



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 02:24 PM BST

PDB ID : 4HEA  
Title : Crystal structure of the entire respiratory complex I from *Thermus thermophilus*  
Authors : Baradaran, R.; Berrisford, J.M.; Minhas, G.S.; Sazanov, L.A.  
Deposited on : 2012-10-03  
Resolution : 3.30 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	:	<b>FAILED</b>
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

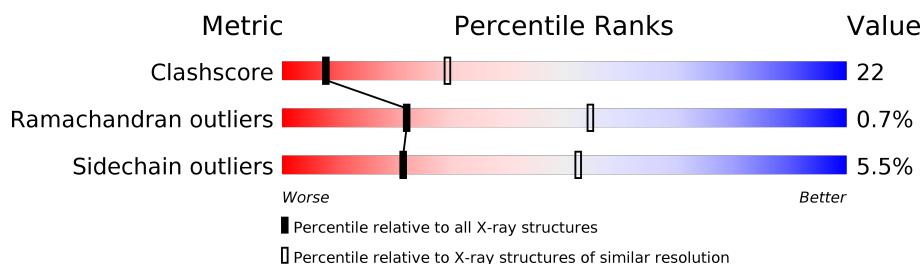
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)



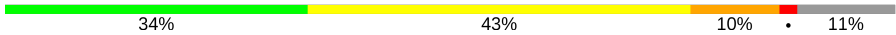
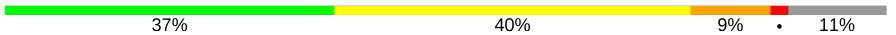




















The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	
1	B	438	
2	2	181	
2	C	181	
3	3	783	
3	D	783	
4	4	409	
4	E	409	

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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	6	201	-	-	X	-
17	SF4	9	201	-	-	X	-
17	SF4	9	202	-	-	X	-
17	SF4	B	501	-	-	X	-
17	SF4	G	201	-	-	X	-
17	SF4	O	201	-	-	X	-
17	SF4	O	202	-	-	X	-
19	FES	D	804	-	-	X	-

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 73998 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	161	Total	C	N	O	S	0	0	0
			1245	787	227	218	13			
6	G	161	Total	C	N	O	S	0	0	0
			1245	787	227	218	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 Putative uncharacterized protein TTHA1528.

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			

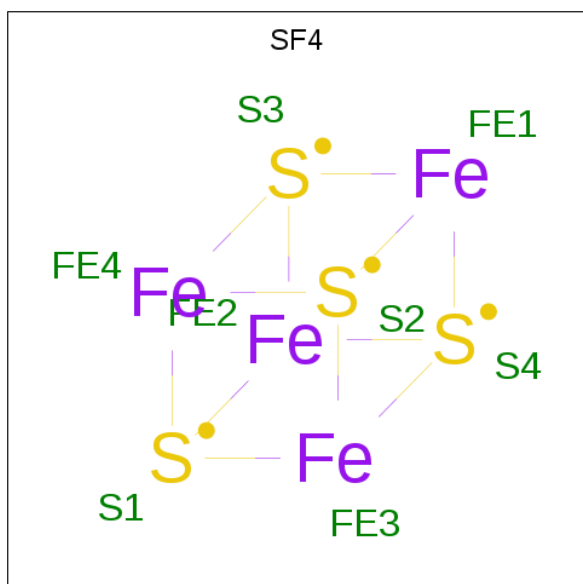
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

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: Fe<sub>4</sub>S<sub>4</sub>).



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		

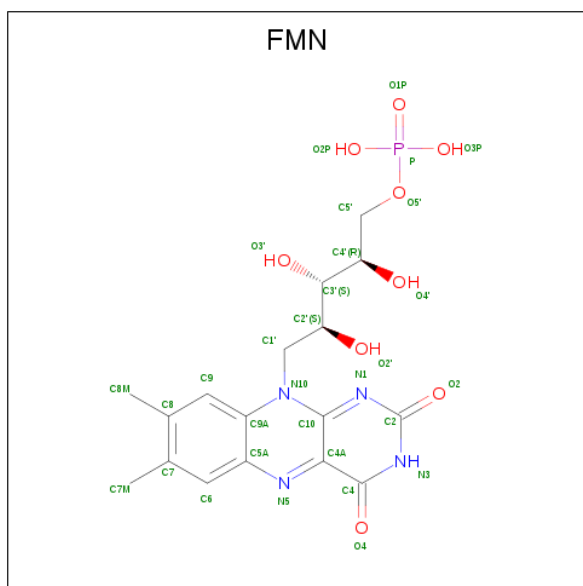
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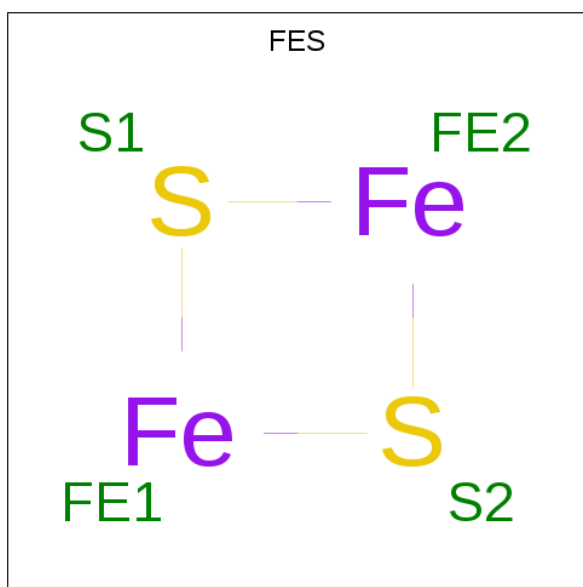
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	D	1	Total	Fe	S	0	0
			8	4	4		
17	D	1	Total	Fe	S	0	0
			8	4	4		
17	G	1	Total	Fe	S	0	0
			8	4	4		
17	O	1	Total	Fe	S	0	0
			8	4	4		
17	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 18 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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<sub>2</sub>S<sub>2</sub>).



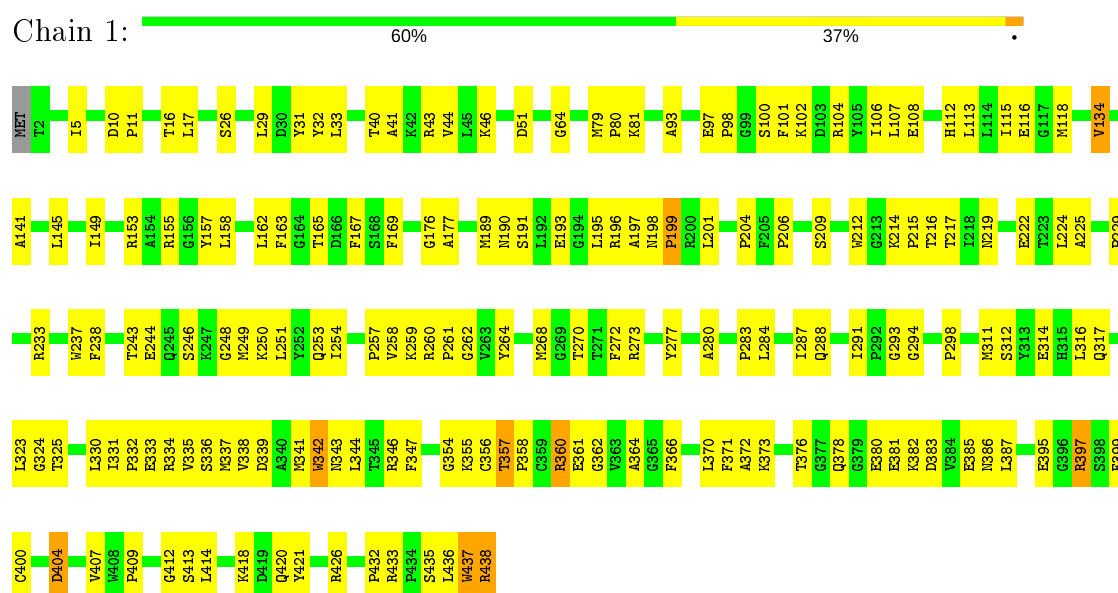
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	2	1	Total	Fe	S	0	0
			4	2	2		
19	3	1	Total	Fe	S	0	0
			4	2	2		
19	C	1	Total	Fe	S	0	0
			4	2	2		
19	D	1	Total	Fe	S	0	0
			4	2	2		

### 3 Residue-property plots

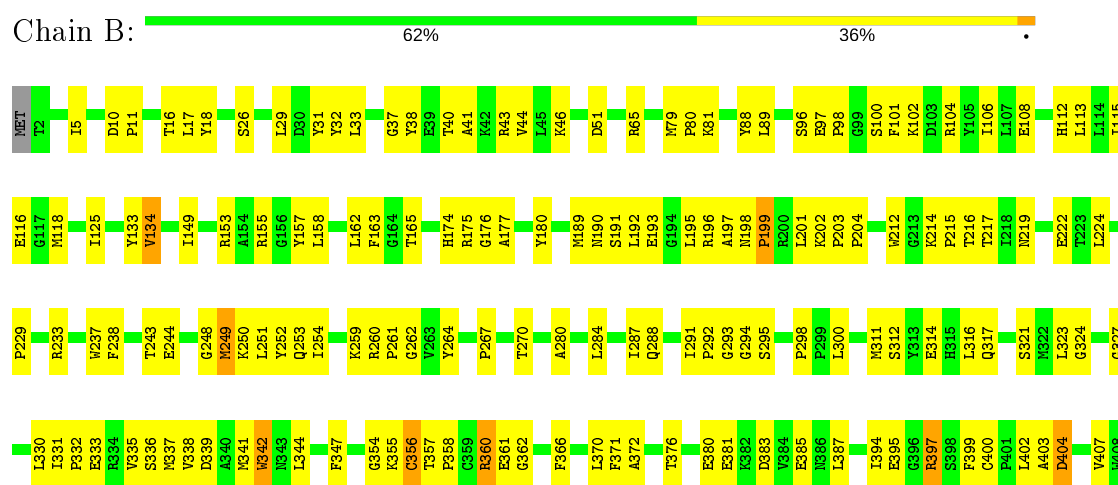
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

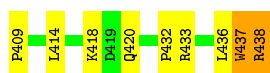
Note EDS failed to run properly.

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

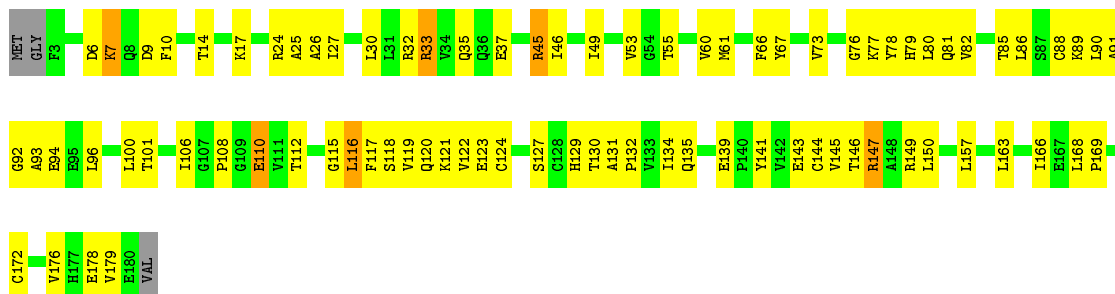


#### • Molecule 1: NADH-quinone oxidoreductase subunit 1

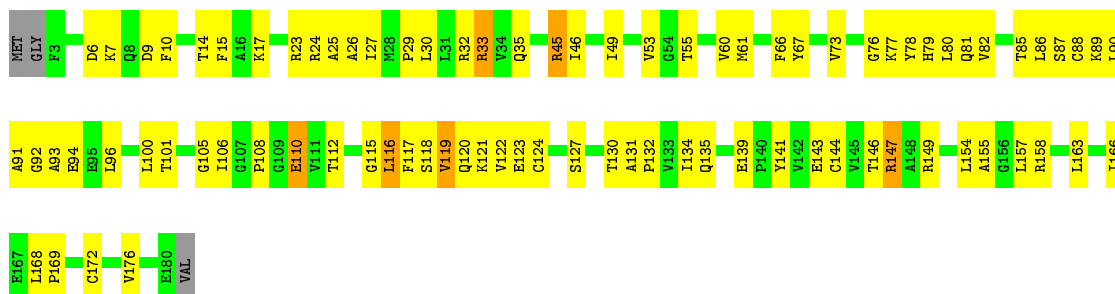




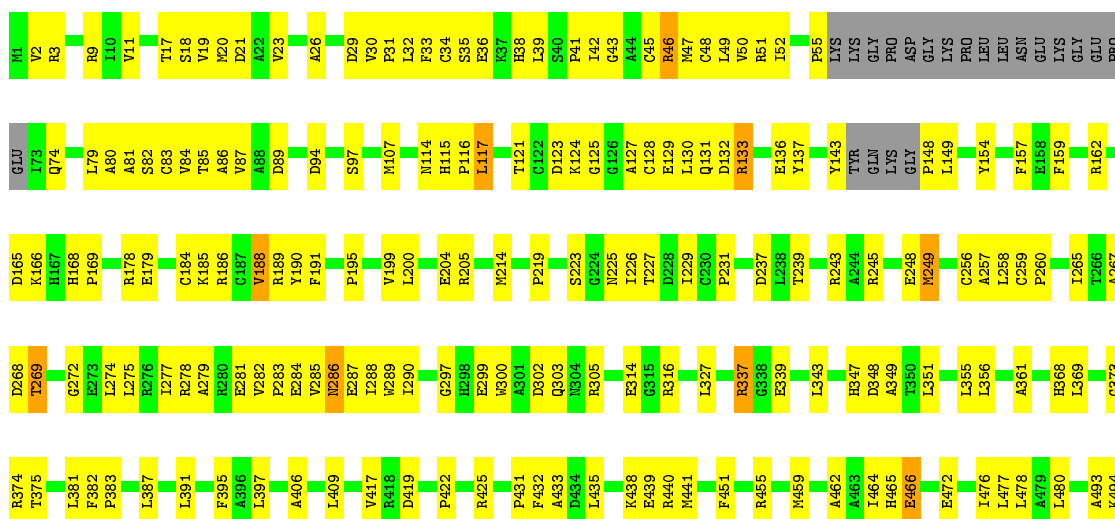
• Molecule 2: NADH-quinone oxidoreductase subunit 2

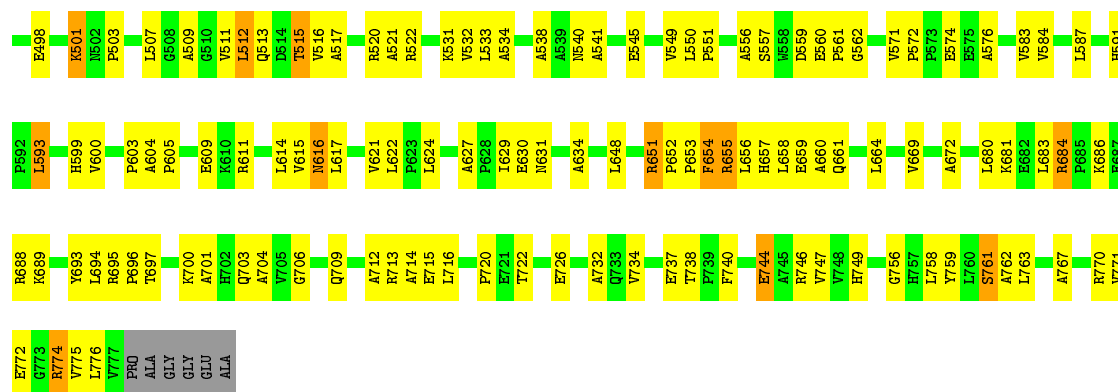


• Molecule 2: NADH-quinone oxidoreductase subunit 2



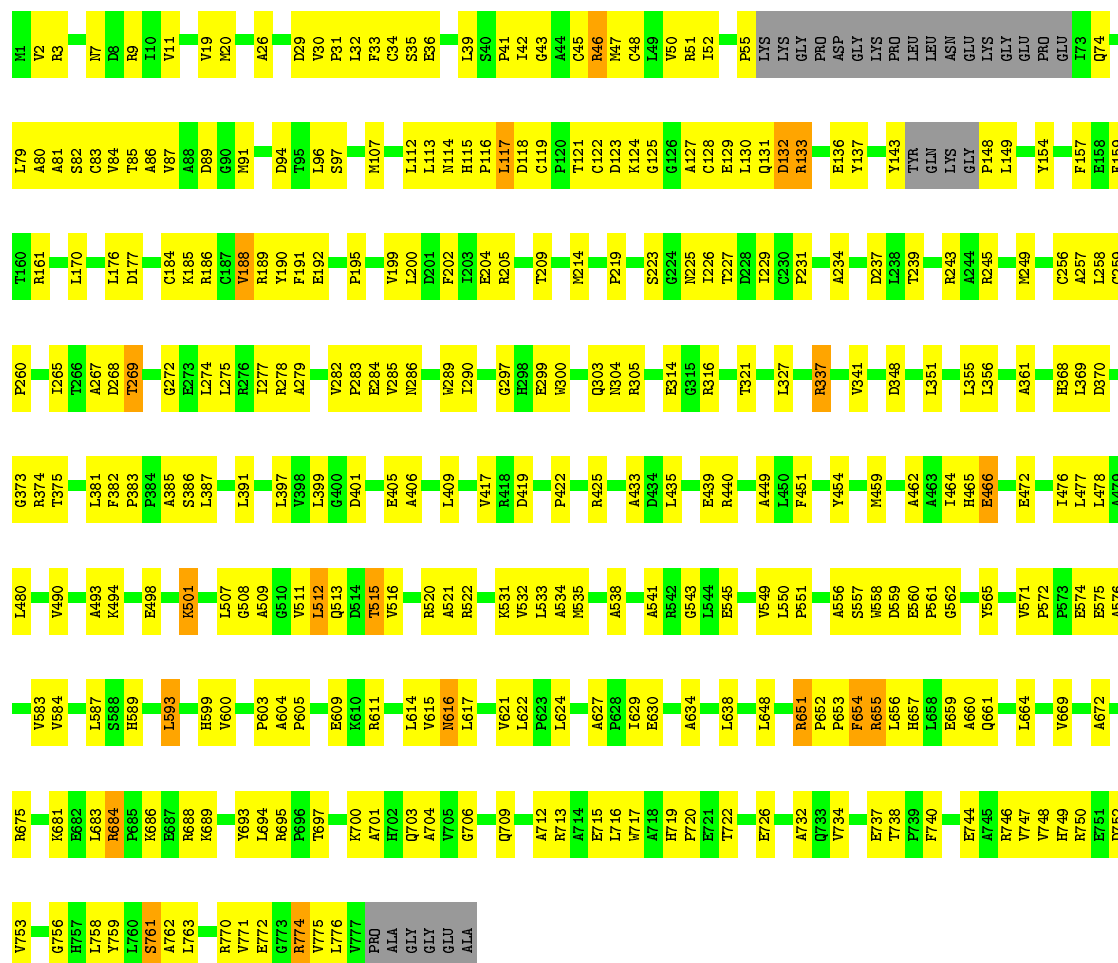
• Molecule 3: NADH-quinone oxidoreductase subunit 3





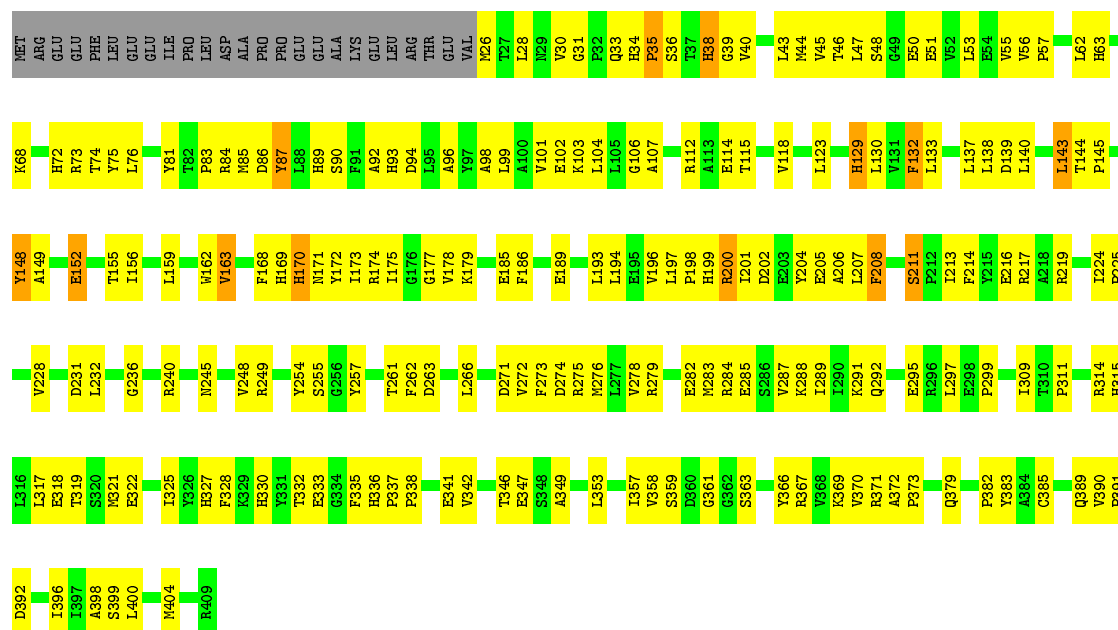
• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain D: 56% 38%



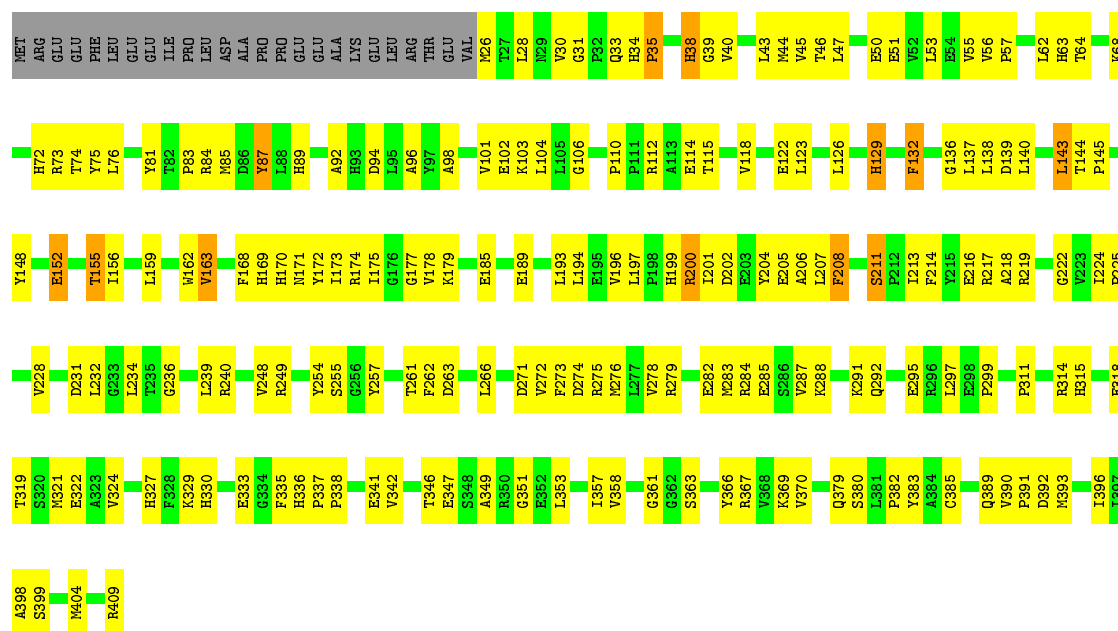
• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain 4: 46% 45% 6%



• Molecule 4: NADH-quinone oxidoreductase subunit 4

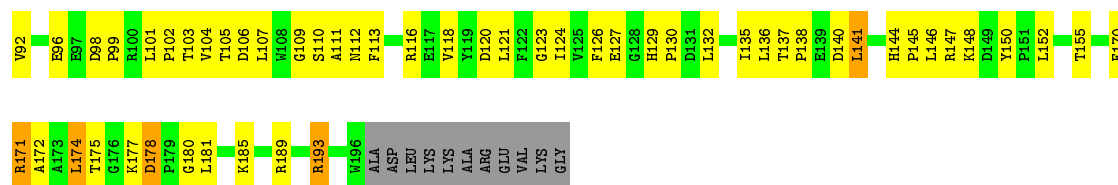
Chain E: 48% 43% 6%



• Molecule 5: NADH-quinone oxidoreductase subunit 5

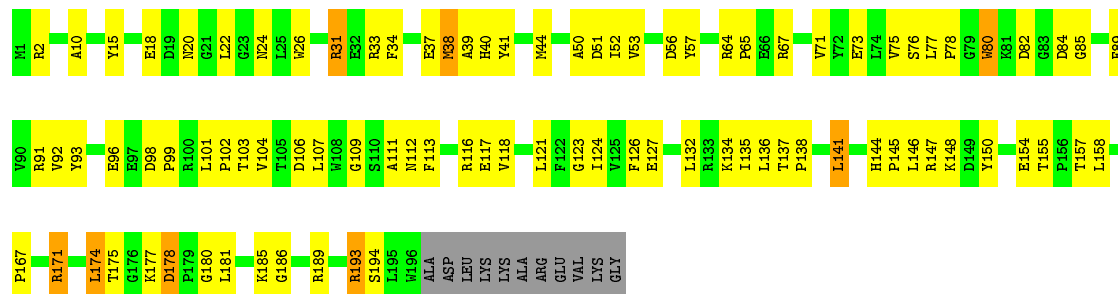
Chain 5: 50% 41% 5%





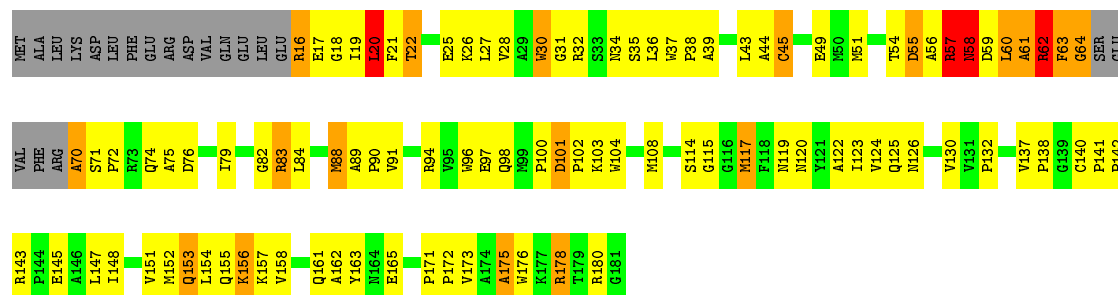
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain F: 51% 40% 5%



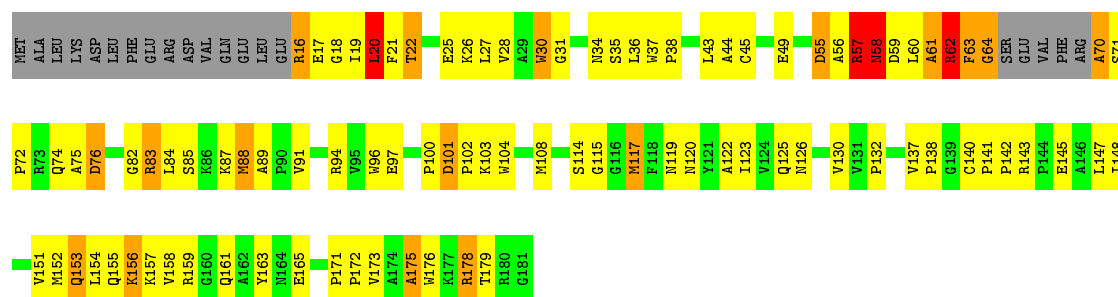
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain 6: 34% 43% 10% 11%



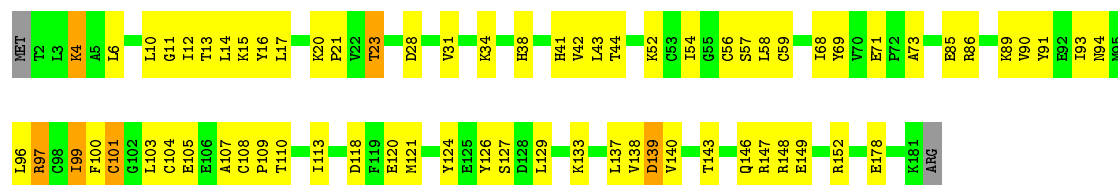
• Molecule 6: NADH-quinone oxidoreductase subunit 6

Chain G: 37% 40% 9% 11%

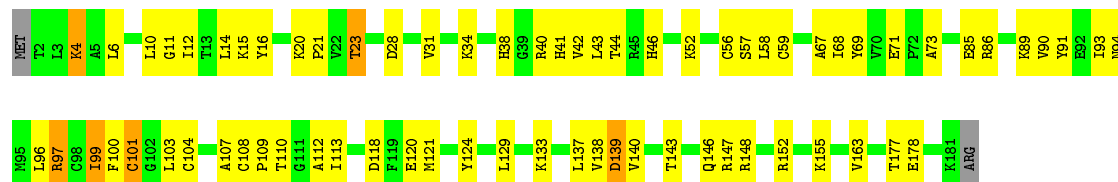


• Molecule 7: NADH-quinone oxidoreductase subunit 9

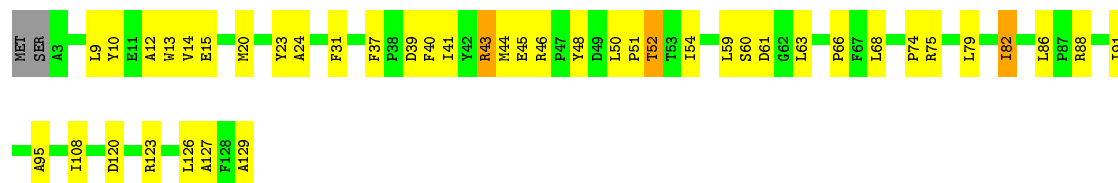
Chain 9: 60% 35% 5%



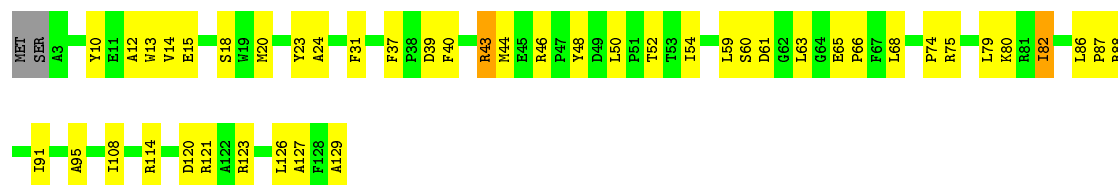
• Molecule 7: NADH-quinone oxidoreductase subunit 9



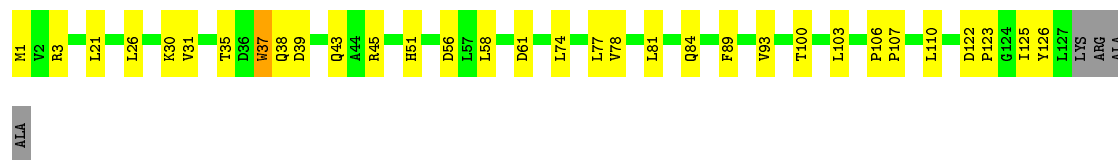
• Molecule 8: NADH-quinone oxidoreductase subunit 15



• Molecule 8: NADH-quinone oxidoreductase subunit 15



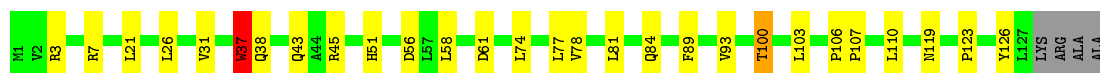
• Molecule 9: Putative uncharacterized protein TTHA1528



• Molecule 9: Putative uncharacterized protein TTHA1528

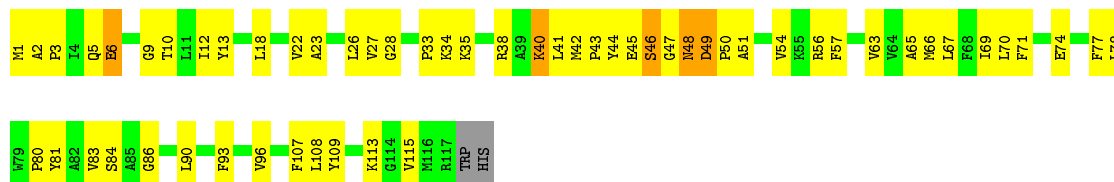






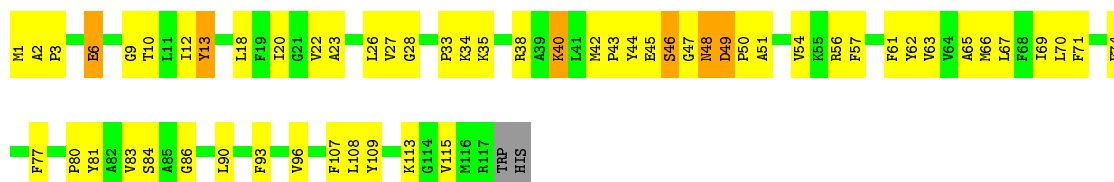
- Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain A:  50% 44% 6%



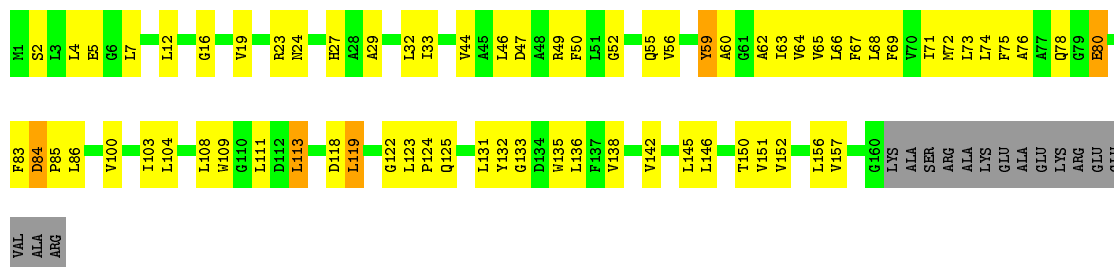
- Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P:  50% 43% 5%



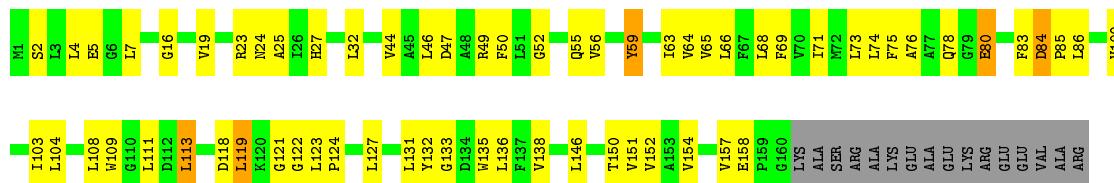
- Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J:  51% 37% • 9%



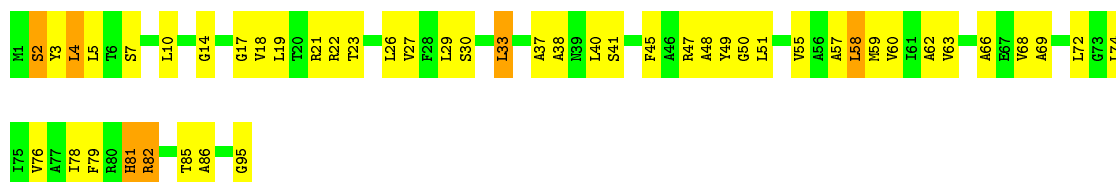
- Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain R:  55% 34% 9%



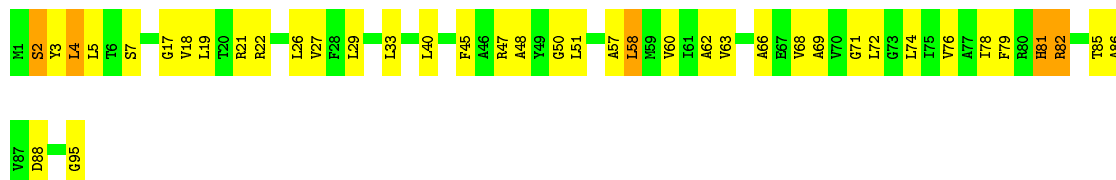
- Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K:  49% 44% 6%



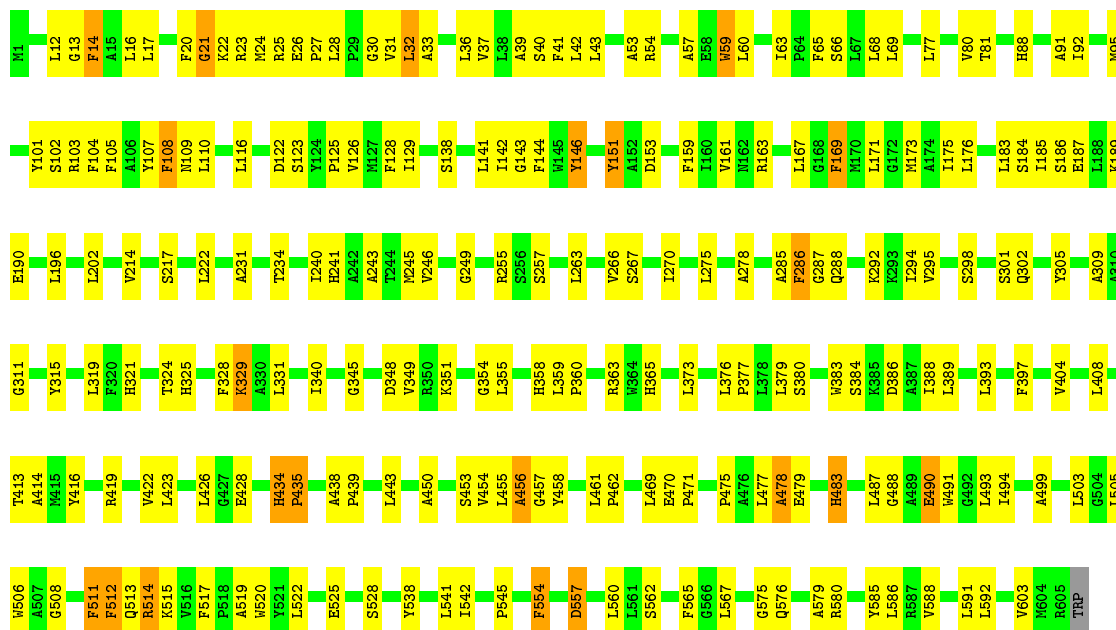
- Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain S: 58% 37% 5%



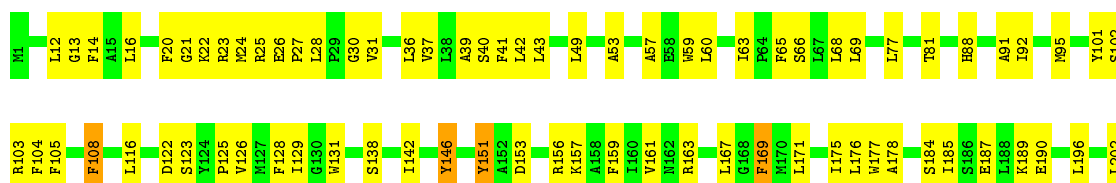
- Molecule 13: NADH-quinone oxidoreductase subunit 12

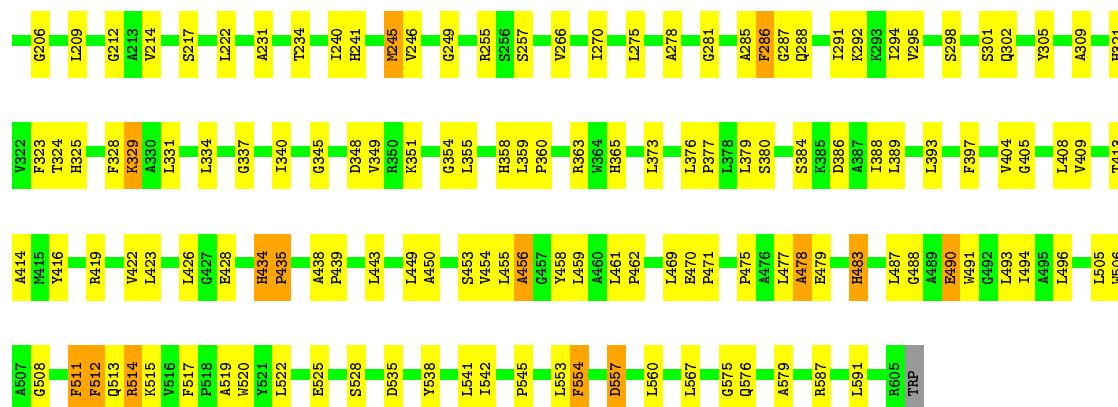
Chain L: 63% 33% 4%



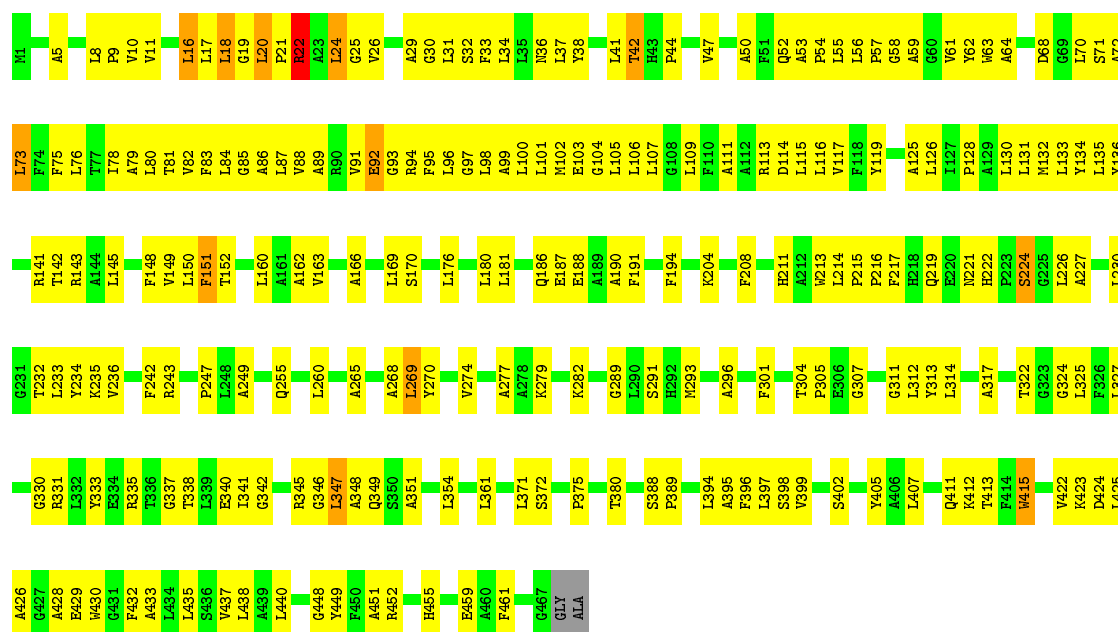
- Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain T: 65% 32% 3%

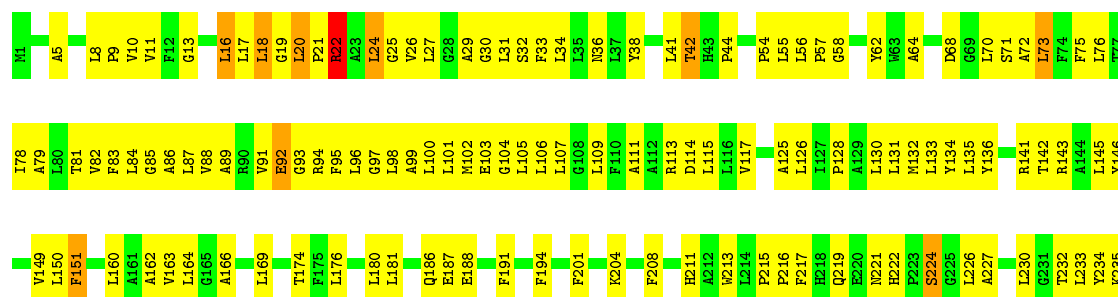


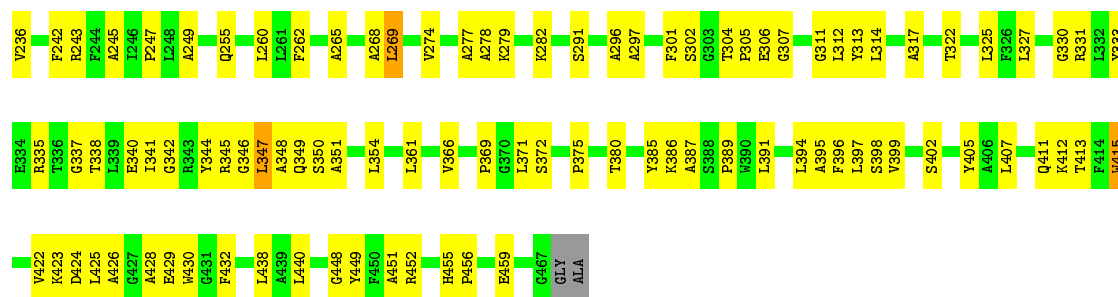


• Molecule 14: NADH-quinone oxidoreductase subunit 13



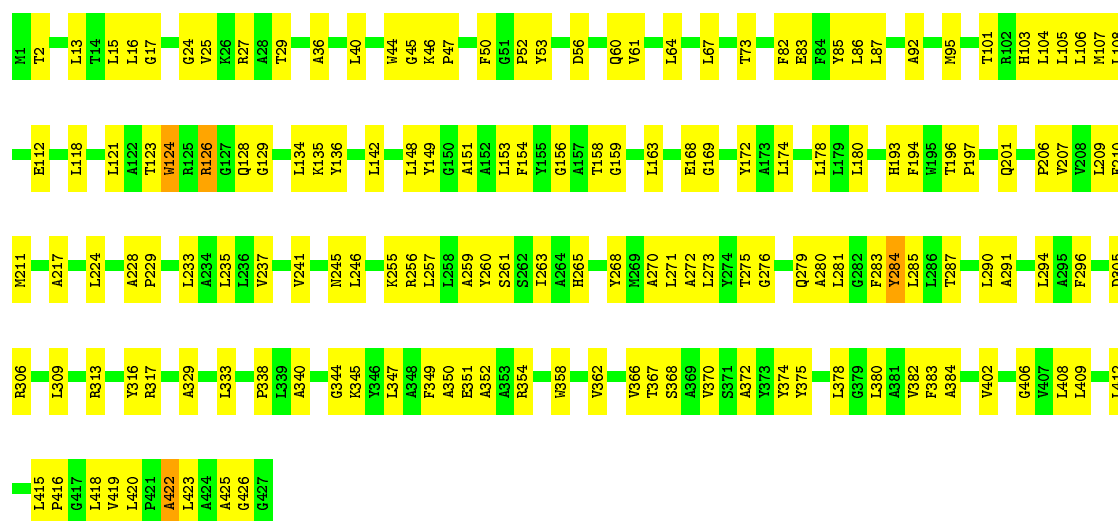
• Molecule 14: NADH-quinone oxidoreductase subunit 13





