2	1.75	0.68
16:H:50:ARG:O	16:H:52:GLY:N	2.21	0.68
9:W:51:HIS:ND1	9:W:56:ASP:OD1	2.26	0.68
10:A:113:LYS:HD3	11:J:154:VAL:HG11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:682:GLU:OE1	3:D:684:ARG:NH2	2.26	0.68
12:K:28:PHE:CZ	12:K:68:VAL:HA	2.28	0.68
1:1:312:SER:OG	1:1:315:HIS:ND1	2.22	0.68
11:J:130:LEU:CD1	12:K:51:LEU:CD2	2.70	0.68
15:N:13:LEU:HD22	15:N:25:VAL:HG13	1.74	0.68
15:N:228:ALA:HB1	15:N:233:LEU:CD1	2.23	0.68
9:X:98:GLU:OE2	9:X:113:ARG:NH1	2.26	0.68
3:3:713:ARG:HH21	3:3:746:ARG:HH21	1.40	0.68
3:3:149:LEU:HD11	4:4:304:ASP:HA	1.76	0.68
3:D:435:LEU:O	3:D:438:LYS:NZ	2.27	0.68
3:D:635:GLU:OE2	9:X:7:ARG:NH1	2.26	0.68
13:T:213:ALA:HB2	13:T:252:LEU:HD23	1.76	0.68
13:T:70:ASP:H	13:T:73:SER:HB2	1.58	0.68
14:U:56:LEU:HB2	14:U:61:VAL:HB	1.75	0.68
4:E:49:GLY:HA2	10:P:58:PRO:HD3	1.76	0.68
1:B:79:MET:SD	1:B:217:THR:OG1	2.51	0.68
16:H:291:ILE:HA	16:H:294:ARG:HG3	1.74	0.68
11:R:152:VAL:HG13	15:V:120:ALA:HB2	1.73	0.68
5:5:73:GLU:OE2	5:5:87:ARG:NH1	2.27	0.68
3:3:169:PRO:HA	3:3:175:ILE:HA	1.76	0.68
4:4:163:VAL:HG13	4:4:164:THR:HG23	1.76	0.68
3:D:195:PRO:O	3:D:410:HIS:NE2	2.27	0.68
16:H:143:SER:HB2	16:H:235:GLU:HG3	1.76	0.68
1:B:260:ARG:NH1	1:B:279:TRP:O	2.25	0.67
3:D:30:VAL:O	5:F:184:TYR:OH	2.12	0.67
13:T:355:LEU:HB3	13:T:359:LEU:HD12	1.76	0.67
13:L:132:GLU:OE2	13:L:163:ARG:NH1	2.27	0.67
13:L:355:LEU:HB3	13:L:359:LEU:HD12	1.76	0.67
14:M:115:LEU:HD13	14:M:163:VAL:HG23	1.75	0.67
14:M:115:LEU:HD12	14:M:180:LEU:HD13	1.76	0.67
13:L:572:ARG:NH2	15:N:373:TYR:OH	2.25	0.67
15:N:38:ALA:HA	15:N:41:LEU:HD12	1.77	0.67
3:3:551:PRO:HB2	3:3:555:GLY:HA2	1.75	0.67
6:6:138:PRO:HG2	7:9:121:MET:HG3	1.76	0.67
1:B:353:CYS:SG	17:B:501:SF4:FE4	1.86	0.67
1:B:259:LYS:NZ	2:C:178:GLU:OE2	2.26	0.67
5:F:35:LYS:NZ	5:F:103:THR:O	2.25	0.67
13:L:147:LYS:NZ	14:M:349:GLN:OE1	2.26	0.67
15:V:53:TYR:HA	15:V:101:THR:HG22	1.76	0.67
16:H:205:VAL:HG21	16:H:317:ALA:HB2	1.76	0.67
15:N:290:LEU:HD11	15:N:408:LEU:HD23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:168:GLU:HG2	15:V:169:GLY:H	1.59	0.67
10:P:35:LYS:O	10:P:40:LYS:NZ	2.24	0.67
1:1:165:THR:HG23	1:1:167:PHE:H	1.58	0.67
1:1:354:GLY:O	1:1:360:ARG:NH1	2.27	0.67
4:4:33:GLN:HE22	20:4:501:DCQ:H8A	1.59	0.67
14:U:208:PHE:O	14:U:211:HIS:ND1	2.27	0.67
4:4:205:GLU:OE1	4:4:284:ARG:NH2	2.27	0.67
3:D:186:ARG:HD3	3:D:229:ILE:HG22	1.75	0.67
10:P:95:GLY:HA3	11:R:136:LEU:HD11	1.77	0.67
10:A:41:LEU:HD22	16:H:75:ALA:H	1.59	0.67
6:G:143:ARG:NE	6:G:145:GLU:OE1	2.28	0.66
8:I:23:TYR:OH	8:I:123:ARG:NH1	2.24	0.66
7:9:75:ASN:ND2	7:9:84:GLY:O	2.28	0.66
1:B:288:GLN:NE2	1:B:335:VAL:O	2.28	0.66
3:D:474:ARG:O	3:D:520:ARG:NH1	2.27	0.66
3:D:587:LEU:O	3:D:604:ALA:N	2.28	0.66
4:E:138:LEU:CD1	4:E:143:LEU:CD2	2.66	0.66
6:6:62:ARG:HG2	16:H:48:PRO:HA	1.77	0.66
2:2:42:ARG:HB2	2:2:45:ARG:HG2	1.78	0.66
4:4:194:LEU:HD21	4:4:290:ILE:HG22	1.78	0.66
15:N:44:TRP:HE1	15:N:422:ALA:HB1	1.58	0.66
13:T:419:ARG:NH2	13:T:525:GLU:OE2	2.27	0.66
14:U:157:LEU:HB3	15:V:365:LEU:HB3	1.77	0.66
6:6:50:MET:O	6:6:53:SER:OG	2.13	0.66
3:D:414:SER:OG	3:D:443:ARG:NH2	2.28	0.66
13:L:70:ASP:H	13:L:73:SER:HB2	1.61	0.66
1:B:165:THR:HG23	1:B:167:PHE:H	1.61	0.66
10:A:34:LYS:N	16:H:70:GLU:OE1	2.27	0.66
15:N:309:LEU:HD22	15:N:378:LEU:HD11	1.78	0.66
13:T:328:PHE:O	13:T:332:LEU:CD1	2.44	0.66
4:4:147:PHE:HE2	16:H:45:ARG:HD3	1.60	0.66
15:N:128:GLN:OE1	15:N:306:ARG:NH2	2.29	0.66
2:2:77:LYS:H	2:2:116:LEU:HA	1.59	0.66
4:4:87:TYR:HB3	6:6:45:CYS:HB3	1.77	0.66
10:A:62:TYR:CD2	11:J:66:LEU:HD11	2.31	0.66
16:H:212:ALA:HA	16:H:218:PRO:HG3	1.77	0.66
13:T:214:VAL:HG13	13:T:219:GLN:HB2	1.77	0.66
13:T:359:LEU:HD23	13:T:437:GLU:HB3	1.79	0.66
3:D:723:ALA:HA	3:D:728:LEU:HD12	1.78	0.65
4:E:208:PHE:HE2	4:E:214:PHE:CZ	2.14	0.65
13:T:151:TYR:HB3	13:T:231:ALA:HB1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:94:ASP:OD2	3:D:97:SER:OG	2.10	0.65
8:I:49:ASP:OD1	8:I:75:ARG:NE	2.28	0.65
16:Q:332:LEU:HB2	16:Q:333:PRO:HD3	1.78	0.65
7:9:40:ARG:NH2	7:9:118:ASP:OD1	2.29	0.65
3:D:373:GLY:HA3	3:D:538:ALA:HB2	1.77	0.65
11:J:157:VAL:HG12	11:J:159:PRO:HD3	1.79	0.65
13:L:325:HIS:NE2	13:L:329:LYS:HG3	2.11	0.65
15:N:168:GLU:HG2	15:N:169:GLY:H	1.61	0.65
14:U:332:LEU:O	14:U:336:THR:OG1	2.08	0.65
3:3:576:ALA:O	3:3:580:LYS:NZ	2.28	0.65
13:L:63:ILE:HG21	13:L:125:PRO:HG2	1.77	0.65
3:3:185:LYS:HB3	3:3:189:ARG:HH11	1.61	0.65
6:6:119:ASN:HA	6:6:125:GLN:HE22	1.61	0.65
13:L:422:VAL:HG22	13:L:426:LEU:HD22	1.77	0.65
15:N:136:TYR:OH	15:N:186:LYS:NZ	2.30	0.65
11:R:22:LEU:O	12:S:21:ARG:NH2	2.29	0.65
15:V:294:LEU:HD11	15:V:325:ALA:HB1	1.79	0.65
1:1:288:GLN:HE21	1:1:331:ILE:HG22	1.62	0.65
3:3:175:ILE:O	3:3:235:LEU:HA	1.96	0.65
7:9:43:LEU:HB2	7:9:137:LEU:HD12	1.78	0.65
4:E:163:VAL:HG13	4:E:164:THR:HG23	1.79	0.65
5:F:68:PHE:HB2	5:F:94:VAL:HB	1.77	0.65
6:G:106:ILE:HD11	6:G:154:LEU:HD22	1.79	0.65
13:L:105:PHE:O	13:L:109:ASN:ND2	2.30	0.65
11:J:130:LEU:HD12	12:K:51:LEU:CD2	2.26	0.65
13:T:334:LEU:HD12	13:T:449:LEU:HD11	1.78	0.65
13:L:214:VAL:HG13	13:L:219:GLN:HB2	1.79	0.65
4:4:161:GLU:HG2	7:9:34:LYS:HB2	1.79	0.65
1:B:380:GLU:N	1:B:383:ASP:OD2	2.30	0.65
7:O:117:TYR:HE2	7:O:166:VAL:HG12	1.62	0.65
3:D:690:GLY:HA2	3:D:770:ARG:HB3	1.79	0.64
8:I:44:MET:HE2	8:I:46:ARG:HH22	1.62	0.64
15:N:262:SER:OG	15:N:288:TYR:OH	2.14	0.64
14:U:151:PHE:HD1	14:U:203:ILE:HD11	1.61	0.64
3:D:233:GLY:HA2	3:D:236:LEU:HD21	1.79	0.64
3:D:621:VAL:HG23	3:D:672:ALA:HA	1.79	0.64
16:Q:216:ARG:HB2	16:Q:294:ARG:HD2	1.79	0.64
3:3:228:ASP:OD2	3:3:295:ARG:NH2	2.28	0.64
4:4:84:ARG:O	6:6:83:ARG:NH2	2.28	0.64
16:Q:267:TRP:CG	16:Q:268:THR:N	2.66	0.64
13:T:314:ALA:HB1	13:T:317:VAL:HB	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:288:GLN:NE2	13:T:528:SER:O	2.31	0.64
3:3:285:VAL:HG13	3:3:286:ASN:H	1.61	0.64
3:D:34:CYS:O	3:D:189:ARG:NH2	2.30	0.64
4:E:208:PHE:CE2	4:E:214:PHE:CZ	2.86	0.64
14:U:12:PHE:HB3	14:U:100:LEU:HD13	1.79	0.64
1:1:104:ARG:NH1	1:1:108:GLU:OE2	2.31	0.64
1:1:5:ILE:H	1:1:12:ARG:HH22	1.45	0.64
4:4:81:TYR:OH	6:6:117:MET:O	2.12	0.64
7:9:71:GLU:HB2	7:9:90:VAL:HB	1.79	0.64
3:D:125:GLY:HA2	3:D:245:ARG:HH21	1.63	0.64
4:4:200:ARG:NH1	7:9:16:TYR:OH	2.31	0.64
4:E:138:LEU:HD12	4:E:143:LEU:HD23	1.77	0.64
13:T:246:VAL:HB	13:T:303:LEU:HD21	1.78	0.64
1:B:190:ASN:ND2	1:B:198:ASN:O	2.30	0.64
5:F:31:ARG:NH2	5:F:98:ASP:OD2	2.31	0.64
16:H:211:MET:HG3	16:H:218:PRO:HD3	1.80	0.64
8:I:74:PRO:HG2	8:I:77:ALA:HB2	1.78	0.64
8:I:98:GLU:HG2	8:I:104:VAL:HG21	1.79	0.64
4:4:40:VAL:HG21	6:6:88:MET:HE2	1.80	0.64
16:H:267:TRP:CG	16:H:268:THR:N	2.66	0.64
10:A:100:THR:HG21	16:H:322:LEU:HD11	1.79	0.64
8:7:88:ARG:HH21	8:7:126:LEU:HB3	1.63	0.63
14:U:235:LYS:HD3	14:U:293:MET:HG3	1.80	0.63
16:H:141:TRP:HE3	16:H:149:LEU:HD21	1.63	0.63
1:B:425:ALA:O	1:B:428:LYS:NZ	2.30	0.63
7:9:10:LEU:HD12	16:H:296:THR:HG21	1.81	0.63
6:G:50:MET:O	6:G:53:SER:OG	2.15	0.63
13:L:151:TYR:HB3	13:L:231:ALA:HB1	1.81	0.63
11:R:119:LEU:HD21	12:S:47:ARG:HA	1.81	0.63
13:T:305:TYR:OH	13:T:406:ALA:O	2.14	0.63
15:V:261:SER:HG	15:V:375:TYR:HH	1.44	0.63
15:V:343:TRP:CE2	15:V:416:PRO:HG3	2.34	0.63
3:D:226:ILE:HD12	3:D:235:LEU:HD13	1.80	0.63
11:R:64:VAL:HG13	16:Q:134:TYR:OH	1.97	0.63
10:P:62:TYR:HD2	11:R:66:LEU:HD11	1.64	0.63
4:E:173:ILE:O	4:E:174:ARG:NH1	2.31	0.63
11:J:130:LEU:HD11	12:K:51:LEU:HD22	1.81	0.63
13:T:105:PHE:O	13:T:109:ASN:ND2	2.32	0.63
15:V:103:HIS:CE1	15:V:161:LEU:HB2	2.34	0.63
4:4:333:GLU:OE2	4:4:336:HIS:NE2	2.32	0.63
6:G:58:ASN:ND2	6:G:145:GLU:OE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:359:LEU:HD23	13:L:437:GLU:HB3	1.81	0.63
15:N:234:ALA:HB1	15:N:360:VAL:HG21	1.80	0.63
11:R:64:VAL:HA	11:R:67:PHE:HB2	1.81	0.63
15:V:92:ALA:HA	15:V:95:MET:HE2	1.79	0.63
1:1:184:GLU:OE1	1:1:186:THR:OG1	2.13	0.63
2:2:24:ARG:HH21	2:2:59:GLU:HB3	1.64	0.63
6:6:53:SER:O	6:6:60:LEU:N	2.31	0.63
6:6:94:ARG:O	6:6:98:GLN:N	2.32	0.63
3:D:203:ILE:HG22	3:D:204:GLU:HG3	1.80	0.63
1:B:293:GLY:O	1:B:327:GLY:N	2.31	0.62
4:E:143:LEU:HD21	16:Q:226:GLN:HE21	1.63	0.62
11:J:130:LEU:CD1	12:K:51:LEU:HD23	2.29	0.62
14:M:268:ALA:HA	14:M:291:SER:HA	1.79	0.62
7:O:18:PHE:O	7:O:20:LYS:NZ	2.32	0.62
4:4:261:THR:H	4:4:292:GLN:HE22	1.47	0.62
15:N:317:ARG:NH1	15:N:384:ALA:O	2.32	0.62
3:3:697:THR:OG1	3:3:762:ALA:O	2.16	0.62
14:M:16:LEU:HD22	14:M:97:GLY:H	1.65	0.62
3:3:120:PRO:HA	4:4:328:PHE:HE2	1.62	0.62
4:4:336:HIS:ND1	5:5:189:ARG:O	2.31	0.62
6:6:60:LEU:HG	6:6:65:SER:HB2	1.81	0.62
7:9:68:ILE:HG12	7:9:93:ILE:HG12	1.80	0.62
4:E:343:TYR:HB2	4:E:356:TYR:HD1	1.63	0.62
4:E:48:SER:H	4:E:53:LEU:HD23	1.64	0.62
4:E:73:ARG:NE	4:E:81:TYR:OH	2.33	0.62
15:N:53:TYR:HA	15:N:101:THR:HG22	1.82	0.62
14:M:56:LEU:HD11	15:N:416:PRO:HG2	1.81	0.62
13:T:278:ALA:HB1	13:T:409:VAL:HG11	1.79	0.62
13:T:291:ILE:HD12	13:T:336:SER:HB3	1.82	0.62
2:2:71:GLN:NE2	2:2:120:GLN:OE1	2.32	0.62
4:4:112:ARG:NH2	4:4:181:ASP:OD1	2.32	0.62
4:4:314:ARG:NH2	7:9:106:GLU:O	2.33	0.62
4:E:171:ASN:OD1	4:E:174:ARG:NH1	2.30	0.62
16:Q:227:GLU:HB2	16:Q:299:ARG:NH1	2.15	0.62
14:M:332:LEU:O	14:M:336:THR:OG1	2.10	0.62
11:R:29:ALA:O	11:R:33:ILE:HG13	2.00	0.62
1:B:365:GLY:O	1:B:369:ASN:ND2	2.31	0.62
2:C:77:LYS:H	2:C:116:LEU:HA	1.65	0.62
6:G:37:TRP:CZ2	6:G:67:VAL:HB	2.34	0.62
16:H:29:ALA:O	16:H:32:THR:OG1	2.18	0.62
13:L:359:LEU:O	13:L:363:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:114:ASN:HA	3:3:161:ARG:HG2	1.82	0.62
3:3:404:GLU:OE1	3:3:698:MET:N	2.20	0.62
2:C:56:THR:OG1	3:D:198:GLU:O	2.12	0.62
4:E:131:VAL:HG23	4:E:153:ARG:HD2	1.82	0.62
7:O:110:THR:OG1	17:O:202:SF4:S2	2.56	0.62
16:Q:332:LEU:HB2	16:Q:333:PRO:CD	2.29	0.62
3:3:346:ALA:HA	3:3:372:GLN:HB2	1.81	0.62
11:R:93:ALA:HB2	13:T:591:LEU:HD11	1.80	0.62
15:V:73:THR:HB	15:V:209:LEU:HD22	1.80	0.62
1:1:88:TYR:HB2	1:1:216:THR:HG22	1.82	0.61
3:3:256:CYS:HB2	3:3:265:ILE:HD13	1.82	0.61
11:J:22:LEU:HD13	11:J:27:HIS:HB3	1.82	0.61
13:L:163:ARG:HE	14:M:399:VAL:HB	1.64	0.61
11:R:17:VAL:O	11:R:21:THR:OG1	2.16	0.61
15:V:279:GLN:NE2	15:V:420:LEU:O	2.32	0.61
1:1:404:ASP:HA	1:1:407:VAL:HG22	1.81	0.61
3:3:129:GLU:O	3:3:133:ARG:HG2	2.00	0.61
11:J:29:ALA:O	11:J:33:ILE:HG13	2.00	0.61
16:Q:290:PHE:O	16:Q:294:ARG:HG2	1.99	0.61
10:P:113:LYS:NZ	15:V:83:GLU:OE2	2.33	0.61
3:3:287:GLU:OE1	3:3:289:TRP:NE1	2.32	0.61
10:A:109:TYR:OH	10:A:113:LYS:NZ	2.26	0.61
1:B:241:MET:O	1:B:248:GLY:N	2.33	0.61
3:D:404:GLU:OE1	3:D:698:MET:N	2.31	0.61
4:E:315:HIS:HA	8:I:46:ARG:CZ	2.31	0.61
6:6:37:TRP:HB2	16:H:65:LYS:HE2	1.80	0.61
15:N:24:GLY:HA2	15:N:27:ARG:HD2	1.81	0.61
4:4:341:GLU:HG2	4:4:358:VAL:HG22	1.83	0.61
3:D:40:SER:O	3:D:189:ARG:NE	2.27	0.61
4:E:62:LEU:HD21	6:G:43:LEU:HB3	1.82	0.61
11:J:133:GLY:H	11:J:136:LEU:HB2	1.65	0.61
2:2:110:GLU:OE2	8:7:114:ARG:NE	2.26	0.61
5:5:121:LEU:HA	5:5:145:PRO:HD2	1.82	0.61
1:B:305:GLU:O	1:B:309:THR:OG1	2.17	0.61
3:D:29:ASP:OD2	5:F:187:GLY:N	2.28	0.61
3:3:42:ILE:HD12	3:3:42:ILE:O	2.00	0.61
6:G:69:ARG:NH2	16:Q:225:GLU:OE2	2.34	0.61
13:L:502:LEU:HD23	13:L:505:LEU:HD12	1.82	0.61
10:P:57:PHE:HB3	10:P:58:PRO:HD2	1.81	0.61
13:T:171:LEU:HB3	13:T:208:LEU:HD13	1.82	0.61
1:1:60:SER:HB2	1:1:230:ILE:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:59:ASP:OD1	6:6:62:ARG:NH2	2.33	0.61
16:H:198:TYR:O	16:H:341:SER:OG	2.17	0.61
8:7:98:GLU:HG2	8:7:104:VAL:HG21	1.83	0.61
1:B:104:ARG:NH1	1:B:108:GLU:OE2	2.33	0.61
3:D:349:ALA:O	3:D:540:ASN:ND2	2.29	0.61
14:M:304:THR:O	14:M:307:GLY:N	2.33	0.61
10:A:105:VAL:HG13	15:N:15:LEU:HD21	1.81	0.61
3:D:285:VAL:HG13	3:D:286:ASN:H	1.66	0.61
4:E:373:PRO:O	4:E:377:ASN:ND2	2.34	0.61
6:6:30:TRP:O	6:6:34:ASN:ND2	2.34	0.61
10:A:65:ALA:O	10:A:69:ILE:HG23	2.01	0.61
11:J:83:PHE:O	12:K:22:ARG:NH1	2.33	0.61
2:2:130:THR:HB	2:2:143:GLU:HB3	1.83	0.60
6:6:160:GLY:O	6:6:169:ARG:NH1	2.33	0.60
2:C:28:MET:O	2:C:70:TYR:OH	2.17	0.60
3:D:46:ARG:HH22	3:D:81:ALA:HB2	1.66	0.60
4:E:72:HIS:HB3	5:F:171:ARG:HE	1.66	0.60
13:L:255:ARG:HA	13:L:477:LEU:HD23	1.83	0.60
12:S:94:ARG:NH2	13:T:585:TYR:OH	2.28	0.60
9:X:46:TYR:HB2	9:X:63:PHE:HB2	1.82	0.60
1:1:212:TRP:HE1	2:2:22:GLY:HA3	1.66	0.60
3:3:382:PHE:HB3	3:3:532:VAL:HB	1.83	0.60
10:A:57:PHE:HB3	10:A:58:PRO:HD2	1.82	0.60
4:E:367:ARG:HH12	4:E:369:LYS:HB2	1.66	0.60
5:F:13:LYS:NZ	5:F:37:GLU:OE2	2.28	0.60
14:U:427:GLY:HA2	14:U:430:TRP:HD1	1.65	0.60
4:4:152:GLU:OE2	4:4:200:ARG:NE	2.34	0.60
6:G:74:GLN:NE2	16:Q:233:HIS:HB2	2.16	0.60
10:A:3:PRO:HD2	16:H:2:THR:HB	1.83	0.60
16:Q:17:ALA:O	16:Q:21:VAL:HG23	2.02	0.60
3:3:715:GLU:H	3:3:761:SER:HB2	1.65	0.60
6:6:56:ALA:HA	16:H:45:ARG:HB2	1.82	0.60
6:G:134:ASP:OD1	6:G:157:LYS:NZ	2.32	0.60
13:T:139:PHE:HB2	13:T:159:PHE:HB2	1.83	0.60
13:T:356:TRP:HB2	13:T:425:PHE:HB3	1.83	0.60
1:1:274:GLU:HG3	1:1:278:GLU:HG3	1.82	0.60
3:3:165:ASP:HB2	8:7:66:PRO:HG2	1.83	0.60
14:M:49:HIS:HD2	14:M:67:LEU:HD22	1.66	0.60
14:U:313:TYR:OH	14:U:443:MET:O	2.18	0.60
5:F:151:PRO:HD3	9:X:112:LYS:HE2	1.83	0.60
4:4:254:TYR:OH	4:4:346:THR:OG1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:7:TYR:OH	16:H:119:ASP:OD1	2.20	0.60
1:B:63:ARG:O	1:B:65:ARG:NE	2.32	0.60
3:D:48:CYS:SG	3:D:83:CYS:N	2.75	0.60
11:J:50:PHE:HB2	11:J:124:PRO:HD3	1.83	0.60
16:Q:177:VAL:HG11	16:Q:185:ILE:HG12	1.83	0.60
6:6:39:ALA:HB2	6:6:75:ALA:HB3	1.84	0.60
1:B:372:ALA:O	1:B:376:THR:OG1	2.14	0.60
1:B:388:GLU:OE2	1:B:418:LYS:NZ	2.34	0.60
15:V:132:ALA:HB1	15:V:199:VAL:HA	1.84	0.60
1:1:92:ASN:HB3	1:1:220:ASN:HA	1.84	0.60
4:4:45:VAL:HG13	4:4:55:VAL:HG22	1.83	0.60
6:G:165:GLU:HG2	7:O:148:ARG:NH1	2.17	0.60
10:P:52:GLY:O	16:Q:146:LYS:NZ	2.27	0.60
15:V:33:LEU:HB2	15:V:71:LEU:HD21	1.82	0.60
3:3:587:LEU:O	3:3:604:ALA:N	2.35	0.60
3:3:611:ARG:HA	3:3:624:LEU:O	2.02	0.60
8:I:88:ARG:HH21	8:I:126:LEU:HB3	1.67	0.60
13:L:419:ARG:NH2	13:L:525:GLU:OE2	2.29	0.60
13:T:286:PHE:O	13:T:419:ARG:NH1	2.34	0.60
13:T:358:HIS:ND1	13:T:429:GLU:OE2	2.32	0.60
1:1:95:GLU:OE2	1:1:102:LYS:N	2.34	0.60
4:4:236:GLY:N	4:4:377:ASN:OD1	2.26	0.60
4:E:333:GLU:OE2	4:E:336:HIS:NE2	2.34	0.60
13:L:162:ASN:OD1	13:L:216:LYS:NZ	2.34	0.60
14:M:221:ASN:ND2	14:M:228:ASP:OD1	2.35	0.60
11:R:68:LEU:HD23	11:R:71:ILE:HD11	1.84	0.60
14:U:56:LEU:HD11	15:V:416:PRO:HG2	1.82	0.60
1:1:354:GLY:HA2	1:1:360:ARG:HB2	1.85	0.59
3:3:208:HIS:O	8:7:85:ARG:NH2	2.25	0.59
11:J:69:PHE:CZ	16:H:156:SER:HB3	2.38	0.59
16:H:17:ALA:O	16:H:21:VAL:HG23	2.02	0.59
13:L:17:LEU:HB2	13:L:106:ALA:HB2	1.84	0.59
16:Q:39:LEU:O	16:Q:43:GLN:HG2	2.02	0.59
14:U:304:THR:O	14:U:307:GLY:N	2.35	0.59
1:1:4:PRO:HA	1:1:12:ARG:HH12	1.68	0.59
2:2:107:GLY:H	2:2:110:GLU:HG3	1.66	0.59
3:D:551:PRO:HB2	3:D:555:GLY:HA2	1.83	0.59
16:Q:168:LEU:HD12	16:Q:314:PHE:HB3	1.84	0.59
14:U:157:LEU:HD12	15:V:369:ALA:HB2	1.84	0.59
1:1:15:ARG:HH22	1:1:279:TRP:HH2	1.50	0.59
4:E:87:TYR:CB	6:G:45:CYS:HB3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:189:GLN:HG2	16:Q:195:LEU:H	1.67	0.59
13:T:490:GLU:O	13:T:494:ILE:HG12	2.02	0.59
1:B:201:LEU:HG	1:B:203:PRO:HD2	1.84	0.59
4:4:201:ILE:HG21	4:4:284:ARG:HG3	1.83	0.59
1:B:338:VAL:HG21	1:B:424:LEU:HD22	1.85	0.59
3:D:190:TYR:OH	3:D:222:PHE:O	2.16	0.59
16:H:332:LEU:HB2	16:H:333:PRO:CD	2.31	0.59
13:L:314:ALA:HB1	13:L:317:VAL:HB	1.83	0.59
10:A:5:GLN:OE1	16:H:10:TYR:OH	2.19	0.59
3:D:8:ASP:OD2	3:D:28:TYR:OH	2.20	0.59
7:O:13:THR:HB	16:Q:42:PHE:CE1	2.38	0.59
13:T:487:LEU:HA	13:T:490:GLU:HG2	1.84	0.59
14:U:237:GLY:O	14:U:241:PHE:N	2.28	0.59
4:4:367:ARG:NH1	4:4:369:LYS:HB2	2.18	0.59
3:D:274:LEU:H	3:D:302:ASP:HB3	1.68	0.59
4:E:30:VAL:HB	4:E:43:LEU:HB2	1.84	0.59
7:O:45:ARG:NH2	7:O:137:LEU:HD23	2.18	0.59
6:G:73:ARG:NH2	10:P:42:MET:O	2.34	0.59
13:T:103:ARG:NH2	13:T:144:PHE:O	2.31	0.59
14:U:345:ARG:HG2	14:U:412:LYS:O	2.03	0.59
15:V:102:ARG:HD3	15:V:163:LEU:HB2	1.82	0.59
1:1:259:LYS:NZ	2:2:178:GLU:OE2	2.35	0.59
10:A:66:MET:O	10:A:69:ILE:HG12	2.03	0.59
1:B:316:LEU:HD13	1:B:323:LEU:HB2	1.83	0.59
6:G:61:ALA:HA	6:G:66:GLU:HB2	1.84	0.59
5:5:59:THR:HG22	5:5:59:THR:O	2.02	0.59
13:L:377:PRO:HG3	13:L:498:ALA:HB1	1.84	0.59
7:O:10:LEU:O	7:O:13:THR:OG1	2.20	0.59
16:Q:205:VAL:HG21	16:Q:317:ALA:HB2	1.85	0.59
1:1:365:GLY:O	1:1:369:ASN:ND2	2.35	0.59
3:3:34:CYS:O	3:3:189:ARG:NH2	2.34	0.59
3:D:297:GLY:O	3:D:703:GLN:NE2	2.34	0.59
14:U:85:GLY:O	14:U:89:ALA:HB2	2.01	0.59
4:4:87:TYR:CB	6:6:45:CYS:HB3	2.33	0.58
7:9:63:CYS:HA	17:9:201:SF4:S2	2.43	0.58
10:A:74:GLU:HB2	10:A:103:LEU:HD22	1.85	0.58
3:D:198:GLU:OE2	3:D:440:ARG:NH1	2.28	0.58
3:D:399:LEU:O	3:D:508:GLY:N	2.35	0.58
3:D:311:VAL:HG23	3:D:600:VAL:HG22	1.85	0.58
4:E:167:ARG:HD3	6:G:143:ARG:NH1	2.18	0.58
10:P:64:VAL:HA	10:P:67:LEU:HD22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:150:LEU:O	16:Q:154:ARG:HG3	2.03	0.58
15:V:234:ALA:HB1	15:V:360:VAL:HG21	1.85	0.58
1:1:239:ALA:HA	1:1:247:LYS:HB3	1.83	0.58
3:3:109:GLU:OE1	3:3:156:ARG:NH2	2.36	0.58
3:D:455:ARG:HH21	3:D:750:ARG:NH2	1.99	0.58
16:Q:271:VAL:HG12	16:Q:272:LEU:HG	1.83	0.58
1:B:83:ASP:OD2	1:B:87:HIS:NE2	2.37	0.58
3:D:694:LEU:HB3	3:D:762:ALA:HB2	1.86	0.58
4:E:217:ARG:HD2	16:Q:301:ARG:HH11	1.68	0.58
13:L:149:PRO:HG3	14:M:416:GLU:HG2	1.84	0.58
14:M:338:THR:HG22	14:M:340:GLU:H	1.68	0.58
15:V:119:TYR:CZ	15:V:137:PHE:HA	2.38	0.58
15:V:271:LEU:HD23	15:V:352:ALA:HB2	1.84	0.58
1:B:63:ARG:NE	1:B:69:GLY:O	2.37	0.58
3:D:615:VAL:HG22	3:D:621:VAL:HG12	1.85	0.58
14:M:13:GLY:HA2	14:M:97:GLY:HA2	1.84	0.58
14:U:402:SER:HA	14:U:405:TYR:CE2	2.38	0.58
1:1:241:MET:O	1:1:248:GLY:N	2.32	0.58
3:3:186:ARG:HD3	3:3:229:ILE:HG22	1.86	0.58
6:G:54:THR:HA	6:G:60:LEU:H	1.69	0.58
16:H:45:ARG:HG2	16:H:46:MET:N	2.18	0.58
13:L:4:LEU:HG	13:L:8:LEU:HG	1.86	0.58
15:N:185:PHE:O	15:N:195:TRP:NE1	2.36	0.58
16:Q:291:ILE:HA	16:Q:294:ARG:CG	2.33	0.58
13:T:502:LEU:HD23	13:T:505:LEU:HD12	1.86	0.58
3:3:635:GLU:OE2	9:W:7:ARG:NH1	2.37	0.58
4:4:341:GLU:HA	4:4:357:ILE:O	2.04	0.58
4:E:403:VAL:HG12	4:E:406:ASP:H	1.67	0.58
16:H:127:ALA:O	16:H:131:LEU:HG	2.03	0.58
6:6:62:ARG:HD2	16:H:50:ARG:HH21	1.67	0.58
11:R:119:LEU:HD11	12:S:47:ARG:HG3	1.85	0.58
13:T:234:THR:HG23	13:T:292:LYS:HE2	1.86	0.58
1:1:63:ARG:H	1:1:65:ARG:HH21	1.50	0.58
2:2:173:GLY:HA3	2:2:176:VAL:O	2.03	0.58
3:3:384:PRO:HG3	3:3:542:ARG:NH1	2.19	0.58
4:E:62:LEU:HD11	6:G:43:LEU:O	2.03	0.58
11:J:107:GLY:HA3	15:N:174:LEU:HD22	1.86	0.58
13:T:394:THR:HB	13:T:484:HIS:O	2.04	0.58
4:4:30:VAL:HB	4:4:43:LEU:HB2	1.85	0.58
4:E:345:PRO:HB3	5:F:87:ARG:NH1	2.19	0.58
11:J:135:TRP:HZ2	12:K:52:ASP:HB3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:71:GLU:OE1	3:D:527:ARG:HD3	2.03	0.58
3:3:81:ALA:O	3:3:85:THR:OG1	2.15	0.58
3:3:94:ASP:OD2	3:3:97:SER:OG	2.17	0.58
5:5:68:PHE:HB2	5:5:94:VAL:HB	1.85	0.58
4:E:185:GLU:N	4:E:185:GLU:OE1	2.35	0.58
4:E:224:ILE:HD11	4:E:275:ARG:CZ	2.34	0.58
16:Q:96:ALA:HB1	16:Q:125:LEU:HD23	1.86	0.58
3:D:445:THR:HB	3:D:463:ALA:HB2	1.85	0.58
14:M:91:VAL:HG12	14:M:222:HIS:CE1	2.39	0.58
1:1:387:LEU:HA	1:1:390:LEU:HD12	1.86	0.57
3:3:462:ALA:O	3:3:465:HIS:ND1	2.37	0.57
6:G:37:TRP:HH2	16:Q:36:ARG:HH22	1.51	0.57
15:N:6:LEU:HB3	15:N:93:LEU:HD12	1.85	0.57
7:O:51:GLU:OE1	7:O:133:LYS:NZ	2.24	0.57
16:Q:120:LEU:HD22	16:Q:180:LEU:HD12	1.85	0.57
1:1:373:LYS:HA	8:7:79:LEU:HD11	1.86	0.57
3:3:271:SER:HG	7:9:69:TYR:HH	1.51	0.57
3:3:722:THR:HG21	3:3:756:GLY:H	1.69	0.57
7:9:110:THR:OG1	17:9:202:SF4:S2	2.56	0.57
1:B:92:ASN:N	1:B:219:ASN:O	2.28	0.57
1:B:8:GLY:HA2	1:B:270:THR:HG22	1.84	0.57
10:A:69:ILE:HG22	11:J:62:ALA:HB1	1.85	0.57
14:M:333:TYR:O	14:M:337:GLY:N	2.37	0.57
14:M:91:VAL:HG23	14:M:92:GLU:H	1.69	0.57
16:Q:101:PRO:HA	16:Q:114:TRP:HB3	1.86	0.57
1:1:32:TYR:OH	1:1:116:GLU:OE1	2.16	0.57
3:3:226:ILE:HD12	3:3:235:LEU:HD13	1.85	0.57
3:3:494:LYS:O	3:3:498:GLU:HG2	2.03	0.57
1:B:132:ILE:HD11	1:B:171:LEU:HD13	1.85	0.57
4:E:84:ARG:HG3	4:E:169:HIS:CE1	2.40	0.57
13:L:600:LEU:HD11	15:N:232:ALA:HB1	1.85	0.57
3:3:113:LEU:O	3:3:161:ARG:NH1	2.37	0.57
7:9:96:LEU:HD21	7:9:129:LEU:HD13	1.85	0.57
3:D:728:LEU:HB3	3:D:747:VAL:HG11	1.86	0.57
5:F:2:ARG:NH2	5:F:82:ASP:O	2.37	0.57
4:E:252:TYR:OH	5:F:85:GLY:O	2.19	0.57
13:L:103:ARG:NH2	13:L:144:PHE:O	2.37	0.57
2:2:146:THR:HG22	2:2:149:ARG:HB2	1.85	0.57
4:E:103:LYS:NZ	5:F:22:LEU:O	2.21	0.57
11:J:69:PHE:HZ	16:H:156:SER:HB3	1.69	0.57
13:L:234:THR:HG23	13:L:292:LYS:HE2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:59:TYR:O	11:R:64:VAL:HG12	2.05	0.57
7:9:33:LEU:HD11	7:9:119:PHE:HE2	1.70	0.57
3:D:250:GLU:HG3	5:F:169:GLU:HG3	1.86	0.57
16:H:137:PHE:HA	16:H:152:SER:HB2	1.86	0.57
10:P:81:TYR:HB2	11:R:132:TYR:CZ	2.39	0.57
14:U:203:ILE:HG13	14:U:210:LEU:HB3	1.86	0.57
1:1:149:ILE:HG22	1:1:153:ARG:HE	1.70	0.57
3:3:248:GLU:HG2	5:5:170:PHE:CE1	2.40	0.57
5:5:75:VAL:HG13	5:5:87:ARG:HB2	1.87	0.57
13:L:490:GLU:O	13:L:494:ILE:HG12	2.04	0.57
4:E:31:GLY:HA3	10:P:45:GLU:OE2	2.05	0.57
16:Q:141:TRP:CE3	16:Q:149:LEU:HD11	2.40	0.57
3:3:397:LEU:HD21	3:3:480:LEU:HD13	1.87	0.57
15:N:343:TRP:CD1	15:N:413:GLY:HA2	2.39	0.57
15:N:98:LEU:HD23	15:N:218:ALA:HB1	1.87	0.57
7:O:41:HIS:HB3	7:O:113:ILE:HD11	1.86	0.57
13:T:557:ASP:OD1	14:U:211:HIS:NE2	2.32	0.57
13:T:55:PHE:O	13:T:66:SER:HA	2.04	0.57
15:V:340:ALA:HA	15:V:343:TRP:HD1	1.69	0.57
3:3:300:TRP:CD1	3:3:703:GLN:HA	2.39	0.57
4:4:181:ASP:O	7:9:36:ARG:NH2	2.29	0.57
6:6:134:ASP:OD1	6:6:157:LYS:NZ	2.38	0.57
1:B:189:MET:SD	1:B:216:THR:OG1	2.60	0.57
4:E:68:LYS:NZ	5:F:150:TYR:O	2.28	0.57
6:G:60:LEU:HG	6:G:65:SER:HB2	1.87	0.57
16:H:227:GLU:HG2	16:H:228:LEU:H	1.70	0.57
6:G:145:GLU:HG2	7:O:31:VAL:HG21	1.87	0.57
7:9:123:ASP:OD1	7:9:124:TYR:N	2.36	0.57
16:H:136:ILE:HG23	16:H:232:TYR:HD2	1.70	0.57
15:N:92:ALA:HA	15:N:95:MET:HE2	1.86	0.57
13:T:529:ARG:NH2	13:T:530:GLU:OE2	2.38	0.57
14:U:62:TYR:HE2	14:U:174:THR:HG21	1.69	0.56
9:X:37:TRP:HE1	9:X:40:LYS:HD2	1.70	0.56
1:1:238:PHE:CZ	1:1:248:GLY:HA3	2.41	0.56
13:L:66:SER:HB2	13:L:122:ASP:HB3	1.87	0.56
15:N:224:LEU:HD11	15:N:281:LEU:HD23	1.87	0.56
1:1:360:ARG:NE	1:1:361:GLU:OE2	2.38	0.56
3:3:506:ILE:HG12	3:3:533:LEU:HB2	1.87	0.56
6:6:165:GLU:OE2	7:9:148:ARG:NH1	2.38	0.56
1:B:323:LEU:HD11	1:B:326:GLY:HA2	1.86	0.56
5:F:73:GLU:OE2	5:F:87:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:294:LEU:HD12	15:N:405:ALA:HB3	1.87	0.56
10:P:105:VAL:HG11	15:V:11:VAL:HG13	1.87	0.56
16:Q:2:THR:HG23	16:Q:5:TYR:HD2	1.69	0.56
14:U:328:LEU:HD23	14:U:332:LEU:HD23	1.87	0.56
1:1:437:TRP:O	2:2:147:ARG:NH2	2.38	0.56
3:3:740:PHE:HE2	3:3:771:VAL:HG11	1.70	0.56
4:4:48:SER:H	4:4:53:LEU:HD23	1.69	0.56
7:9:120:GLU:OE1	7:9:146:GLN:NE2	2.39	0.56
10:P:1:MET:O	16:Q:2:THR:N	2.39	0.56
3:3:399:LEU:O	3:3:508:GLY:N	2.38	0.56
6:6:54:THR:HA	6:6:59:ASP:HA	1.87	0.56
13:L:328:PHE:O	13:L:332:LEU:CD1	2.54	0.56
15:V:203:SER:HB2	15:V:208:VAL:HG22	1.86	0.56
5:5:18:GLU:HB2	5:5:26:TRP:HB2	1.86	0.56
3:D:261:VAL:HG21	3:D:408:ILE:HG12	1.88	0.56
16:H:5:TYR:OH	16:H:184:ASP:OD1	2.19	0.56
16:H:186:VAL:HG11	16:H:267:TRP:CZ3	2.40	0.56
8:I:82:ILE:HG23	8:I:95:ALA:HB3	1.85	0.56
13:T:373:LEU:HD21	13:T:416:TYR:HE1	1.70	0.56
14:U:349:GLN:NE2	14:U:418:GLY:HA3	2.20	0.56
15:V:279:GLN:HG3	15:V:423:LEU:HB2	1.86	0.56
4:4:73:ARG:NH2	4:4:81:TYR:OH	2.38	0.56
3:D:51:ARG:HB3	3:D:94:ASP:HB3	1.87	0.56
3:D:261:VAL:O	3:D:616:ASN:ND2	2.35	0.56
7:O:30:PRO:HB2	7:O:162:VAL:HG22	1.87	0.56
15:V:115:SER:HA	15:V:118:LEU:HD12	1.88	0.56
1:1:343:ASN:HB2	2:2:89:LYS:HZ3	1.70	0.56
3:3:338:GLY:O	3:3:366:THR:HB	2.06	0.56
3:D:256:CYS:HB2	3:D:265:ILE:HD13	1.88	0.56
3:D:494:LYS:O	3:D:498:GLU:HG2	2.05	0.56
13:L:422:VAL:HA	13:L:426:LEU:HD13	1.86	0.56
11:R:146:LEU:O	11:R:150:THR:HG23	2.06	0.56
3:3:261:VAL:O	3:3:616:ASN:ND2	2.37	0.56
4:4:128:SER:HG	4:4:350:ARG:NH2	2.03	0.56
1:B:274:GLU:HG3	1:B:278:GLU:HG3	1.86	0.56
10:A:56:ARG:HD3	11:J:74:LEU:HA	1.88	0.56
16:Q:45:ARG:HG2	16:Q:46:MET:N	2.21	0.56
13:T:177:TRP:HE3	13:T:183:LEU:HG	1.71	0.56
9:X:74:LEU:HD21	9:X:126:TYR:HB3	1.86	0.56
3:3:51:ARG:HB3	3:3:94:ASP:HB3	1.86	0.56
2:C:40:TRP:CD1	2:C:74:PRO:HA	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:664:LEU:HD22	3:D:669:VAL:HG11	1.87	0.56
3:D:559:ASP:OD2	3:D:686:LYS:NZ	2.38	0.56
4:E:236:GLY:HA2	4:E:351:GLY:HA3	1.87	0.56
16:H:131:LEU:HA	16:H:134:TYR:HB2	1.88	0.56
10:P:68:PHE:CD2	16:Q:164:LEU:HB2	2.41	0.56
15:V:265:HIS:HA	15:V:268:TYR:CD2	2.41	0.56
6:G:178:ARG:NH1	9:X:122:ASP:OD2	2.38	0.56
3:3:474:ARG:O	3:3:520:ARG:NH1	2.39	0.56
4:4:352:GLU:CD	5:5:87:ARG:HH22	2.08	0.56
14:M:102:MET:HB3	14:M:230:LEU:HD23	1.88	0.56
10:P:109:TYR:HE1	15:V:82:PHE:HZ	1.54	0.56
14:U:333:TYR:O	14:U:337:GLY:N	2.39	0.56
15:V:33:LEU:HD22	15:V:67:LEU:HD22	1.87	0.56
3:3:710:GLU:O	3:3:713:ARG:NH1	2.35	0.55
3:3:694:LEU:HB3	3:3:762:ALA:HB2	1.88	0.55
1:B:203:PRO:HB2	1:B:204:PRO:HD3	1.88	0.55
3:D:185:LYS:HB3	3:D:189:ARG:HH11	1.71	0.55
13:T:247:THR:HG22	13:T:322:VAL:HG13	1.88	0.55
4:4:75:TYR:CZ	4:4:337:PRO:HG2	2.41	0.55
1:B:259:LYS:HB3	1:B:281:GLY:HA3	1.87	0.55
3:D:409:LEU:HD12	3:D:535:MET:HE3	1.88	0.55
4:E:84:ARG:CZ	4:E:169:HIS:HB3	2.35	0.55
13:L:409:VAL:HA	13:L:412:LEU:HD12	1.87	0.55
14:M:54:PRO:HA	14:M:62:TYR:HD1	1.70	0.55
11:R:151:VAL:HG11	15:V:90:TYR:HE2	1.71	0.55
13:T:463:HIS:CG	13:T:464:PRO:HD3	2.42	0.55
15:V:275:THR:OG1	15:V:351:GLU:OE1	2.20	0.55
4:4:185:GLU:OE2	7:9:165:TYR:OH	2.18	0.55
3:D:609:GLU:HA	3:D:627:ALA:H	1.71	0.55
3:3:717:TRP:HB2	3:3:759:TYR:HB2	1.87	0.55
9:W:43:GLN:NE2	3:D:522:ARG:HH22	2.05	0.55
10:A:67:LEU:HB3	16:H:310:TRP:HZ2	1.70	0.55
2:C:110:GLU:HA	8:I:121:ARG:HH12	1.71	0.55
10:P:71:PHE:CZ	10:P:107:PHE:HB2	2.41	0.55
1:1:219:ASN:ND2	18:1:502:FMN:O2P	2.40	0.55
4:E:114:GLU:O	4:E:118:VAL:HG13	2.06	0.55
4:E:376:VAL:HA	4:E:379:GLN:HE21	1.72	0.55
5:F:99:PRO:HB2	5:F:124:ILE:HA	1.88	0.55
8:I:60:SER:HA	8:I:66:PRO:HA	1.87	0.55
14:M:126:LEU:HD11	14:M:149:VAL:HG22	1.89	0.55
15:N:209:LEU:HB2	15:N:296:PHE:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:40:ARG:NH2	7:O:118:ASP:OD1	2.38	0.55
13:T:122:ASP:OD2	13:T:184:SER:OG	2.21	0.55
14:U:321:TYR:CE1	14:U:365:MET:HA	2.42	0.55
9:W:37:TRP:CD1	9:W:40:LYS:HD2	2.42	0.55
4:4:148:TYR:HB3	4:4:200:ARG:NH2	2.22	0.55
4:4:86:ASP:HB3	4:4:93:HIS:CD2	2.42	0.55
7:9:40:ARG:HH12	7:9:42:VAL:HG12	1.72	0.55
10:A:68:PHE:CD2	16:H:164:LEU:HB2	2.40	0.55
11:J:130:LEU:HD12	12:K:51:LEU:HD23	1.86	0.55
13:L:160:ILE:O	13:L:164:ILE:HG13	2.07	0.55
14:M:350:SER:HB3	14:M:421:GLY:HA2	1.88	0.55
2:2:74:PRO:HB2	8:7:121:ARG:HE	1.71	0.55
3:3:337:ARG:NH1	3:3:565:TYR:OH	2.38	0.55
3:3:713:ARG:NE	3:3:746:ARG:HE	2.04	0.55
1:B:90:ILE:HD11	1:B:211:LEU:HD22	1.89	0.55
4:E:28:LEU:HD21	16:Q:228:LEU:HD11	1.88	0.55
4:E:352:GLU:CD	5:F:87:ARG:HH22	2.10	0.55
6:G:53:SER:O	6:G:60:LEU:N	2.39	0.55
10:P:65:ALA:HB3	11:R:66:LEU:HD13	1.88	0.55
5:5:38:MET:HA	5:5:41:TYR:HD2	1.71	0.55
7:9:128:ASP:O	7:9:144:LYS:NZ	2.25	0.55
3:D:592:PRO:HA	3:D:595:GLU:HG2	1.89	0.55
4:E:261:THR:H	4:E:292:GLN:HE22	1.55	0.55
6:G:132:PRO:HG2	6:G:175:ALA:HA	1.89	0.55
14:M:235:LYS:HD3	14:M:293:MET:HG3	1.88	0.55
13:T:391:ALA:O	13:T:395:TYR:HB2	2.07	0.55
3:3:194:VAL:HG12	3:3:411:LEU:HD22	1.89	0.55
4:4:234:LEU:O	4:4:239:LEU:HB2	2.07	0.55
10:A:81:TYR:CE2	10:A:96:VAL:HG11	2.42	0.55
4:E:367:ARG:NH1	4:E:369:LYS:HB2	2.22	0.55
6:G:174:ALA:HA	6:G:177:LYS:HE2	1.88	0.55
11:J:130:LEU:HD11	12:K:51:LEU:CD2	2.36	0.55
15:V:294:LEU:HG	15:V:402:VAL:HG13	1.87	0.55
15:V:98:LEU:HD23	15:V:218:ALA:HB1	1.89	0.55
4:4:248:VAL:HG13	4:4:252:TYR:HD2	1.71	0.55
4:4:38:HIS:ND1	4:4:139:ASP:OD2	2.39	0.55
5:5:101:LEU:O	5:5:127:GLU:N	2.33	0.55
1:B:95:GLU:OE2	1:B:102:LYS:N	2.40	0.55
2:C:110:GLU:OE2	8:I:114:ARG:NE	2.39	0.55
