



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:49 AM UTC

PDB ID : 4HEA / pdb_00004hea
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

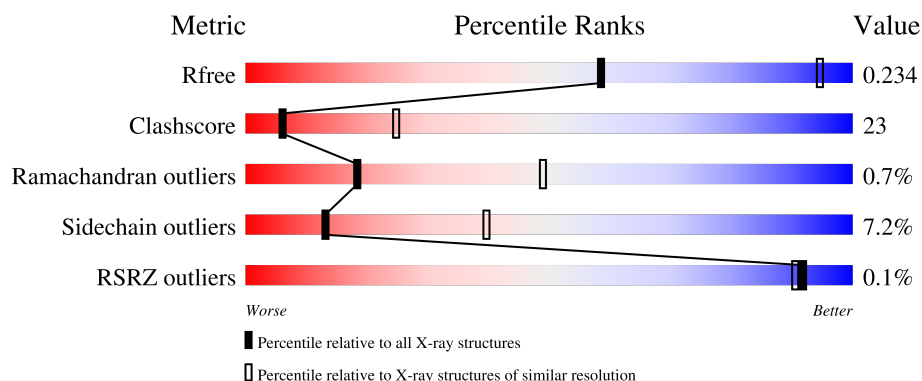
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



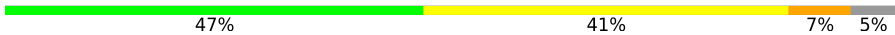
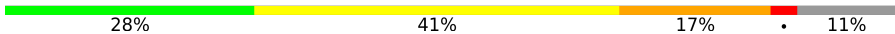
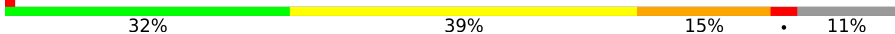
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	1	438	59% 37% .
1	B	438	61% 35% .
2	2	181	51% 41% 6% .
2	C	181	49% 45% 5% .
3	3	783	54% 38% 5% .

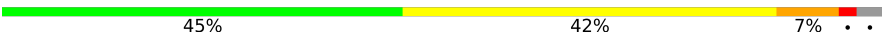
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Mol	Chain	Length	Quality of chain
3	D	783	
4	4	409	
4	E	409	
5	5	207	
5	F	207	
6	6	181	
6	G	181	
7	9	182	
7	O	182	
8	7	129	
8	I	129	
9	W	131	
9	X	131	
10	A	119	
10	P	119	
11	J	176	
11	R	176	
12	K	95	
12	S	95	
13	L	606	
13	T	606	
14	M	469	
14	U	469	
15	N	427	
15	V	427	

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Mol	Chain	Length	Quality of chain
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 criteria:

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			

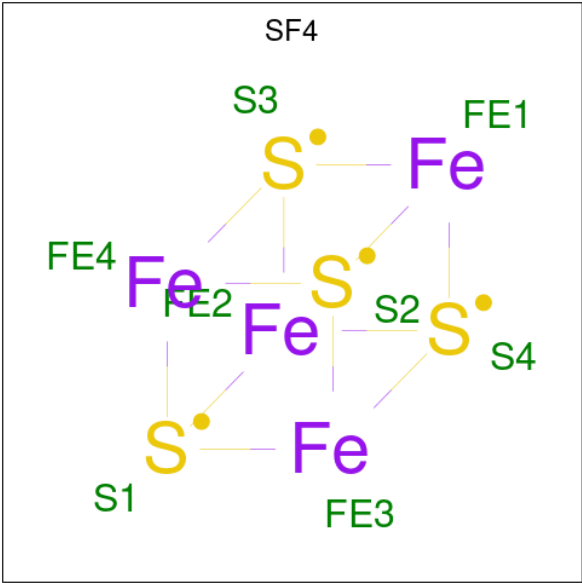
- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 14.

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 (CCD ID: SF4) (formula: Fe₄S₄).



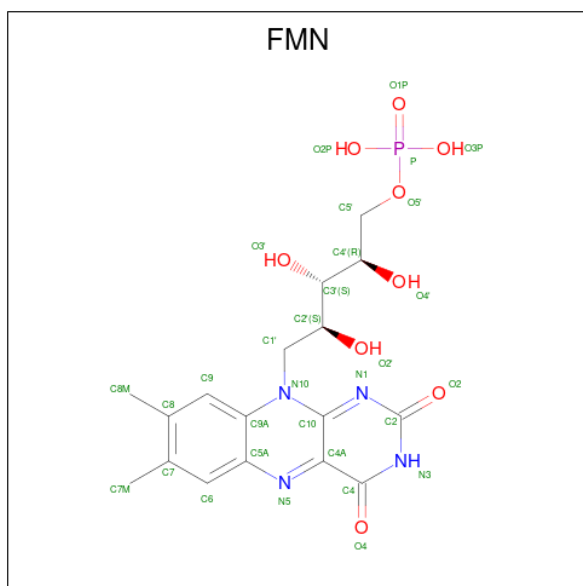
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	1	1	Total	Fe	S	0	0
			8	4	4		
17	3	1	Total	Fe	S	0	0
			8	4	4		
17	3	1	Total	Fe	S	0	0
			8	4	4		
17	3	1	Total	Fe	S	0	0
			8	4	4		
17	6	1	Total	Fe	S	0	0
			8	4	4		
17	9	1	Total	Fe	S	0	0
			8	4	4		
17	9	1	Total	Fe	S	0	0
			8	4	4		
17	B	1	Total	Fe	S	0	0
			8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

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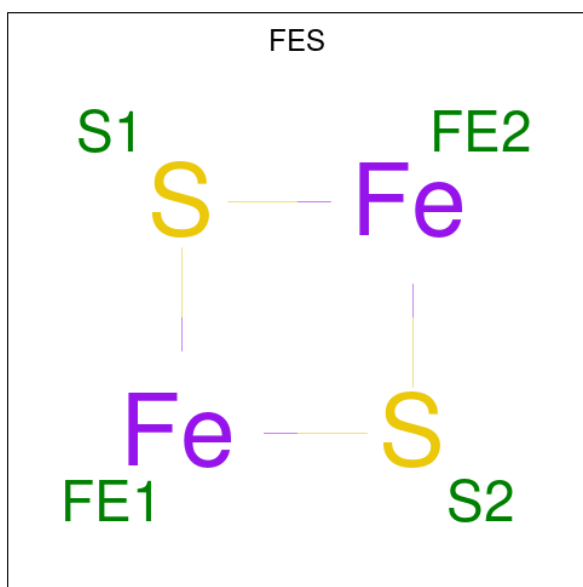
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	D	1	Total	Fe	S	0	0
			8	4	4		
17	D	1	Total	Fe	S	0	0
			8	4	4		
17	G	1	Total	Fe	S	0	0
			8	4	4		
17	O	1	Total	Fe	S	0	0
			8	4	4		
17	O	1	Total	Fe	S	0	0
			8	4	4		

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



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

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

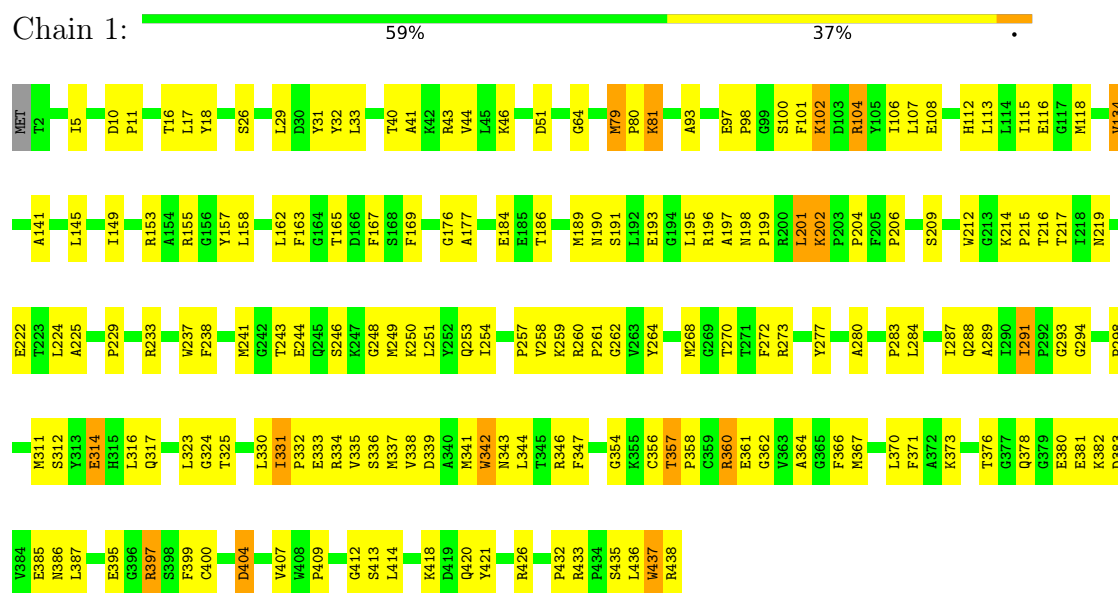


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	2	1	Total	Fe	S	0	0
			4	2	2		
19	3	1	Total	Fe	S	0	0
			4	2	2		
19	C	1	Total	Fe	S	0	0
			4	2	2		
19	D	1	Total	Fe	S	0	0
			4	2	2		

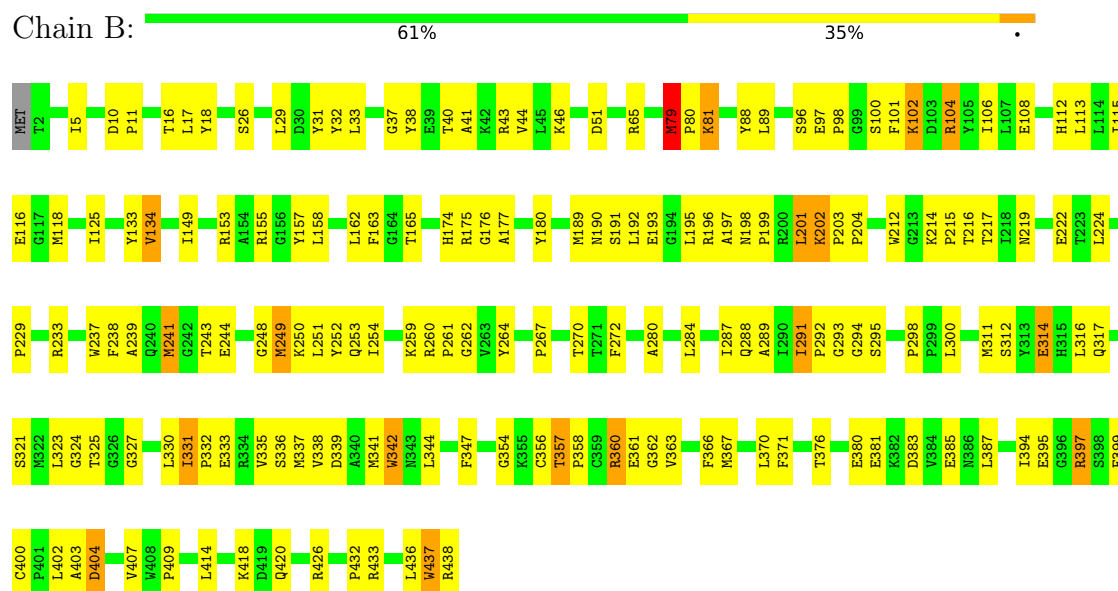
3 Residue-property plots

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

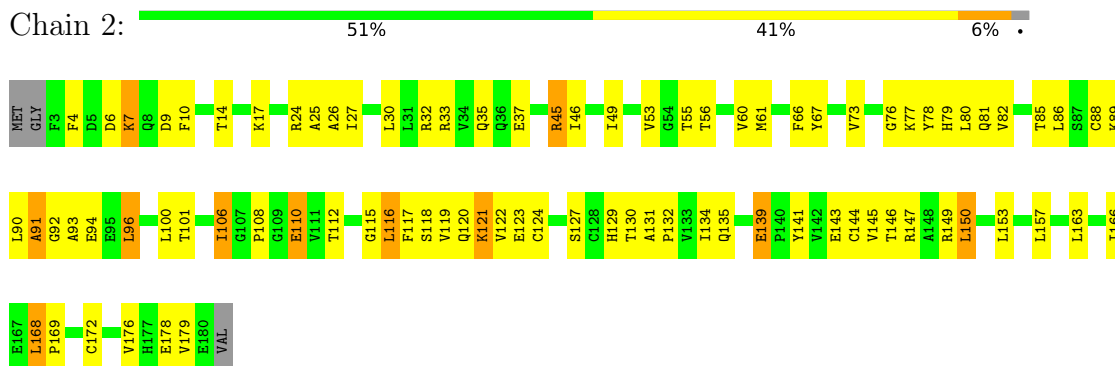
• Molecule 1: NADH-quinone oxidoreductase subunit 1



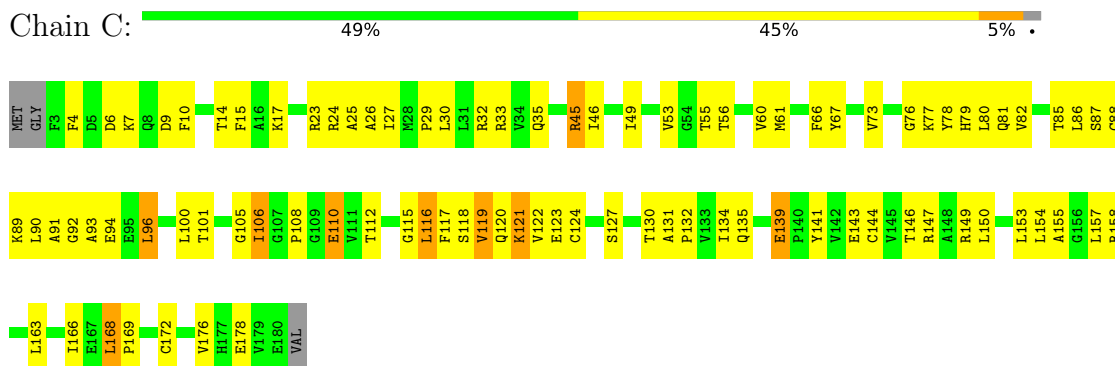
• Molecule 1: NADH-quinone oxidoreductase subunit 1



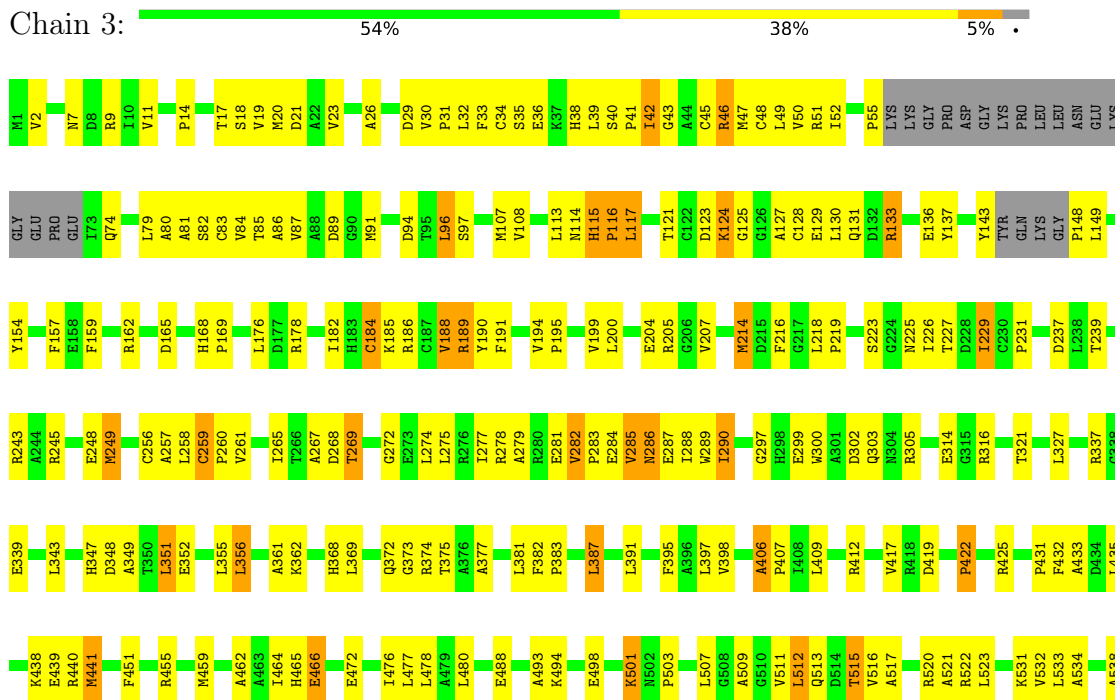
- Molecule 2: NADH-quinone oxidoreductase subunit 2

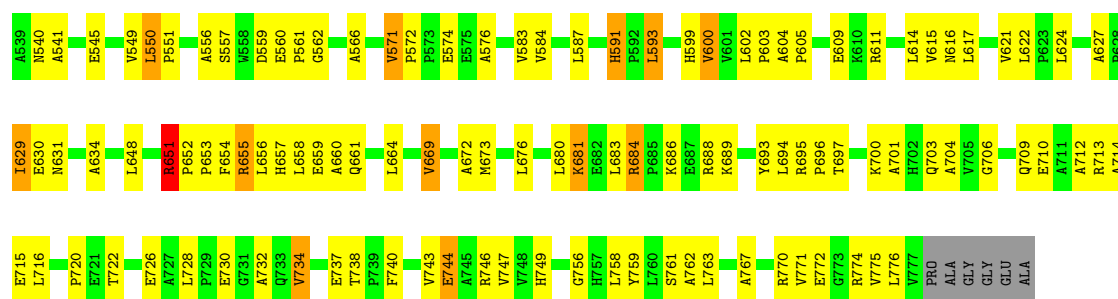


- Molecule 2: NADH-quinone oxidoreductase subunit 2



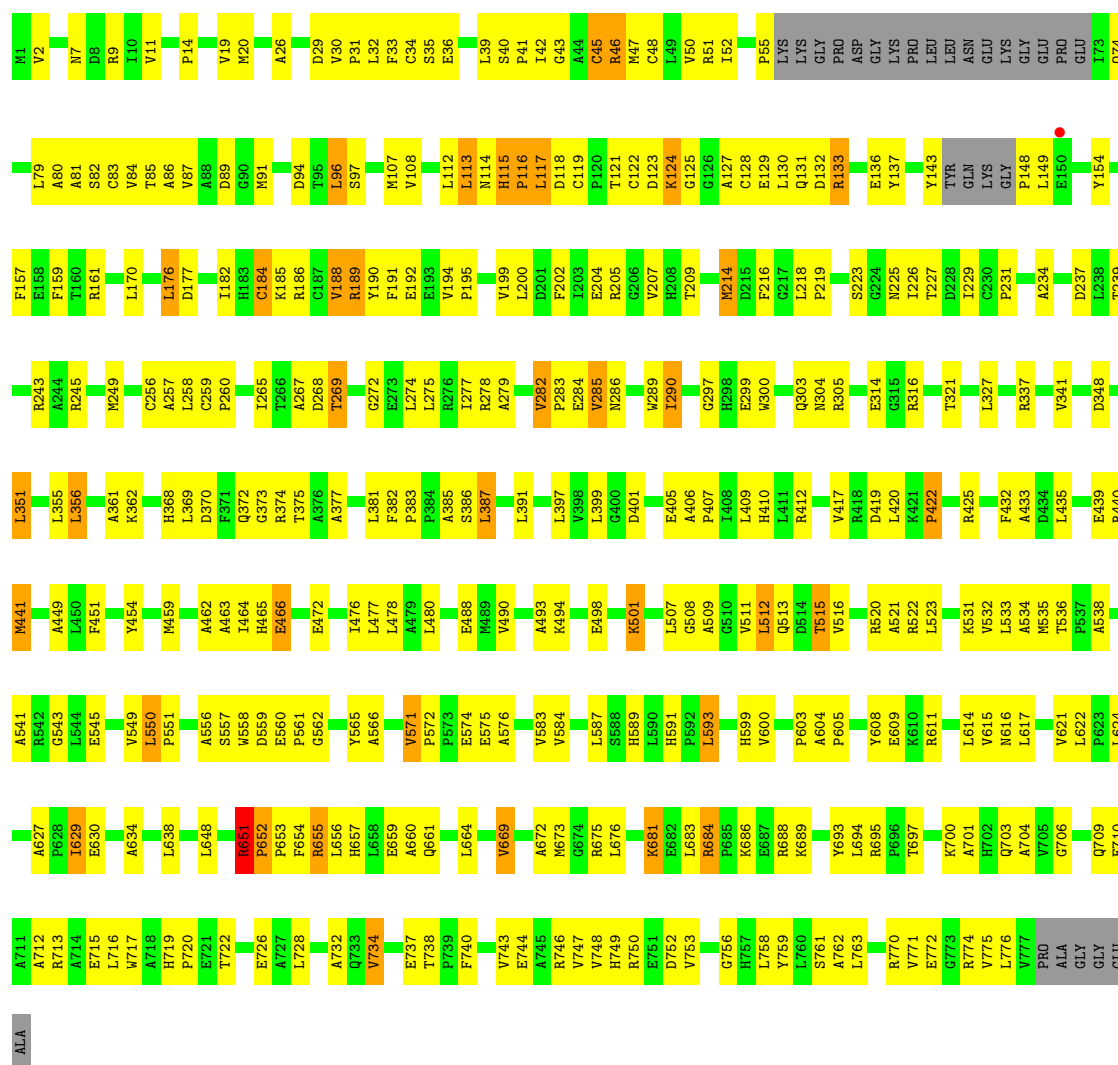
- Molecule 3: NADH-quinone oxidoreductase subunit 3





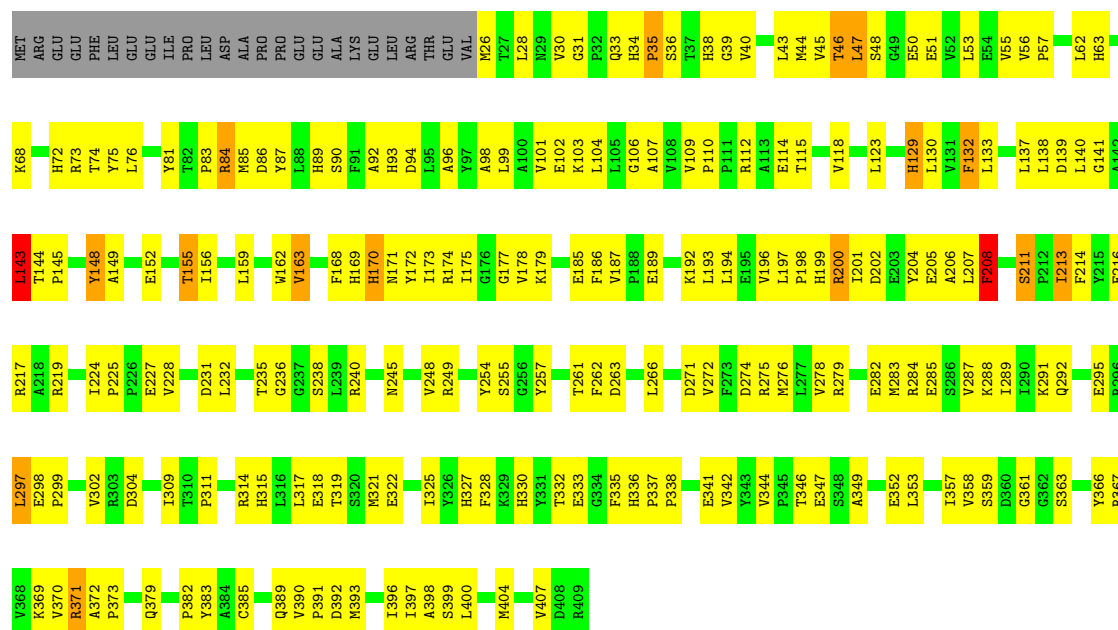
• Molecule 3: NADH-quinone oxidoreductase subunit 3

Chain D: 53% 39% 5%



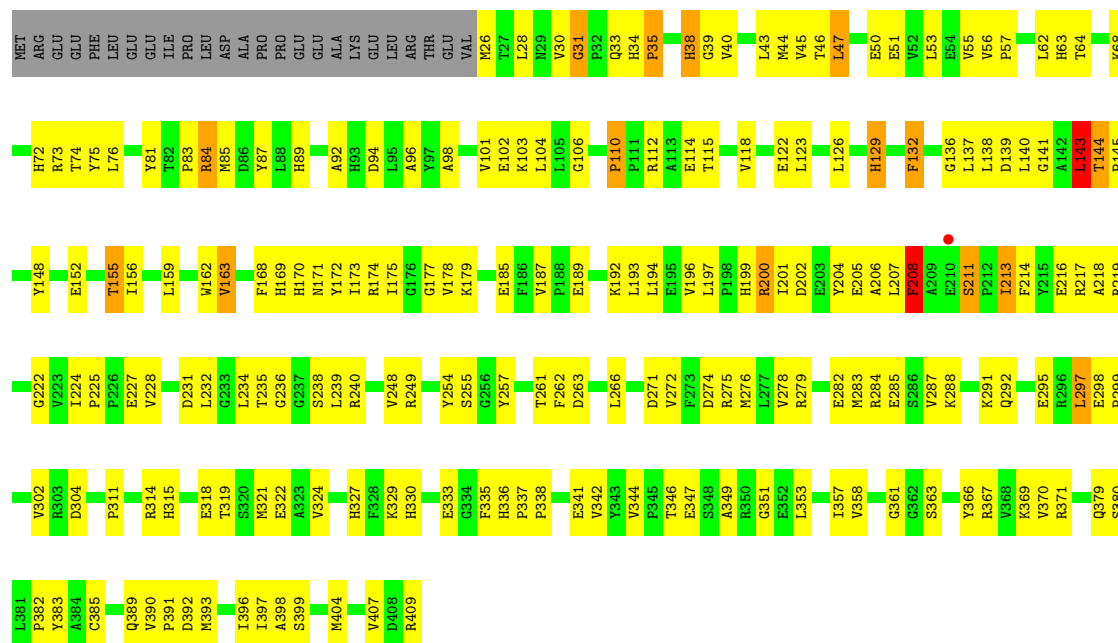
• Molecule 4: NADH-quinone oxidoreductase subunit 4

Chain 4: 42% 47% 6%



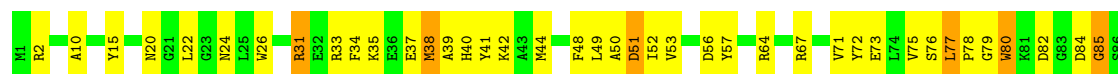
• Molecule 4: NADH-quinone oxidoreductase subunit 4

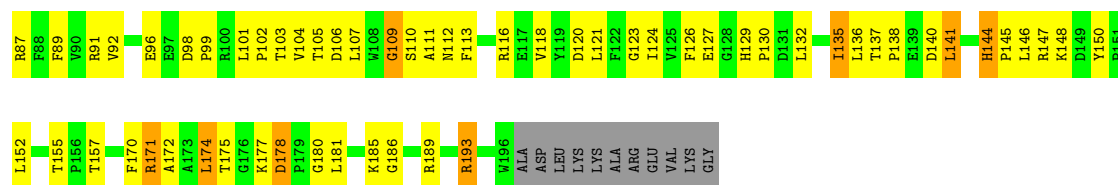
Chain E: 45% 44% 6%



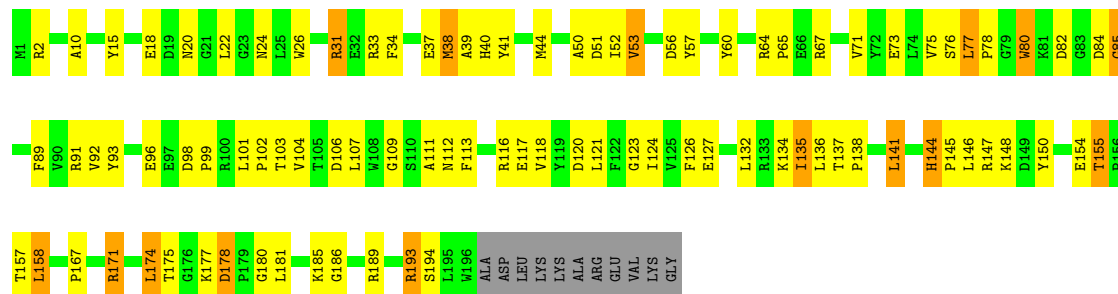
• Molecule 5: NADH-quinone oxidoreductase subunit 5

Chain 5: 47% 41% 7% 5%

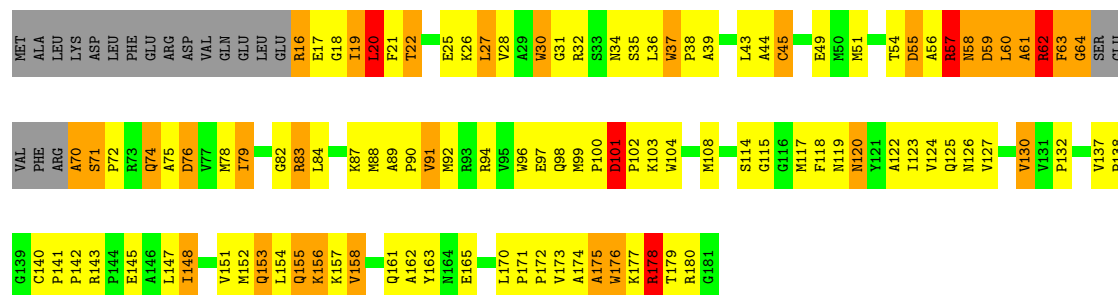




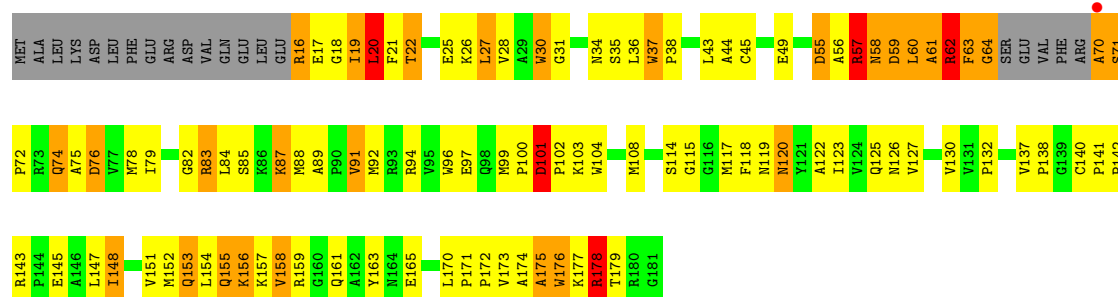
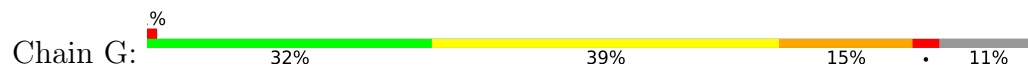
• Molecule 5: NADH-quinone oxidoreductase subunit 5



• Molecule 6: NADH-quinone oxidoreductase subunit 6

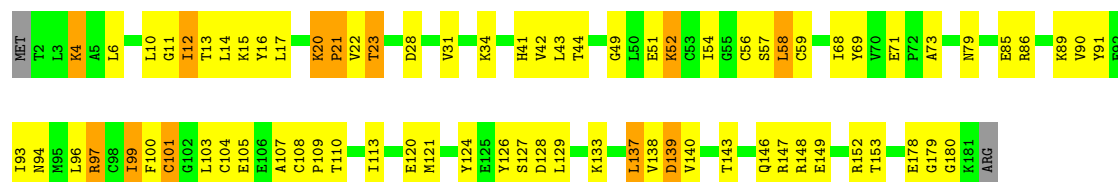


• Molecule 6: NADH-quinone oxidoreductase subunit 6



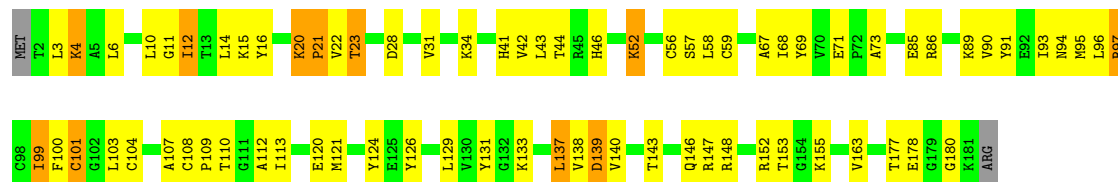
• Molecule 7: NADH-quinone oxidoreductase subunit 9