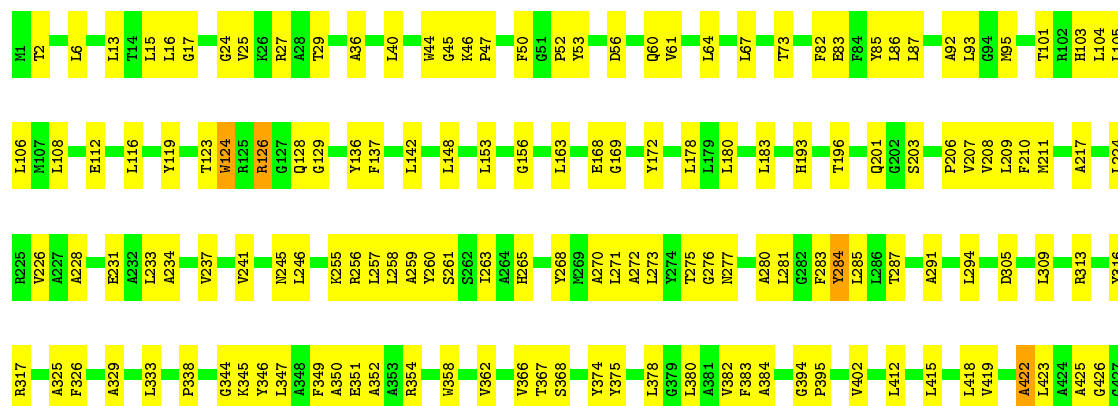
• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain N: 63% 36%



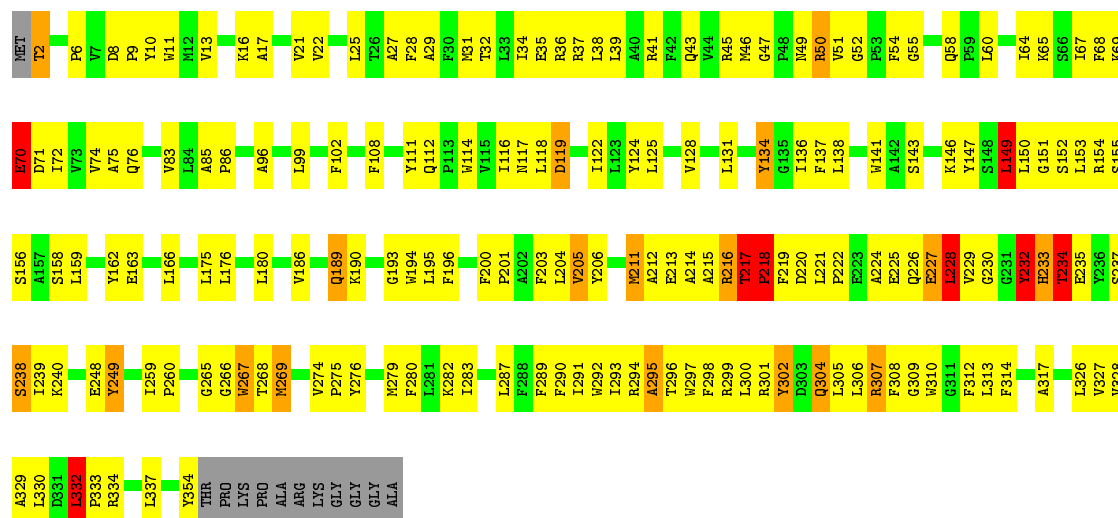
• Molecule 15: NADH-quinone oxidoreductase subunit 14

Chain V: 65% 34%



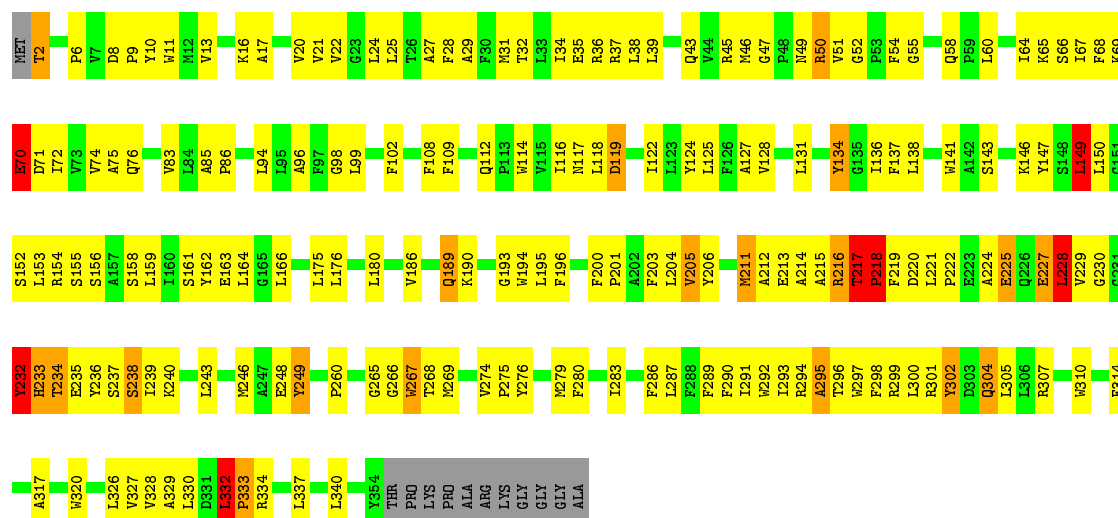
• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain H: 47% 43% 5%



• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q: 46% 44% 5%



## 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, $\alpha$ , $\beta$ , $\gamma$	96.28 Å   340.89 Å   263.30 Å 90.00°   100.57°   90.00°	Depositor
Resolution (Å)	40.00 – 3.30	Depositor
% Data completeness (in resolution range)	93.7 (40.00-3.30)	Depositor
$R_{merge}$	0.25	Depositor
$R_{sym}$	0.25	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 3.32 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1041)	Depositor
R, $R_{free}$	0.202 , 0.239	Depositor
Wilson B-factor (Å <sup>2</sup> )	76.0	Xtriage
Anisotropy	0.003	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.377 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.470 for -h,-k,h+l	Depositor
Outliers	0 of 233384 reflections	Xtriage
Total number of atoms	73998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1	0.34	0/3506	0.61	0/4745
1	B	0.33	1/3506 (0.0%)	0.59	0/4745
2	2	0.39	0/1439	0.63	0/1953
2	C	0.38	0/1439	0.61	0/1953
3	3	0.42	0/6035	0.71	0/8185
3	D	0.41	0/6035	0.71	0/8185
4	4	0.38	0/3150	0.70	1/4284 (0.0%)
4	E	0.37	0/3150	0.67	0/4284
5	5	0.36	0/1656	0.68	0/2246
5	F	0.35	0/1656	0.67	0/2246
6	6	0.57	0/1273	0.93	4/1723 (0.2%)
6	G	0.56	0/1273	0.92	5/1723 (0.3%)
7	9	0.46	0/1423	0.71	0/1933
7	O	0.42	0/1423	0.69	0/1933
8	7	0.37	0/1059	0.66	1/1429 (0.1%)
8	I	0.31	0/1059	0.63	1/1429 (0.1%)
9	W	0.37	0/985	0.62	0/1335
9	X	0.36	0/985	0.61	0/1335
10	A	0.41	0/940	0.70	0/1280
10	P	0.41	0/940	0.69	0/1280
11	J	0.35	0/1206	0.64	0/1649
11	R	0.36	0/1206	0.64	0/1649
12	K	0.37	0/710	0.59	0/962
12	S	0.38	0/710	0.59	0/962
13	L	0.33	0/4741	0.63	1/6460 (0.0%)
13	T	0.33	0/4741	0.62	2/6460 (0.0%)
14	M	0.39	0/3591	0.70	3/4896 (0.1%)
14	U	0.39	0/3591	0.70	3/4896 (0.1%)
15	N	0.34	0/3238	0.59	0/4434
15	V	0.34	0/3238	0.57	0/4434
16	H	0.48	1/2935 (0.0%)	0.79	5/4014 (0.1%)
16	Q	0.48	0/2935	0.79	5/4014 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.39	2/75774 (0.0%)	0.68	31/103056 (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
6	6	0	5
6	G	0	5
7	9	0	3
7	O	0	3
12	K	0	1
12	S	0	1
13	L	0	4
13	T	0	4
14	M	0	1
14	U	0	1
15	N	0	2
15	V	0	2
16	H	0	6
16	Q	0	6
All	All	0	44

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	225	GLU	CG-CD	-5.04	1.44	1.51
1	B	356	CYS	CB-SG	-5.02	1.73	1.81

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	U	22	ARG	NE-CZ-NH2	-12.89	113.85	120.30
14	M	22	ARG	NE-CZ-NH2	-12.73	113.93	120.30
14	U	22	ARG	NE-CZ-NH1	10.89	125.74	120.30
14	M	22	ARG	NE-CZ-NH1	10.39	125.49	120.30
16	Q	149	LEU	CB-CG-CD1	-8.27	96.95	111.00
16	H	149	LEU	CB-CG-CD1	-8.03	97.35	111.00
6	G	64	GLY	N-CA-C	-7.55	94.24	113.10
6	6	64	GLY	N-CA-C	-7.10	95.34	113.10
6	G	62	ARG	N-CA-C	-6.87	92.45	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	6	62	ARG	N-CA-C	-6.75	92.77	111.00
16	Q	149	LEU	CB-CG-CD2	6.49	122.03	111.00
16	Q	332	LEU	CA-CB-CG	6.46	130.15	115.30
6	6	57	ARG	NE-CZ-NH1	6.25	123.43	120.30
6	G	57	ARG	NE-CZ-NH1	6.14	123.37	120.30
13	T	514	ARG	N-CA-C	6.06	127.36	111.00
16	H	149	LEU	CB-CG-CD2	5.96	121.12	111.00
13	L	514	ARG	N-CA-C	5.75	126.52	111.00
8	I	68	LEU	CA-CB-CG	5.63	128.24	115.30
16	H	217	THR	C-N-CD	5.58	140.11	128.40
16	Q	225	GLU	N-CA-C	5.45	125.71	111.00
8	7	68	LEU	CA-CB-CG	5.38	127.68	115.30
14	U	397	LEU	N-CA-C	-5.34	96.57	111.00
14	M	397	LEU	N-CA-C	-5.28	96.76	111.00
16	H	332	LEU	CA-CB-CG	5.26	127.40	115.30
16	H	225	GLU	N-CA-C	5.25	125.17	111.00
6	G	76	ASP	N-CA-C	5.18	125.00	111.00
4	4	236	GLY	N-CA-C	5.09	125.82	113.10
6	6	20	LEU	N-CA-C	5.07	124.69	111.00
6	G	20	LEU	N-CA-C	5.04	124.61	111.00
13	T	245	MET	N-CA-CB	5.04	119.67	110.60
16	Q	217	THR	C-N-CD	5.01	138.93	128.40

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	6	175	ALA	Peptide
6	6	20	LEU	Peptide
6	6	56	ALA	Peptide
6	6	57	ARG	Peptide
6	6	70	ALA	Peptide
7	9	178	GLU	Peptide
7	9	20	LYS	Peptide
7	9	21	PRO	Peptide
6	G	175	ALA	Peptide
6	G	20	LEU	Peptide
6	G	56	ALA	Peptide
6	G	57	ARG	Peptide
6	G	70	ALA	Peptide
16	H	218	PRO	Peptide
16	H	227	GLU	Peptide

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Mol	Chain	Res	Type	Group
16	H	228	LEU	Peptide
16	H	266	GLY	Peptide
16	H	295	ALA	Peptide
16	H	332	LEU	Peptide
12	K	50	GLY	Peptide
13	L	397	PHE	Peptide
13	L	456	ALA	Peptide
13	L	462	PRO	Peptide
13	L	512	PHE	Peptide
14	M	71	SER	Peptide
15	N	123	THR	Peptide
15	N	422	ALA	Peptide
7	O	178	GLU	Peptide
7	O	20	LYS	Peptide
7	O	21	PRO	Peptide
16	Q	218	PRO	Peptide
16	Q	227	GLU	Peptide
16	Q	228	LEU	Peptide
16	Q	266	GLY	Peptide
16	Q	295	ALA	Peptide
16	Q	332	LEU	Peptide
12	S	50	GLY	Peptide
13	T	397	PHE	Peptide
13	T	456	ALA	Peptide
13	T	462	PRO	Peptide
13	T	512	PHE	Peptide
14	U	71	SER	Peptide
15	V	123	THR	Peptide
15	V	422	ALA	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3417	0	3388	144	0
1	B	3417	0	3388	128	0
2	2	1406	0	1373	81	0
2	C	1406	0	1373	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3	5895	0	5930	232	0
3	D	5895	0	5930	236	0
4	4	3067	0	3049	193	0
4	E	3067	0	3049	179	0
5	5	1607	0	1574	99	0
5	F	1607	0	1574	84	0
6	6	1245	0	1255	148	0
6	G	1245	0	1255	139	0
7	9	1388	0	1383	65	0
7	O	1388	0	1383	58	0
8	7	1031	0	1029	42	0
8	I	1031	0	1029	42	0
9	W	967	0	1010	27	0
9	X	967	0	1010	23	0
10	A	910	0	939	79	0
10	P	910	0	939	80	0
11	J	1183	0	1286	69	0
11	R	1183	0	1286	62	0
12	K	703	0	747	47	0
12	S	703	0	747	36	0
13	L	4604	0	4734	164	0
13	T	4604	0	4734	150	0
14	M	3489	0	3606	199	0
14	U	3489	0	3606	184	0
15	N	3154	0	3343	115	0
15	V	3154	0	3343	107	0
16	H	2838	0	2903	208	0
16	Q	2838	0	2903	205	0
17	1	8	0	0	1	0
17	3	24	0	0	0	0
17	6	8	0	0	2	0
17	9	16	0	0	6	0
17	B	8	0	0	2	0
17	D	24	0	0	0	0
17	G	8	0	0	2	0
17	O	16	0	0	7	0
18	1	31	0	19	4	0
18	B	31	0	19	3	0
19	2	4	0	0	1	0
19	3	4	0	0	1	0
19	C	4	0	0	1	0
19	D	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	73998	0	75136	3243	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 22.