2:C:85:THR:HG22	2:C:86:LEU:H	1.72	0.55
14:M:232:THR:HA	14:M:235:LYS:HZ2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:162:TYR:OH	16:Q:305:LEU:O	2.17	0.55
13:T:160:ILE:O	13:T:164:ILE:HG13	2.07	0.55
5:5:100:ARG:NH1	5:5:127:GLU:OE1	2.40	0.54
10:A:61:PHE:HB2	11:J:73:LEU:HD11	1.89	0.54
1:B:72:THR:HG21	1:B:223:THR:HG21	1.90	0.54
2:C:130:THR:HB	2:C:143:GLU:HB3	1.90	0.54
4:4:50:GLU:CD	16:H:154:ARG:HH12	2.10	0.54
12:K:25:ILE:HG12	12:K:75:ILE:HG21	1.89	0.54
7:O:33:LEU:HB2	7:O:163:VAL:HG12	1.89	0.54
6:G:114:SER:OG	7:O:96:LEU:O	2.24	0.54
9:X:29:ALA:HB1	9:X:50:LEU:HD11	1.89	0.54
5:5:120:ASP:OD2	5:5:136:LEU:N	2.39	0.54
13:T:162:ASN:OD1	13:T:216:LYS:NZ	2.38	0.54
13:T:61:PRO:HD3	14:U:448:GLY:HA2	1.88	0.54
2:2:9:ASP:OD1	2:2:9:ASP:N	2.40	0.54
2:C:79:HIS:H	2:C:137:ASN:CG	2.10	0.54
3:D:557:SER:OG	3:D:559:ASP:OD1	2.21	0.54
13:L:463:HIS:CG	13:L:464:PRO:HD3	2.42	0.54
13:L:55:PHE:O	13:L:66:SER:HA	2.08	0.54
13:T:325:HIS:NE2	13:T:329:LYS:HG3	2.23	0.54
4:4:375:PHE:HA	4:4:407:VAL:HG13	1.90	0.54
4:E:144:THR:HG22	4:E:148:TYR:CE1	2.36	0.54
16:Q:122:ILE:HB	16:Q:170:LEU:HD13	1.90	0.54
13:T:119:VAL:O	13:T:251:TYR:OH	2.19	0.54
13:T:490:GLU:HG3	13:T:491:TRP:N	2.23	0.54
14:U:426:ALA:N	14:U:429:GLU:OE1	2.34	0.54
14:U:82:VAL:HG21	14:U:103:GLU:HB2	1.89	0.54
1:1:293:GLY:O	1:1:327:GLY:N	2.40	0.54
16:H:150:LEU:O	16:H:154:ARG:HG3	2.07	0.54
14:M:215:PRO:HG2	14:M:216:PRO:HD3	1.89	0.54
16:Q:33:LEU:HD11	16:Q:56:LEU:HA	1.90	0.54
12:S:93:LEU:HD21	15:V:128:GLN:HB2	1.90	0.54
3:3:337:ARG:HH12	3:3:581:ARG:NH1	2.05	0.54
10:A:61:PHE:HD2	11:J:73:LEU:HD21	1.73	0.54
3:D:444:ARG:NH2	3:D:446:ASP:OD2	2.41	0.54
5:F:116:ARG:O	5:F:120:ASP:N	2.39	0.54
7:O:9:SER:O	7:O:12:ILE:HG13	2.07	0.54
7:O:96:LEU:HD21	7:O:129:LEU:HD13	1.88	0.54
3:3:118:ASP:OD2	3:3:180:ARG:NE	2.34	0.54
1:B:414:LEU:O	1:B:418:LYS:N	2.41	0.54
1:B:343:ASN:HD22	2:C:89:LYS:NZ	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:265:PRO:HB2	4:E:278:VAL:HG13	1.90	0.54
6:G:37:TRP:HH2	16:Q:36:ARG:NH2	2.06	0.54
15:N:294:LEU:HG	15:N:402:VAL:HG13	1.89	0.54
15:N:63:THR:HG22	15:N:96:HIS:HA	1.89	0.54
4:4:129:HIS:HE1	4:4:349:ALA:HB1	1.73	0.54
1:B:393:LEU:HD22	3:D:106:GLY:HA3	1.88	0.54
5:F:121:LEU:HA	5:F:145:PRO:HD2	1.89	0.54
16:H:149:LEU:O	16:H:153:LEU:HG	2.08	0.54
10:P:107:PHE:HE1	16:Q:310:TRP:CD1	2.26	0.54
16:Q:149:LEU:O	16:Q:153:LEU:HG	2.08	0.54
1:1:139:ARG:HD2	2:2:138:ASP:O	2.08	0.54
5:5:31:ARG:HH21	5:5:100:ARG:HB2	1.73	0.54
2:C:106:ILE:HD11	2:C:112:THR:HB	1.90	0.54
2:C:79:HIS:N	2:C:137:ASN:OD1	2.40	0.54
3:D:2:VAL:HG13	3:D:89:ASP:HA	1.90	0.54
11:J:59:TYR:O	11:J:64:VAL:HG12	2.08	0.54
16:Q:274:VAL:HG22	16:Q:275:PRO:HD2	1.88	0.54
6:G:62:ARG:HG2	16:Q:48:PRO:HA	1.88	0.54
14:U:41:LEU:O	14:U:42:THR:HG22	2.07	0.54
3:3:268:ASP:OD2	3:3:278:ARG:NH1	2.40	0.54
6:6:21:PHE:O	6:6:25:GLU:HG2	2.07	0.54
1:B:201:LEU:HD13	3:D:42:ILE:HG22	1.89	0.54
1:B:61:GLY:HA3	1:B:247:LYS:HG3	1.88	0.54
3:D:688:ARG:HB3	3:D:770:ARG:HB2	1.90	0.54
13:L:328:PHE:O	13:L:332:LEU:HD13	2.08	0.54
11:R:152:VAL:O	11:R:156:LEU:HB2	2.07	0.54
13:T:600:LEU:HD13	15:V:236:LEU:HD21	1.89	0.54
15:V:38:ALA:HA	15:V:41:LEU:HD12	1.89	0.54
2:2:82:VAL:HG22	2:2:134:ILE:HG12	1.89	0.53
3:3:48:CYS:HB3	19:3:804:FES:S2	2.48	0.53
13:L:413:THR:HA	13:L:416:TYR:CE2	2.43	0.53
13:L:163:ARG:NE	14:M:399:VAL:HB	2.23	0.53
9:W:1:MET:HG3	9:W:56:ASP:HB2	1.89	0.53
5:F:163:ARG:NH2	7:O:92:GLU:OE2	2.40	0.53
13:T:316:TRP:HA	13:T:319:LEU:HD12	1.90	0.53
14:U:215:PRO:HG2	14:U:216:PRO:HD3	1.89	0.53
1:B:211:LEU:HB2	1:B:216:THR:HG21	1.90	0.53
2:C:9:ASP:N	2:C:9:ASP:OD1	2.40	0.53
2:C:110:GLU:HA	8:I:121:ARG:HH22	1.74	0.53
16:Q:260:PRO:HG3	16:Q:286:PHE:CD2	2.43	0.53
13:T:88:HIS:O	13:T:92:ILE:HG13	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:350:ARG:O	4:4:373:PRO:HB2	2.08	0.53
1:B:288:GLN:HE21	1:B:331:ILE:HG22	1.73	0.53
13:L:490:GLU:HG3	13:L:491:TRP:N	2.22	0.53
14:M:22:ARG:HD2	14:M:22:ARG:C	2.28	0.53
15:N:85:TYR:O	15:N:88:VAL:HB	2.09	0.53
13:T:405:GLY:O	13:T:409:VAL:HG23	2.08	0.53
8:7:86:LEU:HD11	8:7:118:LEU:HD11	1.90	0.53
5:F:174:LEU:HD13	5:F:180:GLY:HA2	1.90	0.53
6:G:96:TRP:CE3	6:G:97:GLU:HG3	2.44	0.53
13:T:98:ASP:HB3	13:T:145:TRP:HE1	1.71	0.53
14:U:318:SER:HA	14:U:321:TYR:CZ	2.44	0.53
13:L:316:TRP:HA	13:L:319:LEU:HD12	1.91	0.53
14:M:205:THR:HG23	14:M:238:VAL:HG23	1.90	0.53
14:M:345:ARG:HG2	14:M:412:LYS:O	2.08	0.53
14:M:49:HIS:HB2	14:M:67:LEU:HD13	1.91	0.53
16:Q:8:ASP:OD2	16:Q:111:TYR:HB3	2.08	0.53
16:Q:170:LEU:HD21	16:Q:262:LEU:HD13	1.91	0.53
16:H:291:ILE:HA	16:H:294:ARG:CG	2.37	0.53
11:J:17:VAL:O	11:J:21:THR:OG1	2.18	0.53
10:P:65:ALA:O	10:P:69:ILE:HG23	2.08	0.53
14:U:13:GLY:HA2	14:U:97:GLY:HA2	1.91	0.53
14:U:56:LEU:HB3	14:U:59:ALA:HB3	1.91	0.53
1:1:260:ARG:NH1	1:1:279:TRP:O	2.36	0.53
1:1:382:LYS:O	1:1:386:ASN:ND2	2.42	0.53
1:B:63:ARG:H	1:B:65:ARG:NH2	2.05	0.53
13:L:380:SER:HA	13:L:383:TRP:HD1	1.73	0.53
14:M:56:LEU:HB3	14:M:59:ALA:HB3	1.90	0.53
16:Q:190:LYS:HD3	16:Q:268:THR:HG22	1.90	0.53
13:T:141:LEU:HB3	13:T:236:VAL:HG11	1.91	0.53
15:V:259:ALA:O	15:V:263:ILE:HG13	2.09	0.53
15:V:128:GLN:OE1	15:V:306:ARG:NH2	2.42	0.53
3:3:716:LEU:HD21	3:3:758:LEU:HD23	1.90	0.53
6:6:96:TRP:CZ2	6:6:103:LYS:HE3	2.43	0.53
10:A:81:TYR:HB2	11:J:132:TYR:CE1	2.43	0.53
3:D:129:GLU:OE2	3:D:186:ARG:NH1	2.40	0.53
3:D:586:HIS:NE2	3:D:603:PRO:O	2.42	0.53
11:J:64:VAL:HG13	16:H:134:TYR:OH	2.09	0.53
16:H:290:PHE:O	16:H:294:ARG:HG2	2.09	0.53
14:U:167:ARG:NH2	14:U:173:PRO:O	2.26	0.53
6:G:124:VAL:HG22	9:X:120:PRO:HD2	1.91	0.53
1:1:342:TRP:HZ3	1:1:346:ARG:HE	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:124:PRO:HA	11:J:127:LEU:HB2	1.90	0.53
13:T:386:ASP:OD2	13:T:494:ILE:HA	2.09	0.53
15:V:181:VAL:HA	15:V:192:PHE:CE2	2.44	0.53
15:V:207:VAL:O	15:V:211:MET:HG3	2.10	0.53
3:3:190:TYR:OH	3:3:222:PHE:O	2.20	0.52
4:4:232:LEU:HD23	5:5:109:GLY:HA3	1.90	0.52
1:B:63:ARG:HD3	1:B:313:TYR:HD2	1.75	0.52
4:E:201:ILE:HA	4:E:204:TYR:HD2	1.73	0.52
16:H:37:ARG:NH2	16:H:54:PHE:O	2.41	0.52
14:M:318:SER:HA	14:M:321:TYR:CE1	2.44	0.52
13:T:586:LEU:HB2	15:V:135:LYS:HZ2	1.74	0.52
14:U:151:PHE:CD1	14:U:203:ILE:HD11	2.41	0.52
14:U:90:ARG:HG2	14:U:334:GLU:HG3	1.91	0.52
1:1:243:THR:HG22	1:1:244:GLU:H	1.74	0.52
3:3:50:VAL:HG22	3:3:82:SER:HB3	1.91	0.52
8:7:74:PRO:HG2	8:7:77:ALA:HB2	1.92	0.52
1:B:238:PHE:CZ	1:B:248:GLY:HA3	2.44	0.52
2:C:108:PRO:HA	2:C:119:VAL:HG23	1.90	0.52
3:D:31:PRO:HB2	3:D:47:MET:HB3	1.92	0.52
4:E:128:SER:OG	4:E:350:ARG:NH2	2.42	0.52
4:E:128:SER:OG	4:E:350:ARG:NH1	2.41	0.52
6:G:56:ALA:HB1	16:Q:44:VAL:HG12	1.91	0.52
6:G:40:THR:N	6:G:68:PHE:HE1	2.06	0.52
1:1:288:GLN:NE2	1:1:332:PRO:O	2.42	0.52
3:3:413:LEU:HA	3:3:416:PHE:HB3	1.90	0.52
3:3:444:ARG:NH2	3:3:446:ASP:OD2	2.42	0.52
2:2:110:GLU:HA	8:7:121:ARG:HH22	1.72	0.52
8:7:82:ILE:HG23	8:7:95:ALA:HB3	1.89	0.52
1:B:96:SER:HB2	1:B:180:TYR:HD1	1.73	0.52
6:G:143:ARG:HG3	6:G:144:PRO:HD2	1.91	0.52
11:J:123:LEU:HD22	16:H:120:LEU:HD21	1.91	0.52
13:T:128:PHE:CZ	13:T:166:ASP:HB3	2.44	0.52
13:T:365:HIS:HD2	13:T:450:ALA:HB2	1.73	0.52
1:B:90:ILE:O	1:B:218:ILE:HA	2.10	0.52
3:D:159:PHE:HE2	8:I:79:LEU:HD22	1.74	0.52
3:D:515:THR:HG23	3:D:683:LEU:HB3	1.91	0.52
5:F:38:MET:HA	5:F:41:TYR:HD2	1.74	0.52
1:B:373:LYS:HA	8:I:79:LEU:HD11	1.91	0.52
13:L:141:LEU:HB3	13:L:236:VAL:HG21	1.91	0.52
14:M:85:GLY:O	14:M:89:ALA:HB2	2.09	0.52
16:Q:236:TYR:CD1	16:Q:240:LYS:HD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:208:PHE:CE2	4:E:214:PHE:CE2	2.98	0.52
6:G:81:ALA:HA	6:G:108:MET:HB3	1.90	0.52
16:H:224:ALA:HB2	16:H:233:HIS:CE1	2.44	0.52
14:M:309:MET:HG3	14:M:454:LEU:HD12	1.92	0.52
13:L:159:PHE:HD2	14:M:407:LEU:HD11	1.74	0.52
14:M:70:LEU:HD13	14:M:454:LEU:HD21	1.90	0.52
15:N:14:THR:HA	15:N:86:LEU:HD21	1.92	0.52
13:T:434:HIS:HB3	13:T:435:PRO:HD3	1.91	0.52
15:V:283:PHE:O	15:V:287:THR:HG23	2.08	0.52
3:3:110:PHE:O	3:3:113:LEU:HB2	2.10	0.52
6:6:119:ASN:HA	6:6:125:GLN:NE2	2.25	0.52
7:9:54:ILE:HG12	7:9:110:THR:HG21	1.92	0.52
3:D:115:HIS:HB3	4:E:321:MET:HE3	1.92	0.52
16:H:40:ALA:HB2	16:H:45:ARG:HH21	1.75	0.52
10:P:68:PHE:CE2	16:Q:164:LEU:HB2	2.45	0.52
13:T:380:SER:HA	13:T:383:TRP:HD1	1.73	0.52
13:T:384:SER:O	13:T:388:ILE:HG13	2.10	0.52
15:V:102:ARG:NH1	15:V:225:ARG:O	2.42	0.52
16:H:90:VAL:HG21	16:H:243:LEU:HB3	1.90	0.52
13:L:360:PRO:HA	13:L:363:ARG:HH12	1.73	0.52
15:N:283:PHE:O	15:N:287:THR:HG23	2.08	0.52
13:T:324:THR:HG22	13:T:380:SER:HB2	1.90	0.52
3:3:115:HIS:HB3	4:4:321:MET:CE	2.40	0.52
6:6:40:THR:H	6:6:68:PHE:HE1	1.58	0.52
6:6:40:THR:HB	6:6:68:PHE:CZ	2.45	0.52
1:B:111:PRO:HB3	1:B:145:LEU:HD23	1.92	0.52
3:D:694:LEU:HD12	3:D:769:LEU:HB2	1.92	0.52
6:G:59:ASP:OD1	6:G:62:ARG:NH2	2.43	0.52
16:H:274:VAL:HG12	16:H:278:TRP:HD1	1.66	0.52
16:Q:300:LEU:O	16:Q:301:ARG:HG2	2.10	0.52
7:9:72:PRO:HG3	7:9:86:ARG:NH2	2.25	0.52
1:B:17:LEU:HD22	1:B:113:LEU:HD21	1.92	0.52
2:C:23:ARG:NH1	2:C:52:LEU:O	2.32	0.52
3:D:227:THR:HG21	3:D:237:ASP:HB2	1.90	0.52
4:E:211:SER:O	7:O:2:THR:OG1	2.27	0.52
11:J:59:TYR:CE2	12:K:61:ILE:HG23	2.45	0.52
13:L:512:PHE:HE1	13:L:521:TYR:HH	1.57	0.52
13:L:564:TYR:OH	14:M:209:PRO:O	2.25	0.52
10:P:23:ALA:O	10:P:27:VAL:HG23	2.09	0.52
13:T:361:GLN:HB2	13:T:443:LEU:HD23	1.91	0.52
13:T:459:LEU:O	13:T:468:VAL:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:6:LEU:HG	1:1:240:GLN:HE21	1.75	0.52
5:5:77:LEU:O	5:5:83:GLY:HA3	2.10	0.52
14:M:41:LEU:O	14:M:42:THR:CG2	2.52	0.52
13:T:454:VAL:HB	13:T:455:LEU:HD22	1.91	0.52
9:W:114:VAL:HA	9:W:117:ILE:HG12	1.93	0.52
1:1:287:ILE:HG22	1:1:302:PHE:HB2	1.92	0.51
4:4:222:GLY:HA3	4:4:275:ARG:NH2	2.23	0.51
10:A:71:PHE:CZ	10:A:107:PHE:HB2	2.45	0.51
4:E:341:GLU:OE1	4:E:356:TYR:OH	2.27	0.51
13:L:291:ILE:O	13:L:295:VAL:HG23	2.10	0.51
13:T:293:LYS:O	13:T:297:TYR:HD1	1.93	0.51
13:T:309:ALA:HB2	13:T:388:ILE:HD13	1.92	0.51
3:3:225:ASN:O	3:3:229:ILE:HG13	2.10	0.51
3:3:715:GLU:OE1	3:3:717:TRP:NE1	2.43	0.51
7:9:18:PHE:O	7:9:20:LYS:NZ	2.43	0.51
2:C:45:ARG:O	2:C:49:ILE:HG13	2.10	0.51
6:G:153:GLN:HG3	7:O:124:TYR:CZ	2.44	0.51
13:T:103:ARG:HH12	13:T:144:PHE:HA	1.75	0.51
14:U:9:PRO:HG2	14:U:107:LEU:HD12	1.92	0.51
2:2:85:THR:HG22	2:2:86:LEU:H	1.74	0.51
4:4:173:ILE:O	4:4:174:ARG:NH1	2.43	0.51
6:6:101:ASP:OD2	10:A:35:LYS:HB2	2.10	0.51
6:6:179:THR:HB	9:W:127:LEU:HB2	1.91	0.51
3:D:113:LEU:O	3:D:161:ARG:NH1	2.42	0.51
3:D:283:PRO:O	3:D:412:ARG:NH2	2.43	0.51
4:E:84:ARG:NH2	4:E:169:HIS:HB3	2.25	0.51
4:E:196:VAL:HG22	4:E:200:ARG:HG2	1.92	0.51
16:H:227:GLU:HB2	16:H:299:ARG:NH1	2.26	0.51
13:L:143:GLY:HA3	14:M:415:TRP:CH2	2.46	0.51
16:Q:221:LEU:N	16:Q:222:PRO:HA	2.24	0.51
1:1:297:THR:HG22	1:1:322:MET:HG3	1.92	0.51
2:2:83:CYS:HA	2:2:122:VAL:O	2.11	0.51
3:3:469:ARG:HD3	3:3:757:HIS:HE1	1.75	0.51
3:3:376:ALA:N	3:3:513:GLN:OE1	2.31	0.51
3:3:691:ALA:HB3	3:3:772:GLU:HA	1.93	0.51
1:B:219:ASN:HD22	18:B:502:FMN:P	2.33	0.51
1:B:106:ILE:HD11	1:B:251:LEU:HD21	1.92	0.51
1:B:297:THR:HG21	1:B:324:GLY:H	1.75	0.51
3:D:114:ASN:HA	3:D:161:ARG:HG2	1.92	0.51
4:E:98:ALA:O	4:E:102:GLU:HG3	2.11	0.51
4:E:285:GLU:O	4:E:289:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:341:GLU:OE1	5:F:91:ARG:NH2	2.44	0.51
6:G:99:MET:HG2	6:G:100:PRO:HD2	1.91	0.51
16:H:86:PRO:HG3	16:H:244:PHE:CE2	2.45	0.51
1:1:253:GLN:HG2	1:1:327:GLY:HA2	1.92	0.51
3:3:248:GLU:HB3	3:3:270:ARG:NH1	2.26	0.51
4:4:169:HIS:NE2	6:6:45:CYS:HB2	2.25	0.51
7:9:138:VAL:HA	7:9:173:PHE:HD1	1.75	0.51
1:B:63:ARG:HA	1:B:71:PRO:HA	1.92	0.51
4:4:35:PRO:HG3	16:H:147:TYR:OH	2.10	0.51
11:J:59:TYR:CE1	11:J:63:ILE:HD12	2.46	0.51
13:L:331:LEU:HD12	13:L:446:ASN:OD1	2.10	0.51
13:L:600:LEU:HD13	15:N:236:LEU:HD21	1.93	0.51
14:U:91:VAL:HG23	14:U:92:GLU:H	1.75	0.51
2:2:98:ASP:HB3	8:7:107:LYS:NZ	2.26	0.51
1:B:118:MET:HG2	1:B:224:LEU:HD13	1.92	0.51
4:E:43:LEU:HD13	4:E:55:VAL:HG11	1.92	0.51
16:H:206:TYR:HE1	16:H:259:ILE:HG12	1.74	0.51
16:H:39:LEU:O	16:H:43:GLN:HG2	2.11	0.51
8:I:10:TYR:O	8:I:14:VAL:HG23	2.11	0.51
13:L:87:ILE:HD12	13:L:239:LEU:HD13	1.92	0.51
14:M:219:GLN:HA	14:M:282:LYS:HG3	1.92	0.51
13:T:53:ALA:HB3	13:T:69:LEU:HB3	1.91	0.51
14:U:201:PHE:O	14:U:205:THR:N	2.44	0.51
1:1:18:TYR:OH	1:1:102:LYS:O	2.27	0.51
3:3:455:ARG:HH21	3:3:750:ARG:NH2	2.09	0.51
3:3:706:GLY:O	3:3:709:GLN:HB2	2.11	0.51
4:4:26:MET:N	10:A:54:VAL:HG21	2.26	0.51
4:4:46:THR:O	4:4:53:LEU:HB2	2.10	0.51
3:D:182:ILE:HG23	3:D:232:VAL:HG11	1.91	0.51
3:D:329:LEU:HD21	3:D:644:LEU:HA	1.93	0.51
4:E:129:HIS:CE1	4:E:349:ALA:HB1	2.46	0.51
6:G:36:LEU:HD13	6:G:154:LEU:HD23	1.91	0.51
16:H:189:GLN:O	16:H:193:GLY:HA2	2.10	0.51
12:K:79:PHE:CG	12:K:85:THR:HA	2.46	0.51
13:L:246:VAL:HB	13:L:303:LEU:HD21	1.93	0.51
13:L:33:ALA:HA	13:L:36:LEU:HD12	1.91	0.51
13:L:539:ASN:HA	13:L:543:VAL:HB	1.93	0.51
7:O:45:ARG:HH21	7:O:137:LEU:HD23	1.75	0.51
14:U:91:VAL:HB	14:U:95:PHE:HE1	1.76	0.51
15:V:237:VAL:O	15:V:241:VAL:HG23	2.11	0.51
3:3:274:LEU:H	3:3:302:ASP:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:201:ILE:HA	4:4:204:TYR:HD2	1.76	0.51
5:5:154:GLU:OE2	5:5:167:PRO:HB2	2.11	0.51
3:D:451:PHE:CD1	3:D:466:GLU:HB3	2.46	0.51
6:G:80:VAL:HG11	6:G:127:VAL:HG21	1.93	0.51
11:J:146:LEU:O	11:J:150:THR:HG23	2.11	0.51
3:D:245:ARG:HG3	7:O:57:SER:HB3	1.92	0.51
10:P:105:VAL:HG13	15:V:15:LEU:HD21	1.93	0.51
14:U:331:ARG:HA	14:U:331:ARG:HH11	1.75	0.51
2:2:98:ASP:HB3	8:7:107:LYS:HZ2	1.75	0.51
3:3:198:GLU:OE2	3:3:440:ARG:NH1	2.44	0.51
3:3:438:LYS:O	3:3:441:MET:HG3	2.11	0.51
8:7:33:LYS:HG3	8:7:54:ILE:HD12	1.91	0.51
10:A:90:LEU:HD12	16:H:330:LEU:HD21	1.91	0.51
1:B:74:LEU:HD12	1:B:77:SER:OG	2.11	0.51
3:D:229:ILE:HD11	3:D:289:TRP:HZ3	1.76	0.51
3:D:34:CYS:SG	3:D:35:SER:N	2.84	0.51
13:L:302:GLN:O	13:L:306:MET:HG3	2.11	0.51
15:N:207:VAL:O	15:N:211:MET:HG3	2.10	0.51
10:P:88:LEU:HD23	11:R:132:TYR:HB2	1.93	0.51
14:U:128:PRO:O	14:U:132:MET:HG2	2.10	0.51
4:4:148:TYR:HB3	4:4:200:ARG:HH21	1.75	0.51
1:B:18:TYR:OH	1:B:102:LYS:O	2.27	0.51
16:Q:174:VAL:O	16:Q:178:GLY:N	2.35	0.51
16:Q:189:GLN:O	16:Q:193:GLY:HA2	2.11	0.51
11:R:94:ALA:O	11:R:97:ALA:HB3	2.11	0.51
13:T:373:LEU:HD21	13:T:416:TYR:CE1	2.46	0.51
15:V:73:THR:OG1	15:V:206:PRO:O	2.24	0.51
3:3:323:GLU:OE1	9:W:11:ARG:NH1	2.44	0.51
3:3:384:PRO:O	3:3:675:ARG:NH2	2.44	0.50
5:5:160:ARG:HB2	5:5:163:ARG:HH21	1.75	0.50
1:B:3:GLY:O	1:B:5:ILE:N	2.42	0.50
4:E:148:TYR:O	4:E:151:ARG:HB3	2.11	0.50
4:E:89:HIS:CE1	4:E:92:ALA:HB2	2.47	0.50
10:P:2:ALA:HB2	16:Q:119:ASP:HB3	1.92	0.50
14:U:221:ASN:ND2	14:U:228:ASP:OD1	2.44	0.50
1:1:323:LEU:HD11	1:1:326:GLY:HA2	1.93	0.50
1:1:66:GLY:HA3	18:1:502:FMN:H3'	1.92	0.50
4:4:87:TYR:CZ	4:4:403:VAL:HG13	2.47	0.50
1:B:6:LEU:HD11	1:B:240:GLN:HE21	1.75	0.50
3:D:715:GLU:OE1	3:D:717:TRP:NE1	2.36	0.50
12:K:46:ALA:HB2	12:K:53:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:29:LEU:HD23	1:1:155:ARG:NH1	2.25	0.50
1:1:87:HIS:HD2	1:1:215:PRO:HD2	1.75	0.50
2:2:110:GLU:HA	8:7:121:ARG:NH1	2.25	0.50
3:D:695:ARG:NH1	3:D:761:SER:OG	2.44	0.50
20:E:501:DCQ:H7	6:G:42:GLY:HA3	1.94	0.50
16:H:213:GLU:N	16:H:213:GLU:OE1	2.44	0.50
11:R:123:LEU:HD13	11:R:124:PRO:HD2	1.93	0.50
14:U:331:ARG:O	14:U:335:ARG:HG2	2.11	0.50
1:1:249:MET:HA	1:1:267:PRO:HA	1.93	0.50
4:4:285:GLU:O	4:4:289:ILE:HG12	2.12	0.50
4:E:47:LEU:HD13	4:E:52:VAL:HA	1.92	0.50
5:F:120:ASP:OD2	5:F:136:LEU:N	2.41	0.50
6:G:120:ASN:HD22	6:G:122:ALA:H	1.58	0.50
16:Q:232:TYR:HB2	16:Q:244:PHE:CE1	2.46	0.50
14:U:424:ASP:O	14:U:425:LEU:HD12	2.12	0.50
9:X:37:TRP:NE1	9:X:40:LYS:HD2	2.26	0.50
1:1:219:ASN:HD22	18:1:502:FMN:P	2.35	0.50
12:K:79:PHE:CD2	12:K:85:THR:HA	2.47	0.50
14:M:127:ILE:HB	14:M:128:PRO:HD3	1.93	0.50
15:N:181:VAL:HA	15:N:192:PHE:CE2	2.47	0.50
4:4:47:LEU:HD13	4:4:51:GLU:O	2.11	0.50
10:A:33:PRO:HD2	16:H:70:GLU:HB2	1.93	0.50
3:D:123:ASP:OD2	3:D:241:ARG:HA	2.11	0.50
3:D:260:PRO:HB2	3:D:617:LEU:HB3	1.94	0.50
14:M:93:GLY:O	14:M:136:TYR:OH	2.20	0.50
14:U:338:THR:HG22	14:U:340:GLU:H	1.75	0.50
9:X:51:HIS:CE1	9:X:111:LEU:HD21	2.47	0.50
4:4:162:TRP:N	7:9:34:LYS:HG3	2.25	0.50
3:D:186:ARG:NH1	3:D:229:ILE:O	2.36	0.50
4:E:38:HIS:HA	20:E:501:DCQ:H8	1.94	0.50
4:E:390:VAL:HB	4:E:391:PRO:HD3	1.94	0.50
16:H:196:PHE:N	16:H:263:PHE:O	2.41	0.50
14:M:36:ASN:HD22	14:M:39:LEU:HD12	1.77	0.50
7:O:40:ARG:HH22	7:O:173:PHE:HE1	1.59	0.50
11:R:53:PHE:CE2	16:Q:120:LEU:HB2	2.47	0.50
10:P:109:TYR:HE2	11:R:154:VAL:HG11	1.76	0.50
14:U:350:SER:HB3	14:U:422:VAL:H	1.76	0.50
9:W:7:ARG:NE	9:W:61:ASP:OD2	2.45	0.50
2:2:101:THR:HG23	2:2:106:ILE:O	2.12	0.50
3:3:166:LYS:NZ	3:3:179:GLU:OE1	2.30	0.50
3:3:21:ASP:OD1	3:3:432:PHE:N	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:156:ILE:O	4:4:159:LEU:HB2	2.12	0.50
4:E:211:SER:HB3	4:E:214:PHE:HD2	1.77	0.50
16:H:119:ASP:OD1	16:H:120:LEU:HG	2.12	0.50
16:H:274:VAL:CG2	16:H:275:PRO:HD2	2.42	0.50
11:J:93:ALA:O	11:J:97:ALA:N	2.30	0.50
15:V:95:MET:SD	15:V:214:SER:HB3	2.52	0.50
1:1:253:GLN:O	1:1:327:GLY:HA2	2.12	0.50
2:2:146:THR:HG23	2:2:149:ARG:H	1.77	0.50
3:3:459:MET:HA	3:3:462:ALA:HB3	1.94	0.50
4:4:122:GLU:HB2	4:4:290:ILE:HD11	1.94	0.50
4:4:250:LYS:HE2	4:4:262:PHE:HB3	1.92	0.50
5:5:113:PHE:O	5:5:116:ARG:HB2	2.12	0.50
3:D:157:PHE:CE1	3:D:159:PHE:HB2	2.46	0.50
5:F:186:GLY:HA2	5:F:190:LYS:HD3	1.93	0.50
8:I:89:ALA:O	8:I:91:ILE:HG13	2.12	0.50
11:J:99:GLY:O	11:J:103:ILE:HG22	2.12	0.50
13:L:84:GLY:O	13:L:88:HIS:ND1	2.39	0.50
14:M:90:ARG:HB2	14:M:331:ARG:CZ	2.42	0.50
16:Q:177:VAL:HG21	16:Q:185:ILE:HG12	1.94	0.50
16:Q:226:GLN:C	16:Q:299:ARG:HH12	2.16	0.50
1:1:250:LYS:HB3	1:1:252:TYR:CE1	2.47	0.49
7:9:9:SER:O	7:9:12:ILE:HG13	2.11	0.49
1:B:260:ARG:HA	2:C:177:HIS:O	2.12	0.49
15:N:340:ALA:HA	15:N:343:TRP:HD1	1.77	0.49
13:T:392:THR:HG22	13:T:399:GLY:HA3	1.94	0.49
1:1:259:LYS:HE3	1:1:260:ARG:HH21	1.76	0.49
3:3:33:PHE:HB2	3:3:45:CYS:SG	2.52	0.49
6:6:37:TRP:HB3	6:6:75:ALA:HA	1.94	0.49
10:A:113:LYS:HG3	15:N:18:PHE:HE1	1.77	0.49
3:D:576:ALA:O	3:D:580:LYS:NZ	2.42	0.49
16:H:117:ASN:O	16:H:181:ASN:ND2	2.45	0.49
16:H:221:LEU:N	16:H:222:PRO:HA	2.26	0.49
16:H:224:ALA:HA	16:H:229:VAL:HA	1.93	0.49
14:M:313:TYR:OH	14:M:443:MET:O	2.22	0.49
15:N:62:PHE:CE2	15:N:285:LEU:HD22	2.47	0.49
16:Q:122:ILE:HA	16:Q:125:LEU:HD12	1.92	0.49
16:Q:213:GLU:N	16:Q:213:GLU:OE1	2.45	0.49
15:V:24:GLY:HA2	15:V:27:ARG:HD2	1.93	0.49
1:1:5:ILE:O	1:1:12:ARG:NH2	2.45	0.49
1:B:356:CYS:N	17:B:501:SF4:S3	2.73	0.49
1:B:264:TYR:CZ	2:C:176:VAL:HG11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:54:THR:HG22	6:G:60:LEU:HB3	1.94	0.49
16:H:185:ILE:HG22	16:H:189:GLN:OE1	2.12	0.49
11:J:23:ARG:HD2	11:J:80:GLU:N	2.28	0.49
13:L:255:ARG:HD2	13:L:477:LEU:HD23	1.95	0.49
13:L:487:LEU:HA	13:L:490:GLU:HG2	1.95	0.49
14:M:131:LEU:O	14:M:135:LEU:HD23	2.11	0.49
15:N:87:LEU:O	15:N:91:ALA:N	2.26	0.49
16:Q:35:GLU:HG3	16:Q:291:ILE:HG23	1.94	0.49
15:V:204:PRO:O	15:V:208:VAL:HG23	2.12	0.49
9:W:59:VAL:HG11	9:W:63:PHE:HE2	1.77	0.49
1:1:201:LEU:HG	1:1:203:PRO:HD2	1.95	0.49
1:1:291:ILE:HD11	1:1:331:ILE:HD11	1.94	0.49
1:B:437:TRP:HB3	2:C:92:GLY:HA3	1.95	0.49
3:D:8:ASP:OD1	3:D:9:ARG:HG3	2.13	0.49
13:L:88:HIS:O	13:L:92:ILE:HG13	2.12	0.49
15:N:204:PRO:O	15:N:208:VAL:HG23	2.13	0.49
13:T:9:LEU:HB2	13:T:10:PRO:HD3	1.95	0.49
1:1:372:ALA:O	1:1:376:THR:OG1	2.20	0.49
2:2:74:PRO:HB2	8:7:121:ARG:NE	2.26	0.49
3:3:165:ASP:OD2	3:3:168:HIS:HB2	2.12	0.49
4:4:211:SER:HB3	4:4:214:PHE:HD2	1.78	0.49
7:9:164:PRO:HA	7:9:178:GLU:HB2	1.94	0.49
1:B:342:TRP:HE1	1:B:372:ALA:HA	1.77	0.49
16:H:161:SER:HG	16:H:310:TRP:HZ3	1.60	0.49
16:H:35:GLU:OE1	16:H:249:TYR:OH	2.19	0.49
14:M:385:TYR:CE1	14:M:389:PRO:HB3	2.46	0.49
10:P:22:VAL:O	10:P:26:LEU:HG	2.13	0.49
10:P:77:PHE:O	10:P:80:PRO:HD2	2.12	0.49
16:Q:265:GLY:O	16:Q:282:LYS:NZ	2.28	0.49
14:U:186:GLN:HG2	14:U:187:GLU:H	1.77	0.49
14:U:238:VAL:HA	14:U:241:PHE:HB2	1.93	0.49
4:4:103:LYS:HE3	5:5:22:LEU:HB3	1.94	0.49
4:4:158:ASP:OD1	6:6:57:ARG:NH1	2.46	0.49
7:9:111:GLY:N	8:7:44:MET:HG2	2.27	0.49
3:D:185:LYS:O	3:D:189:ARG:HB2	2.11	0.49
13:L:405:GLY:O	13:L:409:VAL:HG23	2.12	0.49
15:N:59:SER:OG	15:N:100:SER:OG	2.19	0.49
16:Q:154:ARG:HD3	16:Q:222:PRO:HG3	1.95	0.49
14:U:218:HIS:O	14:U:282:LYS:NZ	2.37	0.49
15:V:251:GLN:OE1	15:V:256:ARG:HD3	2.13	0.49
4:4:224:ILE:HG22	4:4:229:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:80:TRP:HA	5:5:80:TRP:CE3	2.48	0.49
3:D:186:ARG:HD2	3:D:231:PRO:HD3	1.95	0.49
10:A:62:TYR:HD2	11:J:66:LEU:HD11	1.78	0.49
14:M:237:GLY:O	14:M:241:PHE:N	2.37	0.49
15:N:248:ALA:HB2	15:N:260:TYR:HB3	1.94	0.49
14:U:451:ALA:HA	14:U:454:LEU:HG	1.95	0.49
15:V:153:LEU:HD22	15:V:171:LEU:HD11	1.93	0.49
1:1:220:ASN:N	18:1:502:FMN:O3P	2.30	0.49
6:6:114:SER:OG	7:9:96:LEU:O	2.31	0.49
3:D:190:TYR:O	3:D:195:PRO:HD2	2.12	0.49
16:Q:236:TYR:HD1	16:Q:240:LYS:HD2	1.77	0.49
1:1:203:PRO:HB2	1:1:204:PRO:HD3	1.94	0.49
2:2:42:ARG:HB3	2:2:44:GLU:OE1	2.13	0.49
4:4:156:ILE:HA	4:4:159:LEU:HD12	1.95	0.49
2:C:4:PHE:N	2:C:48:GLU:OE2	2.38	0.49
3:D:300:TRP:CD1	3:D:703:GLN:HA	2.48	0.49
4:E:333:GLU:O	4:E:363:SER:OG	2.26	0.49
4:E:73:ARG:NH2	7:O:64:PRO:O	2.46	0.49
13:L:325:HIS:CE1	13:L:329:LYS:HG3	2.48	0.49
15:V:62:PHE:CE2	15:V:285:LEU:HD22	2.48	0.49
8:7:71:ASP:OD2	8:7:81:ARG:NH2	2.44	0.49
7:9:33:LEU:HD11	7:9:119:PHE:CE2	2.46	0.49
1:B:291:ILE:O	1:B:328:VAL:HA	2.13	0.49
1:B:94:ASP:O	18:B:502:FMN:N3	2.38	0.49
13:L:9:LEU:HB2	13:L:10:PRO:HD3	1.94	0.49
14:M:327:LEU:O	14:M:331:ARG:HG2	2.12	0.49
15:N:249:LEU:HD23	15:N:374:TYR:HD2	1.77	0.49
11:R:100:VAL:HA	13:T:598:LEU:HD21	1.95	0.49
13:T:90:TYR:OH	13:T:338:SER:N	2.46	0.49
14:U:22:ARG:HD2	14:U:23:ALA:CA	2.42	0.49
7:O:126:TYR:HB3	9:X:39:ASP:CG	2.34	0.49
1:B:92:ASN:ND2	18:B:502:FMN:HO3'	2.08	0.48
3:D:631:ASN:HD22	3:D:634:ALA:HB3	1.78	0.48
14:M:224:SER:HA	14:M:330:GLY:HA3	1.94	0.48
15:N:217:ALA:HA	15:N:285:LEU:HD23	1.95	0.48
7:O:43:LEU:O	7:O:138:VAL:HG13	2.13	0.48
16:Q:119:ASP:OD1	16:Q:120:LEU:HG	2.13	0.48
16:Q:186:VAL:HG11	16:Q:267:TRP:CZ3	2.48	0.48
13:T:298:SER:O	13:T:302:GLN:HG2	2.13	0.48
13:T:60:LEU:HD21	14:U:375:PRO:HB3	1.95	0.48
9:X:78:VAL:HB	9:X:127:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:114:GLU:O	4:4:118:VAL:HG13	2.13	0.48
6:6:33:SER:O	6:6:36:LEU:HG	2.13	0.48
6:6:74:GLN:NE2	16:H:233:HIS:HB2	2.28	0.48
4:E:26:MET:N	10:P:54:VAL:HG21	2.28	0.48
5:F:80:TRP:CE3	5:F:80:TRP:HA	2.47	0.48
8:I:86:LEU:HB2	8:I:91:ILE:HB	1.93	0.48
11:J:5:GLU:O	11:J:9:LEU:HG	2.13	0.48
11:J:63:ILE:O	11:J:66:LEU:N	2.46	0.48
13:T:4:LEU:HG	13:T:8:LEU:HG	1.95	0.48
15:V:96:HIS:CE1	15:V:100:SER:HG	2.31	0.48
4:4:194:LEU:HD11	4:4:290:ILE:HG21	1.95	0.48
1:B:87:HIS:HD2	1:B:215:PRO:HD2	1.78	0.48
3:D:516:VAL:O	3:D:520:ARG:HG3	2.14	0.48
14:M:22:ARG:HD2	14:M:23:ALA:CA	2.42	0.48
15:N:163:LEU:HD13	15:N:226:VAL:HA	1.94	0.48
13:T:104:PHE:HZ	13:T:235:PRO:HG2	1.78	0.48
13:T:427:GLY:O	13:T:428:GLU:HG2	2.12	0.48
4:4:64:THR:HB	4:4:66:PHE:CE1	2.49	0.48
8:7:89:ALA:O	8:7:91:ILE:HG13	2.14	0.48
7:9:102:GLY:HA2	7:9:115:LEU:HD11	1.95	0.48
3:D:300:TRP:O	3:D:589:HIS:NE2	2.44	0.48
13:L:1:MET:HA	13:L:55:PHE:CD2	2.48	0.48
16:Q:146:LYS:CA	16:Q:149:LEU:HB2	2.37	0.48
16:Q:333:PRO:HG2	16:Q:336:TYR:CD1	2.48	0.48
13:T:291:ILE:HG13	13:T:292:LYS:N	2.29	0.48
15:V:283:PHE:HB2	15:V:420:LEU:HD13	1.94	0.48
1:1:339:ASP:OD1	1:1:433:ARG:NH2	2.46	0.48
2:2:112:THR:HG22	2:2:117:PHE:H	1.77	0.48
3:3:182:ILE:HG23	3:3:232:VAL:HG11	1.95	0.48
3:3:345:LEU:O	3:3:372:GLN:N	2.46	0.48
5:5:53:VAL:HG13	5:5:71:VAL:HB	1.95	0.48
1:B:44:VAL:HG13	1:B:48:LYS:HD2	1.94	0.48
4:E:158:ASP:OD2	6:G:57:ARG:NH2	2.46	0.48
4:E:225:PRO:HG2	4:E:228:VAL:HB	1.95	0.48
10:P:93:PHE:O	10:P:96:VAL:HG12	2.14	0.48
16:Q:40:ALA:HB2	16:Q:45:ARG:HH21	1.78	0.48
10:P:62:TYR:CD2	11:R:66:LEU:HD11	2.47	0.48
13:T:214:VAL:O	13:T:218:ALA:N	2.47	0.48
13:T:313:GLY:HA2	13:T:315:TYR:CZ	2.49	0.48
13:T:328:PHE:O	13:T:331:LEU:HB3	2.14	0.48
13:T:501:ALA:O	13:T:505:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:167:ARG:HG3	14:U:172:SER:HB3	1.95	0.48
14:U:55:LEU:HD13	14:U:63:TRP:HE1	1.79	0.48
1:1:363:VAL:O	1:1:368:VAL:HG12	2.13	0.48
1:B:104:ARG:NH2	1:B:105:TYR:OH	2.41	0.48
3:D:497:TRP:O	3:D:528:LYS:HE3	2.14	0.48
4:E:363:SER:HB3	5:F:173:ALA:HB1	1.94	0.48
4:E:64:THR:OG1	6:G:83:ARG:HD2	2.13	0.48
16:H:326:LEU:HD12	16:H:330:LEU:HD23	1.96	0.48
13:L:90:TYR:CE2	13:L:334:LEU:HB3	2.49	0.48
14:M:33:PHE:HA	14:M:79:ALA:HB1	1.96	0.48
10:P:68:PHE:HE1	11:R:62:ALA:HA	1.79	0.48
11:R:19:VAL:HG23	11:R:28:ALA:O	2.13	0.48
13:T:136:LEU:O	13:T:140:LEU:HG	2.13	0.48
13:T:219:GLN:O	13:T:223:MET:N	2.46	0.48
13:T:376:LEU:HB3	13:T:379:LEU:HD12	1.95	0.48
13:T:604:MET:HG2	15:V:232:ALA:HB2	1.95	0.48
14:U:346:GLY:HA2	14:U:416:GLU:O	2.13	0.48
1:1:39:GLU:O	1:1:43:ARG:HG2	2.14	0.48
5:5:99:PRO:HB2	5:5:124:ILE:HA	1.96	0.48
7:9:40:ARG:HH22	7:9:173:PHE:HZ	1.59	0.48
1:B:101:PHE:CE1	1:B:253:GLN:HB2	2.49	0.48
1:B:243:THR:HG21	1:B:315:HIS:HE1	1.79	0.48
3:D:413:LEU:HA	3:D:416:PHE:HB3	1.94	0.48
16:H:177:VAL:HA	16:H:188:TRP:CD1	2.49	0.48
16:H:274:VAL:CG1	16:H:278:TRP:CD1	2.88	0.48
13:L:263:LEU:HB3	13:L:266:VAL:HB	1.95	0.48
14:M:187:GLU:HG2	14:M:188:GLU:N	2.28	0.48
10:P:20:ILE:HD12	16:Q:21:VAL:HG11	1.95	0.48
14:U:443:MET:HA	14:U:450:PHE:CE2	2.49	0.48
9:W:38:GLN:HG3	9:W:93:VAL:HG11	1.95	0.48
1:1:106:ILE:HD11	1:1:251:LEU:HD21	1.94	0.48
3:3:185:LYS:O	3:3:189:ARG:HB2	2.14	0.48
3:3:316:ARG:HD3	3:D:675:ARG:HD3	1.96	0.48
3:3:36:GLU:HB3	3:3:39:LEU:HB2	1.96	0.48
3:3:568:TYR:CD1	3:3:572:PRO:HG3	2.49	0.48
4:4:288:LYS:HA	4:4:288:LYS:HD3	1.56	0.48
1:B:342:TRP:CD1	1:B:371:PHE:HB3	2.49	0.48
1:B:427:GLU:OE1	1:B:429:ARG:NH1	2.47	0.48
11:J:16:GLY:HA2	11:J:19:VAL:HG12	1.95	0.48
15:V:62:PHE:HE2	15:V:285:LEU:HD22	1.78	0.48
5:5:163:ARG:NH1	7:9:90:VAL:HG11	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:LYS:NZ	1:B:325:THR:O	2.39	0.48
4:E:91:PHE:CZ	4:E:173:ILE:HB	2.49	0.48
4:E:352:GLU:HB3	4:E:371:ARG:NE	2.28	0.48
6:G:112:ALA:O	6:G:127:VAL:HG23	2.13	0.48
4:E:168:PHE:CE1	6:G:141:PRO:HG3	2.49	0.48
13:T:59:TRP:CH2	13:T:129:ILE:HD11	2.49	0.48
13:T:214:VAL:HG12	13:T:222:LEU:HB2	1.95	0.48
1:1:48:LYS:O	1:1:123:TYR:OH	2.13	0.48
3:3:168:HIS:N	3:3:176:LEU:O	2.36	0.48
4:4:143:LEU:HD23	4:4:143:LEU:H	1.78	0.48
1:B:350:HIS:O	3:D:205:ARG:NH1	2.45	0.48
13:L:90:TYR:OH	13:L:338:SER:OG	2.19	0.48
15:N:422:ALA:O	15:N:423:LEU:HD23	2.14	0.48
7:O:51:GLU:N	7:O:81:VAL:O	2.46	0.48
16:Q:37:ARG:NH2	16:Q:54:PHE:O	2.41	0.48
13:T:355:LEU:H	13:T:425:PHE:HA	1.78	0.48
15:V:103:HIS:HE1	15:V:161:LEU:HB2	1.76	0.48
5:5:105:THR:HA	5:5:108:TRP:O	2.13	0.47
6:6:120:ASN:HD22	6:6:122:ALA:H	1.62	0.47
6:6:163:TYR:CD1	7:9:152:ARG:HD2	2.49	0.47
7:9:6:LEU:HD23	16:H:297:TRP:CE2	2.48	0.47
3:D:48:CYS:HB3	19:D:804:FES:S2	2.53	0.47
4:E:133:LEU:HD11	4:E:149:ALA:HB2	1.96	0.47
4:E:214:PHE:HA	4:E:217:ARG:HB2	1.96	0.47
16:H:293:ILE:HD12	16:H:297:TRP:CZ3	2.49	0.47
14:M:109:LEU:HD21	14:M:236:VAL:HG21	1.96	0.47
14:M:335:ARG:NH2	14:M:429:GLU:OE2	2.47	0.47
15:N:216:LYS:NZ	15:N:266:ALA:HB2	2.29	0.47
16:Q:31:MET:SD	16:Q:287:LEU:HD13	2.54	0.47
18:1:502:FMN:H9	18:1:502:FMN:H1'1	1.60	0.47
4:4:208:PHE:CE2	4:4:276:MET:HG2	2.48	0.47
5:5:159:PHE:HB2	5:5:163:ARG:HB2	1.95	0.47
3:D:36:GLU:HB3	3:D:39:LEU:HB2	1.95	0.47
4:E:166:GLN:OE1	4:E:170:HIS:HA	2.14	0.47
4:E:27:THR:H	10:P:54:VAL:HG11	1.79	0.47
4:E:33:GLN:HE22	20:E:501:DCQ:H10A	1.79	0.47
4:E:86:ASP:HB3	4:E:93:HIS:HD2	1.79	0.47
6:G:39:ALA:HB2	6:G:75:ALA:HB3	1.94	0.47
6:6:70:ALA:N	16:H:225:GLU:OE2	2.26	0.47
16:H:306:LEU:O	16:H:310:TRP:HB2	2.14	0.47
4:E:318:GLU:HB2	8:I:39:ASP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:147:MET:O	11:R:150:THR:OG1	2.26	0.47