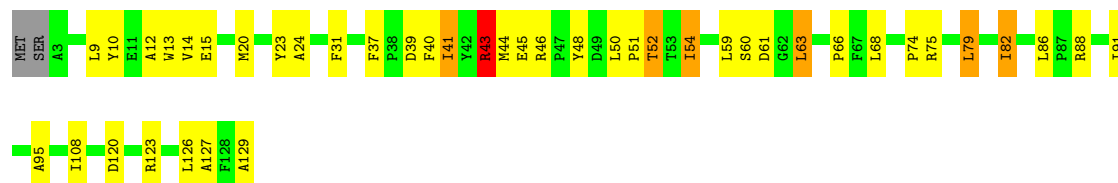
• Molecule 7: NADH-quinone oxidoreductase subunit 9

Chain O: 58% 35% 6% •



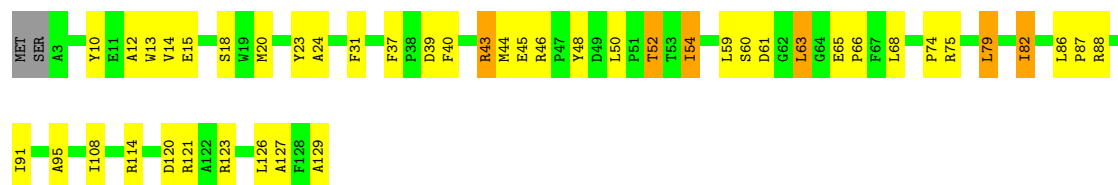
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain 7: 65% 28% 5% ••



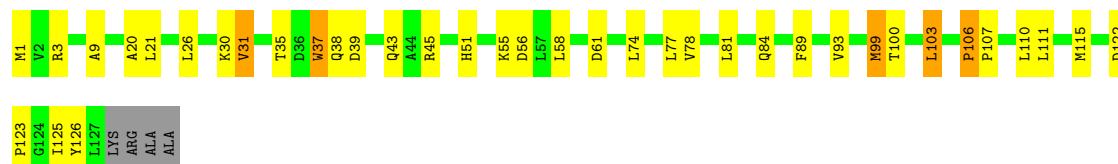
• Molecule 8: NADH-quinone oxidoreductase subunit 15

Chain I: 64% 30% 5% •



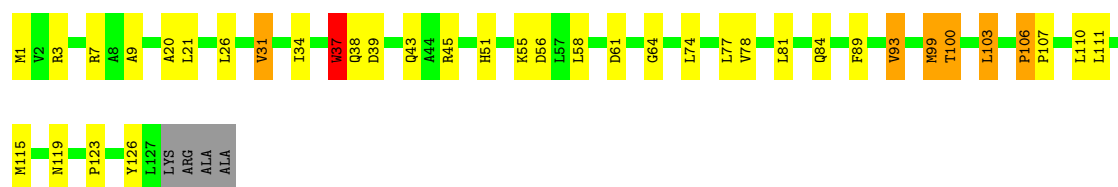
• Molecule 9: Putative uncharacterized protein TTHA1528

Chain W: 68% 25% ••



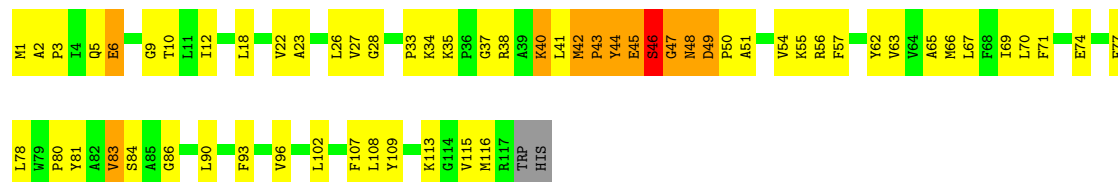
• Molecule 9: Putative uncharacterized protein TTHA1528

Chain X: 68% 24% 5% ••



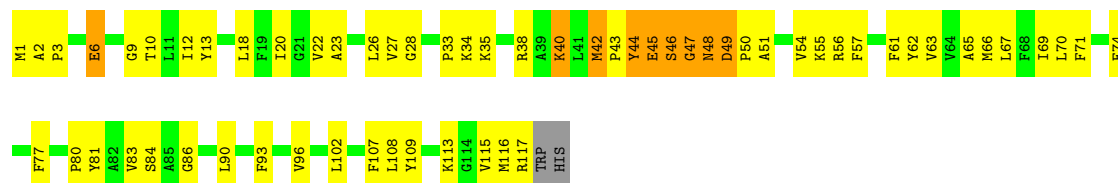
- Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain A: 47% 42% 8% ..



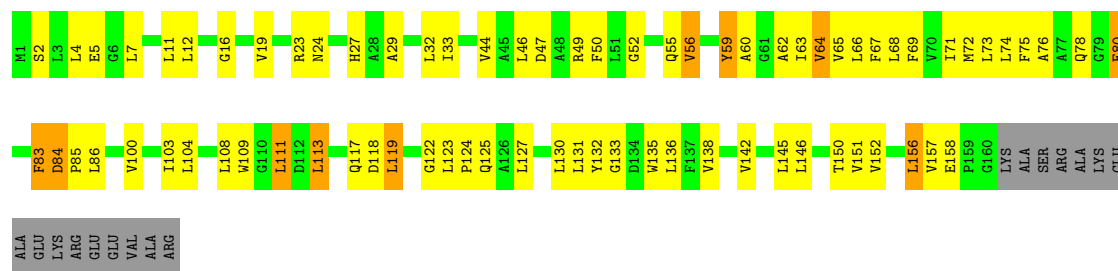
- Molecule 10: NADH-quinone oxidoreductase subunit 7

Chain P: 47% 44% 8% .



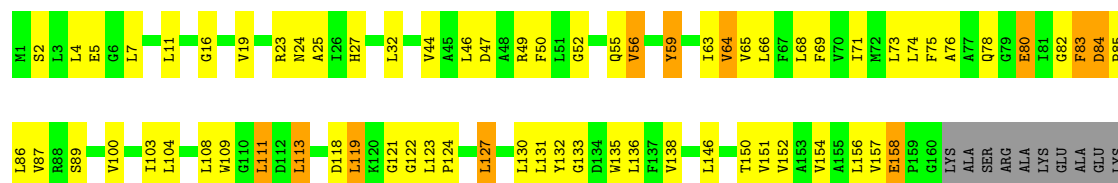
- Molecule 11: NADH-quinone oxidoreductase subunit 10

Chain J: 48% 37% 6% 9%



- Molecule 11: NADH-quinone oxidoreductase subunit 10

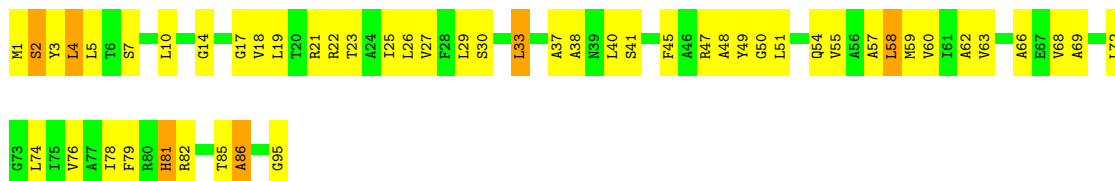
Chain R: 51% 34% 6% 9%



ARG
GLU
GLU
VAL
ALA
ARG

• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain K: 46% 47% 6%



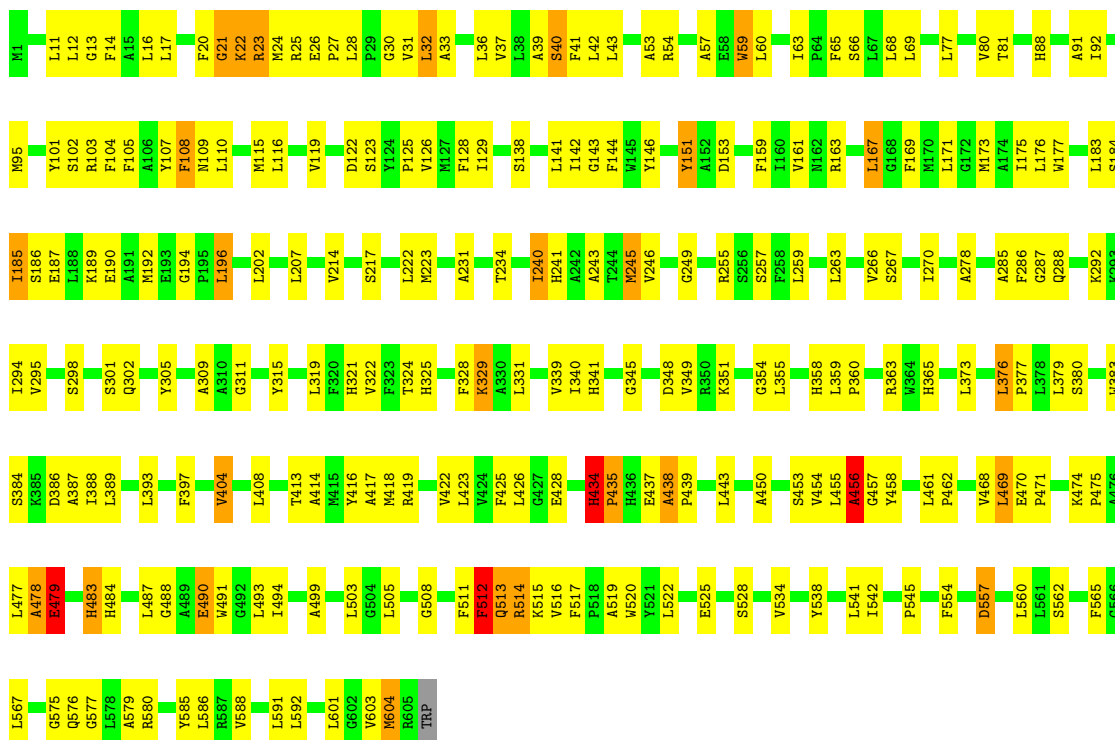
• Molecule 12: NADH-quinone oxidoreductase subunit 11

Chain S: 56% 39% 5%



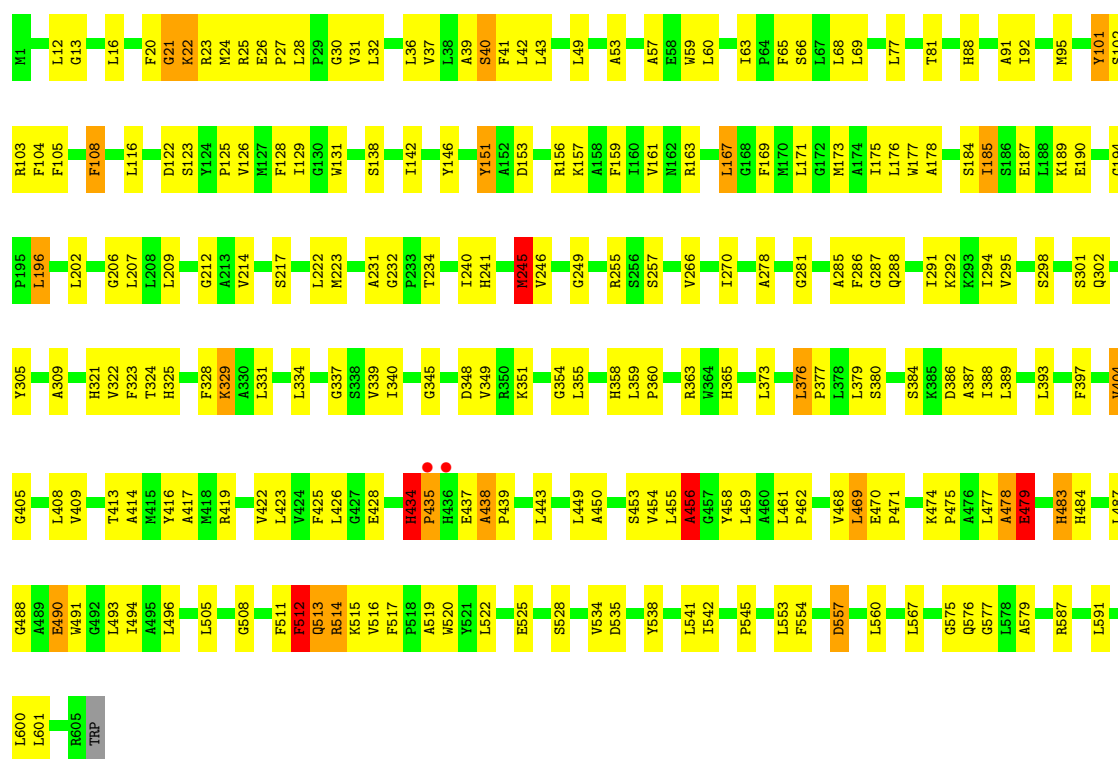
• Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain L: 59% 35% 6%



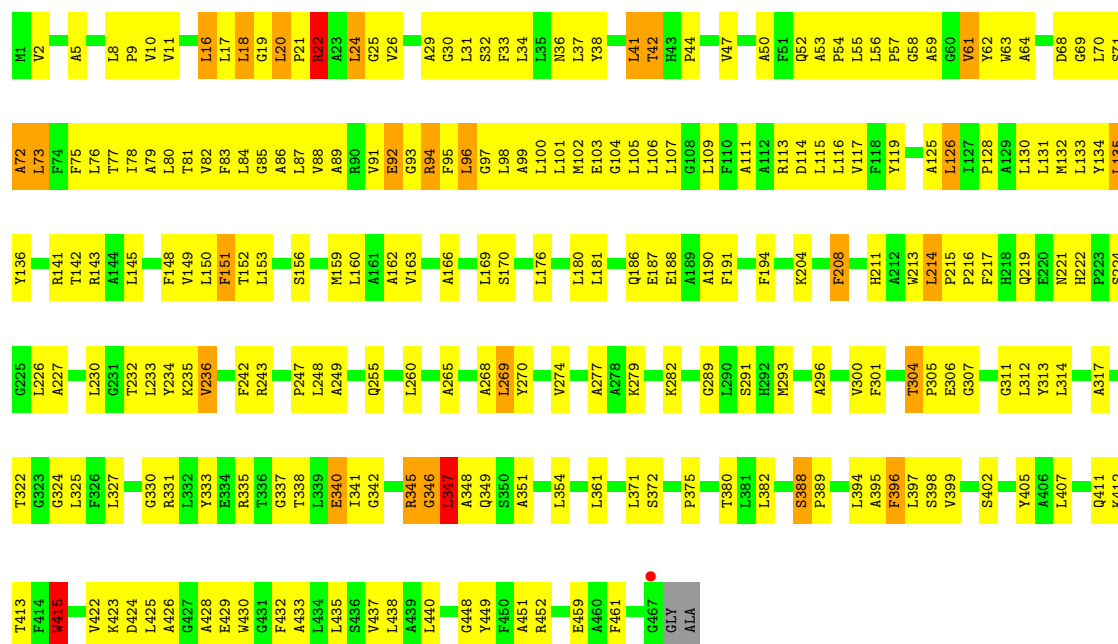
• Molecule 13: NADH-quinone oxidoreductase subunit 12

Chain T:  62% 33% . .



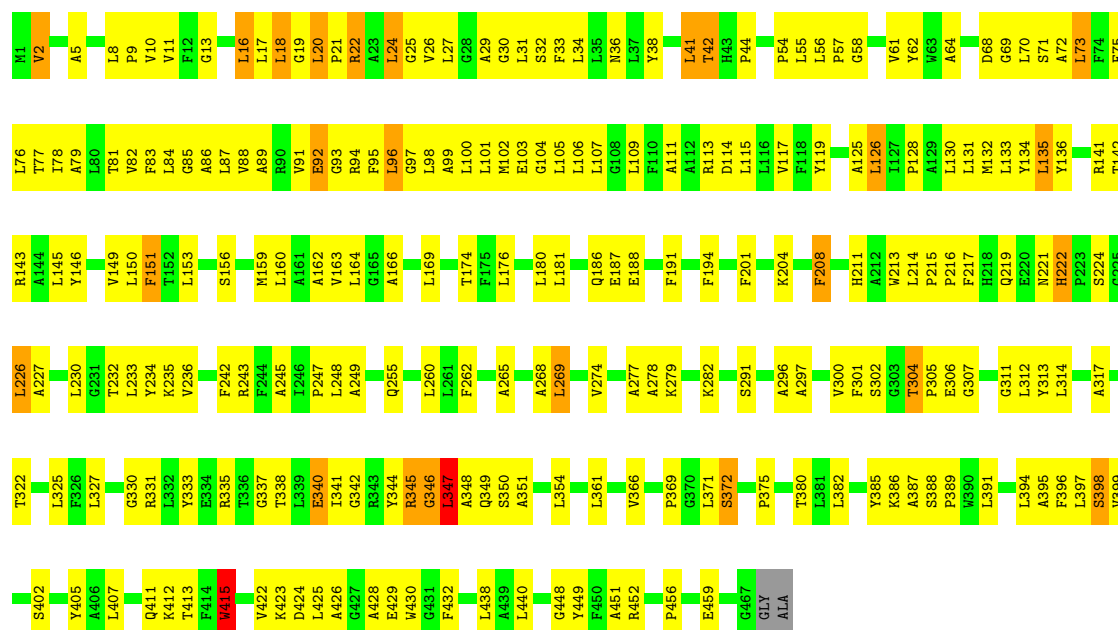
• Molecule 14: NADH-quinone oxidoreductase subunit 13

Chain M:  49% 44% 5% .



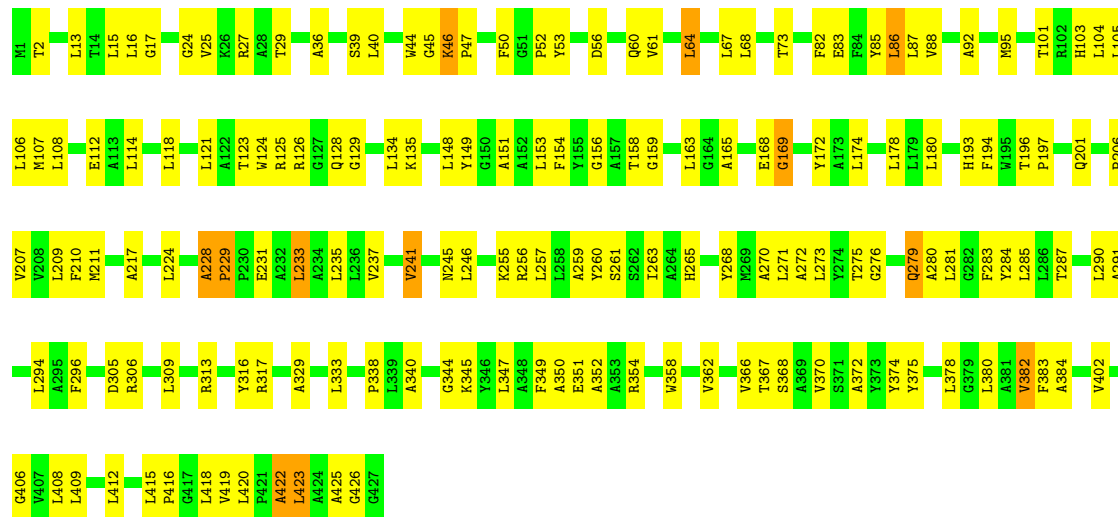
• Molecule 14: NADH-quinone oxidoreductase subunit 13

Chain U:  49% 45% 5%



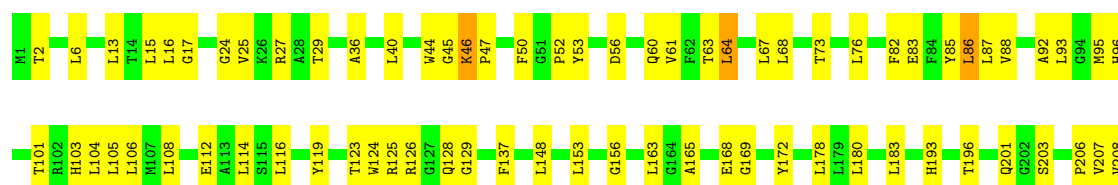
• Molecule 15: NADH-quinone oxidoreductase subunit 14

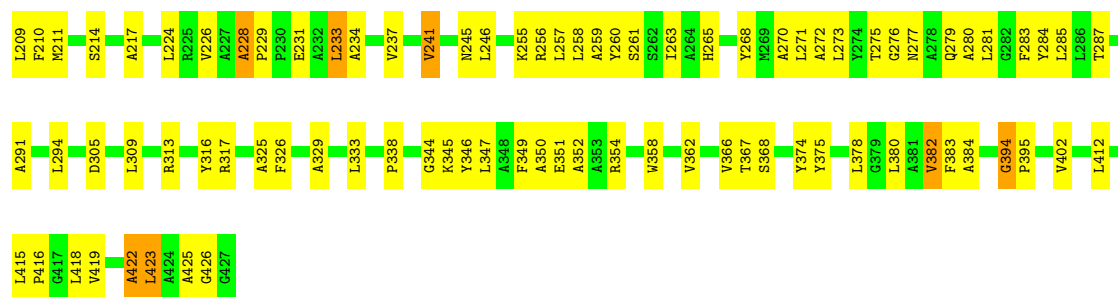
Chain N:  62% 35% 3%



• Molecule 15: NADH-quinone oxidoreductase subunit 14

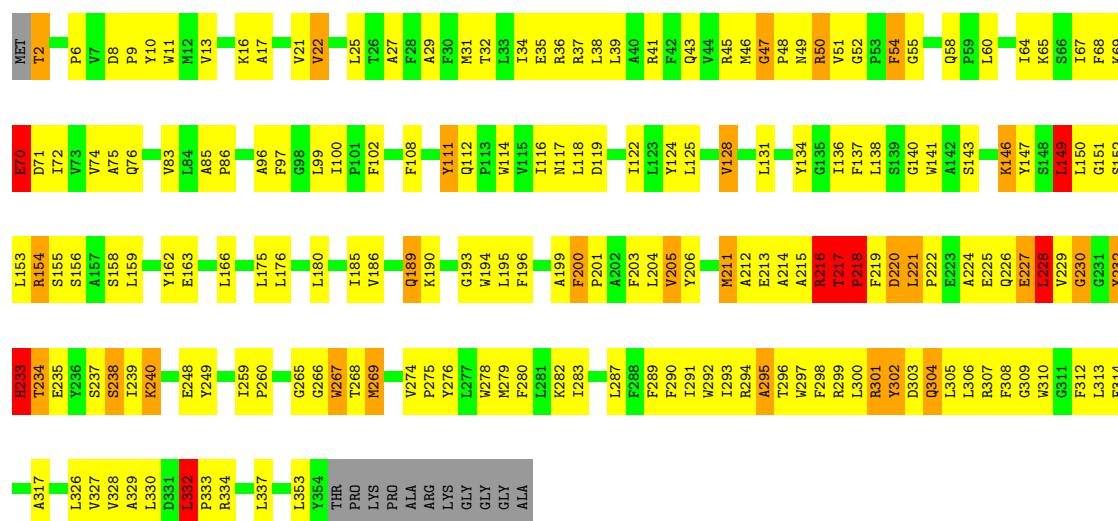
Chain V:  63% 35% 2%





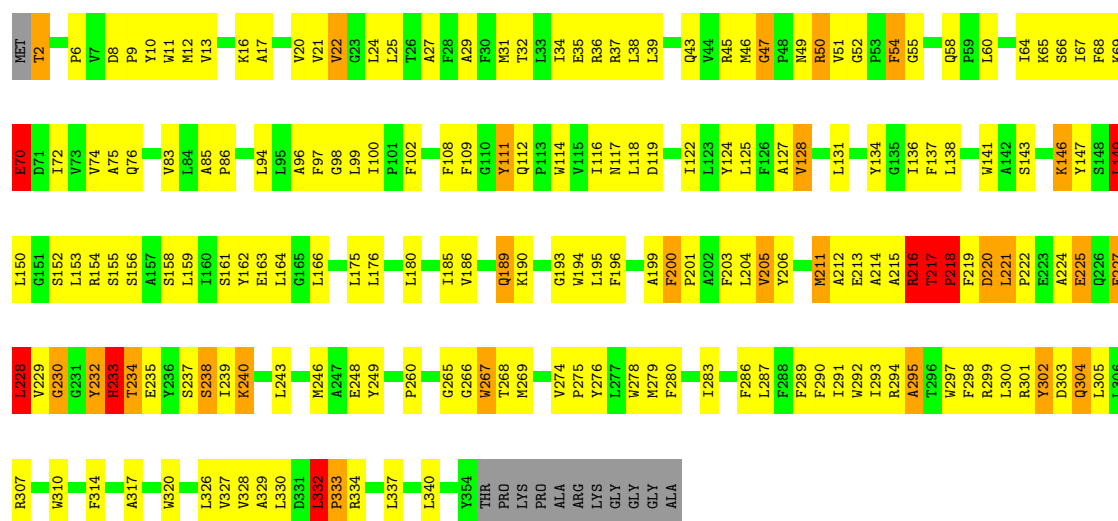
• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain H: 45% 42% 7% . .



• Molecule 16: NADH-quinone oxidoreductase subunit 8

Chain Q: 45% 42% 7% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.28Å 340.89Å 263.30Å 90.00° 100.57° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 40.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.7 (40.00-3.30) 93.7 (40.00-3.30)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1041)	Depositor
R, R_{free}	0.202 , 0.239 0.202 , 0.234	Depositor DCC
R_{free} test set	2417 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 16.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.377 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.470 for -h,-k,h+1	Depositor
Outliers	0 of 233384 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	73998	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.45	0/3506	0.98	7/4745 (0.1%)
1	B	0.44	0/3506	0.97	8/4745 (0.2%)
2	2	0.51	0/1439	1.05	8/1953 (0.4%)
2	C	0.50	0/1439	1.03	7/1953 (0.4%)
3	3	0.59	0/6035	1.17	51/8185 (0.6%)
3	D	0.57	0/6035	1.15	45/8185 (0.5%)
4	4	0.54	0/3150	1.14	24/4284 (0.6%)
4	E	0.52	0/3150	1.11	25/4284 (0.6%)
5	5	0.48	0/1656	1.10	7/2246 (0.3%)
5	F	0.45	0/1656	1.07	10/2246 (0.4%)
6	6	0.76	1/1273 (0.1%)	1.46	24/1723 (1.4%)
6	G	0.77	1/1273 (0.1%)	1.45	23/1723 (1.3%)
7	9	0.64	0/1423	1.19	12/1933 (0.6%)
7	O	0.59	0/1423	1.15	7/1933 (0.4%)
8	7	0.50	0/1059	1.00	3/1429 (0.2%)
8	I	0.43	0/1059	0.96	1/1429 (0.1%)
9	W	0.52	0/985	1.10	7/1335 (0.5%)
9	X	0.52	0/985	1.10	10/1335 (0.7%)
10	A	0.53	0/940	1.14	10/1280 (0.8%)
10	P	0.52	0/940	1.12	6/1280 (0.5%)
11	J	0.50	0/1206	0.97	2/1649 (0.1%)
11	R	0.54	0/1206	0.97	2/1649 (0.1%)
12	K	0.51	0/710	0.96	0/962
12	S	0.50	0/710	0.95	0/962
13	L	0.47	0/4741	1.05	25/6460 (0.4%)
13	T	0.46	0/4741	1.04	23/6460 (0.4%)
14	M	0.52	0/3591	1.08	21/4896 (0.4%)
14	U	0.54	0/3591	1.07	22/4896 (0.4%)
15	N	0.48	1/3238 (0.0%)	1.05	13/4434 (0.3%)
15	V	0.47	0/3238	1.02	14/4434 (0.3%)
16	H	0.63	1/2935 (0.0%)	1.16	21/4014 (0.5%)
16	Q	0.63	1/2935 (0.0%)	1.16	18/4014 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.53	5/75774 (0.0%)	1.10	456/103056 (0.4%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	149	LEU	CA-C	-6.12	1.45	1.52
6	G	63	PHE	CA-C	-5.87	1.45	1.52
15	N	229	PRO	CA-C	5.78	1.55	1.51
6	6	63	PHE	CA-C	-5.16	1.46	1.52
16	H	149	LEU	CA-C	-5.06	1.46	1.52