All (3243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:57:ARG:CD	6:6:60:LEU:HD11	1.35	1.55
6:G:57:ARG:CD	6:G:60:LEU:HD11	1.43	1.49
6:6:57:ARG:HD2	6:6:60:LEU:CD1	1.46	1.46
6:G:57:ARG:HD2	6:G:60:LEU:CD1	1.52	1.40
6:6:57:ARG:CD	6:6:60:LEU:CD1	2.05	1.20
6:G:57:ARG:CD	6:G:60:LEU:CD1	2.11	1.17
6:G:57:ARG:NE	6:G:60:LEU:HD11	1.67	1.09
6:6:57:ARG:CG	6:6:60:LEU:HD11	1.84	1.08
6:6:57:ARG:NE	6:6:60:LEU:HD11	1.69	1.07
6:G:57:ARG:HD2	6:G:60:LEU:HD12	1.37	1.04
1:1:437:TRP:HB3	2:2:92:GLY:HA3	1.40	1.03
16:H:302:TYR:HA	16:H:305:LEU:HB3	1.42	1.02
6:6:57:ARG:HD2	6:6:60:LEU:HD12	1.37	1.00
6:6:57:ARG:CZ	6:6:60:LEU:HD21	1.91	1.00
6:G:57:ARG:CG	6:G:60:LEU:HD11	1.95	0.96
1:B:437:TRP:HB3	2:C:92:GLY:HA3	1.47	0.96
16:Q:227:GLU:HG2	16:Q:228:LEU:N	1.78	0.94
16:Q:302:TYR:HA	16:Q:305:LEU:HB3	1.47	0.94
6:6:57:ARG:CG	6:6:60:LEU:CD1	2.43	0.93
16:H:227:GLU:HG2	16:H:228:LEU:N	1.80	0.93
6:G:57:ARG:CZ	6:G:60:LEU:HD11	1.98	0.93
3:D:722:THR:HG21	3:D:756:GLY:H	1.33	0.91
10:A:35:LYS:O	10:A:40:LYS:NZ	2.06	0.89
11:J:119:LEU:HD11	12:K:47:ARG:HA	1.52	0.89
3:D:694:LEU:HB3	3:D:762:ALA:HB2	1.56	0.88
14:M:99:ALA:HB2	14:M:226:LEU:HD21	1.55	0.86
6:G:57:ARG:CG	6:G:60:LEU:CD1	2.51	0.86
7:O:96:LEU:HD21	7:O:129:LEU:HD13	1.57	0.86
3:3:722:THR:HG21	3:3:756:GLY:H	1.42	0.85
7:9:96:LEU:HD21	7:9:129:LEU:HD13	1.58	0.85
16:Q:222:PRO:HD2	16:Q:230:GLY:HA2	1.57	0.85
4:E:261:THR:H	4:E:292:GLN:HE22	1.24	0.84
11:R:111:LEU:HD11	11:R:113:LEU:HD12	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:397:LEU:HD21	3:3:480:LEU:HD13	1.59	0.84
6:6:57:ARG:CZ	6:6:60:LEU:HD11	2.06	0.84
6:G:57:ARG:CZ	6:G:60:LEU:HD21	2.07	0.84
6:G:64:GLY:O	6:G:75:ALA:HB2	1.78	0.84
10:A:70:LEU:HD13	11:J:150:THR:HG22	1.61	0.83
4:4:338:PRO:HG3	5:5:193:ARG:HB2	1.59	0.82
14:U:305:PRO:HB3	14:U:459:GLU:HA	1.61	0.82
13:L:298:SER:OG	13:L:329:LYS:NZ	2.11	0.82
1:1:287:ILE:HG12	1:1:330:LEU:HB3	1.59	0.82
10:P:35:LYS:O	10:P:40:LYS:NZ	2.12	0.82
11:J:111:LEU:HD11	11:J:113:LEU:HD12	1.61	0.82
4:E:39:GLY:O	4:E:404:MET:HG3	1.79	0.81
16:Q:45:ARG:HG3	16:Q:46:MET:H	1.45	0.81
15:V:92:ALA:HA	15:V:95:MET:HE2	1.60	0.81
3:D:397:LEU:HD21	3:D:480:LEU:HD13	1.61	0.81
16:H:72:ILE:HG22	16:H:237:SER:HB3	1.62	0.81
13:T:298:SER:OG	13:T:329:LYS:NZ	2.13	0.81
4:4:103:LYS:NZ	5:5:22:LEU:O	2.12	0.81
6:6:64:GLY:O	6:6:75:ALA:HB2	1.80	0.81
4:4:200:ARG:NH1	7:9:16:TYR:OH	2.14	0.81
4:E:333:GLU:O	4:E:363:SER:OG	1.99	0.81
10:P:90:LEU:HD12	16:Q:330:LEU:HD11	1.61	0.81
12:K:63:VAL:HG13	15:N:112:GLU:HG3	1.62	0.81
16:Q:224:ALA:HA	16:Q:230:GLY:H	1.46	0.80
10:P:6:GLU:OE1	16:Q:117:ASN:N	2.15	0.80
6:G:119:ASN:HA	6:G:125:GLN:HE22	1.43	0.80
10:P:70:LEU:HD13	11:R:150:THR:HG22	1.63	0.80
3:D:621:VAL:HG23	3:D:672:ALA:HA	1.62	0.80
6:G:57:ARG:HG3	6:G:57:ARG:HH11	1.47	0.80
14:M:224:SER:HA	14:M:330:GLY:HA3	1.63	0.80
11:R:119:LEU:HD11	12:S:47:ARG:HA	1.64	0.80
3:D:268:ASP:OD2	3:D:278:ARG:NH1	2.15	0.80
4:E:103:LYS:NZ	5:F:22:LEU:O	2.14	0.80
3:3:694:LEU:HB3	3:3:762:ALA:HB2	1.63	0.79
8:7:50:LEU:HD11	8:7:75:ARG:HB2	1.63	0.79
4:4:31:GLY:HA3	10:A:45:GLU:HG2	1.64	0.79
10:A:57:PHE:HE2	16:H:149:LEU:HD23	1.45	0.79
4:4:333:GLU:O	4:4:363:SER:OG	2.00	0.79
6:6:34:ASN:HB3	16:H:51:VAL:HG21	1.64	0.79
3:3:501:LYS:H	3:3:501:LYS:HD2	1.47	0.79
4:E:200:ARG:NH1	7:O:16:TYR:OH	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:224:ALA:HA	16:H:230:GLY:H	1.46	0.79
10:A:3:PRO:HD2	16:H:2:THR:HB	1.63	0.79
16:H:45:ARG:HG3	16:H:46:MET:H	1.48	0.79
3:D:501:LYS:H	3:D:501:LYS:HD2	1.47	0.79
4:E:338:PRO:HG3	5:F:193:ARG:HB2	1.63	0.79
3:D:655:ARG:HH12	3:D:659:GLU:HG3	1.47	0.79
6:6:60:LEU:O	6:6:60:LEU:HD12	1.83	0.78
6:G:60:LEU:HD12	6:G:60:LEU:O	1.83	0.78
16:Q:72:ILE:HG22	16:Q:237:SER:HB3	1.65	0.78
13:L:189:LYS:HZ1	13:L:479:GLU:HB2	1.47	0.78
3:3:538:ALA:HB3	3:3:541:ALA:HB2	1.64	0.78
4:4:205:GLU:OE1	4:4:284:ARG:NH2	2.15	0.78
10:P:113:LYS:NZ	15:V:83:GLU:OE2	2.15	0.78
2:C:146:THR:HG22	2:C:149:ARG:HB2	1.65	0.78
13:T:386:ASP:HA	13:T:389:LEU:HB2	1.66	0.78
13:L:575:GLY:HA2	15:N:246:LEU:HB3	1.66	0.78
4:4:261:THR:H	4:4:292:GLN:HE22	1.29	0.78
6:6:119:ASN:HA	6:6:125:GLN:HE22	1.49	0.78
4:4:333:GLU:OE2	4:4:336:HIS:NE2	2.17	0.78
10:A:57:PHE:CE2	16:H:149:LEU:HD23	2.19	0.78
4:4:216:GLU:OE2	16:H:304:GLN:NE2	2.17	0.77
4:E:50:GLU:O	4:E:389:GLN:NE2	2.15	0.77
16:H:222:PRO:HD2	16:H:230:GLY:HA2	1.66	0.77
14:U:224:SER:HA	14:U:330:GLY:HA3	1.67	0.77
6:6:57:ARG:HG3	6:6:57:ARG:HH11	1.50	0.77
5:5:102:PRO:HA	5:5:127:GLU:HB2	1.67	0.77
6:6:156:LYS:HG2	6:6:161:GLN:HB3	1.64	0.77
6:6:132:PRO:HG3	6:6:178:ARG:HE	1.50	0.77
4:E:205:GLU:OE1	4:E:284:ARG:NH2	2.18	0.77
6:6:57:ARG:HG3	6:6:60:LEU:HD11	1.67	0.77
4:4:28:LEU:HD21	16:H:228:LEU:HD21	1.67	0.77
4:4:50:GLU:O	4:4:389:GLN:NE2	2.17	0.77
6:6:57:ARG:HD2	6:6:60:LEU:CG	2.14	0.76
4:4:83:PRO:HB2	4:4:169:HIS:HA	1.67	0.76
9:X:3:ARG:NH1	9:X:103:LEU:O	2.18	0.76
3:3:269:THR:HG21	3:3:629:ILE:HG12	1.67	0.76
4:4:26:MET:HB2	4:4:47:LEU:O	1.85	0.76
6:G:34:ASN:HB3	16:Q:51:VAL:HG21	1.67	0.76
3:D:609:GLU:HA	3:D:627:ALA:H	1.50	0.76
6:G:63:PHE:HB3	6:G:70:ALA:HB3	1.68	0.76
14:U:347:LEU:HD23	14:U:413:THR:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:34:CYS:HA	3:D:184:CYS:HB2	1.67	0.76
13:T:414:ALA:HB1	13:T:505:LEU:HD23	1.68	0.76
14:U:99:ALA:HB2	14:U:226:LEU:HD21	1.66	0.76
4:E:85:MET:HE1	4:E:370:VAL:HG21	1.67	0.76
6:G:57:ARG:HB3	6:G:60:LEU:O	1.85	0.76
4:E:31:GLY:HA3	10:P:45:GLU:HG2	1.68	0.76
6:6:76:ASP:OD1	16:H:65:LYS:NZ	2.19	0.76
3:3:34:CYS:SG	3:3:35:SER:N	2.59	0.75
16:H:300:LEU:O	16:H:301:ARG:HG2	1.87	0.75
14:M:91:VAL:HG21	14:M:226:LEU:HD22	1.68	0.75
6:6:132:PRO:HG2	6:6:175:ALA:HB2	1.69	0.75
4:4:318:GLU:HB2	8:7:39:ASP:HA	1.68	0.75
2:2:24:ARG:HA	2:2:53:VAL:HG22	1.69	0.75
3:3:609:GLU:HA	3:3:627:ALA:H	1.52	0.75
5:5:126:PHE:H	5:5:132:LEU:HD11	1.52	0.75
1:1:361:GLU:OE1	3:3:114:ASN:ND2	2.20	0.75
13:L:414:ALA:HB1	13:L:505:LEU:HD23	1.69	0.75
10:P:57:PHE:HE2	16:Q:149:LEU:HD23	1.52	0.75
3:3:621:VAL:HG23	3:3:672:ALA:HA	1.69	0.75
1:B:79:MET:HE3	1:B:80:PRO:HD2	1.69	0.75
3:D:584:VAL:HG12	3:D:600:VAL:HB	1.69	0.75
16:H:150:LEU:HD22	16:H:228:LEU:HD12	1.67	0.75
3:3:655:ARG:HH12	3:3:659:GLU:HG3	1.52	0.74
6:G:132:PRO:HG2	6:G:175:ALA:HB2	1.66	0.74
1:1:79:MET:HE3	1:1:80:PRO:HD2	1.69	0.74
3:3:584:VAL:HG12	3:3:600:VAL:HB	1.70	0.74
1:B:190:ASN:ND2	1:B:198:ASN:O	2.19	0.74
10:P:3:PRO:HD2	16:Q:2:THR:HB	1.68	0.74
16:Q:300:LEU:O	16:Q:301:ARG:HG2	1.87	0.74
14:U:21:PRO:HD2	14:U:24:LEU:HG	1.67	0.74
16:Q:39:LEU:HD22	16:Q:295:ALA:HB2	1.69	0.74
10:A:6:GLU:OE1	16:H:117:ASN:N	2.20	0.74
14:M:347:LEU:HD23	14:M:413:THR:O	1.86	0.74
3:3:297:GLY:O	3:3:300:TRP:NE1	2.20	0.74
4:E:216:GLU:OE2	16:Q:304:GLN:NE2	2.20	0.74
9:X:78:VAL:HG21	9:X:126:TYR:HB2	1.70	0.74
3:3:268:ASP:OD2	3:3:278:ARG:NH1	2.20	0.74
3:3:561:PRO:HB3	3:3:576:ALA:HA	1.70	0.74
14:M:305:PRO:HB3	14:M:459:GLU:HA	1.68	0.74
3:D:185:LYS:HB3	3:D:189:ARG:HD3	1.68	0.74
6:G:156:LYS:HG2	6:G:161:GLN:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:21:PRO:HD2	14:M:24:LEU:HG	1.67	0.74
16:Q:155:SER:OG	16:Q:156:SER:N	2.20	0.74
6:6:132:PRO:HA	6:6:178:ARG:HH21	1.53	0.74
11:J:119:LEU:HD23	12:K:51:LEU:HD12	1.68	0.74
3:3:557:SER:H	3:3:560:GLU:HB2	1.53	0.73
16:Q:141:TRP:HA	16:Q:149:LEU:HD11	1.70	0.73
4:E:83:PRO:HB2	4:E:169:HIS:HA	1.69	0.73
6:G:76:ASP:OD1	16:Q:65:LYS:NZ	2.21	0.73
1:B:287:ILE:HG12	1:B:330:LEU:HB3	1.70	0.73
11:R:119:LEU:HD23	12:S:51:LEU:HD12	1.70	0.73
1:B:104:ARG:HH21	2:C:127:SER:HB3	1.53	0.73
13:L:60:LEU:HD21	14:M:375:PRO:HB3	1.71	0.73
9:W:3:ARG:NH1	9:W:103:LEU:O	2.22	0.73
10:A:63:VAL:HG11	10:A:115:VAL:HG21	1.69	0.73
10:A:90:LEU:HD12	16:H:330:LEU:HD11	1.71	0.73
15:N:294:LEU:HG	15:N:402:VAL:HG13	1.69	0.73
10:A:113:LYS:NZ	15:N:83:GLU:OE2	2.19	0.73
6:6:57:ARG:HG3	6:6:60:LEU:CD1	2.18	0.73
14:U:91:VAL:HG21	14:U:226:LEU:HD22	1.71	0.73
12:S:81:HIS:CD2	12:S:81:HIS:H	2.04	0.72
16:H:155:SER:OG	16:H:156:SER:N	2.21	0.72
4:E:318:GLU:HB2	8:I:39:ASP:HA	1.71	0.72
12:K:81:HIS:H	12:K:81:HIS:CD2	2.05	0.72
4:E:28:LEU:HD21	16:Q:228:LEU:HD21	1.71	0.72
6:G:132:PRO:HA	6:G:178:ARG:HH21	1.53	0.72
16:H:302:TYR:HA	16:H:305:LEU:CB	2.19	0.72
3:3:127:ALA:HB2	5:5:181:LEU:HB3	1.70	0.72
2:C:76:GLY:N	2:C:118:SER:OG	2.18	0.72
3:D:9:ARG:NH1	3:D:26:ALA:O	2.23	0.72
4:E:26:MET:HB2	4:E:47:LEU:O	1.89	0.72
14:U:16:LEU:HD12	14:U:25:GLY:HA3	1.69	0.72
6:6:57:ARG:HB3	6:6:60:LEU:O	1.88	0.72
3:3:716:LEU:HD21	3:3:758:LEU:HD23	1.72	0.72
2:C:112:THR:HG23	2:C:115:GLY:H	1.53	0.72
16:Q:31:MET:HA	16:Q:34:ILE:HD12	1.70	0.72
15:V:196:THR:HG22	15:V:259:ALA:HB1	1.70	0.72
2:2:146:THR:HG22	2:2:149:ARG:HB2	1.72	0.72
2:2:46:ILE:HG23	2:2:60:VAL:HG12	1.71	0.72
6:6:153:GLN:HG3	7:9:124:TYR:CZ	2.24	0.72
6:G:132:PRO:HG3	6:G:178:ARG:HE	1.54	0.72
3:3:41:PRO:HB3	3:3:433:ALA:HB1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:185:LYS:HB3	3:3:189:ARG:HD3	1.71	0.71
16:H:152:SER:O	16:H:155:SER:OG	2.05	0.71
8:I:50:LEU:HD11	8:I:75:ARG:HB2	1.72	0.71
5:5:103:THR:HG22	5:5:126:PHE:HB3	1.72	0.71
3:D:655:ARG:HB2	3:D:655:ARG:HH11	1.55	0.71
13:L:386:ASP:HA	13:L:389:LEU:HB2	1.72	0.71
14:M:81:THR:HB	14:M:233:LEU:HD11	1.71	0.71
15:N:280:ALA:HA	15:N:347:LEU:HD13	1.70	0.71
6:G:57:ARG:NH1	6:G:60:LEU:HD11	2.04	0.71
14:M:16:LEU:HD12	14:M:25:GLY:HA3	1.70	0.71
13:T:575:GLY:HA2	15:V:246:LEU:HB3	1.73	0.71
3:3:34:CYS:HA	3:3:184:CYS:HB2	1.71	0.71
14:M:82:VAL:HG11	14:M:103:GLU:HB2	1.72	0.71
16:Q:65:LYS:O	16:Q:69:LYS:HB2	1.90	0.71
16:H:162:TYR:CE1	16:H:305:LEU:HG	2.25	0.71
13:L:355:LEU:HB3	13:L:359:LEU:HD12	1.72	0.71
14:U:115:LEU:HD13	14:U:163:VAL:HG23	1.72	0.71
14:M:91:VAL:HB	14:M:95:PHE:CE1	2.26	0.71
7:O:28:ASP:OD2	16:Q:50:ARG:NH1	2.24	0.71
13:L:458:TYR:HB3	13:L:461:LEU:HD11	1.73	0.71
16:Q:35:GLU:OE1	16:Q:249:TYR:OH	2.05	0.71
13:L:419:ARG:HB2	13:L:512:PHE:CD2	2.25	0.70
7:O:120:GLU:OE1	7:O:146:GLN:NE2	2.23	0.70
3:D:716:LEU:HD21	3:D:758:LEU:HD23	1.72	0.70
15:N:92:ALA:HA	15:N:95:MET:HE2	1.71	0.70
16:H:141:TRP:HA	16:H:149:LEU:HD11	1.71	0.70
7:O:41:HIS:HB3	7:O:113:ILE:HD11	1.73	0.70
13:T:434:HIS:HB3	13:T:435:PRO:HD3	1.71	0.70
6:6:61:ALA:O	6:6:62:ARG:HD3	1.91	0.70
1:B:176:GLY:O	2:C:32:ARG:NH2	2.19	0.70
10:P:57:PHE:CE2	16:Q:149:LEU:HD23	2.26	0.70
14:U:265:ALA:HA	14:U:395:ALA:HB2	1.72	0.70
6:G:61:ALA:O	6:G:62:ARG:HD3	1.91	0.70
13:L:434:HIS:HB3	13:L:435:PRO:HD3	1.72	0.70
4:4:39:GLY:O	4:4:404:MET:HG3	1.91	0.70
10:A:109:TYR:OH	10:A:113:LYS:NZ	2.25	0.70
4:4:84:ARG:CZ	4:4:169:HIS:HB3	2.21	0.70
2:C:73:VAL:HG21	8:I:91:ILE:HD11	1.73	0.70
13:T:419:ARG:HB2	13:T:512:PHE:CD2	2.26	0.70
9:W:78:VAL:HG21	9:W:126:TYR:HB2	1.74	0.70
1:B:361:GLU:OE1	3:D:114:ASN:ND2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:102:GLU:HG2	4:4:175:ILE:O	1.92	0.69
3:D:722:THR:HG21	3:D:756:GLY:N	2.06	0.69
15:N:196:THR:HG22	15:N:259:ALA:HB1	1.74	0.69
12:K:7:SER:HB3	12:K:40:LEU:HD23	1.74	0.69
6:G:57:ARG:HD2	6:G:60:LEU:CG	2.22	0.69
16:H:176:LEU:HD21	16:H:337:LEU:HD12	1.74	0.69
1:1:337:MET:O	1:1:341:MET:HG2	1.93	0.69
2:C:46:ILE:HG23	2:C:60:VAL:HG12	1.73	0.69
3:3:117:LEU:HG	4:4:321:MET:HE1	1.74	0.69
4:4:389:GLN:HG3	4:4:391:PRO:HD2	1.74	0.69
6:G:64:GLY:C	6:G:74:GLN:HB2	2.13	0.69
10:A:51:ALA:HB1	16:H:146:LYS:HB2	1.73	0.69
4:4:341:GLU:OE2	5:5:57:TYR:OH	2.09	0.69
1:B:243:THR:HG22	1:B:244:GLU:H	1.58	0.69
3:D:538:ALA:HB3	3:D:541:ALA:HB2	1.73	0.69
4:E:338:PRO:HG2	5:F:193:ARG:HH11	1.58	0.69
14:M:73:LEU:O	14:M:76:LEU:N	2.26	0.69
14:U:128:PRO:O	14:U:132:MET:HG2	1.93	0.69
1:1:243:THR:HG22	1:1:244:GLU:H	1.58	0.69
11:J:113:LEU:HD22	12:K:48:ALA:HB1	1.75	0.69
16:H:31:MET:HA	16:H:34:ILE:HD12	1.75	0.69
10:P:63:VAL:HG11	10:P:115:VAL:HG21	1.73	0.69
13:T:189:LYS:HZ1	13:T:479:GLU:HB2	1.56	0.69
14:M:33:PHE:HA	14:M:79:ALA:HB1	1.75	0.68
16:Q:227:GLU:HG2	16:Q:228:LEU:H	1.58	0.68
5:5:50:ALA:HB3	5:5:73:GLU:HB3	1.76	0.68
6:G:57:ARG:HG3	6:G:60:LEU:CD1	2.24	0.68
13:L:122:ASP:O	13:L:185:ILE:N	2.25	0.68
4:4:72:HIS:HB3	5:5:171:ARG:HH21	1.58	0.68
7:9:120:GLU:OE1	7:9:146:GLN:NE2	2.25	0.68
15:V:294:LEU:HG	15:V:402:VAL:HG13	1.74	0.68
6:6:64:GLY:C	6:6:74:GLN:HB2	2.14	0.68
6:6:94:ARG:HD2	10:A:46:SER:HA	1.76	0.68
11:J:50:PHE:HE2	12:K:58:LEU:HD11	1.58	0.68
16:Q:237:SER:OG	16:Q:238:SER:N	2.25	0.68
6:6:132:PRO:HG3	6:6:178:ARG:NE	2.09	0.68
2:C:106:ILE:HD11	2:C:112:THR:HB	1.76	0.68
13:L:187:GLU:HA	13:L:190:GLU:HG2	1.74	0.68
7:O:43:LEU:HD12	7:O:133:LYS:HG3	1.76	0.68
3:3:615:VAL:HG22	3:3:621:VAL:HG12	1.76	0.68
4:E:72:HIS:HB3	5:F:171:ARG:HH21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:219:PHE:C	16:H:221:LEU:H	1.97	0.68
2:2:112:THR:HG23	2:2:115:GLY:H	1.58	0.68
3:3:715:GLU:H	3:3:761:SER:HB2	1.58	0.68
3:D:494:LYS:O	3:D:498:GLU:HG2	1.94	0.68
4:E:333:GLU:OE2	4:E:336:HIS:NE2	2.27	0.68
11:R:68:LEU:HD23	11:R:71:ILE:HD11	1.76	0.68
13:T:458:TYR:HB3	13:T:461:LEU:HD11	1.76	0.68
3:3:494:LYS:O	3:3:498:GLU:HG2	1.93	0.67
4:E:389:GLN:HG3	4:E:391:PRO:HD2	1.75	0.67
14:M:84:LEU:O	14:M:88:VAL:HG12	1.94	0.67
7:O:73:ALA:HB2	7:O:89:LYS:HB2	1.75	0.67
9:W:51:HIS:ND1	9:W:56:ASP:OD1	2.27	0.67
3:3:115:HIS:CG	3:3:116:PRO:HD2	2.30	0.67
6:6:61:ALA:O	6:6:62:ARG:NH1	2.26	0.67
1:B:337:MET:O	1:B:341:MET:HG2	1.95	0.67
4:E:123:LEU:HG	4:E:156:ILE:HG23	1.75	0.67
6:G:61:ALA:O	6:G:62:ARG:NH1	2.26	0.67
15:N:108:LEU:HD22	15:N:148:LEU:HD13	1.77	0.67
6:G:57:ARG:HG3	6:G:60:LEU:HD11	1.75	0.67
16:H:227:GLU:HG2	16:H:228:LEU:H	1.60	0.67
16:H:39:LEU:HD22	16:H:295:ALA:HB2	1.77	0.67
13:T:355:LEU:HB3	13:T:359:LEU:HD12	1.76	0.67
14:U:29:ALA:HB1	14:U:83:PHE:HA	1.76	0.67
3:3:373:GLY:HA3	3:3:538:ALA:HB2	1.75	0.67
3:D:615:VAL:HG22	3:D:621:VAL:HG12	1.76	0.67
3:3:655:ARG:HB2	3:3:655:ARG:HH11	1.59	0.67
13:T:122:ASP:O	13:T:185:ILE:N	2.27	0.67
4:4:314:ARG:NH2	8:7:44:MET:SD	2.68	0.67
16:H:158:SER:HA	16:H:306:LEU:HD21	1.77	0.67
14:M:333:TYR:O	14:M:337:GLY:N	2.27	0.67
14:M:29:ALA:HB1	14:M:83:PHE:HA	1.76	0.67
16:Q:302:TYR:HA	16:Q:305:LEU:CB	2.23	0.67
1:1:395:GLU:HB2	1:1:407:VAL:HG21	1.75	0.67
1:B:106:ILE:HD11	1:B:251:LEU:HD21	1.76	0.67
3:D:616:ASN:HD22	3:D:622:LEU:HD11	1.60	0.67
13:L:13:GLY:HA3	13:L:36:LEU:HD13	1.77	0.67
14:M:265:ALA:HA	14:M:395:ALA:HB2	1.76	0.67
2:C:24:ARG:HA	2:C:53:VAL:HG22	1.77	0.67
11:J:68:LEU:HD23	11:J:71:ILE:HD11	1.76	0.67
16:Q:176:LEU:HD21	16:Q:337:LEU:HD12	1.77	0.67
14:U:73:LEU:O	14:U:76:LEU:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:91:VAL:HG12	14:U:222:HIS:ND1	2.10	0.67
1:1:436:LEU:HD23	2:2:90:LEU:HA	1.75	0.66
11:J:47:ASP:O	11:J:122:GLY:N	2.29	0.66
16:Q:150:LEU:HD22	16:Q:228:LEU:HD12	1.76	0.66
3:3:722:THR:HG21	3:3:756:GLY:N	2.09	0.66
15:V:25:VAL:HG11	15:V:82:PHE:HB2	1.77	0.66
14:M:91:VAL:HG12	14:M:222:HIS:ND1	2.11	0.66
3:3:285:VAL:HA	3:3:387:LEU:HD12	1.77	0.66
3:D:127:ALA:HB2	5:F:181:LEU:HB3	1.76	0.66
6:G:94:ARG:HD2	10:P:46:SER:HA	1.77	0.66
16:H:60:LEU:O	16:H:64:ILE:HG13	1.96	0.66
14:M:128:PRO:O	14:M:132:MET:HG2	1.96	0.66
12:S:7:SER:HB3	12:S:40:LEU:HD23	1.76	0.66
5:5:104:VAL:HG23	5:5:111:ALA:HB2	1.77	0.66
6:G:153:GLN:HG3	7:O:124:TYR:CZ	2.30	0.66
4:E:102:GLU:HG2	4:E:175:ILE:O	1.96	0.66
11:J:133:GLY:H	11:J:136:LEU:HB2	1.59	0.66
13:L:163:ARG:HE	14:M:399:VAL:HB	1.61	0.66
13:L:419:ARG:NH2	13:L:525:GLU:OE2	2.28	0.66
3:3:713:ARG:HH21	3:3:746:ARG:HH21	1.42	0.66
3:D:713:ARG:HH21	3:D:746:ARG:HH21	1.42	0.66
6:G:37:TRP:O	6:G:75:ALA:HB1	1.96	0.66
16:Q:216:ARG:HB2	16:Q:294:ARG:HD2	1.78	0.66
11:R:50:PHE:HE2	12:S:58:LEU:HD11	1.60	0.66
1:1:190:ASN:ND2	1:1:198:ASN:O	2.29	0.65
10:P:56:ARG:HB3	11:R:73:LEU:O	1.96	0.65
16:Q:162:TYR:CE1	16:Q:305:LEU:HG	2.30	0.65
4:4:263:ASP:HB2	4:4:285:GLU:HG3	1.78	0.65
14:M:347:LEU:CD1	14:M:422:VAL:HG21	2.26	0.65
15:N:280:ALA:HB1	15:N:347:LEU:HB3	1.78	0.65
16:Q:219:PHE:C	16:Q:221:LEU:H	1.97	0.65
1:1:201:LEU:HD12	1:1:399:PHE:HE1	1.61	0.65
4:4:337:PRO:O	4:4:361:GLY:HA2	1.97	0.65
6:6:57:ARG:NH1	6:6:60:LEU:HD11	2.11	0.65
4:E:118:VAL:HB	4:E:257:TYR:HE1	1.61	0.65
13:L:278:ALA:HA	13:L:301:SER:HA	1.78	0.65
12:S:63:VAL:HG13	15:V:112:GLU:HG3	1.76	0.65
6:6:63:PHE:HB3	6:6:70:ALA:HB3	1.78	0.65
4:E:213:ILE:HD13	16:Q:298:PHE:HB2	1.78	0.65
4:4:118:VAL:HB	4:4:257:TYR:HE1	1.62	0.65
6:G:154:LEU:O	6:G:158:VAL:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:113:LEU:HD22	12:S:48:ALA:HB1	1.79	0.65
14:U:335:ARG:NH1	14:U:423:LYS:O	2.30	0.65
13:L:413:THR:HA	13:L:416:TYR:CE2	2.32	0.65
3:D:459:MET:HG2	3:D:465:HIS:HB2	1.79	0.65
13:L:393:LEU:HD12	13:L:493:LEU:HD11	1.78	0.65
14:M:188:GLU:HA	14:M:191:PHE:HB3	1.78	0.65
14:M:331:ARG:HB3	14:M:429:GLU:OE2	1.96	0.65
13:T:393:LEU:HD12	13:T:493:LEU:HD11	1.78	0.65
1:I:341:MET:HB2	1:I:371:PHE:CE2	2.31	0.65
6:G:132:PRO:HG3	6:G:178:ARG:NE	2.12	0.65
8:I:60:SER:HA	8:I:66:PRO:HA	1.78	0.65
14:M:448:GLY:O	14:M:452:ARG:HG2	1.97	0.65
4:4:338:PRO:HG2	5:5:193:ARG:HH11	1.62	0.65
5:5:80:TRP:CE3	5:5:80:TRP:HA	2.32	0.65
8:7:44:MET:HE2	8:7:46:ARG:HH22	1.61	0.65
13:L:159:PHE:HD2	14:M:407:LEU:HD11	1.62	0.65
7:O:71:GLU:HB2	7:O:90:VAL:HB	1.78	0.65
3:3:9:ARG:NH1	3:3:26:ALA:O	2.30	0.65
10:A:47:GLY:O	10:A:48:ASN:ND2	2.23	0.65
16:H:162:TYR:HA	16:H:314:PHE:CZ	2.32	0.65
1:B:287:ILE:HA	1:B:332:PRO:HA	1.78	0.64
13:L:487:LEU:HD12	13:L:488:GLY:H	1.62	0.64
13:T:126:VAL:HA	13:T:129:ILE:HD12	1.79	0.64
12:K:19:LEU:HD22	13:L:591:LEU:HD12	1.78	0.64
2:2:73:VAL:HG21	8:7:91:ILE:HD11	1.80	0.64
6:6:96:TRP:HZ2	6:6:175:ALA:HB1	1.63	0.64
7:9:71:GLU:HB2	7:9:90:VAL:HB	1.77	0.64
3:D:509:ALA:O	3:D:513:GLN:N	2.30	0.64
14:M:115:LEU:HD13	14:M:163:VAL:HG23	1.79	0.64
15:N:193:HIS:HB2	15:N:263:ILE:HD13	1.80	0.64
16:H:189:GLN:O	16:H:193:GLY:HA2	1.98	0.64
14:M:347:LEU:O	14:M:351:ALA:N	2.24	0.64
14:U:151:PHE:HD2	14:U:213:TRP:HB3	1.62	0.64
8:7:37:PHE:CE1	8:7:74:PRO:HA	2.32	0.64
10:A:56:ARG:HB3	11:J:73:LEU:O	1.97	0.64
3:D:128:CYS:HB3	3:D:131:GLN:HB2	1.80	0.64
3:D:557:SER:H	3:D:560:GLU:HB2	1.62	0.64
4:E:341:GLU:HG2	4:E:358:VAL:HG22	1.80	0.64
14:M:115:LEU:HD12	14:M:180:LEU:HD13	1.80	0.64
15:N:25:VAL:HG11	15:N:82:PHE:HB2	1.79	0.64
13:T:187:GLU:HA	13:T:190:GLU:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:656:LEU:HD21	9:W:3:ARG:HD3	1.77	0.64
1:B:356:CYS:HB3	1:B:358:PRO:HD2	1.79	0.64
1:B:436:LEU:HD23	2:C:90:LEU:HA	1.79	0.64
2:2:106:ILE:HD11	2:2:112:THR:HB	1.80	0.64
1:1:104:ARG:HH21	2:2:127:SER:HB3	1.62	0.64
3:3:186:ARG:HD3	3:3:229:ILE:HG22	1.80	0.64
4:4:261:THR:H	4:4:292:GLN:NE2	1.96	0.64
1:B:395:GLU:HB2	1:B:407:VAL:HG21	1.79	0.64
13:L:380:SER:HB3	13:L:456:ALA:HB3	1.79	0.64
10:P:47:GLY:O	10:P:48:ASN:ND2	2.24	0.64
10:P:109:TYR:OH	10:P:113:LYS:NZ	2.31	0.64
1:1:106:ILE:HD11	1:1:251:LEU:HD21	1.80	0.64
3:D:515:THR:HG23	3:D:683:LEU:HD13	1.80	0.64
5:F:102:PRO:HA	5:F:127:GLU:HB2	1.80	0.64
10:A:33:PRO:HD2	16:H:70:GLU:HB3	1.80	0.64
14:M:84:LEU:HB3	14:M:432:PHE:CD1	2.33	0.64
10:P:51:ALA:HB1	16:Q:146:LYS:HB2	1.79	0.64
14:U:91:VAL:HB	14:U:95:PHE:CE1	2.33	0.64
3:D:34:CYS:SG	3:D:35:SER:N	2.71	0.64
5:F:103:THR:HG22	5:F:126:PHE:HB3	1.80	0.64
13:L:126:VAL:HA	13:L:129:ILE:HD12	1.80	0.64
11:J:50:PHE:HB2	11:J:124:PRO:HD3	1.80	0.63
3:3:46:ARG:HG2	3:3:46:ARG:HH11	1.63	0.63
3:D:186:ARG:HD3	3:D:229:ILE:HG22	1.80	0.63
15:N:168:GLU:H	15:N:172:TYR:HB2	1.64	0.63
6:6:37:TRP:O	6:6:75:ALA:HB1	1.99	0.63
3:D:656:LEU:HD21	9:X:3:ARG:HD3	1.81	0.63
14:U:333:TYR:O	14:U:337:GLY:N	2.31	0.63
14:U:346:GLY:O	14:U:348:ALA:N	2.31	0.63
13:T:60:LEU:HD21	14:U:375:PRO:HB3	1.80	0.63
1:B:201:LEU:HD12	1:B:399:PHE:HE1	1.63	0.63
3:3:2:VAL:HG13	3:3:89:ASP:HA	1.80	0.63
5:5:67:ARG:HD3	5:5:96:GLU:HG3	1.81	0.63
1:B:438:ARG:OXT	2:C:146:THR:OG1	2.17	0.63
13:L:189:LYS:NZ	13:L:479:GLU:HB2	2.13	0.63
6:6:154:LEU:O	6:6:158:VAL:HG13	1.98	0.63
14:U:105:LEU:HD13	14:U:125:ALA:HA	1.81	0.63
7:9:113:ILE:HB	17:9:202:SF4:S4	2.38	0.63
13:L:63:ILE:HG21	13:L:125:PRO:HG2	1.80	0.63
14:M:335:ARG:NH1	14:M:423:LYS:O	2.32	0.63
13:T:458:TYR:HD1	13:T:461:LEU:HD21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:57:ARG:NH2	6:6:60:LEU:HD21	2.14	0.63
6:G:63:PHE:HB3	6:G:70:ALA:CB	2.29	0.63
13:T:163:ARG:HE	14:U:399:VAL:HB	1.64	0.63
6:6:153:GLN:O	6:6:157:LYS:N	2.32	0.62
11:J:19:VAL:O	12:K:21:ARG:NH2	2.28	0.62
13:L:348:ASP:HB3	13:L:351:LYS:HB2	1.79	0.62
11:R:133:GLY:H	11:R:136:LEU:HB2	1.64	0.62
13:T:487:LEU:HD12	13:T:488:GLY:H	1.63	0.62
3:D:115:HIS:CG	3:D:116:PRO:HD2	2.35	0.62
3:D:561:PRO:HB3	3:D:576:ALA:HA	1.82	0.62
16:H:134:TYR:HA	16:H:137:PHE:CE2	2.33	0.62
11:J:75:PHE:HZ	11:J:78:GLN:HG2	1.64	0.62
14:U:82:VAL:HG11	14:U:103:GLU:HB2	1.81	0.62
3:D:720:PRO:HG3	3:D:749:HIS:HB3	1.80	0.62
3:D:664:LEU:HD22	3:D:669:VAL:HG11	1.80	0.62
16:H:124:TYR:O	16:H:128:VAL:HG13	1.99	0.62
16:H:216:ARG:HB2	16:H:294:ARG:HD2	1.82	0.62
13:L:458:TYR:HD1	13:L:461:LEU:HD21	1.64	0.62
16:Q:211:MET:HA	16:Q:215:ALA:HB3	1.81	0.62
13:T:419:ARG:NH2	13:T:525:GLU:OE2	2.31	0.62
1:1:438:ARG:OXT	2:2:146:THR:OG1	2.18	0.62
4:E:201:ILE:HA	4:E:204:TYR:HD2	1.65	0.62
7:9:28:ASP:OD2	16:H:50:ARG:NH1	2.33	0.62
13:T:217:SER:HB3	13:T:249:GLY:HA3	1.80	0.62
15:V:47:PRO:HB3	15:V:56:ASP:HA	1.80	0.62
3:D:605:PRO:HB2	3:D:609:GLU:HG3	1.82	0.62
8:I:44:MET:HE2	8:I:46:ARG:HH22	1.62	0.62
14:M:126:LEU:HD11	14:M:149:VAL:HG22	1.80	0.62
11:R:2:SER:HA	11:R:5:GLU:HB3	1.81	0.62
12:S:19:LEU:HD22	13:T:591:LEU:HD12	1.80	0.62
13:T:240:ILE:HG22	13:T:241:HIS:HD2	1.63	0.62
14:U:448:GLY:O	14:U:452:ARG:HG2	1.99	0.62
3:3:605:PRO:HB2	3:3:609:GLU:HG3	1.81	0.62
16:Q:290:PHE:O	16:Q:294:ARG:HG2	2.00	0.62
16:Q:37:ARG:NH2	16:Q:54:PHE:O	2.33	0.62
16:H:35:GLU:OE1	16:H:249:TYR:OH	2.12	0.62
14:M:346:GLY:O	14:M:348:ALA:N	2.32	0.62
14:M:54:PRO:HA	14:M:62:TYR:HD1	1.64	0.62
16:Q:124:TYR:O	16:Q:128:VAL:HG13	1.99	0.62
14:U:84:LEU:O	14:U:88:VAL:HG12	2.00	0.62
5:5:39:ALA:HA	5:5:107:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:56:ASP:OD2	5:5:148:LYS:N	2.30	0.62
3:D:2:VAL:HG13	3:D:89:ASP:HA	1.82	0.62
16:Q:52:GLY:HA2	16:Q:55:GLY:H	1.64	0.62
1:B:46:LYS:HE2	1:B:163:PHE:HB3	1.81	0.61
16:Q:152:SER:O	16:Q:155:SER:OG	2.09	0.61
4:4:240:ARG:NH1	4:4:282:GLU:OE2	2.33	0.61
4:E:272:VAL:HG13	4:E:399:SER:HB3	1.81	0.61
6:G:104:TRP:NE1	6:G:172:PRO:O	2.33	0.61
6:6:57:ARG:CZ	6:6:60:LEU:CD2	2.73	0.61
3:D:46:ARG:HG2	3:D:46:ARG:HH11	1.65	0.61
5:F:67:ARG:HD3	5:F:96:GLU:HG3	1.83	0.61
11:J:69:PHE:HZ	16:H:156:SER:HG	1.47	0.61
16:H:65:LYS:O	16:H:69:LYS:HB2	1.99	0.61
3:D:19:VAL:HG21	3:D:52:ILE:HD11	1.80	0.61
13:L:102:SER:OG	13:L:103:ARG:N	2.33	0.61
14:M:84:LEU:HB3	14:M:432:PHE:HD1	1.64	0.61
14:U:347:LEU:HD12	14:U:422:VAL:HG21	1.82	0.61
2:2:24:ARG:HA	2:2:53:VAL:CG2	2.30	0.61
1:B:344:LEU:HD21	2:C:86:LEU:HD22	1.83	0.61
3:D:199:VAL:HG11	3:D:219:PRO:HD2	1.83	0.61
3:D:269:THR:HG21	3:D:629:ILE:HG12	1.82	0.61
16:Q:227:GLU:CG	16:Q:228:LEU:N	2.59	0.61
7:9:4:LYS:H	7:9:4:LYS:HD2	1.66	0.61
4:4:213:ILE:HD13	16:H:298:PHE:HB2	1.82	0.61
13:T:454:VAL:HB	13:T:455:LEU:HD22	1.83	0.61
4:4:143:LEU:HD23	4:4:143:LEU:H	1.63	0.61
8:7:37:PHE:HE1	8:7:74:PRO:HA	1.66	0.61
1:B:100:SER:HA	1:B:253:GLN:HE21	1.65	0.61
13:L:288:GLN:NE2	13:L:528:SER:O	2.34	0.61
7:O:68:ILE:HG12	7:O:93:ILE:HG12	1.83	0.61
11:R:75:PHE:HZ	11:R:78:GLN:HG2	1.64	0.61
13:T:324:THR:HB	13:T:380:SER:HB2	1.83	0.61
1:1:259:LYS:HA	1:1:284:LEU:HD21	1.83	0.61
6:G:125:GLN:O	9:X:38:GLN:NE2	2.34	0.61
15:N:265:HIS:NE2	15:N:333:LEU:O	2.33	0.61
14:U:8:LEU:HD21	14:U:31:LEU:HB3	1.83	0.61
16:H:158:SER:HB2	16:H:305:LEU:HD23	1.83	0.61
14:U:5:ALA:HB1	14:U:36:ASN:ND2	2.15	0.61
15:V:280:ALA:HA	15:V:347:LEU:HD13	1.81	0.61
13:L:12:LEU:O	13:L:16:LEU:HG	2.00	0.61
15:N:168:GLU:HG2	15:N:169:GLY:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:201:ILE:HA	4:4:204:TYR:HD2	1.66	0.60
1:B:341:MET:HB2	1:B:371:PHE:CE2	2.36	0.60
3:D:237:ASP:OD1	3:D:239:THR:HG22	2.01	0.60
4:E:240:ARG:NH1	4:E:282:GLU:OE2	2.34	0.60
4:E:84:ARG:CZ	4:E:169:HIS:HB3	2.31	0.60
16:H:237:SER:OG	16:H:238:SER:N	2.31	0.60
16:H:29:ALA:O	16:H:32:THR:OG1	2.11	0.60
11:J:75:PHE:CZ	11:J:78:GLN:HG2	2.36	0.60
14:M:79:ALA:HA	14:M:103:GLU:OE1	2.01	0.60
15:V:193:HIS:HB2	15:V:263:ILE:HD13	1.83	0.60
2:2:76:GLY:N	2:2:118:SER:OG	2.28	0.60
6:G:30:TRP:CD1	6:G:31:GLY:N	2.69	0.60
13:T:13:GLY:HA3	13:T:36:LEU:HD13	1.84	0.60
3:3:19:VAL:HG21	3:3:52:ILE:HD11	1.81	0.60
3:D:51:ARG:HB3	3:D:94:ASP:HB3	1.83	0.60
3:D:657:HIS:O	3:D:661:GLN:HG2	2.00	0.60
13:L:454:VAL:HB	13:L:455:LEU:HD22	1.83	0.60
3:D:406:ALA:O	3:D:409:LEU:HB2	2.02	0.60
7:O:43:LEU:HB2	7:O:137:LEU:HD12	1.82	0.60
1:1:356:CYS:HB3	1:1:358:PRO:HD2	1.82	0.60
4:4:254:TYR:HD1	4:4:255:SER:H	1.48	0.60
2:C:76:GLY:H	2:C:118:SER:HG	1.48	0.60
4:E:392:ASP:OD2	16:Q:301:ARG:NH1	2.29	0.60
4:4:367:ARG:NH1	4:4:369:LYS:HB2	2.16	0.60
3:D:688:ARG:HB3	3:D:770:ARG:HB2	1.82	0.60
4:E:143:LEU:H	4:E:143:LEU:HD23	1.65	0.60
13:L:349:VAL:HG13	13:L:423:LEU:HB3	1.84	0.60
14:M:91:VAL:HG13	14:M:224:SER:OG	2.02	0.60
14:U:84:LEU:HB3	14:U:432:PHE:CD1	2.36	0.60
9:W:31:VAL:HG11	9:W:81:LEU:HD13	1.83	0.60
4:4:224:ILE:HD11	4:4:275:ARG:NH1	2.17	0.60
3:D:734:VAL:HG13	3:D:775:VAL:HG13	1.84	0.60
4:E:261:THR:H	4:E:292:GLN:NE2	1.97	0.60
4:E:367:ARG:NH1	4:E:369:LYS:HB2	2.16	0.60
16:H:227:GLU:CG	16:H:228:LEU:N	2.61	0.60
16:H:74:VAL:HG12	16:H:75:ALA:O	2.01	0.60
10:P:57:PHE:HE2	16:Q:149:LEU:CD2	2.15	0.60
9:X:45:ARG:NH1	9:X:61:ASP:OD2	2.32	0.60
1:1:201:LEU:HD12	1:1:399:PHE:CE1	2.36	0.60
10:A:69:ILE:HD11	12:K:69:ALA:HB2	1.84	0.60
3:D:297:GLY:O	3:D:300:TRP:NE1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:101:VAL:HB	4:E:175:ILE:HD12	1.83	0.60
6:G:34:ASN:O	6:G:59:ASP:HB3	2.01	0.60
14:M:186:GLN:HG2	14:M:187:GLU:H	1.67	0.60
14:M:93:GLY:HA3	14:M:95:PHE:HD1	1.66	0.60
13:T:12:LEU:O	13:T:16:LEU:HG	2.02	0.60
3:3:31:PRO:HG3	3:3:137:TYR:CD2	2.36	0.60
3:D:136:GLU:HG2	5:F:189:ARG:HG2	1.83	0.60
3:D:373:GLY:HA3	3:D:538:ALA:HB2	1.83	0.60
3:D:31:PRO:HB2	3:D:47:MET:HB3	1.84	0.60
3:D:80:ALA:HB1	3:D:85:THR:OG1	2.02	0.60
4:E:341:GLU:OE2	5:F:57:TYR:OH	2.17	0.60
5:F:80:TRP:HA	5:F:80:TRP:CE3	2.37	0.60
10:P:65:ALA:HB3	11:R:66:LEU:HD13	1.83	0.60
11:R:85:PRO:HA	12:S:22:ARG:HH12	1.65	0.60
1:1:100:SER:HA	1:1:253:GLN:HE21	1.66	0.60
5:F:50:ALA:HB3	5:F:73:GLU:HB3	1.84	0.60
13:L:217:SER:HB3	13:L:249:GLY:HA3	1.83	0.60
14:M:101:LEU:HD23	14:M:128:PRO:HG3	1.83	0.60
14:M:91:VAL:HG23	14:M:92:GLU:H	1.66	0.60
14:M:95:PHE:HB3	14:M:136:TYR:CE2	2.36	0.60
14:U:402:SER:HA	14:U:405:TYR:CE2	2.36	0.60
6:6:76:ASP:HB2	6:6:104:TRP:CE3	2.36	0.59
4:E:74:THR:HG22	4:E:76:LEU:H	1.67	0.59
14:M:89:ALA:HB1	14:M:92:GLU:OE2	2.02	0.59
14:U:347:LEU:O	14:U:351:ALA:N	2.27	0.59
6:6:125:GLN:O	9:W:38:GLN:NE2	2.35	0.59
8:7:40:PHE:O	8:7:43:ARG:HD3	2.02	0.59
8:I:23:TYR:OH	8:I:123:ARG:NH1	2.34	0.59
15:V:168:GLU:H	15:V:172:TYR:HB2	1.67	0.59
4:4:137:LEU:HD23	4:4:145:PRO:HG2	1.82	0.59
4:4:123:LEU:HG	4:4:156:ILE:HG23	1.83	0.59
4:4:327:HIS:NE2	7:9:107:ALA:O	2.35	0.59
6:G:101:ASP:H	16:Q:70:GLU:HG2	1.67	0.59
14:U:317:ALA:HB1	14:U:372:SER:HB3	1.83	0.59
7:9:41:HIS:HB3	7:9:113:ILE:HD11	1.84	0.59
3:D:33:PHE:HB2	3:D:45:CYS:SG	2.42	0.59
3:D:616:ASN:ND2	3:D:622:LEU:HD11	2.18	0.59
10:P:66:MET:O	10:P:69:ILE:HG12	2.02	0.59
16:Q:39:LEU:O	16:Q:43:GLN:HG2	2.02	0.59
13:T:413:THR:HA	13:T:416:TYR:CE2	2.38	0.59
4:4:272:VAL:HG13	4:4:399:SER:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:GLY:HA3	1:B:324:GLY:H	1.66	0.59
4:E:225:PRO:HG2	4:E:228:VAL:HB	1.84	0.59
15:N:347:LEU:O	15:N:351:GLU:HG2	2.03	0.59
16:Q:36:ARG:HH12	16:Q:58:GLN:HG2	1.66	0.59
13:T:286:PHE:O	13:T:419:ARG:NH1	2.36	0.59
14:U:268:ALA:HA	14:U:291:SER:HA	1.84	0.59
6:G:96:TRP:HZ2	6:G:175:ALA:HB1	1.67	0.59
11:R:75:PHE:CZ	11:R:78:GLN:HG2	2.38	0.59
14:U:81:THR:HB	14:U:233:LEU:HD11	1.85	0.59
3:3:697:THR:HG21	3:3:761:SER:OG	2.03	0.59
4:E:45:VAL:HG13	4:E:55:VAL:HG22	1.83	0.59
6:G:57:ARG:NH1	6:G:60:LEU:CD1	2.66	0.59
11:J:2:SER:HA	11:J:5:GLU:HB3	1.85	0.59
13:T:159:PHE:HD2	14:U:407:LEU:HD11	1.66	0.59
1:1:344:LEU:HD21	2:2:86:LEU:HD22	1.85	0.59
7:9:108:CYS:HB2	7:9:113:ILE:HG22	1.84	0.59
2:C:24:ARG:HA	2:C:53:VAL:CG2	2.32	0.59
3:D:129:GLU:O	3:D:133:ARG:HB2	2.03	0.59
16:H:211:MET:HA	16:H:215:ALA:HB3	1.84	0.59
10:P:108:LEU:HD23	15:V:15:LEU:HD22	1.83	0.59
13:T:278:ALA:HA	13:T:301:SER:HA	1.83	0.59
1:1:287:ILE:HA	1:1:332:PRO:HA	1.83	0.59
3:3:459:MET:HG2	3:3:465:HIS:HB2	1.85	0.59
4:4:152:GLU:OE2	4:4:204:TYR:OH	2.20	0.59
6:6:44:ALA:H	6:6:82:GLY:HA3	1.68	0.59
1:1:41:ALA:HB2	1:1:116:GLU:HG3	1.83	0.59
3:3:774:ARG:HG2	3:3:776:LEU:HD23	1.84	0.59
3:D:149:LEU:HD11	4:E:110:PRO:HG3	1.84	0.59
16:H:290:PHE:O	16:H:294:ARG:HG2	2.03	0.59
12:S:74:LEU:O	12:S:78:ILE:HG13	2.03	0.59
6:6:27:LEU:O	6:6:30:TRP:HD1	1.86	0.58
15:N:224:LEU:HD11	15:N:281:LEU:HD23	1.85	0.58
7:O:4:LYS:H	7:O:4:LYS:HD2	1.68	0.58
16:Q:29:ALA:O	16:Q:32:THR:OG1	2.15	0.58
16:Q:37:ARG:HG2	16:Q:47:GLY:HA3	1.83	0.58
14:U:91:VAL:HG13	14:U:224:SER:OG	2.03	0.58
4:E:254:TYR:HD1	4:E:255:SER:H	1.49	0.58
16:H:217:THR:O	16:H:300:LEU:HD13	2.03	0.58
15:V:168:GLU:HG2	15:V:169:GLY:H	1.68	0.58
15:V:237:VAL:O	15:V:241:VAL:HG23	2.04	0.58
3:3:686:LYS:HD3	3:3:688:ARG:NH2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:314:ARG:HB3	8:7:44:MET:HE1	1.85	0.58
1:B:259:LYS:HA	1:B:284:LEU:HD21	1.85	0.58
3:D:285:VAL:HA	3:D:387:LEU:HD12	1.85	0.58
11:J:135:TRP:HZ3	15:N:105:LEU:HD22	1.66	0.58
13:T:365:HIS:CE1	13:T:443:LEU:HG	2.38	0.58
14:U:162:ALA:O	14:U:166:ALA:N	2.34	0.58
14:U:347:LEU:CD1	14:U:422:VAL:HG21	2.33	0.58
1:1:46:LYS:HE2	1:1:163:PHE:HB3	1.84	0.58
3:3:551:PRO:HG2	3:3:684:ARG:HD2	1.85	0.58
4:4:98:ALA:O	4:4:102:GLU:HG3	2.02	0.58
8:7:23:TYR:OH	8:7:123:ARG:NH1	2.37	0.58
3:D:451:PHE:CD1	3:D:466:GLU:HB3	2.38	0.58
4:E:314:ARG:NH2	8:I:44:MET:SD	2.76	0.58
13:L:103:ARG:NH2	13:L:144:PHE:O	2.35	0.58
14:M:102:MET:HB3	14:M:230:LEU:HD23	1.86	0.58
14:M:56:LEU:O	14:M:58:GLY:N	2.37	0.58
16:Q:102:PHE:CE1	16:Q:279:MET:HG2	2.38	0.58
3:3:94:ASP:OD2	3:3:97:SER:OG	2.16	0.58
4:4:114:GLU:O	4:4:118:VAL:HG13	2.03	0.58
2:C:112:THR:HG22	2:C:117:PHE:H	1.68	0.58
3:D:715:GLU:H	3:D:761:SER:HB2	1.67	0.58
14:M:402:SER:HA	14:M:405:TYR:CE2	2.38	0.58
1:1:354:GLY:O	1:1:360:ARG:NH1	2.34	0.58
6:6:104:TRP:CE2	6:6:173:VAL:HG22	2.39	0.58
7:9:43:LEU:HB2	7:9:137:LEU:HD12	1.85	0.58
16:H:39:LEU:O	16:H:43:GLN:HG2	2.03	0.58
14:U:33:PHE:HA	14:U:79:ALA:HB1	1.85	0.58
15:V:347:LEU:O	15:V:351:GLU:HG2	2.04	0.58
9:X:51:HIS:ND1	9:X:56:ASP:OD1	2.37	0.58
3:D:299:GLU:O	3:D:303:GLN:HB2	2.04	0.58
3:D:50:VAL:HG22	3:D:82:SER:HB3	1.85	0.58
15:N:53:TYR:HA	15:N:101:THR:HG22	1.86	0.58
6:G:114:SER:OG	7:O:96:LEU:O	2.21	0.58
16:Q:74:VAL:HG12	16:Q:75:ALA:O	2.03	0.58
14:U:101:LEU:HD23	14:U:128:PRO:HG3	1.86	0.58
3:3:159:PHE:HE2	8:7:79:LEU:HD13	1.69	0.58
3:3:305:ARG:NH1	3:3:609:GLU:OE1	2.36	0.58
15:N:128:GLN:NE2	15:N:305:ASP:OD1	2.36	0.58
16:Q:60:LEU:O	16:Q:64:ILE:HG13	2.04	0.58
13:T:153:ASP:OD1	14:U:411:GLN:NE2	2.32	0.58
13:T:380:SER:HB3	13:T:456:ALA:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:176:GLY:O	2:2:32:ARG:NH2	2.21	0.58
4:4:94:ASP:HB3	4:4:173:ILE:HG21	1.86	0.58
1:B:354:GLY:O	1:B:360:ARG:NH1	2.35	0.58
1:B:201:LEU:HD12	1:B:399:PHE:CE1	2.38	0.58
16:H:162:TYR:HE1	16:H:305:LEU:HG	1.66	0.58
11:J:146:LEU:HD23	12:K:66:ALA:HB2	1.84	0.58
13:L:379:LEU:HD22	13:L:454:VAL:HA	1.86	0.58
14:M:8:LEU:HD21	14:M:31:LEU:HB3	1.86	0.58
10:P:33:PRO:HD2	16:Q:70:GLU:HB3	1.86	0.58
11:R:50:PHE:HB2	11:R:124:PRO:HD3	1.85	0.58
13:T:376:LEU:HB3	13:T:379:LEU:HD12	1.85	0.58
11:R:151:VAL:HG11	15:V:86:LEU:HD23	1.86	0.58
8:7:60:SER:HA	8:7:66:PRO:HA	1.85	0.58
16:H:147:TYR:CD1	16:H:229:VAL:HG22	2.38	0.58
14:M:232:THR:HA	14:M:235:LYS:HZ3	1.69	0.58
14:M:88:VAL:HA	14:M:428:ALA:HB1	1.84	0.58
6:6:30:TRP:CD1	6:6:31:GLY:N	2.71	0.57
6:G:153:GLN:O	6:G:157:LYS:N	2.37	0.57
13:T:189:LYS:NZ	13:T:479:GLU:HB2	2.19	0.57
14:U:232:THR:HA	14:U:235:LYS:HZ3	1.69	0.57
1:1:196:ARG:NH2	3:3:204:GLU:O	2.38	0.57
4:4:115:THR:O	4:4:118:VAL:HG22	2.05	0.57
3:D:686:LYS:HD3	3:D:688:ARG:NH2	2.20	0.57
6:G:76:ASP:HB2	6:G:104:TRP:CZ3	2.39	0.57
14:M:5:ALA:HB1	14:M:36:ASN:ND2	2.19	0.57
15:N:415:LEU:HB3	15:N:418:LEU:HD13	1.85	0.57
16:Q:162:TYR:HE1	16:Q:305:LEU:HG	1.68	0.57
16:Q:70:GLU:O	16:Q:237:SER:OG	2.20	0.57
10:P:56:ARG:NH1	11:R:75:PHE:HB2	2.19	0.57
15:V:317:ARG:NH1	15:V:384:ALA:O	2.36	0.57
1:1:32:TYR:OH	1:1:116:GLU:OE1	2.16	0.57
4:4:87:TYR:HB3	4:4:169:HIS:HE1	1.69	0.57
6:6:76:ASP:HB2	6:6:104:TRP:CZ3	2.40	0.57
6:6:44:ALA:HB3	17:6:201:SF4:S4	2.44	0.57
16:H:189:GLN:HG2	16:H:195:LEU:H	1.68	0.57
8:I:23:TYR:HH	8:I:123:ARG:NH1	2.02	0.57
13:L:286:PHE:O	13:L:419:ARG:NH1	2.37	0.57
10:P:69:ILE:HD11	12:S:69:ALA:HB2	1.86	0.57
14:U:91:VAL:HG23	14:U:92:GLU:H	1.68	0.57
15:V:265:HIS:HA	15:V:268:TYR:CD2	2.38	0.57
1:1:314:GLU:HA	1:1:317:GLN:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:31:PRO:HB2	3:3:47:MET:HB3	1.87	0.57
6:6:115:GLY:HA3	6:6:125:GLN:OE1	2.03	0.57
6:6:34:ASN:O	6:6:59:ASP:HB3	2.05	0.57
6:6:57:ARG:CD	6:6:60:LEU:HD12	2.12	0.57
14:M:88:VAL:CG2	14:M:331:ARG:HG3	2.33	0.57
15:N:47:PRO:HB3	15:N:56:ASP:HA	1.85	0.57
14:U:186:GLN:HG2	14:U:187:GLU:H	1.70	0.57
15:V:280:ALA:HB1	15:V:347:LEU:HB3	1.86	0.57
3:3:664:LEU:HD22	3:3:669:VAL:HG11	1.86	0.57
4:4:389:GLN:HB3	4:4:392:ASP:HB2	1.86	0.57
5:5:38:MET:HA	5:5:41:TYR:HD2	1.68	0.57
7:9:52:LYS:NZ	8:7:44:MET:O	2.33	0.57
7:9:94:ASN:HB3	7:9:97:ARG:HB2	1.86	0.57
2:C:101:THR:HG23	2:C:106:ILE:O	2.04	0.57
16:H:224:ALA:HA	16:H:230:GLY:N	2.19	0.57
16:H:274:VAL:HG22	16:H:275:PRO:HD2	1.86	0.57
16:H:37:ARG:NH2	16:H:54:PHE:O	2.37	0.57
15:N:412:LEU:HD13	15:N:419:VAL:HG21	1.84	0.57
15:V:265:HIS:NE2	15:V:333:LEU:O	2.37	0.57
4:4:211:SER:HB3	4:4:214:PHE:HD2	1.68	0.57
4:E:224:ILE:HD11	4:E:275:ARG:NH1	2.19	0.57
16:H:219:PHE:HD2	16:H:299:ARG:HE	1.53	0.57
14:M:95:PHE:HB2	14:M:98:LEU:HD12	1.87	0.57
15:V:270:ALA:O	15:V:273:LEU:HB2	2.04	0.57
1:1:259:LYS:NZ	2:2:178:GLU:OE2	2.31	0.57
2:2:89:LYS:HG3	2:2:94:GLU:HG2	1.85	0.57
6:G:57:ARG:CZ	6:G:60:LEU:CD1	2.80	0.57
6:G:82:GLY:HA2	17:G:201:SF4:S4	2.44	0.57
16:H:222:PRO:O	16:H:230:GLY:HA3	2.04	0.57
16:H:310:TRP:HA	16:H:314:PHE:CD2	2.40	0.57
16:H:70:GLU:O	16:H:237:SER:OG	2.20	0.57
14:M:224:SER:HA	14:M:330:GLY:CA	2.33	0.57
6:G:138:PRO:HG2	7:O:121:MET:HG3	1.86	0.57
11:R:47:ASP:O	11:R:122:GLY:N	2.37	0.57
11:R:146:LEU:HD23	12:S:66:ALA:HB2	1.87	0.57
13:T:102:SER:OG	13:T:103:ARG:N	2.37	0.57
6:6:63:PHE:HB3	6:6:70:ALA:CB	2.35	0.57
10:A:71:PHE:O	10:A:74:GLU:HB3	2.05	0.57
2:C:130:THR:HB	2:C:143:GLU:HB3	1.87	0.57
3:D:20:MET:HE1	3:D:83:CYS:HB2	1.86	0.57
5:F:38:MET:HA	5:F:41:TYR:HD2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:151:PHE:HD2	14:M:213:TRP:HB3	1.70	0.57
16:Q:189:GLN:O	16:Q:193:GLY:HA2	2.05	0.57
14:U:188:GLU:HA	14:U:191:PHE:HB3	1.85	0.57
14:U:88:VAL:HA	14:U:428:ALA:HB1	1.86	0.57
3:3:574:GLU:HB2	3:3:593:LEU:HD11	1.86	0.57
2:C:135:GLN:HB2	2:C:141:TYR:HD1	1.70	0.57
16:H:36:ARG:HH12	16:H:58:GLN:HG2	1.69	0.57
12:K:2:SER:HA	12:K:5:LEU:HD12	1.87	0.57
13:T:63:ILE:HG21	13:T:125:PRO:HG2	1.86	0.57
4:4:68:LYS:HB2	5:5:146:LEU:HD23	1.87	0.57
7:O:6:LEU:HD23	16:Q:297:TRP:CE2	2.40	0.57
6:6:114:SER:OG	7:9:96:LEU:O	2.22	0.56
5:F:20:ASN:HD21	5:F:24:ASN:HB2	1.70	0.56
13:T:483:HIS:ND1	13:T:483:HIS:O	2.38	0.56
1:1:291:ILE:HG22	1:1:294:GLY:O	2.06	0.56
4:4:45:VAL:HG13	4:4:55:VAL:HG22	1.86	0.56
12:K:95:GLY:HA2	15:N:256:ARG:HE	1.68	0.56
13:L:324:THR:HB	13:L:380:SER:HB2	1.87	0.56
15:V:128:GLN:NE2	15:V:305:ASP:OD1	2.38	0.56
15:V:345:LYS:HB3	15:V:349:PHE:CE2	2.40	0.56
5:5:80:TRP:HE3	5:5:80:TRP:HA	1.70	0.56
15:N:309:LEU:HD22	15:N:378:LEU:HD11	1.86	0.56
11:R:69:PHE:HZ	16:Q:156:SER:HG	1.53	0.56
6:G:115:GLY:HA3	6:G:125:GLN:OE1	2.05	0.56
4:4:50:GLU:OE2	16:H:154:ARG:NH2	2.38	0.56
3:3:299:GLU:O	3:3:303:GLN:HB2	2.06	0.56
8:7:120:ASP:OD1	8:7:123:ARG:NH1	2.35	0.56
16:H:75:ALA:O	16:H:76:GLN:HB2	2.06	0.56
13:L:123:SER:HA	13:L:184:SER:HA	1.87	0.56
11:R:59:TYR:O	11:R:64:VAL:HG12	2.05	0.56
1:1:337:MET:HB2	1:1:420:GLN:OE1	2.05	0.56
3:3:738:THR:HG22	3:3:740:PHE:H	1.70	0.56
3:D:41:PRO:HB3	3:D:433:ALA:HB1	1.87	0.56
6:G:43:LEU:HB2	6:G:82:GLY:HA3	1.87	0.56
16:Q:75:ALA:O	16:Q:76:GLN:HB2	2.06	0.56
9:W:45:ARG:NH1	9:W:61:ASP:OD2	2.36	0.56
5:F:155:THR:HG23	9:X:93:VAL:HB	1.87	0.56
3:3:737:GLU:HB3	3:3:774:ARG:HD3	1.87	0.56
6:6:28:VAL:HA	16:H:64:ILE:HG21	1.87	0.56
4:E:263:ASP:HB2	4:E:285:GLU:HG3	1.88	0.56
16:H:99:LEU:HA	16:H:116:ILE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:126:LEU:HD11	14:U:149:VAL:HG22	1.87	0.56
7:9:69:TYR:HE1	7:9:71:GLU:HG3	1.71	0.56
10:A:71:PHE:CZ	10:A:107:PHE:HB2	2.41	0.56
4:E:137:LEU:HD23	4:E:145:PRO:HG2	1.86	0.56
10:P:71:PHE:CZ	10:P:107:PHE:HB2	2.41	0.56
15:V:13:LEU:HA	15:V:16:LEU:HB2	1.88	0.56