11:R:16:GLY:HA2	11:R:19:VAL:HG12	1.96	0.47
10:P:56:ARG:HD3	11:R:74:LEU:HA	1.96	0.47
14:U:172:SER:OG	14:U:174:THR:O	2.28	0.47
3:3:364:LEU:HD13	3:3:648:LEU:HD13	1.96	0.47
3:3:463:ALA:O	3:3:465:HIS:ND1	2.47	0.47
3:3:688:ARG:HD3	3:3:688:ARG:HA	1.49	0.47
4:4:390:VAL:HB	4:4:391:PRO:HD3	1.96	0.47
4:4:384:ALA:HB1	4:4:396:ILE:HD11	1.96	0.47
6:G:41:PHE:CE2	6:G:43:LEU:HD21	2.50	0.47
6:G:94:ARG:O	6:G:98:GLN:N	2.47	0.47
16:H:216:ARG:CG	16:H:294:ARG:HD2	2.45	0.47
15:N:245:ASN:OD1	15:N:374:TYR:OH	2.32	0.47
3:3:256:CYS:O	3:3:262:GLY:HA2	2.14	0.47
3:3:337:ARG:H	3:3:337:ARG:CD	2.26	0.47
1:B:123:TYR:HA	1:B:167:PHE:CE1	2.48	0.47
1:B:205:PHE:HB2	1:B:208:GLN:OE1	2.14	0.47
1:B:230:ILE:HG23	1:B:235:ALA:HA	1.96	0.47
3:D:706:GLY:O	3:D:709:GLN:HB2	2.15	0.47
4:E:381:LEU:HB3	4:E:382:PRO:HD3	1.95	0.47
13:L:372:ALA:O	13:L:381:GLY:HA3	2.14	0.47
14:M:148:PHE:O	14:M:152:THR:HG23	2.15	0.47
10:P:75:VAL:HG11	16:Q:167:GLY:HA3	1.95	0.47
16:Q:65:LYS:HZ2	16:Q:69:LYS:HE2	1.79	0.47
14:U:306:GLU:O	14:U:379:LEU:HB3	2.14	0.47
14:U:325:LEU:HG	14:U:361:LEU:HB3	1.96	0.47
14:U:43:HIS:NE2	14:U:67:LEU:O	2.32	0.47
3:3:40:SER:HB3	3:3:437:ILE:HG22	1.95	0.47
6:6:33:SER:HB2	6:6:155:GLN:HG2	1.97	0.47
1:B:343:ASN:HD22	2:C:89:LYS:HZ2	1.61	0.47
16:H:147:TYR:CD1	16:H:229:VAL:HG22	2.48	0.47
13:L:380:SER:HB3	13:L:457:GLY:H	1.80	0.47
14:M:316:ALA:O	14:M:320:VAL:HG23	2.15	0.47
13:T:263:LEU:HB3	13:T:266:VAL:HB	1.95	0.47
14:U:127:ILE:HB	14:U:128:PRO:HD3	1.94	0.47
3:3:371:PHE:CZ	3:3:374:ARG:HA	2.49	0.47
6:6:96:TRP:CE3	6:6:97:GLU:HG3	2.50	0.47
7:9:91:TYR:HB3	7:9:133:LYS:HB2	1.97	0.47
2:C:71:GLN:NE2	2:C:120:GLN:OE1	2.46	0.47
3:D:351:LEU:HD11	3:D:615:VAL:HG23	1.95	0.47
3:D:505:LEU:HD21	3:D:507:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:405:GLU:OE1	3:D:509:ALA:N	2.47	0.47
16:H:111:TYR:O	16:H:112:GLN:NE2	2.47	0.47
16:H:260:PRO:HG3	16:H:286:PHE:CD2	2.49	0.47
12:K:15:VAL:O	12:K:19:LEU:HG	2.14	0.47
13:L:444:TRP:O	13:L:447:HIS:HB2	2.14	0.47
10:P:106:GLY:O	10:P:109:TYR:HB3	2.15	0.47
1:1:223:THR:O	1:1:227:VAL:HG23	2.14	0.47
3:3:177:ASP:HB3	3:3:234:ALA:HA	1.96	0.47
4:4:356:TYR:CE2	5:5:55:LEU:HD11	2.49	0.47
6:G:35:SER:OG	16:Q:65:LYS:HD3	2.14	0.47
16:H:274:VAL:HG22	16:H:275:PRO:HD2	1.95	0.47
13:L:293:LYS:O	13:L:297:TYR:HD1	1.98	0.47
13:L:291:ILE:HD12	13:L:336:SER:HB3	1.97	0.47
12:S:15:VAL:O	12:S:19:LEU:HG	2.14	0.47
13:T:512:PHE:HA	13:T:517:PHE:HE1	1.79	0.47
4:4:318:GLU:HB2	8:7:39:ASP:HA	1.97	0.47
1:B:291:ILE:HG12	1:B:299:PRO:HB3	1.97	0.47
16:H:225:GLU:HB3	16:H:226:GLN:HG2	1.97	0.47
8:I:71:ASP:OD2	8:I:81:ARG:NH2	2.46	0.47
16:Q:65:LYS:NZ	16:Q:69:LYS:HE2	2.30	0.47
14:U:157:LEU:HD23	14:U:157:LEU:HA	1.70	0.47
15:V:108:LEU:HA	15:V:111:LEU:HD12	1.96	0.47
1:1:137:GLU:O	2:2:141:TYR:OH	2.26	0.47
3:3:29:ASP:OD1	3:3:29:ASP:N	2.48	0.47
4:4:148:TYR:O	4:4:151:ARG:HB3	2.15	0.47
4:4:254:TYR:HH	4:4:346:THR:HG1	1.51	0.47
3:D:459:MET:HA	3:D:462:ALA:HB3	1.97	0.47
16:H:260:PRO:HG3	16:H:286:PHE:CE2	2.49	0.47
16:H:70:GLU:O	16:H:237:SER:OG	2.28	0.47
11:J:61:GLY:O	11:J:65:VAL:HG21	2.15	0.47
13:L:26:GLU:HB3	13:L:27:PRO:HD3	1.97	0.47
13:T:433:HIS:CG	13:T:433:HIS:O	2.67	0.47
15:V:316:TYR:HB2	15:V:382:VAL:HG12	1.97	0.47
15:V:40:LEU:HD13	15:V:64:LEU:HB2	1.96	0.47
4:4:236:GLY:HA2	4:4:351:GLY:CA	2.41	0.47
7:9:149:GLU:HA	7:9:152:ARG:NE	2.29	0.47
1:B:243:THR:HG22	1:B:244:GLU:H	1.80	0.47
1:B:344:LEU:HD21	2:C:86:LEU:HD22	1.97	0.47
1:B:382:LYS:O	1:B:386:ASN:ND2	2.48	0.47
3:D:165:ASP:OD2	3:D:168:HIS:HB2	2.14	0.47
3:D:19:VAL:HG23	3:D:85:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:48:CYS:O	3:D:82:SER:OG	2.18	0.47
3:D:395:PHE:HB3	3:D:503:PRO:HB3	1.97	0.47
6:G:34:ASN:HB3	16:Q:51:VAL:HG21	1.96	0.47
16:H:232:TYR:HB2	16:H:244:PHE:CD1	2.50	0.47
15:N:201:GLN:OE1	15:N:256:ARG:NH1	2.48	0.47
10:P:66:MET:O	10:P:69:ILE:HG12	2.15	0.47
16:Q:227:GLU:HG2	16:Q:228:LEU:N	2.30	0.47
16:Q:324:THR:O	16:Q:328:VAL:HG23	2.15	0.47
14:U:363:LEU:HD22	14:U:368:LEU:HD13	1.96	0.47
9:W:91:GLU:OE1	9:W:126:TYR:OH	2.22	0.47
3:3:115:HIS:HB3	4:4:321:MET:HE2	1.97	0.47
10:A:106:GLY:O	10:A:109:TYR:HB3	2.15	0.47
1:B:104:ARG:O	1:B:108:GLU:HG3	2.14	0.47
1:B:404:ASP:HA	1:B:407:VAL:HG22	1.95	0.47
3:D:36:GLU:OE1	3:D:37:LYS:N	2.46	0.47
3:D:387:LEU:O	3:D:390:LEU:HB3	2.14	0.47
3:D:439:GLU:HG2	3:D:440:ARG:HG2	1.97	0.47
3:D:582:PHE:HA	3:D:599:HIS:ND1	2.30	0.47
4:E:118:VAL:O	4:E:122:GLU:HG2	2.15	0.47
4:E:80:THR:HG21	7:O:64:PRO:HG3	1.97	0.47
6:G:63:PHE:HA	16:Q:50:ARG:HG2	1.97	0.47
11:R:24:ASN:HA	11:R:77:ALA:O	2.15	0.47
13:T:413:THR:HA	13:T:416:TYR:CE2	2.50	0.47
14:U:448:GLY:O	14:U:452:ARG:HG2	2.15	0.47
15:V:262:SER:OG	15:V:288:TYR:OH	2.27	0.47
1:1:63:ARG:O	1:1:65:ARG:NE	2.46	0.46
4:4:209:ALA:HB2	4:4:277:LEU:HD21	1.96	0.46
7:9:68:ILE:HD11	17:9:201:SF4:S1	2.55	0.46
3:D:133:ARG:NE	3:D:136:GLU:OE2	2.32	0.46
4:E:343:TYR:HB2	4:E:356:TYR:CD1	2.48	0.46
5:F:67:ARG:NH1	5:F:96:GLU:OE2	2.47	0.46
12:K:90:LEU:HB3	15:N:131:GLU:HG3	1.96	0.46
14:M:75:PHE:CZ	14:M:111:ALA:HB2	2.50	0.46
14:M:204:LYS:HE3	14:M:234:TYR:O	2.14	0.46
14:M:371:LEU:HD12	14:M:440:LEU:HB3	1.96	0.46
15:N:87:LEU:HB3	15:N:117:PRO:HB2	1.96	0.46
13:L:586:LEU:HD13	15:N:138:LEU:HD12	1.96	0.46
16:Q:72:ILE:HG22	16:Q:237:SER:HB3	1.97	0.46
14:U:22:ARG:C	14:U:22:ARG:HD2	2.34	0.46
14:U:341:ILE:HG13	14:U:342:GLY:N	2.28	0.46
1:1:53:VAL:O	1:1:57:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:63:HIS:O	6:6:122:ALA:HB1	2.14	0.46
1:B:140:ARG:HB2	2:C:140:PRO:HG3	1.96	0.46
1:B:174:HIS:ND1	2:C:18:TYR:OH	2.42	0.46
3:D:170:LEU:HD11	3:D:176:LEU:HD22	1.97	0.46
4:E:38:HIS:HB2	20:E:501:DCQ:C4	2.44	0.46
5:F:71:VAL:HG11	5:F:89:PHE:HD2	1.79	0.46
16:H:103:GLY:HA2	16:H:267:TRP:CE2	2.50	0.46
13:L:142:ILE:HA	13:L:232:GLY:HA3	1.97	0.46
12:K:88:ASP:OD1	13:L:587:ARG:HG3	2.15	0.46
14:M:91:VAL:HB	14:M:95:PHE:CE1	2.50	0.46
15:N:299:LEU:HD21	15:N:312:LEU:HD11	1.97	0.46
15:N:318:LYS:HD3	15:N:391:PHE:CG	2.51	0.46
15:N:411:ALA:O	15:N:415:LEU:N	2.35	0.46
6:G:138:PRO:HG2	7:O:121:MET:HG3	1.97	0.46
16:Q:143:SER:HB2	16:Q:235:GLU:HG3	1.98	0.46
11:R:19:VAL:HG21	11:R:32:LEU:HB2	1.97	0.46
13:T:108:PHE:HE1	13:T:236:VAL:HG22	1.81	0.46
15:V:52:PRO:HB3	15:V:103:HIS:HB2	1.97	0.46
3:3:232:VAL:HA	17:3:801:SF4:S2	2.56	0.46
4:4:127:ALA:HB1	4:4:153:ARG:NH1	2.30	0.46
4:4:112:ARG:NH1	4:4:181:ASP:OD2	2.46	0.46
5:5:28:VAL:HA	5:5:91:ARG:O	2.15	0.46
1:B:253:GLN:HA	1:B:262:GLY:O	2.15	0.46
4:E:213:ILE:O	4:E:217:ARG:HG2	2.16	0.46
13:L:192:MET:SD	13:L:258:PHE:HE1	2.39	0.46
13:L:422:VAL:O	13:L:426:LEU:N	2.47	0.46
11:R:138:VAL:HG22	15:V:106:LEU:HD22	1.98	0.46
1:1:93:ALA:HB3	1:1:133:TYR:O	2.16	0.46
3:3:722:THR:HG21	3:3:756:GLY:N	2.28	0.46
6:6:99:MET:HG2	6:6:100:PRO:HD2	1.98	0.46
2:C:79:HIS:H	2:C:137:ASN:ND2	2.13	0.46
4:E:216:GLU:O	16:Q:301:ARG:NH1	2.48	0.46
5:F:82:ASP:N	5:F:82:ASP:OD1	2.49	0.46
13:L:163:ARG:HD3	14:M:399:VAL:O	2.15	0.46
14:M:349:GLN:NE2	14:M:418:GLY:HA3	2.30	0.46
14:M:7:LEU:O	14:M:11:VAL:HG12	2.16	0.46
15:N:61:VAL:O	15:N:65:LEU:HG	2.16	0.46
12:S:28:PHE:CE1	12:S:68:VAL:HA	2.46	0.46
15:V:313:ARG:HB2	15:V:384:ALA:HB3	1.97	0.46
2:2:24:ARG:NH2	2:2:59:GLU:HB3	2.31	0.46
4:4:370:VAL:HB	4:4:409:ARG:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:158:VAL:HA	6:6:172:PRO:HB3	1.96	0.46
6:6:39:ALA:HB2	6:6:75:ALA:CB	2.46	0.46
8:7:40:PHE:HA	8:7:43:ARG:HG2	1.97	0.46
7:9:44:THR:HG22	7:9:138:VAL:HG11	1.96	0.46
1:B:190:ASN:OD1	1:B:200:ARG:NE	2.43	0.46
3:D:356:LEU:HD13	3:D:654:PHE:HB2	1.97	0.46
16:Q:131:LEU:HA	16:Q:134:TYR:HB2	1.98	0.46
16:Q:200:PHE:N	16:Q:341:SER:OG	2.46	0.46
13:T:90:TYR:OH	13:T:334:LEU:O	2.15	0.46
13:T:77:LEU:HD12	13:T:116:LEU:HD22	1.98	0.46
15:V:237:VAL:HG11	15:V:271:LEU:HD11	1.97	0.46
15:V:294:LEU:HD12	15:V:405:ALA:HB3	1.97	0.46
1:1:373:LYS:NZ	1:1:383:ASP:OD1	2.44	0.46
3:3:139:LEU:HD12	4:4:326:TYR:CZ	2.51	0.46
4:4:154:GLU:OE2	4:4:167:ARG:NH2	2.47	0.46
2:C:173:GLY:HA3	2:C:176:VAL:O	2.16	0.46
3:D:274:LEU:H	3:D:302:ASP:CB	2.27	0.46
14:M:206:PRO:HD2	14:M:293:MET:HG3	1.98	0.46
15:N:237:VAL:O	15:N:241:VAL:HG23	2.16	0.46
13:T:461:LEU:N	13:T:467:ASN:OD1	2.45	0.46
3:3:38:HIS:ND1	3:3:287:GLU:OE2	2.48	0.46
8:7:86:LEU:HB2	8:7:91:ILE:HB	1.96	0.46
4:4:80:THR:HG21	7:9:64:PRO:HG3	1.98	0.46
3:D:46:ARG:N	19:D:804:FES:S1	2.88	0.46
16:H:190:LYS:HB2	16:H:268:THR:HG21	1.98	0.46
11:J:97:ALA:O	11:J:100:VAL:HG12	2.16	0.46
13:L:433:HIS:O	13:L:433:HIS:CG	2.69	0.46
15:N:262:SER:HG	15:N:288:TYR:HH	1.57	0.46
15:N:317:ARG:NH2	15:N:383:PHE:O	2.49	0.46
13:T:210:PHE:CD1	13:T:270:ILE:HG12	2.51	0.46
13:T:541:LEU:C	13:T:545:PRO:HG2	2.35	0.46
14:U:148:PHE:O	14:U:152:THR:HG23	2.16	0.46
1:1:409:PRO:O	1:1:413:SER:HB3	2.16	0.46
3:3:149:LEU:HD12	4:4:108:VAL:HG23	1.98	0.46
4:4:379:GLN:HG2	5:5:113:PHE:CD2	2.51	0.46
4:4:40:VAL:O	4:4:404:MET:HG3	2.16	0.46
5:5:82:ASP:N	5:5:82:ASP:OD1	2.47	0.46
10:A:29:ALA:O	10:A:34:LYS:NZ	2.28	0.46
10:A:2:ALA:HB3	16:H:119:ASP:OD2	2.16	0.46
4:4:31:GLY:HA3	10:A:45:GLU:OE2	2.16	0.46
6:G:140:CYS:SG	7:O:99:ILE:HG13	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:67:LEU:HD23	16:H:310:TRP:CZ2	2.51	0.46
14:M:54:PRO:HA	14:M:62:TYR:CD1	2.50	0.46
15:N:115:SER:HB2	15:N:119:TYR:CZ	2.50	0.46
15:N:126:ARG:HD2	15:N:128:GLN:HG2	1.97	0.46
13:L:586:LEU:HD11	15:N:135:LYS:HA	1.98	0.46
13:T:90:TYR:CE2	13:T:334:LEU:HB3	2.51	0.46
15:V:155:TYR:HB2	15:V:161:LEU:HD21	1.98	0.46
15:V:63:THR:HG21	15:V:96:HIS:ND1	2.31	0.46
9:X:48:LEU:O	9:X:58:LEU:HD12	2.16	0.46
4:4:247:ASP:OD1	4:4:249:ARG:HG3	2.16	0.46
8:7:49:ASP:OD1	8:7:75:ARG:NE	2.38	0.46
1:B:4:PRO:HA	1:B:12:ARG:HH22	1.80	0.46
2:C:162:ARG:NE	2:C:164:GLU:OE2	2.35	0.46
2:C:78:TYR:CZ	2:C:157:LEU:HD22	2.50	0.46
3:D:119:CYS:HB2	3:D:120:PRO:HD3	1.97	0.46
3:D:37:LYS:HB3	3:D:430:THR:HG21	1.97	0.46
3:D:454:TYR:HB2	3:D:752:ASP:OD2	2.16	0.46
4:E:366:TYR:HE1	5:F:59:THR:HB	1.80	0.46
16:H:333:PRO:HB2	16:H:335:THR:H	1.80	0.46
13:L:469:LEU:HA	13:L:469:LEU:HD12	1.72	0.46
14:M:106:LEU:O	14:M:110:PHE:HD1	1.99	0.46
14:M:331:ARG:HA	14:M:331:ARG:HH11	1.81	0.46
7:O:117:TYR:CZ	7:O:163:VAL:HG11	2.51	0.46
1:1:291:ILE:HG12	1:1:299:PRO:HB3	1.97	0.46
2:2:58:THR:HG23	3:3:213:THR:HA	1.98	0.46
3:3:254:THR:OG1	3:3:624:LEU:HD23	2.16	0.46
4:4:352:GLU:OE2	5:5:87:ARG:NH1	2.42	0.46
4:E:66:PHE:HZ	6:G:83:ARG:HH12	1.63	0.46
13:L:198:ASN:ND2	13:L:201:LEU:HB2	2.31	0.46
13:L:291:ILE:HG13	13:L:292:LYS:N	2.31	0.46
14:M:186:GLN:HG2	14:M:187:GLU:H	1.81	0.46
13:T:348:ASP:OD1	13:T:349:VAL:N	2.47	0.46
13:T:403:TYR:CZ	13:T:493:LEU:HD13	2.51	0.46
13:T:84:GLY:O	13:T:88:HIS:ND1	2.45	0.46
14:U:78:ILE:HG22	14:U:103:GLU:HG3	1.98	0.46
3:3:464:ILE:HG21	3:3:493:ALA:HB2	1.97	0.45
3:3:735:ALA:HA	3:3:744:GLU:HA	1.98	0.45
4:4:356:TYR:HE2	5:5:55:LEU:HD11	1.81	0.45
7:9:33:LEU:HD12	7:9:161:TYR:CG	2.51	0.45
4:E:148:TYR:HE2	7:O:16:TYR:CG	2.34	0.45
4:E:190:LEU:HD23	4:E:294:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:246:TYR:HD1	5:F:78:PRO:HD2	1.81	0.45
13:L:70:ASP:OD2	13:L:73:SER:OG	2.27	0.45
7:O:102:GLY:HA2	7:O:115:LEU:HD11	1.97	0.45
16:Q:227:GLU:HG2	16:Q:228:LEU:H	1.80	0.45
16:Q:276:TYR:HD2	16:Q:280:PHE:HE2	1.64	0.45
16:Q:35:GLU:HA	16:Q:291:ILE:HD13	1.97	0.45
16:Q:301:ARG:NH2	16:Q:304:GLN:HB2	2.31	0.45
16:Q:35:GLU:OE1	16:Q:249:TYR:OH	2.26	0.45
1:1:157:TYR:O	1:1:158:LEU:HD23	2.16	0.45
1:1:222:GLU:OE2	1:1:250:LYS:HD2	2.16	0.45
3:3:115:HIS:O	3:3:161:ARG:HD3	2.15	0.45
4:4:367:ARG:HH12	4:4:369:LYS:HB2	1.79	0.45
1:B:18:TYR:CD2	1:B:21:VAL:HG21	2.51	0.45
3:D:281:GLU:HA	3:D:287:GLU:O	2.15	0.45
3:D:409:LEU:HA	3:D:409:LEU:HD23	1.59	0.45
16:H:308:PHE:O	16:H:312:PHE:HB3	2.16	0.45
13:L:414:ALA:HB1	13:L:505:LEU:HD23	1.96	0.45
15:N:17:GLY:HA3	15:N:82:PHE:CE2	2.51	0.45
16:Q:146:LYS:HG2	16:Q:149:LEU:HD12	1.98	0.45
16:Q:218:PRO:C	16:Q:220:ASP:H	2.20	0.45
11:R:65:VAL:HG11	16:Q:160:ILE:CD1	2.45	0.45
11:R:75:PHE:O	11:R:77:ALA:N	2.50	0.45
14:U:75:PHE:HZ	14:U:111:ALA:HB2	1.81	0.45
15:V:280:ALA:HA	15:V:347:LEU:HD13	1.98	0.45
1:1:254:ILE:HG23	1:1:261:PRO:HA	1.97	0.45
3:3:224:GLY:O	3:3:227:THR:HB	2.17	0.45
3:3:29:ASP:OD2	5:5:187:GLY:N	2.31	0.45
1:B:197:ALA:HB3	2:C:66:PHE:CZ	2.51	0.45
4:E:112:ARG:NH2	4:E:181:ASP:OD1	2.49	0.45
4:E:261:THR:H	4:E:292:GLN:NE2	2.12	0.45
16:H:33:LEU:HD11	16:H:56:LEU:HA	1.98	0.45
13:L:391:ALA:O	13:L:395:TYR:HB2	2.16	0.45
15:N:294:LEU:O	15:N:298:VAL:HG23	2.17	0.45
16:Q:216:ARG:CG	16:Q:294:ARG:HD2	2.46	0.45
11:R:155:ALA:O	15:V:81:ARG:NH1	2.48	0.45
14:U:7:LEU:O	14:U:11:VAL:HG12	2.17	0.45
1:1:195:LEU:HD23	2:2:24:ARG:HH12	1.81	0.45
1:1:401:PRO:HB2	18:1:502:FMN:HM82	1.98	0.45
3:3:33:PHE:HZ	3:3:130:LEU:HA	1.81	0.45
3:3:713:ARG:HE	3:3:746:ARG:HE	1.64	0.45
4:4:382:PRO:O	4:4:386:LYS:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:74:GLU:O	10:A:78:LEU:HG	2.16	0.45
1:B:18:TYR:CZ	1:B:263:VAL:HG11	2.52	0.45
4:E:211:SER:HB2	4:E:214:PHE:HB3	1.97	0.45
11:J:33:ILE:HG12	11:J:64:VAL:HG11	1.97	0.45
13:L:263:LEU:HD13	13:L:266:VAL:HG21	1.99	0.45
13:L:380:SER:HA	13:L:457:GLY:HA2	1.99	0.45
14:M:113:ARG:HH21	14:M:178:GLU:HB2	1.82	0.45
16:Q:204:LEU:HD12	16:Q:348:LEU:HD13	1.99	0.45
16:Q:234:THR:HG22	16:Q:234:THR:O	2.16	0.45
4:4:131:VAL:HG23	4:4:153:ARG:HD2	1.99	0.45
10:A:61:PHE:HB3	11:J:69:PHE:CD2	2.52	0.45
1:B:184:GLU:OE1	1:B:186:THR:OG1	2.19	0.45
3:D:29:ASP:N	3:D:29:ASP:OD1	2.49	0.45
3:D:387:LEU:HA	3:D:387:LEU:HD23	1.76	0.45
4:E:247:ASP:OD1	4:E:249:ARG:HG3	2.16	0.45
13:L:454:VAL:HB	13:L:455:LEU:HD22	1.98	0.45
14:M:302:SER:O	14:M:304:THR:HG23	2.16	0.45
15:N:237:VAL:HG22	15:N:270:ALA:HB3	1.98	0.45
14:U:318:SER:HA	14:U:321:TYR:CE1	2.51	0.45
4:4:211:SER:HB2	4:4:215:TYR:N	2.32	0.45
1:B:53:VAL:O	1:B:57:VAL:HG23	2.16	0.45
4:E:371:ARG:HG3	5:F:51:ASP:OD1	2.15	0.45
5:F:64:ARG:HA	5:F:64:ARG:HD3	1.73	0.45
16:H:271:VAL:HG12	16:H:272:LEU:HG	1.99	0.45
13:L:419:ARG:HD2	13:L:512:PHE:CZ	2.51	0.45
12:K:27:VAL:HG11	15:N:138:LEU:HD13	1.98	0.45
16:Q:163:GLU:O	16:Q:166:LEU:HB2	2.17	0.45
4:4:185:GLU:OE1	4:4:185:GLU:N	2.46	0.45
4:4:62:LEU:HD11	6:6:43:LEU:O	2.17	0.45
7:9:40:ARG:HH21	7:9:118:ASP:CG	2.18	0.45
2:C:50:ALA:HA	2:C:53:VAL:HG12	1.99	0.45
4:E:260:TYR:HA	4:E:292:GLN:NE2	2.32	0.45
4:E:400:LEU:HA	4:E:400:LEU:HD23	1.81	0.45
6:G:37:TRP:CH2	16:Q:36:ARG:NH2	2.85	0.45
16:H:103:GLY:O	16:H:113:PRO:HG2	2.15	0.45
16:H:331:ASP:CG	16:H:334:ARG:HH22	2.20	0.45
10:A:65:ALA:HB1	11:J:66:LEU:HB2	1.99	0.45
11:J:75:PHE:O	11:J:77:ALA:N	2.50	0.45
13:L:328:PHE:O	13:L:331:LEU:HB3	2.16	0.45
14:M:208:PHE:N	14:M:267:SER:OG	2.48	0.45
14:M:318:SER:HA	14:M:321:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:217:ARG:HD2	16:Q:301:ARG:NH1	2.32	0.45
16:Q:37:ARG:HD3	16:Q:47:GLY:HA3	1.98	0.45
4:4:349:ALA:HB3	4:4:350:ARG:HH12	1.82	0.45
1:B:363:VAL:O	1:B:368:VAL:HG12	2.17	0.45
4:E:263:ASP:O	4:E:285:GLU:HG3	2.16	0.45
16:H:274:VAL:HG12	16:H:278:TRP:NE1	2.31	0.45
16:H:32:THR:O	16:H:36:ARG:HG3	2.17	0.45
13:L:427:GLY:O	13:L:428:GLU:HG2	2.17	0.45
14:M:385:TYR:CD1	14:M:389:PRO:HB3	2.52	0.45
16:Q:216:ARG:NH1	16:Q:294:ARG:HB3	2.31	0.45
16:Q:332:LEU:H	16:Q:332:LEU:HD12	1.81	0.45
13:T:575:GLY:HA2	15:V:246:LEU:HB3	1.98	0.45
14:U:305:PRO:O	14:U:309:MET:HB3	2.17	0.45
15:V:340:ALA:HA	15:V:343:TRP:CD1	2.51	0.45
15:V:76:LEU:HD12	15:V:206:PRO:HB3	1.99	0.45
5:5:153:GLY:HA2	9:W:113:ARG:NH2	2.31	0.45
1:1:238:PHE:CE2	1:1:248:GLY:HA3	2.52	0.45
1:1:17:LEU:HD12	1:1:251:LEU:HD11	1.99	0.45
4:4:171:ASN:ND2	4:4:174:ARG:HH22	2.15	0.45
1:B:419:ASP:O	1:B:423:ALA:N	2.36	0.45
3:D:165:ASP:HB3	3:D:178:ARG:HD2	1.99	0.45
3:D:248:GLU:HB3	3:D:270:ARG:NH1	2.31	0.45
3:D:248:GLU:HG2	5:F:170:PHE:CE1	2.52	0.45
3:D:478:LEU:HD12	3:D:520:ARG:NH2	2.32	0.45
4:E:33:GLN:N	4:E:40:VAL:HG23	2.31	0.45
6:G:154:LEU:O	6:G:158:VAL:HG13	2.17	0.45
16:H:140:GLY:HA3	16:H:152:SER:HB3	1.99	0.45
13:L:335:ALA:O	13:L:339:VAL:HG23	2.16	0.45
15:N:95:MET:HA	15:N:114:LEU:HD22	1.99	0.45
15:N:203:SER:HB2	15:N:208:VAL:HG22	1.98	0.45
10:P:105:VAL:HG22	15:V:15:LEU:HD11	1.99	0.45
10:P:62:TYR:OH	12:S:73:GLY:N	2.50	0.45
16:Q:237:SER:OG	16:Q:238:SER:N	2.49	0.45
13:T:41:PHE:HB2	13:T:81:THR:HB	1.98	0.45
14:U:347:LEU:HB2	14:U:414:PHE:HA	1.98	0.45
14:U:68:ASP:OD2	14:U:243:ARG:NH2	2.50	0.45
9:W:32:TYR:OH	9:W:115:MET:HG2	2.17	0.45
9:X:90:TYR:HB3	9:X:118:ALA:HB1	1.99	0.45
4:4:283:MET:O	4:4:287:VAL:HG23	2.17	0.45
1:B:107:LEU:O	1:B:111:PRO:HG3	2.17	0.45
1:B:157:TYR:O	1:B:158:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:THR:HG23	2:C:149:ARG:H	1.82	0.45
3:D:128:CYS:HB3	3:D:131:GLN:HB2	1.99	0.45
4:E:41:LEU:HD12	4:E:42:ARG:H	1.82	0.45
11:J:5:GLU:OE2	12:K:3:TYR:OH	2.31	0.45
13:L:108:PHE:CE1	13:L:236:VAL:HG22	2.52	0.45
14:M:114:ASP:HB3	14:M:176:LEU:HD23	1.99	0.45
14:M:69:GLY:O	14:M:73:LEU:CD2	2.57	0.45
10:P:110:GLU:O	10:P:114:GLY:N	2.49	0.45
16:Q:267:TRP:O	16:Q:269:MET:N	2.50	0.45
15:V:321:LEU:HD13	15:V:403:VAL:HG21	1.98	0.45
4:4:381:LEU:HB3	4:4:382:PRO:HD3	1.98	0.44
10:A:96:VAL:HA	10:A:99:PHE:HB3	1.99	0.44
1:B:243:THR:N	1:B:246:SER:O	2.50	0.44
1:B:96:SER:HA	1:B:135:ARG:NH1	2.31	0.44
2:C:93:ALA:HA	2:C:96:LEU:HB3	1.99	0.44
3:D:237:ASP:OD1	3:D:239:THR:HG22	2.17	0.44
3:D:618:GLU:OE2	3:D:620:ARG:NE	2.49	0.44
3:D:681:LYS:HB3	3:D:681:LYS:HE3	1.70	0.44
3:D:688:ARG:HA	3:D:688:ARG:HD3	1.76	0.44
4:E:288:LYS:HD3	4:E:288:LYS:HA	1.76	0.44
16:H:69:LYS:HB3	16:H:238:SER:HA	1.99	0.44
16:H:266:GLY:HA2	16:H:279:MET:HE1	1.98	0.44
6:G:148:ILE:HG21	7:O:26:TYR:HD2	1.80	0.44
13:T:13:GLY:O	13:T:17:LEU:HG	2.17	0.44
13:T:549:LEU:O	13:T:553:LEU:HG	2.17	0.44
3:3:421:LYS:N	3:3:436:GLN:OE1	2.46	0.44
3:3:378:PRO:HD2	3:3:683:LEU:HD23	1.99	0.44
3:3:19:VAL:HG23	3:3:85:THR:O	2.17	0.44
4:4:193:LEU:HA	4:4:196:VAL:HG12	1.99	0.44
4:4:72:HIS:HB3	5:5:171:ARG:CZ	2.47	0.44
7:9:123:ASP:HB3	7:9:129:LEU:HG	1.98	0.44
7:9:40:ARG:NH2	7:9:173:PHE:HZ	2.15	0.44
10:A:56:ARG:HB3	11:J:73:LEU:O	2.17	0.44
1:B:62:LEU:HD11	1:B:223:THR:HG23	1.98	0.44
16:H:304:GLN:HE22	16:H:307:ARG:HD2	1.81	0.44
13:T:461:LEU:HB3	13:T:465:LEU:HB2	1.99	0.44
14:U:106:LEU:O	14:U:110:PHE:HD1	2.00	0.44
14:U:75:PHE:CZ	14:U:111:ALA:HB2	2.52	0.44
14:U:302:SER:O	14:U:304:THR:HG23	2.18	0.44
14:U:463:LYS:HA	14:U:463:LYS:HD2	1.77	0.44
1:1:241:MET:HG2	1:1:267:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:164:ASN:HD22	6:6:170:LEU:HD21	1.82	0.44
1:B:259:LYS:O	2:C:179:VAL:N	2.35	0.44
6:G:105:VAL:HB	6:G:132:PRO:O	2.17	0.44
16:H:36:ARG:NH2	16:H:62:ASP:OD2	2.50	0.44
13:L:90:TYR:CD2	13:L:334:LEU:HD13	2.53	0.44
14:M:146:TYR:HE1	15:N:376:LEU:HB3	1.82	0.44
14:M:172:SER:OG	14:M:174:THR:O	2.33	0.44
14:M:69:GLY:HA3	14:M:453:GLY:HA3	1.99	0.44
16:Q:12:MET:HG2	16:Q:111:TYR:CD2	2.52	0.44
16:Q:147:TYR:CD1	16:Q:229:VAL:HG22	2.52	0.44
16:Q:222:PRO:HG2	16:Q:230:GLY:HA2	1.99	0.44
14:U:54:PRO:HA	14:U:62:TYR:CD1	2.43	0.44
12:S:63:VAL:HG13	15:V:112:GLU:HG3	1.99	0.44
1:1:343:ASN:O	1:1:346:ARG:HG2	2.18	0.44
3:3:406:ALA:O	3:3:409:LEU:HB2	2.18	0.44
3:3:149:LEU:HG	4:4:305:PRO:HD2	2.00	0.44
4:4:73:ARG:HH11	5:5:171:ARG:HH21	1.66	0.44
1:B:293:GLY:HA3	1:B:297:THR:HG21	1.98	0.44
1:B:66:GLY:HA3	18:B:502:FMN:H3'	2.00	0.44
2:C:31:LEU:HD22	2:C:41:ILE:HD13	2.00	0.44
1:B:364:ALA:HB3	3:D:207:VAL:HG13	2.00	0.44
16:H:202:ALA:O	16:H:205:VAL:HG22	2.18	0.44
12:K:1:MET:HG3	12:K:5:LEU:HD11	2.00	0.44
15:N:345:LYS:NZ	15:N:368:SER:OG	2.49	0.44
4:E:180:GLU:HG3	7:O:36:ARG:HH12	1.83	0.44
16:Q:226:GLN:HB2	16:Q:299:ARG:HH22	1.83	0.44
11:R:97:ALA:HB2	12:S:16:TYR:HB2	2.00	0.44
15:V:175:ALA:O	15:V:179:LEU:HG	2.18	0.44
4:4:130:LEU:HD22	4:4:149:ALA:HB1	1.99	0.44
4:4:375:PHE:HB2	4:4:407:VAL:HA	1.98	0.44
5:5:75:VAL:HG21	5:5:87:ARG:HH21	1.82	0.44
2:C:81:GLN:NE2	2:C:135:GLN:OE1	2.50	0.44
3:D:729:PRO:HD2	3:D:732:ALA:HB3	1.98	0.44
4:E:353:LEU:HD12	4:E:354:GLY:H	1.82	0.44
11:J:23:ARG:HG2	11:J:80:GLU:HG2	1.99	0.44
14:M:402:SER:HA	14:M:405:TYR:CE2	2.52	0.44
13:T:129:ILE:HG12	14:U:369:PRO:HB2	1.98	0.44
13:T:365:HIS:CD2	13:T:450:ALA:HB2	2.52	0.44
15:V:95:MET:HB3	15:V:218:ALA:HB2	1.99	0.44
1:1:107:LEU:O	1:1:111:PRO:HG3	2.18	0.44
2:2:83:CYS:SG	2:2:124:CYS:HA	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:276:MET:O	4:4:280:ILE:HG13	2.18	0.44
10:A:109:TYR:HE2	11:J:154:VAL:HG21	1.82	0.44
3:D:337:ARG:H	3:D:337:ARG:CD	2.31	0.44
4:E:159:LEU:O	4:E:163:VAL:HG12	2.17	0.44
4:E:73:ARG:HG2	4:E:81:TYR:CE1	2.52	0.44
4:E:75:TYR:HA	4:E:78:ASN:HD22	1.83	0.44
4:E:147:PHE:HD2	6:G:56:ALA:HB2	1.82	0.44
4:E:158:ASP:CG	6:G:57:ARG:HH22	2.21	0.44
10:A:70:LEU:HD13	11:J:150:THR:HG22	2.00	0.44
14:M:55:LEU:HD22	14:M:63:TRP:CE2	2.52	0.44
15:N:362:VAL:O	15:N:366:VAL:HG23	2.17	0.44
15:N:87:LEU:HB3	15:N:117:PRO:CB	2.47	0.44
5:F:163:ARG:NH1	7:O:90:VAL:HG11	2.33	0.44
16:Q:96:ALA:HB2	16:Q:128:VAL:HG21	2.00	0.44
16:Q:260:PRO:HG3	16:Q:286:PHE:CE2	2.53	0.44
15:V:128:GLN:NE2	15:V:305:ASP:OD1	2.50	0.44
15:V:45:GLY:HA3	15:V:425:ALA:O	2.17	0.44
1:1:356:CYS:HB3	1:1:358:PRO:HG2	1.99	0.44
6:6:171:PRO:HA	6:6:172:PRO:HD3	1.87	0.44
6:6:37:TRP:O	6:6:75:ALA:HB1	2.18	0.44
11:J:109:TRP:CE3	11:J:109:TRP:HA	2.53	0.44
13:L:139:PHE:CD2	13:L:155:ALA:HB1	2.52	0.44
13:L:288:GLN:NE2	13:L:529:ARG:O	2.51	0.44
13:L:463:HIS:NE2	13:L:487:LEU:HD13	2.33	0.44
15:N:103:HIS:O	15:N:107:MET:HB2	2.17	0.44
16:Q:159:LEU:O	16:Q:163:GLU:HB2	2.18	0.44
16:Q:269:MET:HG3	16:Q:270:PRO:HD2	2.00	0.44
16:Q:216:ARG:CB	16:Q:294:ARG:HD2	2.46	0.44
3:3:616:ASN:OD1	3:3:617:LEU:HD23	2.18	0.44
4:4:346:THR:HG22	4:4:353:LEU:O	2.18	0.44
5:5:64:ARG:HD3	5:5:64:ARG:HA	1.64	0.44
6:6:44:ALA:CB	6:6:83:ARG:HE	2.31	0.44
7:9:33:LEU:HG	7:9:161:TYR:HB2	2.00	0.44
7:9:40:ARG:HD2	7:9:131:TYR:HE2	1.83	0.44
1:B:223:THR:O	1:B:227:VAL:HG23	2.17	0.44
1:B:381:GLU:HG3	1:B:422:LEU:HD22	2.00	0.44
5:F:167:PRO:HA	5:F:170:PHE:HB3	1.99	0.44
16:H:150:LEU:HD23	16:H:154:ARG:HD2	1.99	0.44
13:T:342:ALA:HA	13:T:436:HIS:CE1	2.53	0.44
13:T:491:TRP:HA	13:T:494:ILE:HG12	1.99	0.44
14:U:141:ARG:HG3	14:U:142:THR:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:343:ARG:HB3	14:U:344:TYR:HD1	1.83	0.44
15:V:3:LEU:HD13	15:V:96:HIS:HD2	1.83	0.44
4:4:134:GLY:HA3	4:4:146:PHE:HD1	1.82	0.44
4:4:358:VAL:O	4:4:366:TYR:N	2.51	0.44
10:A:23:ALA:O	10:A:27:VAL:HG23	2.18	0.44
3:D:110:PHE:O	3:D:113:LEU:HB2	2.17	0.44
3:D:135:VAL:HA	4:E:326:TYR:CZ	2.53	0.44
4:E:73:ARG:HG3	4:E:77:GLN:OE1	2.18	0.44
6:G:40:THR:HB	6:G:68:PHE:CZ	2.53	0.44
13:L:115:MET:HG2	13:L:244:THR:HG22	1.99	0.44
13:L:323:PHE:CZ	13:L:327:PHE:HE2	2.36	0.44
10:P:109:TYR:HE1	15:V:82:PHE:CZ	2.35	0.44
14:U:204:LYS:HA	14:U:204:LYS:HD2	1.77	0.44
14:U:271:GLY:HA2	14:U:287:TYR:HD1	1.83	0.44
14:U:347:LEU:HD13	14:U:422:VAL:HG21	1.99	0.44
15:V:196:THR:HG22	15:V:259:ALA:HB1	2.00	0.44
1:1:65:ARG:HB2	1:1:223:THR:OG1	2.17	0.43
1:1:393:LEU:HD22	3:3:106:GLY:HA3	2.00	0.43
4:4:353:LEU:HD12	4:4:354:GLY:H	1.82	0.43
5:5:163:ARG:NE	7:9:92:GLU:OE1	2.51	0.43
7:9:56:CYS:SG	7:9:58:LEU:HG	2.57	0.43
10:A:93:PHE:O	10:A:96:VAL:HG12	2.18	0.43
1:B:357:THR:N	1:B:358:PRO:HD2	2.32	0.43
3:D:21:ASP:OD1	3:D:432:PHE:N	2.44	0.43
4:E:276:MET:O	4:E:280:ILE:HG13	2.18	0.43
13:L:41:PHE:HD2	13:L:42:LEU:HD12	1.83	0.43
14:M:426:ALA:O	14:M:430:TRP:N	2.50	0.43
10:P:71:PHE:CE2	10:P:107:PHE:HB2	2.53	0.43
11:R:5:GLU:O	11:R:9:LEU:HG	2.18	0.43
15:V:201:GLN:HA	15:V:255:LYS:HE3	2.00	0.43
15:V:385:ARG:HH12	15:V:387:GLU:HG2	1.83	0.43
9:X:80:LEU:O	9:X:84:GLN:HG2	2.18	0.43
3:3:283:PRO:HA	3:3:287:GLU:HA	2.01	0.43
4:4:221:VAL:HG11	4:4:392:ASP:CG	2.38	0.43
5:5:154:GLU:HG2	6:6:119:ASN:O	2.18	0.43
4:4:81:TYR:CZ	6:6:117:MET:HG3	2.53	0.43
7:9:2:THR:OG1	7:9:2:THR:O	2.36	0.43
10:A:110:GLU:OE1	16:H:310:TRP:NE1	2.38	0.43
1:B:201:LEU:O	1:B:204:PRO:HD2	2.18	0.43
1:B:262:GLY:HA3	2:C:176:VAL:HG12	2.00	0.43
5:F:71:VAL:HA	5:F:90:VAL:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:93:PHE:CE2	16:Q:326:LEU:HD13	2.53	0.43
13:T:463:HIS:CD2	13:T:464:PRO:HD3	2.52	0.43
13:T:287:GLY:HA3	13:T:528:SER:HB2	2.01	0.43
9:X:21:LEU:HD12	9:X:24:LEU:HB3	1.98	0.43
1:1:205:PHE:HB2	1:1:208:GLN:HE22	1.83	0.43
1:1:273:ARG:NH2	1:1:304:GLU:OE1	2.44	0.43
1:1:41:ALA:HB2	1:1:116:GLU:HG3	2.01	0.43
3:3:370:ASP:OD2	3:3:558:TRP:HD1	2.02	0.43
3:3:415:GLU:HA	3:3:420:LEU:HD12	2.01	0.43
4:4:191:LYS:HE2	4:4:294:LEU:HD21	2.00	0.43
4:4:50:GLU:OE1	16:H:154:ARG:NH1	2.33	0.43
8:7:27:LYS:HA	8:7:27:LYS:HD3	1.91	0.43
10:A:48:ASN:OD1	10:A:49:ASP:HB2	2.18	0.43
1:B:112:HIS:CE1	1:B:148:ALA:HB1	2.54	0.43
1:B:184:GLU:HG2	18:B:502:FMN:C8	2.48	0.43
18:B:502:FMN:H1'1	18:B:502:FMN:H9	1.67	0.43
2:C:29:PRO:O	2:C:32:ARG:HB3	2.18	0.43
4:E:346:THR:HG22	4:E:353:LEU:O	2.19	0.43
5:F:163:ARG:CZ	7:O:90:VAL:HG11	2.48	0.43
5:F:49:LEU:HD21	5:F:52:ILE:HD11	1.99	0.43
6:G:39:ALA:HB2	6:G:75:ALA:CB	2.49	0.43
4:E:314:ARG:O	8:I:46:ARG:NH2	2.51	0.43
7:O:149:GLU:O	7:O:153:THR:CB	2.67	0.43
16:Q:141:TRP:HE3	16:Q:149:LEU:HD11	1.81	0.43
9:X:37:TRP:CD1	9:X:40:LYS:HB2	2.41	0.43
4:4:28:LEU:HA	10:A:50:PRO:O	2.19	0.43
1:B:404:ASP:OD1	1:B:404:ASP:N	2.51	0.43
1:B:436:LEU:HD23	2:C:90:LEU:O	2.18	0.43
2:C:89:LYS:HA	2:C:93:ALA:HB3	2.00	0.43
3:D:184:CYS:SG	3:D:185:LYS:N	2.90	0.43
3:D:224:GLY:O	3:D:227:THR:HB	2.17	0.43
16:H:217:THR:HG23	16:H:298:PHE:O	2.19	0.43
16:H:267:TRP:O	16:H:269:MET:N	2.51	0.43
13:L:219:GLN:NE2	13:L:277:THR:HG21	2.33	0.43
16:Q:224:ALA:HA	16:Q:229:VAL:HA	2.01	0.43
13:T:325:HIS:CD2	13:T:329:LYS:HG3	2.53	0.43
13:T:329:LYS:HA	13:T:332:LEU:HD13	2.00	0.43
14:U:134:TYR:O	14:U:141:ARG:HD3	2.17	0.43
14:U:21:PRO:HD2	14:U:24:LEU:HG	2.00	0.43
1:1:170:ASP:OD1	1:1:171:LEU:N	2.51	0.43
4:4:272:VAL:N	4:4:275:ARG:HH21	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:317:LEU:HA	4:4:317:LEU:HD12	1.81	0.43
6:6:62:ARG:HA	16:H:48:PRO:HA	2.00	0.43
2:C:42:ARG:HB2	2:C:45:ARG:HG2	2.00	0.43
4:E:148:TYR:HB3	4:E:200:ARG:NH2	2.33	0.43
5:F:101:LEU:HD23	5:F:126:PHE:CE2	2.53	0.43
4:E:72:HIS:ND1	5:F:152:LEU:HD22	2.33	0.43
14:M:209:PRO:HD3	14:M:263:LEU:HD22	1.99	0.43
14:M:367:GLY:O	14:M:374:PHE:HB2	2.18	0.43
15:N:13:LEU:HD21	15:N:28:ALA:HB3	2.00	0.43
16:Q:287:LEU:O	16:Q:291:ILE:HG13	2.18	0.43
11:R:2:SER:HA	11:R:5:GLU:HB3	2.00	0.43
13:T:328:PHE:O	13:T:332:LEU:HD13	2.18	0.43
13:T:586:LEU:HB2	15:V:135:LYS:NZ	2.33	0.43
14:U:331:ARG:HA	14:U:331:ARG:HD2	1.78	0.43
14:U:43:HIS:CD2	14:U:48:ALA:HB2	2.54	0.43
14:U:43:HIS:NE2	14:U:45:GLY:O	2.51	0.43
15:V:124:TRP:O	15:V:125:ARG:HB2	2.19	0.43
15:V:119:TYR:CE2	15:V:137:PHE:HA	2.53	0.43
3:3:297:GLY:O	3:3:300:TRP:NE1	2.50	0.43
10:A:71:PHE:HZ	10:A:107:PHE:HB2	1.83	0.43
3:D:33:PHE:HZ	3:D:130:LEU:HA	1.84	0.43
3:D:414:SER:O	3:D:418:ARG:NE	2.33	0.43
6:G:46:CYS:SG	6:G:109:GLY:HA3	2.59	0.43
16:H:289:PHE:O	16:H:293:ILE:HG12	2.18	0.43
13:L:107:TYR:CD2	13:L:140:LEU:HB3	2.53	0.43
14:M:452:ARG:HA	14:M:452:ARG:HD3	1.73	0.43
15:N:177:GLY:O	15:N:181:VAL:HG23	2.18	0.43
16:Q:333:PRO:HB2	16:Q:335:THR:H	1.83	0.43
14:U:238:VAL:O	14:U:241:PHE:HB2	2.18	0.43
14:U:270:TYR:O	14:U:274:VAL:HG23	2.19	0.43
3:3:118:ASP:O	3:3:122:CYS:N	2.52	0.43
3:3:385:ALA:O	3:3:533:LEU:HD21	2.18	0.43
4:4:183:PRO:HB2	4:4:185:GLU:OE1	2.19	0.43
4:4:214:PHE:HA	4:4:217:ARG:HB2	2.00	0.43
4:4:41:LEU:HD13	4:4:59:ILE:HG22	2.00	0.43
8:7:50:LEU:HA	8:7:51:PRO:HD3	1.88	0.43
1:B:39:GLU:O	1:B:43:ARG:HG2	2.17	0.43
3:D:129:GLU:O	3:D:133:ARG:HG2	2.19	0.43
3:D:133:ARG:HH21	3:D:136:GLU:CD	2.19	0.43
3:D:570:PHE:O	3:D:572:PRO:HD3	2.19	0.43
3:D:616:ASN:HD22	3:D:622:LEU:HD11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:83:CYS:SG	3:D:84:VAL:HG13	2.58	0.43
4:E:272:VAL:N	4:E:275:ARG:HH21	2.17	0.43