All (456) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	228	ALA	CA-C-N	14.85	130.50	119.66
15	N	228	ALA	C-N-CA	14.85	130.50	119.66
6	6	59	ASP	N-CA-C	-14.55	98.03	114.62
6	G	59	ASP	N-CA-C	-14.53	98.06	114.62
15	V	228	ALA	CA-C-N	13.95	129.84	119.66
15	V	228	ALA	C-N-CA	13.95	129.84	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	218	LEU	CA-C-N	11.54	131.24	119.24
3	D	218	LEU	C-N-CA	11.54	131.24	119.24
6	G	76	ASP	N-CA-C	11.36	125.00	111.82
3	3	115	HIS	CA-C-N	11.28	131.15	119.19
3	3	115	HIS	C-N-CA	11.28	131.15	119.19
4	4	208	PHE	N-CA-C	10.99	123.00	111.14
6	6	76	ASP	N-CA-C	10.87	124.43	111.82
6	G	62	ARG	N-CA-C	-10.83	92.45	109.23
3	D	571	VAL	CA-C-N	10.69	131.39	120.38
3	D	571	VAL	C-N-CA	10.69	131.39	120.38
6	6	62	ARG	N-CA-C	-10.62	92.77	109.23
4	E	208	PHE	N-CA-C	10.53	122.51	111.14
10	P	116	MET	N-CA-C	-10.28	100.00	112.54
3	3	218	LEU	CA-C-N	10.15	129.79	119.24
3	3	218	LEU	C-N-CA	10.15	129.79	119.24
14	M	345	ARG	N-CA-C	9.94	122.19	111.36
6	6	20	LEU	N-CA-C	9.73	124.69	112.24
14	U	345	ARG	N-CA-C	9.72	121.95	111.36
6	G	20	LEU	N-CA-C	9.67	124.61	112.24
1	1	331	ILE	CA-C-N	9.37	129.31	119.85
1	1	331	ILE	C-N-CA	9.37	129.31	119.85
1	B	331	ILE	CA-C-N	9.00	129.68	120.14
1	B	331	ILE	C-N-CA	9.00	129.68	120.14
3	D	115	HIS	CA-C-N	8.93	128.66	119.19
3	D	115	HIS	C-N-CA	8.93	128.66	119.19
10	A	116	MET	N-CA-C	-8.89	101.69	112.54
3	3	651	ARG	CA-C-N	8.86	126.04	119.66
3	3	651	ARG	C-N-CA	8.86	126.04	119.66
15	N	423	LEU	N-CA-C	-8.80	101.51	113.30
10	A	47	GLY	N-CA-C	-8.78	102.34	114.64
4	4	143	LEU	N-CA-C	8.65	120.71	111.28
4	4	238	SER	N-CA-C	-8.63	102.29	113.17
16	Q	220	ASP	N-CA-C	-8.56	99.48	111.81
4	4	302	VAL	N-CA-C	8.55	122.11	113.47
15	V	279	GLN	N-CA-C	-8.54	101.19	111.69
15	N	279	GLN	N-CA-C	-8.48	101.26	111.69
15	V	423	LEU	N-CA-C	-8.44	101.99	113.30
6	6	155	GLN	N-CA-C	-8.39	101.72	111.03
6	G	155	GLN	N-CA-C	-8.31	101.81	111.03
5	5	77	LEU	CA-C-N	8.29	128.01	119.56
5	5	77	LEU	C-N-CA	8.29	128.01	119.56
7	O	3	LEU	N-CA-C	8.29	121.36	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	571	VAL	CA-C-N	8.27	128.90	120.38
3	3	571	VAL	C-N-CA	8.27	128.90	120.38
3	D	651	ARG	CA-C-N	8.25	125.60	119.66
3	D	651	ARG	C-N-CA	8.25	125.60	119.66
4	E	143	LEU	N-CA-C	8.22	120.24	111.28
3	3	728	LEU	CA-C-N	8.21	128.14	119.85
3	3	728	LEU	C-N-CA	8.21	128.14	119.85
16	Q	97	PHE	N-CA-C	-8.19	103.30	113.38
16	H	303	ASP	N-CA-C	-8.17	102.32	111.14
3	D	441	MET	CA-C-N	8.16	127.92	119.76
3	D	441	MET	C-N-CA	8.16	127.92	119.76
13	T	513	GLN	N-CA-C	8.14	121.18	111.33
16	H	217	THR	CA-C-N	-8.09	109.73	119.84
16	H	217	THR	C-N-CA	-8.09	109.73	119.84
16	H	220	ASP	N-CA-C	-8.05	100.21	111.81
10	P	47	GLY	N-CA-C	-8.04	103.38	114.64
11	J	83	PHE	N-CA-C	7.93	121.48	108.08
4	E	238	SER	N-CA-C	-7.92	103.19	113.17
13	T	22	LYS	N-CA-C	-7.85	103.42	113.16
9	X	106	PRO	CA-C-N	7.83	127.38	119.24
9	X	106	PRO	C-N-CA	7.83	127.38	119.24
6	6	120	ASN	N-CA-C	7.78	118.84	107.88
13	T	514	ARG	N-CA-C	7.78	127.36	110.80
11	R	83	PHE	N-CA-C	7.75	121.19	108.08
7	9	21	PRO	N-CA-C	7.74	124.54	113.47
4	E	235	THR	N-CA-C	7.71	119.77	111.36
6	G	174	ALA	N-CA-C	-7.67	99.13	110.48
13	L	22	LYS	N-CA-C	-7.65	103.68	113.16
3	3	116	PRO	N-CA-C	7.64	123.58	113.57
7	O	22	VAL	N-CA-C	7.62	119.66	109.37
3	3	40	SER	CA-C-N	-7.59	112.17	119.76
3	3	40	SER	C-N-CA	-7.59	112.17	119.76
7	9	22	VAL	N-CA-C	7.52	119.53	109.37
6	6	174	ALA	N-CA-C	-7.52	99.36	110.48
7	O	153	THR	N-CA-C	-7.41	103.32	113.18
4	4	235	THR	N-CA-C	7.41	119.44	111.36
13	L	514	ARG	N-CA-C	7.38	126.52	110.80
2	2	168	LEU	CA-C-N	7.37	127.42	119.90
2	2	168	LEU	C-N-CA	7.37	127.42	119.90
6	6	170	LEU	CA-C-N	7.35	127.95	120.38
6	6	170	LEU	C-N-CA	7.35	127.95	120.38
7	9	153	THR	N-CA-C	-7.33	103.44	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	116	PRO	N-CA-C	7.24	123.06	113.57
6	G	120	ASN	N-CA-C	7.24	118.08	107.88
6	6	19	ILE	N-CA-C	7.20	119.19	108.96
9	W	9	ALA	CA-C-N	7.20	126.73	119.24
9	W	9	ALA	C-N-CA	7.20	126.73	119.24
13	L	513	GLN	N-CA-C	7.18	120.02	111.33
6	6	71	SER	N-CA-C	-7.16	100.21	110.08
15	N	228	ALA	N-CA-C	7.15	118.36	109.57
6	G	170	LEU	CA-C-N	7.15	127.74	120.38
6	G	170	LEU	C-N-CA	7.15	127.74	120.38
14	M	304	THR	CA-C-N	7.10	128.72	119.84
14	M	304	THR	C-N-CA	7.10	128.72	119.84
6	G	19	ILE	N-CA-C	7.06	118.99	108.96
7	9	52	LYS	N-CA-C	-7.04	103.66	111.82
16	Q	217	THR	CA-C-N	-7.04	111.05	119.84
16	Q	217	THR	C-N-CA	-7.04	111.05	119.84
16	H	97	PHE	N-CA-C	-7.00	104.77	113.38
16	Q	225	GLU	N-CA-C	7.00	125.71	110.80
4	4	213	ILE	N-CA-C	-7.00	105.54	111.56
6	G	37	TRP	CA-C-N	6.99	127.38	119.83
6	G	37	TRP	C-N-CA	6.99	127.38	119.83
13	T	479	GLU	N-CA-C	6.97	118.53	111.07
5	F	144	HIS	CA-C-N	6.96	126.48	119.24
5	F	144	HIS	C-N-CA	6.96	126.48	119.24
13	T	194	GLY	CA-C-N	6.93	127.08	119.87
13	T	194	GLY	C-N-CA	6.93	127.08	119.87
13	T	456	ALA	N-CA-C	-6.91	103.44	110.97
3	D	591	HIS	CA-C-N	6.90	126.71	119.05
3	D	591	HIS	C-N-CA	6.90	126.71	119.05
13	L	479	GLU	N-CA-C	6.90	118.45	111.07
14	M	415	TRP	N-CA-C	6.90	119.64	111.71
14	U	397	LEU	N-CA-C	-6.89	96.57	108.56
4	4	141	GLY	N-CA-C	-6.89	103.09	112.52
13	L	604	MET	N-CA-C	6.87	119.61	111.71
16	Q	303	ASP	N-CA-C	-6.87	103.72	111.14
14	U	214	LEU	CA-C-N	-6.83	113.34	120.38
14	U	214	LEU	C-N-CA	-6.83	113.34	120.38
4	E	110	PRO	CA-C-N	6.81	126.32	119.24
4	E	110	PRO	C-N-CA	6.81	126.32	119.24
9	W	106	PRO	CA-C-N	6.78	126.29	119.24
9	W	106	PRO	C-N-CA	6.78	126.29	119.24
14	M	397	LEU	N-CA-C	-6.78	96.76	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	H	200	PHE	N-CA-C	6.78	122.71	113.77
5	F	77	LEU	CA-C-N	6.76	126.45	119.56
5	F	77	LEU	C-N-CA	6.76	126.45	119.56
16	H	225	GLU	N-CA-C	6.75	125.17	110.80
3	D	184	CYS	N-CA-C	-6.71	101.86	110.19
7	O	21	PRO	N-CA-C	6.71	123.06	113.47
14	M	388	SER	CA-C-N	6.70	125.94	118.97
14	M	388	SER	C-N-CA	6.70	125.94	118.97
3	D	728	LEU	CA-C-N	6.68	126.59	119.85
3	D	728	LEU	C-N-CA	6.68	126.59	119.85
4	E	304	ASP	CA-C-N	6.67	127.53	120.12
4	E	304	ASP	C-N-CA	6.67	127.53	120.12
4	4	110	PRO	CA-C-N	6.61	126.11	119.24
4	4	110	PRO	C-N-CA	6.61	126.11	119.24
3	D	377	ALA	CA-C-N	6.61	126.64	119.90
3	D	377	ALA	C-N-CA	6.61	126.64	119.90
4	4	397	ILE	N-CA-C	-6.60	105.31	111.45
13	L	456	ALA	N-CA-C	-6.60	103.78	110.97
14	U	304	THR	CA-C-N	6.59	128.08	119.84
14	U	304	THR	C-N-CA	6.59	128.08	119.84
3	3	176	LEU	N-CA-C	6.58	119.13	108.41
14	U	415	TRP	N-CA-C	6.58	119.27	111.71
16	H	230	GLY	N-CA-C	-6.57	104.12	112.54
6	G	64	GLY	N-CA-C	-6.57	94.24	113.30
13	L	194	GLY	CA-C-N	6.57	126.70	119.87
13	L	194	GLY	C-N-CA	6.57	126.70	119.87
7	9	180	GLY	N-CA-C	-6.54	104.89	112.73
4	E	302	VAL	N-CA-C	6.51	120.05	113.47
16	Q	200	PHE	N-CA-C	6.50	122.35	113.77
13	L	387	ALA	N-CA-C	-6.49	104.12	111.07
2	C	168	LEU	CA-C-N	6.49	126.52	119.90
2	C	168	LEU	C-N-CA	6.49	126.52	119.90
14	M	208	PHE	CA-C-N	-6.49	113.00	119.56
14	M	208	PHE	C-N-CA	-6.49	113.00	119.56
14	M	346	GLY	N-CA-C	6.48	120.51	112.73
3	3	216	PHE	N-CA-C	6.48	118.14	111.14
4	E	213	ILE	N-CA-C	-6.47	106.00	111.56
14	U	346	GLY	N-CA-C	6.44	120.46	112.73
14	M	214	LEU	CA-C-N	-6.44	113.75	120.38
14	M	214	LEU	C-N-CA	-6.44	113.75	120.38
3	3	184	CYS	N-CA-C	-6.43	102.21	110.19
15	N	229	PRO	CA-C-N	6.40	126.15	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	229	PRO	C-N-CA	6.40	126.15	119.05
16	H	47	GLY	CA-C-N	6.39	127.83	119.84
16	H	47	GLY	C-N-CA	6.39	127.83	119.84
3	D	176	LEU	N-CA-C	6.39	118.82	108.41
3	3	441	MET	CA-C-N	6.37	126.12	119.76
3	3	441	MET	C-N-CA	6.37	126.12	119.76
5	F	85	GLY	N-CA-C	-6.37	105.57	116.01
14	M	96	LEU	N-CA-C	-6.36	104.63	112.38
15	N	165	ALA	CA-C-N	6.36	125.85	119.24
15	N	165	ALA	C-N-CA	6.36	125.85	119.24
4	E	397	ILE	N-CA-C	-6.35	105.55	111.45
3	3	591	HIS	CA-C-N	6.25	126.44	119.32
3	3	591	HIS	C-N-CA	6.25	126.44	119.32
15	V	394	GLY	CA-C-N	6.24	126.80	120.38
15	V	394	GLY	C-N-CA	6.24	126.80	120.38
4	E	344	VAL	CA-C-N	6.23	126.72	119.99
4	E	344	VAL	C-N-CA	6.23	126.72	119.99
3	D	282	VAL	CA-C-N	6.22	125.91	119.56
3	D	282	VAL	C-N-CA	6.22	125.91	119.56
14	U	96	LEU	N-CA-C	-6.22	104.80	112.38
5	5	144	HIS	CA-C-N	6.20	125.69	119.24
5	5	144	HIS	C-N-CA	6.20	125.69	119.24
6	6	37	TRP	CA-C-N	6.20	126.52	119.83
6	6	37	TRP	C-N-CA	6.20	126.52	119.83
6	6	64	GLY	N-CA-C	-6.19	95.34	113.30
3	3	602	LEU	CA-C-N	6.18	126.39	119.90
3	3	602	LEU	C-N-CA	6.18	126.39	119.90
13	L	474	LYS	N-CA-C	6.18	121.15	112.75
10	P	45	GLU	N-CA-C	6.16	120.37	111.56
8	I	54	ILE	N-CA-C	6.15	116.97	107.99
16	H	54	PHE	N-CA-C	-6.14	105.55	113.16
14	U	208	PHE	CA-C-N	-6.13	113.37	119.56
14	U	208	PHE	C-N-CA	-6.13	113.37	119.56
4	4	298	GLU	CA-C-N	6.11	126.12	119.89
4	4	298	GLU	C-N-CA	6.11	126.12	119.89
2	2	4	PHE	N-CA-C	-6.10	105.59	113.16
3	3	387	LEU	N-CA-C	6.10	118.43	111.11
9	X	9	ALA	CA-C-N	6.09	125.58	119.24
9	X	9	ALA	C-N-CA	6.09	125.58	119.24
2	C	4	PHE	N-CA-C	-6.09	105.61	113.16
4	4	109	VAL	CA-C-N	6.07	126.63	120.38
4	4	109	VAL	C-N-CA	6.07	126.63	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	178	ARG	N-CA-C	-6.06	99.76	108.60
6	G	71	SER	N-CA-C	-6.06	101.72	110.08
13	T	232	GLY	CA-C-N	6.05	126.07	119.90
13	T	232	GLY	C-N-CA	6.05	126.07	119.90
10	P	44	TYR	N-CA-C	6.03	118.87	109.52
3	D	194	VAL	CA-C-N	-6.02	112.32	119.84
3	D	194	VAL	C-N-CA	-6.02	112.32	119.84
13	L	577	GLY	N-CA-C	-6.01	105.08	112.77
6	6	176	TRP	N-CA-C	-6.00	105.95	113.28
16	H	199	ALA	N-CA-C	6.00	120.30	112.92
4	4	344	VAL	CA-C-N	6.00	126.47	119.99
4	4	344	VAL	C-N-CA	6.00	126.47	119.99
10	A	44	TYR	N-CA-C	6.00	118.82	109.52
13	T	474	LYS	N-CA-C	5.99	120.90	112.75
15	V	165	ALA	CA-C-N	5.98	125.46	119.24
15	V	165	ALA	C-N-CA	5.98	125.46	119.24
3	3	362	LYS	N-CA-C	-5.98	104.40	111.03
4	E	141	GLY	N-CA-C	-5.98	104.33	112.52
6	6	74	GLN	N-CA-C	-5.97	104.65	113.61
14	U	22	ARG	NE-CZ-NH2	-5.94	113.85	119.20
6	G	74	GLN	N-CA-C	-5.93	104.71	113.61
14	U	156	SER	N-CA-C	5.93	117.55	111.14
3	D	652	PRO	CA-C-N	5.91	125.61	119.64
3	D	652	PRO	C-N-CA	5.91	125.61	119.64
3	D	216	PHE	N-CA-C	5.91	117.52	111.14
3	3	229	ILE	N-CA-C	5.90	116.08	110.53
2	2	56	THR	CA-C-N	5.90	125.60	119.05
2	2	56	THR	C-N-CA	5.90	125.60	119.05
4	4	304	ASP	CA-C-N	5.90	126.67	120.12
4	4	304	ASP	C-N-CA	5.90	126.67	120.12
13	L	438	ALA	N-CA-C	5.89	120.11	109.44
9	W	20	ALA	N-CA-C	5.89	118.65	111.82
2	2	139	GLU	CA-C-N	5.87	127.17	119.84
2	2	139	GLU	C-N-CA	5.87	127.17	119.84
15	V	228	ALA	N-CA-C	5.87	116.78	109.57
3	D	566	ALA	N-CA-C	5.86	118.31	109.23
14	M	22	ARG	NE-CZ-NH2	-5.85	113.93	119.20
15	V	229	PRO	CA-C-N	5.84	125.54	119.05
15	V	229	PRO	C-N-CA	5.84	125.54	119.05
13	T	387	ALA	N-CA-C	-5.84	104.83	111.07
14	U	2	VAL	N-CA-C	5.84	116.02	110.42
6	G	176	TRP	N-CA-C	-5.83	106.17	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	47	LEU	N-CA-C	5.79	117.69	107.61
3	D	184	CYS	CA-C-N	-5.78	113.58	122.60
3	D	184	CYS	C-N-CA	-5.78	113.58	122.60
3	D	410	HIS	N-CA-C	-5.78	104.98	111.28
10	A	42	MET	CA-C-N	5.77	127.06	119.84
10	A	42	MET	C-N-CA	5.77	127.06	119.84
14	M	94	ARG	N-CA-C	-5.76	104.93	113.40
10	A	45	GLU	N-CA-C	5.75	119.78	111.56
3	3	422	PRO	CA-C-N	5.75	125.72	120.03
3	3	422	PRO	C-N-CA	5.75	125.72	120.03
4	E	298	GLU	CA-C-N	5.75	125.75	119.89
4	E	298	GLU	C-N-CA	5.75	125.75	119.89
13	T	438	ALA	N-CA-C	5.74	119.83	109.44
5	5	85	GLY	N-CA-C	-5.74	106.60	116.01
13	L	240	ILE	N-CA-C	5.73	115.92	110.42
5	F	158	LEU	N-CA-C	5.72	118.72	109.40
7	O	20	LYS	N-CA-C	5.72	122.45	109.81
13	L	512	PHE	N-CA-CB	-5.71	103.00	110.88
3	3	14	PRO	CA-C-N	5.71	125.18	119.24
3	3	14	PRO	C-N-CA	5.71	125.18	119.24
6	6	37	TRP	CB-CA-C	-5.71	104.72	110.65
13	T	512	PHE	N-CA-CB	-5.70	103.02	110.88
16	Q	233	HIS	N-CA-C	-5.69	103.19	110.53
13	L	434	HIS	CA-C-N	-5.69	112.73	119.84
13	L	434	HIS	C-N-CA	-5.69	112.73	119.84
3	3	377	ALA	CA-C-N	5.68	125.70	119.90
3	3	377	ALA	C-N-CA	5.68	125.70	119.90
8	7	41	ILE	CB-CA-C	-5.68	104.43	111.70
3	3	372	GLN	N-CA-C	5.67	119.01	111.75
7	O	52	LYS	N-CA-C	-5.67	105.24	111.82
7	9	20	LYS	N-CA-C	5.67	122.34	109.81
16	H	111	TYR	N-CA-C	5.67	117.14	108.30
16	H	233	HIS	N-CA-C	-5.67	103.22	110.53
3	3	282	VAL	CA-C-N	5.67	125.34	119.56
3	3	282	VAL	C-N-CA	5.67	125.34	119.56
8	7	54	ILE	N-CA-C	5.66	116.26	107.99
1	B	291	ILE	CA-C-N	5.65	126.91	119.84
1	B	291	ILE	C-N-CA	5.65	126.91	119.84
9	X	20	ALA	N-CA-C	5.65	118.37	111.82
8	7	43	ARG	N-CA-C	-5.63	101.70	110.10
3	3	566	ALA	N-CA-C	5.63	117.95	109.23
13	L	376	LEU	CA-C-N	5.63	126.87	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	376	LEU	C-N-CA	5.63	126.87	119.84
6	G	79	ILE	N-CA-C	5.62	115.69	107.37
13	T	40	SER	N-CA-C	-5.60	98.86	110.80
3	D	14	PRO	CA-C-N	5.59	125.06	119.24
3	D	14	PRO	C-N-CA	5.59	125.06	119.24
3	D	387	LEU	N-CA-C	5.59	117.82	111.11
3	3	184	CYS	CA-C-N	-5.58	113.89	122.60
3	3	184	CYS	C-N-CA	-5.58	113.89	122.60
3	D	422	PRO	CA-C-N	5.56	125.53	120.03
3	D	422	PRO	C-N-CA	5.56	125.53	120.03
16	Q	199	ALA	N-CA-C	5.55	119.75	112.92
7	O	180	GLY	N-CA-C	-5.54	106.08	112.73
6	6	178	ARG	N-CA-C	-5.54	100.51	108.60
3	3	730	GLU	N-CA-C	5.54	119.13	112.38
14	M	69	GLY	N-CA-C	-5.53	105.99	113.24
16	Q	332	LEU	CA-C-N	-5.53	112.92	119.84
16	Q	332	LEU	C-N-CA	-5.53	112.92	119.84
2	C	56	THR	CA-C-N	5.53	125.19	119.05
2	C	56	THR	C-N-CA	5.53	125.19	119.05
3	3	42	ILE	N-CA-C	-5.53	100.10	108.17
16	Q	230	GLY	N-CA-C	-5.53	105.47	112.54
14	U	398	SER	N-CA-C	-5.52	99.04	110.80
16	H	332	LEU	CA-C-N	-5.52	112.94	119.84
16	H	332	LEU	C-N-CA	-5.52	112.94	119.84
1	B	363	VAL	N-CA-C	5.51	115.60	110.42
3	D	372	GLN	N-CA-C	5.51	118.81	111.75
6	6	130	VAL	N-CA-C	5.51	117.42	111.58
14	M	156	SER	N-CA-C	5.51	117.09	111.14
3	3	259	CYS	CA-C-N	-5.50	114.10	120.04
3	3	259	CYS	C-N-CA	-5.50	114.10	120.04
16	Q	111	TYR	N-CA-C	5.49	116.86	108.30
16	H	140	GLY	N-CA-C	-5.48	106.14	112.50
10	A	37	GLY	N-CA-C	-5.48	102.80	110.96
3	3	124	LYS	N-CA-C	-5.47	106.56	113.18
3	3	189	ARG	N-CA-C	-5.47	105.22	111.07
7	9	79	ASN	CA-C-N	5.46	125.66	120.31
7	9	79	ASN	C-N-CA	5.46	125.66	120.31
16	H	154	ARG	N-CA-C	-5.46	104.56	111.11
4	E	407	VAL	N-CA-C	5.46	120.69	109.34
7	9	128	ASP	N-CA-C	-5.45	106.13	112.89
3	D	189	ARG	N-CA-C	-5.45	105.23	111.07
5	F	155	THR	N-CA-C	-5.45	101.91	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	40	SER	N-CA-C	-5.45	99.20	110.80
4	E	84	ARG	N-CA-C	5.44	119.67	113.19
13	L	341	HIS	N-CA-C	-5.44	106.15	112.89
13	T	245	MET	N-CA-CB	5.43	119.67	110.49
13	T	434	HIS	CA-C-N	-5.43	113.05	119.84
13	T	434	HIS	C-N-CA	-5.43	113.05	119.84
3	3	406	ALA	CA-C-N	5.42	126.62	119.84
3	3	406	ALA	C-N-CA	5.42	126.62	119.84
7	9	49	GLY	N-CA-C	-5.41	107.89	114.92
7	9	58	LEU	N-CA-C	-5.41	106.52	113.23
6	6	101	ASP	N-CA-C	5.40	121.74	109.81
9	X	31	VAL	N-CA-C	5.39	115.35	107.37
2	2	91	ALA	N-CA-C	-5.38	106.39	113.17
5	5	109	GLY	N-CA-C	-5.38	106.42	115.62
13	L	196	LEU	CB-CA-C	-5.38	108.80	115.89
4	E	38	HIS	N-CA-C	5.37	118.22	110.28
1	1	102	LYS	N-CA-C	5.36	118.28	111.69
4	E	144	THR	CA-C-N	-5.36	114.50	120.45
4	E	144	THR	C-N-CA	-5.36	114.50	120.45
13	T	196	LEU	CB-CA-C	-5.35	108.83	115.89
15	N	169	GLY	CA-C-N	5.34	126.52	119.84
15	N	169	GLY	C-N-CA	5.34	126.52	119.84
16	H	278	TRP	N-CA-C	5.34	117.10	111.28
10	P	42	MET	CA-C-N	5.34	126.51	119.84
10	P	42	MET	C-N-CA	5.34	126.51	119.84
4	4	236	GLY	N-CA-C	5.33	125.82	113.18
9	W	106	PRO	O-C-N	5.33	123.76	121.31
9	X	93	VAL	N-CA-C	5.33	115.53	107.80
4	4	84	ARG	N-CA-C	5.32	119.52	113.19
16	H	301	ARG	N-CA-CB	5.32	119.47	110.49
13	L	23	ARG	N-CA-C	-5.31	106.64	113.02
4	4	47	LEU	N-CA-C	5.30	116.83	107.61
16	Q	47	GLY	CA-C-N	5.29	126.45	119.84
16	Q	47	GLY	C-N-CA	5.29	126.45	119.84
15	V	229	PRO	N-CA-C	5.29	115.55	110.47
16	Q	149	LEU	O-C-N	5.28	127.51	122.07
14	U	69	GLY	N-CA-C	-5.28	106.33	113.24
14	M	72	ALA	N-CA-C	5.27	116.33	108.31
5	5	157	THR	N-CA-C	-5.26	101.95	110.32
1	B	79	MET	CA-C-N	5.26	124.97	119.82
1	B	79	MET	C-N-CA	5.26	124.97	119.82
10	A	46	SER	N-CA-C	5.25	117.58	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	376	LEU	CA-C-N	5.24	126.39	119.84
13	T	376	LEU	C-N-CA	5.24	126.39	119.84
4	4	297	LEU	N-CA-C	5.24	117.16	108.20
3	D	124	LYS	N-CA-C	-5.23	106.85	113.18
13	T	417	ALA	N-CA-C	-5.23	105.58	111.28
14	U	388	SER	CA-C-N	5.23	124.41	118.97
14	U	388	SER	C-N-CA	5.23	124.41	118.97
16	Q	54	PHE	N-CA-C	-5.21	106.69	113.16
13	L	417	ALA	N-CA-C	-5.21	105.60	111.28
9	W	31	VAL	N-CA-C	5.21	115.08	107.37
6	6	27	LEU	N-CA-C	-5.20	105.52	111.14
7	9	179	GLY	N-CA-C	-5.20	107.62	114.95
4	E	31	GLY	CA-C-N	5.20	126.33	119.84
4	E	31	GLY	C-N-CA	5.20	126.33	119.84
15	N	229	PRO	N-CA-C	5.19	115.45	110.47
2	C	139	GLU	CA-C-N	5.19	126.33	119.84
2	C	139	GLU	C-N-CA	5.19	126.33	119.84
5	F	60	TYR	CA-C-N	5.18	125.23	119.32
5	F	60	TYR	C-N-CA	5.18	125.23	119.32
14	U	226	LEU	N-CA-C	-5.18	105.55	111.14
4	4	46	THR	N-CA-C	-5.17	100.65	108.67
3	D	407	PRO	N-CA-C	5.17	123.12	112.47
6	G	37	TRP	CB-CA-C	-5.17	105.28	110.65
6	G	101	ASP	N-CA-C	5.16	121.22	109.81
1	1	291	ILE	CA-C-N	5.16	126.29	119.84
1	1	291	ILE	C-N-CA	5.16	126.29	119.84
15	N	64	LEU	N-CA-C	-5.16	105.55	111.07
6	G	27	LEU	N-CA-C	-5.15	105.58	111.14
11	J	117	GLN	N-CA-C	-5.15	100.91	108.99
4	E	297	LEU	N-CA-C	5.14	117.00	108.20
11	R	82	GLY	N-CA-C	-5.14	108.53	115.21
6	G	60	LEU	CA-C-N	5.13	131.35	121.54
6	G	60	LEU	C-N-CA	5.13	131.35	121.54
9	X	64	GLY	CA-C-N	5.13	124.85	119.82
9	X	64	GLY	C-N-CA	5.13	124.85	119.82
14	U	222	HIS	CA-C-N	5.13	125.42	119.47
14	U	222	HIS	C-N-CA	5.13	125.42	119.47
5	F	53	VAL	N-CA-C	5.12	114.95	107.37
3	3	600	VAL	N-CA-C	5.12	115.41	107.78
3	D	362	LYS	N-CA-C	-5.11	105.36	111.03
10	A	43	PRO	CA-C-N	-5.10	114.58	122.59
10	A	43	PRO	C-N-CA	-5.10	114.58	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	398	VAL	N-CA-C	5.09	115.24	108.11
14	U	372	SER	N-CA-C	5.09	117.50	111.33
9	X	106	PRO	O-C-N	5.08	123.65	121.31
3	3	407	PRO	N-CA-C	5.08	122.94	112.47
6	6	60	LEU	CA-C-N	5.08	131.25	121.54
6	6	60	LEU	C-N-CA	5.08	131.25	121.54
14	M	236	VAL	N-CA-C	5.08	119.92	109.34
16	H	353	LEU	N-CA-C	5.08	119.46	113.16
13	T	101	TYR	N-CA-C	-5.08	105.63	111.07
15	V	64	LEU	N-CA-C	-5.08	105.63	111.07
1	B	102	LYS	N-CA-C	5.08	117.94	111.69
1	1	376	THR	N-CA-C	-5.08	106.77	113.17
14	M	72	ALA	CB-CA-C	-5.08	110.70	116.54
3	3	194	VAL	CA-C-N	-5.07	113.50	119.84
3	3	194	VAL	C-N-CA	-5.07	113.50	119.84
16	Q	278	TRP	N-CA-C	5.07	116.81	111.28
15	V	76	LEU	N-CA-C	5.06	116.88	111.36
1	1	202	LYS	N-CA-C	5.05	120.98	109.81
6	6	79	ILE	N-CA-C	5.05	114.84	107.37
13	T	577	GLY	N-CA-C	-5.05	106.31	112.77
3	D	40	SER	CA-C-N	-5.05	114.71	119.76
3	D	40	SER	C-N-CA	-5.05	114.71	119.76
13	L	512	PHE	N-CA-C	-5.04	107.11	114.12
13	L	11	LEU	N-CA-C	-5.04	100.06	110.80
3	D	45	CYS	N-CA-C	-5.03	106.40	112.54
3	D	608	TYR	N-CA-C	-5.03	105.80	111.28
4	4	407	VAL	N-CA-C	5.03	119.80	109.34
3	3	352	GLU	N-CA-C	-5.02	105.52	111.69
3	D	463	ALA	N-CA-C	-5.02	105.50	110.97
14	M	396	PHE	N-CA-C	5.01	119.03	113.02

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

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Mol	Chain	Res	Type	Group
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
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	150	0
1	B	3417	0	3388	136	0
2	2	1406	0	1373	83	0
2	C	1406	0	1373	80	0
3	3	5895	0	5930	242	0
3	D	5895	0	5930	246	0
4	4	3067	0	3049	200	0
4	E	3067	0	3049	186	0
5	5	1607	0	1574	106	0
5	F	1607	0	1574	89	0
6	6	1245	0	1255	162	0
6	G	1245	0	1255	149	0
7	9	1388	0	1383	67	0
7	O	1388	0	1383	61	0
8	7	1031	0	1029	41	0
8	I	1031	0	1029	43	0
9	W	967	0	1010	30	0
9	X	967	0	1010	27	0
10	A	910	0	939	80	0
10	P	910	0	939	82	0
11	J	1183	0	1286	72	0
11	R	1183	0	1286	64	0
12	K	703	0	747	50	0
12	S	703	0	747	38	0
13	L	4604	0	4734	173	0
13	T	4604	0	4734	159	0
14	M	3489	0	3606	201	0
14	U	3489	0	3606	186	0
15	N	3154	0	3343	118	0
15	V	3154	0	3343	111	0
16	H	2838	0	2903	214	0
16	Q	2838	0	2903	206	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	73998	0	75136	3370	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 23.

