



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 07:50 am BST

PDB ID : 1BGY
Title : CYTOCHROME BC1 COMPLEX FROM BOVINE
Authors : Iwata, S.; Lee, J.W.; Okada, K.; Lee, J.K.; Iwata, M.; Ramaswamy, S.; Jap, B.K.
Deposited on : 1998-06-02
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

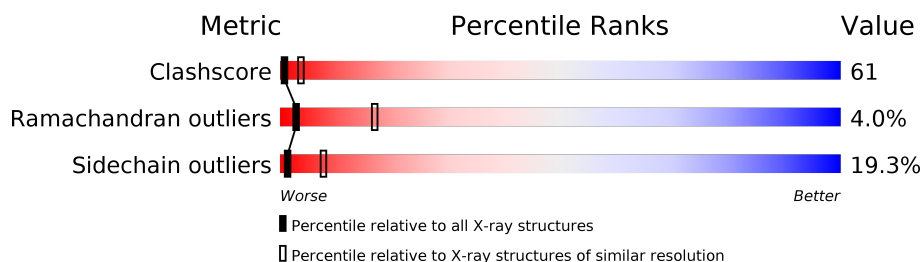
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	446	
1	M	446	
2	B	439	
2	N	439	
3	C	379	
3	O	379	
4	D	241	
4	P	241	

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Mol	Chain	Length	Quality of chain
5	E	196	
5	Q	196	
6	F	110	
6	R	110	
7	G	81	
7	S	81	
8	H	78	
8	T	78	
9	I	78	
9	U	78	
10	J	62	
10	V	62	
11	K	56	
11	W	56	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 31486 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 CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3458	2161	609	668	20			
1	M	446	Total	C	N	O	S	0	0	0
			3458	2161	609	668	20			

- Molecule 2 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3141	1972	556	606	7			
2	N	419	Total	C	N	O	S	0	0	0
			3141	1972	556	606	7			

- Molecule 3 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	379	Total	C	N	O	S	0	0	0
			3011	2018	472	502	19			
3	O	379	Total	C	N	O	S	0	0	0
			3011	2018	472	502	19			

- Molecule 4 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			
4	P	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

- Molecule 5 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	75	Total	C	N	O	S	0	0	0
			566	352	94	118	2			
5	Q	196	Total	C	N	O	S	0	0	0
			1518	956	263	291	8			

- Molecule 6 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	106	Total	C	N	O	S	0	0	0
			916	579	166	169	2			
6	R	106	Total	C	N	O	S	0	0	0
			916	579	166	169	2			

- Molecule 7 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	81	Total	C	N	O	S	0	0	0
			682	441	128	112	1			
7	S	81	Total	C	N	O	S	0	0	0
			682	441	128	112	1			

- Molecule 8 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	64	Total	C	N	O	S	0	0	0
			524	316	96	107	5			
8	T	64	Total	C	N	O	S	0	0	0
			524	316	96	107	5			

- Molecule 9 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	33	Total	C	N	O	S	0	0	0
			248	152	51	44	1			
9	U	33	Total	C	N	O	S	0	0	0
			248	152	51	44	1			

- Molecule 10 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	62	Total	C	N	O	0	0	0
			512	335	89	88			

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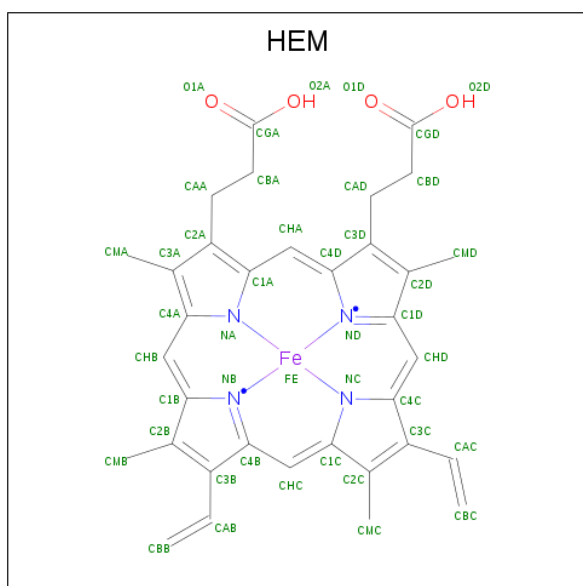
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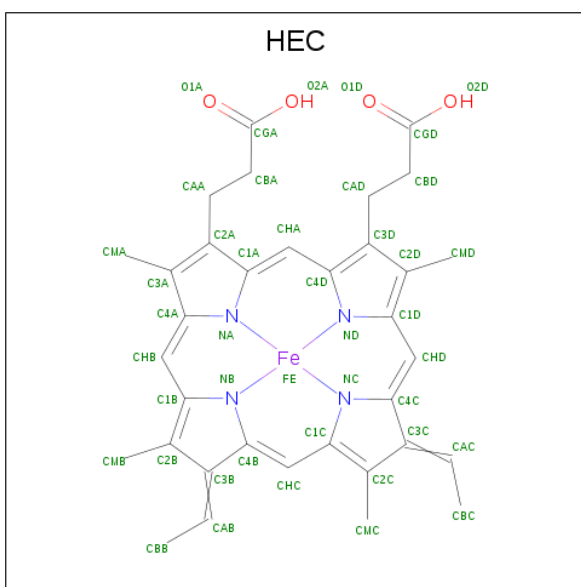
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	V	62	Total	C	N	O	0	0	0
			512	335	89	88			