4:E:87:TYR:CZ	4:E:403:VAL:HG13	2.53	0.43
5:F:120:ASP:OD2	5:F:135:ILE:N	2.50	0.43
6:G:66:GLU:OE1	16:Q:45:ARG:NH1	2.52	0.43
16:H:301:ARG:O	16:H:302:TYR:CD1	2.71	0.43
13:L:119:VAL:O	13:L:251:TYR:OH	2.28	0.43
14:M:201:PHE:CE2	14:M:245:ALA:HB2	2.54	0.43
14:M:341:ILE:HG13	14:M:342:GLY:N	2.32	0.43
13:L:129:ILE:HG12	14:M:369:PRO:HB2	2.01	0.43
16:Q:213:GLU:HG2	16:Q:251:HIS:CE1	2.53	0.43
12:S:25:ILE:HG13	12:S:25:ILE:H	1.61	0.43
13:T:373:LEU:HD23	13:T:417:ALA:HB2	2.00	0.43
14:U:316:ALA:O	14:U:320:VAL:HG23	2.18	0.43
2:2:129:HIS:CD2	2:2:130:THR:HG23	2.54	0.43
3:3:505:LEU:HB3	3:3:532:VAL:HG22	2.01	0.43
3:3:715:GLU:H	3:3:761:SER:CB	2.31	0.43
7:9:44:THR:OG1	7:9:52:LYS:HD2	2.19	0.43
10:A:69:ILE:HA	11:J:62:ALA:HB1	2.01	0.43
1:B:245:GLN:HB2	1:B:314:GLU:OE2	2.19	0.43
3:D:17:THR:HG22	3:D:18:SER:O	2.18	0.43
3:D:654:PHE:CE2	3:D:660:ALA:HA	2.54	0.43
4:E:38:HIS:HE1	4:E:398:ALA:HA	1.84	0.43
4:E:72:HIS:HB3	5:F:171:ARG:HH21	1.84	0.43
11:J:23:ARG:HD2	11:J:80:GLU:H	1.84	0.43
13:L:317:VAL:HG12	13:L:388:ILE:HG12	2.01	0.43
13:L:341:HIS:O	13:L:436:HIS:HE1	2.01	0.43
15:N:21:PRO:O	15:N:25:VAL:HG23	2.18	0.43
10:P:62:TYR:CE2	12:S:72:LEU:HB3	2.54	0.43
14:U:305:PRO:HA	14:U:458:ALA:HB1	2.01	0.43
1:1:50:PRO:HA	1:1:53:VAL:HG12	2.01	0.43
3:3:178:ARG:HH22	8:7:65:GLU:CD	2.22	0.43
3:3:409:LEU:HD23	3:3:409:LEU:HA	1.63	0.43
4:4:169:HIS:CD2	6:6:141:PRO:HD3	2.42	0.43
7:9:33:LEU:O	7:9:163:VAL:HG12	2.19	0.43
7:9:88:ALA:HB3	7:9:133:LYS:NZ	2.33	0.43
10:A:99:PHE:O	10:A:102:LEU:HB2	2.18	0.43
1:B:90:ILE:HA	1:B:131:TYR:O	2.19	0.43
2:C:112:THR:HG23	2:C:115:GLY:H	1.83	0.43
3:D:385:ALA:HB3	3:D:533:LEU:HG	2.01	0.43
3:D:52:ILE:HD12	3:D:80:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:74:LEU:HD12	5:F:88:PHE:CE1	2.53	0.43
8:I:27:LYS:HA	8:I:27:LYS:HD3	1.81	0.43
13:L:434:HIS:HB3	13:L:435:PRO:HD3	2.00	0.43
13:L:501:ALA:O	13:L:505:LEU:HG	2.19	0.43
14:M:347:LEU:HB2	14:M:414:PHE:HA	2.00	0.43
10:P:67:LEU:O	10:P:71:PHE:HD1	2.02	0.43
16:Q:170:LEU:HD23	16:Q:170:LEU:HA	1.83	0.43
16:Q:257:ALA:O	16:Q:260:PRO:HD2	2.19	0.43
13:T:14:PHE:HB2	13:T:109:ASN:HB2	2.01	0.43
13:T:187:GLU:HA	13:T:190:GLU:HG2	2.01	0.43
14:U:17:LEU:HD11	14:U:98:LEU:HD23	2.01	0.43
15:V:143:ALA:HB1	15:V:182:GLY:HA2	2.00	0.43
1:1:113:LEU:HD12	1:1:228:VAL:HG21	2.01	0.43
1:1:302:PHE:CZ	1:1:307:LEU:HD21	2.54	0.43
3:3:28:TYR:CE2	3:3:96:LEU:HD11	2.54	0.43
4:4:166:GLN:OE1	4:4:170:HIS:HA	2.18	0.43
1:B:207:ALA:O	1:B:215:PRO:HB3	2.19	0.43
1:B:312:SER:O	1:B:316:LEU:HD12	2.17	0.43
1:B:433:ARG:NH1	2:C:94:GLU:HG3	2.33	0.43
3:D:735:ALA:HA	3:D:744:GLU:HA	2.01	0.43
6:G:132:PRO:HG3	6:G:178:ARG:NE	2.33	0.43
4:E:61:TYR:O	6:G:85:SER:HB3	2.18	0.43
16:H:267:TRP:HB3	16:H:279:MET:HB2	2.01	0.43
14:M:143:ARG:HA	14:M:143:ARG:HD3	1.81	0.43
14:M:36:ASN:HA	14:M:39:LEU:HD12	2.00	0.43
14:M:352:PRO:HG3	14:M:424:ASP:OD2	2.19	0.43
14:M:424:ASP:O	14:M:425:LEU:HD12	2.18	0.43
15:N:194:PHE:O	15:N:197:PRO:HD2	2.19	0.43
15:N:331:LEU:O	15:N:335:GLY:N	2.51	0.43
7:O:54:ILE:HG12	7:O:110:THR:HG21	2.01	0.43
10:P:64:VAL:O	10:P:67:LEU:HB2	2.19	0.43
16:Q:50:ARG:O	16:Q:52:GLY:N	2.52	0.43
14:U:30:GLY:O	14:U:34:LEU:HG	2.19	0.43
3:3:487:SER:OG	3:3:490:VAL:HG23	2.19	0.42
4:4:249:ARG:HG3	4:4:347:GLU:HB3	2.00	0.42
1:B:273:ARG:O	1:B:277:TYR:HB2	2.19	0.42
3:D:464:ILE:HD12	3:D:464:ILE:H	1.83	0.42
4:E:162:TRP:NE1	7:O:34:LYS:HD2	2.34	0.42
4:E:172:TYR:O	4:E:179:LYS:HB2	2.19	0.42
6:G:83:ARG:HB2	6:G:123:ILE:HD12	2.01	0.42
16:H:156:SER:O	16:H:160:ILE:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:399:GLY:HA2	13:L:402:PHE:CD2	2.53	0.42
16:Q:224:ALA:O	16:Q:229:VAL:HG12	2.19	0.42
13:T:285:ALA:O	13:T:294:ILE:HG13	2.19	0.42
13:T:377:PRO:HG3	13:T:498:ALA:HB1	2.00	0.42
14:U:143:ARG:HA	14:U:143:ARG:HD3	1.65	0.42
14:U:218:HIS:HA	14:U:221:ASN:HD22	1.84	0.42
15:V:87:LEU:O	15:V:90:TYR:HB2	2.18	0.42
1:1:242:GLY:HA2	1:1:268:MET:O	2.18	0.42
4:4:213:ILE:O	4:4:217:ARG:HG2	2.19	0.42
5:5:163:ARG:HB3	7:9:69:TYR:CD2	2.53	0.42
10:A:67:LEU:HB3	16:H:310:TRP:CZ2	2.53	0.42
1:B:437:TRP:CH2	2:C:147:ARG:HG3	2.54	0.42
1:B:72:THR:HG21	1:B:223:THR:CG2	2.49	0.42
3:D:176:LEU:HD13	3:D:235:LEU:CD2	2.49	0.42
4:E:167:ARG:HH11	6:G:143:ARG:HH12	1.65	0.42
16:H:120:LEU:HD22	16:H:180:LEU:HD12	2.02	0.42
16:H:200:PHE:HB3	16:H:201:PRO:HD3	2.00	0.42
16:H:205:VAL:HA	16:H:313:LEU:HD22	2.01	0.42
16:H:227:GLU:HG2	16:H:228:LEU:N	2.33	0.42
13:L:328:PHE:O	13:L:332:LEU:HD12	2.18	0.42
13:L:348:ASP:OD1	13:L:349:VAL:N	2.51	0.42
14:M:204:LYS:HD2	14:M:204:LYS:HA	1.88	0.42
14:M:306:GLU:O	14:M:379:LEU:HB3	2.20	0.42
11:R:65:VAL:HG23	16:Q:134:TYR:CZ	2.54	0.42
15:V:422:ALA:O	15:V:423:LEU:HD23	2.18	0.42
3:3:621:VAL:HG23	3:3:672:ALA:HA	2.00	0.42
3:3:83:CYS:SG	3:3:84:VAL:N	2.92	0.42
4:4:39:GLY:H	20:4:501:DCQ:C2	2.32	0.42
5:5:154:GLU:CD	5:5:171:ARG:HH22	2.23	0.42
4:4:314:ARG:HB3	8:7:44:MET:HE1	2.00	0.42
8:7:61:ASP:OD1	8:7:64:GLY:N	2.52	0.42
1:B:162:LEU:O	1:B:165:THR:HG22	2.18	0.42
1:B:177:ALA:HB3	2:C:67:TYR:CG	2.54	0.42
2:C:8:GLN:HA	2:C:11:LEU:HD12	2.00	0.42
4:E:140:LEU:HG	16:Q:299:ARG:HH11	1.85	0.42
16:H:83:VAL:O	16:H:86:PRO:HD2	2.19	0.42
13:L:219:GLN:O	13:L:223:MET:N	2.52	0.42
13:L:413:THR:HA	13:L:416:TYR:CZ	2.53	0.42
10:P:67:LEU:HD23	16:Q:310:TRP:NE1	2.33	0.42
15:V:228:ALA:HB1	15:V:233:LEU:HD13	2.02	0.42
15:V:388:GLU:OE1	15:V:388:GLU:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:61:VAL:O	15:V:65:LEU:HG	2.18	0.42
6:6:178:ARG:NE	9:W:125:ILE:HG22	2.34	0.42
3:3:83:CYS:SG	3:3:84:VAL:HG13	2.59	0.42
3:D:124:LYS:HG2	3:D:236:LEU:HD21	2.00	0.42
4:E:317:LEU:HA	4:E:317:LEU:HD12	1.82	0.42
16:H:190:LYS:HD3	16:H:268:THR:HG22	2.01	0.42
8:I:36:ASP:HA	8:I:54:ILE:HA	2.01	0.42
11:J:65:VAL:HG11	16:H:160:ILE:CD1	2.49	0.42
14:M:95:PHE:HB3	14:M:136:TYR:CE2	2.54	0.42
12:K:28:PHE:CZ	15:N:137:PHE:HZ	2.38	0.42
11:R:100:VAL:HG23	13:T:598:LEU:HD21	2.01	0.42
13:T:65:PHE:CZ	13:T:67:LEU:HD21	2.54	0.42
15:V:294:LEU:O	15:V:298:VAL:HG23	2.20	0.42
3:3:460:LYS:HB2	3:3:460:LYS:HE2	1.80	0.42
4:4:108:VAL:O	4:4:304:ASP:HB2	2.18	0.42
4:4:61:TYR:O	6:6:85:SER:HB3	2.20	0.42
1:B:4:PRO:HA	1:B:12:ARG:NH2	2.35	0.42
3:D:356:LEU:HD22	3:D:638:LEU:HD12	2.00	0.42
4:E:246:TYR:CD1	5:F:78:PRO:HD2	2.54	0.42
5:F:121:LEU:HD13	5:F:146:LEU:HD12	2.00	0.42
16:H:155:SER:OG	16:H:156:SER:N	2.53	0.42
14:M:159:MET:HG3	14:M:197:PHE:CE1	2.55	0.42
11:R:69:PHE:CZ	16:Q:156:SER:HB3	2.54	0.42
16:Q:201:PRO:HG2	16:Q:320:TRP:CE3	2.55	0.42
13:T:388:ILE:O	13:T:392:THR:OG1	2.36	0.42
13:T:539:ASN:HA	13:T:543:VAL:HB	2.00	0.42
9:X:21:LEU:HD21	9:X:26:LEU:HD11	2.01	0.42
9:X:31:VAL:O	9:X:90:TYR:N	2.45	0.42
1:1:87:HIS:CD2	1:1:215:PRO:HD2	2.53	0.42
3:3:166:LYS:HG3	3:3:177:ASP:OD1	2.18	0.42
3:3:398:VAL:HG11	3:3:402:PRO:HG3	2.00	0.42
3:3:512:LEU:HD21	3:3:534:ALA:HB1	2.01	0.42
7:9:4:LYS:HB3	16:H:352:VAL:HG13	2.01	0.42
7:9:94:ASN:OD1	7:9:97:ARG:N	2.53	0.42
4:E:336:HIS:ND1	5:F:189:ARG:O	2.52	0.42
6:G:135:VAL:HG22	7:O:124:TYR:CD2	2.55	0.42
14:M:157:LEU:HD23	14:M:157:LEU:HA	1.82	0.42
15:N:138:LEU:HA	15:N:138:LEU:HD23	1.84	0.42
15:N:343:TRP:CE2	15:N:416:PRO:HG3	2.54	0.42
15:N:343:TRP:NE1	15:N:413:GLY:O	2.29	0.42
10:P:57:PHE:HB2	11:R:73:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:13:TYR:CZ	16:Q:95:LEU:HA	2.54	0.42
13:T:114:MET:HG3	13:T:133:GLY:HA3	2.02	0.42
15:V:309:LEU:HD22	15:V:378:LEU:HD11	2.00	0.42
15:V:85:TYR:O	15:V:88:VAL:HB	2.20	0.42
3:3:154:TYR:CE1	4:4:307:PRO:HB3	2.54	0.42
3:3:693:TYR:HD1	3:3:770:ARG:HG2	1.83	0.42
4:4:98:ALA:O	4:4:102:GLU:HG3	2.18	0.42
4:4:114:GLU:HA	4:4:117:ARG:HD3	2.02	0.42
4:4:43:LEU:HD13	4:4:55:VAL:HG11	2.02	0.42
1:B:197:ALA:HB3	2:C:66:PHE:CE2	2.55	0.42
16:H:224:ALA:O	16:H:229:VAL:HG12	2.19	0.42
16:H:96:ALA:CB	16:H:128:VAL:HG21	2.49	0.42
3:D:165:ASP:HB2	8:I:66:PRO:HG2	2.01	0.42
13:L:114:MET:HG3	13:L:133:GLY:HA3	2.01	0.42
13:L:136:LEU:O	13:L:140:LEU:HG	2.20	0.42
13:L:477:LEU:HD12	13:L:477:LEU:HA	1.71	0.42
14:M:306:GLU:HG3	14:M:306:GLU:H	1.70	0.42
13:L:164:ILE:HG12	14:M:400:ILE:HG12	2.02	0.42
14:M:78:ILE:O	14:M:82:VAL:HG23	2.19	0.42
15:N:279:GLN:HG3	15:N:423:LEU:HB2	2.02	0.42
10:P:57:PHE:CE2	16:Q:146:LYS:HD2	2.55	0.42
16:Q:231:GLY:C	16:Q:233:HIS:H	2.23	0.42
13:T:380:SER:HB3	13:T:457:GLY:H	1.84	0.42
1:1:198:ASN:HB3	1:1:355:LYS:HD2	2.01	0.42
1:1:380:GLU:N	1:1:383:ASP:OD2	2.41	0.42
3:3:7:ASN:OD1	3:3:94:ASP:HA	2.18	0.42
20:4:501:DCQ:H7	20:4:501:DCQ:H1M	1.76	0.42
6:6:163:TYR:HD1	7:9:152:ARG:HD2	1.82	0.42
8:7:105:THR:HG23	8:7:110:LEU:HB2	2.02	0.42
3:D:656:LEU:HD21	9:X:3:ARG:HD3	2.02	0.42
4:E:142:ALA:HB2	16:Q:297:TRP:O	2.20	0.42
5:F:53:VAL:HG13	5:F:71:VAL:HB	2.01	0.42
5:F:75:VAL:HG13	5:F:87:ARG:HB2	2.02	0.42
16:H:208:ILE:O	16:H:211:MET:HG2	2.19	0.42
13:L:171:LEU:O	13:L:175:ILE:HG13	2.19	0.42
13:L:373:LEU:HD21	13:L:416:TYR:HE1	1.85	0.42
14:M:202:ALA:HB1	14:M:207:LEU:HD12	2.02	0.42
14:M:56:LEU:HB2	14:M:61:VAL:HB	2.00	0.42
15:N:99:ALA:O	15:N:225:ARG:NH1	2.52	0.42
15:N:334:LEU:HD13	15:N:375:TYR:CD2	2.55	0.42
16:Q:224:ALA:HA	16:Q:230:GLY:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:515:LYS:HA	13:T:517:PHE:CZ	2.54	0.42
13:T:70:ASP:OD2	13:T:73:SER:OG	2.34	0.42
14:U:407:LEU:HA	14:U:407:LEU:HD23	1.84	0.42
15:V:177:GLY:O	15:V:181:VAL:HG23	2.20	0.42
15:V:297:ALA:O	15:V:301:GLN:HG3	2.20	0.42
2:2:29:PRO:O	2:2:32:ARG:HB3	2.20	0.42
4:4:91:PHE:HD2	4:4:121:ASN:HB2	1.85	0.42
4:4:159:LEU:O	4:4:163:VAL:HG12	2.20	0.42
4:4:352:GLU:O	4:4:373:PRO:HB3	2.20	0.42
5:5:101:LEU:HD23	5:5:126:PHE:CE2	2.55	0.42
5:5:75:VAL:HG21	5:5:87:ARG:NH2	2.34	0.42
6:6:112:ALA:O	6:6:127:VAL:HG23	2.20	0.42
2:C:110:GLU:OE2	8:I:114:ARG:NH2	2.52	0.42
3:D:272:GLY:O	3:D:630:GLU:N	2.41	0.42
4:E:374:SER:HA	4:E:377:ASN:HB2	2.01	0.42
13:L:194:GLY:HA3	13:L:195:PRO:HD3	1.93	0.42
13:L:513:GLN:O	13:L:515:LYS:HG3	2.20	0.42
15:N:265:HIS:HA	15:N:268:TYR:CD2	2.54	0.42
10:P:71:PHE:HZ	10:P:107:PHE:HB2	1.83	0.42
10:P:63:VAL:O	10:P:67:LEU:HD13	2.20	0.42
15:V:201:GLN:O	15:V:255:LYS:NZ	2.46	0.42
1:1:338:VAL:HG11	1:1:424:LEU:HD22	2.02	0.42
2:2:154:LEU:HD23	2:2:154:LEU:HA	1.95	0.42
5:5:57:TYR:OH	5:5:91:ARG:NH1	2.52	0.42
1:B:167:PHE:CE2	1:B:169:PHE:HB2	2.55	0.42
1:B:254:ILE:HG23	1:B:261:PRO:HA	2.02	0.42
1:B:298:PRO:HG3	1:B:408:TRP:HB3	2.01	0.42
2:C:65:SER:HA	2:C:72:PHE:CZ	2.55	0.42
9:W:43:GLN:HE21	3:D:522:ARG:HH22	1.68	0.42
14:M:8:LEU:HB3	14:M:9:PRO:HD3	2.02	0.42
15:N:116:LEU:HA	15:N:119:TYR:CD2	2.55	0.42
13:T:267:SER:HB3	13:T:311:GLY:O	2.20	0.42
13:T:290:ASP:OD1	13:T:347:GLN:HG2	2.20	0.42
14:U:160:LEU:O	14:U:163:VAL:HG12	2.19	0.42
14:U:202:ALA:O	14:U:206:PRO:HA	2.19	0.42
2:2:66:PHE:CZ	3:3:205:ARG:HD3	2.55	0.41
3:3:79:LEU:HD22	3:3:100:VAL:HG22	2.02	0.41
4:4:321:MET:HB2	4:4:321:MET:HE2	1.78	0.41
4:4:376:VAL:O	4:4:379:GLN:HG3	2.20	0.41
5:5:3:LEU:HB2	5:5:86:SER:HB2	2.02	0.41
1:B:212:TRP:CZ2	2:C:22:GLY:HA3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:371:PHE:CZ	3:D:374:ARG:HA	2.54	0.41
3:D:464:ILE:HA	3:D:489:MET:SD	2.59	0.41
16:H:216:ARG:NH1	16:H:294:ARG:O	2.50	0.41
13:L:433:HIS:O	13:L:433:HIS:ND1	2.52	0.41
16:Q:289:PHE:O	16:Q:293:ILE:HG12	2.19	0.41
11:R:93:ALA:O	11:R:97:ALA:N	2.44	0.41
13:T:309:ALA:HB2	13:T:388:ILE:CD1	2.50	0.41
14:U:55:LEU:HD22	14:U:63:TRP:CE2	2.54	0.41
1:1:18:TYR:OH	1:1:105:TYR:HB2	2.20	0.41
2:2:149:ARG:NE	2:2:169:PRO:O	2.53	0.41
2:2:45:ARG:O	2:2:49:ILE:HG13	2.20	0.41
3:3:114:ASN:OD1	3:3:161:ARG:HA	2.20	0.41
3:3:8:ASP:OD1	3:3:9:ARG:HG3	2.20	0.41
5:5:71:VAL:HG11	5:5:89:PHE:HD2	1.85	0.41
10:A:74:GLU:HB2	10:A:103:LEU:CD2	2.49	0.41
1:B:176:GLY:HA2	2:C:28:MET:HE2	2.02	0.41
3:D:309:PRO:HG2	3:D:320:ALA:O	2.19	0.41
16:H:104:PRO:HD3	16:H:267:TRP:HE1	1.85	0.41
13:L:598:LEU:HA	13:L:598:LEU:HD23	1.91	0.41
13:L:90:TYR:CG	13:L:334:LEU:HD13	2.55	0.41
14:M:128:PRO:O	14:M:132:MET:HG2	2.20	0.41
16:Q:16:LYS:HE3	16:Q:16:LYS:HB2	1.88	0.41
16:Q:208:ILE:O	16:Q:211:MET:HG2	2.20	0.41
13:T:339:VAL:HG22	13:T:359:LEU:HD13	2.02	0.41
14:U:131:LEU:O	14:U:135:LEU:HD23	2.20	0.41
15:V:105:LEU:O	15:V:109:VAL:HG23	2.21	0.41
15:V:84:PHE:HZ	15:V:123:THR:O	2.03	0.41
1:1:104:ARG:O	1:1:108:GLU:HG3	2.20	0.41
1:1:162:LEU:O	1:1:165:THR:HG22	2.19	0.41
1:1:212:TRP:HE1	2:2:22:GLY:CA	2.32	0.41
4:4:147:PHE:O	4:4:151:ARG:N	2.38	0.41
4:4:161:GLU:OE2	6:6:143:ARG:NH2	2.51	0.41
5:5:147:ARG:HG2	5:5:147:ARG:H	1.65	0.41
1:B:160:LYS:H	1:B:160:LYS:HG2	1.66	0.41
1:B:343:ASN:O	1:B:346:ARG:HG2	2.20	0.41
4:E:38:HIS:CE1	4:E:398:ALA:HA	2.55	0.41
4:E:366:TYR:OH	5:F:56:ASP:O	2.24	0.41
6:G:37:TRP:CE2	6:G:67:VAL:HB	2.55	0.41
13:L:187:GLU:HA	13:L:190:GLU:HG2	2.02	0.41
11:J:96:LEU:HD22	13:L:594:VAL:HG12	2.01	0.41
14:M:242:PHE:CZ	14:M:461:PHE:HD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:280:ALA:HA	15:N:347:LEU:HD13	2.03	0.41
12:S:2:SER:HA	12:S:5:LEU:HD12	2.02	0.41
13:T:161:VAL:HG21	13:T:225:TRP:HB3	2.03	0.41
13:T:24:MET:SD	13:T:28:LEU:HD23	2.60	0.41
13:T:526:ALA:HB1	13:T:529:ARG:HH22	1.86	0.41
13:T:542:ILE:O	13:T:546:LEU:HG	2.20	0.41
9:W:90:TYR:HB3	9:W:118:ALA:HB1	2.01	0.41
9:X:110:LEU:HD12	9:X:110:LEU:O	2.20	0.41
1:1:183:GLY:HA3	18:1:502:FMN:O4	2.20	0.41
1:1:356:CYS:SG	1:1:399:PHE:HB2	2.59	0.41
1:1:357:THR:N	1:1:358:PRO:HD2	2.35	0.41
1:1:212:TRP:CZ2	2:2:19:PRO:HD2	2.55	0.41
3:3:369:LEU:HD13	3:3:549:VAL:HA	2.03	0.41
4:4:62:LEU:HD23	4:4:62:LEU:HA	1.77	0.41
4:4:72:HIS:HB3	5:5:171:ARG:NE	2.35	0.41
5:5:140:ASP:OD2	9:W:90:TYR:OH	2.33	0.41
8:7:10:TYR:O	8:7:14:VAL:HG23	2.20	0.41
3:3:247:TRP:NE1	7:9:61:ALA:HB2	2.35	0.41
1:B:230:ILE:HA	1:B:234:GLY:O	2.21	0.41
1:B:381:GLU:HG2	1:B:385:GLU:OE2	2.20	0.41
1:B:219:ASN:ND2	18:B:502:FMN:O2P	2.53	0.41
3:D:175:ILE:HG22	3:D:236:LEU:HB2	2.02	0.41
3:D:225:ASN:O	3:D:229:ILE:HG13	2.20	0.41
4:E:125:ARG:HG3	4:E:349:ALA:HB2	2.01	0.41
4:E:201:ILE:HA	4:E:204:TYR:CD2	2.54	0.41
4:E:236:GLY:HA2	4:E:351:GLY:CA	2.49	0.41
4:E:75:TYR:HA	4:E:78:ASN:ND2	2.35	0.41
16:H:217:THR:HA	16:H:219:PHE:HB2	2.01	0.41
16:H:45:ARG:HG2	16:H:46:MET:H	1.85	0.41
13:L:361:GLN:HB2	13:L:443:LEU:HD23	2.02	0.41
13:L:549:LEU:O	13:L:553:LEU:HG	2.20	0.41
6:G:162:ALA:HB1	7:O:124:TYR:CZ	2.56	0.41
16:Q:120:LEU:HA	16:Q:180:LEU:HB3	2.01	0.41
16:Q:255:ALA:O	16:Q:259:ILE:HG13	2.20	0.41
14:U:224:SER:HA	14:U:330:GLY:CA	2.50	0.41
15:V:126:ARG:HA	15:V:126:ARG:HD2	1.46	0.41
1:1:3:GLY:HA2	1:1:4:PRO:HD3	1.86	0.41
3:3:14:PRO:HG2	3:3:17:THR:OG1	2.20	0.41
3:3:312:ARG:HA	3:3:316:ARG:O	2.21	0.41
3:3:618:GLU:OE2	3:3:620:ARG:NE	2.44	0.41
4:4:84:ARG:O	6:6:83:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:132:LEU:HD23	5:5:132:LEU:HA	1.86	0.41
6:6:34:ASN:HA	6:6:155:GLN:HE21	1.85	0.41
8:7:101:LYS:H	8:7:101:LYS:HG2	1.68	0.41
7:9:163:VAL:O	7:9:178:GLU:N	2.53	0.41
10:A:31:LEU:HD13	16:H:68:PHE:CZ	2.56	0.41
1:B:32:TYR:OH	1:B:116:GLU:OE1	2.24	0.41
2:C:81:GLN:HB3	2:C:122:VAL:HG21	2.01	0.41
4:E:350:ARG:O	4:E:373:PRO:HB2	2.21	0.41
4:E:60:GLY:N	4:E:408:ASP:OD1	2.50	0.41
6:G:99:MET:HB3	6:G:103:LYS:HD3	2.02	0.41
12:K:7:SER:HB3	12:K:40:LEU:HD23	2.02	0.41
13:L:112:ILE:O	13:L:116:LEU:HG	2.21	0.41
14:M:436:SER:O	14:M:440:LEU:HD13	2.21	0.41
14:M:164:LEU:HD21	15:N:346:TYR:HE1	1.85	0.41
7:O:108:CYS:HB2	7:O:113:ILE:HG22	2.03	0.41
16:Q:123:LEU:HD13	16:Q:180:LEU:HD13	2.01	0.41
13:T:242:ALA:HB1	13:T:326:ALA:HA	2.02	0.41
9:X:7:ARG:NH2	9:X:61:ASP:OD1	2.53	0.41
1:1:83:ASP:OD2	1:1:87:HIS:NE2	2.54	0.41
3:3:136:GLU:HG2	5:5:186:GLY:O	2.20	0.41
2:2:66:PHE:O	3:3:205:ARG:NE	2.54	0.41
4:4:312:PRO:HG3	4:4:323:ALA:O	2.19	0.41
4:4:38:HIS:HB2	20:4:501:DCQ:C4	2.50	0.41
6:6:127:VAL:HG12	6:6:131:VAL:HG22	2.02	0.41
6:6:132:PRO:HG2	6:6:175:ALA:HA	2.03	0.41
1:B:214:LYS:O	1:B:216:THR:HG23	2.21	0.41
3:D:320:ALA:HB1	3:D:324:GLU:HB2	2.02	0.41
11:J:142:VAL:HG21	12:K:59:MET:SD	2.61	0.41
13:L:463:HIS:CD2	13:L:464:PRO:HD3	2.56	0.41
13:L:70:ASP:OD1	13:L:72:LEU:N	2.54	0.41
13:L:7:ILE:HG12	13:L:116:LEU:HB2	2.02	0.41
14:M:151:PHE:HD1	14:M:151:PHE:HA	1.74	0.41
14:M:448:GLY:O	14:M:452:ARG:HG2	2.19	0.41
15:N:155:TYR:HB2	15:N:161:LEU:HD21	2.01	0.41
15:N:299:LEU:HD22	15:N:307:VAL:HG11	2.02	0.41
15:N:316:TYR:HB2	15:N:382:VAL:CG1	2.51	0.41
15:N:97:LEU:HA	15:N:97:LEU:HD23	1.93	0.41
12:S:19:LEU:HD11	13:T:594:VAL:HG21	2.02	0.41
13:T:183:LEU:HD23	13:T:183:LEU:HA	1.82	0.41
13:T:302:GLN:O	13:T:306:MET:HG3	2.20	0.41
13:T:433:HIS:ND1	13:T:433:HIS:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:303:GLY:HA3	14:U:465:LEU:HD11	2.03	0.41
14:U:8:LEU:HB3	14:U:9:PRO:HD3	2.03	0.41
3:3:330:LYS:O	3:3:334:LYS:HB2	2.20	0.41
3:3:583:VAL:HG23	3:3:599:HIS:H	1.85	0.41
3:3:582:PHE:HA	3:3:599:HIS:ND1	2.36	0.41
4:4:67:GLU:OE2	4:4:409:ARG:NE	2.54	0.41
4:4:331:TYR:OH	7:9:106:GLU:OE2	2.39	0.41
1:B:211:LEU:CB	1:B:216:THR:HG21	2.50	0.41
3:D:512:LEU:HD21	3:D:534:ALA:HB1	2.03	0.41
4:E:260:TYR:HA	4:E:292:GLN:HE22	1.86	0.41
6:G:115:GLY:HA3	6:G:125:GLN:OE1	2.20	0.41
11:J:91:PRO:O	11:J:94:ALA:HB3	2.20	0.41
13:L:187:GLU:O	13:L:190:GLU:HG2	2.21	0.41
13:L:349:VAL:O	13:L:352:MET:HB2	2.20	0.41
14:M:338:THR:HG21	14:M:343:ARG:NH1	2.35	0.41
7:O:101:CYS:SG	7:O:103:LEU:HD12	2.61	0.41
7:O:72:PRO:HG3	7:O:86:ARG:NH2	2.35	0.41
16:Q:60:LEU:O	16:Q:64:ILE:HG13	2.20	0.41
10:P:56:ARG:HD3	11:R:73:LEU:O	2.20	0.41
14:U:313:TYR:HE1	14:U:450:PHE:HB2	1.85	0.41
1:1:193:GLU:OE1	1:1:200:ARG:NH2	2.54	0.41
2:2:112:THR:HG23	2:2:115:GLY:H	1.84	0.41
3:3:128:CYS:HB3	3:3:131:GLN:HB2	2.02	0.41
3:3:34:CYS:SG	3:3:35:SER:N	2.94	0.41
3:3:516:VAL:O	3:3:520:ARG:HG3	2.21	0.41
4:4:246:TYR:HD1	5:5:78:PRO:HD2	1.85	0.41
4:4:167:ARG:HD3	6:6:143:ARG:NH1	2.35	0.41
6:6:117:MET:CE	7:9:99:ILE:HG12	2.51	0.41
1:B:283:PRO:HB3	1:B:287:ILE:HD13	2.03	0.41
1:B:272:PHE:HB2	1:B:307:LEU:HA	2.03	0.41
3:D:42:ILE:HG21	3:D:439:GLU:OE1	2.21	0.41
4:E:42:ARG:O	4:E:43:LEU:HD23	2.21	0.41
5:F:116:ARG:HD2	5:F:131:ASP:O	2.21	0.41
10:A:14:VAL:HG22	16:H:95:LEU:HD22	2.03	0.41
13:L:426:LEU:HD23	13:L:513:GLN:NE2	2.28	0.41
13:L:1:MET:HA	13:L:55:PHE:HD2	1.86	0.41
13:L:82:GLY:O	13:L:86:LEU:HG	2.21	0.41
14:M:332:LEU:HA	14:M:335:ARG:HG2	2.02	0.41
14:M:347:LEU:HB2	14:M:413:THR:O	2.21	0.41
16:Q:120:LEU:HA	16:Q:180:LEU:CB	2.51	0.41
13:T:291:ILE:O	13:T:295:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:10:VAL:HG23	14:U:104:GLY:HA3	2.01	0.41
14:U:127:ILE:O	14:U:130:LEU:HG	2.20	0.41
3:3:11:VAL:HG21	3:3:26:ALA:HB2	2.02	0.41
4:4:400:LEU:HA	4:4:400:LEU:HD23	1.89	0.41
4:4:42:ARG:O	4:4:43:LEU:HD23	2.21	0.41
16:H:204:LEU:HA	16:H:204:LEU:HD23	1.79	0.41
8:I:105:THR:HG1	8:I:108:ILE:HB	1.85	0.41
14:M:238:VAL:O	14:M:241:PHE:HB2	2.21	0.41
13:L:159:PHE:CD2	14:M:407:LEU:HD11	2.54	0.41
15:N:232:ALA:O	15:N:236:LEU:HG	2.21	0.41
10:P:40:LYS:HE3	10:P:40:LYS:HB2	1.78	0.41
10:P:94:LEU:O	10:P:97:LEU:HB3	2.20	0.41
11:R:22:LEU:HD13	11:R:27:HIS:HB3	2.02	0.41
13:T:269:ALA:O	13:T:273:VAL:HG23	2.21	0.41
15:V:119:TYR:OH	15:V:140:GLY:HA3	2.21	0.41
9:W:59:VAL:HG11	9:W:63:PHE:CE2	2.55	0.41
1:1:338:VAL:O	1:1:342:TRP:HB2	2.21	0.41
1:1:414:LEU:O	1:1:418:LYS:N	2.54	0.41
3:3:297:GLY:HA3	3:3:703:GLN:NE2	2.36	0.41
3:3:329:LEU:CD1	3:3:584:VAL:HG11	2.51	0.41
6:6:115:GLY:HA3	6:6:125:GLN:OE1	2.21	0.41
6:6:154:LEU:O	6:6:158:VAL:HG13	2.21	0.41
6:6:82:GLY:HA2	17:6:201:SF4:S4	2.60	0.41
7:9:17:LEU:HA	16:H:41:ARG:O	2.20	0.41
10:A:59:VAL:HG13	10:A:62:TYR:HB3	2.03	0.41
1:B:195:LEU:HD23	2:C:24:ARG:HH12	1.85	0.41
1:B:369:ASN:HB3	3:D:159:PHE:CE2	2.56	0.41
3:D:360:LEU:O	3:D:364:LEU:HB3	2.20	0.41
4:E:86:ASP:HB3	4:E:93:HIS:CD2	2.55	0.41
16:H:16:LYS:O	16:H:20:VAL:HG23	2.21	0.41
16:H:330:LEU:HB3	16:H:332:LEU:HD11	2.03	0.41
16:H:52:GLY:HA3	16:H:53:PRO:C	2.41	0.41
16:H:65:LYS:O	16:H:69:LYS:HB2	2.21	0.41
12:K:81:HIS:H	12:K:81:HIS:CD2	2.39	0.41
15:N:272:ALA:O	15:N:276:GLY:N	2.47	0.41
15:N:58:VAL:O	15:N:62:PHE:HD1	2.04	0.41
15:N:17:GLY:HA3	15:N:82:PHE:CD2	2.55	0.41
16:Q:201:PRO:HD2	16:Q:320:TRP:CE2	2.56	0.41
13:T:158:ALA:HA	13:T:225:TRP:HB2	2.03	0.41
14:U:103:GLU:O	14:U:107:LEU:HG	2.20	0.41
14:U:307:GLY:HA2	14:U:379:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:347:LEU:HB2	14:U:413:THR:O	2.21	0.41
1:1:145:LEU:HA	1:1:145:LEU:HD23	1.88	0.41
3:3:645:ALA:HB3	3:3:652:PRO:HD3	2.03	0.41
4:4:218:ALA:HB1	4:4:273:PHE:N	2.36	0.41
5:5:153:GLY:HA2	9:W:113:ARG:HH21	1.86	0.41
1:1:373:LYS:N	8:7:79:LEU:HD21	2.36	0.41
7:9:36:ARG:O	7:9:38:HIS:ND1	2.52	0.41
1:B:3:GLY:HA2	1:B:4:PRO:HD3	1.94	0.41
2:C:24:ARG:HA	2:C:53:VAL:CG2	2.51	0.41
4:E:211:SER:CB	4:E:214:PHE:HB3	2.50	0.41
4:E:40:VAL:O	4:E:404:MET:HG3	2.20	0.41
5:F:154:GLU:CD	5:F:171:ARG:HH22	2.25	0.41
13:L:17:LEU:HD22	13:L:29:PRO:HB3	2.02	0.41
15:N:76:LEU:HD12	15:N:206:PRO:HB3	2.03	0.41
7:O:2:THR:OG1	7:O:2:THR:O	2.38	0.41
10:P:1:MET:HG2	10:P:2:ALA:H	1.86	0.41
16:Q:107:SER:OG	16:Q:113:PRO:HG3	2.21	0.41
13:T:194:GLY:HA3	13:T:195:PRO:HD3	1.86	0.41
13:T:75:PHE:CZ	13:T:79:ILE:HD11	2.56	0.41
15:V:98:LEU:HG	15:V:222:ALA:HB2	2.03	0.41
3:3:168:HIS:O	3:3:176:LEU:N	2.51	0.40
4:4:315:HIS:HA	8:7:46:ARG:CZ	2.50	0.40
3:3:250:GLU:HG3	5:5:169:GLU:HG3	2.03	0.40
8:7:13:TRP:HZ3	8:7:70:ALA:HB1	1.86	0.40
1:B:222:GLU:HG3	1:B:251:LEU:HD22	2.03	0.40
1:B:438:ARG:O	2:C:147:ARG:HB2	2.20	0.40
3:D:200:LEU:HD12	3:D:213:THR:HB	2.02	0.40
4:E:132:PHE:CE2	4:E:279:ARG:HD2	2.55	0.40
6:G:40:THR:HB	6:G:68:PHE:CE1	2.56	0.40
16:H:232:TYR:HB2	16:H:244:PHE:CE1	2.56	0.40
11:J:60:ALA:O	11:J:65:VAL:HG23	2.21	0.40
12:K:47:ARG:HE	12:K:47:ARG:HB3	1.69	0.40
13:L:165:GLY:CA	13:L:212:GLY:HA2	2.52	0.40
14:M:17:LEU:HA	14:M:17:LEU:HD23	1.88	0.40
15:N:124:TRP:O	15:N:125:ARG:HB2	2.21	0.40
7:O:101:CYS:HB2	7:O:103:LEU:H	1.86	0.40
7:O:117:TYR:CE2	7:O:163:VAL:HG11	2.56	0.40
7:O:68:ILE:HD11	17:O:201:SF4:S1	2.61	0.40
12:S:32:GLU:O	12:S:36:ASN:ND2	2.42	0.40
12:S:47:ARG:HE	12:S:47:ARG:HB3	1.68	0.40
12:S:79:PHE:CD2	12:S:85:THR:HA	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:20:HIS:CG	1:1:31:TYR:HE1	2.39	0.40
3:3:418:ARG:HG2	3:3:443:ARG:HG2	2.03	0.40
3:3:701:ALA:HB2	3:3:763:LEU:HB2	2.01	0.40
4:4:49:GLY:HA2	10:A:58:PRO:HD3	2.02	0.40
4:4:89:HIS:ND1	4:4:348:SER:HB2	2.35	0.40
5:5:163:ARG:CZ	7:9:90:VAL:HG11	2.51	0.40
5:5:167:PRO:HA	5:5:170:PHE:HB3	2.02	0.40
7:9:34:LYS:HA	7:9:34:LYS:HD3	1.48	0.40
1:B:64:GLY:N	1:B:70:PHE:O	2.37	0.40
3:D:321:THR:HG22	3:D:322:TRP:H	1.85	0.40
3:D:418:ARG:HD3	3:D:443:ARG:CZ	2.52	0.40
5:F:147:ARG:HG2	5:F:147:ARG:H	1.72	0.40
16:H:237:SER:OG	16:H:238:SER:N	2.53	0.40
16:H:162:TYR:OH	16:H:305:LEU:O	2.36	0.40
13:L:280:TYR:OH	13:L:531:ALA:HB1	2.20	0.40
14:M:6:VAL:HG22	14:M:107:LEU:HB3	2.03	0.40
14:M:160:LEU:O	14:M:163:VAL:HG12	2.21	0.40
14:M:331:ARG:HD2	14:M:331:ARG:HA	1.77	0.40
15:N:14:THR:OG1	15:N:90:TYR:OH	2.10	0.40
15:N:95:MET:HB2	15:N:95:MET:HE3	1.87	0.40
16:Q:96:ALA:HA	16:Q:99:LEU:HD13	2.04	0.40
13:T:15:ALA:O	13:T:19:LEU:HG	2.21	0.40
12:S:19:LEU:HD21	13:T:594:VAL:HG21	2.04	0.40
3:3:329:LEU:HA	3:3:329:LEU:HD12	1.85	0.40
3:3:418:ARG:O	3:3:419:ASP:HB2	2.22	0.40
3:3:46:ARG:NH2	3:3:81:ALA:HB2	2.37	0.40
6:6:91:VAL:HG22	10:A:46:SER:HB3	2.02	0.40
6:6:94:ARG:HB3	6:6:98:GLN:NE2	2.37	0.40
7:9:45:ARG:HH21	7:9:137:LEU:HD23	1.85	0.40
2:C:42:ARG:HB3	2:C:44:GLU:OE1	2.22	0.40
3:D:386:SER:HB3	3:D:389:ASP:OD2	2.21	0.40
3:D:382:PHE:HB3	3:D:532:VAL:HB	2.03	0.40
4:E:80:THR:O	4:E:84:ARG:NH1	2.54	0.40
5:F:103:THR:HG22	5:F:126:PHE:HB3	2.03	0.40
13:L:122:ASP:O	13:L:185:ILE:N	2.52	0.40
13:L:59:TRP:HB3	13:L:64:PRO:HA	2.03	0.40
14:M:346:GLY:HA3	14:M:418:GLY:HA2	2.02	0.40
15:N:319:ASP:HB3	15:N:322:LEU:HB2	2.03	0.40
15:N:62:PHE:CD2	15:N:221:ALA:HB2	2.55	0.40
10:P:84:SER:OG	11:R:128:GLY:HA3	2.21	0.40
13:T:41:PHE:HD2	13:T:42:LEU:HD12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:310:GLY:HA2	14:U:376:GLY:HA2	2.03	0.40
1:1:246:SER:OG	1:1:313:TYR:HB2	2.21	0.40
1:1:262:GLY:HA3	2:2:175:HIS:O	2.21	0.40
3:3:142:LYS:HB2	3:3:142:LYS:HE2	1.87	0.40
3:3:240:ALA:CB	3:3:276:ARG:HB2	2.51	0.40
3:3:38:HIS:CD2	3:3:287:GLU:HB3	2.56	0.40
3:3:664:LEU:HD23	3:3:664:LEU:HA	1.96	0.40
4:4:341:GLU:OE2	5:5:57:TYR:OH	2.28	0.40
6:6:30:TRP:O	6:6:33:SER:OG	2.36	0.40
3:D:136:GLU:HG2	5:F:189:ARG:HG2	2.02	0.40
3:D:397:LEU:O	3:D:505:LEU:HD12	2.21	0.40
3:D:385:ALA:HA	3:D:531:LYS:HB3	2.02	0.40
16:H:51:VAL:HG23	16:H:51:VAL:H	1.59	0.40
11:J:94:ALA:O	11:J:97:ALA:HB3	2.22	0.40
13:L:603:VAL:HG21	15:N:235:LEU:HD22	2.03	0.40
14:M:135:LEU:H	14:M:135:LEU:HD23	1.87	0.40
15:N:303:SER:HB3	15:N:307:VAL:HG22	2.01	0.40
7:O:63:CYS:HA	17:O:201:SF4:S2	2.62	0.40
16:Q:226:GLN:HB2	16:Q:299:ARG:NH2	2.37	0.40
16:Q:86:PRO:HG3	16:Q:244:PHE:CE2	2.56	0.40
13:T:586:LEU:HD12	15:V:135:LYS:HG2	2.03	0.40
14:U:70:LEU:O	14:U:73:LEU:HD23	2.21	0.40
15:V:209:LEU:HB2	15:V:296:PHE:HB3	2.03	0.40
9:X:37:TRP:CD1	9:X:40:LYS:HD2	2.56	0.40
1:1:16:THR:H	1:1:265:GLU:CD	2.21	0.40
4:4:162:TRP:CD2	7:9:34:LYS:CD	2.95	0.40
4:4:234:LEU:HD12	4:4:377:ASN:O	2.22	0.40
4:4:371:ARG:HG3	5:5:51:ASP:OD1	2.22	0.40
4:4:246:TYR:CD1	5:5:78:PRO:HD2	2.56	0.40
10:A:95:GLY:HA3	11:J:136:LEU:HD11	2.02	0.40
1:B:176:GLY:O	2:C:32:ARG:NH2	2.30	0.40
3:D:176:LEU:HD13	3:D:235:LEU:HD23	2.02	0.40
4:E:211:SER:HB2	4:E:215:TYR:N	2.36	0.40
4:E:59:ILE:O	6:G:87:LYS:NZ	2.42	0.40
5:F:145:PRO:HA	5:F:150:TYR:CD1	2.56	0.40
5:F:55:LEU:HB2	5:F:69:ALA:O	2.21	0.40
6:G:119:ASN:HA	6:G:125:GLN:NE2	2.31	0.40
6:G:105:VAL:HG11	6:G:131:VAL:HG23	2.04	0.40
16:H:147:TYR:CE1	16:H:228:LEU:HD13	2.57	0.40
16:H:324:THR:O	16:H:328:VAL:HG23	2.22	0.40
8:I:48:TYR:CE2	8:I:50:LEU:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:586:LEU:CD1	15:N:135:LYS:HA	2.51	0.40
14:M:156:SER:O	14:M:159:MET:HB3	2.21	0.40
16:Q:314:PHE:HB2	16:Q:315:PRO:HD3	2.04	0.40
14:U:343:ARG:HB3	14:U:344:TYR:CD1	2.57	0.40
14:U:305:PRO:HD3	14:U:462:ALA:CB	2.52	0.40
14:U:78:ILE:O	14:U:82:VAL:HG23	2.21	0.40
15:V:59:SER:OG	15:V:100:SER:OG	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	435/438 (99%)	408 (94%)	27 (6%)	0	100	100
1	B	435/438 (99%)	407 (94%)	28 (6%)	0	100	100
2	2	176/181 (97%)	165 (94%)	11 (6%)	0	100	100
2	C	176/181 (97%)	165 (94%)	11 (6%)	0	100	100
3	3	750/783 (96%)	695 (93%)	55 (7%)	0	100	100
3	D	750/783 (96%)	698 (93%)	52 (7%)	0	100	100
4	4	382/409 (93%)	357 (94%)	25 (6%)	0	100	100
4	E	382/409 (93%)	357 (94%)	25 (6%)	0	100	100
5	5	194/207 (94%)	183 (94%)	11 (6%)	0	100	100
5	F	194/207 (94%)	180 (93%)	14 (7%)	0	100	100
6	6	164/181 (91%)	149 (91%)	15 (9%)	0	100	100
6	G	164/181 (91%)	152 (93%)	12 (7%)	0	100	100
7	9	178/182 (98%)	170 (96%)	8 (4%)	0	100	100
7	O	178/182 (98%)	169 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	7	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
8	I	125/129 (97%)	119 (95%)	6 (5%)	0	100	100
9	W	125/131 (95%)	121 (97%)	4 (3%)	0	100	100
9	X	125/131 (95%)	121 (97%)	4 (3%)	0	100	100
10	A	115/119 (97%)	103 (90%)	12 (10%)	0	100	100
10	P	115/119 (97%)	104 (90%)	11 (10%)	0	100	100
11	J	158/176 (90%)	146 (92%)	12 (8%)	0	100	100
11	R	158/176 (90%)	145 (92%)	13 (8%)	0	100	100
12	K	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
12	S	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
13	L	603/606 (100%)	562 (93%)	40 (7%)	1 (0%)	47	79
13	T	603/606 (100%)	568 (94%)	34 (6%)	1 (0%)	47	79
14	M	465/469 (99%)	436 (94%)	29 (6%)	0	100	100
14	U	465/469 (99%)	439 (94%)	26 (6%)	0	100	100
15	N	425/427 (100%)	399 (94%)	26 (6%)	0	100	100
15	V	425/427 (100%)	397 (93%)	27 (6%)	1 (0%)	47	79
16	H	351/365 (96%)	302 (86%)	43 (12%)	6 (2%)	9	45
16	Q	351/365 (96%)	307 (88%)	39 (11%)	5 (1%)	11	48
All	All	9478/9796 (97%)	8820 (93%)	644 (7%)	14 (0%)	51	83