All (3370) 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
13:L:189:LYS:HZ1	13:L:479:GLU:HB2	1.27	0.98
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
3:D:115:HIS:HB3	4:E:321:MET:HE3	1.46	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
15:V:92:ALA:HA	15:V:95:MET:HE2	1.52	0.92
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
15:N:92:ALA:HA	15:N:95:MET:HE2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:314:ARG:HB3	8:I:44:MET:HE1	1.54	0.88
4:4:314:ARG:HB3	8:7:44:MET:HE1	1.55	0.88
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
4:4:85:MET:HE1	4:4:370:VAL:HG21	1.57	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
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
13:L:298:SER:OG	13:L:329:LYS:NZ	2.11	0.83
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
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
3:D:117:LEU:N	4:E:321:MET:HE1	1.94	0.81
16:H:72:ILE:HG22	16:H:237:SER:HB3	1.62	0.81
3:D:397:LEU:HD21	3:D:480:LEU:HD13	1.61	0.81
4:E:39:GLY:O	4:E:404:MET:HG3	1.79	0.81
13:T:298:SER:OG	13:T:329:LYS:NZ	2.13	0.81
16:Q:45:ARG:HG3	16:Q:46:MET:H	1.45	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:66:MET:HE2	10:P:67:LEU:HD12	1.63	0.80
10:P:70:LEU:HD13	11:R:150:THR:HG22	1.63	0.80
14:M:224:SER:HA	14:M:330:GLY:HA3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:621:VAL:HG23	3:D:672:ALA:HA	1.62	0.80
6:G:57:ARG:HH11	6:G:57:ARG:HG3	1.47	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
10:P:113:LYS:NZ	15:V:83:GLU:OE2	2.15	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
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
16:H:224:ALA:HA	16:H:230:GLY:H	1.46	0.79
4:E:200:ARG:NH1	7:O:16:TYR:OH	2.15	0.79
3:3:115:HIS:HB3	4:4:321:MET:HE3	1.65	0.79
3:D:117:LEU:H	4:E:321:MET:HE1	1.47	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:HD12	6:6:60:LEU:O	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
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
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
16:H:222:PRO:HD2	16:H:230:GLY:HA2	1.66	0.77
4:E:50:GLU:O	4:E:389:GLN:NE2	2.15	0.77
14:U:224:SER:HA	14:U:330:GLY:HA3	1.67	0.77
6:6:57:ARG:HH11	6:6:57:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:4:28:LEU:HD21	16:H:228:LEU:HD21	1.67	0.77
6:6:57:ARG:HG3	6:6:60:LEU:HD11	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
4:E:85:MET:HE1	4:E:370:VAL:HG21	1.65	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
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
13:L:128:PHE:HB2	13:L:173:MET:HE1	1.66	0.76
14:U:99:ALA:HB2	14:U:226:LEU:HD21	1.66	0.76
4:E:31:GLY:HA3	10:P:45:GLU:HG2	1.68	0.76
6:G:57:ARG:HB3	6:G:60:LEU:O	1.85	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
10:A:66:MET:HE2	10:A:67:LEU:HD12	1.68	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
4:4:318:GLU:HB2	8:7:39:ASP:HA	1.68	0.75
6:6:132:PRO:HG2	6:6:175:ALA:HB2	1.69	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
16:H:150:LEU:HD22	16:H:228:LEU:HD12	1.67	0.75
3:D:584:VAL:HG12	3:D:600:VAL:HB	1.69	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:3:PRO:HD2	16:Q:2:THR:HB	1.68	0.74
14:U:21:PRO:HD2	14:U:24:LEU:HG	1.67	0.74
16:Q:300:LEU:O	16:Q:301:ARG:HG2	1.87	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
3:3:20:MET:HE3	3:3:432:PHE:HB3	1.68	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
6:G:76:ASP:HB3	16:Q:69:LYS:HZ3	1.53	0.74
14:M:21:PRO:HD2	14:M:24:LEU:HG	1.67	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
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
6:G:64:GLY:C	6:G:74:GLN:HB2	2.13	0.73
16:Q:141:TRP:HA	16:Q:149:LEU:HD11	1.70	0.73
3:3:117:LEU:N	4:4:321:MET:HE1	2.03	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
9:W:3:ARG:NH1	9:W:103:LEU:O	2.22	0.73
13:L:60:LEU:HD21	14:M:375:PRO:HB3	1.71	0.73
1:B:104:ARG:HH21	2:C:127:SER:HB3	1.53	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
6:6:64:GLY:C	6:6:74:GLN:HB2	2.14	0.73
10:A:113:LYS:NZ	15:N:83:GLU:OE2	2.19	0.73
15:N:294:LEU:HG	15:N:402:VAL:HG13	1.69	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:H	12:S:81:HIS:CD2	2.04	0.72
12:K:81:HIS:H	12:K:81:HIS:CD2	2.05	0.72
16:H:155:SER:OG	16:H:156:SER:N	2.21	0.72