- Molecule 11 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	22	Total	C	N	O	0	0	0
			159	103	29	27			
11	W	22	Total	C	N	O	0	0	0
			159	103	29	27			

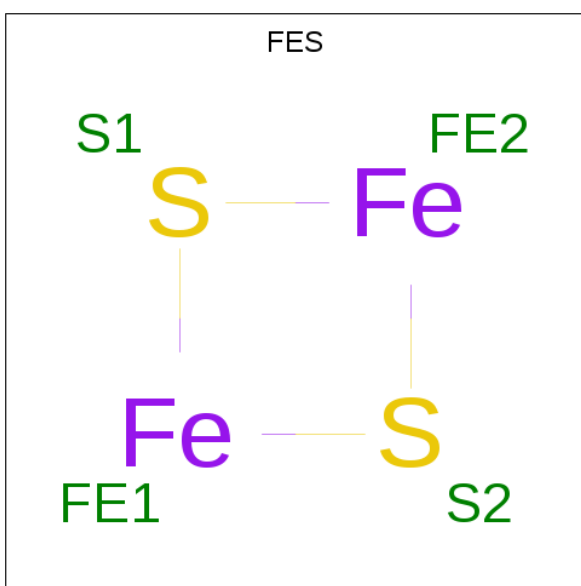
- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



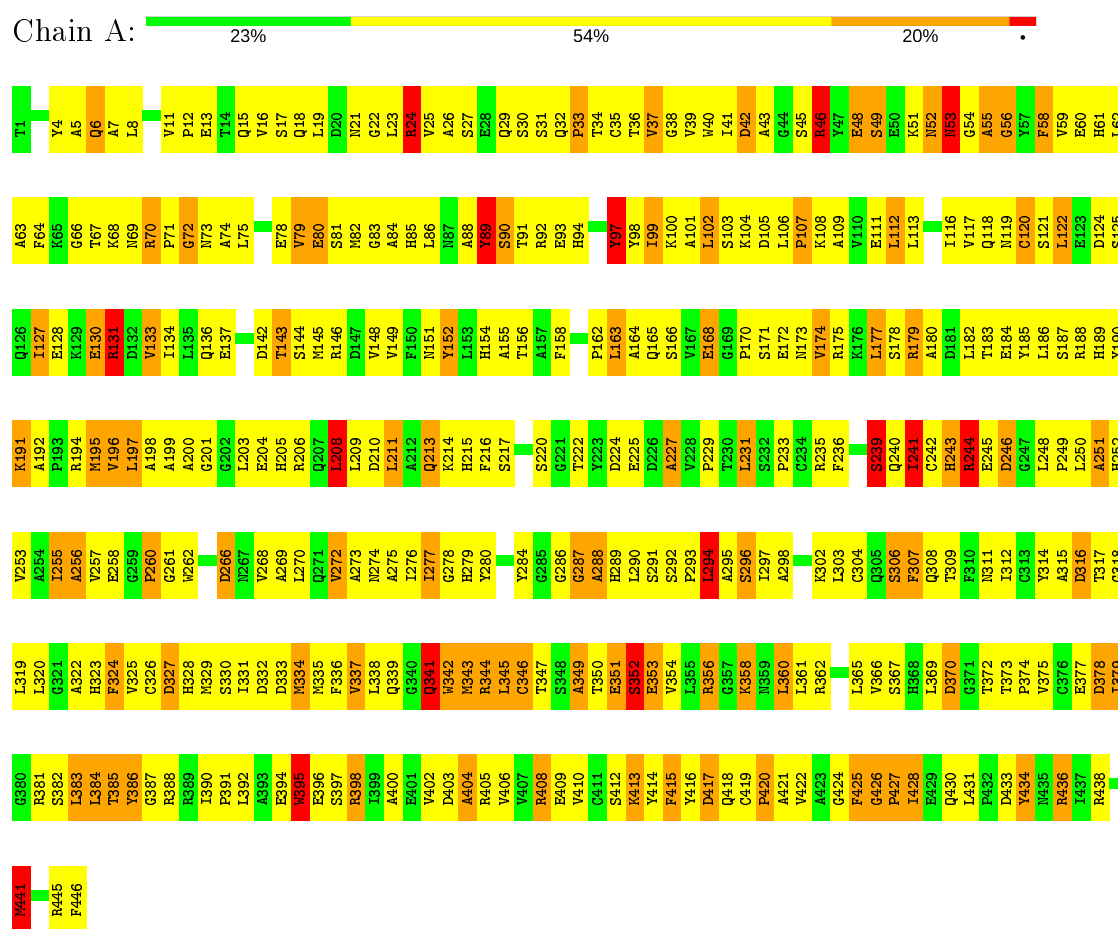
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	Q	1	Total	Fe	S	0	0
			4	2	2		