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	H	51	VAL
16	H	44	VAL
16	Q	51	VAL
16	H	268	THR
16	Q	44	VAL
16	Q	268	THR
16	H	50	ARG
13	T	435	PRO
16	Q	50	ARG
13	L	435	PRO
15	V	425	ALA
16	H	52	GLY
16	Q	218	PRO

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Mol	Chain	Res	Type
16	H	218	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%)	347 (98%)	8 (2%)	50	76
1	B	355/356 (100%)	346 (98%)	9 (2%)	47	75
2	2	150/152 (99%)	144 (96%)	6 (4%)	31	65
2	C	150/152 (99%)	145 (97%)	5 (3%)	38	69
3	3	609/628 (97%)	597 (98%)	12 (2%)	55	79
3	D	609/628 (97%)	600 (98%)	9 (2%)	65	84
4	4	332/355 (94%)	325 (98%)	7 (2%)	53	78
4	E	332/355 (94%)	329 (99%)	3 (1%)	78	90
5	5	167/175 (95%)	162 (97%)	5 (3%)	41	71
5	F	167/175 (95%)	164 (98%)	3 (2%)	59	81
6	6	135/149 (91%)	126 (93%)	9 (7%)	16	50
6	G	135/149 (91%)	125 (93%)	10 (7%)	13	46
7	9	148/150 (99%)	146 (99%)	2 (1%)	67	85
7	O	148/150 (99%)	146 (99%)	2 (1%)	67	85
8	7	104/106 (98%)	103 (99%)	1 (1%)	76	88
8	I	104/106 (98%)	103 (99%)	1 (1%)	76	88
9	W	99/101 (98%)	98 (99%)	1 (1%)	76	88
9	X	99/101 (98%)	98 (99%)	1 (1%)	76	88
10	A	90/92 (98%)	87 (97%)	3 (3%)	38	69
10	P	90/92 (98%)	86 (96%)	4 (4%)	28	63
11	J	118/130 (91%)	115 (98%)	3 (2%)	47	75
11	R	118/130 (91%)	115 (98%)	3 (2%)	47	75
12	K	71/71 (100%)	70 (99%)	1 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	S	71/71 (100%)	69 (97%)	2 (3%)	43	72
13	L	453/454 (100%)	443 (98%)	10 (2%)	52	77
13	T	453/454 (100%)	444 (98%)	9 (2%)	55	79
14	M	332/332 (100%)	325 (98%)	7 (2%)	53	78
14	U	332/332 (100%)	326 (98%)	6 (2%)	59	81
15	N	302/302 (100%)	298 (99%)	4 (1%)	69	86
15	V	302/302 (100%)	297 (98%)	5 (2%)	60	82
16	H	293/300 (98%)	282 (96%)	11 (4%)	33	66
16	Q	293/300 (98%)	285 (97%)	8 (3%)	44	73
All	All	7516/7706 (98%)	7346 (98%)	170 (2%)	50	76