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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	0.72
4:E:318:GLU:HB2	8:I:39:ASP:HA	1.71	0.72
4:E:28:LEU:HD21	16:Q:228:LEU:HD21	1.71	0.72
16:H:302:TYR:HA	16:H:305:LEU:CB	2.19	0.72
6:G:132:PRO:HA	6:G:178:ARG:HH21	1.53	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
15:V:196:THR:HG22	15:V:259:ALA:HB1	1.70	0.72
16:Q:31:MET:HA	16:Q:34:ILE:HD12	1.70	0.72
2:2:46:ILE:HG23	2:2:60:VAL:HG12	1.71	0.72
2:2:146:THR:HG22	2:2:149:ARG:HB2	1.72	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
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:20:MET:HE3	3:D:432:PHE:HB3	1.72	0.71
6:6:96:TRP:HA	6:6:99:MET:HE3	1.71	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
3:D:655:ARG:HB2	3:D:655:ARG:HH11	1.55	0.71
14:M:16:LEU:HD12	14:M:25:GLY:HA3	1.70	0.71
6:G:57:ARG:NH1	6:G:60:LEU:HD11	2.04	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
13:L:355:LEU:HB3	13:L:359:LEU:HD12	1.72	0.71
16:H:162:TYR:CE1	16:H:305:LEU:HG	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
13:L:434:HIS:HB3	13:L:435:PRO:HD3	1.72	0.70
6:G:61:ALA:O	6:G:62:ARG:HD3	1.91	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
9:W:78:VAL:HG21	9:W:126:TYR:HB2	1.74	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
16:Q:219:PHE:C	16:Q:221:LEU:H	1.97	0.70
1:B:361:GLU:OE1	3:D:114:ASN:ND2	2.25	0.69
4:4:102:GLU:HG2	4:4:175:ILE:O	1.92	0.69
15:N:196:THR:HG22	15:N:259:ALA:HB1	1.74	0.69
3:D:722:THR:HG21	3:D:756:GLY:N	2.06	0.69
12:K:7:SER:HB3	12:K:40:LEU:HD23	1.74	0.69
16:H:176:LEU:HD21	16:H:337:LEU:HD12	1.74	0.69
6:G:57:ARG:HD2	6:G:60:LEU:CG	2.22	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
4:4:341:GLU:OE2	5:5:57:TYR:OH	2.09	0.69
4:4:389:GLN:HG3	4:4:391:PRO:HD2	1.74	0.69
10:A:51:ALA:HB1	16:H:146:LYS:HB2	1.73	0.69
14:M:73:LEU:O	14:M:76:LEU:N	2.26	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: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:Q:267:TRP:CD1	16:Q:268:THR:H	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:M:33:PHE:HA	14:M:79:ALA:HB1	1.75	0.68
16:H:267:TRP:CD1	16:H:268:THR:H	2.10	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
13:L:122:ASP:O	13:L:185:ILE:N	2.25	0.68
6:G:57:ARG:HG3	6:G:60:LEU:CD1	2.24	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
2:C:76:GLY:H	2:C:118:SER:HG	1.41	0.68
13:T:128:PHE:HB2	13:T:173:MET:HE1	1.73	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
6:6:132:PRO:HG3	6:6:178:ARG:NE	2.09	0.68
13:L:187:GLU:HA	13:L:190:GLU:HG2	1.74	0.68
2:C:106:ILE:HD11	2:C:112:THR:HB	1.76	0.68
7:O:43:LEU:HD12	7:O:133:LYS:HG3	1.76	0.68
3:3:47:MET:HE1	3:3:108:VAL:HA	1.74	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
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
9:W:51:HIS:ND1	9:W:56:ASP:OD1	2.27	0.67
14:M:84:LEU:O	14:M:88:VAL:HG12	1.94	0.67
4:E:389:GLN:HG3	4:E:391:PRO:HD2	1.75	0.67
7:O:73:ALA:HB2	7:O:89:LYS:HB2	1.75	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
15:N:108:LEU:HD22	15:N:148:LEU:HD13	1.77	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
16:H:39:LEU:HD22	16:H:295:ALA:HB2	1.77	0.67
16:H:227:GLU:HG2	16:H:228:LEU:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:57:ARG:HG3	6:G:60:LEU:HD11	1.75	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
14:M:29:ALA:HB1	14:M:83:PHE:HA	1.76	0.67
14:M:232:THR:HA	14:M:235:LYS:HZ2	1.60	0.67
14:M:333:TYR:O	14:M:337:GLY:N	2.27	0.67
16:H:158:SER:HA	16:H:306:LEU:HD21	1.77	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
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
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
11:J:68:LEU:HD23	11:J:71:ILE:HD11	1.76	0.67
2:C:24:ARG:HA	2:C:53:VAL:HG22	1.77	0.67
14:U:73:LEU:O	14:U:76:LEU:N	2.28	0.67
14:U:91:VAL:HG12	14:U:222:HIS:ND1	2.10	0.67
16:Q:176:LEU:HD21	16:Q:337:LEU:HD12	1.77	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
14:M:128:PRO:O	14:M:132:MET:HG2	1.96	0.66
16:H:60:LEU:O	16:H:64:ILE:HG13	1.96	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
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
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
4:E:102:GLU:HG2	4:E:175:ILE:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:R:50:PHE:HE2	12:S:58:LEU:HD11	1.60	0.66
16:Q:216:ARG:HB2	16:Q:294:ARG:HD2	1.78	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
16:Q:237:SER:OG	16:Q:238:SER:N	2.25	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
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
13:L:278:ALA:HA	13:L:301:SER:HA	1.78	0.65
4:E:118:VAL:HB	4:E:257:TYR:HE1	1.61	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
13:T:189:LYS:HZ1	13:T:479:GLU:HB2	1.59	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
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
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
3:D:459:MET:HG2	3:D:465:HIS:HB2	1.79	0.65
13:T:393:LEU:HD12	13:T:493:LEU:HD11	1.78	0.65
1:1:341:MET:HB2	1:1:371:PHE:CE2	2.31	0.65
14:M:448:GLY:O	14:M:452:ARG:HG2	1.97	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
4:4:338:PRO:HG2	5:5:193:ARG:HH11	1.62	0.65
5:5:80:TRP:HA	5:5:80:TRP:CE3	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:162:TYR:HA	16:H:314:PHE:CZ	2.32	0.65
13:L:487:LEU:HD12	13:L:488:GLY:H	1.62	0.64
1:B:287:ILE:HA	1:B:332:PRO:HA	1.78	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
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
3:D:509:ALA:O	3:D:513:GLN:N	2.30	0.64
14:M:347:LEU:O	14:M:351:ALA:N	2.24	0.64
16:H:189:GLN:O	16:H:193:GLY:HA2	1.98	0.64
14:U:151:PHE:HD2	14:U:213:TRP:HB3	1.62	0.64
3:3:656:LEU:HD21	9:W:3:ARG:HD3	1.77	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
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
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
13:T:187:GLU:HA	13:T:190:GLU:HG2	1.78	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
1:1:104:ARG:HH21	2:2:127:SER:HB3	1.62	0.64
2:2:106:ILE:HD11	2:2:112:THR:HB	1.80	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
13:L:380:SER:HB3	13:L:456:ALA:HB3	1.79	0.64
1:B:395:GLU:HB2	1:B:407:VAL:HG21	1.79	0.64
10:P:47:GLY:O	10:P:48:ASN:ND2	2.24	0.64
1:1:79:MET:HE3	1:1:80:PRO:HD2	1.79	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:126:VAL:HA	13:L:129:ILE:HD12	1.80	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
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
15:N:168:GLU:H	15:N:172:TYR:HB2	1.64	0.63
3:D:186:ARG:HD3	3:D:229:ILE:HG22	1.80	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:79:MET:HE3	1:B:80:PRO:HD2	1.79	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
7:O:52:LYS:NZ	8:I:44:MET:O	2.31	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
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
11:J:75:PHE:HZ	11:J:78:GLN:HG2	1.64	0.62
16:H:134:TYR:HA	16:H:137:PHE:CE2	2.33	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
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
13:L:458:TYR:HD1	13:L:461:LEU:HD21	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:664:LEU:HD22	3:D:669:VAL:HG11	1.80	0.62
13:T:419:ARG:NH2	13:T:525:GLU:OE2	2.31	0.62
16:Q:211:MET:HA	16:Q:215:ALA:HB3	1.81	0.62
1:1:438:ARG:OXT	2:2:146:THR:OG1	2.18	0.62
7:9:28:ASP:OD2	16:H:50:ARG:NH1	2.33	0.62
4:E:201:ILE:HA	4:E:204:TYR:HD2	1.65	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
14:M:126:LEU:HD11	14:M:149:VAL:HG22	1.80	0.62
3:D:605:PRO:HB2	3:D:609:GLU:HG3	1.82	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:37:ARG:NH2	16:Q:54:PHE:O	2.33	0.62
16:Q:290:PHE:O	16:Q:294:ARG:HG2	2.00	0.62
14:M:54:PRO:HA	14:M:62:TYR:HD1	1.64	0.62
14:M:346:GLY:O	14:M:348:ALA:N	2.32	0.62
16:H:35:GLU:OE1	16:H:249:TYR:OH	2.12	0.62
14:U:84:LEU:O	14:U:88:VAL:HG12	2.00	0.62
16:Q:124:TYR:O	16:Q:128:VAL:HG13	1.99	0.62
5:5:39:ALA:HA	5:5:107:LEU:HD21	1.81	0.62
6:6:78:MET:HE1	6:6:92:MET:CG	2.30	0.62
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
16:Q:240:LYS:HB2	16:Q:240:LYS:HZ2	1.64	0.62
6:6:78:MET:HE1	6:6:92:MET:HG3	1.80	0.61
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
16:H:65:LYS:O	16:H:69:LYS:HB2	1.99	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
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
1:B:289:ALA:HB3	1:B:337:MET:HE3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:19:VAL:HG21	3:D:52:ILE:HD11	1.80	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
4:4:213:ILE:HD13	16:H:298:PHE:HB2	1.82	0.61
7:9:4:LYS:H	7:9:4:LYS:HD2	1.66	0.61
4:E:341:GLU:OE2	5:F:57:TYR:OH	2.17	0.61
13:T:454:VAL:HB	13:T:455:LEU:HD22	1.83	0.61
4:4:143:LEU:H	4:4:143:LEU:HD23	1.63	0.61
8:7:37:PHE:HE1	8:7:74:PRO:HA	1.66	0.61
13:L:288:GLN:NE2	13:L:528:SER:O	2.34	0.61
1:B:100:SER:HA	1:B:253:GLN:HE21	1.65	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
15:N:265:HIS:NE2	15:N:333:LEU:O	2.33	0.61
6:G:125:GLN:O	9:X:38:GLN:NE2	2.34	0.61
14:U:8:LEU:HD21	14:U:31:LEU:HB3	1.83	0.61
6:6:78:MET:HB2	6:6:99:MET:HE1	1.81	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
3:3:87:VAL:HG12	3:3:91:MET:HE1	1.82	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
4:4:201:ILE:HA	4:4:204:TYR:HD2	1.66	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
16:H:29:ALA:O	16:H:32:THR:OG1	2.11	0.60
16:H:237:SER:OG	16:H:238:SER:N	2.31	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:84:ARG:CZ	4:E:169:HIS:HB3	2.31	0.60
4:E:240:ARG:NH1	4:E:282:GLU:OE2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:L:454:VAL:HB	13:L:455:LEU:HD22	1.83	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
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
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
9:W:31:VAL:HG11	9:W:81:LEU:HD13	1.83	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
3:D:688:ARG:HB3	3:D:770:ARG:HB2	1.82	0.60
4:E:143:LEU:HD23	4:E:143:LEU:H	1.65	0.60
14:U:84:LEU:HB3	14:U:432:PHE:CD1	2.36	0.60
4:4:224:ILE:HD11	4:4:275:ARG:NH1	2.17	0.60
16:H:74:VAL:HG12	16:H:75:ALA:O	2.01	0.60
16:H:227:GLU:CG	16:H:228:LEU:N	2.61	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
9:X:45:ARG:NH1	9:X:61:ASP:OD2	2.32	0.60
10:P:57:PHE:HE2	16:Q:149:LEU:CD2	2.15	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
14:M:93:GLY:HA3	14:M:95:PHE:HD1	1.66	0.60
14:M:186:GLN:HG2	14:M:187:GLU:H	1.67	0.60
16:H:267:TRP:CG	16:H:268:THR:H	2.20	0.60
3:D:297:GLY:O	3:D:300:TRP:NE1	2.33	0.60
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
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:20:MET:HE2	3:D:433:ALA:HB2	1.84	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
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
5:F:80:TRP:CE3	5:F:80:TRP:HA	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:L:217:SER:HB3	13:L:249:GLY:HA3	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:M:101:LEU:HD23	14:M:128:PRO:HG3	1.83	0.60
5:F:50:ALA:HB3	5:F:73:GLU:HB3	1.84	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
14:M:89:ALA:HB1	14:M:92:GLU:OE2	2.02	0.59
4:E:74:THR:HG22	4:E:76:LEU:H	1.67	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
4:4:123:LEU:HG	4:4:156:ILE:HG23	1.83	0.59
4:4:137:LEU:HD23	4:4:145:PRO:HG2	1.82	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
16:Q:267:TRP:CG	16:Q:268:THR:H	2.20	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
13:T:413:THR:HA	13:T:416:TYR:CE2	2.38	0.59
16:Q:39:LEU:O	16:Q:43:GLN:HG2	2.02	0.59
4:4:272:VAL:HG13	4:4:399:SER:HB3	1.85	0.59
15:N:347:LEU:O	15:N:351:GLU:HG2	2.03	0.59
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
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
16:Q:36:ARG:HH12	16:Q:58:GLN:HG2	1.66	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
11:J:2:SER:HA	11:J:5:GLU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:47:MET:HE1	3:D:108:VAL:HA	1.83	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
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
5:5:26:TRP:NE1	5:5:91:ARG:HH21	2.00	0.59
7:9:108:CYS:HB2	7:9:113:ILE:HG22	1.84	0.59
16:H:211:MET:HA	16:H:215:ALA:HB3	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
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
16:H:220:ASP:CG	16:H:301:ARG:HA	2.28	0.59
16:H:290:PHE:O	16:H:294:ARG:HG2	2.03	0.59
3:D:149:LEU:HD11	4:E:110:PRO:HG3	1.84	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
14:U:91:VAL:HG13	14:U:224:SER:OG	2.03	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
16:H:217:THR:O	16:H:300:LEU:HD13	2.03	0.58
4:E:254:TYR:HD1	4:E:255:SER:H	1.49	0.58
6:G:61:ALA:C	6:G:62:ARG:HH11	2.11	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
7:9:110:THR:C	8:7:44:MET:HG2	2.28	0.58
11:J:135:TRP:HZ3	15:N:105:LEU:HD22	1.66	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:L:103:ARG:NH2	13:L:144:PHE:O	2.35	0.58
14:M:56:LEU:O	14:M:58:GLY:N	2.37	0.58
14:M:102:MET:HB3	14:M:230:LEU:HD23	1.86	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
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
8:7:44:MET:HE2	8:7:46:ARG:HH22	1.69	0.58
14:M:402:SER:HA	14:M:405:TYR:CE2	2.38	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
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
9:X:51:HIS:ND1	9:X:56:ASP:OD1	2.37	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
7:9:52:LYS:NZ	8:7:44:MET:O	2.33	0.58
15:N:53:TYR:HA	15:N:101:THR:HG22	1.86	0.58
3:D:50:VAL:HG22	3:D:82:SER:HB3	1.85	0.58
3:D:299:GLU:O	3:D:303:GLN:HB2	2.04	0.58
6:G:114:SER:OG	7:O:96:LEU:O	2.21	0.58
14:U:101:LEU:HD23	14:U:128:PRO:HG3	1.86	0.58
16:Q:74:VAL:HG12	16:Q:75:ALA:O	2.03	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
3:D:300:TRP:CD1	3:D:300:TRP:H	2.22	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
16:Q:60:LEU:O	16:Q:64:ILE:HG13	2.04	0.58
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:8:LEU:HD21	14:M:31:LEU:HB3	1.86	0.58
16:H:162:TYR:HE1	16:H:305:LEU:HG	1.66	0.58
1:B:201:LEU:HD12	1:B:399:PHE:CE1	2.38	0.58
1:B:354:GLY:O	1:B:360:ARG:NH1	2.35	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
11:R:151:VAL:HG11	15:V:86:LEU:HD23	1.86	0.58
13:T:376:LEU:HB3	13:T:379:LEU:HD12	1.85	0.58
18:1:502:FMN:N1	18:1:502:FMN:O3'	2.34	0.58
8:7:60:SER:HA	8:7:66:PRO:HA	1.85	0.58
14:M:88:VAL:HA	14:M:428:ALA:HB1	1.84	0.58
16:H:147:TYR:CD1	16:H:229:VAL:HG22	2.38	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
1:1:196:ARG:NH2	3:3:204:GLU:O	2.38	0.57
3:3:300:TRP:CD1	3:3:300:TRP:H	2.22	0.57
4:4:115:THR:O	4:4:118:VAL:HG22	2.05	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
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
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
16:Q:70:GLU:O	16:Q:237:SER:OG	2.20	0.57
16:Q:162:TYR:HE1	16:Q:305:LEU:HG	1.68	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
6:6:44:ALA:HB3	17:6:201:SF4:S4	2.44	0.57
6:6:61:ALA:C	6:6:62:ARG:HH11	2.13	0.57
6:6:76:ASP:HB2	6:6:104:TRP:CZ3	2.40	0.57
13:L:286:PHE:O	13:L:419:ARG:NH1	2.37	0.57
16:H:189:GLN:HG2	16:H:195:LEU:H	1.68	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
3:3:31:PRO:HB2	3:3:47:MET:HB3	1.87	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
6:6:115:GLY:HA3	6:6:125:GLN:OE1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:9:94:ASN:HB3	7:9:97:ARG:HB2	1.86	0.57
15:N:2:THR:HG1	15:N:39:SER:HG	1.50	0.57
15:N:412:LEU:HD13	15:N:419:VAL:HG21	1.84	0.57
16:H:37:ARG:NH2	16:H:54:PHE:O	2.37	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
2:C:101:THR:HG23	2:C:106:ILE:O	2.04	0.57
5:F:41:TYR:HA	5:F:44:MET:HE3	1.87	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
14:M:95:PHE:HB2	14:M:98:LEU:HD12	1.87	0.57
16:H:219:PHE:HD2	16:H:299:ARG:HE	1.53	0.57
4:E:224:ILE:HD11	4:E:275:ARG:NH1	2.19	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
14:M:224:SER:HA	14:M:330:GLY:CA	2.33	0.57
16:H:70:GLU:O	16:H:237:SER:OG	2.20	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
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
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
6:6:60:LEU:HD12	6:6:60:LEU:C	2.30	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
14:M:151:PHE:HD2	14:M:213:TRP:HB3	1.70	0.57
2:C:130:THR:HB	2:C:143:GLU:HB3	1.87	0.57
5:F:38:MET:HA	5:F:41:TYR:HD2	1.69	0.57
14:U:88:VAL:HA	14:U:428:ALA:HB1	1.86	0.57
14:U:188:GLU:HA	14:U:191:PHE:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:189:GLN:O	16:Q:193:GLY:HA2	2.05	0.57
3:3:574:GLU:HB2	3:3:593:LEU:HD11	1.86	0.57
12:K:2:SER:HA	12:K:5:LEU:HD12	1.87	0.57
16:H:36:ARG:HH12	16:H:58:GLN:HG2	1.69	0.57
2:C:135:GLN:HB2	2:C:141:TYR:HD1	1.70	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
4:4:50:GLU:OE2	16:H:154:ARG:NH2	2.38	0.56
5:5:80:TRP:HA	5:5:80:TRP:HE3	1.70	0.56
6:6:57:ARG:C	6:6:58:ASN:HD22	2.13	0.56
15:N:309:LEU:HD22	15:N:378:LEU:HD11	1.86	0.56
16:H:240:LYS:HZ2	16:H:240:LYS:HB2	1.69	0.56
6:G:115:GLY:HA3	6:G:125:GLN:OE1	2.05	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
13:L:123:SER:HA	13:L:184:SER:HA	1.87	0.56
16:H:75:ALA:O	16:H:76:GLN:HB2	2.06	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
9:W:45:ARG:NH1	9:W:61:ASP:OD2	2.36	0.56
3:D:41:PRO:HB3	3:D:433:ALA:HB1	1.87	0.56
3:D:87:VAL:HG12	3:D:91:MET:HE1	1.86	0.56
5:F:155:THR:HG23	9:X:93:VAL:HB	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
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
16:H:99:LEU:HA	16:H:116:ILE:O	2.06	0.56
4:E:263:ASP:HB2	4:E:285:GLU:HG3	1.88	0.56
14:U:126:LEU:HD11	14:U:149:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:6:43:LEU:HB2	6:6:82:GLY:HA3	1.88	0.56
6:6:101:ASP:H	16:H:70:GLU:HG2	1.71	0.56
7:9:94:ASN:OD1	7:9:97:ARG:N	2.38	0.56
13:L:483:HIS:ND1	13:L:483:HIS:O	2.39	0.56
16:H:8:ASP:OD1	16:H:112:GLN:HG2	2.06	0.56
3:D:31:PRO:HG3	3:D:137:TYR:CD2	2.41	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
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
4:E:46:THR:O	4:E:53:LEU:HB2	2.06	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
15:N:24:GLY:HA2	15:N:27:ARG:HD2	1.88	0.56
16:H:332:LEU:HD12	16:H:332:LEU:H	1.70	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
8:I:120:ASP:OD1	8:I:123:ARG:NH1	2.34	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
11:J:69:PHE:HZ	16:H:156:SER:HG	1.53	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
14:M:75:PHE:HZ	14:M:111:ALA:HB2	1.71	0.55
6:G:60:LEU:HD12	6:G:60:LEU:C	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:37:PHE:CE1	8:I:74:PRO:HA	2.41	0.55
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
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
2:C:146:THR:HG23	2:C:149:ARG:H	1.70	0.55
4:E:162:TRP:CE2	7:O:34:LYS:HD2	2.41	0.55
6:G:27:LEU:O	6:G:30:TRP:HD1	1.89	0.55
7:O:57:SER:N	17:O:202:SF4:S1	2.75	0.55
7:O:137:LEU:O	7:O:140:VAL:HG12	2.05	0.55
8:I:20:MET:HE3	8:I:59:LEU:HG	1.88	0.55
5:5:171:ARG:HG3	5:5:171:ARG:HH11	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
6:G:117:MET:HE3	6:G:118:PHE:CZ	2.42	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
5:5:52:ILE:HG22	5:5:118:VAL:HG21	1.89	0.55
5:5:155:THR:HG23	9:W:93:VAL:HB	1.88	0.55
6:6:19:ILE:HG12	6:6:20:LEU:H	1.71	0.55
15:N:422:ALA:HB1	15:N:426:GLY:HA2	1.89	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
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
14:M:26:VAL:HA	14:M:86:ALA:HB1	1.87	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
3:D:689:LYS:HD2	3:D:772:GLU:HG2	1.88	0.55
6:G:78:MET:HE1	6:G:92:MET:HG3	1.89	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
11:J:113:LEU:HD21	12:K:49:TYR:CZ	2.41	0.55
16:H:16:LYS:NZ	16:H:114:TRP:O	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:99:PRO:HB2	5:F:124:ILE:HA	1.88	0.55
6:G:126:ASN:HB2	9:X:38:GLN:HE21	1.72	0.55
13:T:288:GLN:NE2	13:T:528:SER:O	2.40	0.55
15:V:309:LEU:HD22	15:V:378:LEU:HD11	1.87	0.55
15:V:350:ALA:O	15:V:354:ARG:HB2	2.07	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
7:9:44:THR:OG1	7:9:52:LYS:HD2	2.07	0.55
7:9:56:CYS:N	17:9:202:SF4:S1	2.79	0.55
9:W:26:LEU:HD12	9:W:84:GLN:HB2	1.89	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
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
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
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
6:G:58:ASN:ND2	16:Q:47:GLY:O	2.40	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
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
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
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:87:TYR:HB3	4:E:169:HIS:HE1	1.72	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
5:5:41:TYR:HA	5:5:44:MET:HE3	1.89	0.54
6:6:104:TRP:NE1	6:6:172:PRO:O	2.40	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:H:52:GLY:HA2	16:H:55:GLY:H	1.72	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
15:V:241:VAL:O	15:V:245:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:38:LEU:HD23	16:Q:291:ILE:HG21	1.89	0.54
1:1:195:LEU:CD2	2:2:24:ARG:HH12	2.20	0.54
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
6:G:78:MET:HE1	6:G:92:MET:CG	2.37	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
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
16:Q:214:ALA:HB1	16:Q:248:GLU:OE2	2.08	0.54
3:3:20:MET:HE2	3:3:433:ALA:HB2	1.90	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
14:M:26:VAL:HG22	14:M:86:ALA:O	2.07	0.54
14:M:78:ILE:HG22	14:M:103:GLU:HG3	1.90	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
6:G:57:ARG:C	6:G:58:ASN:HD22	2.15	0.54
10:P:33:PRO:HD2	16:Q:70:GLU:CB	2.36	0.54
16:Q:217:THR:O	16:Q:300:LEU:HD13	2.06	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
13:L:24:MET:HB3	13:L:28:LEU:HB3	1.90	0.54
1:B:195:LEU:CD2	2:C:24:ARG:HH12	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
16:H:6:PRO:HG2	16:H:112:GLN:NE2	2.22	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
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
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
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:T:348:ASP:HB3	13:T:351:LYS:HB2	1.89	0.54
14:U:20:LEU:H	14:U:20:LEU:HD12	1.71	0.54
16:Q:6:PRO:HG2	16:Q:112:GLN:NE2	2.22	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)
10:A:66:MET:HE3	10:A:70:LEU:HD12	1.90	0.54
13:L:240:ILE:HG22	13:L:241:HIS:HD2	1.73	0.54
13:L:295:VAL:O	13:L:298:SER:OG	2.24	0.54
6:G:76:ASP:HB2	6:G:104:TRP:CE3	2.43	0.54
9:X:31:VAL:HG11	9:X:81:LEU:HD13	1.88	0.54
13:T:123:SER:HA	13:T:184:SER:HA	1.90	0.54
16:Q:224:ALA:HA	16:Q:230:GLY:N	2.19	0.54
1:1:51:ASP:OD1	1:1:81:LYS:HE2	2.08	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
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
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
13:L:57:ALA:HB3	13:L:65:PHE:HB3	1.88	0.53
16:H:131:LEU:O	16:H:134:TYR:HB2	2.08	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
5:F:26:TRP:NE1	5:F:91:ARG:HH21	2.07	0.53
8:I:86:LEU:HB2	8:I:91:ILE:HB	1.90	0.53
13:T:360:PRO:HA	13:T:363:ARG:NH1	2.24	0.53
16:Q:232:TYR:CD1	16:Q:233:HIS:N	2.76	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:38:HIS:HE1	4:E:398:ALA:HA	1.73	0.53
3:3:199:VAL:HG11	3:3:219:PRO:HD2	1.91	0.53
6:6:28:VAL:HA	16:H:64:ILE:CG2	2.38	0.53
6:6:132:PRO:CG	6:6:175:ALA:HB2	2.38	0.53
11:J:151:VAL:HG11	15:N:86:LEU:HD23	1.91	0.53
13:L:37:VAL:HG21	13:L:88:HIS:CE1	2.43	0.53
16:H:70:GLU:O	16:H:70:GLU:HG3	2.08	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
13:T:379:LEU:HD22	13:T:454:VAL:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:538:TYR:O	13:T:542:ILE:HB	2.08	0.53
15:V:180:LEU:HD21	15:V:228:ALA:HB2	1.89	0.53
1:1:289:ALA:HB3	1:1:337:MET:HE3	1.90	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
14:M:91:VAL:CG2	14:M:92:GLU:H	2.21	0.53
14:M:268:ALA:HA	14:M:291:SER:HA	1.90	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:U:151:PHE:CD2	14:U:213:TRP:HB3	2.43	0.53
16:Q:8:ASP:OD1	16:Q:112:GLN:HG2	2.09	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
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
3:D:159:PHE:HE2	8:I:79:LEU:HD13	1.74	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
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
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
6:G:125:GLN:HB2	9:X:119:ASN:HD21	1.74	0.53
14:U:305:PRO:HB3	14:U:459:GLU:CA	2.37	0.53
16:Q:159:LEU:O	16:Q:163:GLU:HB2	2.08	0.53
6:6:102:PRO:HG3	10:A:33:PRO:HG2	1.89	0.53
13:L:576:GLN:HA	13:L:579:ALA:HB3	1.89	0.53
16:H:265:GLY:O	16:H:268:THR:HB	2.08	0.53
4:E:84:ARG:HD3	6:G:117:MET:HE1	1.90	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
14:U:95:PHE:HB3	14:U:136:TYR:CE2	2.43	0.53
16:Q:16:LYS:NZ	16:Q:114:TRP:O	2.40	0.53
4:4:371:ARG:HG3	5:5:51:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:3:656:LEU:HD21	9:W:3:ARG:CD	2.39	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
1:1:293:GLY:HA3	1:1:324:GLY:H	1.74	0.52
1:1:298:PRO:HA	1:1:409:PRO:HA	1.90	0.52
1:1:354:GLY:HA2	1:1:360:ARG:HB2	1.92	0.52
3:3:701:ALA:HB2	3:3:763:LEU:HB2	1.91	0.52
7:9:126:TYR:HB3	9:W:39:ASP:CG	2.34	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
16:H:9:PRO:HB2	16:H:11:TRP:CD1	2.44	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
14:U:89:ALA:HB1	14:U:92:GLU:OE2	2.09	0.52
14:U:260:LEU:HB3	14:U:301:PHE:CD2	2.44	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
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
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
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
3:3:20:MET:N	3:3:82:SER:O	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:347:HIS:HB2	3:3:538:ALA:HA	1.92	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
6:6:163:TYR:CD1	7:9:152:ARG:HD2	2.45	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
16:H:267:TRP:CG	16:H:268:THR:N	2.77	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:71:VAL:HG11	5:F:89:PHE:HD2	1.75	0.52
5:F:171:ARG:HH11	5:F:171:ARG:HG3	1.75	0.52
7:O:108:CYS:HA	17:O:202:SF4:S3	2.49	0.52
14:U:115:LEU:HD12	14:U:180:LEU:HD13	1.92	0.52
16:Q:293:ILE:HD12	16:Q:297:TRP:CZ3	2.44	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
4:4:28:LEU:HD11	16:H:147:TYR:CE2	2.44	0.52
4:4:44:MET:HB2	4:4:56:VAL:HB	1.90	0.52
4:4:162:TRP:CE2	7:9:34:LYS:HD2	2.44	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
10:A:67:LEU:HB3	16:H:310:TRP:CZ2	2.44	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
16:H:147:TYR:HD1	16:H:229:VAL:HG22	1.73	0.52
13:T:151:TYR:HB3	13:T:231:ALA:HB1	1.90	0.52
3:3:549:VAL:C	3:3:550:LEU:HD12	2.34	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
14:M:64:ALA:C	14:M:113:ARG:HB3	2.35	0.52
14:M:88:VAL:HB	14:M:432:PHE:HB2	1.91	0.52
14:M:208:PHE:O	14:M:211:HIS:ND1	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:101:VAL:HB	4:4:175:ILE:HD12	1.92	0.52
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
6:G:57:ARG:HH11	6:G:60:LEU:HD11	1.74	0.52
16:Q:99:LEU:HD12	16:Q:116:ILE:HG13	1.92	0.52
15:N:124:TRP:CZ3	15:N:305:ASP:HB2	2.44	0.52
16:H:37:ARG:NH2	16:H:49:ASN:OD1	2.42	0.52
2:C:9:ASP:OD1	2:C:9:ASP:N	2.43	0.52
3:D:190:TYR:O	3:D:195:PRO:HD2	2.09	0.52
5:F:80:TRP:HA	5:F:80:TRP:HE3	1.75	0.52
5:F:104:VAL:HA	5:F:107:LEU:HD13	1.92	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
14:U:371:LEU:HD12	14:U:440:LEU:HB3	1.90	0.52
16:Q:147:TYR:CD1	16:Q:229:VAL:HG22	2.45	0.52
3:3:373:GLY:CA	3:3:538:ALA:HB2	2.40	0.52
14:M:55:LEU:HG	14:M:56:LEU:HD13	1.91	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
8:I:44:MET:HE2	8:I:46:ARG:HH22	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
16:Q:136:ILE:HG23	16:Q:232:TYR:HD2	1.74	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
7:9:58:LEU:HD12	7:9:109:PRO:HG3	1.91	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
16:H:214:ALA:HB1	16:H:248:GLU:OE2	2.10	0.52
4:E:96:ALA:HB2	4:E:346:THR:HG21	1.90	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
11:R:152:VAL:HG22	15:V:87:LEU:HD22	1.92	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
3:3:191:PHE:HE2	3:3:200:LEU:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:30:VAL:HG13	4:4:35:PRO:HD2	1.93	0.51
13:L:66:SER:HB3	13:L:122:ASP:HB3	1.91	0.51
16:H:293:ILE:HD12	16:H:297:TRP:CZ3	2.45	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
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
4:4:263:ASP:HB2	4:4:285:GLU:CD	2.34	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
16:H:190:LYS:HD3	16:H:268:THR:HG23	1.92	0.51
16:H:292:TRP:CD1	16:H:296:THR:HG1	2.27	0.51
3:D:738:THR:HG23	3:D:771:VAL:HG21	1.90	0.51
10:P:44:TYR:CG	10:P:45:GLU:N	2.78	0.51
14:U:54:PRO:HA	14:U:62:TYR:HD1	1.75	0.51
14:U:70:LEU:HD13	14:U:312:LEU:HD13	1.92	0.51
16:Q:143:SER:HB2	16:Q:235:GLU:HG3	1.91	0.51
16:Q:267:TRP:CG	16:Q:268:THR:N	2.77	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
14:M:70:LEU:HD13	14:M:312:LEU:HD13	1.92	0.51
14:M:87:LEU:HD12	14:M:88:VAL:N	2.26	0.51
14:M:335:ARG:NH2	14:M:429:GLU:OE1	2.42	0.51
3:D:269:THR:HG22	3:D:274:LEU:HA	1.92	0.51
3:D:655:ARG:NH1	3:D:659:GLU:HG3	2.22	0.51
11:R:46:LEU:HD21	12:S:3:TYR:CE2	2.46	0.51
2:2:14:THR:HG22	2:2:17:LYS:NZ	2.26	0.51
2:2:112:THR:HG22	2:2:117:PHE:H	1.75	0.51
4:4:81:TYR:CZ	6:6:117:MET:HG3	2.46	0.51
4:4:263:ASP:HB2	4:4:285:GLU:CG	2.39	0.51
13:L:380:SER:CB	13:L:456:ALA:HB3	2.40	0.51
16:H:38:LEU:HD23	16:H:291:ILE:HG21	1.93	0.51
4:E:159:LEU:O	4:E:163:VAL:HG12	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:18:LEU:O	10:A:22:VAL:HG23	2.11	0.51
10:A:77:PHE:O	10:A:80:PRO:HD2	2.09	0.51
12:K:63:VAL:CG1	15:N:112:GLU:HG3	2.38	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
16:H:307:ARG:HD3	16:H:307:ARG:C	2.35	0.51
3:D:603:PRO:HB2	3:D:634:ALA:HA	1.92	0.51
6:G:108:MET:HE3	6:G:142:PRO:HG2	1.91	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
1:1:341:MET:HE2	1:1:413:SER:HB3	1.92	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
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
16:H:267:TRP:HB2	16:H:275:PRO:O	2.11	0.51
1:B:26:SER:HA	1:B:31:TYR:CG	2.45	0.51
1:B:32:TYR:OH	1:B:116:GLU:OE1	2.14	0.51
1:B:288:GLN:HB3	1:B:333:GLU:CG	2.40	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
4:4:86:ASP:HB3	4:4:93:HIS:CD2	2.46	0.51
9:W:21:LEU:HD21	9:W:26:LEU:HD11	1.92	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
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:32:LEU:HD11	3:D:35:SER:HB2	1.92	0.51
3:D:113:LEU:O	3:D:161:ARG:NH1	2.44	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
6:G:78:MET:HB2	6:G:99:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:100:PHE:HA	17:O:201:SF4:S4	2.51	0.51
12:S:95:GLY:HA2	15:V:256:ARG:HE	1.74	0.51
16:Q:232:TYR:HD1	16:Q:233:HIS:N	2.09	0.51
1:1:258:VAL:HG23	1:1:283:PRO:HA	1.93	0.51
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
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
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
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:HB3	6:6:16:ARG:HH11	1.76	0.51
6:6:91:VAL:HG22	10:A:46:SER:HB2	1.92	0.51
16:H:158:SER:HB2	16:H:305:LEU:CD2	2.40	0.51
16:H:232:TYR:CD1	16:H:233:HIS:N	2.79	0.51
2:C:14:THR:HG22	2:C:17:LYS:NZ	2.26	0.51
2:C:127:SER:HB2	2:C:130:THR:OG1	2.11	0.51
3:D:29:ASP:OD1	3:D:29:ASP:N	2.43	0.51
14:U:18:LEU:HG	14:U:19:GLY:N	2.26	0.51
16:Q:162:TYR:HA	16:Q:314:PHE:CZ	2.46	0.51
16:Q:220:ASP:CG	16:Q:301:ARG:HA	2.35	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
6:6:108:MET:HE3	6:6:142:PRO:HG2	1.91	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
1:B:18:TYR:OH	1:B:102:LYS:O	2.22	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
14:U:93:GLY:HA3	14:U:95:PHE:HD1	1.75	0.51
13:L:68:LEU:HD23	13:L:255:ARG:HH22	1.75	0.50
13:L:557:ASP:CG	14:M:211:HIS:HE2	2.19	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:57:ARG:O	6:G:58:ASN:ND2	2.39	0.50
11:R:23:ARG:HG2	11:R:80:GLU:HG2	1.92	0.50
13:T:177:TRP:HE1	14:U:306:GLU:CD	2.19	0.50
1:1:288:GLN:HB3	1:1:333:GLU:HG2	1.93	0.50
3:3:29:ASP:OD1	3:3:29:ASP:N	2.44	0.50
4:4:287:VAL:O	4:4:291:LYS:HG3	2.12	0.50
11:J:12:LEU:HD22	12:K:10:LEU:HD11	1.93	0.50
13:L:66:SER:CB	13:L:122:ASP:HB3	2.40	0.50
13:L:422:VAL:HG11	13:L:513:GLN:N	2.26	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
16:H:175:LEU:HB3	16:H:328:VAL:HG21	1.93	0.50
2:C:66:PHE:O	3:D:205:ARG:NE	2.44	0.50
4:E:114:GLU:O	4:E:118:VAL:HG13	2.11	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
3:3:46:ARG:HG2	3:3:46:ARG:NH1	2.26	0.50
3:3:451:PHE:CD1	3:3:466:GLU:HB3	2.46	0.50
4:4:162:TRP:NE1	7:9:34:LYS:HD2	2.26	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
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
15:V:283:PHE:O	15:V:287:THR:HG23	2.09	0.50
4:4:84:ARG:HD3	6:6:117:MET:HE1	1.93	0.50
14:M:88:VAL:HG22	14:M:331:ARG:HG3	1.93	0.50
3:D:33:PHE:CE2	3:D:47:MET:HE3	2.47	0.50
4:E:26:MET:HG2	10:P:54:VAL:HB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:J:59:TYR:O	11:J:64:VAL:HG12	2.12	0.50
13:L:30:GLY:HA3	13:L:92:ILE:HG12	1.93	0.50
13:L:151:TYR:HB3	13:L:231:ALA:HB1	1.93	0.50
3:D:20:MET:N	3:D:82:SER:O	2.36	0.50
3:D:55:PRO:HG3	3:D:74:GLN:N	2.25	0.50
3:D:382:PHE:HB3	3:D:532:VAL:HB	1.93	0.50
12:S:57:ALA:O	12:S:60:VAL:HB	2.11	0.50
13:T:138:SER:OG	13:T:245:MET:HE3	2.12	0.50
15:V:45:GLY:C	15:V:47:PRO:HD3	2.35	0.50
16:Q:289:PHE:O	16:Q:293:ILE:HG12	2.12	0.50
4:4:34:HIS:HB2	10:A:45:GLU:OE1	2.12	0.50
4:4:84:ARG:CD	6:6:117:MET:HE1	2.42	0.50
8:7:52:THR:HB	8:7:54:ILE:HG22	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
16:H:96:ALA:HB1	16:H:125:LEU:HD23	1.93	0.50
2:C:77:LYS:H	2:C:116:LEU:HA	1.76	0.50
3:D:19:VAL:HG22	3:D:91:MET:HE1	1.94	0.50
11:R:75:PHE:CG	11:R:76:ALA:N	2.80	0.50
14:U:96:LEU:O	14:U:100:LEU:HG	2.11	0.50
14:U:134:TYR:HB2	14:U:145:LEU:CD1	2.42	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
4:4:63:HIS:O	6:6:122:ALA:HB1	2.12	0.50
4:4:261:THR:N	4:4:292:GLN:HE22	2.02	0.50
6:6:35:SER:O	6:6:37:TRP:HE3	1.95	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
1:B:201:LEU:O	1:B:204:PRO:HD2	2.12	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
14:M:9:PRO:HG3	14:M:32:SER:HB2	1.94	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
6:G:30:TRP:CH2	16:Q:51:VAL:HG13	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:J:50:PHE:CE2	12:K:58:LEU:HD11	2.44	0.50
11:J:146:LEU:O	11:J:150:THR:HG23	2.11	0.50
15:N:313:ARG:HE	15:N:384:ALA:HB3	1.76	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
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
4:E:263:ASP:HB2	4:E:285:GLU:CD	2.37	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
11:R:52:GLY:O	11:R:55:GLN:HB3	2.11	0.50
11:R:65:VAL:HG23	16:Q:134:TYR:CZ	2.46	0.50
16:Q:9:PRO:HB2	16:Q:11:TRP:CD1	2.46	0.50
16:Q:27:ALA:O	16:Q:31:MET:HG2	2.12	0.50
3:3:282:VAL:HG21	3:3:673:MET:HE1	1.94	0.49
4:4:50:GLU:O	4:4:390:VAL:HG23	2.12	0.49
4:4:338:PRO:HG2	5:5:193:ARG:HD3	1.94	0.49
4:4:390:VAL:HG11	16:H:228:LEU:HG	1.94	0.49
8:7:61:ASP:HB3	8:7:127:ALA:HB1	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
10:P:47:GLY:C	10:P:48:ASN:HD22	2.16	0.49
2:2:120:GLN:HG2	2:2:121:LYS:O	2.12	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
4:E:38:HIS:ND1	4:E:139:ASP:OD2	2.44	0.49
4:E:129:HIS:CE1	4:E:349:ALA:HB1	2.47	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
14:U:26:VAL:HA	14:U:86:ALA:HB1	1.93	0.49
14:U:313:TYR:CD1	14:U:451:ALA:HB2	2.46	0.49
2:2:46:ILE:HD13	2:2:61:MET:HA	1.94	0.49
2:2:108:PRO:HA	2:2:119:VAL:O	2.12	0.49
4:4:26:MET:HA	10:A:54:VAL:HG12	1.93	0.49
6:6:31:GLY:O	6:6:35:SER:HB3	2.13	0.49
6:6:91:VAL:HA	10:A:46:SER:HB3	1.94	0.49
8:7:40:PHE:HB2	8:7:48:TYR:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:O:95:MET:HE3	7:O:131:TYR:HB2	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
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
3:D:704:ALA:HB2	3:D:712:ALA:HB3	1.94	0.49
4:E:26:MET:HA	10:P:54:VAL:HG12	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
7:O:110:THR:C	8:I:44:MET:HG2	2.37	0.49
13:T:321:HIS:HD2	13:T:388:ILE:HD12	1.77	0.49
16:Q:310:TRP:HA	16:Q:314:PHE:CD2	2.48	0.49
2:2:127:SER:HB2	2:2:130:THR:OG1	2.12	0.49
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
16:H:327:VAL:HA	16:H:332:LEU:HD13	1.94	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
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
3:3:17:THR:HB	3:3:87:VAL:HG21	1.94	0.49
3:3:337:ARG:H	3:3:337:ARG:CD	2.26	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
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
16:H:136:ILE:HG23	16:H:232:TYR:HD2	1.76	0.49
4:E:64:THR:N	4:E:409:ARG:OXT	2.43	0.49
4:E:274:ASP:O	4:E:278:VAL:HG23	2.12	0.49
13:T:189:LYS:HZ3	13:T:477:LEU:HD12	1.78	0.49
14:U:296:ALA:HB2	14:U:314:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:A:56:ARG:NH1	11:J:75:PHE:HB2	2.28	0.49
11:J:138:VAL:HG22	15:N:106:LEU:HB2	1.94	0.49
14:M:56:LEU:O	14:M:59:ALA:N	2.44	0.49
16:H:99:LEU:HD12	16:H:116:ILE:HG13	1.95	0.49
16:H:287:LEU:O	16:H:291:ILE:HG13	2.12	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:129:HIS:CE1	4:E:279:ARG:HD3	2.47	0.49
4:E:201:ILE:HA	4:E:204:TYR:CD2	2.46	0.49
6:G:108:MET:HA	6:G:137:VAL:HG13	1.94	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
6:6:37:TRP:HD1	6:6:64:GLY:O	1.95	0.49
6:6:104:TRP:CZ2	6:6:173:VAL:HG22	2.47	0.49
10:A:23:ALA:O	10:A:27:VAL:HG23	2.13	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
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:168:PHE:CE1	6:G:141:PRO:HG3	2.47	0.49
4:E:234:LEU:O	4:E:239:LEU:HB2	2.13	0.49
10:P:23:ALA:O	10:P:27:VAL:HG23	2.13	0.49
11:R:109:TRP:HA	11:R:109:TRP:CE3	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
16:Q:211:MET:HG3	16:Q:212:ALA:N	2.26	0.49
16:Q:221:LEU:N	16:Q:222:PRO:HA	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:219:PHE:HB3	16:H:299:ARG:HG2	1.93	0.49
6:G:165:GLU:OE2	7:O:148:ARG:NH1	2.42	0.49
10:P:18:LEU:O	10:P:22:VAL:HG23	2.13	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:17:LEU:HD21	14:U:98:LEU:HG	1.94	0.49
14:U:26:VAL:HG22	14:U:86:ALA:O	2.13	0.49
14:U:134:TYR:CE2	15:V:383:PHE:HB2	2.48	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
16:Q:108:PHE:HB3	16:Q:112:GLN:H	1.77	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
8:7:86:LEU:HB2	8:7:91:ILE:HB	1.95	0.49
13:L:554:PHE:HD2	14:M:277:ALA:HB3	1.77	0.49
14:M:86:ALA:O	14:M:96:LEU:HD11	2.12	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
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: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
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
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
10:A:47:GLY:C	10:A:48:ASN:HD22	2.16	0.48
16:H:17:ALA:O	16:H:21:VAL:HG23	2.12	0.48
6:G:148:ILE:O	6:G:152:MET:HG3	2.13	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
9:W:111:LEU:HG	9:W:115:MET:HE2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:PHE:CZ	2:C:33:ARG:HG3	2.48	0.48
3:D:81:ALA:HB3	3:D:84:VAL:CG2	2.43	0.48
3:D:337:ARG:CD	3:D:337:ARG:H	2.26	0.48
4:E:34:HIS:HB2	10:P:45:GLU:OE1	2.13	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
10:P:62:TYR:CD1	10:P:62:TYR:C	2.91	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
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:96:TRP:HA	6:G:99:MET:HE3	1.94	0.48
6:G:138:PRO:O	6:G:142:PRO:HB3	2.14	0.48
7:O:163:VAL:HG23	7:O:177:THR:HG22	1.95	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
6:6:58:ASN:ND2	16:H:47:GLY:O	2.46	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
10:A:69:ILE:HG22	11:J:62:ALA:HB1	1.96	0.48
11:J:138:VAL:HA	15:N:106:LEU:HD13	1.95	0.48
13:L:263:LEU:HD13	13:L:266:VAL:HG21	1.96	0.48
16:H:143:SER:HB2	16:H:235:GLU:HG3	1.95	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
10:P:77:PHE:O	10:P:80:PRO:HD2	2.12	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
16:Q:21:VAL:HG13	16:Q:94:LEU:HD13	1.94	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
1:1:338:VAL:O	1:1:342:TRP:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:51:ARG:HB3	3:3:94:ASP:HB3	1.95	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
3:3:631: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
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
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
3:D:587:LEU:O	3:D:604:ALA:N	2.46	0.48
6:G:76:ASP:HB3	16:Q:69:LYS:NZ	2.27	0.48
6:G:104:TRP:CE2	6:G:173:VAL:HG22	2.48	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
5:5:26:TRP:CD1	5:5:91:ARG:HH21	2.31	0.48
6:6:57:ARG:HH21	6:6:148:ILE:HA	1.78	0.48
11:J:23:ARG:HG2	11:J:80:GLU:HG2	1.94	0.48
16:H:232:TYR:HD1	16:H:233:HIS:N	2.11	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
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
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
16:Q:267:TRP:HB2	16:Q:275:PRO:O	2.13	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:6:92:MET:HE1	6:6:127:VAL:HG13	1.96	0.48
10:A:10:THR:OG1	16:H:118:LEU:HD21	2.13	0.48
13:L:21:GLY:C	13:L:102:SER:HB3	2.38	0.48
14:M:313:TYR:CD1	14:M:451:ALA:HB2	2.48	0.48
16:H:314:PHE:N	16:H:314:PHE:CD1	2.80	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
8:I:61:ASP:HB2	8:I:129:ALA:OXT	2.13	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
16:Q:186:VAL:HA	16:Q:189:GLN:NE2	2.29	0.48
1:1:149:ILE:HG21	1:1:153:ARG:HH21	1.78	0.48
13:L:603:VAL:HG21	15:N:235:LEU:HD22	1.94	0.48
14:M:86:ALA:HA	14:M:96:LEU:HD11	1.95	0.48
16:H:96:ALA:HB2	16:H:124:TYR:CE2	2.49	0.48
16:H:224:ALA:CA	16:H:230:GLY:H	2.22	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
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
11:J:44:VAL:HG13	11:J:49:ARG:HG2	1.96	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
4:E:84:ARG:CD	6:G:117:MET:HE1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:52:ILE:HG22	5:F:118:VAL:HG21	1.96	0.48
9:X:21:LEU:HD21	9:X:26:LEU:HD11	1.95	0.48
11:R:19:VAL:HG21	11:R:32:LEU:HB2	1.95	0.48
16:Q:221:LEU:HB3	16:Q:222:PRO:HA	1.96	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:H	16:Q:332:LEU:HD12	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
14:M:345:ARG:HG2	14:M:412:LYS:O	2.14	0.47
1:B:288:GLN:HB3	1:B:333:GLU:HG2	1.95	0.47
2:C:45:ARG:O	2:C:49:ILE:HG13	2.14	0.47
3:D:36:GLU:HB3	3:D:39:LEU:HB2	1.96	0.47
3:D:192:GLU:HG3	3:D:440:ARG:HH11	1.79	0.47
3:D:549:VAL:C	3:D:550:LEU:HD12	2.39	0.47
4:E:43:LEU:HD13	4:E:55:VAL:HG11	1.96	0.47
4:E:171:ASN:CG	4:E:174:ARG:HH22	2.22	0.47
14:U:224:SER:CA	14:U:330:GLY:HA3	2.42	0.47
16:Q:131:LEU:O	16:Q:134:TYR:HB2	2.14	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
5:5:140:ASP:HB2	9:W:30:LYS:NZ	2.30	0.47
8:7:45:GLU:CD	8:7:45:GLU:H	2.21	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
16:H:221:LEU:HB3	16:H:222:PRO:HA	1.97	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
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
1:1:316:LEU:HD13	1:1:323:LEU:HB2	1.95	0.47
4:4:40:VAL:HG21	6:6:88:MET:HE2	1.96	0.47
6:6:100:PRO:CG	16:H:69:LYS:HE3	2.44	0.47
9:W:74:LEU:HD12	9:W:77:LEU:HD23	1.96	0.47
11:J:16:GLY:O	11:J:19:VAL:HG12	2.14	0.47
13:L:189:LYS:NZ	13:L:479:GLU:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PRO:HD3	3:D:107:MET:SD	2.54	0.47
1:B:438:ARG:C	2:C:146:THR:HG1	2.22	0.47
2:C:101:THR:O	2:C:105:GLY:N	2.46	0.47
3:D:7:ASN:CG	3:D:96:LEU:HD12	2.40	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:89:HIS:CE1	4:E:92:ALA:HB2	2.48	0.47
4:E:224:ILE:HD11	4:E:275:ARG:CZ	2.43	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
6:G:132:PRO:CG	6:G:175:ALA:HB2	2.41	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
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
10:A:44:TYR:O	10:A:48:ASN:HA	2.14	0.47
14:M:130:LEU:HD13	15:N:380:LEU:HD11	1.95	0.47
14:M:307:GLY:HA2	14:M:380:THR:HA	1.97	0.47
16:H:283:ILE:O	16:H:287:LEU:HB2	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
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
16:Q:122:ILE:HA	16:Q:125:LEU:HD12	1.96	0.47
3:3:655:ARG:HB2	3:3:655:ARG:NH1	2.27	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: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:50:GLU:O	4:E:390:VAL:HG23	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
5:F:134:LYS:NZ	5:F:141:LEU:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:163:TYR:CD1	7:O:152:ARG:HD2	2.50	0.47
14:U:64:ALA:C	14:U:113:ARG:HB3	2.40	0.47
14:U:201:PHE:CD2	14:U:245:ALA:HB2	2.50	0.47
14:U:204:LYS:HE3	14:U:234:TYR:O	2.14	0.47
15:V:29:THR:HG21	15:V:85:TYR:HB3	1.96	0.47
3:3:30:VAL:HG22	3:3:48:CYS:HA	1.97	0.47
3:3:33:PHE:CE2	3:3:47:MET:HE3	2.49	0.47
3:3:50:VAL:HG22	3:3:82:SER:HB3	1.95	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
4:4:86:ASP:HB3	4:4:93:HIS:HD2	1.78	0.47
5:5:34:PHE:CD2	5:5:102:PRO:HG2	2.50	0.47
5:5:116:ARG:HG2	5:5:132:LEU:HD23	1.95	0.47
6:6:72:PRO:HG3	10:A:44:TYR:CE1	2.50	0.47
6:6:97:GLU:O	10:A:40:LYS:HG3	2.15	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
10:A:49:ASP:N	10:A:50:PRO:HD3	2.30	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
15:N:45:GLY:C	15:N:47:PRO:HD3	2.39	0.47
16:H:159:LEU:O	16:H:163:GLU:HB2	2.14	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:HD3	3:D:688:ARG:HA	1.55	0.47
4:E:232:LEU:HD23	5:F:109:GLY:HA3	1.96	0.47
4:E:234:LEU:HD12	4:E:380:SER:HB2	1.95	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
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
9:X:58:LEU:HD21	9:X:103:LEU:HB3	1.96	0.47
10:P:67:LEU:HD23	16:Q:310:TRP:CZ2	2.49	0.47
10:P:67:LEU:HB3	16:Q:310:TRP:HZ2	1.80	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:66:SER:CB	13:T:122:ASP:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:138:SER:O	13:T:142:ILE:HG13	2.14	0.47
13:T:285:ALA:O	13:T:294:ILE:HG13	2.14	0.47
16:Q:96:ALA:HB3	16:Q:128:VAL:HG21	1.96	0.47
16:Q:96:ALA:HB2	16:Q:124:TYR:CE2	2.50	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
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
16:H:215:ALA:O	16:H:216:ARG:HB2	2.14	0.47
6:G:104:TRP:HB3	6:G:154:LEU:HD11	1.97	0.47
8:I:37:PHE:HE1	8:I:74:PRO:HA	1.79	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
5:5:34:PHE:CD1	5:5:92:VAL:HG11	2.50	0.47
14:M:30:GLY:O	14:M:34:LEU:HG	2.15	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:104:LEU:HB2	4:E:342:VAL:HG11	1.97	0.47
4:E:174:ARG:N	4:E:177:GLY:O	2.33	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
10:P:49:ASP:N	10:P:50:PRO:HD3	2.30	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
16:Q:327:VAL:HA	16:Q:332:LEU:HD13	1.95	0.47
3:3:369:LEU:HD12	3:3:369:LEU:O	2.14	0.47
4:4:171:ASN:CG	4:4:174:ARG:HH22	2.23	0.47