1:1:214:LYS:O	1:1:216:THR:HG23	2.06	0.56
4:4:74:THR:HG22	4:4:76:LEU:H	1.70	0.56
6:6:101:ASP:H	16:H:70:GLU:HG2	1.71	0.56
6:6:43:LEU:HB2	6:6:82:GLY:HA3	1.88	0.56
7:9:94:ASN:OD1	7:9:97:ARG:N	2.38	0.56
3:D:31:PRO:HG3	3:D:137:TYR:CD2	2.41	0.56
16:H:8:ASP:OD1	16:H:112:GLN:HG2	2.06	0.56
13:L:483:HIS:ND1	13:L:483:HIS:O	2.39	0.56
11:R:135:TRP:HZ3	15:V:105:LEU:HD22	1.70	0.56
1:1:191:SER:HB2	1:1:197:ALA:HB2	1.86	0.56
4:E:46:THR:O	4:E:53:LEU:HB2	2.06	0.56
14:M:371:LEU:HD12	14:M:440:LEU:HB3	1.86	0.56
15:N:13:LEU:HA	15:N:16:LEU:HB2	1.88	0.56
10:P:10:THR:OG1	16:Q:118:LEU:HD21	2.05	0.56
16:Q:134:TYR:HA	16:Q:137:PHE:CE2	2.40	0.56
16:Q:274:VAL:HG22	16:Q:275:PRO:HD2	1.87	0.56
1:1:195:LEU:HD23	2:2:24:ARG:HH12	1.71	0.56
1:1:397:ARG:HG2	3:3:79:LEU:HD12	1.87	0.56
4:4:366:TYR:CZ	5:5:148:LYS:HE3	2.41	0.56
7:9:73:ALA:HB2	7:9:89:LYS:HB2	1.88	0.56
4:E:132:PHE:CE2	4:E:279:ARG:HD2	2.41	0.56
4:E:341:GLU:OE1	5:F:91:ARG:NH2	2.39	0.56
16:H:332:LEU:HD12	16:H:332:LEU:H	1.70	0.56
8:I:120:ASP:OD1	8:I:123:ARG:NH1	2.34	0.56
15:N:24:GLY:HA2	15:N:27:ARG:HD2	1.88	0.56
4:4:129:HIS:CE1	4:4:279:ARG:HD3	2.41	0.55
8:7:63:LEU:HD13	8:7:129:ALA:HB3	1.87	0.55
10:A:66:MET:O	10:A:69:ILE:HG12	2.06	0.55
5:F:39:ALA:HA	5:F:107:LEU:HD21	1.87	0.55
6:G:119:ASN:HA	6:G:125:GLN:NE2	2.18	0.55
14:U:84:LEU:HB3	14:U:432:PHE:HD1	1.69	0.55
1:1:98:PRO:HA	2:2:124:CYS:SG	2.47	0.55
5:5:137:THR:HB	5:5:141:LEU:HD22	1.87	0.55
8:I:37:PHE:CE1	8:I:74:PRO:HA	2.41	0.55
14:M:75:PHE:HZ	14:M:111:ALA:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:99:LEU:HA	16:Q:116:ILE:O	2.06	0.55
1:1:101:PHE:CE1	1:1:253:GLN:HB2	2.41	0.55
4:4:254:TYR:CE2	4:4:346:THR:HA	2.41	0.55
6:6:57:ARG:HB3	6:6:60:LEU:HD12	1.87	0.55
2:C:146:THR:HG23	2:C:149:ARG:H	1.70	0.55
6:G:27:LEU:O	6:G:30:TRP:HD1	1.89	0.55
14:M:91:VAL:HG23	14:M:92:GLU:N	2.22	0.55
15:N:257:LEU:HD11	15:N:374:TYR:HB2	1.86	0.55
7:O:137:LEU:O	7:O:140:VAL:HG12	2.05	0.55
7:O:57:SER:N	17:O:202:SF4:S1	2.75	0.55
4:E:162:TRP:CE2	7:O:34:LYS:HD2	2.41	0.55
5:5:171:ARG:HH11	5:5:171:ARG:HG3	1.72	0.55
11:J:24:ASN:HB3	11:J:27:HIS:HB2	1.88	0.55
15:N:237:VAL:O	15:N:241:VAL:HG23	2.07	0.55
12:S:79:PHE:HA	12:S:82:ARG:HB3	1.88	0.55
2:2:10:PHE:CZ	2:2:33:ARG:HG3	2.41	0.55
4:4:231:ASP:O	5:5:109:GLY:N	2.40	0.55
5:5:155:THR:HG23	9:W:93:VAL:HB	1.88	0.55
5:5:52:ILE:HG22	5:5:118:VAL:HG21	1.89	0.55
6:6:19:ILE:HG12	6:6:20:LEU:H	1.71	0.55
4:E:98:ALA:O	4:E:102:GLU:HG3	2.06	0.55
6:G:44:ALA:HB3	17:G:201:SF4:S4	2.46	0.55
15:N:422:ALA:HB1	15:N:426:GLY:HA2	1.89	0.55
13:T:490:GLU:HG3	13:T:491:TRP:N	2.22	0.55
14:U:221:ASN:HB3	14:U:227:ALA:HB3	1.88	0.55
2:2:61:MET:SD	3:3:214:MET:HG3	2.47	0.55
3:3:738:THR:HG23	3:3:771:VAL:HG21	1.89	0.55
3:D:689:LYS:HD2	3:D:772:GLU:HG2	1.88	0.55
16:H:102:PHE:CE1	16:H:279:MET:HG2	2.42	0.55
16:H:102:PHE:CD1	16:H:279:MET:HG2	2.42	0.55
14:M:26:VAL:HA	14:M:86:ALA:HB1	1.87	0.55
2:2:101:THR:HG22	8:7:108:ILE:HD11	1.89	0.55
4:4:89:HIS:CE1	4:4:92:ALA:HB2	2.42	0.55
1:B:337:MET:HB2	1:B:420:GLN:OE1	2.06	0.55
3:D:355:LEU:HG	3:D:654:PHE:CZ	2.42	0.55
5:F:99:PRO:HB2	5:F:124:ILE:HA	1.88	0.55
16:H:16:LYS:NZ	16:H:114:TRP:O	2.40	0.55
11:J:113:LEU:HD21	12:K:49:TYR:CZ	2.41	0.55
13:T:288:GLN:NE2	13:T:528:SER:O	2.40	0.55
15:V:350:ALA:O	15:V:354:ARG:HB2	2.07	0.55
15:V:309:LEU:HD22	15:V:378:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:126:ASN:HB2	9:X:38:GLN:HE21	1.72	0.55
1:1:80:PRO:HG2	1:1:215:PRO:HB3	1.89	0.55
2:2:27:ILE:HG13	2:2:53:VAL:HG21	1.88	0.55
7:9:56:CYS:N	17:9:202:SF4:S1	2.79	0.55
7:9:44:THR:OG1	7:9:52:LYS:HD2	2.07	0.55
1:B:133:TYR:HH	1:B:191:SER:HG	1.52	0.55
1:B:254:ILE:HD11	1:B:330:LEU:HD11	1.88	0.55
9:W:26:LEU:HD12	9:W:84:GLN:HB2	1.89	0.55
3:3:515:THR:HG23	3:3:683:LEU:HD13	1.89	0.55
7:9:43:LEU:HD12	7:9:133:LYS:HG3	1.88	0.55
1:B:29:LEU:HD23	1:B:155:ARG:HD2	1.89	0.55
3:D:737:GLU:HB3	3:D:774:ARG:HD3	1.89	0.55
5:F:18:GLU:HB2	5:F:26:TRP:HB2	1.88	0.55
16:H:205:VAL:HG21	16:H:317:ALA:HB2	1.87	0.55
16:H:216:ARG:HD2	16:H:294:ARG:HA	1.88	0.55
16:Q:17:ALA:O	16:Q:21:VAL:HG23	2.05	0.55
16:Q:287:LEU:O	16:Q:291:ILE:HG13	2.06	0.55
6:G:58:ASN:ND2	16:Q:47:GLY:O	2.40	0.55
3:3:243:ARG:NH1	3:3:275:LEU:HA	2.22	0.55
4:4:341:GLU:OE1	5:5:91:ARG:NH2	2.38	0.55
3:D:225:ASN:O	3:D:229:ILE:HG13	2.07	0.55
3:D:243:ARG:HB3	3:D:275:LEU:HD22	1.88	0.55
4:E:314:ARG:HB3	8:I:44:MET:CE	2.37	0.55
4:E:87:TYR:HB3	4:E:169:HIS:HE1	1.72	0.55
8:I:20:MET:HE2	8:I:59:LEU:HG	1.87	0.55
13:L:105:PHE:O	13:L:109:ASN:ND2	2.37	0.55
14:M:347:LEU:HD12	14:M:422:VAL:HG21	1.89	0.55
14:U:91:VAL:HG23	14:U:92:GLU:N	2.22	0.55
3:3:522:ARG:NH1	3:3:681:LYS:HD3	2.21	0.54
6:6:104:TRP:NE1	6:6:172:PRO:O	2.40	0.54
3:D:115:HIS:HB3	4:E:321:MET:HE2	1.88	0.54
3:D:386:SER:HB2	3:D:675:ARG:NH1	2.22	0.54
3:D:738:THR:HG22	3:D:740:PHE:H	1.71	0.54
4:E:367:ARG:HH12	4:E:369:LYS:HB2	1.71	0.54
6:G:57:ARG:NE	6:G:60:LEU:CD1	2.55	0.54
16:H:52:GLY:HA2	16:H:55:GLY:H	1.72	0.54
12:K:57:ALA:O	12:K:60:VAL:HB	2.08	0.54
13:L:360:PRO:HA	13:L:363:ARG:NH1	2.23	0.54
16:Q:38:LEU:HD23	16:Q:291:ILE:HG21	1.89	0.54
15:V:241:VAL:O	15:V:245:ASN:ND2	2.40	0.54
1:1:195:LEU:CD2	2:2:24:ARG:HH12	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:507:LEU:HB3	3:3:511:VAL:HG11	1.88	0.54
7:9:137:LEU:O	7:9:140:VAL:HG12	2.07	0.54
10:A:33:PRO:HD2	16:H:70:GLU:CB	2.37	0.54
10:A:44:TYR:CG	10:A:45:GLU:N	2.75	0.54
6:G:19:ILE:HG12	6:G:20:LEU:H	1.72	0.54
10:P:86:GLY:HA2	16:Q:329:ALA:HA	1.88	0.54
12:S:2:SER:HA	12:S:5:LEU:HD12	1.89	0.54
14:U:208:PHE:O	14:U:211:HIS:ND1	2.41	0.54
3:3:136:GLU:HG2	5:5:189:ARG:HG2	1.88	0.54
14:M:331:ARG:HA	14:M:331:ARG:HH11	1.72	0.54
15:N:294:LEU:HD22	15:N:329:ALA:HB2	1.90	0.54
16:Q:214:ALA:HB1	16:Q:248:GLU:OE2	2.08	0.54
16:Q:292:TRP:HD1	16:Q:296:THR:HG1	1.52	0.54
14:U:55:LEU:HG	14:U:56:LEU:HD13	1.89	0.54
14:U:56:LEU:O	14:U:58:GLY:N	2.40	0.54
15:V:224:LEU:HD11	15:V:281:LEU:HD23	1.89	0.54
3:3:190:TYR:O	3:3:195:PRO:HD2	2.07	0.54
3:3:257:ALA:HB1	3:3:348:ASP:HB2	1.88	0.54
3:3:611:ARG:HA	3:3:624:LEU:O	2.07	0.54
3:D:439:GLU:HG2	3:D:440:ARG:HG2	1.90	0.54
4:E:261:THR:N	4:E:292:GLN:HE22	2.01	0.54
6:G:57:ARG:CD	6:G:60:LEU:HD12	2.11	0.54
14:M:78:ILE:HG22	14:M:103:GLU:HG3	1.90	0.54
14:M:26:VAL:HG22	14:M:86:ALA:O	2.07	0.54
16:Q:217:THR:O	16:Q:300:LEU:HD13	2.06	0.54
10:P:33:PRO:HD2	16:Q:70:GLU:CB	2.36	0.54
1:1:262:GLY:HA3	2:2:176:VAL:HA	1.89	0.54
3:3:279:ALA:HA	3:3:290:ILE:HG12	1.89	0.54
3:3:658:LEU:HD11	9:W:106:PRO:HA	1.90	0.54
3:3:706:GLY:O	3:3:709:GLN:HB2	2.07	0.54
4:4:43:LEU:HD13	4:4:55:VAL:HG11	1.89	0.54
5:5:99:PRO:HB2	5:5:124:ILE:HA	1.89	0.54
1:B:195:LEU:CD2	2:C:24:ARG:HH12	2.21	0.54
13:L:24:MET:HB3	13:L:28:LEU:HB3	1.90	0.54
16:Q:102:PHE:CD1	16:Q:279:MET:HG2	2.43	0.54
2:2:130:THR:HB	2:2:143:GLU:HB3	1.90	0.54
3:D:697:THR:HG21	3:D:761:SER:OG	2.06	0.54
6:G:37:TRP:HD1	6:G:64:GLY:O	1.90	0.54
14:U:306:GLU:OE2	14:U:386:LYS:NZ	2.39	0.54
3:3:36:GLU:HB3	3:3:39:LEU:HB2	1.88	0.54
3:3:272:GLY:O	3:3:630:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:72:HIS:ND1	5:5:152:LEU:HD22	2.23	0.54
6:6:18:GLY:HA2	6:6:28:VAL:HG11	1.89	0.54
7:9:110:THR:C	8:7:44:MET:HG2	2.28	0.54
16:H:220:ASP:CG	16:H:301:ARG:HA	2.28	0.54
13:L:321:HIS:HD2	13:L:388:ILE:HD12	1.71	0.54
10:P:77:PHE:HE2	12:S:62:ALA:HB2	1.70	0.54
13:T:39:ALA:HA	13:T:42:LEU:HB2	1.88	0.54
3:3:616:ASN:HD22	3:3:622:LEU:HD11	1.73	0.54
4:4:392:ASP:OD2	16:H:301:ARG:NH1	2.34	0.54
6:6:57:ARG:NH1	6:6:60:LEU:CD1	2.70	0.54
2:C:120:GLN:HG2	2:C:121:LYS:O	2.07	0.54
3:D:94:ASP:OD2	3:D:97:SER:OG	2.17	0.54
6:G:61:ALA:C	6:G:62:ARG:HH11	2.11	0.54
16:H:6:PRO:HG2	16:H:112:GLN:NE2	2.22	0.54
11:J:85:PRO:HA	12:K:22:ARG:HH12	1.72	0.54
13:L:376:LEU:HB3	13:L:379:LEU:HD12	1.89	0.54
13:L:490:GLU:HG3	13:L:491:TRP:N	2.23	0.54
13:L:511:PHE:O	13:L:514:ARG:HB2	2.08	0.54
15:N:241:VAL:O	15:N:245:ASN:ND2	2.41	0.54
15:N:255:LYS:HE2	15:N:306:ARG:HA	1.90	0.54
15:N:284:TYR:HA	15:N:344:GLY:HA3	1.90	0.54
13:T:234:THR:HG23	13:T:292:LYS:HE2	1.90	0.54
14:U:160:LEU:HA	14:U:163:VAL:HG12	1.88	0.54
3:3:478:LEU:HD12	3:3:520:ARG:CZ	2.37	0.54
6:6:19:ILE:HG12	6:6:20:LEU:N	2.22	0.54
4:4:314:ARG:HB3	8:7:44:MET:CE	2.37	0.54
2:C:27:ILE:HG13	2:C:53:VAL:HG21	1.90	0.54
2:C:96:LEU:HD11	2:C:134:ILE:HD11	1.90	0.54
5:F:137:THR:HB	5:F:141:LEU:HD22	1.89	0.54
13:L:365:HIS:CE1	13:L:443:LEU:HG	2.43	0.54
14:M:317:ALA:HB1	14:M:372:SER:HB3	1.89	0.54
15:N:270:ALA:O	15:N:273:LEU:HB2	2.07	0.54
16:Q:6:PRO:HG2	16:Q:112:GLN:NE2	2.22	0.54
13:T:348:ASP:HB3	13:T:351:LYS:HB2	1.89	0.54
14:U:20:LEU:HD12	14:U:20:LEU:H	1.71	0.54
2:2:26:ALA:O	2:2:30:LEU:HG	2.08	0.54
3:3:688:ARG:HB3	3:3:770:ARG:HB2	1.88	0.54
4:4:225:PRO:HG2	4:4:228:VAL:HB	1.90	0.54
4:4:232:LEU:HD23	5:5:109:GLY:HA3	1.90	0.54
4:4:341:GLU:HG2	4:4:358:VAL:HG22	1.90	0.54
10:A:38:ARG:O	10:A:42:MET:HG3	2.09	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:76:ASP:HB2	6:G:104:TRP:CE3	2.43	0.54
13:L:240:ILE:HG22	13:L:241:HIS:HD2	1.73	0.54
16:Q:224:ALA:HA	16:Q:230:GLY:N	2.19	0.54
13:T:123:SER:HA	13:T:184:SER:HA	1.90	0.54
9:X:31:VAL:HG11	9:X:81:LEU:HD13	1.88	0.54
1:1:51:ASP:OD1	1:1:81:LYS:HE2	2.08	0.53
5:F:126:PHE:H	5:F:132:LEU:HD11	1.72	0.53
6:G:19:ILE:HG12	6:G:20:LEU:N	2.22	0.53
10:A:57:PHE:HE2	16:H:149:LEU:CD2	2.17	0.53
14:M:224:SER:CA	14:M:330:GLY:HA3	2.36	0.53
11:R:100:VAL:O	11:R:104:LEU:HG	2.07	0.53
13:T:349:VAL:HG13	13:T:423:LEU:HB3	1.90	0.53
15:V:53:TYR:HA	15:V:101:THR:HG22	1.90	0.53
5:5:123:GLY:H	5:5:147:ARG:HH11	1.56	0.53
7:9:6:LEU:HD23	16:H:297:TRP:CE2	2.43	0.53
1:B:196:ARG:NH2	3:D:204:GLU:O	2.41	0.53
1:B:291:ILE:HG22	1:B:294:GLY:O	2.09	0.53
1:B:314:GLU:HA	1:B:317:GLN:HB3	1.89	0.53
3:D:154:TYR:HB3	4:E:322:GLU:HB2	1.90	0.53
16:H:131:LEU:O	16:H:134:TYR:HB2	2.08	0.53
8:I:86:LEU:HB2	8:I:91:ILE:HB	1.90	0.53
13:L:57:ALA:HB3	13:L:65:PHE:HB3	1.88	0.53
16:Q:232:TYR:CD1	16:Q:233:HIS:N	2.76	0.53
13:T:360:PRO:HA	13:T:363:ARG:NH1	2.24	0.53
1:1:358:PRO:HD3	3:3:107:MET:SD	2.47	0.53
4:4:46:THR:O	4:4:53:LEU:HB2	2.08	0.53
8:7:10:TYR:O	8:7:14:VAL:HG23	2.08	0.53
10:A:86:GLY:HA2	16:H:329:ALA:HA	1.88	0.53
4:E:314:ARG:HB3	8:I:44:MET:HE1	1.89	0.53
4:E:38:HIS:HE1	4:E:398:ALA:HA	1.73	0.53
16:H:152:SER:C	16:H:155:SER:HG	2.08	0.53
3:3:199:VAL:HG11	3:3:219:PRO:HD2	1.91	0.53
6:6:132:PRO:CG	6:6:175:ALA:HB2	2.38	0.53
6:6:28:VAL:HA	16:H:64:ILE:CG2	2.38	0.53
3:D:356:LEU:HD13	3:D:654:PHE:HB2	1.90	0.53
6:G:36:LEU:O	6:G:38:PRO:HD3	2.07	0.53
16:H:70:GLU:O	16:H:70:GLU:HG3	2.08	0.53
13:L:37:VAL:HG21	13:L:88:HIS:CE1	2.43	0.53
11:J:151:VAL:HG11	15:N:86:LEU:HD23	1.91	0.53
13:T:379:LEU:HD22	13:T:454:VAL:HA	1.91	0.53
13:T:538:TYR:O	13:T:542:ILE:HB	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:180:LEU:HD21	15:V:228:ALA:HB2	1.89	0.53
3:3:369:LEU:HD13	3:3:549:VAL:HG13	1.90	0.53
4:4:155:THR:HB	4:4:193:LEU:HD12	1.90	0.53
5:5:71:VAL:HG11	5:5:89:PHE:HD2	1.74	0.53
3:D:191:PHE:HE2	3:D:200:LEU:HD22	1.73	0.53
3:D:717:TRP:HB2	3:D:759:TYR:HB2	1.90	0.53
4:E:94:ASP:HB3	4:E:173:ILE:HG21	1.90	0.53
14:M:268:ALA:HA	14:M:291:SER:HA	1.90	0.53
14:M:91:VAL:CG2	14:M:92:GLU:H	2.21	0.53
16:Q:8:ASP:OD1	16:Q:112:GLN:HG2	2.09	0.53
14:U:151:PHE:CD2	14:U:213:TRP:HB3	2.43	0.53
3:3:343:LEU:HD12	3:3:361:ALA:HB2	1.89	0.53
3:3:439:GLU:HG2	3:3:440:ARG:HG2	1.90	0.53
4:E:155:THR:HB	4:E:193:LEU:HD12	1.90	0.53
6:G:18:GLY:HA2	6:G:28:VAL:HG11	1.89	0.53
3:D:159:PHE:HE2	8:I:79:LEU:HD13	1.74	0.53
13:L:161:VAL:HG13	13:L:222:LEU:HD22	1.90	0.53
13:L:538:TYR:O	13:L:542:ILE:HB	2.08	0.53
14:M:91:VAL:HG21	14:M:226:LEU:CD2	2.38	0.53
11:R:16:GLY:O	11:R:19:VAL:HG12	2.08	0.53
1:1:335:VAL:HG22	1:1:436:LEU:HD21	1.90	0.53
2:2:77:LYS:H	2:2:116:LEU:HA	1.74	0.53
3:3:237:ASP:OD1	3:3:239:THR:HG22	2.08	0.53
5:5:106:ASP:HB2	5:5:107:LEU:HD12	1.90	0.53
12:K:79:PHE:HA	12:K:82:ARG:HB3	1.90	0.53
13:L:189:LYS:HZ3	13:L:477:LEU:HD12	1.74	0.53
14:M:18:LEU:HG	14:M:19:GLY:N	2.24	0.53
15:N:283:PHE:O	15:N:287:THR:HG23	2.06	0.53
16:Q:159:LEU:O	16:Q:163:GLU:HB2	2.08	0.53
14:U:305:PRO:HB3	14:U:459:GLU:CA	2.37	0.53
6:G:125:GLN:HB2	9:X:119:ASN:HD21	1.74	0.53
6:6:102:PRO:HG3	10:A:33:PRO:HG2	1.89	0.53
4:E:236:GLY:HA2	4:E:351:GLY:HA3	1.90	0.53
5:F:56:ASP:OD2	5:F:148:LYS:N	2.36	0.53
16:H:265:GLY:O	16:H:268:THR:HB	2.08	0.53
13:L:576:GLN:HA	13:L:579:ALA:HB3	1.89	0.53
14:U:95:PHE:HB3	14:U:136:TYR:CE2	2.43	0.53
4:4:371:ARG:HG3	5:5:51:ASP:OD1	2.08	0.53
6:6:61:ALA:C	6:6:62:ARG:HH11	2.13	0.53
1:B:354:GLY:HA2	1:B:360:ARG:HB2	1.90	0.53
13:T:167:LEU:HD21	14:U:396:PHE:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:29:LEU:HD23	1:1:155:ARG:HD2	1.91	0.53
1:1:382:LYS:O	1:1:386:ASN:ND2	2.42	0.53
1:1:433:ARG:NH1	2:2:94:GLU:HG3	2.24	0.53
3:3:734:VAL:HG13	3:3:775:VAL:HG13	1.91	0.53
16:Q:222:PRO:O	16:Q:230:GLY:HA3	2.09	0.53
16:Q:265:GLY:O	16:Q:268:THR:HB	2.09	0.53
3:3:656:LEU:HD21	9:W:3:ARG:CD	2.39	0.53
1:1:293:GLY:HA3	1:1:324:GLY:H	1.74	0.52
1:1:354:GLY:HA2	1:1:360:ARG:HB2	1.92	0.52
1:1:298:PRO:HA	1:1:409:PRO:HA	1.90	0.52
3:3:701:ALA:HB2	3:3:763:LEU:HB2	1.91	0.52
1:B:98:PRO:HA	2:C:124:CYS:SG	2.49	0.52
3:D:128:CYS:SG	3:D:130:LEU:HB3	2.49	0.52
16:H:9:PRO:HB2	16:H:11:TRP:CD1	2.44	0.52
14:M:17:LEU:HD21	14:M:98:LEU:HG	1.90	0.52
15:N:317:ARG:NH1	15:N:384:ALA:O	2.41	0.52
15:N:350:ALA:O	15:N:354:ARG:HB2	2.09	0.52
10:P:66:MET:CE	10:P:67:LEU:HD12	2.39	0.52
14:U:260:LEU:HB3	14:U:301:PHE:CD2	2.44	0.52
14:U:89:ALA:HB1	14:U:92:GLU:OE2	2.09	0.52
3:3:509:ALA:O	3:3:513:GLN:N	2.40	0.52
4:4:159:LEU:O	4:4:163:VAL:HG12	2.09	0.52
4:4:369:LYS:HG3	5:5:53:VAL:HG23	1.92	0.52
7:9:108:CYS:HA	17:9:202:SF4:S3	2.48	0.52
1:B:162:LEU:O	1:B:165:THR:HG22	2.09	0.52
3:D:43:GLY:HA2	19:D:804:FES:S1	2.49	0.52
4:E:162:TRP:NE1	7:O:34:LYS:HD2	2.24	0.52
10:A:67:LEU:HB3	16:H:310:TRP:HZ2	1.75	0.52
11:J:63:ILE:HG23	12:K:68:VAL:HG11	1.91	0.52
12:K:74:LEU:O	12:K:78:ILE:HG13	2.08	0.52
14:U:224:SER:HA	14:U:330:GLY:CA	2.38	0.52
1:1:260:ARG:N	1:1:280:ALA:O	2.35	0.52
1:1:288:GLN:HB3	1:1:333:GLU:CG	2.39	0.52
3:3:129:GLU:O	3:3:133:ARG:HB2	2.10	0.52
3:3:356:LEU:HD13	3:3:654:PHE:HB2	1.90	0.52
3:3:20:MET:N	3:3:82:SER:O	2.38	0.52
14:M:160:LEU:HA	14:M:163:VAL:HG12	1.90	0.52
14:M:221:ASN:HB3	14:M:227:ALA:HB3	1.90	0.52
15:N:265:HIS:HA	15:N:268:TYR:CD2	2.43	0.52
14:U:395:ALA:O	14:U:398:SER:HB2	2.09	0.52
1:1:26:SER:HA	1:1:31:TYR:CG	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:347:HIS:HB2	3:3:538:ALA:HA	1.92	0.52
6:6:163:TYR:CD1	7:9:152:ARG:HD2	2.45	0.52
6:6:55:ASP:OD1	16:H:45:ARG:NH2	2.42	0.52
6:6:57:ARG:O	6:6:58:ASN:ND2	2.37	0.52
3:D:459:MET:HG2	3:D:465:HIS:CD2	2.45	0.52
3:D:464:ILE:HG21	3:D:493:ALA:HB2	1.91	0.52
5:F:171:ARG:HG3	5:F:171:ARG:HH11	1.75	0.52
5:F:71:VAL:HG11	5:F:89:PHE:HD2	1.75	0.52
16:H:267:TRP:CG	16:H:268:THR:N	2.77	0.52
14:M:70:LEU:HD23	14:M:243:ARG:HH21	1.75	0.52
15:N:153:LEU:HD12	15:N:178:LEU:HD12	1.90	0.52
7:O:108:CYS:HA	17:O:202:SF4:S3	2.49	0.52
16:Q:293:ILE:HD12	16:Q:297:TRP:CZ3	2.44	0.52
14:U:115:LEU:HD12	14:U:180:LEU:HD13	1.92	0.52
3:3:33:PHE:HB2	3:3:45:CYS:SG	2.49	0.52
3:3:33:PHE:O	3:3:186:ARG:NE	2.42	0.52
3:3:43:GLY:HA2	19:3:804:FES:S1	2.50	0.52
3:3:459:MET:HG2	3:3:465:HIS:CD2	2.45	0.52
4:4:44:MET:HB2	4:4:56:VAL:HB	1.90	0.52
5:5:104:VAL:HA	5:5:107:LEU:HD13	1.92	0.52
6:6:152:MET:HA	6:6:155:GLN:HB2	1.92	0.52
6:6:60:LEU:C	6:6:60:LEU:HD12	2.30	0.52
4:4:162:TRP:CE2	7:9:34:LYS:HD2	2.44	0.52
10:A:67:LEU:HB3	16:H:310:TRP:CZ2	2.44	0.52
4:4:28:LEU:HD11	16:H:147:TYR:CE2	2.44	0.52
16:H:147:TYR:HD1	16:H:229:VAL:HG22	1.73	0.52
14:M:131:LEU:O	14:M:135:LEU:HD23	2.10	0.52
14:M:181:LEU:HD21	14:M:247:PRO:HB2	1.92	0.52
13:T:151:TYR:HB3	13:T:231:ALA:HB1	1.90	0.52
4:4:172:TYR:O	4:4:179:LYS:N	2.42	0.52
4:4:219:ARG:HD3	4:4:271:ASP:OD2	2.08	0.52
6:6:36:LEU:O	6:6:38:PRO:HD3	2.09	0.52
1:B:101:PHE:CE1	1:B:253:GLN:HB2	2.45	0.52
1:B:380:GLU:N	1:B:383:ASP:OD2	2.31	0.52
3:D:551:PRO:HG2	3:D:684:ARG:HD2	1.91	0.52
3:D:656:LEU:HD21	9:X:3:ARG:CD	2.40	0.52
14:M:208:PHE:O	14:M:211:HIS:ND1	2.43	0.52
14:M:88:VAL:HB	14:M:432:PHE:HB2	1.91	0.52
16:Q:267:TRP:CG	16:Q:268:THR:N	2.77	0.52
4:4:101:VAL:HB	4:4:175:ILE:HD12	1.92	0.52
6:G:57:ARG:HH11	6:G:60:LEU:HD11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:14:LEU:HD12	16:H:292:TRP:CH2	2.45	0.52
14:M:425:LEU:HD22	14:M:430:TRP:CE2	2.45	0.52
16:Q:99:LEU:HD12	16:Q:116:ILE:HG13	1.92	0.52
2:C:9:ASP:N	2:C:9:ASP:OD1	2.43	0.52
3:D:190:TYR:O	3:D:195:PRO:HD2	2.09	0.52
5:F:104:VAL:HA	5:F:107:LEU:HD13	1.92	0.52
5:F:80:TRP:HE3	5:F:80:TRP:HA	1.75	0.52
16:H:37:ARG:NH2	16:H:49:ASN:OD1	2.42	0.52
15:N:124:TRP:CZ3	15:N:305:ASP:HB2	2.44	0.52
16:Q:147:TYR:CD1	16:Q:229:VAL:HG22	2.45	0.52
14:U:371:LEU:HD12	14:U:440:LEU:HB3	1.90	0.52
14:U:91:VAL:CG2	14:U:92:GLU:H	2.22	0.52
14:U:130:LEU:HD13	15:V:380:LEU:HD11	1.91	0.52
3:3:373:GLY:CA	3:3:538:ALA:HB2	2.40	0.52
1:B:397:ARG:HG2	3:D:79:LEU:HD12	1.92	0.52
3:D:406:ALA:HB2	3:D:535:MET:HG2	1.92	0.52
3:D:655:ARG:HH12	3:D:659:GLU:CG	2.20	0.52
16:H:71:ASP:OD1	16:H:240:LYS:NZ	2.34	0.52
14:M:55:LEU:HG	14:M:56:LEU:HD13	1.91	0.52
16:Q:136:ILE:HG23	16:Q:232:TYR:HD2	1.74	0.52
13:T:340:ILE:HB	13:T:345:GLY:HA2	1.91	0.52
13:T:386:ASP:OD2	13:T:494:ILE:HA	2.10	0.52
14:U:217:PHE:O	14:U:221:ASN:ND2	2.43	0.52
14:U:331:ARG:HB3	14:U:429:GLU:OE2	2.10	0.52
1:1:243:THR:HG22	1:1:244:GLU:N	2.22	0.52
1:1:437:TRP:O	2:2:147:ARG:NH2	2.42	0.52
4:4:367:ARG:HH12	4:4:369:LYS:HB2	1.75	0.52
6:6:57:ARG:C	6:6:58:ASN:HD22	2.13	0.52
7:9:58:LEU:HD12	7:9:109:PRO:HG3	1.91	0.52
4:E:172:TYR:O	4:E:179:LYS:N	2.43	0.52
4:E:208:PHE:HE2	4:E:276:MET:HG2	1.75	0.52
4:E:96:ALA:HB2	4:E:346:THR:HG21	1.90	0.52
16:H:214:ALA:HB1	16:H:248:GLU:OE2	2.10	0.52
13:L:167:LEU:HD21	14:M:396:PHE:HB3	1.92	0.52
13:L:321:HIS:HA	13:L:384:SER:HB2	1.91	0.52
14:M:20:LEU:H	14:M:20:LEU:HD12	1.73	0.52
14:U:242:PHE:CD2	14:U:312:LEU:HD11	2.45	0.52
15:V:272:ALA:O	15:V:276:GLY:N	2.43	0.52
11:R:152:VAL:HG22	15:V:87:LEU:HD22	1.92	0.52
3:3:191:PHE:HE2	3:3:200:LEU:HD22	1.75	0.51
4:4:30:VAL:HG13	4:4:35:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:66:MET:HE1	10:A:67:LEU:HD12	1.91	0.51
1:B:243:THR:HG22	1:B:244:GLU:N	2.22	0.51
3:D:693:TYR:HB3	3:D:759:TYR:CD1	2.44	0.51
4:E:196:VAL:HG22	4:E:200:ARG:HG2	1.92	0.51
6:G:152:MET:HA	6:G:155:GLN:HB2	1.92	0.51
16:H:293:ILE:HD12	16:H:297:TRP:CZ3	2.45	0.51
13:L:66:SER:HB3	13:L:122:ASP:HB3	1.91	0.51
1:1:40:THR:O	1:1:44:VAL:HG23	2.10	0.51
1:1:433:ARG:HH12	2:2:94:GLU:HG3	1.75	0.51
3:3:267:ALA:HA	3:3:277:ILE:HD13	1.91	0.51
3:3:516:VAL:O	3:3:520:ARG:HG3	2.10	0.51
5:5:20:ASN:HD21	5:5:24:ASN:HB2	1.74	0.51
6:6:140:CYS:SG	7:9:99:ILE:HG13	2.50	0.51
3:D:738:THR:HG23	3:D:771:VAL:HG21	1.90	0.51
16:H:190:LYS:HD3	16:H:268:THR:HG23	1.92	0.51
10:P:44:TYR:CG	10:P:45:GLU:N	2.78	0.51
16:Q:143:SER:HB2	16:Q:235:GLU:HG3	1.91	0.51
14:U:70:LEU:HD13	14:U:312:LEU:HD13	1.92	0.51
14:U:54:PRO:HA	14:U:62:TYR:HD1	1.75	0.51
1:1:219:ASN:ND2	18:1:502:FMN:O2P	2.43	0.51
3:3:556:ALA:HB2	3:3:562:GLY:HA3	1.93	0.51
3:D:269:THR:HG22	3:D:274:LEU:HA	1.92	0.51
3:D:29:ASP:N	3:D:29:ASP:OD1	2.43	0.51
3:D:655:ARG:NH1	3:D:659:GLU:HG3	2.22	0.51
14:M:70:LEU:HD13	14:M:312:LEU:HD13	1.92	0.51
14:M:335:ARG:NH2	14:M:429:GLU:OE1	2.42	0.51
14:M:87:LEU:HD12	14:M:88:VAL:N	2.26	0.51
11:R:46:LEU:HD21	12:S:3:TYR:CE2	2.46	0.51
2:2:112:THR:HG22	2:2:117:PHE:H	1.75	0.51
2:2:14:THR:HG22	2:2:17:LYS:NZ	2.26	0.51
4:4:263:ASP:HB2	4:4:285:GLU:CG	2.39	0.51
4:4:81:TYR:CZ	6:6:117:MET:HG3	2.46	0.51
8:7:23:TYR:HH	8:7:123:ARG:NH1	2.08	0.51
4:E:159:LEU:O	4:E:163:VAL:HG12	2.10	0.51
16:H:38:LEU:HD23	16:H:291:ILE:HG21	1.93	0.51
13:L:380:SER:CB	13:L:456:ALA:HB3	2.40	0.51
10:P:71:PHE:O	10:P:74:GLU:HB3	2.10	0.51
16:Q:216:ARG:HD2	16:Q:294:ARG:HA	1.92	0.51
3:3:693:TYR:HB3	3:3:759:TYR:CD1	2.46	0.51
4:4:73:ARG:NH2	4:4:81:TYR:OH	2.44	0.51
10:A:18:LEU:O	10:A:22:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:77:PHE:O	10:A:80:PRO:HD2	2.09	0.51
3:D:603:PRO:HB2	3:D:634:ALA:HA	1.92	0.51
13:L:287:GLY:HA3	13:L:528:SER:HB2	1.91	0.51
14:M:114:ASP:HB3	14:M:176:LEU:HD23	1.93	0.51
14:M:395:ALA:O	14:M:398:SER:HB2	2.11	0.51
12:K:63:VAL:CG1	15:N:112:GLU:HG3	2.38	0.51
7:O:113:ILE:HB	17:O:202:SF4:S4	2.50	0.51
11:R:83:PHE:HB3	11:R:85:PRO:HG3	1.93	0.51
14:U:134:TYR:HE2	15:V:383:PHE:HB2	1.75	0.51
2:2:135:GLN:HB2	2:2:141:TYR:HD1	1.75	0.51
6:6:57:ARG:CZ	6:6:60:LEU:CD1	2.84	0.51
6:6:72:PRO:HG3	10:A:44:TYR:HE1	1.74	0.51
1:B:32:TYR:OH	1:B:116:GLU:OE1	2.14	0.51
1:B:26:SER:HA	1:B:31:TYR:CG	2.45	0.51
1:B:288:GLN:HB3	1:B:333:GLU:CG	2.40	0.51
16:H:267:TRP:HB2	16:H:275:PRO:O	2.11	0.51
13:L:508:GLY:O	13:L:512:PHE:HB2	2.11	0.51
15:N:180:LEU:HD21	15:N:228:ALA:HB2	1.92	0.51
15:N:268:TYR:OH	15:N:368:SER:HA	2.10	0.51
7:O:58:LEU:HD12	7:O:109:PRO:HG3	1.92	0.51
11:R:63:ILE:HG23	12:S:68:VAL:HG11	1.93	0.51
13:T:217:SER:HA	13:T:246:VAL:HA	1.93	0.51
14:U:88:VAL:CG2	14:U:331:ARG:HG3	2.40	0.51
14:U:91:VAL:HG21	14:U:226:LEU:CD2	2.40	0.51
15:V:415:LEU:HB3	15:V:418:LEU:HD13	1.92	0.51
1:1:162:LEU:O	1:1:165:THR:HG22	2.10	0.51
3:3:166:LYS:NZ	3:3:179:GLU:OE1	2.35	0.51
4:4:86:ASP:HB3	4:4:93:HIS:CD2	2.46	0.51
1:B:191:SER:HB2	1:B:197:ALA:HB2	1.91	0.51
2:C:88:CYS:HA	2:C:131:ALA:HB1	1.93	0.51
3:D:113:LEU:O	3:D:161:ARG:NH1	2.44	0.51
3:D:32:LEU:HD11	3:D:35:SER:HB2	1.92	0.51
3:D:655:ARG:HB2	3:D:655:ARG:NH1	2.24	0.51
6:G:57:ARG:NH2	6:G:60:LEU:HD21	2.25	0.51
10:A:77:PHE:HE2	12:K:62:ALA:HB2	1.75	0.51
10:A:108:LEU:HD23	15:N:15:LEU:HD22	1.91	0.51
7:O:100:PHE:HA	17:O:201:SF4:S4	2.51	0.51
16:Q:232:TYR:HD1	16:Q:233:HIS:N	2.09	0.51
12:S:95:GLY:HA2	15:V:256:ARG:HE	1.74	0.51
9:W:21:LEU:HD21	9:W:26:LEU:HD11	1.92	0.51
1:1:258:VAL:HG23	1:1:283:PRO:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:57:ARG:CG	6:6:60:LEU:HD12	2.36	0.51
10:A:12:ILE:HD11	16:H:10:TYR:HB3	1.93	0.51
3:D:170:LEU:HD11	3:D:176:LEU:HD22	1.93	0.51
3:D:314:GLU:O	3:D:316:ARG:HG2	2.10	0.51
6:G:35:SER:HG	6:G:37:TRP:HE3	1.57	0.51
10:A:65:ALA:HB3	11:J:66:LEU:HD13	1.93	0.51
14:M:93:GLY:HA3	14:M:136:TYR:CE1	2.46	0.51
1:1:339:ASP:O	1:1:342:TRP:HB3	2.11	0.51
4:4:208:PHE:HE2	4:4:276:MET:HG2	1.74	0.51
6:6:16:ARG:HH11	6:6:16:ARG:HB3	1.76	0.51
6:6:91:VAL:HG22	10:A:46:SER:HB2	1.92	0.51
2:C:127:SER:HB2	2:C:130:THR:OG1	2.11	0.51
2:C:14:THR:HG22	2:C:17:LYS:NZ	2.26	0.51
6:G:60:LEU:HD12	6:G:60:LEU:C	2.31	0.51
16:H:232:TYR:CD1	16:H:233:HIS:N	2.79	0.51
16:H:158:SER:HB2	16:H:305:LEU:CD2	2.40	0.51
16:Q:162:TYR:HA	16:Q:314:PHE:CZ	2.46	0.51
14:U:18:LEU:HG	14:U:19:GLY:N	2.26	0.51
1:1:257:PRO:HG2	1:1:332:PRO:HG3	1.93	0.51
3:3:700:LYS:HA	3:3:763:LEU:O	2.10	0.51
4:4:96:ALA:HB2	4:4:346:THR:HG21	1.91	0.51
5:5:78:PRO:HG3	5:5:85:GLY:HA2	1.93	0.51
3:D:614:LEU:O	3:D:621:VAL:HA	2.10	0.51
5:F:106:ASP:HB2	5:F:107:LEU:HD12	1.93	0.51
5:F:155:THR:N	6:G:119:ASN:OD1	2.31	0.51
8:I:82:ILE:HG23	8:I:95:ALA:HB3	1.93	0.51
11:J:83:PHE:HB3	11:J:85:PRO:HG3	1.93	0.51
14:M:91:VAL:HB	14:M:95:PHE:CZ	2.46	0.51
14:U:93:GLY:HA3	14:U:95:PHE:HD1	1.75	0.51
1:B:40:THR:O	1:B:44:VAL:HG23	2.12	0.50
2:C:89:LYS:HG3	2:C:94:GLU:HG2	1.92	0.50
4:E:118:VAL:HB	4:E:257:TYR:CE1	2.43	0.50
6:G:57:ARG:O	6:G:58:ASN:ND2	2.39	0.50
13:L:68:LEU:HD23	13:L:255:ARG:HH22	1.75	0.50
11:R:23:ARG:HG2	11:R:80:GLU:HG2	1.92	0.50
1:1:288:GLN:HB3	1:1:333:GLU:HG2	1.93	0.50
3:3:29:ASP:N	3:3:29:ASP:OD1	2.44	0.50
4:4:287:VAL:O	4:4:291:LYS:HG3	2.12	0.50
2:C:66:PHE:O	3:D:205:ARG:NE	2.44	0.50
3:D:19:VAL:HG22	3:D:91:MET:HE1	1.93	0.50
4:E:114:GLU:O	4:E:118:VAL:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:175:LEU:HB3	16:H:328:VAL:HG21	1.93	0.50
11:J:12:LEU:HD22	12:K:10:LEU:HD11	1.93	0.50
13:L:422:VAL:HG11	13:L:513:GLN:N	2.26	0.50
13:L:66:SER:CB	13:L:122:ASP:HB3	2.40	0.50
14:M:106:LEU:O	14:M:109:LEU:HB3	2.12	0.50
14:M:169:LEU:HD21	15:N:358:TRP:HZ2	1.77	0.50
7:O:14:LEU:HD12	16:Q:292:TRP:CH2	2.47	0.50
16:Q:190:LYS:HD3	16:Q:268:THR:HG23	1.94	0.50
1:1:17:LEU:HD22	1:1:113:LEU:HD21	1.92	0.50
2:2:88:CYS:HA	2:2:131:ALA:HB1	1.94	0.50
3:3:451:PHE:CD1	3:3:466:GLU:HB3	2.46	0.50
3:3:46:ARG:HG2	3:3:46:ARG:NH1	2.26	0.50
4:4:162:TRP:NE1	7:9:34:LYS:HD2	2.26	0.50
2:C:46:ILE:HD13	2:C:61:MET:HA	1.93	0.50
3:D:30:VAL:HG22	3:D:48:CYS:HA	1.94	0.50
4:E:112:ARG:HG3	4:E:297:LEU:HD11	1.93	0.50
6:G:35:SER:O	6:G:37:TRP:HE3	1.95	0.50
11:J:59:TYR:CD1	11:J:63:ILE:HD12	2.47	0.50
11:J:75:PHE:CG	11:J:76:ALA:N	2.80	0.50
13:L:153:ASP:OD1	14:M:411:GLN:NE2	2.31	0.50
13:L:255:ARG:HD2	13:L:477:LEU:HD23	1.94	0.50
14:M:105:LEU:HD13	14:M:125:ALA:HA	1.94	0.50
14:M:148:PHE:O	14:M:152:THR:HG23	2.12	0.50
15:V:283:PHE:O	15:V:287:THR:HG23	2.09	0.50
1:B:372:ALA:O	1:B:376:THR:OG1	2.23	0.50
4:E:26:MET:HG2	10:P:54:VAL:HB	1.93	0.50
14:M:88:VAL:HG22	14:M:331:ARG:HG3	1.93	0.50
13:T:325:HIS:NE2	13:T:329:LYS:HG3	2.26	0.50
13:T:576:GLN:HA	13:T:579:ALA:HB3	1.92	0.50
15:V:261:SER:HG	15:V:375:TYR:HH	1.56	0.50
3:3:614:LEU:O	3:3:621:VAL:HA	2.11	0.50
3:3:657:HIS:O	3:3:661:GLN:HG2	2.11	0.50
4:4:118:VAL:HB	4:4:257:TYR:CE1	2.44	0.50
6:6:64:GLY:HA2	6:6:71:SER:O	2.11	0.50
3:D:382:PHE:HB3	3:D:532:VAL:HB	1.93	0.50
3:D:55:PRO:HG3	3:D:74:GLN:N	2.25	0.50
3:D:20:MET:N	3:D:82:SER:O	2.36	0.50
11:J:59:TYR:O	11:J:64:VAL:HG12	2.12	0.50
13:L:151:TYR:HB3	13:L:231:ALA:HB1	1.93	0.50
13:L:30:GLY:HA3	13:L:92:ILE:HG12	1.93	0.50
16:Q:211:MET:HG3	16:Q:212:ALA:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:289:PHE:O	16:Q:293:ILE:HG12	2.12	0.50
12:S:57:ALA:O	12:S:60:VAL:HB	2.11	0.50
4:4:34:HIS:HB2	10:A:45:GLU:OE1	2.12	0.50
8:7:52:THR:HB	8:7:54:ILE:HG22	1.93	0.50
2:C:77:LYS:H	2:C:116:LEU:HA	1.76	0.50
16:H:96:ALA:HB1	16:H:125:LEU:HD23	1.93	0.50
14:M:114:ASP:OD1	14:M:117:VAL:HB	2.12	0.50
15:N:40:LEU:HD12	15:N:67:LEU:HD12	1.94	0.50
11:R:75:PHE:CG	11:R:76:ALA:N	2.80	0.50
14:U:134:TYR:HB2	14:U:145:LEU:CD1	2.42	0.50
14:U:96:LEU:O	14:U:100:LEU:HG	2.11	0.50
15:V:61:VAL:O	15:V:64:LEU:HB3	2.12	0.50
1:1:361:GLU:OE2	3:3:162:ARG:NH2	2.44	0.50
4:4:261:THR:N	4:4:292:GLN:HE22	2.02	0.50
4:4:63:HIS:O	6:6:122:ALA:HB1	2.12	0.50
6:6:35:SER:O	6:6:37:TRP:HE3	1.95	0.50
1:B:201:LEU:O	1:B:204:PRO:HD2	2.12	0.50
12:K:60:VAL:HG23	15:N:105:LEU:HD11	1.91	0.50
14:M:17:LEU:HD23	14:M:94:ARG:O	2.11	0.50
11:R:50:PHE:CE2	12:S:58:LEU:HD11	2.44	0.50
3:3:129:GLU:OE2	3:3:186:ARG:NH1	2.43	0.50
10:A:67:LEU:HD23	16:H:310:TRP:CE2	2.47	0.50
1:B:195:LEU:HD23	2:C:24:ARG:HH12	1.75	0.50
2:C:108:PRO:HA	2:C:119:VAL:O	2.11	0.50
4:E:106:GLY:O	5:F:194:SER:HB3	2.11	0.50
14:M:9:PRO:HG3	14:M:32:SER:HB2	1.94	0.50
10:P:93:PHE:CZ	16:Q:326:LEU:HD13	2.46	0.50
16:Q:22:VAL:O	16:Q:25:LEU:HB2	2.12	0.50
6:G:30:TRP:CH2	16:Q:51:VAL:HG13	2.46	0.50
1:1:201:LEU:O	1:1:204:PRO:HD2	2.12	0.50
5:5:53:VAL:HG13	5:5:71:VAL:HB	1.94	0.50
3:D:774:ARG:HG2	3:D:776:LEU:HD23	1.94	0.50
4:E:193:LEU:HA	4:E:196:VAL:HG12	1.94	0.50
5:F:104:VAL:HG23	5:F:111:ALA:HB2	1.94	0.50
6:G:64:GLY:HA2	6:G:71:SER:O	2.12	0.50
6:G:91:VAL:HA	10:P:46:SER:HB3	1.93	0.50
16:H:22:VAL:O	16:H:25:LEU:HB2	2.11	0.50
16:H:37:ARG:HG2	16:H:47:GLY:HA3	1.94	0.50
11:J:146:LEU:O	11:J:150:THR:HG23	2.11	0.50
11:J:50:PHE:CE2	12:K:58:LEU:HD11	2.44	0.50
15:N:313:ARG:HE	15:N:384:ALA:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:65:VAL:HG23	16:Q:134:TYR:CZ	2.46	0.50
16:Q:27:ALA:O	16:Q:31:MET:HG2	2.12	0.50
16:Q:9:PRO:HB2	16:Q:11:TRP:CD1	2.46	0.50
11:R:52:GLY:O	11:R:55:GLN:HB3	2.11	0.50
4:4:338:PRO:HG2	5:5:193:ARG:HD3	1.94	0.49
4:4:50:GLU:O	4:4:390:VAL:HG23	2.12	0.49
8:7:61:ASP:HB3	8:7:127:ALA:HB1	1.94	0.49
4:4:390:VAL:HG11	16:H:228:LEU:HG	1.94	0.49
14:M:217:PHE:O	14:M:221:ASN:ND2	2.45	0.49
15:N:101:THR:HG21	15:N:106:LEU:HD23	1.94	0.49
7:O:23:THR:HB	16:Q:45:ARG:HD3	1.93	0.49
2:2:120:GLN:HG2	2:2:121:LYS:O	2.12	0.49
4:E:129:HIS:CE1	4:E:349:ALA:HB1	2.47	0.49
4:E:38:HIS:ND1	4:E:139:ASP:OD2	2.44	0.49
4:E:214:PHE:HA	4:E:217:ARG:HB2	1.95	0.49
5:F:137:THR:HG21	5:F:145:PRO:HG3	1.95	0.49
6:G:57:ARG:C	6:G:58:ASN:HD22	2.15	0.49
13:L:20:PHE:O	13:L:22:LYS:N	2.33	0.49
13:L:557:ASP:O	13:L:560:LEU:HB3	2.12	0.49
14:U:313:TYR:CD1	14:U:451:ALA:HB2	2.46	0.49
14:U:26:VAL:HA	14:U:86:ALA:HB1	1.93	0.49
2:2:108:PRO:HA	2:2:119:VAL:O	2.12	0.49
2:2:46:ILE:HD13	2:2:61:MET:HA	1.94	0.49
6:6:31:GLY:O	6:6:35:SER:HB3	2.13	0.49
8:7:40:PHE:HB2	8:7:48:TYR:CE1	2.46	0.49
6:6:91:VAL:HA	10:A:46:SER:HB3	1.94	0.49
4:4:26:MET:HA	10:A:54:VAL:HG12	1.93	0.49
1:B:18:TYR:OH	1:B:102:LYS:O	2.22	0.49
3:D:125:GLY:HA2	3:D:245:ARG:HH21	1.77	0.49
3:D:369:LEU:HD13	3:D:549:VAL:HG13	1.94	0.49
15:V:259:ALA:O	15:V:263:ILE:HG13	2.12	0.49
3:3:587:LEU:O	3:3:604:ALA:N	2.45	0.49
3:D:704:ALA:HB2	3:D:712:ALA:HB3	1.94	0.49
4:E:44:MET:HB2	4:E:56:VAL:HB	1.94	0.49
4:E:231:ASP:O	5:F:109:GLY:N	2.46	0.49
16:H:151:GLY:HA3	16:H:229:VAL:O	2.12	0.49
16:H:300:LEU:HD23	16:H:305:LEU:HA	1.94	0.49
4:E:26:MET:HA	10:P:54:VAL:HG12	1.94	0.49
16:Q:310:TRP:HA	16:Q:314:PHE:CD2	2.48	0.49
13:T:321:HIS:HD2	13:T:388:ILE:HD12	1.77	0.49
2:2:127:SER:HB2	2:2:130:THR:OG1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:116:PRO:O	3:3:117:LEU:HB2	2.10	0.49
4:4:208:PHE:CE2	4:4:276:MET:HG2	2.48	0.49
4:4:379:GLN:HG2	5:5:113:PHE:CD2	2.47	0.49
1:B:298:PRO:HA	1:B:409:PRO:HA	1.93	0.49
1:B:414:LEU:O	1:B:418:LYS:HB2	2.11	0.49
2:C:26:ALA:O	2:C:30:LEU:HG	2.13	0.49
3:D:583:VAL:HG23	3:D:599:HIS:H	1.78	0.49
16:H:327:VAL:HA	16:H:332:LEU:HD13	1.94	0.49
4:E:327:HIS:NE2	7:O:107:ALA:O	2.45	0.49
13:T:206:GLY:HA2	13:T:209:LEU:HD12	1.94	0.49
13:T:340:ILE:O	13:T:345:GLY:N	2.39	0.49
13:T:360:PRO:HA	13:T:363:ARG:HH12	1.77	0.49
13:T:511:PHE:O	13:T:514:ARG:HB2	2.13	0.49
14:U:70:LEU:HD23	14:U:243:ARG:HH21	1.78	0.49
2:2:9:ASP:OD1	2:2:9:ASP:N	2.40	0.49
3:3:337:ARG:H	3:3:337:ARG:CD	2.26	0.49
3:3:17:THR:HB	3:3:87:VAL:HG21	1.94	0.49
6:6:57:ARG:NE	6:6:60:LEU:CD1	2.55	0.49
10:A:2:ALA:HB3	16:H:119:ASP:OD2	2.13	0.49
4:E:211:SER:HG	4:E:273:PHE:HE2	1.60	0.49
4:E:274:ASP:O	4:E:278:VAL:HG23	2.12	0.49
4:E:64:THR:N	4:E:409:ARG:OXT	2.43	0.49
16:H:136:ILE:HG23	16:H:232:TYR:HD2	1.76	0.49
13:L:171:LEU:O	13:L:175:ILE:HG13	2.11	0.49
14:M:338:THR:HG22	14:M:340:GLU:H	1.77	0.49
14:U:296:ALA:HB2	14:U:314:LEU:HD22	1.94	0.49
15:V:284:TYR:HA	15:V:344:GLY:HA3	1.94	0.49
15:V:422:ALA:HB1	15:V:426:GLY:HA2	1.95	0.49
2:2:146:THR:HG23	2:2:149:ARG:H	1.78	0.49
3:3:243:ARG:HB3	3:3:275:LEU:HD22	1.94	0.49
3:3:512:LEU:HD21	3:3:534:ALA:HB1	1.94	0.49
5:5:135:ILE:HG22	5:5:136:LEU:HG	1.93	0.49
1:B:262:GLY:HA3	2:C:176:VAL:HA	1.95	0.49
3:D:305:ARG:NH1	3:D:609:GLU:OE1	2.46	0.49
4:E:201:ILE:HA	4:E:204:TYR:CD2	2.46	0.49
4:E:129:HIS:CE1	4:E:279:ARG:HD3	2.47	0.49
6:G:108:MET:HA	6:G:137:VAL:HG13	1.94	0.49
16:H:287:LEU:O	16:H:291:ILE:HG13	2.12	0.49
16:H:99:LEU:HD12	16:H:116:ILE:HG13	1.95	0.49
10:A:56:ARG:NH1	11:J:75:PHE:HB2	2.28	0.49
14:M:56:LEU:O	14:M:59:ALA:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:138:VAL:HG22	15:N:106:LEU:HB2	1.94	0.49
6:G:76:ASP:HB3	16:Q:69:LYS:NZ	2.27	0.49
11:R:83:PHE:HD2	11:R:85:PRO:HG3	1.77	0.49
14:U:88:VAL:HB	14:U:432:PHE:HB2	1.94	0.49
1:1:341:MET:HB2	1:1:371:PHE:HE2	1.76	0.49
3:3:256:CYS:HB2	3:3:265:ILE:HD13	1.93	0.49
6:6:104:TRP:CZ2	6:6:173:VAL:HG22	2.47	0.49
6:6:37:TRP:HD1	6:6:64:GLY:O	1.95	0.49
10:A:23:ALA:O	10:A:27:VAL:HG23	2.13	0.49
2:C:61:MET:SD	3:D:214:MET:HG3	2.53	0.49
2:C:80:LEU:HD13	2:C:100:LEU:HD11	1.95	0.49
4:E:234:LEU:O	4:E:239:LEU:HB2	2.13	0.49
4:E:168:PHE:CE1	6:G:141:PRO:HG3	2.47	0.49
13:L:77:LEU:HD12	13:L:116:LEU:HD22	1.94	0.49
14:M:260:LEU:HB3	14:M:301:PHE:CD2	2.48	0.49
10:P:23:ALA:O	10:P:27:VAL:HG23	2.13	0.49
16:Q:221:LEU:N	16:Q:222:PRO:HA	2.27	0.49
6:G:76:ASP:HB3	16:Q:69:LYS:HZ3	1.76	0.49
11:R:109:TRP:CE3	11:R:109:TRP:HA	2.47	0.49
13:T:321:HIS:HA	13:T:384:SER:HB2	1.93	0.49
14:U:87:LEU:HD12	14:U:88:VAL:N	2.28	0.49
1:1:433:ARG:HH12	2:2:89:LYS:HE3	1.78	0.49
3:3:314:GLU:O	3:3:316:ARG:HG2	2.12	0.49
3:3:559:ASP:OD2	3:3:686:LYS:NZ	2.46	0.49
3:3:700:LYS:O	3:3:703:GLN:HB2	2.13	0.49
2:C:61:MET:HB2	3:D:214:MET:HE3	1.95	0.49
6:G:165:GLU:OE2	7:O:148:ARG:NH1	2.42	0.49
16:H:219:PHE:HB3	16:H:299:ARG:HG2	1.93	0.49
10:A:67:LEU:HD23	16:H:310:TRP:CZ2	2.47	0.49
14:M:29:ALA:CB	14:M:83:PHE:HA	2.41	0.49
10:P:18:LEU:O	10:P:22:VAL:HG23	2.13	0.49
16:Q:108:PHE:HB3	16:Q:112:GLN:H	1.77	0.49
10:P:28:GLY:HA3	16:Q:239:ILE:CG2	2.43	0.49
13:T:30:GLY:HA3	13:T:92:ILE:HG12	1.94	0.49
14:U:134:TYR:CE2	15:V:383:PHE:HB2	2.48	0.49
14:U:26:VAL:HG22	14:U:86:ALA:O	2.13	0.49
14:U:17:LEU:HD21	14:U:98:LEU:HG	1.94	0.49
15:V:201:GLN:HA	15:V:255:LYS:HE3	1.94	0.49
15:V:275:THR:OG1	15:V:351:GLU:HB3	2.12	0.49
2:2:27:ILE:HG12	2:2:53:VAL:HG11	1.95	0.49
2:2:91:ALA:HB1	2:2:132:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:86:LEU:HB2	8:7:91:ILE:HB	1.95	0.49
2:C:146:THR:CG2	2:C:149:ARG:H	2.25	0.49
3:D:289:TRP:O	3:D:290:ILE:HD13	2.13	0.49
13:L:554:PHE:HD2	14:M:277:ALA:HB3	1.77	0.49
14:M:214:LEU:HD21	14:M:235:LYS:HE3	1.95	0.49
14:M:327:LEU:O	14:M:331:ARG:HG2	2.13	0.49
14:M:86:ALA:O	14:M:96:LEU:HD11	2.12	0.49
16:Q:205:VAL:HG21	16:Q:317:ALA:HB2	1.94	0.49
16:Q:219:PHE:HD2	16:Q:299:ARG:HE	1.61	0.49
13:T:57:ALA:HB3	13:T:65:PHE:HB3	1.93	0.49
14:U:169:LEU:HD21	15:V:358:TRP:HZ2	1.78	0.49
1:1:414:LEU:O	1:1:418:LYS:HB2	2.12	0.48
3:3:125:GLY:HA2	3:3:245:ARG:HH21	1.77	0.48
3:3:157:PHE:CZ	3:3:159:PHE:HB2	2.47	0.48
4:4:196:VAL:HG22	4:4:200:ARG:HG2	1.94	0.48
5:5:144:HIS:O	5:5:147:ARG:HG2	2.13	0.48
6:G:148:ILE:O	6:G:152:MET:HG3	2.13	0.48
16:H:17:ALA:O	16:H:21:VAL:HG23	2.12	0.48
7:O:44:THR:OG1	7:O:52:LYS:HD2	2.13	0.48
11:R:83:PHE:CD2	11:R:85:PRO:HG3	2.47	0.48
13:T:471:PRO:O	13:T:475:PRO:HD3	2.12	0.48
15:V:2:THR:HG23	15:V:36:ALA:HB1	1.95	0.48
15:V:124:TRP:CZ3	15:V:305:ASP:HB2	2.48	0.48
6:6:21:PHE:O	6:6:25:GLU:HG2	2.13	0.48
10:A:63:VAL:O	10:A:67:LEU:HD13	2.13	0.48
1:B:339:ASP:O	1:B:342:TRP:HB3	2.13	0.48
2:C:10:PHE:CZ	2:C:33:ARG:HG3	2.48	0.48
3:D:337:ARG:CD	3:D:337:ARG:H	2.26	0.48
3:D:81:ALA:HB3	3:D:84:VAL:CG2	2.43	0.48
4:E:115:THR:O	4:E:118:VAL:HG22	2.14	0.48
4:E:140:LEU:HD21	4:E:217:ARG:NH1	2.28	0.48
4:E:219:ARG:HD3	4:E:271:ASP:OD2	2.13	0.48
4:E:34:HIS:HB2	10:P:45:GLU:OE1	2.13	0.48
14:U:130:LEU:O	14:U:133:LEU:HB3	2.13	0.48
15:V:294:LEU:HD22	15:V:329:ALA:HB2	1.94	0.48
1:1:331:ILE:HD11	2:2:86:LEU:HD21	1.95	0.48
3:3:549:VAL:C	3:3:550:LEU:HD12	2.34	0.48
4:4:132:PHE:CE2	4:4:279:ARG:HD2	2.49	0.48
7:9:139:ASP:OD1	7:9:139:ASP:N	2.44	0.48
5:F:53:VAL:HG13	5:F:71:VAL:HB	1.95	0.48
6:G:138:PRO:O	6:G:142:PRO:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:163:VAL:HG23	7:O:177:THR:HG22	1.95	0.48
16:Q:240:LYS:HZ2	16:Q:240:LYS:HB2	1.78	0.48
11:R:146:LEU:O	11:R:150:THR:HG23	2.13	0.48
14:U:102:MET:HB3	14:U:230:LEU:HD23	1.96	0.48
2:2:45:ARG:O	2:2:49:ILE:HG13	2.13	0.48
3:3:131:GLN:HG2	4:4:325:ILE:HG23	1.96	0.48
3:3:464:ILE:HG21	3:3:493:ALA:HB2	1.95	0.48
3:3:716:LEU:HA	3:3:759:TYR:O	2.13	0.48
6:6:108:MET:HA	6:6:137:VAL:HG13	1.94	0.48
6:6:158:VAL:HA	6:6:172:PRO:HA	1.94	0.48
6:6:58:ASN:ND2	16:H:47:GLY:O	2.46	0.48
7:9:126:TYR:HB3	9:W:39:ASP:CG	2.34	0.48
4:E:211:SER:HB3	4:E:214:PHE:HD2	1.78	0.48
6:G:28:VAL:HA	16:Q:64:ILE:HG21	1.95	0.48
16:H:143:SER:HB2	16:H:235:GLU:HG3	1.95	0.48
10:A:69:ILE:HG22	11:J:62:ALA:HB1	1.96	0.48
13:L:263:LEU:HD13	13:L:266:VAL:HG21	1.96	0.48
11:J:138:VAL:HA	15:N:106:LEU:HD13	1.95	0.48
10:P:77:PHE:O	10:P:80:PRO:HD2	2.12	0.48
16:Q:175:LEU:HB3	16:Q:328:VAL:HG21	1.96	0.48
16:Q:215:ALA:O	16:Q:216:ARG:HB2	2.13	0.48
16:Q:21:VAL:HG13	16:Q:94:LEU:HD13	1.94	0.48
11:R:85:PRO:HA	12:S:22:ARG:NH1	2.28	0.48
13:T:53:ALA:HB3	13:T:69:LEU:HB3	1.95	0.48
14:U:194:PHE:HB2	14:U:249:ALA:HB3	1.95	0.48
14:U:215:PRO:HG2	14:U:216:PRO:HD3	1.95	0.48
1:1:338:VAL:O	1:1:342:TRP:HB2	2.14	0.48
18:1:502:FMN:O3'	18:1:502:FMN:N1	2.34	0.48
3:3:154:TYR:HB3	4:4:322:GLU:HB2	1.95	0.48
3:3:375:THR:HA	3:3:513:GLN:OE1	2.14	0.48
3:3:494:LYS:NZ	3:3:498:GLU:OE2	2.47	0.48
3:3:51:ARG:HB3	3:3:94:ASP:HB3	1.95	0.48
3:3:631:ASN:HB2	3:3:634:ALA:HB3	1.96	0.48
4:4:311:PRO:HD3	4:4:330:HIS:CE1	2.49	0.48
5:5:174:LEU:HD11	5:5:189:ARG:HH21	1.78	0.48
6:6:84:LEU:HD12	6:6:124:VAL:HG21	1.96	0.48
3:D:587:LEU:O	3:D:604:ALA:N	2.46	0.48
6:G:104:TRP:CE2	6:G:173:VAL:HG22	2.48	0.48
11:J:46:LEU:HD21	12:K:3:TYR:CE2	2.48	0.48
13:L:325:HIS:NE2	13:L:329:LYS:HG3	2.28	0.48
13:L:354:GLY:HA3	13:L:428:GLU:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:471:PRO:O	13:L:475:PRO:HD3	2.12	0.48
14:M:37:LEU:HB2	14:M:76:LEU:HD13	1.94	0.48
16:Q:52:GLY:HA2	16:Q:55:GLY:N	2.28	0.48
1:1:341:MET:CE	1:1:409:PRO:HB2	2.44	0.48
3:3:281:GLU:HA	3:3:287:GLU:O	2.14	0.48
4:4:201:ILE:HA	4:4:204:TYR:CD2	2.46	0.48
6:6:57:ARG:HH21	6:6:148:ILE:HA	1.78	0.48