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	249	MET
1	1	337	MET
1	1	342	TRP
1	1	353	CYS
1	1	366	PHE
1	1	397	ARG
1	1	400	CYS
1	1	437	TRP
2	2	6	ASP
2	2	33	ARG
2	2	35	GLN
2	2	45	ARG
2	2	116	LEU
2	2	171	LYS
3	3	76	GLN
3	3	83	CYS
3	3	123	ASP
3	3	124	LYS
3	3	214	MET
3	3	337	ARG
3	3	369	LEU
3	3	425	ARG
3	3	501	LYS
3	3	655	ARG
3	3	761	SER

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Mol	Chain	Res	Type
3	3	774	ARG
4	4	68	LYS
4	4	87	TYR
4	4	129	HIS
4	4	132	PHE
4	4	152	GLU
4	4	208	PHE
4	4	262	PHE
5	5	31	ARG
5	5	38	MET
5	5	147	ARG
5	5	178	ASP
5	5	183	PHE
6	6	37	TRP
6	6	45	CYS
6	6	49	GLU
6	6	55	ASP
6	6	68	PHE
6	6	101	ASP
6	6	153	GLN
6	6	156	LYS
6	6	176	TRP
7	9	34	LYS
7	9	38	HIS
8	7	43	ARG
9	W	37	TRP
10	A	13	TYR
10	A	48	ASN
10	A	49	ASP
11	J	69	PHE
11	J	118	ASP
11	J	119	LEU
12	K	28	PHE
13	L	14	PHE
13	L	56	GLN
13	L	59	TRP
13	L	146	TYR
13	L	169	PHE
13	L	245	MET
13	L	506	TRP
13	L	511	PHE
13	L	554	PHE