8:7:48:TYR:CE2	8:7:50:LEU:HB2	2.49	0.47
15:N:290:LEU:HD13	15:N:408:LEU:HB3	1.97	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
11:R:111:LEU:HD12	12:S:1:MET:HE1	1.97	0.47
14:U:307:GLY:HA2	14:U:380:THR:HA	1.97	0.47
14:U:345:ARG:HG2	14:U:412:LYS:O	2.15	0.47
16:Q:220:ASP:OD2	16:Q:301:ARG:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:L:115:MET:HE3	13:L:119:VAL:HG13	1.96	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
16:H:194:TRP:HE3	16:H:196:PHE:HE1	1.63	0.46
16:H:216:ARG:C	16:H:218:PRO:HD3	2.40	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
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
1:1:339:ASP:OD2	2:2:89:LYS:HE2	2.14	0.46
1:1:367:MET:HE2	1:1:367:MET:HB3	1.82	0.46
3:3:83:CYS:SG	3:3:84:VAL:HG13	2.55	0.46
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
4:4:196:VAL:O	4:4:200:ARG:HB2	2.15	0.46
6:6:35:SER:HG	6:6:37:TRP:HE3	1.62	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
11:J:72:MET:HE1	16:H:153:LEU:HD21	1.97	0.46
14:M:232:THR:HG21	14:M:322:THR:HG21	1.96	0.46
16:H:200:PHE:O	16:H:203:PHE:HB3	2.15	0.46
3:D:522:ARG:NH1	3:D:681:LYS:HD3	2.29	0.46
10:P:66:MET:CE	10:P:67:LEU:HD12	2.39	0.46
14:U:262:PHE:N	14:U:391:LEU:HD13	2.30	0.46
14:U:385:TYR:HA	14:U:389:PRO:HA	1.97	0.46
15:V:271:LEU:HB3	15:V:352:ALA:HB2	1.97	0.46
16:Q:166:LEU:HD22	16:Q:206:TYR:CE2	2.50	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
11:J:65:VAL:HG23	16:H:134:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:101:THR:HG22	8:I:108:ILE:HD11	1.97	0.46
4:E:47:LEU:HD13	4:E:51:GLU:O	2.16	0.46
5:F:2:ARG:HG3	5:F:84:ASP:OD2	2.15	0.46
5:F:185:LYS:HB2	5:F:189:ARG:HG3	1.98	0.46
6:G:72:PRO:HG3	10:P:44:TYR:HE1	1.80	0.46
7:O:11:GLY:O	7:O:15:LYS:HG3	2.15	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
6:6:17:GLU:HA	10:A:33:PRO:HG3	1.98	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
13:L:217:SER:HA	13:L:246:VAL:HA	1.98	0.46
16:H:218:PRO:HB3	16:H:305:LEU:HD13	1.96	0.46
2:C:81:GLN:HB3	2:C:122:VAL:CG2	2.45	0.46
3:D:304:ASN:O	3:D:589:HIS:CD2	2.68	0.46
3:D:477:LEU:CD2	3:D:521:ALA:HB2	2.45	0.46
4:E:40:VAL:HG21	6:G:88:MET:HE2	1.97	0.46
6:G:96:TRP:CZ2	6:G:103:LYS:HE3	2.50	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
4:4:104:LEU:HD21	4:4:359:SER:HB3	1.97	0.46
4:4:200:ARG:HD2	4:4:200:ARG:HA	1.70	0.46
6:6:117:MET:HE3	6:6:118:PHE:CZ	2.51	0.46
12:K:38:ALA:HA	15:N:149:TYR:HD1	1.81	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
13:T:334:LEU:HD12	13:T:449:LEU:CD1	2.46	0.46
16:Q:220:ASP:HA	16:Q:222:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:W:35:THR:O	9:W:93:VAL:HA	2.16	0.46
13:L:376:LEU:HD12	13:L:377:PRO:HD2	1.97	0.46
14:M:70:LEU:HD23	14:M:243:ARG:NH2	2.30	0.46
14:M:219:GLN:HA	14:M:282:LYS:HG3	1.98	0.46
15:N:422:ALA:O	15:N:423:LEU:HD23	2.15	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
6:G:35:SER:O	6:G:36:LEU:C	2.57	0.46
9:X:111:LEU:HG	9:X:115:MET:HE2	1.97	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
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
2:2:82:VAL:HG22	2:2:134:ILE:HG12	1.97	0.46
3:3:688:ARG:HD3	3:3:688:ARG:HA	1.50	0.46
4:4:148:TYR:N	4:4:148:TYR:CD1	2.84	0.46
6:6:35:SER:O	6:6:36:LEU:C	2.57	0.46
6:6:57:ARG:HD2	6:6:60:LEU:HG	1.94	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
16:H:216:ARG:HD2	16:H:294:ARG:CA	2.46	0.46
3:D:55:PRO:HG3	3:D:74:GLN:H	1.80	0.46
3:D:186:ARG:HD2	3:D:231:PRO:HD3	1.97	0.46
3:D:536:THR:OG1	3:D:538:ALA:O	2.27	0.46
4:E:225:PRO:HG3	4:E:383:TYR:OH	2.16	0.46
4:E:337:PRO:O	4:E:361:GLY:HA2	2.15	0.46
7:O:44:THR:HA	7:O:138:VAL:HG13	1.98	0.46
7:O:133:LYS:O	7:O:137:LEU:HD13	2.15	0.46
1:1:381:GLU:CD	1:1:426:ARG:HH21	2.24	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
11:J:104:LEU:O	11:J:108:LEU:HD12	2.16	0.46
13:L:138:SER:OG	13:L:245:MET:HE3	2.15	0.46
13:L:360:PRO:HA	13:L:363:ARG:HH12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:406:GLY:O	15:N:409:LEU:HB2	2.15	0.46
3:D:115:HIS:CB	4:E:321:MET:HE3	2.31	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
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
15:V:294:LEU:HD11	15:V:325:ALA:HB1	1.98	0.46
1:1:225:ALA:O	1:1:229:PRO:HD2	2.16	0.46
18:1:502:FMN:H9	18:1:502:FMN:H1'1	1.51	0.46
3:3:85:THR:HG22	3:3:86:ALA:O	2.16	0.46
3:3:409:LEU:HD23	3:3:409:LEU:HA	1.57	0.46
4:4:38:HIS:ND1	4:4:139:ASP:OD2	2.47	0.46
4:4:288:LYS:HD3	4:4:288:LYS:HA	1.63	0.46
6:6:57:ARG:HH11	6:6:60:LEU:HD11	1.78	0.46
6:6:117:MET:HE2	7:9:99:ILE:HG12	1.97	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
15:N:416:PRO:C	15:N:418:LEU:H	2.23	0.46
16:H:220:ASP:OD2	16:H:301:ARG:HA	2.15	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
13:T:161:VAL:HG13	13:T:222:LEU:HD22	1.98	0.46
13:T:287:GLY:HA3	13:T:528:SER:HB2	1.97	0.46
13:T:325:HIS:CD2	13:T:329:LYS:HG3	2.51	0.46
14:U:75:PHE:HZ	14:U:111:ALA:HB2	1.80	0.46
15:V:231:GLU:CD	15:V:231:GLU:H	2.24	0.46
16:Q:290:PHE:O	16:Q:293:ILE:HB	2.15	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:HD1	4:4:148:TYR:H	1.62	0.46
5:5:42:LYS:NZ	5:5:107:LEU:O	2.40	0.46
15:N:154:PHE:O	15:N:158:THR:HG22	2.16	0.46
16:H:332:LEU:H	16:H:332:LEU:CD1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:O:108:CYS:HB2	7:O:113:ILE:HG22	1.98	0.46
13:T:77:LEU:HD12	13:T:116:LEU:HD22	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
15:V:63:THR:HG21	15:V:96:HIS:HD1	1.81	0.46
16:Q:96:ALA:HB1	16:Q:125:LEU:HD23	1.97	0.46
2:2:163:LEU:HA	2:2:166:ILE:HG13	1.97	0.45
3:3:52:ILE:HD12	3:3:85:THR:HG21	1.98	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
13:L:234:THR:HG23	13:L:292:LYS:HE2	1.98	0.45
13:L:604:MET:HE2	13:L:604:MET:HB3	1.76	0.45
15:N:73:THR:HG21	15:N:210:PHE:HB2	1.98	0.45
16:H:52:GLY:HA2	16:H:55:GLY:CA	2.46	0.45
1:B:88:TYR:HB2	1:B:216:THR:HG22	1.98	0.45
1:B:157:TYR:O	1:B:158:LEU:HD23	2.16	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
7:O:99:ILE:HG22	7:O:101:CYS:SG	2.56	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
16:Q:39:LEU:CD2	16:Q:295:ALA:HB2	2.42	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
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
16:H:52:GLY:HA2	16:H:55:GLY:HA2	1.97	0.45
2:C:82:VAL:HG22	2:C:134:ILE:HG12	1.98	0.45
3:D:272:GLY:O	3:D:630:GLU:N	2.49	0.45
3:D:451:PHE:HD1	3:D:466:GLU:HB3	1.80	0.45
4:E:28:LEU:HD11	16:Q:147:TYR:CE2	2.51	0.45
5:F:75:VAL:HG12	5:F:76:SER:N	2.31	0.45
5:F:101:LEU:HA	5:F:102:PRO:HD2	1.85	0.45
6:G:85:SER:HA	6:G:123:ILE:HD13	1.97	0.45
8:I:88:ARG:NH2	8:I:126:LEU:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:131:TRP:HH2	13:T:212:GLY:C	2.24	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
3:3:117:LEU:H	4:4:321:MET:HE1	1.77	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
6:6:57:ARG:NE	6:6:60:LEU:HD21	2.30	0.45
6:6:96:TRP:CZ2	6:6:103:LYS:HE3	2.52	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
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
9:X:1:MET:HE1	9:X:110:LEU:HD23	1.97	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
16:Q:216:ARG:HG3	16:Q:219:PHE:CE1	2.50	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
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
16:H:85:ALA:HB3	16:H:86:PRO:HD3	1.99	0.45
1:B:199:PRO:HG2	17:B:501:SF4:S2	2.56	0.45
13:T:223:MET:HE3	13:T:534:VAL:HG11	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:345:LYS:NZ	15:V:368:SER:OG	2.49	0.45
16:Q:307:ARG:C	16:Q:307:ARG:HD3	2.42	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
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
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
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
16:Q:83:VAL:O	16:Q:86:PRO:HD2	2.17	0.45
16:Q:216:ARG:C	16:Q:218:PRO:HD3	2.41	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
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
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
18:B:502:FMN:H9	18:B:502:FMN:H1'1	1.53	0.45
4:E:200:ARG:HD2	4:E:200:ARG:HA	1.71	0.45
4:E:338:PRO:HG2	5:F:193:ARG:HD3	1.98	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
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
16:Q:291:ILE:HA	16:Q:294:ARG:CG	2.47	0.45
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
3:3:20:MET:O	3:3:23:VAL:HB	2.17	0.45
3:3:128:CYS:SG	3:3:130:LEU:HB3	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:177:ALA:HB3	2:C:67:TYR:CG	2.51	0.45
2:C:24:ARG:HE	2:C:55:THR:HG21	1.82	0.45
2:C:78:TYR:HD2	2:C:116:LEU:HD12	1.80	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
10:P:38:ARG:O	10:P:42:MET:HG3	2.17	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
4:4:328:PHE:CE2	7:9:58:LEU:HD21	2.52	0.45
5:5:116:ARG:HB3	5:5:135:ILE:HG13	1.98	0.45
14:M:88:VAL:HG11	14:M:432:PHE:CD1	2.52	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
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:H:211:MET:O	16:H:218:PRO:HG3	2.16	0.45
3:D:50:VAL:CG2	3:D:82:SER:HB3	2.47	0.45
3:D:611:ARG:HA	3:D:624:LEU:O	2.17	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
9:X:78:VAL:HG21	9:X:126:TYR:CB	2.45	0.45
14:U:160:LEU:O	14:U:163:VAL:HG12	2.17	0.45
16:Q:189:GLN:HG2	16:Q:195:LEU:H	1.81	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:H:213:GLU:OE1	16:H:213:GLU:N	2.49	0.45
16:H:308:PHE:O	16:H:312:PHE:HB3	2.17	0.45
1:B:336:SER:HB2	1:B:432:PRO:HD2	1.99	0.45
4:E:47:LEU:HA	4:E:53:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:47:LEU:HD21	4:E:390:VAL:HG22	1.98	0.45
6:G:84:LEU:HD11	6:G:89:ALA:HA	1.99	0.45
13:T:425:PHE:C	13:T:426:LEU:HD12	2.42	0.45
14:U:131:LEU:O	14:U:135:LEU:HD23	2.17	0.45
1:1:18:TYR:OH	1:1:102:LYS:O	2.30	0.45
3:3:648:LEU:HD23	3:3:648:LEU:HA	1.81	0.45
4:4:47:LEU:HD21	4:4:390:VAL:HG22	1.98	0.45
4:4:62:LEU:HD23	4:4:62:LEU:HA	1.85	0.45
4:4:185:GLU:O	4:4:189:GLU:HG2	2.17	0.45
9:W:1:MET:HE1	9:W:110:LEU:HD23	1.98	0.45
9:W:78:VAL:HG21	9:W:126:TYR:CB	2.43	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
16:H:176:LEU:HD22	16:H:334:ARG:HD2	1.98	0.45
1:B:239:ALA:C	1:B:241:MET:H	2.25	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:373:GLY:CA	3:D:538:ALA:HB2	2.47	0.45
3:D:409:LEU:HA	3:D:409:LEU:HD23	1.52	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
13:T:214:VAL:HG12	13:T:222:LEU:HB2	1.99	0.45
14:U:68:ASP:O	14:U:72:ALA:HB2	2.16	0.45
14:U:335:ARG:NH2	14:U:429:GLU:OE1	2.49	0.45
3:3:545:GLU:HA	3:3:550:LEU:HD11	1.99	0.44
4:4:87:TYR:HB3	4:4:169:HIS:CE1	2.51	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
11:J:69:PHE:O	11:J:73:LEU:HG	2.17	0.44
11:J:142:VAL:O	11:J:145:LEU:HB3	2.17	0.44
12:K:79:PHE:CD2	12:K:85:THR:HA	2.52	0.44
14:M:85:GLY:HA2	14:M:327:LEU:HD22	1.99	0.44
14:M:166:ALA:O	14:M:170:SER:OG	2.28	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: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
4:E:112:ARG:NH1	4:E:299:PRO:HA	2.31	0.44
6:G:83:ARG:HB2	6:G:123:ILE:HD12	1.99	0.44
13:T:40:SER:OG	13:T:41:PHE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:M:41:LEU:HD23	14:M:449:TYR:OH	2.16	0.44
1:B:104:ARG:NH2	2:C:127:SER:HB3	2.26	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
14:U:114:ASP:OD1	14:U:117:VAL:HB	2.17	0.44
16:Q:314:PHE:N	16:Q:314:PHE:CD1	2.83	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
4:4:47:LEU:HD13	4:4:51:GLU:C	2.42	0.44
4:4:139:ASP:OD2	4:4:398:ALA:HB2	2.17	0.44
4:4:248:VAL:HB	4:4:347:GLU:HB2	2.00	0.44
7:9:149:GLU:HA	7:9:152:ARG:NE	2.32	0.44
10:A:62:TYR:CD1	10:A:62:TYR:C	2.95	0.44
10:A:109:TYR:CD2	11:J:151:VAL:HG22	2.52	0.44
12:K:85:THR:O	12:K:86:ALA:C	2.61	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
16:H:211:MET:HG3	16:H:212:ALA:N	2.32	0.44
1:B:357:THR:N	1:B:358:PRO:HD2	2.33	0.44
4:E:81:TYR:CZ	6:G:117:MET:HG3	2.52	0.44
4:E:138:LEU:HD13	4:E:143:LEU:HA	1.98	0.44
6:G:97:GLU:O	10:P:40:LYS:HG3	2.17	0.44
8:I:123:ARG:O	8:I:127:ALA:HB3	2.17	0.44
13:T:20:PHE:HD1	13:T:23:ARG:HE	1.64	0.44
13:T:359:LEU:HD23	13:T:437:GLU:CD	2.42	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:269:LEU:HD12	14:U:394:LEU:HG	2.00	0.44
14:U:279:LYS:HD3	14:U:279:LYS:HA	1.71	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
15:V:416:PRO:C	15:V:418:LEU:H	2.24	0.44
1:1:64:GLY:HA3	18:1:502:FMN:O1P	2.16	0.44
1:1:184:GLU:OE1	1:1:186:THR:OG1	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:249:ARG:HB3	4:4:257:TYR:CD2	2.52	0.44
6:6:60:LEU:CD1	6:6:60:LEU:C	2.89	0.44
6:6:96:TRP:CE2	6:6:103:LYS:HE3	2.53	0.44
7:9:10:LEU:O	16:H:292:TRP:HZ2	2.01	0.44
8:7:48:TYR:CZ	8:7:50:LEU:HB2	2.52	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:H:9:PRO:HB2	16:H:11:TRP:NE1	2.33	0.44
16:H:152:SER:C	16:H:155:SER:HG	2.10	0.44
16:H:162:TYR:HA	16:H:314:PHE:HZ	1.81	0.44
2:C:78:TYR:CE2	2:C:157:LEU:HB3	2.52	0.44
4:E:288:LYS:HA	4:E:288:LYS:HD3	1.67	0.44
5:F:26:TRP:CD1	5:F:91:ARG:HH21	2.35	0.44
6:G:31:GLY:O	6:G:35:SER:HB3	2.18	0.44
6:G:132:PRO:HG3	6:G:178:ARG:CD	2.48	0.44
8:I:45:GLU:H	8:I:45:GLU:CD	2.25	0.44
13:T:309:ALA:HB2	13:T:388:ILE:HG12	2.00	0.44
13:T:321:HIS:HA	13:T:384:SER:CB	2.48	0.44
15:V:241:VAL:HG12	15:V:367:THR:OG1	2.18	0.44
16:Q:176:LEU:HD22	16:Q:334:ARG:HD2	1.99	0.44
1:1:341:MET:HE1	1:1:409:PRO:HB2	1.98	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
11:J:83:PHE:O	11:J:84:ASP:HB2	2.18	0.44
14:M:9:PRO:HG2	14:M:107:LEU:HD12	2.00	0.44
14:M:88:VAL:HG13	14:M:89:ALA:H	1.82	0.44
3:D:476:ILE:HG23	3:D:490:VAL:HG13	1.99	0.44
4:E:26:MET:HE2	10:P:57:PHE:HD1	1.82	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
10:P:22:VAL:O	10:P:26:LEU:HG	2.17	0.44
14:U:93:GLY:HA3	14:U:136:TYR:CE1	2.53	0.44
14:U:132:MET:SD	14:U:227:ALA:HA	2.57	0.44
14:U:350:SER:HB3	14:U:422:VAL:H	1.82	0.44
14:U:425:LEU:HD22	14:U:430:TRP:CE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:1:43:ARG:HG3	1:1:44:VAL:N	2.33	0.44
1:1:177:ALA:HB3	2:2:67:TYR:CG	2.52	0.44
1:1:272:PHE:CE2	1:1:311:MET:HE3	2.53	0.44
1:1:358:PRO:O	1:1:362:GLY:HA3	2.17	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
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
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
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
16:Q:45:ARG:HG3	16:Q:46:MET:N	2.25	0.44
1:1:101:PHE:H	1:1:253:GLN:HG3	1.83	0.44
2:2:76:GLY:H	2:2:118:SER:HG	1.59	0.44
2:2:80:LEU:HD13	2:2:100:LEU:HD11	2.00	0.44
2:2:100:LEU:HD13	2:2:150:LEU:HD21	2.00	0.44
3:3:21:ASP:OD1	3:3:431:PRO:HA	2.18	0.44
3:3:696:PRO:HB3	3:3:767:ALA:HB1	1.99	0.44
7:9:51:GLU:OE1	7:9:133:LYS:NZ	2.41	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
13:L:425:PHE:C	13:L:426:LEU:HD12	2.42	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
16:H:221:LEU:N	16:H:222:PRO:HA	2.31	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
7:O:59:CYS:HB2	7:O:104:CYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:87:PRO:O	8:I:88:ARG:HB2	2.17	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: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
14:U:331:ARG:HA	14:U:331:ARG:HD2	1.76	0.44
16:Q:66:SER:O	16:Q:238:SER:OG	2.25	0.44
16:Q:224:ALA:CA	16:Q:230:GLY:H	2.23	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
9:W:1:MET:HB3	9:W:107:PRO:HB3	1.99	0.44
10:A:77:PHE:CE2	12:K:62:ALA:HB2	2.51	0.44
12:K:55:VAL:O	12:K:59:MET:HG2	2.18	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
16:H:8:ASP:OD2	16:H:111:TYR:HB3	2.18	0.44
1:B:43:ARG:HG3	1:B:44:VAL:N	2.33	0.44
1:B:381:GLU:CD	1:B:426:ARG:HH21	2.25	0.44
5:F:135:ILE:HG22	5:F:136:LEU:HG	1.99	0.44
7:O:94:ASN:HB3	7:O:97:ARG:HB2	2.00	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
1:1:258:VAL:HB	1:1:330:LEU:HD12	1.99	0.44
3:3:149:LEU:O	3:3:149:LEU:HD23	2.18	0.44
3:3:462:ALA:O	3:3:465:HIS:ND1	2.51	0.44
4:4:57:PRO:HD3	4:4:382:PRO:HG3	1.99	0.44
4:4:104:LEU:HB2	4:4:342:VAL:HG11	2.00	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
14:M:88:VAL:HG13	14:M:89:ALA:N	2.32	0.44
14:M:296:ALA:HA	14:M:311:GLY:HA2	1.99	0.44
15:N:272:ALA:HB3	15:N:281:LEU:HD13	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:390:VAL:HG11	16:Q:228:LEU:HG	1.99	0.44
6:G:102:PRO:HG3	10:P:33:PRO:HG2	1.99	0.44
7:O:126:TYR:HB3	9:X:39:ASP:CG	2.43	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
3:3:55:PRO:HG3	3:3:74:GLN:H	1.82	0.43
4:4:26:MET:HG2	10:A:54:VAL:HB	1.99	0.43
4:4:173:ILE:O	4:4:174:ARG:NH1	2.51	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
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: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
14:M:269:LEU:HD12	14:M:394:LEU:HG	2.00	0.43
14:M:270:TYR:CE1	14:M:274:VAL:HG21	2.53	0.43
15:N:126:ARG:O	15:N:129:GLY:N	2.51	0.43
16:H:218:PRO:C	16:H:220:ASP:H	2.25	0.43
16:H:228:LEU:HD22	16:H:228:LEU:HA	1.60	0.43
1:B:96:SER:HB2	1:B:180:TYR:HD1	1.81	0.43
1:B:270:THR:O	1:B:311:MET:HG3	2.18	0.43
5:F:144:HIS:O	5:F:147:ARG:HG2	2.18	0.43
9:X:26:LEU:HD12	9:X:84:GLN:HB2	1.98	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
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
5:5:40:HIS:NE2	5:5:44:MET:HE2	2.33	0.43
9:W:81:LEU:HD13	9:W:89:PHE:HE1	1.82	0.43
11:J:46:LEU:HD23	11:J:46:LEU:HA	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
1:B:331:ILE:HA	1:B:332:PRO:HD2	1.73	0.43
2:C:154:LEU:HD23	2:C:154:LEU:HA	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:282:VAL:HG21	3:D:673:MET:HE1	2.00	0.43
3:D:695:ARG:O	3:D:697:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:U:88:VAL:HG13	14:U:89:ALA:N	2.33	0.43
14:U:296:ALA:HA	14:U:311:GLY:HA2	1.99	0.43
15:V:83:GLU:O	15:V:87:LEU:HG	2.17	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
16:Q:218:PRO:C	16:Q:220:ASP:H	2.25	0.43
3:3:689:LYS:HD2	3:3:772:GLU:HG2	1.99	0.43
5:5:2:ARG:HG3	5:5:84:ASP:OD2	2.18	0.43
5:5:120:ASP:OD2	5:5:136:LEU:N	2.44	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
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
16:H:215:ALA:C	16:H:294:ARG:HH11	2.26	0.43
1:B:259:LYS:NZ	2:C:178:GLU:OE2	2.45	0.43
2:C:61:MET:HB2	3:D:214:MET:HE3	2.01	0.43
3:D:556:ALA:HB2	3:D:562:GLY:HA3	2.00	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
7:O:139:ASP:OD1	7:O:139:ASP:N	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
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
15:N:231:GLU:CD	15:N:231:GLU:H	2.26	0.43
16:H:290:PHE:O	16:H:293:ILE:HB	2.17	0.43
1:B:404:ASP:OD1	1:B:404:ASP:N	2.50	0.43
3:D:159:PHE:CE2	8:I:79:LEU:HD13	2.53	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
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
8:I:52:THR:HB	8:I:54:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:477:LEU:HD12	13:T:477:LEU:HA	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
3:3:159:PHE:CE2	8:7:79:LEU:HD13	2.49	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
6:6:34:ASN:HB3	16:H:51:VAL:CG2	2.42	0.43
6:6:76:ASP:H	16:H:65:LYS:HZ1	1.65	0.43
10:A:74:GLU:O	10:A:78:LEU:HG	2.19	0.43
11:J:72:MET:SD	16:H:137:PHE:HD1	2.40	0.43
12:K:45:PHE:CD1	15:N:156:GLY:HA2	2.54	0.43
13:L:418:MET:HE3	13:L:505:LEU:HB3	2.00	0.43
14:M:55:LEU:HB3	14:M:61:VAL:O	2.19	0.43
14:M:143:ARG:HD3	14:M:143:ARG:HA	1.81	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: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:HA	14:U:331:ARG:HH11	1.84	0.43
15:V:206:PRO:O	15:V:209:LEU:HB3	2.18	0.43
16:Q:52:GLY:HA2	16:Q:55:GLY:CA	2.49	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
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
3:3:285:VAL:HG22	3:3:286:ASN:N	2.33	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
6:6:58:ASN:CG	16:H:48:PRO:HA	2.44	0.43
7:9:23:THR:HB	16:H:45:ARG:HD3	2.00	0.43
7:9:143:THR:O	7:9:147:ARG:HG3	2.19	0.43
11:J:4:LEU:O	11:J:7:LEU:HB3	2.18	0.43
11:J:64:VAL:HA	11:J:67:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
16:H:27:ALA:O	16:H:31:MET:HG2	2.19	0.43
16:H:67:ILE:O	16:H:68:PHE:HB2	2.18	0.43
16:H:108:PHE:HB3	16:H:112:GLN:H	1.82	0.43
1:B:219:ASN:ND2	18:B:502:FMN:O2P	2.51	0.43
3:D:85:THR:HG22	3:D:86:ALA:O	2.19	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
4:E:104:LEU:HA	5:F:22:LEU:CD1	2.49	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
13:T:95:MET:O	13:T:101:TYR:HE1	2.02	0.43
13:T:281:GLY:O	13:T:285:ALA:HB2	2.19	0.43
14:U:78:ILE:HG22	14:U:103:GLU:HG3	2.01	0.43
15:V:258:LEU:HD23	15:V:258:LEU:HA	1.85	0.43
1:1:102:LYS:HE2	1:1:222:GLU:OE1	2.19	0.43
3:3:20:MET:HE1	3:3:35:SER:HB2	2.00	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
9:W:99:MET:HE2	9:W:99:MET:HB2	1.70	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:91:VAL:CG2	14:M:92:GLU:N	2.80	0.43
14:M:194:PHE:HB2	14:M:249:ALA:HB3	1.99	0.43
15:N:44:TRP:CZ3	15:N:60:GLN:HB3	2.54	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:60:LEU:CD1	6:G:60:LEU:C	2.91	0.43
6:G:104:TRP:CZ2	6:G:173:VAL:HG22	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
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
16:Q:276:TYR:HD2	16:Q:280:PHE:HE2	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:284:LEU:HD11	2:2:179:VAL:HB	2.00	0.43
3:3:714:ALA:HB3	3:3:744:GLU:O	2.19	0.43
3:3:732:ALA:O	3:3:747:VAL:HG23	2.18	0.43
4:4:171:ASN:OD1	4:4:174:ARG:NH1	2.50	0.43
4:4:232:LEU:CD2	5:5:109:GLY:HA3	2.49	0.43
4:4:372:ALA:HA	4:4:373:PRO:HD2	1.85	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
11:J:135:TRP:HB3	12:K:59:MET:HE3	2.00	0.43
12:K:7:SER:O	12:K:37:ALA:HB1	2.18	0.43
13:L:54:ARG:CZ	13:L:68:LEU:HD13	2.49	0.43
13:L:450:ALA:O	13:L:453:SER:HB3	2.18	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
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
3:D:46:ARG:HG2	3:D:46:ARG:NH1	2.32	0.43
3:D:260:PRO:HB2	3:D:617:LEU:HB3	2.01	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
10:P:109:TYR:CD2	11:R:151:VAL:HG22	2.53	0.43
13:T:541:LEU:HA	13:T:545:PRO:HG2	2.00	0.43
14:U:95:PHE:HB2	14:U:98:LEU:HD12	2.01	0.43
14:U:424:ASP:O	14:U:425:LEU:HD12	2.19	0.43
15:V:374:TYR:O	15:V:378:LEU:HD13	2.19	0.43
16:Q:147:TYR:HD1	16:Q:229:VAL:HG22	1.82	0.43
16:Q:221:LEU:HB3	16:Q:222:PRO:CA	2.49	0.43
1:1:162:LEU:HD11	1:1:169:PHE:HB3	2.01	0.43
1:1:199:PRO:HG2	17:1:501:SF4:S2	2.59	0.43
1:1:336:SER:HB3	1:1:339:ASP:HB2	2.00	0.43
3:3:38:HIS:O	3:3:39:LEU:HD23	2.18	0.43
3:3:349:ALA:O	3:3:540:ASN:ND2	2.40	0.43
5:5:75:VAL:HG12	5:5:76:SER:N	2.33	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:53:ALA:HB3	13:L:69:LEU:HB3	2.00	0.43
13:L:340:ILE:O	13:L:345:GLY:N	2.45	0.43
14:M:119:TYR:CD2	14:M:159:MET:HE3	2.54	0.43
15:N:2:THR:HG23	15:N:36:ALA:HB1	2.01	0.43
16:H:150:LEU:O	16:H:154:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:MET:HE1	1:B:409:PRO:HB2	2.00	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
8:I:12:ALA:O	8:I:15:GLU:HB3	2.19	0.43
12:S:45:PHE:CD1	15:V:156:GLY:HA2	2.54	0.43
14:U:8:LEU:HD23	14:U:32:SER:HA	2.00	0.43
14:U:9:PRO:HG3	14:U:32:SER:HB2	2.01	0.43
15:V:422:ALA:O	15:V:423:LEU:HD23	2.18	0.43
16:Q:85:ALA:HB3	16:Q:86:PRO:HD3	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
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
10:A:54:VAL:HG22	16:H:146:LYS:HD2	2.00	0.43
11:J:100:VAL:O	11:J:104:LEU:HG	2.19	0.43
14:M:33:PHE:HA	14:M:79:ALA:CB	2.47	0.43
14:M:242:PHE:CZ	14:M:461:PHE:HD2	2.37	0.43
16:H:39:LEU:CD2	16:H:295:ALA:HB2	2.46	0.43
16:H:221:LEU:HB3	16:H:222:PRO:CA	2.49	0.43
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:H	3:D:337:ARG:HD2	1.82	0.43
4:E:185:GLU:O	4:E:189:GLU:HG2	2.19	0.43
4:E:276:MET:HE2	4:E:276:MET:HB2	1.79	0.43
6:G:18:GLY:CA	6:G:28:VAL:HG11	2.48	0.43
9:X:99:MET:HE2	9:X:99:MET:HB2	1.78	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
16:Q:125:LEU:O	16:Q:128:VAL:HG22	2.19	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:H	3:3:689:LYS:HG2	1.48	0.42
4:4:317:LEU:HD12	4:4:317:LEU:HA	1.74	0.42
6:6:76:ASP:HB3	16:H:69:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:L:257:SER:OG	13:L:478:ALA:HA	2.19	0.42
14:M:324:GLY:O	14:M:432:PHE:HZ	2.02	0.42
14:M:330:GLY:O	14:M:333:TYR:HB3	2.19	0.42
16:H:186:VAL:HA	16:H:189:GLN:NE2	2.34	0.42
16:H:204:LEU:HD23	16:H:204:LEU:HA	1.85	0.42
16:H:211:MET:HE1	16:H:300:LEU:HD22	2.00	0.42
1:B:51:ASP:OD1	1:B:81:LYS:HE2	2.19	0.42
1:B:203:PRO:HB2	1:B:204:PRO:HD3	2.01	0.42
1:B:367:MET:HE2	1:B:367:MET:HB3	1.92	0.42
2:C:85:THR:OG1	2:C:124:CYS:N	2.52	0.42
3:D:420:LEU:HD21	3:D:441:MET:HE1	2.01	0.42
4:E:311:PRO:HD3	4:E:330:HIS:CE1	2.54	0.42
4:E:315:HIS:HA	8:I:46:ARG:NH1	2.34	0.42
4:E:409:ARG:NH2	5:F:117:GLU:OE2	2.51	0.42
13:T:302:GLN:O	13:T:305:TYR:HB2	2.19	0.42
13:T:323:PHE:CE2	13:T:459:LEU:HD12	2.54	0.42
13:T:405:GLY:O	13:T:409:VAL:HG23	2.19	0.42
13:T:557:ASP:CG	14:U:211:HIS:HE2	2.27	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
14:U:219:GLN:HA	14:U:282:LYS:HG3	2.01	0.42
3:3:136:GLU:CD	5:5:186:GLY:H	2.28	0.42
3:3:227:THR:HG21	3:3:237:ASP:HB2	1.99	0.42
4:4:40:VAL:O	4:4:40:VAL:HG22	2.18	0.42
4:4:213:ILE:HG22	4:4:217:ARG:HG2	2.01	0.42
5:5:185:LYS:HB2	5:5:189:ARG:HG3	2.00	0.42
6:6:104:TRP:HE1	6:6:172:PRO:C	2.27	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:155:THR:HB	4:E:193:LEU:CD1	2.49	0.42
5:F:10:ALA:HB1	5:F:15:TYR:HB2	2.01	0.42
5:F:132:LEU:HD23	5:F:132:LEU:HA	1.90	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:88:VAL:HG22	14:U:331:ARG:HG3	2.01	0.42
14:U:98:LEU:HB3	14:U:132:MET:HE3	2.01	0.42
14:U:114:ASP:HB3	14:U:176:LEU:HD23	2.01	0.42
15:V:40:LEU:HD12	15:V:67:LEU:HD12	2.01	0.42
15:V:317:ARG:HH12	15:V:383:PHE:C	2.27	0.42
4:4:107:ALA:HB2	4:4:309:ILE:HD13	2.02	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
4:4:342:VAL:HG12	4:4:357:ILE:HB	2.01	0.42
9:W:89:PHE:CD2	9:W:123:PRO:HB3	2.54	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
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:40:HIS:NE2	5:F:44:MET:HE2	2.34	0.42
5:F:121:LEU:HA	5:F:145:PRO:HD2	2.00	0.42
6:G:92:MET:HE1	6:G:127:VAL:HG13	2.00	0.42
6:G:100:PRO:CG	16:Q:69:LYS:HE3	2.49	0.42
10:P:13:TYR:HE2	16:Q:98:GLY:HA3	1.83	0.42
10:P:44:TYR:O	10:P:48:ASN:HA	2.18	0.42
11:R:121:GLY:C	11:R:123:LEU:H	2.26	0.42
12:S:17:GLY:O	12:S:21:ARG:HG2	2.19	0.42
12:S:18:VAL:HG13	12:S:27:VAL:HG13	1.99	0.42
13:T:91:ALA:HB1	13:T:104:PHE:HE2	1.83	0.42
16:Q:332:LEU:HB3	16:Q:333:PRO:HD3	2.02	0.42
1:1:101:PHE:CZ	2:2:129:HIS:HB3	2.54	0.42
1:1:145:LEU:HD23	1:1:145:LEU:HA	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
3:3:477:LEU:HD22	3:3:517:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:533:LEU:HA	3:3:533:LEU:HD23	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
11:J:152:VAL:HG22	15:N:87:LEU:HD22	2.01	0.42
13:L:20:PHE:C	13:L:22:LYS:H	2.24	0.42
13:L:40:SER:OG	13:L:41:PHE:N	2.52	0.42
13:L:146:TYR:HB2	14:M:415:TRP:O	2.20	0.42
13:L:177:TRP:HE1	14:M:306:GLU:CD	2.28	0.42
13:L:192:MET:HE1	13:L:259:LEU:HA	2.01	0.42
13:L:359:LEU:HD23	13:L:437:GLU:CD	2.44	0.42
13:L:586:LEU:HD11	15:N:135:LYS:HA	2.01	0.42
14:M:95:PHE:C	14:M:97:GLY:N	2.73	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
16:H:220:ASP:HA	16:H:222:PRO:HB3	2.01	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:120:ASP:CG	5:F:134:LYS:HG3	2.44	0.42
5:F:145:PRO:HA	5:F:150:TYR:CD1	2.54	0.42
7:O:91:TYR:HE1	7:O:93:ILE:HD11	1.85	0.42
7:O:112:ALA:HB3	17:O:202:SF4:S4	2.58	0.42
10:P:2:ALA:HB3	16:Q:119:ASP:OD2	2.20	0.42
10:P:63:VAL:O	10:P:67:LEU:HD13	2.20	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
16:Q:20:VAL:O	16:Q:24:LEU:HD13	2.19	0.42
16:Q:200:PHE:O	16:Q:203:PHE:HB3	2.19	0.42
1:1:370:LEU:HD12	1:1:387:LEU:HB2	2.02	0.42
3:3:327:LEU:HD23	3:3:327:LEU:HA	1.73	0.42
4:4:38:HIS:HE1	4:4:398:ALA:HA	1.84	0.42
4:4:138:LEU:HD13	4:4:143:LEU:HA	2.00	0.42
4:4:393:MET:HE2	4:4:393:MET:HB3	1.89	0.42
5:5:31:ARG:NH2	5:5:98:ASP:OD2	2.52	0.42
9:W:78:VAL:HA	9:W:81:LEU:HD12	2.00	0.42
11:J:52:GLY:O	11:J:56:VAL:HG23	2.19	0.42
13:L:41:PHE:HB2	13:L:81:THR:HB	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:83:VAL:O	16:H:86:PRO:HD2	2.20	0.42
16:H:301:ARG:O	16:H:302:TYR:HD1	2.02	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
8:I:48:TYR:CE2	8:I:50:LEU:HB2	2.54	0.42
11:R:4:LEU:HG	11:R:7:LEU:HD22	2.02	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:291:ILE:O	13:T:295:VAL:HG23	2.18	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:6:LEU:HD13	15:V:93:LEU:HA	2.00	0.42
15:V:281:LEU:HD12	15:V:281:LEU:HA	1.82	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:HA	5:5:64:ARG:HD3	1.88	0.42
6:6:38:PRO:O	6:6:63:PHE:HD1	2.02	0.42
12:K:49:TYR:CD1	15:N:159:GLY:HA2	2.55	0.42
13:L:223:MET:HE3	13:L:534:VAL:HG11	2.00	0.42
13:L:373:LEU:HD21	13:L:416:TYR:HE1	1.85	0.42
14:M:73:LEU:H	14:M:73:LEU:HD23	1.85	0.42
14:M:424:ASP:O	14:M:425:LEU:HD12	2.20	0.42
15:N:260:TYR:HA	15:N:263:ILE:HD12	2.00	0.42
16:H:153:LEU:HD23	16:H:153:LEU:HA	1.73	0.42
16:H:292:TRP:HD1	16:H:296:THR:HG1	1.67	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:57:PRO:HD3	4:E:382:PRO:HG3	2.00	0.42
4:E:254:TYR:CE2	4:E:346:THR:HA	2.54	0.42
4:E:329:LYS:HD2	4:E:329:LYS:HA	1.82	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
8:I:20:MET:HE2	8:I:20:MET:HB3	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:119:TYR:CD2	14:U:159:MET:HE3	2.55	0.42
15:V:52:PRO:HB3	15:V:103:HIS:HB2	2.00	0.42
16:Q:161:SER:O	16:Q:164:LEU:HB3	2.19	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
4:4:276:MET:HE2	4:4:276:MET:HB2	1.85	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
7:9:59:CYS:SG	7:9:91:TYR:OH	2.71	0.42
7:9:100:PHE:HA	17:9:201:SF4:S4	2.60	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
16:H:52:GLY:HA2	16:H:55:GLY:N	2.33	0.42
1:B:174:HIS:CE1	2:C:29:PRO:HD3	2.54	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
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
10:P:67:LEU:HD23	16:Q:310:TRP:NE1	2.35	0.42
13:T:21:GLY:C	13:T:102:SER:HB3	2.44	0.42
13:T:49:LEU:HD23	13:T:49:LEU:HA	1.94	0.42
13:T:156:ARG:HG3	14:U:407:LEU:HB3	2.02	0.42
13:T:189:LYS:HZ3	13:T:477:LEU:CD1	2.33	0.42
13:T:519:ALA:HB3	13:T:520:TRP:CE3	2.55	0.42
14:U:27:LEU:O	14:U:31:LEU:HD13	2.20	0.42
14:U:85:GLY:HA2	14:U:327:LEU:HD22	2.00	0.42
14:U:143:ARG:HA	14:U:143:ARG:HD3	1.75	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
4:4:90:SER:O	4:4:93:HIS:HB2	2.20	0.42
4:4:197:LEU:N	4:4:198:PRO:HD2	2.34	0.42
5:5:112:ASN:O	5:5:129:HIS:NE2	2.53	0.42
6:6:76:ASP:HB3	16:H:69:LYS:HZ3	1.84	0.42
6:6:94:ARG:O	6:6:98:GLN:N	2.49	0.42
9:W:21:LEU:HD11	9:W:26:LEU:HD21	2.02	0.42
14:M:10:VAL:HG23	14:M:104:GLY:HA3	2.02	0.42
15:N:29:THR:HG21	15:N:85:TYR:HB3	2.01	0.42
15:N:46:LYS:N	15:N:47:PRO:HD3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:559:ASP:OD2	3:D:686:LYS:NZ	2.52	0.42
4:E:47:LEU:HD13	4:E:51:GLU:C	2.45	0.42
11:R:25:ALA:HB2	12:S:26:LEU:HD11	2.01	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
13:T:325:HIS:HA	13:T:328:PHE:CE2	2.55	0.42
14:U:296:ALA:HB2	14:U:314:LEU:CD2	2.49	0.42
15:V:24:GLY:HA2	15:V:27:ARG:HD2	2.01	0.42
15:V:241:VAL:HG12	15:V:245:ASN:ND2	2.34	0.42
16:Q:260:PRO:HG3	16:Q:286:PHE:CD2	2.54	0.42
1:1:112:HIS:HA	1:1:115:ILE:HD12	2.00	0.42
3:3:17:THR:HG22	3:3:18:SER:O	2.20	0.42
3:3:168:HIS:HA	3:3:169:PRO:HD2	1.86	0.42
3:3:501:LYS:HD2	3:3:501:LYS:N	2.25	0.42
3:3:689:LYS:HG3	3:3:771:VAL:HA	2.01	0.42
4:4:314:ARG:HB3	8:7:44:MET:CE	2.37	0.42
5:5:105:THR:HG21	5:5:130:PRO:CD	2.50	0.42
5:5:112:ASN:O	5:5:129:HIS:CE1	2.73	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
11:J:156:LEU:HD12	11:J:156:LEU:HA	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
16:H:216:ARG:HG3	16:H:219:PHE:CE1	2.54	0.42
1:B:272:PHE:CE2	1:B:311:MET:HE3	2.55	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
6:G:72:PRO:HG3	10:P:44:TYR:CE1	2.55	0.42
7:O:67:ALA:HB2	7:O:97:ARG:HB3	2.02	0.42
8:I:10:TYR:O	8:I:14:VAL:HG23	2.20	0.42
9:X:89:PHE:CD2	9:X:123:PRO:HB3	2.55	0.42
9:X:106:PRO:HA	9:X:107:PRO:HD3	1.90	0.42
10:P:1:MET:HG2	10:P:2:ALA:H	1.85	0.42
11:R:87:VAL:C	11:R:89:SER:N	2.78	0.42
13:T:554:PHE:HD2	14:U:277:ALA:HB3	1.85	0.42
15:V:17:GLY:HA3	15:V:82:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:104:LEU:HD21	15:V:163:LEU:HD21	2.00	0.42
16:Q:136:ILE:HD12	16:Q:159:LEU:HD22	2.00	0.42
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
4:4:36:SER:HB2	16:H:226:GLN:HA	2.02	0.42
4:4:129:HIS:CE1	4:4:349:ALA:HB1	2.55	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
15:N:345:LYS:HB3	15:N:349:PHE:CE2	2.55	0.42
1:B:344:LEU:O	1:B:347:PHE:HB3	2.20	0.42
4:E:314:ARG:HB3	8:I:44:MET:CE	2.37	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
12:S:85:THR:O	12:S:86:ALA:C	2.63	0.42
13:T:278:ALA:HB1	13:T:409:VAL:HG11	2.02	0.42
13:T:554:PHE:HE2	14:U:278:ALA:HA	1.85	0.42
14:U:181:LEU:HD21	14:U:247:PRO:HB2	2.02	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
2:2:89:LYS:C	2:2:92:GLY:H	2.27	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
4:4:48:SER:H	4:4:53:LEU:HD23	1.85	0.41
4:4:291:LYS:O	4:4:295:GLU:HG3	2.20	0.41
5:5:49:LEU:HD21	5:5:52:ILE:HD11	2.01	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
6:6:108:MET:HA	6:6:137:VAL:CG1	2.50	0.41
12:K:45:PHE:CG	15:N:156:GLY:HA2	2.54	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
14:M:304:THR:HA	14:M:305:PRO:HD2	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:82:ASP:OD1	5:F:82:ASP:N	2.51	0.41
7:O:6:LEU:HB3	16:Q:297:TRP:CZ2	2.55	0.41
15:V:380:LEU:HD23	15:V:380:LEU:HA	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
4:4:245:ASN:O	5:5:79:GLY:HA3	2.20	0.41
4:4:352:GLU:CD	5:5:87:ARG:HH22	2.28	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
6:6:57:ARG:HG3	6:6:57:ARG:NH1	2.24	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
8:7:24:ALA:HB2	8:7:31:PHE:HB2	2.01	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
16:H:216:ARG:NH1	16:H:294:ARG:HB3	2.35	0.41
1:B:17:LEU:HD22	1:B:113:LEU:HD21	2.00	0.41
1:B:89:LEU:HD13	1:B:125:ILE:HD11	2.01	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:HD23	3:D:648:LEU:HA	1.75	0.41
5:F:157:THR:C	5:F:158:LEU:HD23	2.45	0.41
7:O:46:HIS:NE2	7:O:52:LYS:HA	2.35	0.41
15:V:44:TRP:CZ3	15:V:60:GLN:HB3	2.55	0.41
15:V:207:VAL:O	15:V:210:PHE:HB3	2.19	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:N	3:3:654:PHE:CD1	2.87	0.41
4:4:74:THR:HG22	4:4:75:TYR:N	2.36	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
7:9:97:ARG:HA	7:9:97:ARG:HD3	1.32	0.41
10:A:9:GLY:O	10:A:12:ILE:HB	2.20	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
14:M:134:TYR:HB2	14:M:145:LEU:CD1	2.50	0.41
15:N:241:VAL:HG12	15:N:245:ASN:ND2	2.34	0.41
15:N:317:ARG:HH12	15:N:383:PHE:C	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:260:PRO:HB3	16:H:282:LYS:HD3	2.02	0.41
3:D:454:TYR:HB2	3:D:752:ASP:OD2	2.21	0.41
3:D:719:HIS:HA	3:D:720:PRO:HD3	1.97	0.41
6:G:137:VAL:HA	6:G:138:PRO:HD2	1.82	0.41
7:O:101:CYS:N	17:O:201:SF4:S4	2.93	0.41
8:I:86:LEU:HA	8:I:87:PRO:HD2	1.91	0.41
13:T:450:ALA:O	13:T:453:SER:HB3	2.19	0.41
14:U:95:PHE:C	14:U:97:GLY:N	2.74	0.41
15:V:326:PHE:HE2	15:V:378:LEU:HB3	1.86	0.41
16:Q:58:GLN:O	16:Q:58:GLN:HG3	2.20	0.41
4:4:156:ILE:O	4:4:159:LEU:HB2	2.19	0.41
4:4:332:THR:HB	5:5:172:ALA:HB1	2.02	0.41
4:4:385:CYS:HA	4:4:396:ILE:HD13	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
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
16:H:218:PRO:HB3	16:H:305:LEU:CD1	2.50	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:HD2	3:D:501:LYS:N	2.25	0.41
5:F:157:THR:O	5:F:158:LEU:HD23	2.21	0.41
7:O:155:LYS:HA	7:O:155:LYS:HD2	1.91	0.41
8:I:15:GLU:O	8:I:18:SER:HB3	2.20	0.41
14:U:9:PRO:HG2	14:U:107:LEU:HD12	2.03	0.41
14:U:82:VAL:HG13	14:U:230:LEU:HD11	2.02	0.41
14:U:304:THR:HA	14:U:305:PRO:HD2	1.74	0.41
16:Q:218:PRO:HB3	16:Q:305:LEU:HD13	2.02	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
6:6:82:GLY:HA2	17:6:201:SF4:S4	2.61	0.41
16:H:166:LEU:HD22	16:H:206:TYR:CE2	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:59:CYS:SG	7:O:91:TYR:OH	2.71	0.41
10:P:2:ALA:CB	16:Q:119:ASP:HB3	2.50	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:83:GLU:HA	15:V:86:LEU:HB2	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
16:Q:216:ARG:NH1	16:Q:294:ARG:HB3	2.36	0.41
1:1:259:LYS:HE3	1:1:260:ARG:HH21	1.86	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
3:3:557:SER:OG	3:3:559:ASP:OD1	2.38	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
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:541:LEU:C	13:L:545:PRO:HG2	2.46	0.41
13:L:562:SER:HA	13:L:565:PHE:CD2	2.56	0.41
14:M:47:VAL:HG13	14:M:50:ALA:HB2	2.03	0.41
14:M:134:TYR:CE2	15:N:383:PHE:HB2	2.55	0.41
14:M:150:LEU:HD21	15:N:372:ALA:HB3	2.02	0.41
15:N:201:GLN:HA	15:N:255:LYS:HE3	2.02	0.41
16:H:309:GLY:HA2	16:H:313:LEU:HB2	2.03	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:30:VAL:HG13	4:E:35:PRO:HD2	2.03	0.41
4:E:346:THR:HG22	4:E:353:LEU:O	2.21	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
14:U:88:VAL:HG11	14:U:432:PHE:CD1	2.56	0.41
16:Q:12:MET:HE2	16:Q:111:TYR:HD2	1.86	0.41
16:Q:108:PHE:O	16:Q:109:PHE:HB2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:168:PHE:CE1	6:6:141:PRO:HG3	2.55	0.41
4:4:173:ILE:HA	4:4:178:VAL:HG12	2.03	0.41
5:5:82:ASP:OD1	5:5:82:ASP:N	2.51	0.41
7:9:113:ILE:HD12	7:9:113:ILE:HA	1.94	0.41
11:J:46:LEU:HD11	12:K:3:TYR:CG	2.56	0.41
11:J:111:LEU:HD12	12:K:1:MET:HE1	2.02	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
1:B:250:LYS:NZ	1:B:325:THR:O	2.52	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:R:83:PHE:HB3	11:R:85:PRO:CD	2.51	0.41
11:R:138:VAL:HG22	15:V:106:LEU:HB2	2.01	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
16:Q:67:ILE:O	16:Q:68:PHE:HB2	2.20	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
3:3:7:ASN:CG	3:3:96:LEU:HD12	2.46	0.41
3:3:80:ALA:HB1	3:3:85:THR:OG1	2.21	0.41
4:4:75:TYR:CZ	4:4:337:PRO:HG2	2.56	0.41
4:4:84:ARG:NE	4:4:169:HIS:HB3	2.36	0.41
5:5:44:MET:HE3	5:5:44:MET:HB2	1.88	0.41
8:7:14:VAL:HG21	8:7:51:PRO:HB2	2.01	0.41
8:7:20:MET:HE3	8:7:59:LEU:HG	2.02	0.41
12:K:47:ARG:HE	12:K:47:ARG:HB3	1.60	0.41
13:L:17:LEU:HD21	13:L:32:LEU:HD12	2.02	0.41
13:L:122:ASP:OD1	13:L:186:SER:HB3	2.21	0.41
14:M:68:ASP:O	14:M:72:ALA:HB2	2.19	0.41
14:M:98:LEU:HB3	14:M:132:MET:HE3	2.03	0.41
14:M:190:ALA:HB1	14:M:249:ALA:HB1	2.03	0.41
15:N:261:SER:OG	15:N:375:TYR:OH	2.25	0.41
16:H:71:ASP:OD1	16:H:240:LYS:NZ	2.34	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
10:P:66:MET:HA	11:R:66:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:46:LEU:HD11	12:S:3:TYR:CG	2.56	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
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
16:Q:215:ALA:C	16:Q:294:ARG:HH11	2.28	0.41
1:1:437:TRP:HB3	2:2:92:GLY:CA	2.30	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
4:4:208:PHE:HE1	16:H:298:PHE:CE2	2.39	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
4:4:390:VAL:HB	4:4:391:PRO:HD3	2.01	0.41
5:5:112:ASN:HA	5:5:129:HIS:NE2	2.36	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
12:K:4:LEU:HD12	12:K:41:SER:HA	2.03	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: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
13:L:490:GLU:O	13:L:494:ILE:HG12	2.21	0.41
14:M:9:PRO:HG3	14:M:32:SER:CB	2.51	0.41
14:M:36:ASN:HB3	14:M:75:PHE:HB3	2.02	0.41
14:M:75:PHE:HA	14:M:107:LEU:CD2	2.51	0.41
14:M:438:LEU:HD12	14:M:438:LEU:HA	1.74	0.41
15:N:104:LEU:HD23	15:N:104:LEU:HA	1.86	0.41
16:H:259:ILE:HB	16:H:260:PRO:HD3	2.02	0.41
16:H:269:MET:SD	16:H:282:LYS:HE3	2.60	0.41
1:B:16:THR:HG21	1:B:229:PRO:HB3	2.03	0.41
1:B:37:GLY:O	1:B:38:TYR:HB2	2.19	0.41
1:B:253:GLN:O	1:B:327:GLY:HA2	2.21	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
3:D:401:ASP:O	3:D:405:GLU:HG3	2.21	0.41
4:E:103:LYS:HE3	4:E:103:LYS:HB3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:108:MET:HA	6:G:137:VAL:CG1	2.51	0.41
6:G:140:CYS:SG	7:O:99:ILE:HG13	2.60	0.41
6:G:165:GLU:HG2	7:O:148:ARG:NH1	2.36	0.41
7:O:10:LEU:O	16:Q:292:TRP:HZ2	2.04	0.41
8:I:61:ASP:HB3	8:I:127:ALA:HB1	2.02	0.41
9:X:7:ARG:NH2	9:X:100:THR:HA	2.35	0.41
10:P:61:PHE:HE1	16:Q:302:TYR:OH	2.04	0.41
10:P:83:VAL:HG23	10:P:84:SER:H	1.85	0.41
13:T:373:LEU:HD21	13:T:416:TYR:HE1	1.86	0.41
13:T:541:LEU:C	13:T:545:PRO:HG2	2.46	0.41
13:T:553:LEU:HB2	14:U:274:VAL:HG22	2.02	0.41
14:U:5:ALA:HB1	14:U:36:ASN:HD21	1.86	0.41
14:U:86:ALA:O	14:U:96:LEU:HD11	2.21	0.41
15:V:291:ALA:O	15:V:294:LEU:HB3	2.21	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
1:1:29:LEU:O	1:1:33:LEU:HG	2.21	0.41
3:3:41:PRO:HB2	3:3:84:VAL:HG13	2.02	0.41
3:3:290:ILE:HD13	3:3:290:ILE:HA	1.84	0.41
5:5:132:LEU:HD23	5:5:132:LEU:HA	1.91	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
6:6:115:GLY:HA2	6:6:125:GLN:HA	2.03	0.41
7:9:127:SER:OG	9:W:39:ASP:OD2	2.33	0.41
8:7:9:LEU:HD11	8:7:82:ILE:HG22	2.03	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: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
1:B:336:SER:HB3	1:B:339:ASP:HB2	2.03	0.41
2:C:14:THR:HG22	2:C:17:LYS:HZ2	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
9:X:58:LEU:HD22	9:X:110:LEU:HD21	2.03	0.41
10:P:115:VAL:C	10:P:117:ARG:H	2.26	0.41
12:S:81:HIS:H	12:S:81:HIS:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:Q:243:LEU:O	16:Q:246:MET:HB3	2.21	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
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
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
3:D:20:MET:HE1	3:D:35:SER:HB2	2.02	0.40
3:D:81:ALA:HB3	3:D:84:VAL:HG22	2.03	0.40
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
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
4:E:342:VAL:HG12	4:E:357:ILE:HB	2.03	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
9:X:74:LEU:HD12	9:X:77:LEU:HD23	2.03	0.40
10:P:20:ILE:HD12	16:Q:21:VAL:HG11	2.03	0.40
14:U:62:TYR:HE2	14:U:174:THR:HG21	1.85	0.40
14:U:452:ARG:HD3	14:U:452:ARG:HA	1.78	0.40
15:V:183:LEU:HD13	15:V:226:VAL:HG21	2.03	0.40
16:Q:66:SER:O	16:Q:69:LYS:HB3	2.21	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
7:9:54:ILE:HG21	8:7:41:ILE:HG23	2.03	0.40
8:7:12:ALA:O	8:7:15:GLU:HB3	2.21	0.40
13:L:255:ARG:HD2	13:L:255:ARG:HA	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:197:LEU:HA	4:E:200:ARG:HB2	2.03	0.40
4:E:201:ILE:HG12	4:E:283:MET:HE3	2.02	0.40
5:F:178:ASP:O	5:F:185:LYS:HE2	2.21	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
14:U:398:SER:O	14:U:402:SER:N	2.43	0.40
15:V:95:MET:HE1	15:V:214:SER:HB3	2.03	0.40
1:1:331:ILE:HA	1:1:332:PRO:HD2	1.75	0.40
4:4:26:MET:HE2	10:A:57:PHE:HD1	1.86	0.40
4:4:169:HIS:NE2	6:6:45:CYS:SG	2.93	0.40
4:4:174:ARG:N	4:4:177:GLY:O	2.38	0.40
5:5:121:LEU:HA	5:5:145:PRO:HD2	2.02	0.40
5:5:123:GLY:HA2	5:5:144:HIS:CE1	2.57	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
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:109:LEU:HD21	14:M:236:VAL:HG21	2.03	0.40
14:M:186:GLN:HG2	14:M:187:GLU:N	2.34	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
1:B:16:THR:HG23	1:B:233:ARG:HH21	1.86	0.40
1:B:29:LEU:O	1:B:33:LEU:HG	2.22	0.40
1:B:97:GLU:HG3	1:B:98:PRO:HD2	2.03	0.40
1:B:214:LYS:HA	1:B:215:PRO:HD3	1.93	0.40
1:B:233:ARG:O	1:B:237:TRP:HB3	2.21	0.40
1:B:338:VAL:O	1:B:342:TRP:HB2	2.22	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
9:X:21:LEU:HD11	9:X:26:LEU:HD21	2.04	0.40
10:P:54:VAL:HG22	16:Q:146:LYS:HD2	2.02	0.40
14:U:41:LEU:HD23	14:U:449:TYR:OH	2.20	0.40
16:Q:221:LEU:N	16:Q:222:PRO:CA	2.83	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
7:9:59:CYS:HB2	7:9:104:CYS:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:13:TRP:HE3	8:7:82:ILE:HD12	1.87	0.40
9:W:122:ASP:O	9:W:125:ILE:HG12	2.21	0.40
11:J:104:LEU:HA	15:N:174:LEU:HD21	2.02	0.40
13:L:59:TRP:CH2	13:L:129:ILE:HD11	2.56	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
14:M:347:LEU:HD13	14:M:422:VAL:HG21	2.00	0.40
2:C:110:GLU:HA	8:I:121:ARG:HH12	1.86	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
6:G:35:SER:O	6:G:35:SER:OG	2.40	0.40
6:G:96:TRP:HE3	6:G:97:GLU:HG3	1.86	0.40
11:R:52:GLY:O	11:R:56:VAL:HG23	2.21	0.40
11:R:104:LEU:O	11:R:108:LEU:HD12	2.21	0.40
12:S:88:ASP:OD2	13:T:587:ARG:NH1	2.55	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
14:U:164:LEU:HD21	15:V:346:TYR:CE1	2.57	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
6:6:83:ARG:HB2	6:6:123:ILE:HD12	2.03	0.40
6:6:171:PRO:HA	6:6:172:PRO:HD3	1.97	0.40
7:9:101:CYS:HB2	7:9:103:LEU:H	1.86	0.40
8:7:88:ARG:NH2	8:7:126:LEU:HB3	2.36	0.40
10:A:45:GLU:O	10:A:45:GLU:HG3	2.21	0.40
13:L:59:TRP:O	14:M:452:ARG:NH2	2.55	0.40
14:M:452:ARG:HD3	14:M:452:ARG:HA	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ARG:NH1	1:B:249:MET:O	2.54	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
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:73:ARG:NH2	4:E:81:TYR:OH	2.55	0.40
4:E:74:THR:HG22	4:E:75:TYR:N	2.37	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
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
11:R:46:LEU:HD23	11:R:46:LEU:HA	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
16:Q:108:PHE:O	16:Q:108:PHE:CG	2.74	0.40
16:Q:153:LEU:HD23	16:Q:153:LEU:HA	1.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	435/438 (99%)	405 (93%)	28 (6%)	2 (0%)	24	55
1	B	435/438 (99%)	406 (93%)	27 (6%)	2 (0%)	24	55
2	2	176/181 (97%)	164 (93%)	11 (6%)	1 (1%)	21	52
2	C	176/181 (97%)	164 (93%)	11 (6%)	1 (1%)	21	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	750/783 (96%)	695 (93%)	54 (7%)	1 (0%)	48	75
3	D	750/783 (96%)	695 (93%)	54 (7%)	1 (0%)	48	75
4	4	382/409 (93%)	351 (92%)	29 (8%)	2 (0%)	24	55
4	E	382/409 (93%)	351 (92%)	29 (8%)	2 (0%)	24	55
5	5	194/207 (94%)	182 (94%)	12 (6%)	0	100	100
5	F	194/207 (94%)	182 (94%)	12 (6%)	0	100	100
6	6	157/181 (87%)	140 (89%)	15 (10%)	2 (1%)	9	35
6	G	157/181 (87%)	141 (90%)	14 (9%)	2 (1%)	9	35
7	9	178/182 (98%)	166 (93%)	11 (6%)	1 (1%)	21	52
7	O	178/182 (98%)	167 (94%)	10 (6%)	1 (1%)	21	52
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%)	16	45
9	X	125/131 (95%)	121 (97%)	3 (2%)	1 (1%)	16	45
10	A	115/119 (97%)	105 (91%)	7 (6%)	3 (3%)	4	23
10	P	115/119 (97%)	105 (91%)	7 (6%)	3 (3%)	4	23
11	J	158/176 (90%)	143 (90%)	14 (9%)	1 (1%)	21	52
11	R	158/176 (90%)	142 (90%)	15 (10%)	1 (1%)	21	52
12	K	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	11	39
12	S	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	11	39
13	L	603/606 (100%)	555 (92%)	43 (7%)	5 (1%)	16	45
13	T	603/606 (100%)	555 (92%)	43 (7%)	5 (1%)	16	45
14	M	465/469 (99%)	428 (92%)	33 (7%)	4 (1%)	14	43
14	U	465/469 (99%)	428 (92%)	33 (7%)	4 (1%)	14	43
15	N	425/427 (100%)	398 (94%)	25 (6%)	2 (0%)	24	55
15	V	425/427 (100%)	396 (93%)	27 (6%)	2 (0%)	24	55
16	H	351/365 (96%)	309 (88%)	33 (9%)	9 (3%)	4	23
16	Q	351/365 (96%)	309 (88%)	33 (9%)	9 (3%)	4	23
All	All	9464/9796 (97%)	8730 (92%)	664 (7%)	70 (1%)	18	49