1:B:214:LYS:O	1:B:216:THR:HG23	2.13	0.48
3:D:116:PRO:O	3:D:117:LEU:HB2	2.11	0.48
3:D:115:HIS:HB3	4:E:321:MET:CE	2.43	0.48
5:F:155:THR:O	6:G:119:ASN:ND2	2.43	0.48
6:G:57:ARG:HB3	6:G:60:LEU:HD12	1.94	0.48
16:H:232:TYR:HD1	16:H:233:HIS:N	2.11	0.48
11:J:23:ARG:HG2	11:J:80:GLU:HG2	1.94	0.48
16:Q:267:TRP:HB2	16:Q:275:PRO:O	2.13	0.48
13:T:557:ASP:O	13:T:560:LEU:HB3	2.14	0.48
15:V:257:LEU:HD11	15:V:374:TYR:HB2	1.93	0.48
2:2:79:HIS:ND1	2:2:118:SER:HB2	2.29	0.48
3:3:256:CYS:SG	3:3:258:LEU:HB2	2.54	0.48
3:3:720:PRO:HG3	3:3:749:HIS:HB3	1.95	0.48
10:A:28:GLY:HA3	16:H:239:ILE:CG2	2.43	0.48
1:B:212:TRP:HZ2	2:C:25:ALA:HB2	1.79	0.48
3:D:508:GLY:O	3:D:512:LEU:HB2	2.13	0.48
4:E:173:ILE:HA	4:E:178:VAL:HG12	1.96	0.48
5:F:78:PRO:HG3	5:F:85:GLY:HA2	1.96	0.48
16:H:292:TRP:HD1	16:H:296:THR:HG1	1.61	0.48
12:K:72:LEU:O	12:K:76:VAL:HG23	2.13	0.48
15:N:104:LEU:HD13	15:N:151:ALA:HA	1.95	0.48
7:O:69:TYR:HE1	7:O:71:GLU:HG3	1.79	0.48
13:T:25:ARG:HG2	13:T:28:LEU:HB2	1.95	0.48
13:T:508:GLY:O	13:T:512:PHE:HB2	2.14	0.48
2:2:33:ARG:HH21	2:2:37:GLU:HG3	1.77	0.48
1:B:41:ALA:HB2	1:B:116:GLU:HG3	1.94	0.48
3:D:223:SER:O	3:D:226:ILE:HG12	2.13	0.48
3:D:267:ALA:HA	3:D:277:ILE:HD13	1.96	0.48
3:D:512:LEU:HD21	3:D:534:ALA:HB1	1.96	0.48
6:G:16:ARG:HB3	6:G:16:ARG:HH11	1.79	0.48
10:A:10:THR:OG1	16:H:118:LEU:HD21	2.13	0.48
16:H:314:PHE:CD1	16:H:314:PHE:N	2.80	0.48
8:I:61:ASP:HB2	8:I:129:ALA:OXT	2.13	0.48
14:M:313:TYR:CD1	14:M:451:ALA:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:186:VAL:HA	16:Q:189:GLN:NE2	2.29	0.48
16:Q:219:PHE:C	16:Q:221:LEU:N	2.67	0.48
10:P:1:MET:HA	11:R:123:LEU:HD11	1.96	0.48
13:T:39:ALA:HB1	13:T:43:LEU:HG	1.96	0.48
13:T:41:PHE:HB2	13:T:81:THR:HB	1.96	0.48
14:U:232:THR:HG23	14:U:235:LYS:HD2	1.94	0.48
15:V:217:ALA:HA	15:V:285:LEU:HD23	1.96	0.48
1:1:149:ILE:HG21	1:1:153:ARG:HH21	1.78	0.48
1:B:260:ARG:N	1:B:280:ALA:O	2.38	0.48
3:D:383:PRO:HG2	3:D:531:LYS:HA	1.95	0.48
4:E:366:TYR:CZ	5:F:148:LYS:HE3	2.49	0.48
6:G:57:ARG:CG	6:G:60:LEU:HD12	2.37	0.48
16:H:96:ALA:HB2	16:H:124:TYR:CE2	2.49	0.48
16:H:219:PHE:C	16:H:221:LEU:N	2.67	0.48
16:H:224:ALA:CA	16:H:230:GLY:H	2.22	0.48
14:M:86:ALA:HA	14:M:96:LEU:HD11	1.95	0.48
13:L:603:VAL:HG21	15:N:235:LEU:HD22	1.94	0.48
11:R:127:LEU:HD12	12:S:51:LEU:HD21	1.96	0.48
12:S:63:VAL:CG1	15:V:112:GLU:HG3	2.42	0.48
1:1:409:PRO:O	1:1:413:SER:N	2.47	0.48
2:2:122:VAL:HG12	2:2:123:GLU:O	2.13	0.48
5:5:138:PRO:HG2	5:5:141:LEU:HD13	1.96	0.48
6:6:132:PRO:CG	6:6:178:ARG:HE	2.25	0.48
1:B:312:SER:H	1:B:316:LEU:HD12	1.78	0.48
2:C:122:VAL:HG12	2:C:123:GLU:O	2.14	0.48
3:D:716:LEU:HA	3:D:759:TYR:O	2.14	0.48
5:F:52:ILE:HG22	5:F:118:VAL:HG21	1.96	0.48
11:J:44:VAL:HG13	11:J:49:ARG:HG2	1.96	0.48
16:Q:221:LEU:HB3	16:Q:222:PRO:HA	1.96	0.48
11:R:19:VAL:HG21	11:R:32:LEU:HB2	1.95	0.48
9:X:21:LEU:HD21	9:X:26:LEU:HD11	1.95	0.48
1:1:336:SER:HB2	1:1:432:PRO:HD2	1.96	0.47
3:3:655:ARG:HH12	3:3:659:GLU:CG	2.25	0.47
4:4:207:LEU:HD11	7:9:12:ILE:HG12	1.96	0.47
1:B:341:MET:CE	1:B:409:PRO:HB2	2.44	0.47
4:E:196:VAL:O	4:E:200:ARG:HB2	2.13	0.47
5:F:138:PRO:HG2	5:F:141:LEU:HD13	1.96	0.47
16:Q:332:LEU:HD12	16:Q:332:LEU:H	1.77	0.47
1:1:254:ILE:HG23	1:1:261:PRO:HA	1.95	0.47
5:5:174:LEU:HB3	5:5:178:ASP:HB3	1.95	0.47
1:B:288:GLN:HB3	1:B:333:GLU:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:45:ARG:O	2:C:49:ILE:HG13	2.14	0.47
3:D:192:GLU:HG3	3:D:440:ARG:HH11	1.79	0.47
3:D:36:GLU:HB3	3:D:39:LEU:HB2	1.96	0.47
4:E:43:LEU:HD13	4:E:55:VAL:HG11	1.96	0.47
14:M:345:ARG:HG2	14:M:412:LYS:O	2.14	0.47
16:Q:131:LEU:O	16:Q:134:TYR:HB2	2.14	0.47
13:T:189:LYS:HZ3	13:T:477:LEU:HD12	1.79	0.47
14:U:224:SER:CA	14:U:330:GLY:HA3	2.42	0.47
2:2:24:ARG:HD2	2:2:55:THR:HB	1.95	0.47
4:4:47:LEU:HD13	4:4:51:GLU:O	2.15	0.47
1:B:339:ASP:OD2	2:C:89:LYS:HE2	2.13	0.47
6:G:55:ASP:OD1	16:Q:45:ARG:NH2	2.47	0.47
16:H:221:LEU:HB3	16:H:222:PRO:HA	1.97	0.47
11:J:19:VAL:HG11	12:K:33:LEU:HD13	1.95	0.47
11:J:19:VAL:HG21	11:J:32:LEU:HB2	1.96	0.47
15:N:83:GLU:HA	15:N:86:LEU:HB2	1.95	0.47
10:P:67:LEU:HD23	16:Q:310:TRP:CE2	2.49	0.47
13:T:171:LEU:O	13:T:175:ILE:HG13	2.14	0.47
5:5:140:ASP:HB2	9:W:30:LYS:NZ	2.30	0.47
1:1:316:LEU:HD13	1:1:323:LEU:HB2	1.95	0.47
6:6:100:PRO:CG	16:H:69:LYS:HE3	2.44	0.47
2:C:101:THR:O	2:C:105:GLY:N	2.46	0.47
1:B:358:PRO:HD3	3:D:107:MET:SD	2.54	0.47
3:D:35:SER:OG	3:D:83:CYS:SG	2.72	0.47
3:D:375:THR:HA	3:D:513:GLN:OE1	2.13	0.47
3:D:476:ILE:O	3:D:480:LEU:HG	2.15	0.47
3:D:516:VAL:O	3:D:520:ARG:HG3	2.14	0.47
4:E:224:ILE:HD11	4:E:275:ARG:CZ	2.43	0.47
4:E:89:HIS:CE1	4:E:92:ALA:HB2	2.48	0.47
6:G:132:PRO:CG	6:G:175:ALA:HB2	2.41	0.47
6:G:44:ALA:H	6:G:82:GLY:HA3	1.79	0.47
6:G:91:VAL:HG22	10:P:46:SER:HB2	1.96	0.47
11:J:16:GLY:O	11:J:19:VAL:HG12	2.14	0.47
7:O:56:CYS:N	17:O:202:SF4:S1	2.88	0.47
10:P:12:ILE:HD11	16:Q:10:TYR:HB3	1.96	0.47
15:V:277:ASN:HB3	15:V:280:ALA:HB3	1.96	0.47
9:W:74:LEU:HD12	9:W:77:LEU:HD23	1.96	0.47
1:1:118:MET:HG2	1:1:224:LEU:HD13	1.97	0.47
2:2:88:CYS:HB3	2:2:93:ALA:HB2	1.96	0.47
3:3:477:LEU:CD2	3:3:521:ALA:HB2	2.44	0.47
3:3:20:MET:HE1	3:3:83:CYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:44:TYR:O	10:A:48:ASN:HA	2.14	0.47
3:D:507:LEU:HD22	3:D:511:VAL:HG11	1.96	0.47
4:E:136:GLY:HA2	4:E:398:ALA:HB1	1.96	0.47
5:F:175:THR:HG23	5:F:177:LYS:H	1.79	0.47
6:G:21:PHE:O	6:G:25:GLU:HG2	2.14	0.47
16:H:283:ILE:O	16:H:287:LEU:HB2	2.14	0.47
14:M:64:ALA:C	14:M:113:ARG:HB3	2.35	0.47
14:M:307:GLY:HA2	14:M:380:THR:HA	1.97	0.47
14:M:130:LEU:HD13	15:N:380:LEU:HD11	1.95	0.47
16:Q:122:ILE:HA	16:Q:125:LEU:HD12	1.96	0.47
16:Q:220:ASP:CG	16:Q:301:ARG:HA	2.35	0.47
13:T:157:LYS:NZ	13:T:535:ASP:OD2	2.47	0.47
14:U:86:ALA:HA	14:U:96:LEU:HD11	1.96	0.47
3:3:655:ARG:HB2	3:3:655:ARG:NH1	2.27	0.47
3:D:157:PHE:CZ	3:D:159:PHE:HB2	2.49	0.47
3:D:472:GLU:O	3:D:476:ILE:HD12	2.14	0.47
3:D:652:PRO:HA	3:D:653:PRO:HD3	1.77	0.47
3:D:706:GLY:O	3:D:709:GLN:HB2	2.14	0.47
4:E:202:ASP:O	4:E:206:ALA:N	2.40	0.47
4:E:389:GLN:HB3	4:E:392:ASP:HB2	1.96	0.47
4:E:50:GLU:O	4:E:390:VAL:HG23	2.14	0.47
5:F:134:LYS:NZ	5:F:141:LEU:O	2.47	0.47
6:G:163:TYR:CD1	7:O:152:ARG:HD2	2.50	0.47
10:P:66:MET:HE2	10:P:67:LEU:HD12	1.95	0.47
14:U:204:LYS:HE3	14:U:234:TYR:O	2.14	0.47
14:U:201:PHE:CD2	14:U:245:ALA:HB2	2.50	0.47
15:V:29:THR:HG21	15:V:85:TYR:HB3	1.96	0.47
9:W:58:LEU:HD21	9:W:103:LEU:HB3	1.96	0.47
9:W:58:LEU:HD22	9:W:110:LEU:HD21	1.96	0.47
3:3:274:LEU:H	3:3:302:ASP:CB	2.28	0.47
3:3:355:LEU:HD22	3:3:664:LEU:HD23	1.97	0.47
3:3:383:PRO:HG2	3:3:531:LYS:HA	1.96	0.47
5:5:34:PHE:CD2	5:5:102:PRO:HG2	2.50	0.47
4:E:232:LEU:HD23	5:F:109:GLY:HA3	1.96	0.47
5:F:65:PRO:HD2	5:F:93:TYR:CE2	2.50	0.47
6:G:57:ARG:CZ	6:G:60:LEU:CD2	2.87	0.47
16:H:159:LEU:O	16:H:163:GLU:HB2	2.14	0.47
13:L:138:SER:O	13:L:142:ILE:HG13	2.14	0.47
14:M:82:VAL:HG21	14:M:103:GLU:HB2	1.97	0.47
13:T:138:SER:O	13:T:142:ILE:HG13	2.14	0.47
9:X:58:LEU:HD21	9:X:103:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:30:VAL:HG22	3:3:48:CYS:HA	1.97	0.47
3:3:50:VAL:HG22	3:3:82:SER:HB3	1.95	0.47
4:4:86:ASP:HB3	4:4:93:HIS:HD2	1.78	0.47
5:5:116:ARG:HG2	5:5:132:LEU:HD23	1.95	0.47
6:6:101:ASP:O	6:6:103:LYS:N	2.48	0.47
7:9:101:CYS:N	17:9:201:SF4:S4	2.87	0.47
6:6:97:GLU:O	10:A:40:LYS:HG3	2.15	0.47
6:6:72:PRO:HG3	10:A:44:TYR:CE1	2.50	0.47
10:A:49:ASP:N	10:A:50:PRO:HD3	2.30	0.47
1:B:149:ILE:HG21	1:B:153:ARG:HH21	1.80	0.47
1:B:254:ILE:HG23	1:B:261:PRO:HA	1.96	0.47
1:B:260:ARG:HG3	1:B:264:TYR:OH	2.15	0.47
3:D:507:LEU:HB3	3:D:511:VAL:HG11	1.95	0.47
3:D:605:PRO:CB	3:D:609:GLU:HG3	2.44	0.47
3:D:688:ARG:HA	3:D:688:ARG:HD3	1.55	0.47
4:E:234:LEU:HD12	4:E:380:SER:HB2	1.95	0.47
6:G:155:GLN:O	6:G:159:ARG:HG3	2.15	0.47
7:O:43:LEU:CD1	7:O:133:LYS:HG3	2.42	0.47
10:P:67:LEU:HB3	16:Q:310:TRP:HZ2	1.80	0.47
10:P:67:LEU:HD23	16:Q:310:TRP:CZ2	2.49	0.47
16:Q:96:ALA:HB2	16:Q:124:TYR:CE2	2.50	0.47
16:Q:96:ALA:HB3	16:Q:128:VAL:HG21	1.96	0.47
11:R:44:VAL:HG13	11:R:49:ARG:HG2	1.97	0.47
13:T:25:ARG:CG	13:T:28:LEU:HB2	2.44	0.47
13:T:285:ALA:O	13:T:294:ILE:HG13	2.14	0.47
13:T:66:SER:CB	13:T:122:ASP:HB3	2.44	0.47
1:1:254:ILE:HD11	1:1:330:LEU:HD11	1.96	0.47
3:3:477:LEU:HD23	3:3:521:ALA:HB2	1.97	0.47
4:4:140:LEU:HD21	4:4:217:ARG:NH1	2.30	0.47
6:G:104:TRP:HB3	6:G:154:LEU:HD11	1.97	0.47
16:H:215:ALA:O	16:H:216:ARG:HB2	2.14	0.47
8:I:37:PHE:HE1	8:I:74:PRO:HA	1.79	0.47
13:L:39:ALA:HB1	13:L:43:LEU:HG	1.97	0.47
14:M:38:TYR:O	14:M:41:LEU:O	2.33	0.47
15:N:194:PHE:O	15:N:197:PRO:HD2	2.14	0.47
11:R:24:ASN:HB3	11:R:27:HIS:HB2	1.97	0.47
1:1:10:ASP:OD1	1:1:11:PRO:HD2	2.15	0.47
1:1:270:THR:O	1:1:311:MET:HG3	2.15	0.47
2:2:101:THR:HG23	2:2:106:ILE:O	2.15	0.47
3:3:351:LEU:HA	3:3:351:LEU:HD12	1.68	0.47
4:4:263:ASP:HB2	4:4:285:GLU:CD	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:34:PHE:CD1	5:5:92:VAL:HG11	2.50	0.47
1:B:112:HIS:HA	1:B:115:ILE:HD12	1.97	0.47
2:C:81:GLN:HB3	2:C:122:VAL:HG21	1.97	0.47
4:E:174:ARG:N	4:E:177:GLY:O	2.33	0.47
3:D:117:LEU:H	4:E:321:MET:HE3	1.79	0.47
4:E:104:LEU:HB2	4:E:342:VAL:HG11	1.97	0.47
6:G:84:LEU:HD22	6:G:88:MET:HG3	1.97	0.47
8:I:63:LEU:HD13	8:I:129:ALA:HB3	1.96	0.47
14:M:30:GLY:O	14:M:34:LEU:HG	2.15	0.47
10:P:49:ASP:N	10:P:50:PRO:HD3	2.30	0.47
16:Q:327:VAL:HA	16:Q:332:LEU:HD13	1.95	0.47
14:U:29:ALA:CB	14:U:83:PHE:HA	2.43	0.47
15:V:412:LEU:HD13	15:V:419:VAL:HG21	1.96	0.47
3:3:369:LEU:HD12	3:3:369:LEU:O	2.14	0.47
3:3:20:MET:HE3	3:3:432:PHE:HB3	1.97	0.47
8:7:48:TYR:CE2	8:7:50:LEU:HB2	2.49	0.47
1:B:29:LEU:CD2	1:B:155:ARG:HD2	2.45	0.47
3:D:256:CYS:SG	3:D:258:LEU:HB2	2.55	0.47
4:E:152:GLU:OE2	4:E:204:TYR:OH	2.26	0.47
15:N:290:LEU:HD13	15:N:408:LEU:HB3	1.97	0.47
16:Q:220:ASP:OD2	16:Q:301:ARG:HA	2.15	0.47
14:U:345:ARG:HG2	14:U:412:LYS:O	2.15	0.47
14:U:307:GLY:HA2	14:U:380:THR:HA	1.97	0.47
1:1:16:THR:HG23	1:1:233:ARG:HH21	1.80	0.46
1:1:312:SER:H	1:1:316:LEU:HD12	1.80	0.46
3:3:605:PRO:CB	3:3:609:GLU:HG3	2.44	0.46
4:4:315:HIS:HA	8:7:46:ARG:CZ	2.45	0.46
5:5:178:ASP:O	5:5:185:LYS:HE2	2.15	0.46
7:9:10:LEU:O	7:9:13:THR:OG1	2.28	0.46
3:D:574:GLU:HB2	3:D:593:LEU:HD11	1.97	0.46
4:E:208:PHE:CE2	4:E:276:MET:HG2	2.50	0.46
4:E:379:GLN:HG2	5:F:113:PHE:CD2	2.50	0.46
5:F:33:ARG:O	5:F:37:GLU:HB2	2.15	0.46
16:H:194:TRP:HE3	16:H:196:PHE:HE1	1.63	0.46
13:L:285:ALA:O	13:L:294:ILE:HG13	2.15	0.46
14:M:204:LYS:HE3	14:M:234:TYR:O	2.15	0.46
14:M:305:PRO:HB3	14:M:459:GLU:CA	2.42	0.46
14:U:17:LEU:HD23	14:U:94:ARG:O	2.15	0.46
14:U:338:THR:HG22	14:U:340:GLU:H	1.80	0.46
1:1:372:ALA:O	1:1:376:THR:OG1	2.26	0.46
1:1:339:ASP:OD2	2:2:89:LYS:HE2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:165:ASP:HB3	3:3:178:ARG:HD2	1.97	0.46
3:3:289:TRP:O	3:3:290:ILE:HD13	2.15	0.46
3:3:83:CYS:SG	3:3:84:VAL:HG13	2.55	0.46
4:4:196:VAL:O	4:4:200:ARG:HB2	2.15	0.46
6:6:148:ILE:O	6:6:152:MET:HG3	2.16	0.46
10:A:22:VAL:O	10:A:26:LEU:HG	2.15	0.46
3:D:522:ARG:NH1	3:D:681:LYS:HD3	2.29	0.46
16:H:200:PHE:O	16:H:203:PHE:HB3	2.15	0.46
14:M:232:THR:HG21	14:M:322:THR:HG21	1.96	0.46
16:Q:166:LEU:HD22	16:Q:206:TYR:CE2	2.50	0.46
14:U:385:TYR:HA	14:U:389:PRO:HA	1.97	0.46
14:U:262:PHE:N	14:U:391:LEU:HD13	2.30	0.46
15:V:271:LEU:HB3	15:V:352:ALA:HB2	1.97	0.46
1:1:357:THR:N	1:1:358:PRO:HD2	2.31	0.46
3:3:55:PRO:HG3	3:3:74:GLN:N	2.31	0.46
5:5:10:ALA:HB1	5:5:15:TYR:HB2	1.97	0.46
10:A:57:PHE:CE2	16:H:149:LEU:CD2	2.95	0.46
4:E:47:LEU:HD13	4:E:51:GLU:O	2.16	0.46
5:F:185:LYS:HB2	5:F:189:ARG:HG3	1.98	0.46
5:F:2:ARG:HG3	5:F:84:ASP:OD2	2.15	0.46
16:H:122:ILE:HA	16:H:125:LEU:HD12	1.97	0.46
16:H:289:PHE:O	16:H:293:ILE:HG12	2.15	0.46
16:H:307:ARG:C	16:H:307:ARG:HD3	2.35	0.46
2:C:101:THR:HG22	8:I:108:ILE:HD11	1.97	0.46
11:J:65:VAL:HG23	16:H:134:TYR:CZ	2.50	0.46
13:L:30:GLY:HA2	13:L:105:PHE:CD1	2.51	0.46
15:N:271:LEU:HB3	15:N:352:ALA:HB2	1.96	0.46
7:O:11:GLY:O	7:O:15:LYS:HG3	2.15	0.46
6:G:72:PRO:HG3	10:P:44:TYR:HE1	1.80	0.46
13:T:324:THR:CB	13:T:380:SER:HB2	2.45	0.46
13:T:331:LEU:HD22	13:T:450:ALA:HA	1.97	0.46
13:T:469:LEU:HD12	13:T:469:LEU:HA	1.78	0.46
2:2:24:ARG:HE	2:2:55:THR:HG21	1.81	0.46
3:3:382:PHE:HB3	3:3:532:VAL:HB	1.97	0.46
3:3:603:PRO:HB2	3:3:634:ALA:HA	1.98	0.46
3:3:654:PHE:CD2	3:3:660:ALA:HA	2.50	0.46
6:6:138:PRO:HG2	7:9:121:MET:HG3	1.96	0.46
7:9:11:GLY:O	7:9:15:LYS:HG3	2.15	0.46
6:6:17:GLU:HA	10:A:33:PRO:HG3	1.98	0.46
2:C:81:GLN:HB3	2:C:122:VAL:CG2	2.45	0.46
3:D:477:LEU:CD2	3:D:521:ALA:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:304:ASN:O	3:D:589:HIS:CD2	2.68	0.46
6:G:96:TRP:CZ2	6:G:103:LYS:HE3	2.50	0.46
16:H:218:PRO:HB3	16:H:305:LEU:HD13	1.96	0.46
13:L:217:SER:HA	13:L:246:VAL:HA	1.98	0.46
10:P:67:LEU:HB3	16:Q:310:TRP:CZ2	2.50	0.46
13:T:354:GLY:HA3	13:T:428:GLU:O	2.15	0.46
13:T:358:HIS:O	13:T:360:PRO:HD3	2.15	0.46
1:1:260:ARG:HG3	1:1:264:TYR:OH	2.16	0.46
2:2:78:TYR:HD2	2:2:116:LEU:HD12	1.80	0.46
3:3:406:ALA:O	3:3:409:LEU:HB2	2.16	0.46
4:4:200:ARG:HD2	4:4:200:ARG:HA	1.70	0.46
4:4:211:SER:HG	4:4:273:PHE:HE2	1.62	0.46
4:4:104:LEU:HD21	4:4:359:SER:HB3	1.97	0.46
5:F:34:PHE:CD1	5:F:92:VAL:HG11	2.51	0.46
6:G:101:ASP:O	6:G:103:LYS:N	2.49	0.46
12:K:38:ALA:HA	15:N:149:TYR:HD1	1.81	0.46
16:Q:220:ASP:HA	16:Q:222:PRO:HB3	1.97	0.46
13:T:334:LEU:HD12	13:T:449:LEU:CD1	2.46	0.46
3:3:20:MET:SD	3:3:32:LEU:HD13	2.56	0.46
3:3:395:PHE:HB3	3:3:503:PRO:HB3	1.96	0.46
3:3:655:ARG:NH1	3:3:659:GLU:HG3	2.27	0.46
8:7:82:ILE:HG23	8:7:95:ALA:HB3	1.97	0.46
1:B:10:ASP:OD1	1:B:11:PRO:HD2	2.16	0.46
3:D:256:CYS:HB2	3:D:265:ILE:HD13	1.97	0.46
13:L:376:LEU:HD12	13:L:377:PRO:HD2	1.97	0.46
14:M:219:GLN:HA	14:M:282:LYS:HG3	1.98	0.46
14:M:70:LEU:HD23	14:M:243:ARG:NH2	2.30	0.46
15:N:422:ALA:O	15:N:423:LEU:HD23	2.15	0.46
16:Q:150:LEU:O	16:Q:154:ARG:HG3	2.16	0.46
16:Q:216:ARG:HD2	16:Q:294:ARG:CA	2.46	0.46
12:S:72:LEU:O	12:S:76:VAL:HG23	2.15	0.46
13:T:66:SER:HB3	13:T:122:ASP:HB3	1.97	0.46
14:U:208:PHE:O	14:U:211:HIS:CE1	2.69	0.46
9:W:35:THR:O	9:W:93:VAL:HA	2.16	0.46
2:2:82:VAL:HG22	2:2:134:ILE:HG12	1.97	0.46
3:3:688:ARG:HA	3:3:688:ARG:HD3	1.50	0.46
4:4:148:TYR:CD1	4:4:148:TYR:N	2.84	0.46
6:6:35:SER:HG	6:6:37:TRP:HE3	1.64	0.46
6:6:57:ARG:HD2	6:6:60:LEU:HG	1.94	0.46
3:D:186:ARG:HD2	3:D:231:PRO:HD3	1.97	0.46
3:D:55:PRO:HG3	3:D:74:GLN:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:337:PRO:O	4:E:361:GLY:HA2	2.15	0.46
4:E:225:PRO:HG3	4:E:383:TYR:OH	2.16	0.46
16:H:216:ARG:HD2	16:H:294:ARG:CA	2.46	0.46
13:L:331:LEU:HD22	13:L:450:ALA:HA	1.97	0.46
13:L:426:LEU:HD23	13:L:513:GLN:NE2	2.31	0.46
14:M:162:ALA:O	14:M:166:ALA:N	2.40	0.46
15:N:104:LEU:HD21	15:N:163:LEU:HD21	1.96	0.46
7:O:133:LYS:O	7:O:137:LEU:HD13	2.15	0.46
7:O:44:THR:HA	7:O:138:VAL:HG13	1.98	0.46
4:4:197:LEU:HA	4:4:200:ARG:HB2	1.98	0.46
5:5:180:GLY:HA3	5:5:189:ARG:HH22	1.80	0.46
4:E:379:GLN:OE1	5:F:112:ASN:HB3	2.16	0.46
5:F:116:ARG:HB3	5:F:135:ILE:HG13	1.98	0.46
6:G:57:ARG:HH11	6:G:60:LEU:CD1	2.26	0.46
11:J:104:LEU:O	11:J:108:LEU:HD12	2.16	0.46
13:L:360:PRO:HA	13:L:363:ARG:HH12	1.80	0.46
13:L:557:ASP:CG	14:M:211:HIS:HE2	2.19	0.46
15:N:406:GLY:O	15:N:409:LEU:HB2	2.15	0.46
10:P:57:PHE:CE2	16:Q:149:LEU:CD2	2.95	0.46
10:P:77:PHE:CE2	12:S:62:ALA:HB2	2.50	0.46
13:T:20:PHE:O	13:T:22:LYS:N	2.37	0.46
13:T:177:TRP:HE1	14:U:306:GLU:CD	2.19	0.46
15:V:294:LEU:HD11	15:V:325:ALA:HB1	1.98	0.46
15:V:45:GLY:C	15:V:47:PRO:HD3	2.35	0.46
1:1:225:ALA:O	1:1:229:PRO:HD2	2.16	0.46
18:1:502:FMN:H1'1	18:1:502:FMN:H9	1.51	0.46
3:3:409:LEU:HD23	3:3:409:LEU:HA	1.57	0.46
3:3:85:THR:HG22	3:3:86:ALA:O	2.16	0.46
4:4:38:HIS:ND1	4:4:139:ASP:OD2	2.47	0.46
4:4:288:LYS:HA	4:4:288:LYS:HD3	1.63	0.46
6:6:57:ARG:HH11	6:6:60:LEU:HD11	1.78	0.46
1:B:316:LEU:HD13	1:B:323:LEU:HB2	1.97	0.46
1:B:356:CYS:HB3	1:B:358:PRO:CD	2.45	0.46
3:D:185:LYS:O	3:D:189:ARG:HB2	2.16	0.46
16:H:220:ASP:OD2	16:H:301:ARG:HA	2.15	0.46
11:J:83:PHE:HD2	11:J:85:PRO:HG3	1.80	0.46
12:K:38:ALA:HA	15:N:149:TYR:CD1	2.51	0.46
13:L:14:PHE:CD1	13:L:110:LEU:HB2	2.51	0.46
13:L:386:ASP:OD2	13:L:494:ILE:HA	2.16	0.46
13:L:576:GLN:O	13:L:580:ARG:HB2	2.16	0.46
14:M:279:LYS:HD3	14:M:279:LYS:HA	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:290:PHE:O	16:Q:293:ILE:HB	2.15	0.46
13:T:161:VAL:HG13	13:T:222:LEU:HD22	1.98	0.46
13:T:325:HIS:CD2	13:T:329:LYS:HG3	2.51	0.46
13:T:287:GLY:HA3	13:T:528:SER:HB2	1.97	0.46
14:U:75:PHE:HZ	14:U:111:ALA:HB2	1.80	0.46
1:1:157:TYR:O	1:1:158:LEU:HD23	2.16	0.46
1:1:250:LYS:NZ	1:1:325:THR:O	2.47	0.46
2:2:85:THR:HB	19:2:201:FES:S2	2.56	0.46
4:4:148:TYR:H	4:4:148:TYR:HD1	1.62	0.46
2:C:87:SER:HB2	19:C:201:FES:S2	2.57	0.46
3:D:149:LEU:O	3:D:149:LEU:HD23	2.16	0.46
3:D:177:ASP:HB3	3:D:234:ALA:HA	1.98	0.46
16:H:332:LEU:H	16:H:332:LEU:CD1	2.29	0.46
15:N:154:PHE:O	15:N:158:THR:HG22	2.16	0.46
7:O:108:CYS:HB2	7:O:113:ILE:HG22	1.98	0.46
16:Q:96:ALA:HB1	16:Q:125:LEU:HD23	1.97	0.46
13:T:376:LEU:HD12	13:T:377:PRO:HD2	1.98	0.46
13:T:426:LEU:HD23	13:T:513:GLN:NE2	2.31	0.46
13:T:77:LEU:HD12	13:T:116:LEU:HD22	1.97	0.46
2:2:163:LEU:HA	2:2:166:ILE:HG13	1.97	0.45
3:3:128:CYS:HB3	3:3:131:GLN:HB2	1.97	0.45
3:3:185:LYS:HG2	3:3:188:VAL:HG22	1.97	0.45
3:3:52:ILE:HD12	3:3:85:THR:HG21	1.98	0.45
10:A:66:MET:CE	10:A:67:LEU:HD12	2.46	0.45
1:B:157:TYR:O	1:B:158:LEU:HD23	2.16	0.45
1:B:88:TYR:HB2	1:B:216:THR:HG22	1.98	0.45
3:D:478:LEU:HD12	3:D:520:ARG:CZ	2.47	0.45
4:E:287:VAL:O	4:E:291:LYS:HG3	2.17	0.45
16:H:233:HIS:O	16:H:234:THR:OG1	2.32	0.45
16:H:52:GLY:HA2	16:H:55:GLY:CA	2.46	0.45
13:L:234:THR:HG23	13:L:292:LYS:HE2	1.98	0.45
15:N:73:THR:HG21	15:N:210:PHE:HB2	1.98	0.45
7:O:99:ILE:HG22	7:O:101:CYS:SG	2.56	0.45
16:Q:39:LEU:CD2	16:Q:295:ALA:HB2	2.42	0.45
14:U:297:ALA:HB1	14:U:301:PHE:CE2	2.51	0.45
15:V:362:VAL:O	15:V:366:VAL:HG23	2.16	0.45
3:3:478:LEU:HD12	3:3:520:ARG:NH2	2.32	0.45
3:3:571:VAL:HA	3:3:572:PRO:HD3	1.66	0.45
4:4:202:ASP:OD1	4:4:284:ARG:NE	2.50	0.45
5:5:35:LYS:HD3	5:5:102:PRO:HB2	1.99	0.45
7:9:6:LEU:HB3	16:H:297:TRP:CZ2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:82:VAL:HG22	2:C:134:ILE:HG12	1.98	0.45
3:D:451:PHE:HD1	3:D:466:GLU:HB3	1.80	0.45
3:D:272:GLY:O	3:D:630:GLU:N	2.49	0.45
4:E:28:LEU:HD11	16:Q:147:TYR:CE2	2.51	0.45
5:F:101:LEU:HA	5:F:102:PRO:HD2	1.85	0.45
5:F:75:VAL:HG12	5:F:76:SER:N	2.31	0.45
6:G:85:SER:HA	6:G:123:ILE:HD13	1.97	0.45
16:H:52:GLY:HA2	16:H:55:GLY:HA2	1.97	0.45
8:I:88:ARG:NH2	8:I:126:LEU:HB3	2.31	0.45
11:J:83:PHE:CD2	11:J:85:PRO:HG3	2.51	0.45
13:L:358:HIS:O	13:L:360:PRO:HD3	2.16	0.45
13:T:163:ARG:NH2	14:U:366:VAL:O	2.49	0.45
13:T:380:SER:CB	13:T:456:ALA:HB3	2.46	0.45
3:3:476:ILE:O	3:3:480:LEU:HG	2.17	0.45
3:3:583:VAL:HG23	3:3:599:HIS:H	1.82	0.45
4:4:225:PRO:HG3	4:4:383:TYR:OH	2.16	0.45
5:5:38:MET:HA	5:5:41:TYR:CD2	2.50	0.45
6:6:96:TRP:CZ2	6:6:103:LYS:HE3	2.52	0.45
6:6:57:ARG:NE	6:6:60:LEU:HD21	2.30	0.45
1:B:250:LYS:HB3	1:B:252:TYR:CE1	2.50	0.45
3:D:46:ARG:N	19:D:804:FES:S1	2.86	0.45
8:I:13:TRP:HE3	8:I:82:ILE:HD12	1.81	0.45
13:L:128:PHE:HD1	13:L:169:PHE:CD2	2.35	0.45
13:L:196:LEU:HD23	13:L:202:LEU:HD23	1.98	0.45
13:L:214:VAL:HG12	13:L:222:LEU:HB2	1.99	0.45
13:L:419:ARG:HB2	13:L:512:PHE:HD2	1.77	0.45
14:M:296:ALA:HB2	14:M:314:LEU:HD22	1.98	0.45
14:M:325:LEU:HG	14:M:361:LEU:HD23	1.98	0.45
14:M:331:ARG:HA	14:M:331:ARG:HD2	1.68	0.45
15:N:259:ALA:O	15:N:263:ILE:HG13	2.17	0.45
15:N:275:THR:OG1	15:N:351:GLU:HB3	2.16	0.45
16:Q:216:ARG:HG3	16:Q:219:PHE:CE1	2.50	0.45
11:R:83:PHE:O	11:R:84:ASP:HB2	2.17	0.45
14:U:232:THR:HG21	14:U:322:THR:HG21	1.98	0.45
15:V:207:VAL:O	15:V:211:MET:HG3	2.17	0.45
1:1:344:LEU:O	1:1:347:PHE:HB3	2.17	0.45
1:1:373:LYS:HA	8:7:79:LEU:HD11	1.98	0.45
5:5:171:ARG:HG3	5:5:171:ARG:NH1	2.31	0.45
5:5:175:THR:HG23	5:5:177:LYS:H	1.81	0.45
6:6:132:PRO:HG3	6:6:178:ARG:CD	2.47	0.45
1:B:199:PRO:HG2	17:B:501:SF4:S2	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:85:ALA:HB3	16:H:86:PRO:HD3	1.99	0.45
13:L:25:ARG:HG2	13:L:28:LEU:HB2	1.97	0.45
13:L:340:ILE:HB	13:L:345:GLY:HA2	1.98	0.45
13:L:541:LEU:HA	13:L:545:PRO:HG2	1.97	0.45
15:N:52:PRO:HB3	15:N:103:HIS:HB2	1.98	0.45
13:T:255:ARG:HD2	13:T:477:LEU:HD23	1.98	0.45
13:T:490:GLU:O	13:T:493:LEU:HB2	2.16	0.45
15:V:345:LYS:NZ	15:V:368:SER:OG	2.49	0.45
5:5:33:ARG:O	5:5:37:GLU:HB2	2.17	0.45
6:6:101:ASP:OD1	6:6:180:ARG:NH2	2.50	0.45
7:9:68:ILE:HG12	7:9:93:ILE:HG12	1.99	0.45
1:B:192:LEU:O	2:C:25:ALA:HA	2.17	0.45
4:E:38:HIS:CE1	4:E:398:ALA:HA	2.51	0.45
5:F:38:MET:HA	5:F:41:TYR:CD2	2.51	0.45
14:M:8:LEU:HD23	14:M:32:SER:HA	1.98	0.45
15:N:61:VAL:O	15:N:64:LEU:HB3	2.16	0.45
16:Q:222:PRO:CD	16:Q:230:GLY:HA2	2.39	0.45
16:Q:320:TRP:HH2	16:Q:340:LEU:HB3	1.82	0.45
16:Q:83:VAL:O	16:Q:86:PRO:HD2	2.17	0.45
10:P:81:TYR:HB2	11:R:132:TYR:CE1	2.51	0.45
11:R:69:PHE:O	11:R:73:LEU:HG	2.16	0.45
12:S:79:PHE:CD2	12:S:85:THR:HA	2.52	0.45
14:U:88:VAL:HG13	14:U:89:ALA:H	1.81	0.45
1:1:212:TRP:HZ2	2:2:25:ALA:HB2	1.82	0.45
3:3:297:GLY:O	3:3:703:GLN:NE2	2.48	0.45
3:3:337:ARG:H	3:3:337:ARG:HD2	1.81	0.45
5:5:40:HIS:O	5:5:44:MET:N	2.50	0.45
6:6:57:ARG:CB	6:6:60:LEU:HD12	2.46	0.45
18:B:502:FMN:H9	18:B:502:FMN:H1'1	1.53	0.45
4:E:200:ARG:HA	4:E:200:ARG:HD2	1.71	0.45
4:E:390:VAL:HB	4:E:391:PRO:HD3	1.98	0.45
5:F:34:PHE:CD2	5:F:102:PRO:HG2	2.52	0.45
4:E:338:PRO:HG2	5:F:193:ARG:HD3	1.98	0.45
7:O:110:THR:C	8:I:44:MET:HG2	2.37	0.45
14:M:91:VAL:HG12	14:M:222:HIS:CG	2.50	0.45
15:N:291:ALA:O	15:N:294:LEU:HB3	2.17	0.45
16:Q:291:ILE:HA	16:Q:294:ARG:CG	2.47	0.45
13:T:24:MET:HB3	13:T:28:LEU:HB3	1.99	0.45
13:T:496:LEU:HD12	13:T:496:LEU:HA	1.81	0.45
14:U:10:VAL:HG23	14:U:104:GLY:HA3	1.97	0.45
15:V:316:TYR:HB2	15:V:382:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:380:GLU:N	1:1:383:ASP:OD2	2.38	0.45
2:2:147:ARG:HE	2:2:147:ARG:HB2	1.67	0.45
3:3:128:CYS:SG	3:3:130:LEU:HB3	2.56	0.45
3:3:20:MET:O	3:3:23:VAL:HB	2.17	0.45
4:4:335:PHE:O	4:4:363:SER:HA	2.17	0.45
6:6:140:CYS:HB3	7:9:99:ILE:O	2.17	0.45
1:B:177:ALA:HB3	2:C:67:TYR:CG	2.51	0.45
2:C:78:TYR:HD2	2:C:116:LEU:HD12	1.80	0.45
2:C:24:ARG:HE	2:C:55:THR:HG21	1.82	0.45
3:D:52:ILE:HD12	3:D:85:THR:HG21	1.98	0.45
4:E:62:LEU:HD11	6:G:43:LEU:O	2.16	0.45
14:M:53:ALA:O	14:M:62:TYR:HB3	2.17	0.45
15:N:287:THR:HG22	15:N:340:ALA:HB1	1.98	0.45
15:N:316:TYR:HB2	15:N:382:VAL:HG13	1.99	0.45
10:P:38:ARG:O	10:P:42:MET:HG3	2.17	0.45
10:P:47:GLY:C	10:P:48:ASN:HD22	2.16	0.45
11:R:154:VAL:O	11:R:158:GLU:HB2	2.17	0.45
13:T:196:LEU:HD23	13:T:202:LEU:HD23	1.99	0.45
13:T:257:SER:OG	13:T:478:ALA:HA	2.17	0.45
15:V:116:LEU:HD23	15:V:119:TYR:CE2	2.52	0.45
1:1:29:LEU:CD2	1:1:155:ARG:HD2	2.47	0.45
3:3:186:ARG:HD2	3:3:231:PRO:HD3	1.97	0.45
3:3:355:LEU:HG	3:3:654:PHE:CZ	2.51	0.45
4:4:112:ARG:HG3	4:4:297:LEU:HD11	1.98	0.45
4:4:283:MET:O	4:4:287:VAL:HG23	2.17	0.45
5:5:116:ARG:HB3	5:5:135:ILE:HG13	1.98	0.45
4:4:328:PHE:CE2	7:9:58:LEU:HD21	2.52	0.45
3:D:611:ARG:HA	3:D:624:LEU:O	2.17	0.45
3:D:50:VAL:CG2	3:D:82:SER:HB3	2.47	0.45
5:F:64:ARG:HA	5:F:64:ARG:HD3	1.83	0.45
5:F:77:LEU:HA	5:F:78:PRO:HD3	1.74	0.45
16:H:211:MET:O	16:H:218:PRO:HG3	2.16	0.45
14:M:169:LEU:HD21	15:N:358:TRP:CZ2	2.52	0.45
14:M:289:GLY:O	14:M:293:MET:HG2	2.16	0.45
14:M:88:VAL:HG11	14:M:432:PHE:CD1	2.52	0.45
15:N:118:LEU:HD23	15:N:121:LEU:HD12	1.99	0.45
15:N:207:VAL:O	15:N:211:MET:HG3	2.17	0.45
16:Q:189:GLN:HG2	16:Q:195:LEU:H	1.81	0.45
16:Q:71:ASP:OD1	16:Q:240:LYS:NZ	2.41	0.45
14:U:160:LEU:O	14:U:163:VAL:HG12	2.17	0.45
9:X:78:VAL:HG21	9:X:126:TYR:CB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:SER:HB2	1:B:432:PRO:HD2	1.99	0.45
4:E:47:LEU:HD21	4:E:390:VAL:HG22	1.98	0.45
4:E:47:LEU:HA	4:E:53:LEU:HD23	1.99	0.45
6:G:84:LEU:HD11	6:G:89:ALA:HA	1.99	0.45
16:H:213:GLU:N	16:H:213:GLU:OE1	2.49	0.45
16:H:240:LYS:HZ2	16:H:240:LYS:HB2	1.81	0.45
16:H:308:PHE:O	16:H:312:PHE:HB3	2.17	0.45
11:J:52:GLY:O	11:J:55:GLN:HB3	2.16	0.45
13:L:26:GLU:O	13:L:101:TYR:CE2	2.70	0.45
13:L:490:GLU:O	13:L:493:LEU:HB2	2.17	0.45
14:M:130:LEU:O	14:M:133:LEU:HB3	2.17	0.45
16:Q:236:TYR:HD1	16:Q:240:LYS:HZ2	1.65	0.45
14:U:131:LEU:O	14:U:135:LEU:HD23	2.17	0.45
3:3:648:LEU:HD23	3:3:648:LEU:HA	1.81	0.45
4:4:185:GLU:O	4:4:189:GLU:HG2	2.17	0.45
4:4:47:LEU:HD21	4:4:390:VAL:HG22	1.98	0.45
4:4:62:LEU:HA	4:4:62:LEU:HD23	1.85	0.45
1:B:404:ASP:HA	1:B:407:VAL:HG22	1.99	0.45
3:D:112:LEU:HD22	4:E:321:MET:HG2	1.99	0.45
3:D:409:LEU:HA	3:D:409:LEU:HD23	1.52	0.45
3:D:373:GLY:CA	3:D:538:ALA:HB2	2.47	0.45
5:F:101:LEU:O	5:F:126:PHE:HA	2.17	0.45
6:G:57:ARG:HG3	6:G:57:ARG:NH1	2.21	0.45
16:H:176:LEU:HD22	16:H:334:ARG:HD2	1.98	0.45
13:L:266:VAL:O	13:L:270:ILE:HG13	2.16	0.45
13:L:309:ALA:HB2	13:L:388:ILE:HG12	1.99	0.45
15:N:206:PRO:O	15:N:209:LEU:HB3	2.17	0.45
13:T:214:VAL:HG12	13:T:222:LEU:HB2	1.99	0.45
14:U:335:ARG:NH2	14:U:429:GLU:OE1	2.49	0.45
14:U:68:ASP:O	14:U:72:ALA:HB2	2.16	0.45
9:W:78:VAL:HG21	9:W:126:TYR:CB	2.43	0.45
3:3:545:GLU:HA	3:3:550:LEU:HD11	1.99	0.44
4:4:112:ARG:NH1	4:4:299:PRO:HA	2.32	0.44
4:4:159:LEU:HB3	4:4:186:PHE:HE1	1.82	0.44
4:4:87:TYR:HB3	4:4:169:HIS:CE1	2.51	0.44
1:B:118:MET:HG2	1:B:224:LEU:HD13	1.99	0.44
3:D:654:PHE:CD2	3:D:660:ALA:HA	2.52	0.44
4:E:112:ARG:NH1	4:E:299:PRO:HA	2.31	0.44
4:E:31:GLY:HA3	10:P:45:GLU:CG	2.45	0.44
4:E:68:LYS:HB2	5:F:146:LEU:HD23	1.99	0.44
6:G:83:ARG:HB2	6:G:123:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:142:VAL:O	11:J:145:LEU:HB3	2.17	0.44
11:J:69:PHE:O	11:J:73:LEU:HG	2.17	0.44
12:K:79:PHE:CD2	12:K:85:THR:HA	2.52	0.44
14:M:166:ALA:O	14:M:170:SER:OG	2.28	0.44
14:M:85:GLY:HA2	14:M:327:LEU:HD22	1.99	0.44
13:T:40:SER:OG	13:T:41:PHE:N	2.50	0.44
15:V:268:TYR:OH	15:V:368:SER:HA	2.17	0.44
3:3:223:SER:O	3:3:226:ILE:HG12	2.17	0.44
4:4:99:LEU:HD23	4:4:102:GLU:OE1	2.17	0.44
4:4:133:LEU:O	4:4:137:LEU:HD13	2.17	0.44
4:4:85:MET:HE1	4:4:370:VAL:HG21	1.99	0.44
1:B:104:ARG:NH2	2:C:127:SER:HB3	2.26	0.44
14:M:98:LEU:HB3	14:M:132:MET:HE3	2.00	0.44
14:M:41:LEU:HD23	14:M:449:TYR:OH	2.16	0.44
4:E:207:LEU:HD11	7:O:12:ILE:HG12	2.00	0.44
10:P:9:GLY:O	10:P:12:ILE:HB	2.16	0.44
16:Q:314:PHE:N	16:Q:314:PHE:CD1	2.83	0.44
14:U:114:ASP:OD1	14:U:117:VAL:HB	2.17	0.44
1:1:104:ARG:NH2	2:2:127:SER:HB3	2.31	0.44
3:3:121:THR:HA	7:9:86:ARG:HD3	1.99	0.44
3:3:361:ALA:CB	3:3:369:LEU:HD23	2.47	0.44
4:4:248:VAL:HB	4:4:347:GLU:HB2	2.00	0.44
4:4:139:ASP:OD2	4:4:398:ALA:HB2	2.17	0.44
7:9:149:GLU:HA	7:9:152:ARG:NE	2.32	0.44
1:B:357:THR:N	1:B:358:PRO:HD2	2.33	0.44
4:E:138:LEU:HD13	4:E:143:LEU:HA	1.98	0.44
4:E:81:TYR:CZ	6:G:117:MET:HG3	2.52	0.44
6:G:97:GLU:O	10:P:40:LYS:HG3	2.17	0.44
16:H:211:MET:HG3	16:H:212:ALA:N	2.32	0.44
8:I:123:ARG:O	8:I:127:ALA:HB3	2.17	0.44
10:A:109:TYR:CD2	11:J:151:VAL:HG22	2.52	0.44
14:M:151:PHE:CD2	14:M:213:TRP:HB3	2.52	0.44
15:N:209:LEU:HB2	15:N:296:PHE:HB3	1.98	0.44
13:T:20:PHE:HD1	13:T:23:ARG:HE	1.64	0.44
13:T:511:PHE:O	13:T:511:PHE:HD1	2.00	0.44
14:U:13:GLY:HA2	14:U:97:GLY:HA2	1.99	0.44
14:U:279:LYS:HD3	14:U:279:LYS:HA	1.71	0.44
14:U:269:LEU:HD12	14:U:394:LEU:HG	2.00	0.44
14:U:426:ALA:HB3	14:U:429:GLU:HG3	1.99	0.44
15:V:233:LEU:HD12	15:V:233:LEU:HA	1.82	0.44
7:9:127:SER:OG	9:W:39:ASP:OD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:64:GLY:HA3	18:1:502:FMN:O1P	2.16	0.44
3:3:438:LYS:O	3:3:441:MET:HG3	2.16	0.44
4:4:193:LEU:HA	4:4:196:VAL:HG12	1.99	0.44
4:4:249:ARG:HB3	4:4:257:TYR:CD2	2.52	0.44
6:6:96:TRP:CE2	6:6:103:LYS:HE3	2.53	0.44
8:7:48:TYR:CZ	8:7:50:LEU:HB2	2.52	0.44
2:C:78:TYR:CE2	2:C:157:LEU:HB3	2.52	0.44
4:E:288:LYS:HD3	4:E:288:LYS:HA	1.67	0.44
6:G:132:PRO:HG3	6:G:178:ARG:CD	2.48	0.44
6:G:31:GLY:O	6:G:35:SER:HB3	2.18	0.44
16:H:9:PRO:HB2	16:H:11:TRP:NE1	2.33	0.44
16:H:162:TYR:HA	16:H:314:PHE:HZ	1.81	0.44
7:9:10:LEU:O	16:H:292:TRP:HZ2	2.01	0.44
13:L:511:PHE:O	13:L:511:PHE:HD1	2.00	0.44
15:N:233:LEU:HD12	15:N:233:LEU:HA	1.82	0.44
16:Q:176:LEU:HD22	16:Q:334:ARG:HD2	1.99	0.44
13:T:321:HIS:HA	13:T:384:SER:CB	2.48	0.44
13:T:309:ALA:HB2	13:T:388:ILE:HG12	2.00	0.44
15:V:241:VAL:HG12	15:V:367:THR:OG1	2.18	0.44
4:4:274:ASP:O	4:4:278:VAL:HG23	2.17	0.44
4:4:379:GLN:NE2	5:5:110:SER:HA	2.32	0.44
5:5:103:THR:HG23	5:5:127:GLU:O	2.17	0.44
5:5:145:PRO:HA	5:5:150:TYR:CD1	2.52	0.44
6:6:17:GLU:CG	10:A:33:PRO:HA	2.48	0.44
6:6:17:GLU:HG3	10:A:33:PRO:HA	2.00	0.44
6:6:26:LYS:HA	6:6:26:LYS:HD3	1.80	0.44
7:9:57:SER:N	17:9:202:SF4:S1	2.77	0.44
3:D:476:ILE:HG23	3:D:490:VAL:HG13	1.99	0.44
4:E:318:GLU:OE1	8:I:46:ARG:NE	2.39	0.44
4:E:369:LYS:HG3	5:F:53:VAL:HG23	2.00	0.44
11:J:83:PHE:O	11:J:84:ASP:HB2	2.18	0.44
14:M:88:VAL:HG13	14:M:89:ALA:H	1.82	0.44
14:M:9:PRO:HG2	14:M:107:LEU:HD12	2.00	0.44
10:P:22:VAL:O	10:P:26:LEU:HG	2.17	0.44
16:Q:283:ILE:O	16:Q:287:LEU:HB2	2.17	0.44
16:Q:300:LEU:HD23	16:Q:305:LEU:HA	1.98	0.44
16:Q:37:ARG:NH2	16:Q:49:ASN:OD1	2.50	0.44
16:Q:70:GLU:O	16:Q:70:GLU:HG3	2.18	0.44
14:U:132:MET:SD	14:U:227:ALA:HA	2.57	0.44
14:U:93:GLY:HA3	14:U:136:TYR:CE1	2.53	0.44
14:U:350:SER:HB3	14:U:422:VAL:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:425:LEU:HD22	14:U:430:TRP:CE2	2.51	0.44
1:1:177:ALA:HB3	2:2:67:TYR:CG	2.52	0.44
1:1:358:PRO:O	1:1:362:GLY:HA3	2.17	0.44
1:1:43:ARG:HG3	1:1:44:VAL:N	2.33	0.44
3:3:260:PRO:HB2	3:3:617:LEU:HB3	1.99	0.44
4:4:249:ARG:HB3	4:4:257:TYR:HD2	1.83	0.44
10:A:1:MET:HG2	10:A:2:ALA:H	1.83	0.44
10:A:3:PRO:HB2	10:A:5:GLN:H	1.82	0.44
1:B:80:PRO:HG2	1:B:215:PRO:HB3	1.99	0.44
2:C:110:GLU:OE2	8:I:114:ARG:NH2	2.45	0.44
3:D:351:LEU:HD12	3:D:351:LEU:HA	1.76	0.44
12:K:18:VAL:HG13	12:K:27:VAL:HG13	1.98	0.44
13:L:88:HIS:O	13:L:92:ILE:HG13	2.18	0.44
13:L:95:MET:O	13:L:101:TYR:HE1	2.00	0.44
16:Q:45:ARG:HG3	16:Q:46:MET:N	2.25	0.44
11:R:121:GLY:O	11:R:123:LEU:N	2.47	0.44
13:T:128:PHE:HD1	13:T:169:PHE:CD2	2.36	0.44
1:1:101:PHE:H	1:1:253:GLN:HG3	1.83	0.44
2:2:100:LEU:HD13	2:2:150:LEU:HD21	2.00	0.44
2:2:80:LEU:HD13	2:2:100:LEU:HD11	2.00	0.44
3:3:21:ASP:OD1	3:3:431:PRO:HA	2.18	0.44
3:3:285:VAL:HG22	3:3:286:ASN:N	2.33	0.44
3:3:696:PRO:HB3	3:3:767:ALA:HB1	1.99	0.44
8:7:10:TYR:OH	8:7:75:ARG:HA	2.18	0.44
10:A:83:VAL:HG23	10:A:84:SER:H	1.82	0.44
3:D:387:LEU:HD21	3:D:409:LEU:HD21	2.00	0.44
3:D:656:LEU:HD11	9:X:3:ARG:HD3	1.98	0.44
3:D:700:LYS:O	3:D:703:GLN:HB2	2.17	0.44
5:F:154:GLU:OE2	5:F:167:PRO:HB2	2.18	0.44
5:F:171:ARG:HG3	5:F:171:ARG:NH1	2.32	0.44
5:F:174:LEU:HB3	5:F:178:ASP:HB3	1.99	0.44
16:H:221:LEU:N	16:H:222:PRO:HA	2.31	0.44
8:I:87:PRO:O	8:I:88:ARG:HB2	2.17	0.44
14:M:91:VAL:HA	14:M:222:HIS:CE1	2.53	0.44
15:N:17:GLY:HA3	15:N:82:PHE:CD2	2.53	0.44
7:O:59:CYS:HB2	7:O:104:CYS:HB2	1.99	0.44
16:Q:224:ALA:CA	16:Q:230:GLY:H	2.23	0.44
11:R:83:PHE:HB3	11:R:85:PRO:HD3	1.99	0.44
13:T:422:VAL:HG11	13:T:513:GLN:N	2.33	0.44
13:T:438:ALA:HA	13:T:439:PRO:HD3	1.85	0.44
14:U:331:ARG:HD2	14:U:331:ARG:HA	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:38:TYR:O	14:U:41:LEU:O	2.36	0.44
14:U:84:LEU:HA	14:U:87:LEU:HG	2.00	0.44
14:U:91:VAL:HG12	14:U:222:HIS:CG	2.53	0.44
1:1:260:ARG:HA	1:1:261:PRO:HD2	1.90	0.44
1:1:381:GLU:O	1:1:385:GLU:HG3	2.17	0.44
3:3:225:ASN:O	3:3:229:ILE:HG13	2.18	0.44
4:4:102:GLU:O	4:4:106:GLY:N	2.51	0.44
6:6:126:ASN:HB2	9:W:38:GLN:HE21	1.83	0.44
6:6:138:PRO:O	6:6:142:PRO:HB3	2.18	0.44
10:A:47:GLY:C	10:A:48:ASN:HD22	2.16	0.44
1:B:43:ARG:HG3	1:B:44:VAL:N	2.33	0.44
4:E:263:ASP:HB2	4:E:285:GLU:CD	2.37	0.44
5:F:135:ILE:HG22	5:F:136:LEU:HG	1.99	0.44
16:H:8:ASP:OD2	16:H:111:TYR:HB3	2.18	0.44
12:K:55:VAL:O	12:K:59:MET:HG2	2.18	0.44
10:A:77:PHE:CE2	12:K:62:ALA:HB2	2.51	0.44
13:L:302:GLN:O	13:L:305:TYR:HB2	2.18	0.44
13:L:477:LEU:HA	13:L:477:LEU:HD12	1.71	0.44
13:L:517:PHE:O	13:L:522:LEU:HG	2.17	0.44
7:O:94:ASN:HB3	7:O:97:ARG:HB2	2.00	0.44
10:P:62:TYR:CD1	10:P:62:TYR:C	2.91	0.44
13:T:68:LEU:HD23	13:T:255:ARG:HH22	1.82	0.44
15:V:73:THR:HG21	15:V:210:PHE:HB2	1.99	0.44
9:W:1:MET:HB3	9:W:107:PRO:HB3	1.99	0.44
1:1:258:VAL:HB	1:1:330:LEU:HD12	1.99	0.44
3:3:149:LEU:HD23	3:3:149:LEU:O	2.18	0.44
3:3:462:ALA:O	3:3:465:HIS:ND1	2.51	0.44
4:4:104:LEU:HB2	4:4:342:VAL:HG11	2.00	0.44
4:4:57:PRO:HD3	4:4:382:PRO:HG3	1.99	0.44
8:7:61:ASP:HB2	8:7:129:ALA:OXT	2.16	0.44
10:A:2:ALA:CB	16:H:119:ASP:HB3	2.48	0.44
3:D:549:VAL:C	3:D:550:LEU:HD12	2.39	0.44
3:D:571:VAL:HA	3:D:572:PRO:HD3	1.64	0.44
4:E:75:TYR:CZ	4:E:337:PRO:HG2	2.53	0.44
6:G:102:PRO:HG3	10:P:33:PRO:HG2	1.99	0.44
14:M:296:ALA:HA	14:M:311:GLY:HA2	1.99	0.44
14:M:88:VAL:HG13	14:M:89:ALA:N	2.32	0.44
15:N:272:ALA:HB3	15:N:281:LEU:HD13	2.00	0.44
4:E:390:VAL:HG11	16:Q:228:LEU:HG	1.99	0.44
1:1:104:ARG:O	1:1:108:GLU:HG3	2.18	0.43
2:2:146:THR:CG2	2:2:149:ARG:H	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:55:PRO:HG3	3:3:74:GLN:H	1.82	0.43
4:4:173:ILE:O	4:4:174:ARG:NH1	2.51	0.43
4:4:26:MET:HG2	10:A:54:VAL:HB	1.99	0.43
5:5:155:THR:N	6:6:119:ASN:OD1	2.37	0.43
7:9:54:ILE:HG23	7:9:110:THR:HG21	1.99	0.43
1:B:270:THR:O	1:B:311:MET:HG3	2.18	0.43
1:B:96:SER:HB2	1:B:180:TYR:HD1	1.81	0.43
5:F:144:HIS:O	5:F:147:ARG:HG2	2.18	0.43
16:H:228:LEU:HD22	16:H:228:LEU:HA	1.60	0.43
13:L:105:PHE:HA	13:L:108:PHE:HB2	2.00	0.43
13:L:519:ALA:HB3	13:L:520:TRP:CE3	2.53	0.43
13:L:585:TYR:O	13:L:588:VAL:HB	2.18	0.43
14:M:270:TYR:CE1	14:M:274:VAL:HG21	2.53	0.43
14:M:269:LEU:HD12	14:M:394:LEU:HG	2.00	0.43
14:M:52:GLN:HA	14:M:63:TRP:O	2.18	0.43
14:M:96:LEU:O	14:M:100:LEU:HG	2.18	0.43
15:N:126:ARG:O	15:N:129:GLY:N	2.51	0.43
13:T:26:GLU:O	13:T:101:TYR:CE2	2.71	0.43
13:T:490:GLU:O	13:T:494:ILE:HG12	2.18	0.43
9:X:26:LEU:HD12	9:X:84:GLN:HB2	1.98	0.43
1:1:233:ARG:O	1:1:237:TRP:HB3	2.18	0.43
4:4:228:VAL:HA	4:4:231:ASP:HB3	2.00	0.43
5:5:20:ASN:OD1	5:5:22:LEU:HB2	2.19	0.43
8:7:20:MET:HE3	8:7:59:LEU:HG	2.00	0.43
1:B:331:ILE:HA	1:B:332:PRO:HD2	1.73	0.43
2:C:154:LEU:HA	2:C:154:LEU:HD23	1.90	0.43
2:C:163:LEU:HA	2:C:166:ILE:HG13	1.99	0.43
3:D:33:PHE:CZ	3:D:130:LEU:HA	2.52	0.43
3:D:695:ARG:O	3:D:697:THR:HG23	2.18	0.43
4:E:228:VAL:HA	4:E:231:ASP:HB3	2.00	0.43
6:G:151:VAL:O	6:G:155:GLN:HB2	2.19	0.43
11:J:46:LEU:HA	11:J:46:LEU:HD23	1.69	0.43
14:M:119:TYR:OH	14:M:160:LEU:HB2	2.17	0.43
14:M:215:PRO:HG2	14:M:216:PRO:HD3	1.99	0.43
15:N:217:ALA:HA	15:N:285:LEU:HD23	2.00	0.43
14:U:296:ALA:HA	14:U:311:GLY:HA2	1.99	0.43
14:U:88:VAL:HG13	14:U:89:ALA:N	2.33	0.43
15:V:260:TYR:HA	15:V:263:ILE:HD12	2.00	0.43
15:V:272:ALA:HB3	15:V:281:LEU:HD13	1.99	0.43
15:V:83:GLU:O	15:V:87:LEU:HG	2.17	0.43
9:W:81:LEU:HD13	9:W:89:PHE:HE1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:689:LYS:HD2	3:3:772:GLU:HG2	1.99	0.43
5:5:120:ASP:OD2	5:5:136:LEU:N	2.44	0.43
5:5:2:ARG:HG3	5:5:84:ASP:OD2	2.18	0.43
10:A:63:VAL:HG11	10:A:115:VAL:HG11	1.99	0.43
10:A:67:LEU:HD23	16:H:310:TRP:NE1	2.33	0.43
3:D:556:ALA:HB2	3:D:562:GLY:HA3	2.00	0.43
4:E:171:ASN:CG	4:E:174:ARG:HH22	2.22	0.43
4:E:202:ASP:OD1	4:E:284:ARG:NE	2.51	0.43
5:F:138:PRO:HB3	6:G:87:LYS:HB2	2.00	0.43
6:G:143:ARG:NE	6:G:145:GLU:OE1	2.52	0.43
13:L:21:GLY:C	13:L:102:SER:HB3	2.38	0.43
13:L:469:LEU:HA	13:L:469:LEU:HD12	1.72	0.43
13:L:562:SER:O	13:L:565:PHE:HB2	2.18	0.43
7:O:139:ASP:N	7:O:139:ASP:OD1	2.42	0.43
13:T:286:PHE:HD2	13:T:416:TYR:HB3	1.83	0.43
15:V:394:GLY:HA2	15:V:395:PRO:HD3	1.85	0.43
2:2:168:LEU:HA	2:2:169:PRO:HD2	1.65	0.43
3:3:19:VAL:O	3:3:23:VAL:HG23	2.18	0.43
5:5:37:GLU:O	5:5:40:HIS:HB3	2.18	0.43
1:B:404:ASP:N	1:B:404:ASP:OD1	2.50	0.43
3:D:279:ALA:HA	3:D:290:ILE:HG12	1.99	0.43
4:E:283:MET:O	4:E:287:VAL:HG23	2.19	0.43
4:E:335:PHE:O	4:E:363:SER:HA	2.19	0.43
16:H:290:PHE:O	16:H:293:ILE:HB	2.17	0.43
8:I:52:THR:HB	8:I:54:ILE:HG22	1.99	0.43
3:D:159:PHE:CE2	8:I:79:LEU:HD13	2.53	0.43
11:J:29:ALA:O	11:J:33:ILE:HG13	2.19	0.43
12:K:59:MET:O	12:K:63:VAL:HG23	2.19	0.43
13:L:321:HIS:HA	13:L:384:SER:CB	2.48	0.43
6:G:17:GLU:HA	10:P:33:PRO:HG3	2.00	0.43
6:G:28:VAL:HA	16:Q:64:ILE:CG2	2.48	0.43
13:T:477:LEU:HA	13:T:477:LEU:HD12	1.73	0.43
15:V:108:LEU:HD22	15:V:148:LEU:HD13	1.99	0.43
15:V:153:LEU:HD12	15:V:178:LEU:HD12	2.00	0.43
15:V:313:ARG:HE	15:V:384:ALA:HB3	1.82	0.43
1:1:343:ASN:O	1:1:346:ARG:HG2	2.18	0.43
2:2:81:GLN:HB3	2:2:122:VAL:HG21	1.99	0.43
4:4:338:PRO:CG	5:5:193:ARG:HD3	2.48	0.43
4:4:400:LEU:HD23	4:4:400:LEU:HA	1.89	0.43
5:5:101:LEU:O	5:5:126:PHE:HA	2.19	0.43
5:5:121:LEU:O	5:5:144:HIS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:34:ASN:HB3	16:H:51:VAL:CG2	2.42	0.43
3:3:159:PHE:CE2	8:7:79:LEU:HD13	2.49	0.43
10:A:74:GLU:O	10:A:78:LEU:HG	2.19	0.43
1:B:98:PRO:HB2	1:B:295:SER:HB2	1.99	0.43
3:D:202:PHE:HB3	3:D:209:THR:HG23	1.99	0.43
4:E:156:ILE:O	4:E:159:LEU:HB2	2.18	0.43
11:J:72:MET:SD	16:H:137:PHE:HD1	2.40	0.43
13:L:295:VAL:O	13:L:298:SER:OG	2.24	0.43
14:M:143:ARG:HD3	14:M:143:ARG:HA	1.81	0.43