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Mol	Chain	Res	Type
13	L	557	ASP
14	M	22	ARG
14	M	73	LEU
14	M	115	LEU
14	M	241	PHE
14	M	255	GLN
14	M	326	PHE
14	M	455	HIS
15	N	9	PHE
15	N	50	PHE
15	N	126	ARG
15	N	284	TYR
16	H	28	PHE
16	H	54	PHE
16	H	119	ASP
16	H	134	TYR
16	H	147	TYR
16	H	233	HIS
16	H	298	PHE
16	H	302	TYR
16	H	307	ARG
16	H	310	TRP
16	H	332	LEU
1	B	244	GLU
1	B	249	MET
1	B	302	PHE
1	B	337	MET
1	B	342	TRP
1	B	366	PHE
1	B	397	ARG
1	B	400	CYS
1	B	437	TRP
2	C	6	ASP
2	C	33	ARG
2	C	35	GLN
2	C	45	ARG
2	C	116	LEU
3	D	83	CYS
3	D	123	ASP
3	D	184	CYS
3	D	337	ARG
3	D	369	LEU

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Mol	Chain	Res	Type
3	D	628	PRO
3	D	655	ARG
3	D	761	SER
3	D	774	ARG
4	E	132	PHE
4	E	208	PHE
4	E	262	PHE
5	F	31	ARG
5	F	97	GLU
5	F	147	ARG
6	G	37	TRP
6	G	45	CYS
6	G	49	GLU
6	G	55	ASP
6	G	68	PHE
6	G	117	MET
6	G	120	ASN
6	G	156	LYS
6	G	176	TRP
6	G	177	LYS
7	O	4	LYS
7	O	38	HIS
8	I	43	ARG
9	X	37	TRP
10	P	48	ASN
10	P	49	ASP
10	P	66	MET
10	P	110	GLU
11	R	59	TYR
11	R	69	PHE
11	R	84	ASP
12	S	28	PHE
12	S	82	ARG
13	T	14	PHE
13	T	59	TRP
13	T	169	PHE
13	T	245	MET
13	T	329	LYS
13	T	506	TRP
13	T	511	PHE
13	T	554	PHE
13	T	557	ASP