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
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

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Mol	Chain	Res	Type
16	H	70	GLU
16	H	234	THR
4	E	33	GLN
9	X	37	TRP
14	U	57	PRO
16	Q	70	GLU
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%)	338 (95%)	17 (5%)	23	52
1	B	355/356 (100%)	337 (95%)	18 (5%)	21	50
2	2	150/152 (99%)	137 (91%)	13 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	150/152 (99%)	136 (91%)	14 (9%)	8	30
3	3	609/628 (97%)	559 (92%)	50 (8%)	10	35
3	D	609/628 (97%)	560 (92%)	49 (8%)	11	36
4	4	332/355 (94%)	313 (94%)	19 (6%)	18	47
4	E	332/355 (94%)	313 (94%)	19 (6%)	18	47
5	5	167/175 (95%)	157 (94%)	10 (6%)	17	46
5	F	167/175 (95%)	157 (94%)	10 (6%)	17	46
6	6	130/149 (87%)	108 (83%)	22 (17%)	2	10
6	G	130/149 (87%)	108 (83%)	22 (17%)	2	10
7	9	148/150 (99%)	138 (93%)	10 (7%)	14	42
7	O	148/150 (99%)	138 (93%)	10 (7%)	14	42
8	7	104/106 (98%)	98 (94%)	6 (6%)	18	47
8	I	104/106 (98%)	98 (94%)	6 (6%)	18	47
9	W	99/101 (98%)	93 (94%)	6 (6%)	17	45
9	X	99/101 (98%)	92 (93%)	7 (7%)	13	40
10	A	90/92 (98%)	83 (92%)	7 (8%)	11	36
10	P	90/92 (98%)	84 (93%)	6 (7%)	15	42
11	J	118/130 (91%)	100 (85%)	18 (15%)	3	13
11	R	118/130 (91%)	100 (85%)	18 (15%)	3	13
12	K	71/71 (100%)	63 (89%)	8 (11%)	5	21
12	S	71/71 (100%)	64 (90%)	7 (10%)	7	27
13	L	453/454 (100%)	430 (95%)	23 (5%)	21	50
13	T	453/454 (100%)	429 (95%)	24 (5%)	20	49
14	M	332/332 (100%)	305 (92%)	27 (8%)	11	36
14	U	332/332 (100%)	306 (92%)	26 (8%)	11	36
15	N	302/302 (100%)	292 (97%)	10 (3%)	33	59
15	V	302/302 (100%)	292 (97%)	10 (3%)	33	59
16	H	293/300 (98%)	268 (92%)	25 (8%)	10	33
16	Q	293/300 (98%)	268 (92%)	25 (8%)	10	33
All	All	7506/7706 (97%)	6964 (93%)	542 (7%)	13	40

All (542) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	79	MET
1	1	81	LYS
1	1	104	ARG
1	1	134	VAL
1	1	201	LEU
1	1	202	LYS
1	1	217	THR
1	1	241	MET
1	1	249	MET
1	1	314	GLU
1	1	342	TRP
1	1	357	THR
1	1	366	PHE
1	1	397	ARG
1	1	400	CYS
1	1	404	ASP
1	1	437	TRP
2	2	7	LYS
2	2	35	GLN
2	2	45	ARG
2	2	96	LEU
2	2	106	ILE
2	2	110	GLU
2	2	116	LEU
2	2	121	LYS
2	2	139	GLU
2	2	144	CYS
2	2	150	LEU
2	2	153	LEU
2	2	172	CYS
3	3	11	VAL
3	3	42	ILE
3	3	46	ARG
3	3	96	LEU
3	3	113	LEU
3	3	123	ASP
3	3	124	LYS
3	3	133	ARG
3	3	182	ILE
3	3	188	VAL
3	3	207	VAL
3	3	214	MET
3	3	249	MET

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Mol	Chain	Res	Type
3	3	259	CYS
3	3	261	VAL
3	3	269	THR
3	3	284	GLU
3	3	285	VAL
3	3	286	ASN
3	3	290	ILE
3	3	321	THR
3	3	351	LEU
3	3	356	LEU
3	3	368	HIS
3	3	374	ARG
3	3	412	ARG
3	3	417	VAL
3	3	419	ASP
3	3	425	ARG
3	3	435	LEU
3	3	466	GLU
3	3	488	GLU
3	3	501	LYS
3	3	512	LEU
3	3	515	THR
3	3	523	LEU
3	3	550	LEU
3	3	593	LEU
3	3	629	ILE
3	3	651	ARG
3	3	655	ARG
3	3	669	VAL
3	3	676	LEU
3	3	681	LYS
3	3	684	ARG
3	3	710	GLU
3	3	726	GLU
3	3	734	VAL
3	3	743	VAL
3	3	744	GLU
4	4	129	HIS
4	4	132	PHE
4	4	143	LEU
4	4	144	THR
4	4	148	TYR