14:M:55:LEU:HB3	14:M:61:VAL:O	2.19	0.43
12:K:45:PHE:CD1	15:N:156:GLY:HA2	2.54	0.43
16:Q:194:TRP:HE3	16:Q:196:PHE:HE1	1.67	0.43
16:Q:225:GLU:O	16:Q:299:ARG:NH2	2.43	0.43
16:Q:52:GLY:HA2	16:Q:55:GLY:CA	2.49	0.43
11:R:4:LEU:O	11:R:7:LEU:HB3	2.18	0.43
13:T:454:VAL:HG12	13:T:455:LEU:HD13	1.99	0.43
14:U:141:ARG:HG3	14:U:142:THR:N	2.34	0.43
14:U:331:ARG:HH11	14:U:331:ARG:HA	1.84	0.43
15:V:206:PRO:O	15:V:209:LEU:HB3	2.18	0.43
1:1:334:ARG:NH1	1:1:435:SER:O	2.45	0.43
2:2:106:ILE:HG23	2:2:110:GLU:HB2	1.99	0.43
3:3:249:MET:H	3:3:249:MET:HG2	1.51	0.43
3:3:391:LEU:HD12	3:3:422:PRO:HG3	2.00	0.43
5:5:105:THR:HG21	5:5:130:PRO:HD3	2.00	0.43
7:9:143:THR:O	7:9:147:ARG:HG3	2.19	0.43
1:B:219:ASN:ND2	18:B:502:FMN:O2P	2.51	0.43
3:D:119:CYS:HB2	4:E:324:VAL:HG12	2.00	0.43
3:D:375:THR:HB	3:D:512:LEU:O	2.18	0.43
3:D:381:LEU:HD12	3:D:522:ARG:CD	2.48	0.43
3:D:85:THR:HG22	3:D:86:ALA:O	2.19	0.43
4:E:263:ASP:HB2	4:E:285:GLU:CG	2.47	0.43
5:F:123:GLY:H	5:F:147:ARG:HH11	1.65	0.43
4:E:104:LEU:HA	5:F:22:LEU:CD1	2.49	0.43
16:H:108:PHE:HB3	16:H:112:GLN:H	1.82	0.43
16:H:27:ALA:O	16:H:31:MET:HG2	2.19	0.43
7:9:23:THR:HB	16:H:45:ARG:HD3	2.00	0.43
16:H:67:ILE:O	16:H:68:PHE:HB2	2.18	0.43
11:J:64:VAL:HA	11:J:67:PHE:HB2	2.00	0.43
11:J:4:LEU:O	11:J:7:LEU:HB3	2.18	0.43
11:J:135:TRP:CG	12:K:55:VAL:HG11	2.53	0.43
13:L:438:ALA:HA	13:L:439:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:470:GLU:N	13:L:471:PRO:HD2	2.33	0.43
14:M:114:ASP:CB	14:M:176:LEU:HA	2.49	0.43
13:T:281:GLY:O	13:T:285:ALA:HB2	2.19	0.43
13:T:95:MET:O	13:T:101:TYR:HE1	2.02	0.43
14:U:78:ILE:HG22	14:U:103:GLU:HG3	2.01	0.43
15:V:258:LEU:HA	15:V:258:LEU:HD23	1.85	0.43
1:1:102:LYS:HE2	1:1:222:GLU:OE1	2.19	0.43
4:4:168:PHE:HA	4:4:170:HIS:CE1	2.53	0.43
4:4:327:HIS:CE1	7:9:107:ALA:O	2.72	0.43
1:B:238:PHE:CZ	1:B:248:GLY:HA3	2.53	0.43
1:B:335:VAL:HG22	1:B:436:LEU:HD21	2.01	0.43
2:C:81:GLN:HA	2:C:120:GLN:O	2.19	0.43
3:D:509:ALA:O	3:D:512:LEU:N	2.52	0.43
3:D:713:ARG:HH21	3:D:746:ARG:NH2	2.12	0.43
6:G:104:TRP:CZ2	6:G:173:VAL:HG22	2.54	0.43
11:J:109:TRP:HA	11:J:109:TRP:CE3	2.54	0.43
13:L:315:TYR:O	13:L:319:LEU:HG	2.18	0.43
14:M:194:PHE:HB2	14:M:249:ALA:HB3	1.99	0.43
14:M:91:VAL:CG2	14:M:92:GLU:N	2.80	0.43
15:N:44:TRP:CZ3	15:N:60:GLN:HB3	2.54	0.43
7:O:143:THR:O	7:O:147:ARG:HG3	2.19	0.43
10:P:71:PHE:HZ	10:P:107:PHE:HB2	1.84	0.43
16:Q:276:TYR:HD2	16:Q:280:PHE:HE2	1.66	0.43
14:U:169:LEU:HD21	15:V:358:TRP:CZ2	2.53	0.43
15:V:46:LYS:N	15:V:47:PRO:HD3	2.34	0.43
1:1:284:LEU:HD11	2:2:179:VAL:HB	2.00	0.43
3:3:732:ALA:O	3:3:747:VAL:HG23	2.18	0.43
3:3:714:ALA:HB3	3:3:744:GLU:O	2.19	0.43
4:4:171:ASN:OD1	4:4:174:ARG:NH1	2.50	0.43
4:4:372:ALA:HA	4:4:373:PRO:HD2	1.85	0.43
4:4:232:LEU:CD2	5:5:109:GLY:HA3	2.49	0.43
6:6:57:ARG:HH11	6:6:60:LEU:CD1	2.29	0.43
10:A:93:PHE:CZ	16:H:326:LEU:HD13	2.54	0.43
3:D:260:PRO:HB2	3:D:617:LEU:HB3	2.01	0.43
3:D:46:ARG:NH1	3:D:46:ARG:HG2	2.32	0.43
3:D:305:ARG:HH22	3:D:605:PRO:HA	1.84	0.43
4:E:83:PRO:CB	4:E:169:HIS:HA	2.44	0.43
4:E:222:GLY:HA2	4:E:396:ILE:HD11	2.01	0.43
16:H:186:VAL:HG11	16:H:267:TRP:CZ3	2.53	0.43
16:H:201:PRO:O	16:H:205:VAL:HG13	2.18	0.43
12:K:7:SER:O	12:K:37:ALA:HB1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:450:ALA:O	13:L:453:SER:HB3	2.18	0.43
13:L:54:ARG:CZ	13:L:68:LEU:HD13	2.49	0.43
14:M:80:LEU:HD11	14:M:435:LEU:HG	1.99	0.43
15:N:103:HIS:O	15:N:107:MET:HB2	2.19	0.43
10:P:109:TYR:CD2	11:R:151:VAL:HG22	2.53	0.43
16:Q:221:LEU:HB3	16:Q:222:PRO:CA	2.49	0.43
16:Q:147:TYR:HD1	16:Q:229:VAL:HG22	1.82	0.43
13:T:541:LEU:HA	13:T:545:PRO:HG2	2.00	0.43
14:U:424:ASP:O	14:U:425:LEU:HD12	2.19	0.43
14:U:95:PHE:HB2	14:U:98:LEU:HD12	2.01	0.43
15:V:374:TYR:O	15:V:378:LEU:HD13	2.19	0.43
1:1:162:LEU:HD11	1:1:169:PHE:HB3	2.01	0.43
1:1:336:SER:HB3	1:1:339:ASP:HB2	2.00	0.43
1:1:199:PRO:HG2	17:1:501:SF4:S2	2.59	0.43
3:3:349:ALA:O	3:3:540:ASN:ND2	2.40	0.43
3:3:38:HIS:O	3:3:39:LEU:HD23	2.18	0.43
4:4:85:MET:CE	4:4:370:VAL:HG21	2.48	0.43
5:5:75:VAL:HG12	5:5:76:SER:N	2.33	0.43
1:B:358:PRO:O	1:B:362:GLY:HA3	2.18	0.43
1:B:381:GLU:O	1:B:385:GLU:HG3	2.18	0.43
4:E:213:ILE:HG22	4:E:217:ARG:HG2	2.01	0.43
5:F:31:ARG:NH2	5:F:98:ASP:OD2	2.52	0.43
6:G:17:GLU:HG3	10:P:33:PRO:HA	2.01	0.43
16:H:150:LEU:O	16:H:154:ARG:HG3	2.19	0.43
8:I:12:ALA:O	8:I:15:GLU:HB3	2.19	0.43
11:J:56:VAL:O	11:J:60:ALA:HB3	2.19	0.43
11:J:83:PHE:HB3	11:J:85:PRO:HD3	2.00	0.43
13:L:340:ILE:O	13:L:345:GLY:N	2.45	0.43
13:L:53:ALA:HB3	13:L:69:LEU:HB3	2.00	0.43
15:N:2:THR:HG23	15:N:36:ALA:HB1	2.01	0.43
16:Q:201:PRO:O	16:Q:205:VAL:HG13	2.18	0.43
16:Q:204:LEU:HD23	16:Q:204:LEU:HA	1.86	0.43
16:Q:85:ALA:HB3	16:Q:86:PRO:HD3	2.01	0.43
14:U:9:PRO:HG3	14:U:32:SER:HB2	2.01	0.43
14:U:8:LEU:HD23	14:U:32:SER:HA	2.00	0.43
12:S:45:PHE:CD1	15:V:156:GLY:HA2	2.54	0.43
15:V:422:ALA:O	15:V:423:LEU:HD23	2.18	0.43
1:1:343:ASN:HA	1:1:346:ARG:HG2	2.00	0.43
3:3:305:ARG:HH22	3:3:605:PRO:HA	1.83	0.43
4:4:285:GLU:O	4:4:289:ILE:HG12	2.19	0.43
8:7:45:GLU:H	8:7:45:GLU:CD	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ARG:HA	1:B:261:PRO:HD2	1.91	0.43
2:C:168:LEU:HA	2:C:169:PRO:HD2	1.69	0.43
3:D:143:TYR:HE1	3:D:148:PRO:HD3	1.84	0.43
3:D:337:ARG:HD2	3:D:337:ARG:H	1.82	0.43
4:E:185:GLU:O	4:E:189:GLU:HG2	2.19	0.43
6:G:18:GLY:CA	6:G:28:VAL:HG11	2.48	0.43
10:A:54:VAL:HG22	16:H:146:LYS:HD2	2.00	0.43
16:H:221:LEU:HB3	16:H:222:PRO:CA	2.49	0.43
16:H:39:LEU:CD2	16:H:295:ALA:HB2	2.46	0.43
11:J:100:VAL:O	11:J:104:LEU:HG	2.19	0.43
14:M:242:PHE:CZ	14:M:461:PHE:HD2	2.37	0.43
14:M:33:PHE:HA	14:M:79:ALA:CB	2.47	0.43
16:Q:125:LEU:O	16:Q:128:VAL:HG22	2.19	0.43
13:T:419:ARG:HB2	13:T:512:PHE:HD2	1.79	0.43
14:U:91:VAL:CG2	14:U:92:GLU:N	2.81	0.43
1:1:97:GLU:OE2	1:1:294:GLY:HA3	2.19	0.42
3:3:248:GLU:HG2	5:5:170:PHE:CE1	2.54	0.42
3:3:455:ARG:HA	3:3:459:MET:SD	2.59	0.42
3:3:616:ASN:ND2	3:3:622:LEU:HD11	2.34	0.42
3:3:689:LYS:HG2	3:3:689:LYS:H	1.48	0.42
4:4:317:LEU:HA	4:4:317:LEU:HD12	1.74	0.42
6:6:143:ARG:NE	6:6:145:GLU:OE1	2.52	0.42
7:9:99:ILE:HD12	7:9:99:ILE:HA	1.86	0.42
1:B:203:PRO:HB2	1:B:204:PRO:HD3	2.01	0.42
1:B:51:ASP:OD1	1:B:81:LYS:HE2	2.19	0.42
2:C:85:THR:OG1	2:C:124:CYS:N	2.52	0.42
3:D:7:ASN:CG	3:D:96:LEU:HD12	2.40	0.42
4:E:311:PRO:HD3	4:E:330:HIS:CE1	2.54	0.42
4:E:409:ARG:NH2	5:F:117:GLU:OE2	2.51	0.42
16:H:186:VAL:HA	16:H:189:GLN:NE2	2.34	0.42
16:H:204:LEU:HA	16:H:204:LEU:HD23	1.85	0.42
6:6:76:ASP:HB3	16:H:69:LYS:NZ	2.34	0.42
4:E:315:HIS:HA	8:I:46:ARG:NH1	2.34	0.42
13:L:257:SER:OG	13:L:478:ALA:HA	2.19	0.42
14:M:330:GLY:O	14:M:333:TYR:HB3	2.19	0.42
14:M:324:GLY:O	14:M:432:PHE:HZ	2.02	0.42
13:T:302:GLN:O	13:T:305:TYR:HB2	2.19	0.42
13:T:405:GLY:O	13:T:409:VAL:HG23	2.19	0.42
13:T:323:PHE:CE2	13:T:459:LEU:HD12	2.54	0.42
14:U:109:LEU:HD21	14:U:236:VAL:HG21	2.01	0.42
14:U:146:TYR:O	14:U:150:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:219:GLN:HA	14:U:282:LYS:HG3	2.01	0.42
3:3:227:THR:HG21	3:3:237:ASP:HB2	1.99	0.42
4:4:213:ILE:HG22	4:4:217:ARG:HG2	2.01	0.42
4:4:40:VAL:O	4:4:40:VAL:HG22	2.18	0.42
5:5:185:LYS:HB2	5:5:189:ARG:HG3	2.00	0.42
1:B:433:ARG:HH12	2:C:89:LYS:HE3	1.84	0.42
2:C:106:ILE:HG23	2:C:110:GLU:HB2	2.00	0.42
3:D:185:LYS:HG2	3:D:188:VAL:HG22	2.01	0.42
3:D:282:VAL:HA	3:D:283:PRO:HD2	1.91	0.42
3:D:732:ALA:O	3:D:747:VAL:HG23	2.19	0.42
4:E:155:THR:HB	4:E:193:LEU:CD1	2.49	0.42
5:F:132:LEU:HD23	5:F:132:LEU:HA	1.90	0.42
5:F:10:ALA:HB1	5:F:15:TYR:HB2	2.01	0.42
16:H:159:LEU:HD11	16:H:221:LEU:CD2	2.49	0.42
16:H:276:TYR:HD2	16:H:280:PHE:HE2	1.66	0.42
13:L:39:ALA:HA	13:L:42:LEU:HB2	2.00	0.42
13:L:91:ALA:HB1	13:L:104:PHE:CE2	2.54	0.42
14:M:61:VAL:HG13	14:M:116:LEU:HB3	2.01	0.42
14:M:141:ARG:HG3	14:M:142:THR:N	2.34	0.42
14:M:208:PHE:O	14:M:211:HIS:CE1	2.72	0.42
13:T:178:ALA:HA	14:U:386:LYS:HE2	2.01	0.42
13:T:266:VAL:O	13:T:270:ILE:HG13	2.18	0.42
14:U:114:ASP:HB3	14:U:176:LEU:HD23	2.01	0.42
14:U:88:VAL:HG22	14:U:331:ARG:HG3	2.01	0.42
15:V:40:LEU:HD12	15:V:67:LEU:HD12	2.01	0.42
4:4:217:ARG:CZ	16:H:301:ARG:HB3	2.48	0.42
4:4:224:ILE:HD11	4:4:275:ARG:CZ	2.49	0.42
4:4:107:ALA:HB2	4:4:309:ILE:HD13	2.02	0.42
4:4:342:VAL:HG12	4:4:357:ILE:HB	2.01	0.42
1:B:437:TRP:O	2:C:147:ARG:NH2	2.52	0.42
2:C:79:HIS:ND1	2:C:118:SER:HB2	2.34	0.42
2:C:88:CYS:HB3	2:C:93:ALA:HB2	2.01	0.42
5:F:121:LEU:HA	5:F:145:PRO:HD2	2.00	0.42
6:G:100:PRO:CG	16:Q:69:LYS:HE3	2.49	0.42
11:J:132:TYR:HA	11:J:136:LEU:HD13	2.01	0.42
12:K:17:GLY:O	12:K:21:ARG:HG2	2.19	0.42
12:K:72:LEU:HD23	12:K:72:LEU:HA	1.84	0.42
13:L:404:VAL:O	13:L:408:LEU:HG	2.19	0.42
14:M:388:SER:HA	14:M:389:PRO:HD2	1.74	0.42
10:P:44:TYR:O	10:P:48:ASN:HA	2.18	0.42
16:Q:332:LEU:HB3	16:Q:333:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:13:TYR:HE2	16:Q:98:GLY:HA3	1.83	0.42
12:S:18:VAL:HG13	12:S:27:VAL:HG13	1.99	0.42
12:S:17:GLY:O	12:S:21:ARG:HG2	2.19	0.42
13:T:91:ALA:HB1	13:T:104:PHE:HE2	1.83	0.42
14:U:64:ALA:C	14:U:113:ARG:HB3	2.40	0.42
9:W:89:PHE:CD2	9:W:123:PRO:HB3	2.54	0.42
1:1:145:LEU:HA	1:1:145:LEU:HD23	1.89	0.42
1:1:167:PHE:CE2	1:1:169:PHE:HB2	2.55	0.42
1:1:272:PHE:CE1	1:1:311:MET:HG2	2.54	0.42
1:1:360:ARG:O	1:1:364:ALA:HB3	2.19	0.42
1:1:404:ASP:HA	1:1:407:VAL:HG22	2.01	0.42
1:1:101:PHE:CZ	2:2:129:HIS:HB3	2.54	0.42
3:3:477:LEU:HD22	3:3:517:ALA:O	2.20	0.42
3:3:533:LEU:HD23	3:3:533:LEU:HA	1.72	0.42
3:3:652:PRO:HA	3:3:653:PRO:HD3	1.82	0.42
6:6:96:TRP:HE3	6:6:97:GLU:HG3	1.84	0.42
1:B:356:CYS:O	1:B:360:ARG:HB3	2.19	0.42
3:D:399:LEU:HD22	3:D:477:LEU:HD11	2.01	0.42
5:F:145:PRO:HA	5:F:150:TYR:CD1	2.54	0.42
5:F:41:TYR:HA	5:F:44:MET:HE3	2.01	0.42
16:H:220:ASP:HA	16:H:222:PRO:HB3	2.01	0.42
13:L:146:TYR:HB2	14:M:415:TRP:O	2.20	0.42
13:L:189:LYS:HZ3	13:L:477:LEU:CD1	2.33	0.42
13:L:40:SER:OG	13:L:41:PHE:N	2.52	0.42
14:M:132:MET:SD	14:M:227:ALA:HA	2.59	0.42
14:M:160:LEU:O	14:M:163:VAL:HG12	2.19	0.42
14:M:341:ILE:HG13	14:M:342:GLY:N	2.35	0.42
13:L:586:LEU:HD11	15:N:135:LYS:HA	2.01	0.42
11:J:152:VAL:HG22	15:N:87:LEU:HD22	2.01	0.42
7:O:112:ALA:HB3	17:O:202:SF4:S4	2.58	0.42
7:O:91:TYR:HE1	7:O:93:ILE:HD11	1.85	0.42
10:P:63:VAL:O	10:P:67:LEU:HD13	2.20	0.42
10:P:2:ALA:HB3	16:Q:119:ASP:OD2	2.20	0.42
16:Q:200:PHE:O	16:Q:203:PHE:HB3	2.19	0.42
16:Q:20:VAL:O	16:Q:24:LEU:HD13	2.19	0.42
12:S:60:VAL:HG23	15:V:105:LEU:HD11	2.01	0.42
13:T:146:TYR:HB2	14:U:415:TRP:O	2.20	0.42
1:1:370:LEU:HD12	1:1:387:LEU:HB2	2.02	0.42
3:3:327:LEU:HA	3:3:327:LEU:HD23	1.73	0.42
4:4:138:LEU:HD13	4:4:143:LEU:HA	2.00	0.42
4:4:38:HIS:HE1	4:4:398:ALA:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:31:ARG:NH2	5:5:98:ASP:OD2	2.52	0.42
2:C:147:ARG:HE	2:C:147:ARG:HB2	1.61	0.42
3:D:243:ARG:NH1	3:D:275:LEU:HA	2.35	0.42
4:E:291:LYS:O	4:E:295:GLU:HG3	2.20	0.42
16:H:301:ARG:O	16:H:302:TYR:HD1	2.02	0.42
16:H:83:VAL:O	16:H:86:PRO:HD2	2.20	0.42
8:I:48:TYR:CE2	8:I:50:LEU:HB2	2.54	0.42
11:J:52:GLY:O	11:J:56:VAL:HG23	2.19	0.42
13:L:143:GLY:HA3	14:M:415:TRP:CH2	2.55	0.42
13:L:324:THR:CB	13:L:380:SER:HB2	2.49	0.42
13:L:41:PHE:HB2	13:L:81:THR:HB	2.01	0.42
14:M:75:PHE:CZ	14:M:111:ALA:HB2	2.53	0.42
14:M:426:ALA:HB3	14:M:429:GLU:HG3	2.01	0.42
15:N:45:GLY:C	15:N:47:PRO:HD3	2.39	0.42
11:R:4:LEU:HG	11:R:7:LEU:HD22	2.02	0.42
13:T:291:ILE:O	13:T:295:VAL:HG23	2.18	0.42
13:T:27:PRO:O	13:T:31:VAL:HG23	2.19	0.42
13:T:234:THR:HG21	13:T:337:GLY:CA	2.49	0.42
13:T:404:VAL:O	13:T:408:LEU:HG	2.20	0.42
14:U:341:ILE:HG13	14:U:342:GLY:N	2.35	0.42
14:U:344:TYR:O	14:U:347:LEU:HD21	2.20	0.42
15:V:281:LEU:HA	15:V:281:LEU:HD12	1.82	0.42
15:V:6:LEU:HD13	15:V:93:LEU:HA	2.00	0.42
9:W:78:VAL:HA	9:W:81:LEU:HD12	2.00	0.42
1:1:93:ALA:HB3	1:1:134:VAL:HA	2.00	0.42
1:1:246:SER:HB3	1:1:268:MET:HG2	2.01	0.42
3:3:185:LYS:O	3:3:189:ARG:HB2	2.19	0.42
4:4:379:GLN:OE1	5:5:112:ASN:HB3	2.20	0.42
5:5:64:ARG:HD3	5:5:64:ARG:HA	1.88	0.42
6:6:38:PRO:O	6:6:63:PHE:HD1	2.02	0.42
1:B:101:PHE:H	1:B:253:GLN:HG3	1.84	0.42
3:D:136:GLU:HG2	5:F:186:GLY:O	2.19	0.42
3:D:381:LEU:HD12	3:D:522:ARG:HD3	2.00	0.42
3:D:713:ARG:NH2	3:D:746:ARG:HH21	2.15	0.42
4:E:329:LYS:HA	4:E:329:LYS:HD2	1.82	0.42
4:E:254:TYR:CE2	4:E:346:THR:HA	2.54	0.42
4:E:57:PRO:HD3	4:E:382:PRO:HG3	2.00	0.42
5:F:116:ARG:HG2	5:F:132:LEU:HD23	2.00	0.42
6:G:17:GLU:CG	10:P:33:PRO:HA	2.50	0.42
16:H:153:LEU:HD23	16:H:153:LEU:HA	1.73	0.42
12:K:49:TYR:CD1	15:N:159:GLY:HA2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:373:LEU:HD21	13:L:416:TYR:HE1	1.85	0.42
14:M:424:ASP:O	14:M:425:LEU:HD12	2.20	0.42
14:M:73:LEU:HD23	14:M:73:LEU:H	1.85	0.42
15:N:260:TYR:HA	15:N:263:ILE:HD12	2.00	0.42
16:Q:161:SER:O	16:Q:164:LEU:HB3	2.19	0.42
12:S:71:GLY:HA3	15:V:137:PHE:CZ	2.55	0.42
13:T:105:PHE:HA	13:T:108:PHE:HB2	2.02	0.42
15:V:52:PRO:HB3	15:V:103:HIS:HB2	2.00	0.42
1:1:397:ARG:H	1:1:397:ARG:HD2	1.84	0.42
2:2:81:GLN:HB3	2:2:122:VAL:CG2	2.50	0.42
3:3:143:TYR:HE1	3:3:148:PRO:HD3	1.84	0.42
3:3:339:GLU:OE1	3:3:339:GLU:N	2.52	0.42
5:5:72:TYR:OH	5:5:126:PHE:HE2	2.02	0.42
6:6:147:LEU:O	6:6:151:VAL:HG13	2.19	0.42
7:9:100:PHE:HA	17:9:201:SF4:S4	2.60	0.42
7:9:59:CYS:SG	7:9:91:TYR:OH	2.71	0.42
1:B:394:ILE:HG22	1:B:403:ALA:HB1	2.01	0.42
18:B:502:FMN:N1	18:B:502:FMN:O3'	2.37	0.42
1:B:174:HIS:CE1	2:C:29:PRO:HD3	2.54	0.42
3:D:227:THR:HG21	3:D:237:ASP:HB2	2.01	0.42
3:D:459:MET:HG2	3:D:465:HIS:CB	2.47	0.42
16:H:52:GLY:HA2	16:H:55:GLY:N	2.33	0.42
13:L:20:PHE:HD1	13:L:23:ARG:HE	1.67	0.42
13:L:25:ARG:CG	13:L:28:LEU:HB2	2.50	0.42
15:N:279:GLN:HG2	15:N:420:LEU:HD12	2.01	0.42
10:P:67:LEU:HD23	16:Q:310:TRP:NE1	2.35	0.42
13:T:49:LEU:HD23	13:T:49:LEU:HA	1.94	0.42
13:T:519:ALA:HB3	13:T:520:TRP:CE3	2.55	0.42
14:U:143:ARG:HA	14:U:143:ARG:HD3	1.75	0.42
14:U:27:LEU:O	14:U:31:LEU:HD13	2.20	0.42
13:T:156:ARG:HG3	14:U:407:LEU:HB3	2.02	0.42
14:U:85:GLY:HA2	14:U:327:LEU:HD22	2.00	0.42
15:V:101:THR:HG21	15:V:106:LEU:HD23	2.02	0.42
2:2:66:PHE:O	3:3:205:ARG:NE	2.53	0.42
4:4:171:ASN:CG	4:4:174:ARG:HH22	2.23	0.42
4:4:197:LEU:N	4:4:198:PRO:HD2	2.34	0.42
4:4:90:SER:O	4:4:93:HIS:HB2	2.20	0.42
5:5:112:ASN:O	5:5:129:HIS:NE2	2.53	0.42
6:6:94:ARG:O	6:6:98:GLN:N	2.49	0.42
1:B:402:LEU:HD13	17:B:501:SF4:S1	2.60	0.42
3:D:361:ALA:CB	3:D:369:LEU:HD23	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:559:ASP:OD2	3:D:686:LYS:NZ	2.52	0.42
6:6:76:ASP:H	16:H:65:LYS:HZ1	1.66	0.42
6:6:76:ASP:HB3	16:H:69:LYS:HZ3	1.84	0.42
14:M:10:VAL:HG23	14:M:104:GLY:HA3	2.02	0.42
15:N:46:LYS:N	15:N:47:PRO:HD3	2.35	0.42
15:N:29:THR:HG21	15:N:85:TYR:HB3	2.01	0.42
16:Q:16:LYS:NZ	16:Q:114:TRP:O	2.40	0.42
16:Q:260:PRO:HG3	16:Q:286:PHE:CD2	2.54	0.42
11:R:25:ALA:HB2	12:S:26:LEU:HD11	2.01	0.42
13:T:325:HIS:HA	13:T:328:PHE:CE2	2.55	0.42
13:T:37:VAL:HG21	13:T:88:HIS:CE1	2.55	0.42
13:T:88:HIS:O	13:T:92:ILE:HG13	2.20	0.42
14:U:296:ALA:HB2	14:U:314:LEU:CD2	2.49	0.42
15:V:241:VAL:HG12	15:V:245:ASN:ND2	2.34	0.42
15:V:24:GLY:HA2	15:V:27:ARG:HD2	2.01	0.42
9:W:21:LEU:HD11	9:W:26:LEU:HD21	2.02	0.42
1:1:112:HIS:HA	1:1:115:ILE:HD12	2.00	0.42
3:3:168:HIS:HA	3:3:169:PRO:HD2	1.86	0.42
3:3:17:THR:HG22	3:3:18:SER:O	2.20	0.42
3:3:501:LYS:N	3:3:501:LYS:HD2	2.25	0.42
3:3:689:LYS:HG3	3:3:771:VAL:HA	2.01	0.42
5:5:112:ASN:O	5:5:129:HIS:CE1	2.73	0.42
5:5:105:THR:HG21	5:5:130:PRO:CD	2.50	0.42
5:5:121:LEU:HD13	5:5:146:LEU:HD12	2.01	0.42
6:6:22:THR:O	6:6:26:LYS:HG2	2.19	0.42
1:B:37:GLY:O	1:B:38:TYR:HB2	2.19	0.42
3:D:132:ASP:O	3:D:136:GLU:HG3	2.19	0.42
4:E:63:HIS:O	6:G:122:ALA:HB1	2.20	0.42
5:F:180:GLY:HA3	5:F:189:ARG:HH22	1.85	0.42
6:G:37:TRP:HB2	6:G:76:ASP:OD1	2.20	0.42
16:H:216:ARG:HG3	16:H:219:PHE:CE1	2.54	0.42
16:H:216:ARG:C	16:H:218:PRO:HD3	2.40	0.42
8:I:10:TYR:O	8:I:14:VAL:HG23	2.20	0.42
11:J:156:LEU:HA	11:J:156:LEU:HD12	1.93	0.42
12:K:78:ILE:CD1	15:N:134:LEU:HB2	2.50	0.42
13:L:163:ARG:NE	14:M:399:VAL:HB	2.33	0.42
15:N:241:VAL:HG12	15:N:367:THR:OG1	2.20	0.42
7:O:67:ALA:HB2	7:O:97:ARG:HB3	2.02	0.42
10:P:1:MET:HG2	10:P:2:ALA:H	1.85	0.42
6:G:72:PRO:HG3	10:P:44:TYR:CE1	2.55	0.42
16:Q:136:ILE:HD12	16:Q:159:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:138:LEU:HD23	16:Q:138:LEU:HA	1.93	0.42
16:Q:213:GLU:N	16:Q:213:GLU:OE1	2.52	0.42
16:Q:332:LEU:HB3	16:Q:333:PRO:CD	2.49	0.42
13:T:554:PHE:HD2	14:U:277:ALA:HB3	1.85	0.42
15:V:104:LEU:HD21	15:V:163:LEU:HD21	2.00	0.42
15:V:17:GLY:HA3	15:V:82:PHE:CD2	2.54	0.42
9:X:106:PRO:HA	9:X:107:PRO:HD3	1.90	0.42
9:X:89:PHE:CD2	9:X:123:PRO:HB3	2.55	0.42
4:4:129:HIS:CE1	4:4:349:ALA:HB1	2.55	0.42
4:4:36:SER:HB2	16:H:226:GLN:HA	2.02	0.42
5:5:38:MET:HE2	5:5:104:VAL:HG11	2.00	0.42
5:5:77:LEU:HA	5:5:78:PRO:HD3	1.67	0.42
6:6:37:TRP:HB2	6:6:76:ASP:OD1	2.20	0.42
6:6:162:ALA:HB1	7:9:124:TYR:CZ	2.54	0.42
10:A:81:TYR:CE2	10:A:96:VAL:HG11	2.55	0.42
1:B:344:LEU:O	1:B:347:PHE:HB3	2.20	0.42
15:N:345:LYS:HB3	15:N:349:PHE:CE2	2.55	0.42
7:O:101:CYS:HB2	7:O:103:LEU:H	1.85	0.42
11:R:59:TYR:CD1	11:R:63:ILE:HD12	2.55	0.42
13:T:278:ALA:HB1	13:T:409:VAL:HG11	2.02	0.42
14:U:181:LEU:HD21	14:U:247:PRO:HB2	2.02	0.42
13:T:554:PHE:HE2	14:U:278:ALA:HA	1.85	0.42
1:1:273:ARG:O	1:1:277:TYR:HB2	2.19	0.41
2:2:78:TYR:CE2	2:2:157:LEU:HB3	2.55	0.41
3:3:591:HIS:ND1	3:3:593:LEU:HB2	2.35	0.41
3:3:651:ARG:HA	3:3:652:PRO:HD2	1.91	0.41
3:3:713:ARG:NH2	3:3:746:ARG:HH21	2.14	0.41
4:4:291:LYS:O	4:4:295:GLU:HG3	2.20	0.41
4:4:48:SER:H	4:4:53:LEU:HD23	1.85	0.41
5:5:49:LEU:HD21	5:5:52:ILE:HD11	2.01	0.41
6:6:108:MET:HA	6:6:137:VAL:CG1	2.50	0.41
6:6:38:PRO:HB3	6:6:79:ILE:HD12	2.02	0.41
6:6:84:LEU:HD22	6:6:88:MET:HG3	2.01	0.41
2:C:46:ILE:HG23	2:C:60:VAL:CG1	2.46	0.41
3:D:118:ASP:O	3:D:122:CYS:N	2.53	0.41
3:D:356:LEU:HD22	3:D:638:LEU:HD12	2.01	0.41
3:D:462:ALA:O	3:D:465:HIS:ND1	2.53	0.41
5:F:82:ASP:N	5:F:82:ASP:OD1	2.51	0.41
13:L:286:PHE:HB2	13:L:419:ARG:CD	2.50	0.41
13:L:325:HIS:CD2	13:L:329:LYS:HG3	2.55	0.41
13:L:592:LEU:HB3	15:N:194:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:304:THR:HA	14:M:305:PRO:HD2	1.74	0.41
12:K:45:PHE:CG	15:N:156:GLY:HA2	2.54	0.41
7:O:6:LEU:HB3	16:Q:297:TRP:CZ2	2.55	0.41
15:V:380:LEU:HA	15:V:380:LEU:HD23	1.90	0.41
1:1:206:PRO:HA	1:1:209:SER:O	2.19	0.41
2:2:46:ILE:HG23	2:2:60:VAL:CG1	2.45	0.41
4:4:202:ASP:O	4:4:206:ALA:N	2.47	0.41
5:5:101:LEU:HA	5:5:102:PRO:HD2	1.90	0.41
5:5:121:LEU:HD13	5:5:146:LEU:CD1	2.50	0.41
4:4:245:ASN:O	5:5:79:GLY:HA3	2.20	0.41
6:6:100:PRO:O	6:6:103:LYS:HD3	2.20	0.41
6:6:165:GLU:OE2	7:9:148:ARG:NH1	2.52	0.41
6:6:57:ARG:HG3	6:6:57:ARG:NH1	2.24	0.41
8:7:24:ALA:HB2	8:7:31:PHE:HB2	2.01	0.41
1:B:89:LEU:HD13	1:B:125:ILE:HD11	2.01	0.41
1:B:17:LEU:HD22	1:B:113:LEU:HD21	2.00	0.41
1:B:102:LYS:HE2	1:B:222:GLU:OE1	2.21	0.41
1:B:267:PRO:O	1:B:270:THR:HG23	2.20	0.41
3:D:648:LEU:HA	3:D:648:LEU:HD23	1.75	0.41
16:H:216:ARG:NH1	16:H:294:ARG:HB3	2.35	0.41
11:J:108:LEU:O	11:J:111:LEU:HB3	2.21	0.41
13:L:66:SER:O	13:L:122:ASP:N	2.25	0.41
14:M:20:LEU:HA	14:M:21:PRO:HA	1.80	0.41
15:N:272:ALA:O	15:N:276:GLY:N	2.52	0.41
7:O:40:ARG:HB2	7:O:121:MET:HE1	2.01	0.41
7:O:46:HIS:NE2	7:O:52:LYS:HA	2.35	0.41
15:V:207:VAL:O	15:V:210:PHE:HB3	2.19	0.41
15:V:44:TRP:CZ3	15:V:60:GLN:HB3	2.55	0.41
3:3:282:VAL:HA	3:3:283:PRO:HD2	1.94	0.41
3:3:472:GLU:O	3:3:476:ILE:HD12	2.20	0.41
3:3:654:PHE:CD1	3:3:654:PHE:N	2.87	0.41
4:4:103:LYS:HE3	4:4:103:LYS:HB3	1.81	0.41
4:4:240:ARG:HB2	4:4:266:LEU:HD23	2.01	0.41
4:4:74:THR:HG22	4:4:75:TYR:N	2.36	0.41
7:9:97:ARG:HD3	7:9:97:ARG:HA	1.32	0.41
10:A:9:GLY:O	10:A:12:ILE:HB	2.20	0.41
3:D:719:HIS:HA	3:D:720:PRO:HD3	1.97	0.41
3:D:454:TYR:HB2	3:D:752:ASP:OD2	2.21	0.41
6:G:137:VAL:HA	6:G:138:PRO:HD2	1.82	0.41
16:H:260:PRO:HB3	16:H:282:LYS:HD3	2.02	0.41
8:I:86:LEU:HA	8:I:87:PRO:HD2	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:134:TYR:HB2	14:M:145:LEU:CD1	2.50	0.41
14:M:22:ARG:HG3	14:M:92:GLU:HG3	2.02	0.41
14:M:82:VAL:HG22	14:M:230:LEU:HG	2.02	0.41
15:N:241:VAL:HG12	15:N:245:ASN:ND2	2.34	0.41
7:O:101:CYS:N	17:O:201:SF4:S4	2.93	0.41
16:Q:58:GLN:O	16:Q:58:GLN:HG3	2.20	0.41
13:T:450:ALA:O	13:T:453:SER:HB3	2.19	0.41
15:V:326:PHE:HE2	15:V:378:LEU:HB3	1.86	0.41
4:4:156:ILE:O	4:4:159:LEU:HB2	2.19	0.41
4:4:385:CYS:HA	4:4:396:ILE:HD13	2.02	0.41
4:4:332:THR:HB	5:5:172:ALA:HB1	2.02	0.41
6:6:39:ALA:HB2	6:6:75:ALA:HB3	2.02	0.41
10:A:41:LEU:O	16:H:74:VAL:HG13	2.20	0.41
1:B:370:LEU:HD12	1:B:387:LEU:HB2	2.03	0.41
3:D:121:THR:HA	7:O:86:ARG:HD3	2.02	0.41
3:D:501:LYS:N	3:D:501:LYS:HD2	2.25	0.41
5:F:157:THR:O	5:F:158:LEU:HD23	2.21	0.41
6:G:35:SER:O	6:G:36:LEU:C	2.57	0.41
16:H:218:PRO:HB3	16:H:305:LEU:CD1	2.50	0.41
8:I:15:GLU:O	8:I:18:SER:HB3	2.20	0.41
13:L:325:HIS:HA	13:L:328:PHE:CE2	2.56	0.41
14:M:85:GLY:HA2	14:M:327:LEU:CD2	2.50	0.41
15:N:228:ALA:HA	15:N:229:PRO:HD3	1.64	0.41
7:O:155:LYS:HA	7:O:155:LYS:HD2	1.91	0.41
16:Q:218:PRO:HB3	16:Q:305:LEU:HD13	2.02	0.41
14:U:304:THR:HA	14:U:305:PRO:HD2	1.74	0.41
14:U:82:VAL:HG13	14:U:230:LEU:HD11	2.02	0.41
14:U:9:PRO:HG2	14:U:107:LEU:HD12	2.03	0.41
1:1:238:PHE:CZ	1:1:248:GLY:HA3	2.56	0.41
1:1:298:PRO:HB3	1:1:412:GLY:HA3	2.03	0.41
1:1:347:PHE:CE2	2:2:123:GLU:HB3	2.55	0.41
3:3:46:ARG:O	3:3:49:LEU:HG	2.20	0.41
3:3:704:ALA:HB2	3:3:712:ALA:HB3	2.03	0.41
5:5:48:PHE:CZ	5:5:50:ALA:HA	2.56	0.41
6:6:18:GLY:CA	6:6:28:VAL:HG11	2.50	0.41
6:6:35:SER:O	6:6:36:LEU:C	2.57	0.41
6:6:82:GLY:HA2	17:6:201:SF4:S4	2.61	0.41
4:E:122:GLU:O	4:E:126:LEU:HG	2.20	0.41
4:E:248:VAL:HB	4:E:347:GLU:HB2	2.03	0.41
4:E:385:CYS:HA	4:E:396:ILE:HD13	2.03	0.41
16:H:166:LEU:HD22	16:H:206:TYR:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:128:PHE:HB2	13:L:173:MET:HE1	2.03	0.41
10:P:2:ALA:CB	16:Q:119:ASP:HB3	2.50	0.41
16:Q:216:ARG:NH1	16:Q:294:ARG:HB3	2.36	0.41
11:R:108:LEU:HD22	12:S:4:LEU:HB3	2.01	0.41
13:T:91:ALA:HB1	13:T:104:PHE:CE2	2.55	0.41
14:U:325:LEU:HG	14:U:361:LEU:HD23	2.02	0.41
15:V:203:SER:HB2	15:V:208:VAL:HG22	2.02	0.41
15:V:241:VAL:HG12	15:V:245:ASN:HD21	1.86	0.41
15:V:83:GLU:HA	15:V:86:LEU:HB2	2.02	0.41
1:1:259:LYS:HE3	1:1:260:ARG:HH21	1.86	0.41
1:1:381:GLU:CD	1:1:426:ARG:HH21	2.24	0.41
2:2:77:LYS:HB3	2:2:116:LEU:HB2	2.03	0.41
3:3:81:ALA:HB3	3:3:84:VAL:CG2	2.51	0.41
7:9:17:LEU:HA	16:H:41:ARG:O	2.20	0.41
7:9:99:ILE:HG22	7:9:101:CYS:SG	2.61	0.41
1:B:17:LEU:HD12	1:B:251:LEU:HD11	2.03	0.41
1:B:291:ILE:HA	1:B:292:PRO:HD2	1.91	0.41
1:B:300:LEU:HD21	1:B:321:SER:HB2	2.02	0.41
3:D:327:LEU:HD23	3:D:327:LEU:HA	1.84	0.41
3:D:545:GLU:HA	3:D:550:LEU:HD11	2.02	0.41
4:E:346:THR:HG22	4:E:353:LEU:O	2.21	0.41
4:E:30:VAL:HG13	4:E:35:PRO:HD2	2.03	0.41
5:F:37:GLU:O	5:F:40:HIS:HB3	2.20	0.41
6:G:171:PRO:HA	6:G:172:PRO:HD3	1.89	0.41
16:H:309:GLY:HA2	16:H:313:LEU:HB2	2.03	0.41
12:K:23:THR:OG1	12:K:26:LEU:HD13	2.20	0.41
13:L:107:TYR:HB3	13:L:141:LEU:HG	2.03	0.41
13:L:267:SER:HB3	13:L:311:GLY:O	2.21	0.41
13:L:562:SER:HA	13:L:565:PHE:CD2	2.56	0.41
14:M:134:TYR:CE2	15:N:383:PHE:HB2	2.55	0.41
14:M:47:VAL:HG13	14:M:50:ALA:HB2	2.03	0.41
15:N:201:GLN:HA	15:N:255:LYS:HE3	2.02	0.41
14:M:150:LEU:HD21	15:N:372:ALA:HB3	2.02	0.41
16:Q:108:PHE:O	16:Q:109:PHE:HB2	2.20	0.41
14:U:88:VAL:HG11	14:U:432:PHE:CD1	2.56	0.41
15:V:231:GLU:CD	15:V:231:GLU:H	2.24	0.41
1:1:107:LEU:HB3	1:1:141:ALA:HB1	2.02	0.41
1:1:260:ARG:O	1:1:264:TYR:OH	2.29	0.41
1:1:371:PHE:CE2	1:1:421:TYR:HE2	2.38	0.41
3:3:21:ASP:OD1	3:3:432:PHE:N	2.38	0.41
4:4:173:ILE:HA	4:4:178:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:82:ASP:N	5:5:82:ASP:OD1	2.51	0.41
4:4:168:PHE:CE1	6:6:141:PRO:HG3	2.55	0.41
7:9:113:ILE:HD12	7:9:113:ILE:HA	1.94	0.41
2:C:15:PHE:HE1	2:C:23:ARG:HB3	1.86	0.41
3:D:701:ALA:HB2	3:D:763:LEU:HB2	2.02	0.41
6:G:147:LEU:O	6:G:151:VAL:HG13	2.20	0.41
8:I:108:ILE:N	8:I:108:ILE:HD12	2.36	0.41
11:J:46:LEU:HD11	12:K:3:TYR:CG	2.56	0.41
13:L:80:VAL:HG22	13:L:243:ALA:O	2.20	0.41
14:M:16:LEU:HB3	14:M:97:GLY:CA	2.51	0.41
16:Q:67:ILE:O	16:Q:68:PHE:HB2	2.20	0.41
11:R:83:PHE:HB3	11:R:85:PRO:CD	2.51	0.41
14:U:79:ALA:HA	14:U:103:GLU:OE1	2.20	0.41
14:U:106:LEU:O	14:U:109:LEU:HB3	2.21	0.41
11:R:138:VAL:HG22	15:V:106:LEU:HB2	2.01	0.41
1:1:199:PRO:O	1:1:399:PHE:HE2	2.04	0.41
2:2:7:LYS:H	2:2:7:LYS:HD2	1.84	0.41
3:3:80:ALA:HB1	3:3:85:THR:OG1	2.21	0.41
4:4:84:ARG:NE	4:4:169:HIS:HB3	2.36	0.41
4:4:75:TYR:CZ	4:4:337:PRO:HG2	2.56	0.41
8:7:14:VAL:HG21	8:7:51:PRO:HB2	2.01	0.41
1:B:134:VAL:HG22	1:B:175:ARG:HG2	2.03	0.41
3:D:370:ASP:OD2	3:D:558:TRP:HD1	2.03	0.41
4:E:171:ASN:OD1	4:E:174:ARG:NH1	2.49	0.41
5:F:137:THR:CG2	5:F:145:PRO:HG3	2.51	0.41
6:G:115:GLY:HA2	6:G:125:GLN:HA	2.02	0.41
12:K:47:ARG:HE	12:K:47:ARG:HB3	1.60	0.41
13:L:122:ASP:OD1	13:L:186:SER:HB3	2.21	0.41
13:L:17:LEU:HD21	13:L:32:LEU:HD12	2.02	0.41
14:M:190:ALA:HB1	14:M:249:ALA:HB1	2.03	0.41
14:M:68:ASP:O	14:M:72:ALA:HB2	2.19	0.41
15:N:261:SER:OG	15:N:375:TYR:OH	2.25	0.41
15:N:416:PRO:C	15:N:418:LEU:H	2.23	0.41
16:Q:127:ALA:O	16:Q:131:LEU:HG	2.21	0.41
16:Q:158:SER:HB2	16:Q:305:LEU:HD23	2.03	0.41
11:R:46:LEU:HD11	12:S:3:TYR:CG	2.56	0.41
10:P:66:MET:HA	11:R:66:LEU:HD22	2.03	0.41
13:T:163:ARG:HD3	14:U:399:VAL:O	2.20	0.41
14:U:452:ARG:O	14:U:456:PRO:HD3	2.20	0.41
15:V:126:ARG:O	15:V:129:GLY:N	2.52	0.41
1:1:437:TRP:HB3	2:2:92:GLY:CA	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:208:PHE:HE1	16:H:298:PHE:CE2	2.39	0.41
4:4:390:VAL:HB	4:4:391:PRO:HD3	2.01	0.41
6:6:32:ARG:O	6:6:36:LEU:N	2.53	0.41
7:9:44:THR:HA	7:9:138:VAL:HG13	2.03	0.41
2:C:91:ALA:HB1	2:C:132:PRO:HD3	2.03	0.41
3:D:48:CYS:SG	3:D:83:CYS:HB3	2.60	0.41
4:E:140:LEU:HD21	4:E:217:ARG:HH12	1.85	0.41
4:E:208:PHE:HE1	16:Q:298:PHE:HE2	1.68	0.41
6:G:140:CYS:SG	7:O:99:ILE:HG13	2.60	0.41
16:H:269:MET:SD	16:H:282:LYS:HE3	2.60	0.41
8:I:61:ASP:HB3	8:I:127:ALA:HB1	2.02	0.41
12:K:4:LEU:HD12	12:K:41:SER:HA	2.03	0.41
13:L:183:LEU:HA	13:L:183:LEU:HD23	1.78	0.41
13:L:454:VAL:HG12	13:L:455:LEU:HD13	2.02	0.41
14:M:75:PHE:HA	14:M:107:LEU:CD2	2.51	0.41
15:N:104:LEU:HD23	15:N:104:LEU:HA	1.86	0.41
7:O:10:LEU:O	16:Q:292:TRP:HZ2	2.04	0.41
10:P:83:VAL:HG23	10:P:84:SER:H	1.85	0.41
16:Q:64:ILE:O	16:Q:67:ILE:O	2.39	0.41
16:Q:86:PRO:HG2	16:Q:240:LYS:HD2	2.02	0.41
14:U:86:ALA:O	14:U:96:LEU:HD11	2.21	0.41
9:X:7:ARG:NH2	9:X:100:THR:HA	2.35	0.41
2:2:78:TYR:CE1	2:2:157:LEU:HD22	2.55	0.41
3:3:286:ASN:ND2	3:3:289:TRP:O	2.54	0.41
3:3:695:ARG:HA	3:3:696:PRO:HD2	1.95	0.41
4:4:214:PHE:HA	4:4:217:ARG:HB2	2.03	0.41
4:4:332:THR:OG1	4:4:333:GLU:N	2.53	0.41
5:5:112:ASN:HA	5:5:129:HIS:NE2	2.36	0.41
1:B:16:THR:HG21	1:B:229:PRO:HB3	2.03	0.41
1:B:253:GLN:O	1:B:327:GLY:HA2	2.21	0.41
3:D:401:ASP:O	3:D:405:GLU:HG3	2.21	0.41
4:E:103:LYS:HB3	4:E:103:LYS:HE3	1.81	0.41
6:G:108:MET:HA	6:G:137:VAL:CG1	2.51	0.41
16:H:259:ILE:HB	16:H:260:PRO:HD3	2.02	0.41
13:L:17:LEU:O	13:L:102:SER:HB2	2.21	0.41
13:L:27:PRO:O	13:L:31:VAL:HG23	2.21	0.41
13:L:33:ALA:HB2	13:L:105:PHE:HB3	2.02	0.41
13:L:490:GLU:O	13:L:494:ILE:HG12	2.21	0.41
14:M:438:LEU:HD12	14:M:438:LEU:HA	1.74	0.41
14:M:36:ASN:HB3	14:M:75:PHE:HB3	2.02	0.41
14:M:9:PRO:HG3	14:M:32:SER:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:165:GLU:HG2	7:O:148:ARG:NH1	2.36	0.41
10:P:61:PHE:HE1	16:Q:302:TYR:OH	2.04	0.41
13:T:373:LEU:HD21	13:T:416:TYR:HE1	1.86	0.41
13:T:553:LEU:HB2	14:U:274:VAL:HG22	2.02	0.41
14:U:422:VAL:HG12	14:U:423:LYS:N	2.36	0.41
14:U:5:ALA:HB1	14:U:36:ASN:HD21	1.86	0.41
15:V:291:ALA:O	15:V:294:LEU:HB3	2.21	0.41
1:1:29:LEU:O	1:1:33:LEU:HG	2.21	0.41
3:3:290:ILE:HA	3:3:290:ILE:HD13	1.84	0.41
3:3:41:PRO:HB2	3:3:84:VAL:HG13	2.02	0.41
5:5:132:LEU:HA	5:5:132:LEU:HD23	1.91	0.41
6:6:115:GLY:HA2	6:6:125:GLN:HA	2.03	0.41
6:6:34:ASN:HA	6:6:155:GLN:HE21	1.86	0.41
6:6:51:MET:HA	6:6:54:THR:HG23	2.03	0.41
8:7:9:LEU:HD11	8:7:82:ILE:HG22	2.03	0.41
1:B:336:SER:HB3	1:B:339:ASP:HB2	2.03	0.41
2:C:14:THR:HG22	2:C:17:LYS:HZ1	1.85	0.41
3:D:112:LEU:HD22	4:E:321:MET:CG	2.51	0.41
3:D:391:LEU:HD12	3:D:422:PRO:HG3	2.03	0.41
16:H:108:PHE:O	16:H:108:PHE:CG	2.73	0.41
16:H:138:LEU:HD23	16:H:138:LEU:HA	1.95	0.41
10:A:83:VAL:HB	11:J:125:GLN:OE1	2.21	0.41
15:N:103:HIS:HB3	15:N:106:LEU:HB3	2.03	0.41
15:N:362:VAL:O	15:N:366:VAL:HG23	2.21	0.41
16:Q:243:LEU:O	16:Q:246:MET:HB3	2.21	0.41
12:S:81:HIS:HD2	12:S:81:HIS:H	1.63	0.41
13:T:129:ILE:HG12	14:U:369:PRO:HB2	2.03	0.41
14:U:20:LEU:HA	14:U:21:PRO:HA	1.81	0.41
14:U:22:ARG:HG3	14:U:92:GLU:HG3	2.03	0.41
14:U:30:GLY:O	14:U:34:LEU:HG	2.21	0.41
14:U:302:SER:O	14:U:387:ALA:HB2	2.21	0.41
15:V:231:GLU:O	15:V:234:ALA:HB3	2.21	0.41
9:X:58:LEU:HD22	9:X:110:LEU:HD21	2.03	0.41
1:1:373:LYS:CG	1:1:378:GLN:HB2	2.51	0.40
3:3:381:LEU:HD12	3:3:522:ARG:CD	2.52	0.40
3:3:381:LEU:HD13	3:3:680:LEU:O	2.21	0.40
4:4:130:LEU:HD22	4:4:149:ALA:HA	2.03	0.40
4:4:315:HIS:HA	8:7:46:ARG:NH1	2.35	0.40
1:B:40:THR:HA	1:B:43:ARG:HG2	2.03	0.40
2:C:24:ARG:HD2	2:C:55:THR:HB	2.02	0.40
3:D:19:VAL:HG22	3:D:87:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:449:ALA:HA	3:D:464:ILE:O	2.22	0.40
3:D:543:GLY:CA	3:D:615:VAL:HB	2.51	0.40
3:D:81:ALA:HB3	3:D:84:VAL:HG22	2.03	0.40
4:E:342:VAL:HG12	4:E:357:ILE:HB	2.03	0.40
4:E:40:VAL:O	4:E:40:VAL:HG22	2.20	0.40
4:E:50:GLU:OE2	16:Q:154:ARG:NH2	2.48	0.40
8:I:24:ALA:HB2	8:I:31:PHE:HB2	2.03	0.40
8:I:40:PHE:O	8:I:43:ARG:HD3	2.21	0.40
8:I:75:ARG:C	8:I:80:LYS:HZ1	2.24	0.40
12:K:14:GLY:O	12:K:30:SER:HB3	2.21	0.40
13:L:499:ALA:O	13:L:503:LEU:HG	2.21	0.40
10:P:20:ILE:HD12	16:Q:21:VAL:HG11	2.03	0.40
16:Q:66:SER:O	16:Q:69:LYS:HB3	2.21	0.40
14:U:62:TYR:HE2	14:U:174:THR:HG21	1.85	0.40
14:U:452:ARG:HA	14:U:452:ARG:HD3	1.78	0.40
15:V:183:LEU:HD13	15:V:226:VAL:HG21	2.03	0.40
9:X:74:LEU:HD12	9:X:77:LEU:HD23	2.03	0.40
1:1:40:THR:HA	1:1:43:ARG:HG2	2.03	0.40
2:2:132:PRO:HG2	2:2:145:VAL:O	2.21	0.40
5:5:123:GLY:H	5:5:147:ARG:NH1	2.19	0.40
5:5:137:THR:HG21	5:5:145:PRO:HG3	2.03	0.40
6:6:89:ALA:N	6:6:90:PRO:HD2	2.35	0.40
8:7:12:ALA:O	8:7:15:GLU:HB3	2.21	0.40
7:9:54:ILE:HG21	8:7:41:ILE:HG23	2.03	0.40
1:B:189:MET:O	1:B:193:GLU:HB2	2.21	0.40
3:D:341:VAL:HA	3:D:565:TYR:O	2.21	0.40
3:D:385:ALA:O	3:D:533:LEU:HD21	2.21	0.40
4:E:197:LEU:HA	4:E:200:ARG:HB2	2.03	0.40
5:F:178:ASP:O	5:F:185:LYS:HE2	2.21	0.40
6:G:76:ASP:H	16:Q:65:LYS:HZ1	1.69	0.40
13:L:255:ARG:HA	13:L:255:ARG:HD2	1.91	0.40
13:L:286:PHE:HD2	13:L:416:TYR:HB3	1.87	0.40
14:M:64:ALA:HB1	14:M:113:ARG:HB3	2.03	0.40
14:M:95:PHE:C	14:M:97:GLY:N	2.73	0.40
7:O:67:ALA:O	7:O:93:ILE:HA	2.22	0.40
10:P:65:ALA:O	10:P:69:ILE:HG23	2.21	0.40
10:P:81:TYR:CE2	10:P:96:VAL:HG11	2.56	0.40
13:T:131:TRP:HH2	13:T:212:GLY:C	2.24	0.40
14:U:398:SER:O	14:U:402:SER:N	2.43	0.40
1:1:331:ILE:HA	1:1:332:PRO:HD2	1.75	0.40
4:4:174:ARG:N	4:4:177:GLY:O	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:123:GLY:HA2	5:5:144:HIS:CE1	2.57	0.40
5:5:121:LEU:HA	5:5:145:PRO:HD2	2.02	0.40
4:4:169:HIS:NE2	6:6:45:CYS:SG	2.93	0.40
7:9:105:GLU:HA	7:9:113:ILE:HG23	2.02	0.40
10:A:1:MET:HA	11:J:123:LEU:HD11	2.03	0.40
4:4:26:MET:HE2	10:A:57:PHE:HD1	1.86	0.40
1:B:214:LYS:HA	1:B:215:PRO:HD3	1.93	0.40
1:B:16:THR:HG23	1:B:233:ARG:HH21	1.86	0.40
1:B:233:ARG:O	1:B:237:TRP:HB3	2.21	0.40
1:B:29:LEU:O	1:B:33:LEU:HG	2.22	0.40
1:B:338:VAL:O	1:B:342:TRP:HB2	2.22	0.40
1:B:97:GLU:HG3	1:B:98:PRO:HD2	2.03	0.40
4:E:249:ARG:HB3	4:E:257:TYR:HD2	1.86	0.40
6:G:22:THR:O	6:G:26:LYS:HG2	2.20	0.40
13:L:383:TRP:HD1	13:L:457:GLY:HA2	1.85	0.40
13:L:477:LEU:O	13:L:478:ALA:HB3	2.22	0.40
14:M:186:GLN:HG2	14:M:187:GLU:N	2.34	0.40
14:M:109:LEU:HD21	14:M:236:VAL:HG21	2.03	0.40
14:M:433:ALA:O	14:M:437:VAL:HG23	2.21	0.40
15:N:105:LEU:O	15:N:108:LEU:HB3	2.21	0.40
15:N:367:THR:O	15:N:370:VAL:HB	2.20	0.40
15:N:380:LEU:HD23	15:N:380:LEU:HA	1.96	0.40
10:P:54:VAL:HG22	16:Q:146:LYS:HD2	2.02	0.40
16:Q:221:LEU:N	16:Q:222:PRO:CA	2.83	0.40
14:U:41:LEU:HD23	14:U:449:TYR:OH	2.20	0.40
9:X:21:LEU:HD11	9:X:26:LEU:HD21	2.04	0.40
2:2:96:LEU:HD11	2:2:134:ILE:HD11	2.03	0.40
3:3:507:LEU:HD11	3:3:521:ALA:HB1	2.03	0.40
4:4:346:THR:HG22	4:4:353:LEU:O	2.22	0.40
6:6:76:ASP:H	16:H:65:LYS:NZ	2.19	0.40
8:7:13:TRP:HE3	8:7:82:ILE:HD12	1.87	0.40
7:9:59:CYS:HB2	7:9:104:CYS:HB2	2.02	0.40
2:C:155:ALA:HA	2:C:158:ARG:HB2	2.03	0.40
3:D:202:PHE:HB3	3:D:209:THR:CG2	2.51	0.40
3:D:257:ALA:HB1	3:D:348:ASP:HB2	2.02	0.40
3:D:459:MET:HG2	3:D:465:HIS:CG	2.57	0.40
3:D:700:LYS:HA	3:D:763:LEU:O	2.21	0.40
3:D:717:TRP:CD1	3:D:748:VAL:HB	2.56	0.40
4:E:272:VAL:HG13	4:E:399:SER:CB	2.49	0.40
4:E:393:MET:HA	4:E:396:ILE:HG22	2.02	0.40
5:F:136:LEU:HD23	5:F:136:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:35:SER:OG	6:G:35:SER:O	2.40	0.40
6:G:96:TRP:HE3	6:G:97:GLU:HG3	1.86	0.40
2:C:110:GLU:HA	8:I:121:ARG:HH12	1.86	0.40
13:L:59:TRP:CH2	13:L:129:ILE:HD11	2.56	0.40
14:M:347:LEU:HD13	14:M:422:VAL:HG21	2.00	0.40
14:M:86:ALA:CB	14:M:96:LEU:HD21	2.51	0.40
14:M:88:VAL:HA	14:M:428:ALA:CB	2.51	0.40
11:J:104:LEU:HA	15:N:174:LEU:HD21	2.02	0.40
16:Q:216:ARG:C	16:Q:218:PRO:HD3	2.41	0.40
11:R:104:LEU:O	11:R:108:LEU:HD12	2.21	0.40
11:R:52:GLY:O	11:R:56:VAL:HG23	2.21	0.40
13:T:286:PHE:HB2	13:T:419:ARG:CD	2.52	0.40
13:T:470:GLU:N	13:T:471:PRO:HD2	2.36	0.40
12:S:88:ASP:OD2	13:T:587:ARG:NH1	2.55	0.40
14:U:164:LEU:HD21	15:V:346:TYR:CE1	2.57	0.40
9:W:122:ASP:O	9:W:125:ILE:HG12	2.21	0.40
1:1:16:THR:HG21	1:1:229:PRO:HB3	2.03	0.40
1:1:189:MET:O	1:1:193:GLU:HB2	2.21	0.40
1:1:288:GLN:HG2	1:1:331:ILE:O	2.22	0.40
1:1:404:ASP:OD1	1:1:404:ASP:N	2.54	0.40
2:2:14:THR:HG22	2:2:17:LYS:HZ2	1.86	0.40
3:3:225:ASN:ND2	3:3:289:TRP:HB3	2.36	0.40
3:3:281:GLU:HB2	3:3:288:ILE:HG22	2.03	0.40
4:4:279:ARG:O	4:4:282:GLU:HB2	2.21	0.40
5:5:34:PHE:HD2	5:5:102:PRO:HG2	1.86	0.40
6:6:171:PRO:HA	6:6:172:PRO:HD3	1.97	0.40
6:6:83:ARG:HB2	6:6:123:ILE:HD12	2.03	0.40
8:7:88:ARG:NH2	8:7:126:LEU:HB3	2.36	0.40
7:9:101:CYS:HB2	7:9:103:LEU:H	1.86	0.40
10:A:45:GLU:O	10:A:45:GLU:HG3	2.21	0.40
1:B:104:ARG:O	1:B:108:GLU:HG3	2.21	0.40
1:B:201:LEU:HD11	3:D:84:VAL:HG11	2.02	0.40
1:B:202:LYS:N	1:B:203:PRO:HD2	2.36	0.40
1:B:65:ARG:NH1	1:B:249:MET:O	2.54	0.40
3:D:561:PRO:HB3	3:D:575:GLU:O	2.22	0.40
3:D:651:ARG:HA	3:D:652:PRO:HD2	1.91	0.40
3:D:750:ARG:HB2	3:D:753:VAL:HG23	2.02	0.40
4:E:152:GLU:OE2	4:E:200:ARG:HG3	2.22	0.40
4:E:214:PHE:O	4:E:218:ALA:N	2.38	0.40
4:E:240:ARG:HB2	4:E:266:LEU:HD23	2.02	0.40
4:E:73:ARG:NH2	4:E:81:TYR:OH	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:74:THR:HG22	4:E:75:TYR:N	2.37	0.40
5:F:158:LEU:HD11	9:X:37:TRP:HA	2.03	0.40
6:G:57:ARG:CB	6:G:60:LEU:HD12	2.51	0.40
8:I:65:GLU:HA	8:I:66:PRO:HD3	1.83	0.40
14:M:452:ARG:HD3	14:M:452:ARG:HA	1.77	0.40
13:L:59:TRP:O	14:M:452:ARG:NH2	2.55	0.40
16:Q:108:PHE:CG	16:Q:108:PHE:O	2.74	0.40
16:Q:153:LEU:HA	16:Q:153:LEU:HD23	1.72	0.40
11:R:46:LEU:HA	11:R:46:LEU:HD23	1.76	0.40
13:T:517:PHE:O	13:T:522:LEU:HG	2.21	0.40
14:U:426:ALA:N	14:U:429:GLU:OE1	2.36	0.40
14:U:438:LEU:HA	14:U:438:LEU:HD12	1.81	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	435/438 (99%)	405 (93%)	28 (6%)	2 (0%)	29	61
1	B	435/438 (99%)	406 (93%)	27 (6%)	2 (0%)	29	61
2	2	176/181 (97%)	164 (93%)	11 (6%)	1 (1%)	25	57
2	C	176/181 (97%)	164 (93%)	11 (6%)	1 (1%)	25	57
3	3	750/783 (96%)	695 (93%)	54 (7%)	1 (0%)	51	81
3	D	750/783 (96%)	695 (93%)	54 (7%)	1 (0%)	51	81
4	4	382/409 (93%)	351 (92%)	29 (8%)	2 (0%)	29	61
4	E	382/409 (93%)	351 (92%)	29 (8%)	2 (0%)	29	61
5	5	194/207 (94%)	182 (94%)	12 (6%)	0	100	100
5	F	194/207 (94%)	182 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	6	157/181 (87%)	140 (89%)	15 (10%)	2 (1%)	12	40
6	G	157/181 (87%)	141 (90%)	14 (9%)	2 (1%)	12	40
7	9	178/182 (98%)	166 (93%)	11 (6%)	1 (1%)	25	57
7	O	178/182 (98%)	167 (94%)	10 (6%)	1 (1%)	25	57
8	7	125/129 (97%)	116 (93%)	9 (7%)	0	100	100
8	I	125/129 (97%)	116 (93%)	9 (7%)	0	100	100
9	W	125/131 (95%)	121 (97%)	3 (2%)	1 (1%)	19	51
9	X	125/131 (95%)	121 (97%)	3 (2%)	1 (1%)	19	51
10	A	115/119 (97%)	105 (91%)	7 (6%)	3 (3%)	5	27
10	P	115/119 (97%)	105 (91%)	7 (6%)	3 (3%)	5	27
11	J	158/176 (90%)	143 (90%)	14 (9%)	1 (1%)	25	57
11	R	158/176 (90%)	142 (90%)	15 (10%)	1 (1%)	25	57
12	K	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	14	45
12	S	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	14	45
13	L	603/606 (100%)	555 (92%)	43 (7%)	5 (1%)	19	51
13	T	603/606 (100%)	555 (92%)	43 (7%)	5 (1%)	19	51
14	M	465/469 (99%)	428 (92%)	33 (7%)	4 (1%)	17	48
14	U	465/469 (99%)	428 (92%)	33 (7%)	4 (1%)	17	48
15	N	425/427 (100%)	398 (94%)	25 (6%)	2 (0%)	29	61
15	V	425/427 (100%)	396 (93%)	27 (6%)	2 (0%)	29	61
16	H	351/365 (96%)	309 (88%)	33 (9%)	9 (3%)	5	27
16	Q	351/365 (96%)	309 (88%)	33 (9%)	9 (3%)	5	27
All	All	9464/9796 (97%)	8730 (92%)	664 (7%)	70 (1%)	22	54