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Mol	Chain	Res	Type
14	U	22	ARG
14	U	135	LEU
14	U	151	PHE
14	U	241	PHE
14	U	255	GLN
14	U	455	HIS
15	V	9	PHE
15	V	50	PHE
15	V	78	ARG
15	V	126	ARG
15	V	284	TYR
16	Q	28	PHE
16	Q	119	ASP
16	Q	147	TYR
16	Q	196	PHE
16	Q	233	HIS
16	Q	302	TYR
16	Q	307	ARG
16	Q	332	LEU

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

Mol	Chain	Res	Type
1	1	240	GLN
1	1	288	GLN
2	2	35	GLN
2	2	71	GLN
2	2	120	GLN
3	3	25	HIS
3	3	104	GLN
3	3	168	HIS
3	3	347	HIS
3	3	709	GLN
4	4	33	GLN
4	4	129	HIS
4	4	169	HIS
4	4	292	GLN
5	5	129	HIS
6	6	98	GLN
6	6	120	ASN
6	6	155	GLN
8	7	76	HIS

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Mol	Chain	Res	Type
9	W	43	GLN
10	A	60	HIS
11	J	117	GLN
11	J	125	GLN
13	L	432	HIS
13	L	436	HIS
13	L	447	HIS
13	L	513	GLN
14	M	49	HIS
14	M	52	GLN
14	M	221	ASN
15	N	245	ASN
15	N	277	ASN
16	H	49	ASN
16	H	117	ASN
16	H	181	ASN
16	H	183	ASN
16	H	233	HIS
16	H	304	GLN
1	B	20	HIS
1	B	161	ASN
1	B	219	ASN
1	B	240	GLN
1	B	245	GLN
1	B	288	GLN
1	B	343	ASN
1	B	350	HIS
1	B	386	ASN
2	C	35	GLN
3	D	104	GLN
3	D	208	HIS
3	D	347	HIS
3	D	468	HIS
3	D	631	ASN
3	D	709	GLN
4	E	78	ASN
4	E	379	GLN
5	F	112	ASN
5	F	129	HIS
6	G	74	GLN
6	G	120	ASN
6	G	125	GLN

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Mol	Chain	Res	Type
8	I	76	HIS
9	X	43	GLN
9	X	84	GLN
10	P	60	HIS
11	R	55	GLN
12	S	81	HIS
13	T	150	GLN
13	T	302	GLN
13	T	325	HIS
13	T	365	HIS
14	U	221	ASN
14	U	349	GLN
15	V	103	HIS
15	V	245	ASN
15	V	277	ASN
16	Q	112	GLN
16	Q	226	GLN
16	Q	233	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

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	$\# Z  > 2$
17	SF4	D	802	3	0,12,12	0.00	-	-		
20	DCQ	4	501	-	23,23,23	0.22	0	26,29,29	0.84	1 (3%)
17	SF4	B	501	1	0,12,12	0.00	-	-		
17	SF4	3	802	3	0,12,12	0.00	-	-		
17	SF4	9	201	7	0,12,12	0.00	-	-		
17	SF4	D	803	3	0,12,12	0.00	-	-		
17	SF4	1	501	1	0,12,12	0.00	-	-		
19	FES	2	201	2	0,4,4	0.00	-	-		
17	SF4	9	202	7	0,12,12	0.00	-	-		
20	DCQ	E	501	-	23,23,23	0.18	0	26,29,29	0.86	1 (3%)
19	FES	C	201	2	0,4,4	0.00	-	-		
18	FMN	1	502	-	31,33,33	1.44	4 (12%)	40,50,50	1.76	7 (17%)
19	FES	3	804	3	0,4,4	0.00	-	-		
17	SF4	D	801	3	0,12,12	0.00	-	-		
17	SF4	O	201	7	0,12,12	0.00	-	-		
17	SF4	3	801	3	0,12,12	0.00	-	-		
19	FES	D	804	3	0,4,4	0.00	-	-		
17	SF4	G	201	6	0,12,12	0.00	-	-		
17	SF4	3	803	3	0,12,12	0.00	-	-		
17	SF4	6	201	6	0,12,12	0.00	-	-		
18	FMN	B	502	-	31,33,33	1.42	4 (12%)	40,50,50	1.60	7 (17%)
17	SF4	O	202	7	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
17	SF4	D	802	3	-	-	0/6/5/5
20	DCQ	4	501	-	-	4/14/38/38	0/1/1/1
17	SF4	B	501	1	-	-	0/6/5/5
17	SF4	3	802	3	-	-	0/6/5/5
17	SF4	9	201	7	-	-	0/6/5/5
17	SF4	D	803	3	-	-	0/6/5/5
17	SF4	1	501	1	-	-	0/6/5/5
19	FES	2	201	2	-	-	0/1/1/1
17	SF4	9	202	7	-	-	0/6/5/5
20	DCQ	E	501	-	-	4/14/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	FES	C	201	2	-	-	0/1/1/1
18	FMN	1	502	-	-	8/18/18/18	0/3/3/3
19	FES	3	804	3	-	-	0/1/1/1
17	SF4	D	801	3	-	-	0/6/5/5
17	SF4	O	201	7	-	-	0/6/5/5
17	SF4	3	801	3	-	-	0/6/5/5
19	FES	D	804	3	-	-	0/1/1/1
17	SF4	G	201	6	-	-	0/6/5/5
17	SF4	3	803	3	-	-	0/6/5/5
17	SF4	6	201	6	-	-	0/6/5/5
18	FMN	B	502	-	-	8/18/18/18	0/3/3/3
17	SF4	O	202	7	-	-	0/6/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	502	FMN	C10-N1	4.00	1.38	1.33
18	1	502	FMN	C10-N1	3.96	1.38	1.33
18	1	502	FMN	C4A-N5	3.38	1.38	1.33
18	B	502	FMN	C4A-N5	3.23	1.37	1.33
18	1	502	FMN	C1'-N10	3.13	1.51	1.48
18	B	502	FMN	C1'-N10	3.01	1.51	1.48
18	B	502	FMN	C4-N3	3.00	1.38	1.33
18	1	502	FMN	C4-N3	2.97	1.38	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	502	FMN	C1'-N10-C10	6.10	123.87	118.41
18	1	502	FMN	C4-N3-C2	5.31	119.62	115.14
18	B	502	FMN	C4-N3-C2	5.12	119.47	115.14
18	B	502	FMN	C1'-N10-C10	4.76	122.67	118.41
18	1	502	FMN	C5A-C9A-N10	4.19	120.75	117.72
18	B	502	FMN	C5A-C9A-N10	3.74	120.42	117.72
18	B	502	FMN	C4A-N5-C5A	3.12	119.89	116.77
18	1	502	FMN	C4A-N5-C5A	3.06	119.83	116.77
18	B	502	FMN	C5'-C4'-C3'	-2.90	106.61	112.20
18	1	502	FMN	C5'-C4'-C3'	-2.69	107.01	112.20
18	1	502	FMN	C4A-C4-N3	-2.48	120.03	123.43
20	4	501	DCQ	C4M-O4-C4	2.31	124.66	116.47
20	E	501	DCQ	C4M-O4-C4	2.28	124.55	116.47
18	B	502	FMN	C4A-C4-N3	-2.27	120.32	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	502	FMN	C9A-N10-C10	-2.16	119.08	121.91
18	B	502	FMN	C9A-N10-C10	-2.06	119.21	121.91

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	1	502	FMN	N10-C1'-C2'-O2'
18	1	502	FMN	N10-C1'-C2'-C3'
18	1	502	FMN	C1'-C2'-C3'-O3'
18	1	502	FMN	C1'-C2'-C3'-C4'
18	1	502	FMN	C3'-C4'-C5'-O5'
18	1	502	FMN	O4'-C4'-C5'-O5'
18	B	502	FMN	N10-C1'-C2'-O2'
18	B	502	FMN	N10-C1'-C2'-C3'
18	B	502	FMN	C1'-C2'-C3'-O3'
18	B	502	FMN	C1'-C2'-C3'-C4'
18	B	502	FMN	C3'-C4'-C5'-O5'
18	B	502	FMN	O4'-C4'-C5'-O5'
20	4	501	DCQ	C6-C7-C8-C9
20	E	501	DCQ	C6-C7-C8-C9
18	B	502	FMN	O2'-C2'-C3'-C4'
18	B	502	FMN	O2'-C2'-C3'-O3'
18	1	502	FMN	O2'-C2'-C3'-C4'
20	4	501	DCQ	C9-C10-C11-C12
20	E	501	DCQ	C9-C10-C11-C12
20	4	501	DCQ	C12-C13-C14-C15
20	E	501	DCQ	C12-C13-C14-C15
18	1	502	FMN	O2'-C2'-C3'-O3'
20	E	501	DCQ	C11-C10-C9-C8
20	4	501	DCQ	C11-C10-C9-C8

There are no ring outliers.

15 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	501	DCQ	4	0
17	B	501	SF4	3	0
17	9	201	SF4	2	0
17	D	803	SF4	2	0
17	9	202	SF4	1	0

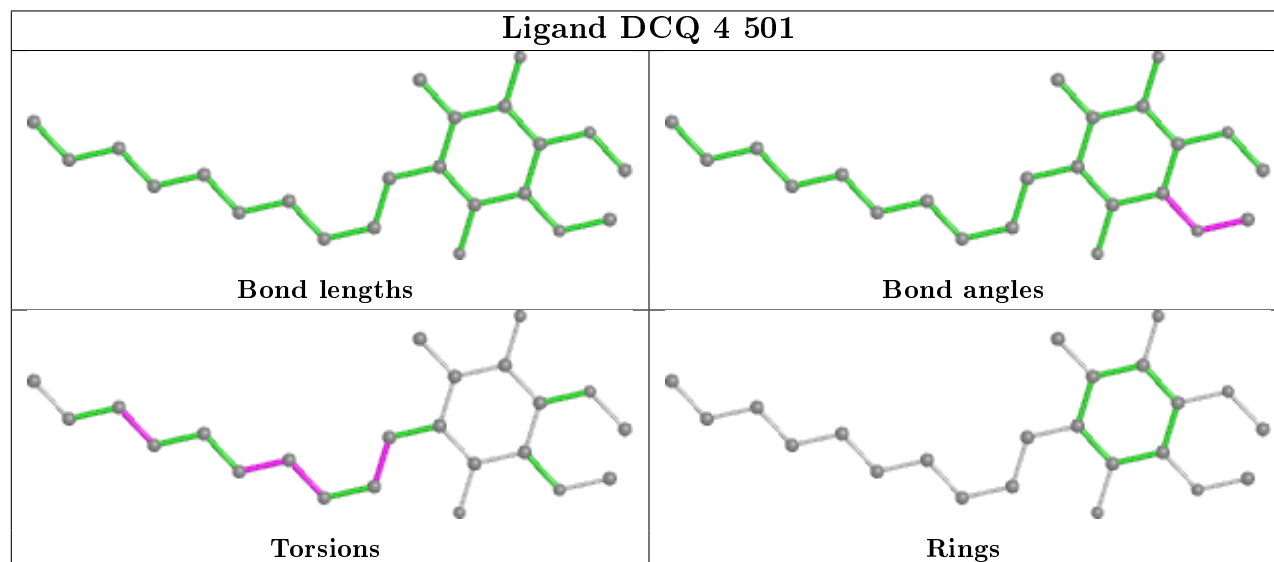
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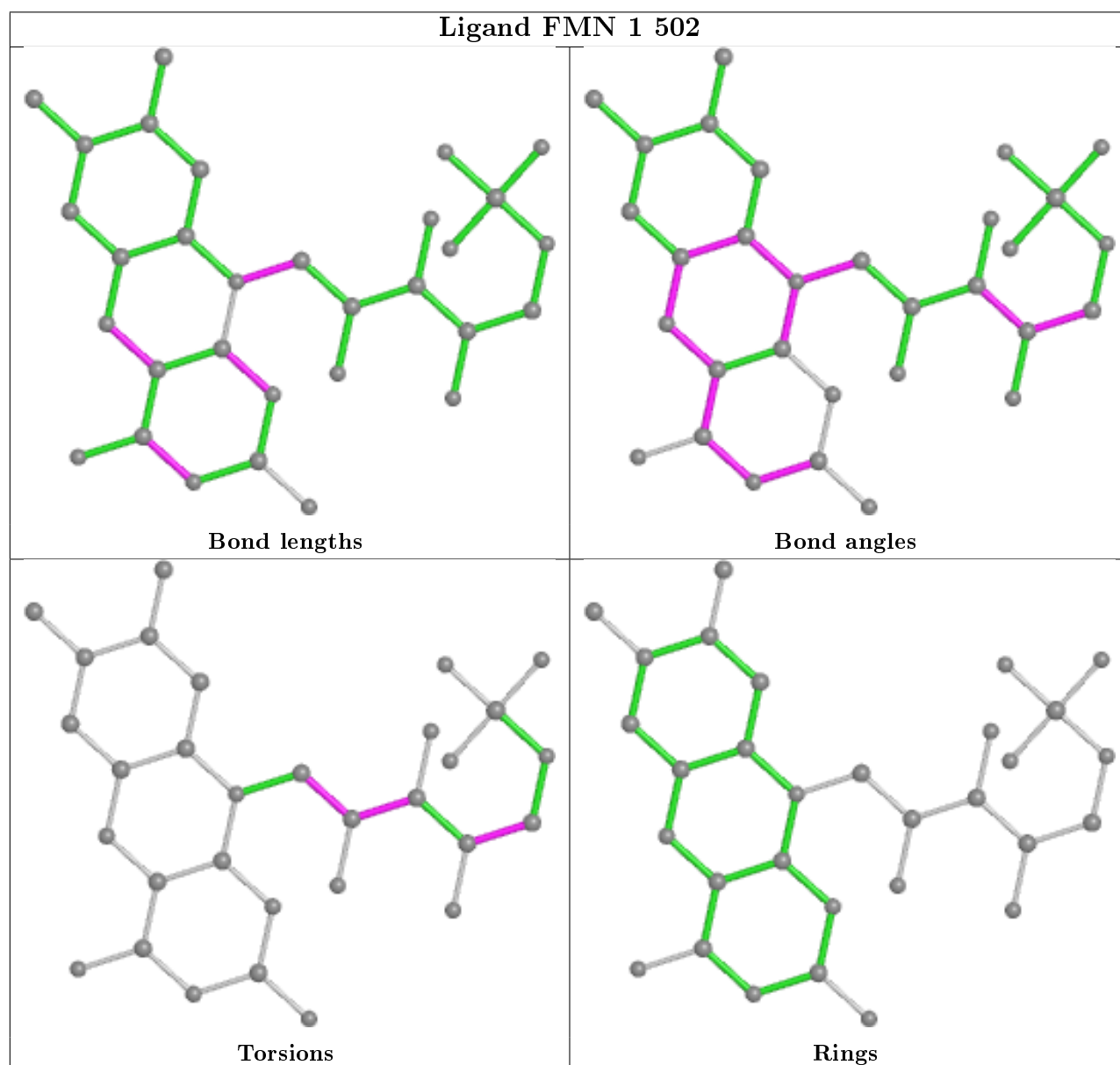
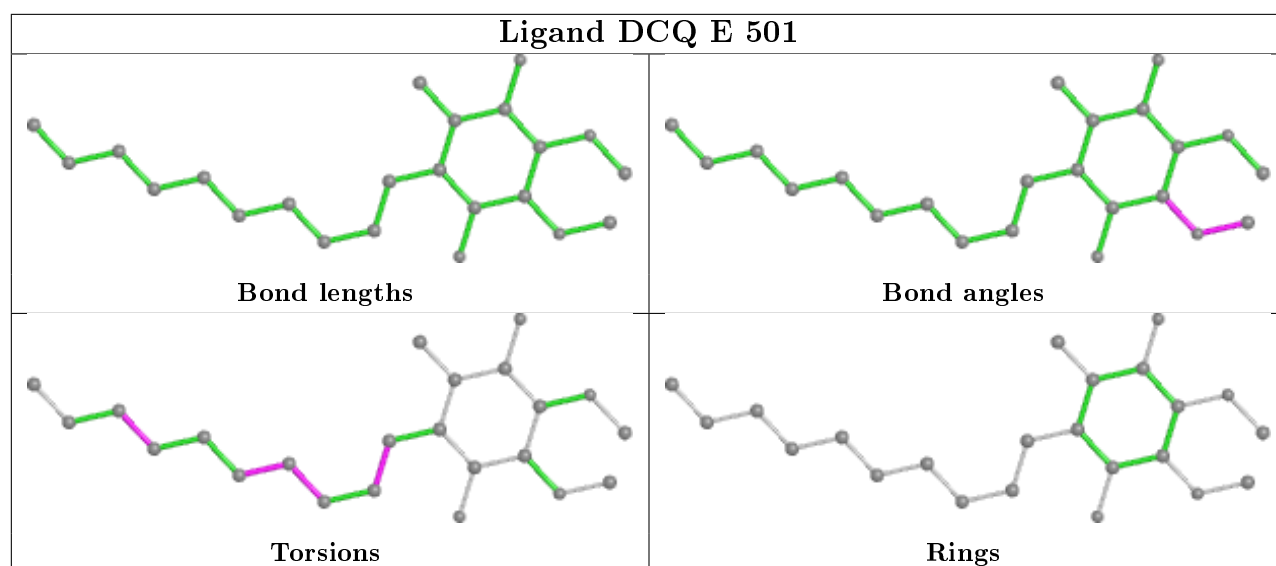


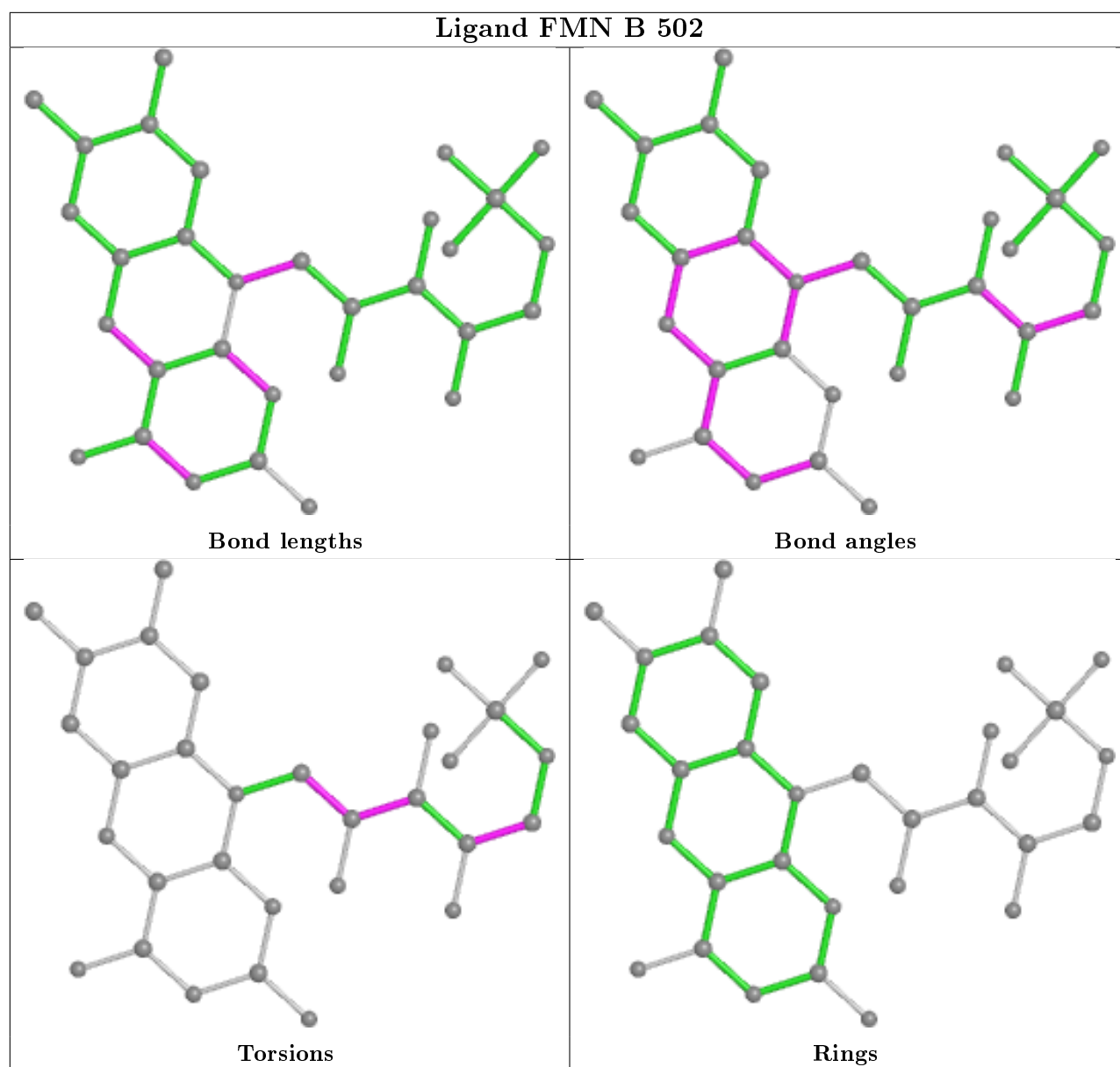
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	E	501	DCQ	4	0
18	1	502	FMN	9	0
19	3	804	FES	1	0
17	O	201	SF4	2	0
17	3	801	SF4	1	0
19	D	804	FES	2	0
17	3	803	SF4	2	0
17	6	201	SF4	1	0
18	B	502	FMN	9	0
17	O	202	SF4	1	0

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.