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Mol	Chain	Res	Type
4	4	155	THR
4	4	163	VAL
4	4	170	HIS
4	4	187	VAL
4	4	192	LYS
4	4	194	LEU
4	4	199	HIS
4	4	200	ARG
4	4	208	PHE
4	4	211	SER
4	4	227	GLU
4	4	262	PHE
4	4	319	THR
4	4	371	ARG
5	5	31	ARG
5	5	38	MET
5	5	51	ASP
5	5	80	TRP
5	5	135	ILE
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
6	6	55	ASP
6	6	57	ARG
6	6	62	ARG
6	6	83	ARG
6	6	87	LYS
6	6	91	VAL
6	6	101	ASP
6	6	120	ASN
6	6	130	VAL
6	6	148	ILE
6	6	153	GLN
6	6	156	LYS
6	6	158	VAL

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Mol	Chain	Res	Type
6	6	176	TRP
6	6	177	LYS
6	6	178	ARG
6	6	179	THR
7	9	4	LYS
7	9	12	ILE
7	9	31	VAL
7	9	42	VAL
7	9	85	GLU
7	9	97	ARG
7	9	99	ILE
7	9	101	CYS
7	9	137	LEU
7	9	139	ASP
8	7	43	ARG
8	7	52	THR
8	7	63	LEU
8	7	68	LEU
8	7	79	LEU
8	7	82	ILE
9	W	37	TRP
9	W	43	GLN
9	W	55	LYS
9	W	99	MET
9	W	100	THR
9	W	103	LEU
10	A	6	GLU
10	A	40	LYS
10	A	46	SER
10	A	48	ASN
10	A	55	LYS
10	A	83	VAL
10	A	102	LEU
11	J	11	LEU
11	J	56	VAL
11	J	59	TYR
11	J	64	VAL
11	J	74	LEU
11	J	80	GLU
11	J	84	ASP
11	J	86	LEU
11	J	103	ILE

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Mol	Chain	Res	Type
11	J	111	LEU
11	J	113	LEU
11	J	118	ASP
11	J	119	LEU
11	J	127	LEU
11	J	130	LEU
11	J	131	LEU
11	J	156	LEU
11	J	158	GLU
12	K	2	SER
12	K	4	LEU
12	K	25	ILE
12	K	29	LEU
12	K	33	LEU
12	K	54	GLN
12	K	58	LEU
12	K	81	HIS
13	L	32	LEU
13	L	59	TRP
13	L	108	PHE
13	L	151	TYR
13	L	167	LEU
13	L	176	LEU
13	L	185	ILE
13	L	207	LEU
13	L	245	MET
13	L	322	VAL
13	L	329	LYS
13	L	339	VAL
13	L	404	VAL
13	L	468	VAL
13	L	469	LEU
13	L	479	GLU
13	L	483	HIS
13	L	484	HIS
13	L	490	GLU
13	L	516	VAL
13	L	557	ASP
13	L	567	LEU
13	L	601	LEU
14	M	2	VAL
14	M	11	VAL

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Mol	Chain	Res	Type
14	M	16	LEU
14	M	18	LEU
14	M	20	LEU
14	M	22	ARG
14	M	24	LEU
14	M	41	LEU
14	M	42	THR
14	M	61	VAL
14	M	73	LEU
14	M	77	THR
14	M	92	GLU
14	M	126	LEU
14	M	135	LEU
14	M	151	PHE
14	M	153	LEU
14	M	248	LEU
14	M	255	GLN
14	M	269	LEU
14	M	300	VAL
14	M	340	GLU
14	M	347	LEU
14	M	349	GLN
14	M	354	LEU
14	M	382	LEU
14	M	415	TRP
15	N	46	LYS
15	N	50	PHE
15	N	68	LEU
15	N	86	LEU
15	N	88	VAL
15	N	114	LEU
15	N	125	ARG
15	N	233	LEU
15	N	241	VAL
15	N	382	VAL
16	H	2	THR
16	H	13	VAL
16	H	22	VAL
16	H	50	ARG
16	H	70	GLU
16	H	100	ILE
16	H	128	VAL

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Mol	Chain	Res	Type
16	H	146	LYS
16	H	149	LEU
16	H	180	LEU
16	H	185	ILE
16	H	189	GLN
16	H	205	VAL
16	H	211	MET
16	H	216	ARG
16	H	221	LEU
16	H	228	LEU
16	H	233	HIS
16	H	234	THR
16	H	240	LYS
16	H	267	TRP
16	H	269	MET
16	H	302	TYR
16	H	304	GLN
16	H	332	LEU
1	B	79	MET
1	B	81	LYS
1	B	104	ARG
1	B	134	VAL
1	B	201	LEU
1	B	202	LYS
1	B	217	THR
1	B	241	MET
1	B	249	MET
1	B	314	GLU
1	B	342	TRP
1	B	357	THR
1	B	366	PHE
1	B	376	THR
1	B	397	ARG
1	B	400	CYS
1	B	404	ASP
1	B	437	TRP
2	C	7	LYS
2	C	35	GLN
2	C	45	ARG
2	C	96	LEU
2	C	106	ILE
2	C	110	GLU

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Mol	Chain	Res	Type
2	C	116	LEU
2	C	119	VAL
2	C	121	LYS
2	C	139	GLU
2	C	144	CYS
2	C	150	LEU
2	C	153	LEU
2	C	172	CYS
3	D	11	VAL
3	D	42	ILE
3	D	46	ARG
3	D	96	LEU
3	D	113	LEU
3	D	123	ASP
3	D	124	LYS
3	D	133	ARG
3	D	182	ILE
3	D	188	VAL
3	D	207	VAL
3	D	214	MET
3	D	249	MET
3	D	259	CYS
3	D	269	THR
3	D	284	GLU
3	D	285	VAL
3	D	286	ASN
3	D	290	ILE
3	D	321	THR
3	D	351	LEU
3	D	356	LEU
3	D	368	HIS
3	D	374	ARG
3	D	412	ARG
3	D	417	VAL
3	D	419	ASP
3	D	425	ARG
3	D	435	LEU
3	D	466	GLU
3	D	488	GLU
3	D	501	LYS
3	D	512	LEU
3	D	515	THR

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Mol	Chain	Res	Type
3	D	523	LEU
3	D	550	LEU
3	D	593	LEU
3	D	629	ILE
3	D	651	ARG
3	D	655	ARG
3	D	669	VAL
3	D	676	LEU
3	D	681	LYS
3	D	684	ARG
3	D	710	GLU
3	D	726	GLU
3	D	734	VAL
3	D	743	VAL
3	D	744	GLU
4	E	129	HIS
4	E	132	PHE
4	E	143	LEU
4	E	144	THR
4	E	148	TYR
4	E	155	THR
4	E	163	VAL
4	E	170	HIS
4	E	187	VAL
4	E	192	LYS
4	E	194	LEU
4	E	199	HIS
4	E	200	ARG
4	E	208	PHE
4	E	211	SER
4	E	227	GLU
4	E	262	PHE
4	E	319	THR
4	E	371	ARG
5	F	31	ARG
5	F	38	MET
5	F	51	ASP
5	F	80	TRP
5	F	135	ILE
5	F	141	LEU
5	F	171	ARG
5	F	174	LEU

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Mol	Chain	Res	Type
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
6	G	55	ASP
6	G	57	ARG
6	G	62	ARG
6	G	83	ARG
6	G	87	LYS
6	G	91	VAL
6	G	101	ASP
6	G	120	ASN
6	G	130	VAL
6	G	148	ILE
6	G	153	GLN
6	G	156	LYS
6	G	158	VAL
6	G	176	TRP
6	G	177	LYS
6	G	178	ARG
6	G	179	THR
7	O	4	LYS
7	O	12	ILE
7	O	31	VAL
7	O	42	VAL
7	O	85	GLU
7	O	97	ARG
7	O	99	ILE
7	O	101	CYS
7	O	137	LEU
7	O	139	ASP
8	I	43	ARG
8	I	52	THR
8	I	63	LEU
8	I	68	LEU
8	I	79	LEU
8	I	82	ILE
9	X	34	ILE
9	X	37	TRP

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Mol	Chain	Res	Type
9	X	43	GLN
9	X	55	LYS
9	X	99	MET
9	X	100	THR
9	X	103	LEU
10	P	6	GLU
10	P	40	LYS
10	P	46	SER
10	P	48	ASN
10	P	55	LYS
10	P	102	LEU
11	R	11	LEU
11	R	56	VAL
11	R	59	TYR
11	R	64	VAL
11	R	74	LEU
11	R	80	GLU
11	R	84	ASP
11	R	86	LEU
11	R	103	ILE
11	R	111	LEU
11	R	113	LEU
11	R	118	ASP
11	R	119	LEU
11	R	127	LEU
11	R	130	LEU
11	R	131	LEU
11	R	156	LEU
11	R	158	GLU
12	S	2	SER
12	S	4	LEU
12	S	29	LEU
12	S	33	LEU
12	S	54	GLN
12	S	58	LEU
12	S	81	HIS
13	T	32	LEU
13	T	59	TRP
13	T	108	PHE
13	T	151	TYR
13	T	167	LEU
13	T	176	LEU

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Mol	Chain	Res	Type
13	T	185	ILE
13	T	207	LEU
13	T	245	MET
13	T	322	VAL
13	T	329	LYS
13	T	339	VAL
13	T	404	VAL
13	T	468	VAL
13	T	469	LEU
13	T	479	GLU
13	T	483	HIS
13	T	484	HIS
13	T	490	GLU
13	T	516	VAL
13	T	557	ASP
13	T	567	LEU
13	T	600	LEU
13	T	601	LEU
14	U	2	VAL
14	U	11	VAL
14	U	16	LEU
14	U	18	LEU
14	U	20	LEU
14	U	24	LEU
14	U	41	LEU
14	U	42	THR
14	U	61	VAL
14	U	73	LEU
14	U	77	THR
14	U	92	GLU
14	U	126	LEU
14	U	135	LEU
14	U	151	PHE
14	U	153	LEU
14	U	248	LEU
14	U	255	GLN
14	U	269	LEU
14	U	300	VAL
14	U	340	GLU
14	U	347	LEU
14	U	349	GLN
14	U	354	LEU

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Mol	Chain	Res	Type
14	U	382	LEU
14	U	415	TRP
15	V	46	LYS
15	V	50	PHE
15	V	68	LEU
15	V	86	LEU
15	V	88	VAL
15	V	114	LEU
15	V	125	ARG
15	V	233	LEU
15	V	241	VAL
15	V	382	VAL
16	Q	2	THR
16	Q	13	VAL
16	Q	22	VAL
16	Q	50	ARG
16	Q	70	GLU
16	Q	100	ILE
16	Q	128	VAL
16	Q	146	LYS
16	Q	149	LEU
16	Q	180	LEU
16	Q	185	ILE
16	Q	189	GLN
16	Q	205	VAL
16	Q	211	MET
16	Q	216	ARG
16	Q	221	LEU
16	Q	228	LEU
16	Q	233	HIS
16	Q	234	THR
16	Q	240	LYS
16	Q	267	TRP
16	Q	269	MET
16	Q	302	TYR
16	Q	304	GLN
16	Q	332	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	86	GLN

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Mol	Chain	Res	Type
1	1	92	ASN
1	1	112	HIS
1	1	172	HIS
1	1	198	ASN
1	1	386	ASN
1	1	416	HIS
2	2	135	GLN
3	3	38	HIS
3	3	167	HIS
3	3	657	HIS
3	3	709	GLN
4	4	292	GLN
5	5	112	ASN
5	5	129	HIS
6	6	155	GLN
9	W	43	GLN
12	K	81	HIS
13	L	432	HIS
15	N	245	ASN
1	B	86	GLN
1	B	112	HIS
1	B	172	HIS
1	B	198	ASN
1	B	386	ASN
1	B	416	HIS
2	C	71	GLN
3	D	410	HIS
3	D	616	ASN
3	D	709	GLN
4	E	292	GLN
5	F	47	ASN
6	G	153	GLN
9	X	38	GLN
9	X	43	GLN
12	S	81	HIS
13	T	432	HIS
16	Q	183	ASN
16	Q	251	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	6	201	6	0,12,12	-	-	-		
17	SF4	9	202	7	0,12,12	-	-	-		
18	FMN	1	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.45	11 (22%)
17	SF4	3	801	3	0,12,12	-	-	-		
17	SF4	D	801	3	0,12,12	-	-	-		
17	SF4	B	501	1	0,12,12	-	-	-		
17	SF4	O	201	7	0,12,12	-	-	-		
19	FES	2	201	2	0,4,4	-	-	-		
17	SF4	G	201	6	0,12,12	-	-	-		
19	FES	D	804	3	0,4,4	-	-	-		
19	FES	3	804	3	0,4,4	-	-	-		
18	FMN	B	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.37	9 (18%)
17	SF4	1	501	1	0,12,12	-	-	-		
17	SF4	3	802	3	0,12,12	-	-	-		
17	SF4	9	201	7	0,12,12	-	-	-		
19	FES	C	201	2	0,4,4	-	-	-		
17	SF4	D	803	3	0,12,12	-	-	-		
17	SF4	O	202	7	0,12,12	-	-	-		
17	SF4	3	803	3	0,12,12	-	-	-		
17	SF4	D	802	3	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	FMN	1	502	-	-	8/18/18/18	0/3/3/3
17	SF4	6	201	6	-	-	0/6/5/5
17	SF4	9	202	7	-	-	0/6/5/5
17	SF4	3	801	3	-	-	0/6/5/5
17	SF4	D	801	3	-	-	0/6/5/5
17	SF4	B	501	1	-	-	0/6/5/5
17	SF4	O	201	7	-	-	0/6/5/5
19	FES	2	201	2	-	-	0/1/1/1
17	SF4	G	201	6	-	-	0/6/5/5
19	FES	D	804	3	-	-	0/1/1/1
19	FES	3	804	3	-	-	0/1/1/1
18	FMN	B	502	-	-	9/18/18/18	0/3/3/3
17	SF4	1	501	1	-	-	0/6/5/5
17	SF4	3	802	3	-	-	0/6/5/5
17	SF4	9	201	7	-	-	0/6/5/5
19	FES	C	201	2	-	-	0/1/1/1
17	SF4	D	803	3	-	-	0/6/5/5
17	SF4	O	202	7	-	-	0/6/5/5
17	SF4	3	803	3	-	-	0/6/5/5
17	SF4	D	802	3	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	502	FMN	C4A-N5	3.36	1.38	1.30
18	1	502	FMN	C4A-N5	3.31	1.37	1.30
18	B	502	FMN	C10-N1	2.74	1.38	1.33
18	1	502	FMN	C10-N1	2.65	1.38	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	502	FMN	C4-N3-C2	-3.56	119.32	125.64
18	B	502	FMN	C4-N3-C2	-3.53	119.37	125.64
18	1	502	FMN	C5A-C9A-N10	3.08	120.75	117.97
18	1	502	FMN	C4A-C10-N1	-2.77	117.80	124.59
18	B	502	FMN	C5A-C9A-N10	2.74	120.44	117.97
18	B	502	FMN	C4A-C10-N1	-2.71	117.95	124.59
18	B	502	FMN	C4A-C4-N3	2.69	120.10	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	502	FMN	C1'-N10-C9A	-2.67	115.44	120.63
18	1	502	FMN	C4A-C4-N3	2.64	119.98	113.25
18	B	502	FMN	C1'-N10-C9A	-2.51	115.76	120.63
18	1	502	FMN	C4A-C10-N10	2.42	119.95	116.48
18	1	502	FMN	C4-C4A-C10	2.41	121.06	116.93
18	B	502	FMN	O4-C4-C4A	-2.40	120.19	126.53
18	1	502	FMN	O4-C4-C4A	-2.36	120.29	126.53
18	B	502	FMN	C4-C4A-C10	2.36	120.98	116.93
18	B	502	FMN	C4A-C10-N10	2.20	119.63	116.48
18	1	502	FMN	C10-C4A-N5	-2.18	120.35	124.81
18	B	502	FMN	C10-C4A-N5	-2.14	120.43	124.81
18	1	502	FMN	C9A-C5A-N5	-2.03	120.30	122.45
18	1	502	FMN	C10-N1-C2	2.02	121.23	116.85

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	1	502	FMN	C2'-C1'-N10-C10
18	1	502	FMN	N10-C1'-C2'-O2'
18	1	502	FMN	N10-C1'-C2'-C3'
18	1	502	FMN	C1'-C2'-C3'-O3'
18	1	502	FMN	C1'-C2'-C3'-C4'
18	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	B	502	FMN	C2'-C1'-N10-C10

There are no ring outliers.

14 monomers are involved in 32 short contacts:

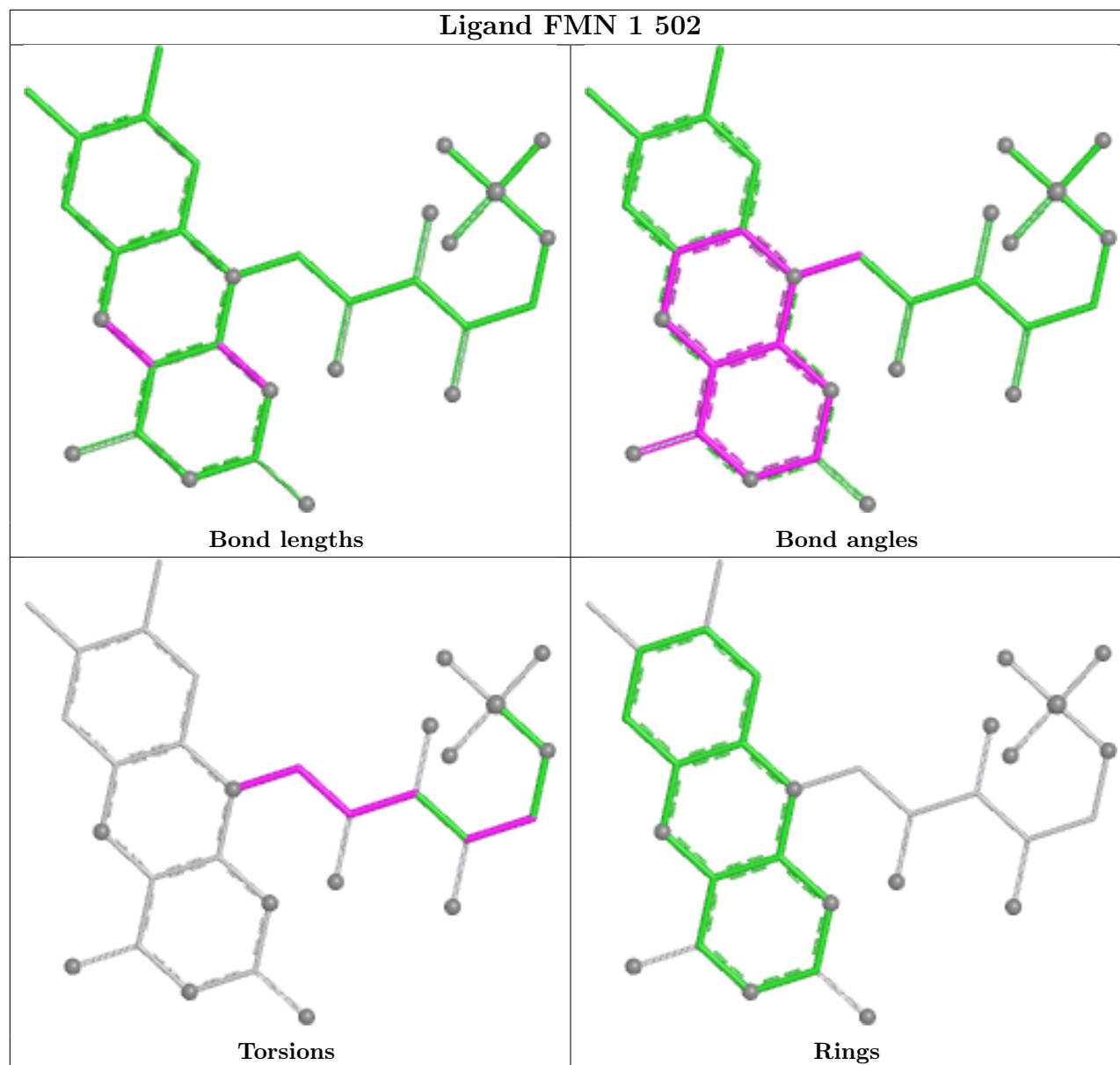
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	6	201	SF4	2	0

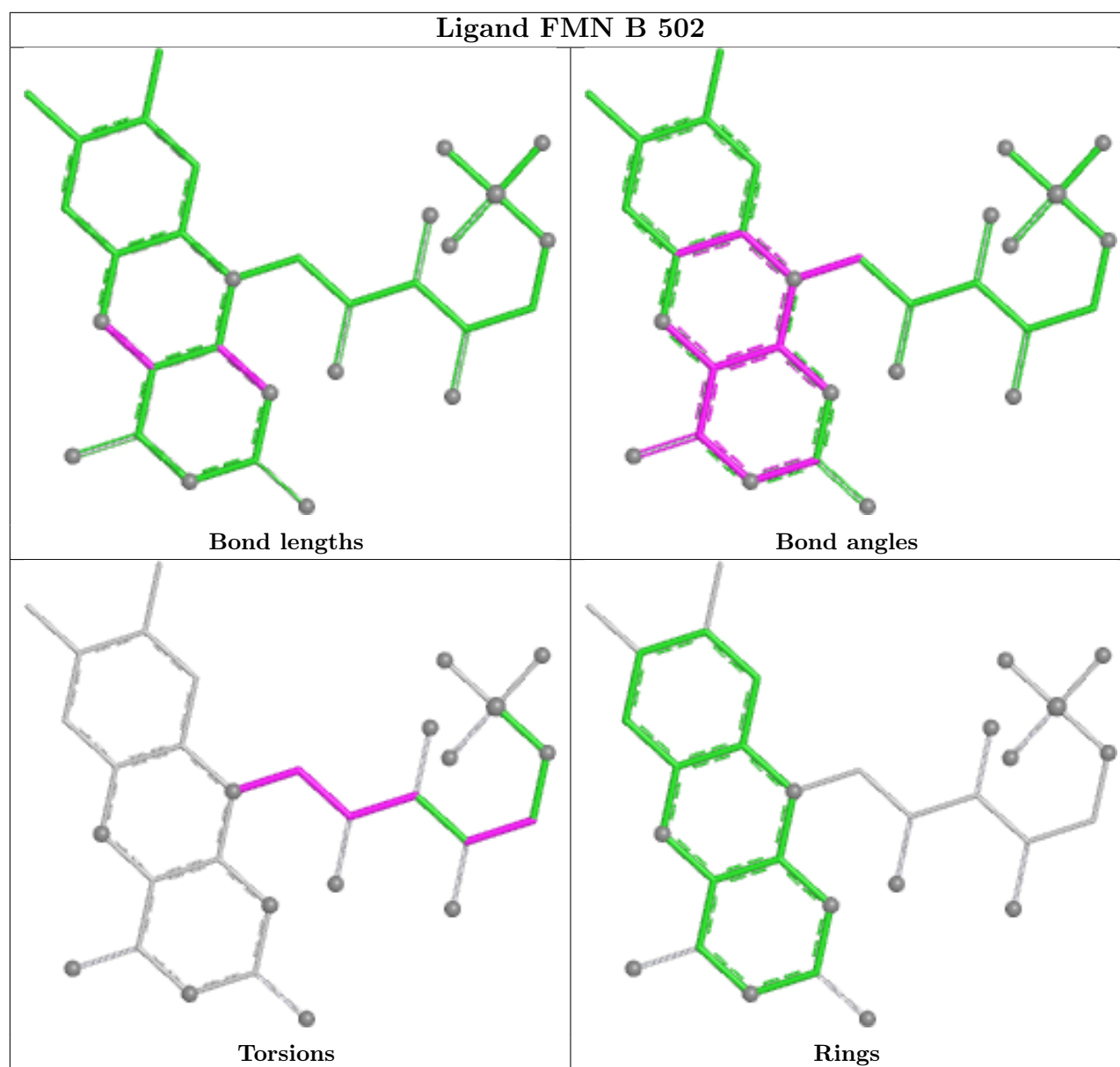
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	9	202	SF4	4	0
18	1	502	FMN	4	0
17	B	501	SF4	2	0
17	O	201	SF4	2	0
19	2	201	FES	1	0
17	G	201	SF4	2	0
19	D	804	FES	2	0
19	3	804	FES	1	0
18	B	502	FMN	3	0
17	1	501	SF4	1	0
17	9	201	SF4	2	0
19	C	201	FES	1	0
17	O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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	437/438 (99%)	-1.50	0 100 100	22, 85, 158, 280	0
1	B	437/438 (99%)	-1.46	0 100 100	20, 89, 156, 270	0
2	2	178/181 (98%)	-1.48	0 100 100	17, 73, 132, 165	0
2	C	178/181 (98%)	-1.49	0 100 100	18, 76, 134, 188	0
3	3	756/783 (96%)	-1.62	0 100 100	4, 39, 102, 257	0
3	D	756/783 (96%)	-1.57	1 (0%) 92 90	5, 41, 105, 245	0
4	4	384/409 (93%)	-1.50	0 100 100	6, 63, 135, 222	0
4	E	384/409 (93%)	-1.48	1 (0%) 90 82	15, 64, 140, 218	0
5	5	196/207 (94%)	-1.54	0 100 100	9, 62, 134, 204	0
5	F	196/207 (94%)	-1.59	0 100 100	7, 67, 138, 180	0
6	6	161/181 (88%)	-1.60	0 100 100	11, 38, 131, 255	0
6	G	161/181 (88%)	-1.49	1 (0%) 85 73	11, 44, 133, 256	0
7	9	180/182 (98%)	-1.59	0 100 100	9, 41, 105, 178	0
7	O	180/182 (98%)	-1.50	0 100 100	9, 47, 120, 191	0
8	7	127/129 (98%)	-1.61	0 100 100	14, 61, 121, 150	0
8	I	127/129 (98%)	-1.48	0 100 100	16, 70, 123, 150	0
9	W	127/131 (96%)	-1.51	0 100 100	15, 84, 155, 290	0
9	X	127/131 (96%)	-1.31	0 100 100	10, 82, 164, 294	0
10	A	117/119 (98%)	-1.44	0 100 100	12, 70, 190, 274	0
10	P	117/119 (98%)	-1.38	0 100 100	21, 74, 190, 299	0
11	J	160/176 (90%)	-1.48	0 100 100	17, 61, 131, 173	0
11	R	160/176 (90%)	-1.54	0 100 100	17, 61, 125, 170	0
12	K	95/95 (100%)	-1.41	0 100 100	15, 60, 129, 170	0
12	S	95/95 (100%)	-1.57	0 100 100	15, 54, 121, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	L	605/606 (99%)	-1.35	0 100 100	24, 90, 181, 382	0
13	T	605/606 (99%)	-1.41	2 (0%) 90 82	23, 92, 181, 381	0
14	M	467/469 (99%)	-1.34	1 (0%) 91 86	21, 74, 142, 186	0
14	U	467/469 (99%)	-1.43	0 100 100	23, 75, 145, 195	0
15	N	427/427 (100%)	-1.45	0 100 100	23, 68, 122, 203	0
15	V	427/427 (100%)	-1.44	0 100 100	21, 61, 128, 211	0
16	H	353/365 (96%)	-1.43	0 100 100	17, 76, 138, 220	0
16	Q	353/365 (96%)	-1.44	0 100 100	21, 76, 144, 222	0
All	All	9540/9796 (97%)	-1.48	6 (0%) 92 90	4, 68, 145, 382	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	T	435	PRO	4.0
3	D	150	GLU	3.3
6	G	70	ALA	2.8
14	M	467	GLY	2.6
4	E	210	GLU	2.1
13	T	436	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
18	FMN	B	502	31/31	0.99	0.05	176,200,223,231	0

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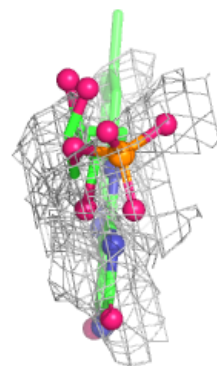
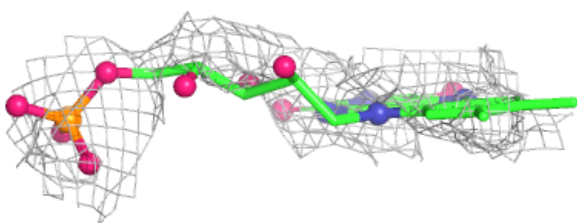
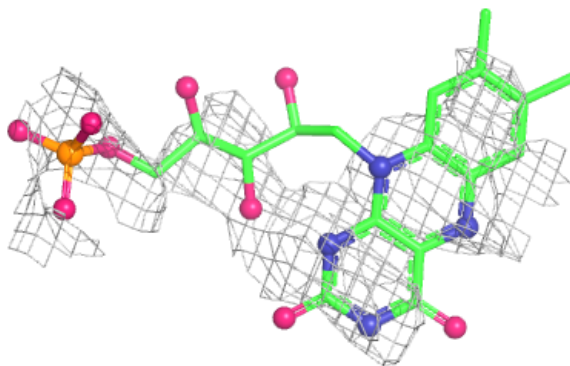
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	SF4	3	801	8/8	1.00	0.01	14,14,14,14	0
17	SF4	3	802	8/8	1.00	0.01	21,21,21,21	0
17	SF4	3	803	8/8	1.00	0.01	5,5,5,5	0
17	SF4	6	201	8/8	1.00	0.01	22,22,22,22	0
17	SF4	9	201	8/8	1.00	0.01	8,8,8,8	0
17	SF4	9	202	8/8	1.00	0.01	10,10,10,10	0
17	SF4	B	501	8/8	1.00	0.02	46,46,46,46	0
17	SF4	D	801	8/8	1.00	0.01	8,8,8,8	0
17	SF4	D	802	8/8	1.00	0.01	7,7,7,7	0
17	SF4	D	803	8/8	1.00	0.01	27,27,27,27	0
17	SF4	G	201	8/8	1.00	0.02	32,32,32,32	0
17	SF4	O	201	8/8	1.00	0.01	8,8,8,8	0
17	SF4	O	202	8/8	1.00	0.01	16,16,16,16	0
18	FMN	1	502	31/31	1.00	0.03	0,37,61,71	0
17	SF4	1	501	8/8	1.00	0.02	36,36,36,36	0
19	FES	2	201	4/4	1.00	0.01	37,37,37,37	0
19	FES	3	804	4/4	1.00	0.01	21,21,21,21	0
19	FES	C	201	4/4	1.00	0.02	74,74,74,74	0
19	FES	D	804	4/4	1.00	0.01	20,20,20,20	0

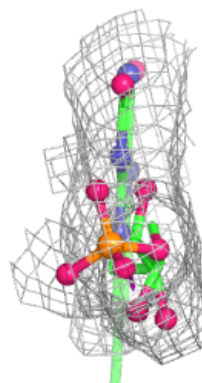
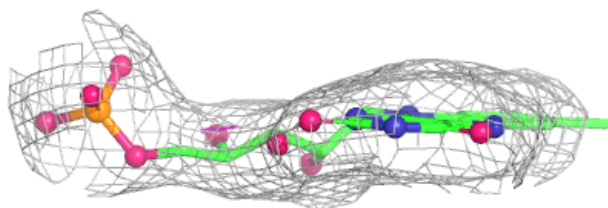
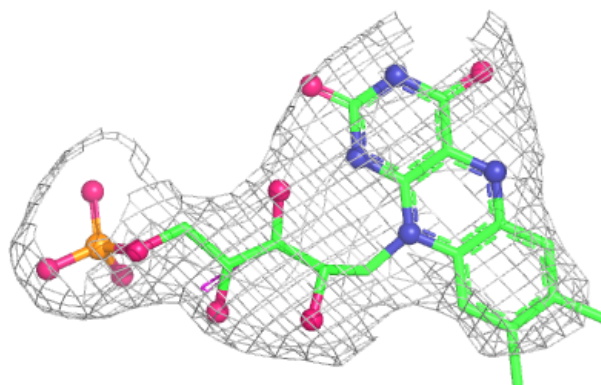
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN B 502:

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

**Electron density around FMN 1 502:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.