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	5	ILE
6	6	61	ALA
7	9	23	THR
10	A	43	PRO
13	L	434	HIS
13	L	435	PRO
14	M	347	LEU

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Mol	Chain	Res	Type
16	H	217	THR
16	H	218	PRO
16	H	232	TYR
16	H	332	LEU
1	B	5	ILE
6	G	61	ALA
7	O	23	THR
10	P	43	PRO
13	T	434	HIS
13	T	435	PRO
14	U	347	LEU
16	Q	217	THR
16	Q	218	PRO
16	Q	232	TYR
16	Q	332	LEU
6	6	58	ASN
12	K	86	ALA
13	L	478	ALA
6	G	58	ASN
12	S	86	ALA
13	T	478	ALA
3	3	117	LEU
10	A	34	LYS
14	M	42	THR
16	H	216	ARG
16	H	238	SER
16	H	333	PRO
3	D	117	LEU
10	P	34	LYS
14	U	42	THR
16	Q	216	ARG
16	Q	238	SER
16	Q	333	PRO
4	4	33	GLN
13	L	515	LYS
14	M	57	PRO
16	H	70	GLU
16	H	234	THR
4	E	33	GLN
9	X	37	TRP
14	U	57	PRO
16	Q	70	GLU

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Mol	Chain	Res	Type
16	Q	234	THR
1	1	360	ARG
2	2	6	ASP
9	W	37	TRP
1	B	360	ARG
2	C	6	ASP
13	T	515	LYS
15	N	425	ALA
15	V	425	ALA
10	A	49	ASP
11	J	157	VAL
10	P	49	ASP
11	R	157	VAL
14	U	44	PRO
14	M	44	PRO
13	L	21	GLY
13	T	21	GLY
4	4	35	PRO
4	E	35	PRO
15	N	338	PRO
15	V	338	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%)	342 (96%)	13 (4%)	34	63
1	B	355/356 (100%)	343 (97%)	12 (3%)	37	65
2	2	150/152 (99%)	140 (93%)	10 (7%)	16	45
2	C	150/152 (99%)	139 (93%)	11 (7%)	14	41
3	3	609/628 (97%)	574 (94%)	35 (6%)	20	51
3	D	609/628 (97%)	573 (94%)	36 (6%)	19	49
4	4	332/355 (94%)	315 (95%)	17 (5%)	24	54
4	E	332/355 (94%)	314 (95%)	18 (5%)	22	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	5	167/175 (95%)	158 (95%)	9 (5%)	22	53
5	F	167/175 (95%)	158 (95%)	9 (5%)	22	53
6	6	130/149 (87%)	109 (84%)	21 (16%)	2	10
6	G	130/149 (87%)	109 (84%)	21 (16%)	2	10
7	9	148/150 (99%)	138 (93%)	10 (7%)	16	44
7	O	148/150 (99%)	138 (93%)	10 (7%)	16	44
8	7	104/106 (98%)	101 (97%)	3 (3%)	42	69
8	I	104/106 (98%)	102 (98%)	2 (2%)	57	77
9	W	99/101 (98%)	96 (97%)	3 (3%)	41	68
9	X	99/101 (98%)	96 (97%)	3 (3%)	41	68
10	A	90/92 (98%)	85 (94%)	5 (6%)	21	52
10	P	90/92 (98%)	85 (94%)	5 (6%)	21	52
11	J	118/130 (91%)	108 (92%)	10 (8%)	10	35
11	R	118/130 (91%)	108 (92%)	10 (8%)	10	35
12	K	71/71 (100%)	64 (90%)	7 (10%)	8	28
12	S	71/71 (100%)	64 (90%)	7 (10%)	8	28
13	L	453/454 (100%)	434 (96%)	19 (4%)	30	60
13	T	453/454 (100%)	435 (96%)	18 (4%)	31	61
14	M	332/332 (100%)	315 (95%)	17 (5%)	24	54
14	U	332/332 (100%)	315 (95%)	17 (5%)	24	54
15	N	302/302 (100%)	296 (98%)	6 (2%)	55	76
15	V	302/302 (100%)	296 (98%)	6 (2%)	55	76
16	H	293/300 (98%)	270 (92%)	23 (8%)	12	38
16	Q	293/300 (98%)	271 (92%)	22 (8%)	13	39
All	All	7506/7706 (97%)	7091 (94%)	415 (6%)	21	52

All (415) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	134	VAL
1	1	199	PRO
1	1	217	THR
1	1	249	MET
1	1	342	TRP

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Mol	Chain	Res	Type
1	1	355	LYS
1	1	357	THR
1	1	366	PHE
1	1	397	ARG
1	1	400	CYS
1	1	404	ASP
1	1	437	TRP
1	1	438	ARG
2	2	7	LYS
2	2	33	ARG
2	2	35	GLN
2	2	45	ARG
2	2	110	GLU
2	2	116	LEU
2	2	139	GLU
2	2	144	CYS
2	2	147	ARG
2	2	172	CYS
3	3	3	ARG
3	3	11	VAL
3	3	42	ILE
3	3	46	ARG
3	3	123	ASP
3	3	124	LYS
3	3	132	ASP
3	3	133	ARG
3	3	188	VAL
3	3	249	MET
3	3	259	CYS
3	3	269	THR
3	3	284	GLU
3	3	286	ASN
3	3	337	ARG
3	3	368	HIS
3	3	374	ARG
3	3	417	VAL
3	3	419	ASP
3	3	425	ARG
3	3	435	LEU
3	3	466	GLU
3	3	501	LYS
3	3	512	LEU

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Mol	Chain	Res	Type
3	3	515	THR
3	3	593	LEU
3	3	616	ASN
3	3	651	ARG
3	3	654	PHE
3	3	655	ARG
3	3	684	ARG
3	3	726	GLU
3	3	744	GLU
3	3	761	SER
3	3	774	ARG
4	4	38	HIS
4	4	87	TYR
4	4	129	HIS
4	4	132	PHE
4	4	143	LEU
4	4	144	THR
4	4	148	TYR
4	4	152	GLU
4	4	163	VAL
4	4	170	HIS
4	4	194	LEU
4	4	199	HIS
4	4	200	ARG
4	4	208	PHE
4	4	211	SER
4	4	262	PHE
4	4	319	THR
5	5	31	ARG
5	5	38	MET
5	5	51	ASP
5	5	80	TRP
5	5	141	LEU
5	5	171	ARG
5	5	174	LEU
5	5	178	ASP
5	5	193	ARG
6	6	16	ARG
6	6	22	THR
6	6	30	TRP
6	6	45	CYS
6	6	49	GLU

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Mol	Chain	Res	Type
6	6	55	ASP
6	6	57	ARG
6	6	58	ASN
6	6	60	LEU
6	6	62	ARG
6	6	63	PHE
6	6	83	ARG
6	6	88	MET
6	6	101	ASP
6	6	117	MET
6	6	120	ASN
6	6	130	VAL
6	6	153	GLN
6	6	156	LYS
6	6	176	TRP
6	6	178	ARG
7	9	4	LYS
7	9	31	VAL
7	9	38	HIS
7	9	42	VAL
7	9	85	GLU
7	9	97	ARG
7	9	99	ILE
7	9	101	CYS
7	9	118	ASP
7	9	139	ASP
8	7	43	ARG
8	7	52	THR
8	7	82	ILE
9	W	37	TRP
9	W	43	GLN
9	W	100	THR
10	A	6	GLU
10	A	13	TYR
10	A	40	LYS
10	A	46	SER
10	A	48	ASN
11	J	59	TYR
11	J	74	LEU
11	J	80	GLU
11	J	84	ASP
11	J	86	LEU

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Mol	Chain	Res	Type
11	J	103	ILE
11	J	113	LEU
11	J	118	ASP
11	J	119	LEU
11	J	131	LEU
12	K	2	SER
12	K	4	LEU
12	K	29	LEU
12	K	33	LEU
12	K	58	LEU
12	K	81	HIS
12	K	82	ARG
13	L	14	PHE
13	L	32	LEU
13	L	59	TRP
13	L	108	PHE
13	L	146	TYR
13	L	151	TYR
13	L	169	PHE
13	L	176	LEU
13	L	245	MET
13	L	275	LEU
13	L	286	PHE
13	L	329	LYS
13	L	483	HIS
13	L	490	GLU
13	L	506	TRP
13	L	511	PHE
13	L	554	PHE
13	L	557	ASP
13	L	567	LEU
14	M	11	VAL
14	M	16	LEU
14	M	18	LEU
14	M	20	LEU
14	M	22	ARG
14	M	24	LEU
14	M	42	THR
14	M	73	LEU
14	M	92	GLU
14	M	151	PHE
14	M	224	SER

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Mol	Chain	Res	Type
14	M	255	GLN
14	M	269	LEU
14	M	349	GLN
14	M	354	LEU
14	M	415	TRP
14	M	455	HIS
15	N	50	PHE
15	N	124	TRP
15	N	126	ARG
15	N	136	TYR
15	N	142	LEU
15	N	284	TYR
16	H	2	THR
16	H	13	VAL
16	H	28	PHE
16	H	50	ARG
16	H	70	GLU
16	H	119	ASP
16	H	134	TYR
16	H	149	LEU
16	H	180	LEU
16	H	189	GLN
16	H	205	VAL
16	H	211	MET
16	H	228	LEU
16	H	232	TYR
16	H	233	HIS
16	H	234	THR
16	H	249	TYR
16	H	267	TRP
16	H	269	MET
16	H	302	TYR
16	H	304	GLN
16	H	307	ARG
16	H	354	TYR
1	B	134	VAL
1	B	199	PRO
1	B	217	THR
1	B	249	MET
1	B	342	TRP
1	B	355	LYS
1	B	366	PHE

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Mol	Chain	Res	Type
1	B	397	ARG
1	B	400	CYS
1	B	404	ASP
1	B	437	TRP
1	B	438	ARG
2	C	7	LYS
2	C	33	ARG
2	C	35	GLN
2	C	45	ARG
2	C	110	GLU
2	C	116	LEU
2	C	119	VAL
2	C	139	GLU
2	C	144	CYS
2	C	147	ARG
2	C	172	CYS
3	D	3	ARG
3	D	11	VAL
3	D	42	ILE
3	D	46	ARG
3	D	123	ASP
3	D	124	LYS
3	D	132	ASP
3	D	133	ARG
3	D	188	VAL
3	D	249	MET
3	D	259	CYS
3	D	269	THR
3	D	284	GLU
3	D	286	ASN
3	D	321	THR
3	D	337	ARG
3	D	368	HIS
3	D	374	ARG
3	D	417	VAL
3	D	419	ASP
3	D	425	ARG
3	D	435	LEU
3	D	466	GLU
3	D	501	LYS
3	D	512	LEU
3	D	515	THR

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Mol	Chain	Res	Type
3	D	593	LEU
3	D	616	ASN
3	D	651	ARG
3	D	654	PHE
3	D	655	ARG
3	D	684	ARG
3	D	726	GLU
3	D	744	GLU
3	D	761	SER
3	D	774	ARG
4	E	38	HIS
4	E	87	TYR
4	E	129	HIS
4	E	132	PHE
4	E	143	LEU
4	E	144	THR
4	E	148	TYR
4	E	152	GLU
4	E	155	THR
4	E	163	VAL
4	E	170	HIS
4	E	194	LEU
4	E	199	HIS
4	E	200	ARG
4	E	208	PHE
4	E	211	SER
4	E	262	PHE
4	E	319	THR
5	F	31	ARG
5	F	38	MET
5	F	51	ASP
5	F	80	TRP
5	F	141	LEU
5	F	171	ARG
5	F	174	LEU
5	F	178	ASP
5	F	193	ARG
6	G	16	ARG
6	G	22	THR
6	G	30	TRP
6	G	45	CYS
6	G	49	GLU

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Mol	Chain	Res	Type
6	G	55	ASP
6	G	57	ARG
6	G	58	ASN
6	G	62	ARG
6	G	63	PHE
6	G	83	ARG
6	G	88	MET
6	G	101	ASP
6	G	117	MET
6	G	120	ASN
6	G	130	VAL
6	G	153	GLN
6	G	156	LYS
6	G	176	TRP
6	G	178	ARG
6	G	179	THR
7	O	4	LYS
7	O	31	VAL
7	O	38	HIS
7	O	42	VAL
7	O	85	GLU
7	O	97	ARG
7	O	99	ILE
7	O	101	CYS
7	O	118	ASP
7	O	139	ASP
8	I	43	ARG
8	I	82	ILE
9	X	37	TRP
9	X	43	GLN
9	X	100	THR
10	P	6	GLU
10	P	13	TYR
10	P	40	LYS
10	P	46	SER
10	P	48	ASN
11	R	59	TYR
11	R	74	LEU
11	R	80	GLU
11	R	84	ASP
11	R	86	LEU
11	R	103	ILE

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Mol	Chain	Res	Type
11	R	113	LEU
11	R	118	ASP
11	R	119	LEU
11	R	131	LEU
12	S	2	SER
12	S	4	LEU
12	S	29	LEU
12	S	33	LEU
12	S	58	LEU
12	S	81	HIS
12	S	82	ARG
13	T	14	PHE
13	T	59	TRP
13	T	108	PHE
13	T	146	TYR
13	T	151	TYR
13	T	169	PHE
13	T	176	LEU
13	T	245	MET
13	T	275	LEU
13	T	286	PHE
13	T	329	LYS
13	T	483	HIS
13	T	490	GLU
13	T	506	TRP
13	T	511	PHE
13	T	554	PHE
13	T	557	ASP
13	T	567	LEU
14	U	11	VAL
14	U	16	LEU
14	U	18	LEU
14	U	20	LEU
14	U	22	ARG
14	U	24	LEU
14	U	42	THR
14	U	73	LEU
14	U	92	GLU
14	U	151	PHE
14	U	224	SER
14	U	255	GLN
14	U	269	LEU

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Mol	Chain	Res	Type
14	U	349	GLN
14	U	354	LEU
14	U	415	TRP
14	U	455	HIS
15	V	50	PHE
15	V	124	TRP
15	V	126	ARG
15	V	136	TYR
15	V	142	LEU
15	V	284	TYR
16	Q	2	THR
16	Q	13	VAL
16	Q	28	PHE
16	Q	50	ARG
16	Q	70	GLU
16	Q	119	ASP
16	Q	134	TYR
16	Q	149	LEU
16	Q	180	LEU
16	Q	189	GLN
16	Q	205	VAL
16	Q	211	MET
16	Q	228	LEU
16	Q	232	TYR
16	Q	233	HIS
16	Q	234	THR
16	Q	249	TYR
16	Q	267	TRP
16	Q	269	MET
16	Q	302	TYR
16	Q	304	GLN
16	Q	307	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	386	ASN
3	3	104	GLN
3	3	167	HIS
4	4	292	GLN
6	6	34	ASN
6	6	155	GLN

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Mol	Chain	Res	Type
12	K	81	HIS
15	N	245	ASN
1	B	386	ASN
2	C	71	GLN
2	C	120	GLN
3	D	410	HIS
3	D	616	ASN
4	E	292	GLN
6	G	34	ASN
9	X	38	GLN
12	S	81	HIS
15	V	245	ASN

### 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](#)

20 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	3	801	3	0,12,12	0.00	-	-		
17	SF4	9	201	7	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	SF4	B	501	1	0,12,12	0.00	-	-		
17	SF4	3	802	3	0,12,12	0.00	-	-		
17	SF4	6	201	6	0,12,12	0.00	-	-		
17	SF4	D	801	3	0,12,12	0.00	-	-		
19	FES	C	201	2	0,4,4	0.00	-	-		
17	SF4	G	201	6	0,12,12	0.00	-	-		
17	SF4	O	202	7	0,12,12	0.00	-	-		
17	SF4	1	501	1	0,12,12	0.00	-	-		
18	FMN	1	502	-	31,33,33	1.46	4 (12%)	40,50,50	2.02	7 (17%)
19	FES	D	804	3	0,4,4	0.00	-	-		
19	FES	2	201	2	0,4,4	0.00	-	-		
17	SF4	O	201	7	0,12,12	0.00	-	-		
17	SF4	D	803	3	0,12,12	0.00	-	-		
17	SF4	D	802	3	0,12,12	0.00	-	-		
19	FES	3	804	3	0,4,4	0.00	-	-		
18	FMN	B	502	-	31,33,33	1.44	4 (12%)	40,50,50	1.86	6 (15%)
17	SF4	3	803	3	0,12,12	0.00	-	-		
17	SF4	9	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	3	801	3	-	-	0/6/5/5
17	SF4	9	201	7	-	-	0/6/5/5
17	SF4	B	501	1	-	-	0/6/5/5
17	SF4	3	802	3	-	-	0/6/5/5
17	SF4	6	201	6	-	-	0/6/5/5
17	SF4	D	801	3	-	-	0/6/5/5
19	FES	C	201	2	-	-	0/1/1/1
17	SF4	9	202	7	-	-	0/6/5/5
17	SF4	G	201	6	-	-	0/6/5/5
17	SF4	O	202	7	-	-	0/6/5/5
17	SF4	1	501	1	-	-	0/6/5/5
18	FMN	1	502	-	-	9/18/18/18	0/3/3/3
19	FES	D	804	3	-	-	0/1/1/1
19	FES	2	201	2	-	-	0/1/1/1
17	SF4	O	201	7	-	-	0/6/5/5
17	SF4	D	803	3	-	-	0/6/5/5
17	SF4	D	802	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	FES	3	804	3	-	-	0/1/1/1
17	SF4	3	803	3	-	-	0/6/5/5
18	FMN	B	502	-	-	9/18/18/18	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	502	FMN	C10-N1	4.28	1.38	1.33
18	1	502	FMN	C10-N1	4.13	1.38	1.33
18	1	502	FMN	C1'-N10	3.41	1.51	1.48
18	B	502	FMN	C4A-N5	3.28	1.38	1.33
18	1	502	FMN	C4A-N5	3.19	1.37	1.33
18	B	502	FMN	C1'-N10	3.03	1.51	1.48
18	1	502	FMN	C4-N3	3.03	1.38	1.33
18	B	502	FMN	C4-N3	2.83	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	502	FMN	C1'-N10-C10	8.19	125.74	118.41
18	B	502	FMN	C1'-N10-C10	7.29	124.94	118.41
18	B	502	FMN	C4-N3-C2	5.01	119.37	115.14
18	1	502	FMN	C4-N3-C2	4.95	119.32	115.14
18	1	502	FMN	C5A-C9A-N10	4.19	120.75	117.72
18	B	502	FMN	C5A-C9A-N10	3.76	120.44	117.72
18	1	502	FMN	C1'-N10-C9A	-3.63	115.44	118.29
18	B	502	FMN	C1'-N10-C9A	-3.22	115.76	118.29
18	B	502	FMN	C4A-N5-C5A	3.06	119.83	116.77
18	1	502	FMN	C4A-N5-C5A	3.05	119.82	116.77
18	1	502	FMN	C4A-C4-N3	-2.52	119.98	123.43
18	B	502	FMN	C4A-C4-N3	-2.44	120.10	123.43
18	1	502	FMN	C9A-N10-C10	-2.36	118.82	121.91

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	1	502	FMN	C2'-C1'-N10-C9A
18	1	502	FMN	C2'-C1'-N10-C10
18	1	502	FMN	N10-C1'-C2'-O2'
18	1	502	FMN	C1'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
18	1	502	FMN	C1'-C2'-C3'-C4'
18	B	502	FMN	C2'-C1'-N10-C9A
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	O4'-C4'-C5'-O5'
18	1	502	FMN	O2'-C2'-C3'-C4'
18	1	502	FMN	O2'-C2'-C3'-O3'
18	B	502	FMN	O2'-C2'-C3'-C4'
18	B	502	FMN	C3'-C4'-C5'-O5'
18	1	502	FMN	O4'-C4'-C5'-O5'
18	B	502	FMN	O2'-C2'-C3'-O3'
18	1	502	FMN	N10-C1'-C2'-C3'

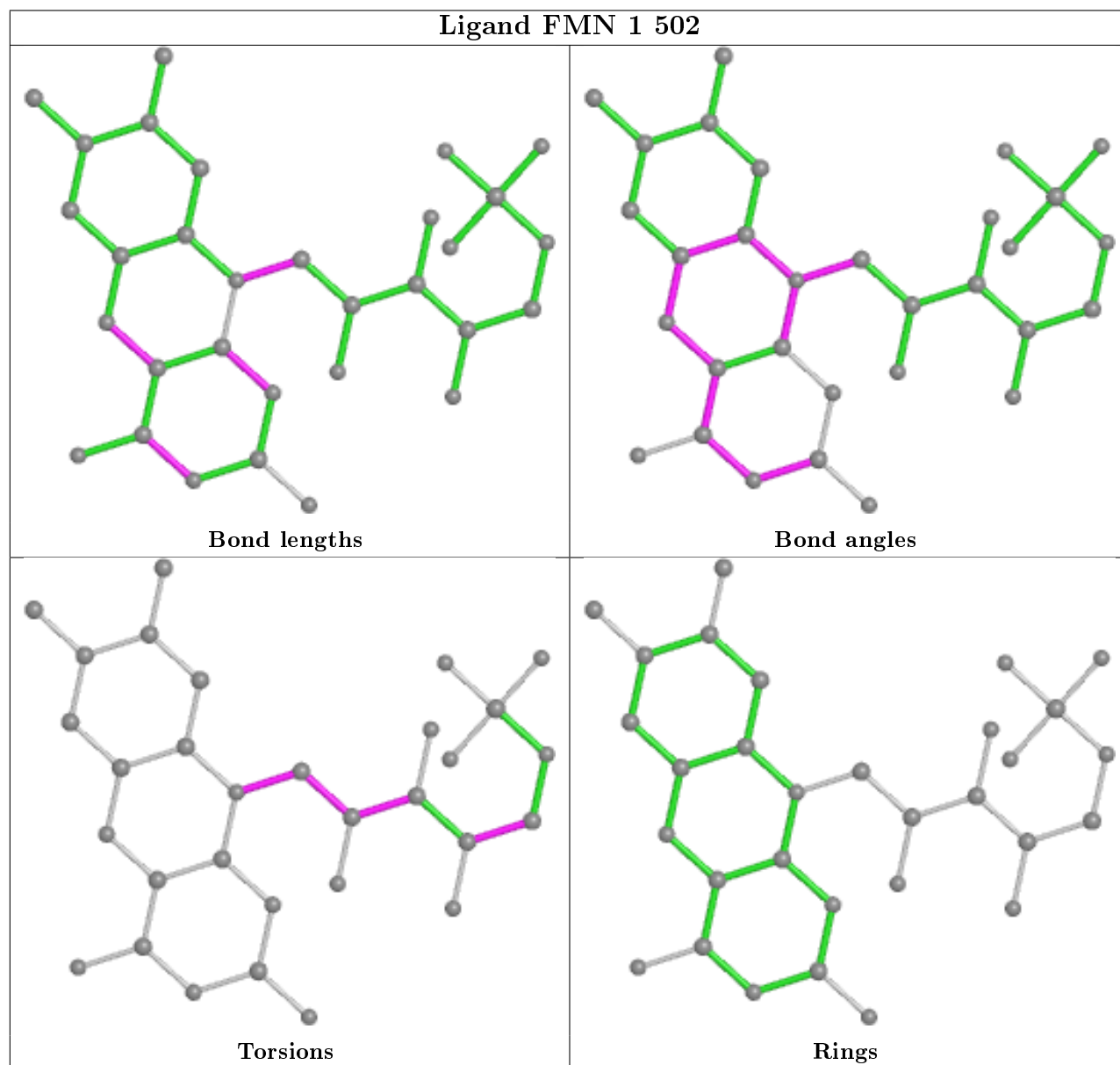
There are no ring outliers.

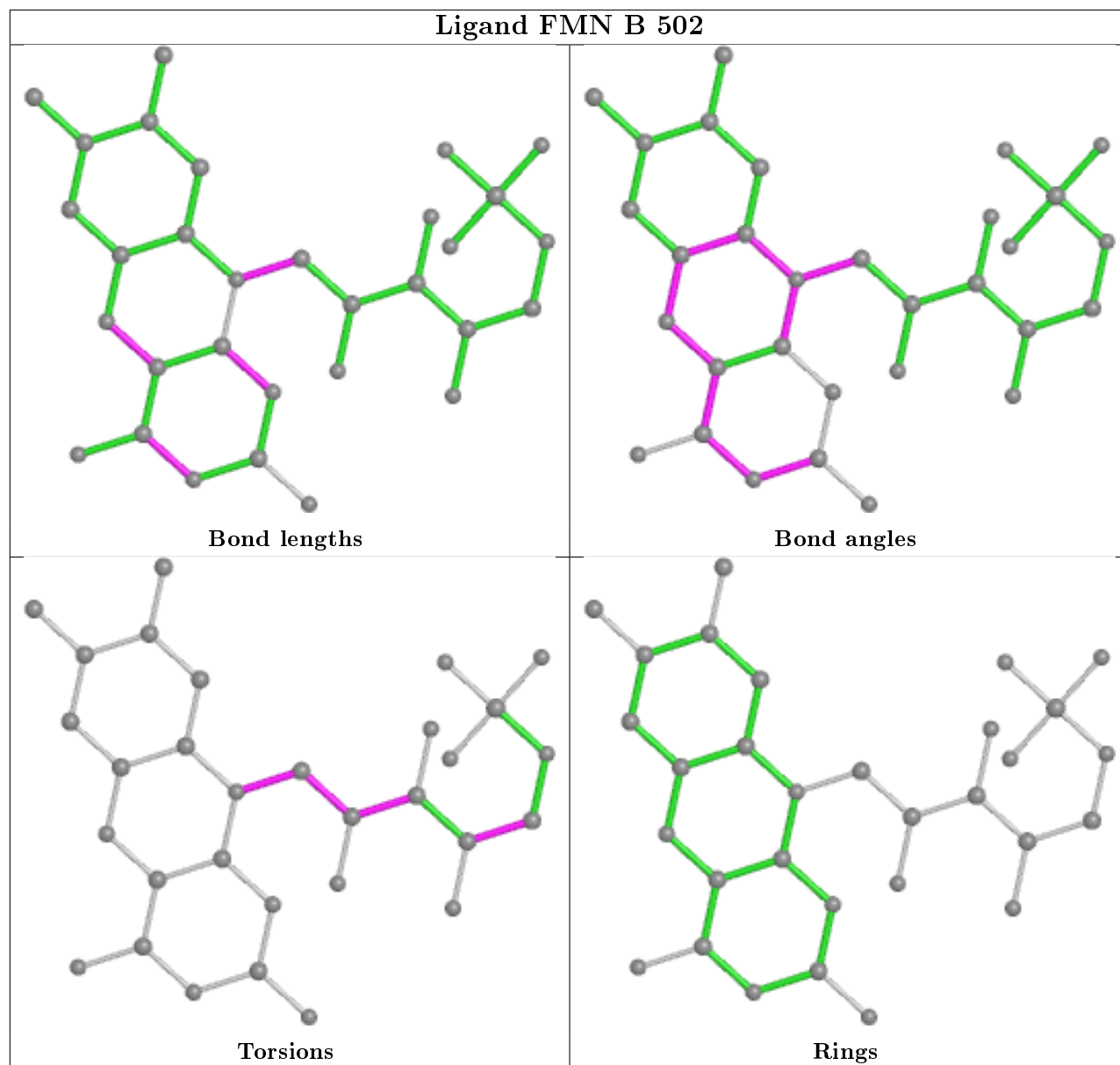
14 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	9	201	SF4	2	0
17	B	501	SF4	2	0
17	6	201	SF4	2	0
19	C	201	FES	1	0
17	G	201	SF4	2	0
17	O	202	SF4	5	0
17	1	501	SF4	1	0
18	1	502	FMN	4	0
19	D	804	FES	2	0
19	2	201	FES	1	0
17	O	201	SF4	2	0
19	3	804	FES	1	0
18	B	502	FMN	3	0
17	9	202	SF4	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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