3 Residue-property plots

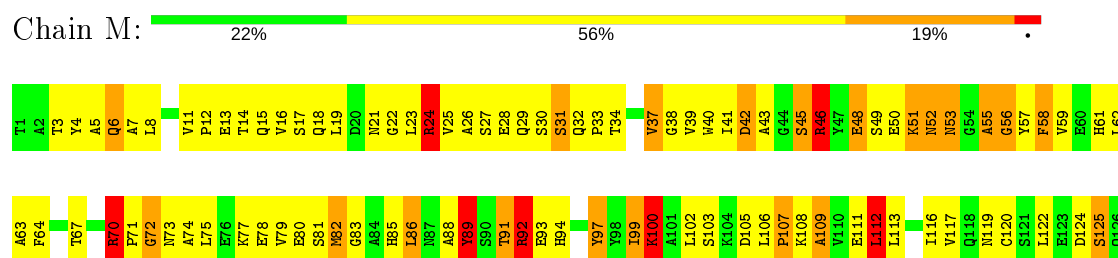
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

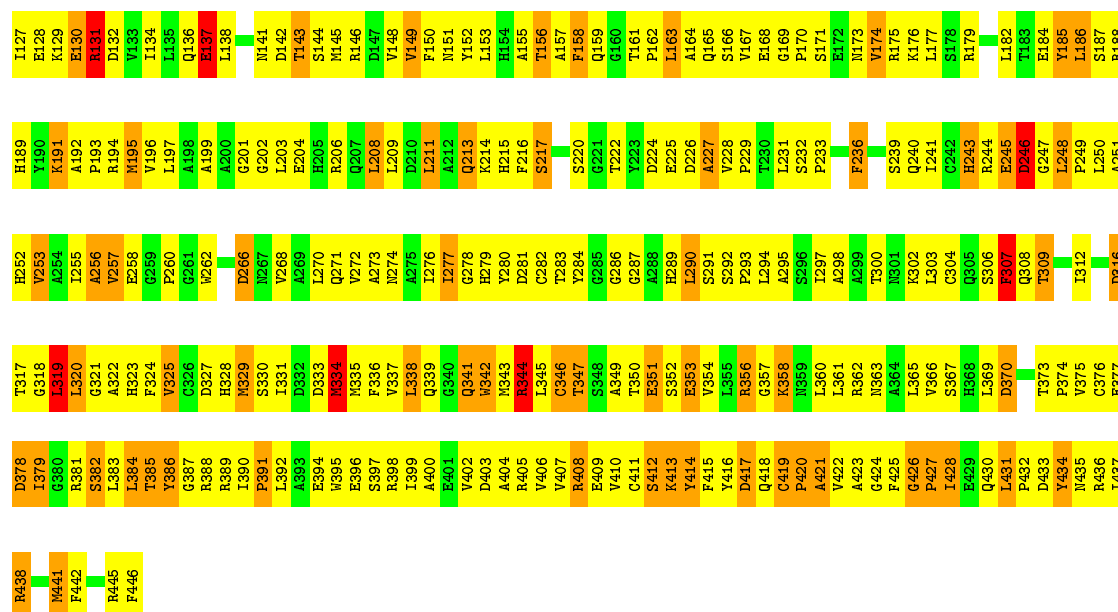
Note EDS was not executed.

- Molecule 1: CYTOCHROME BC1 COMPLEX



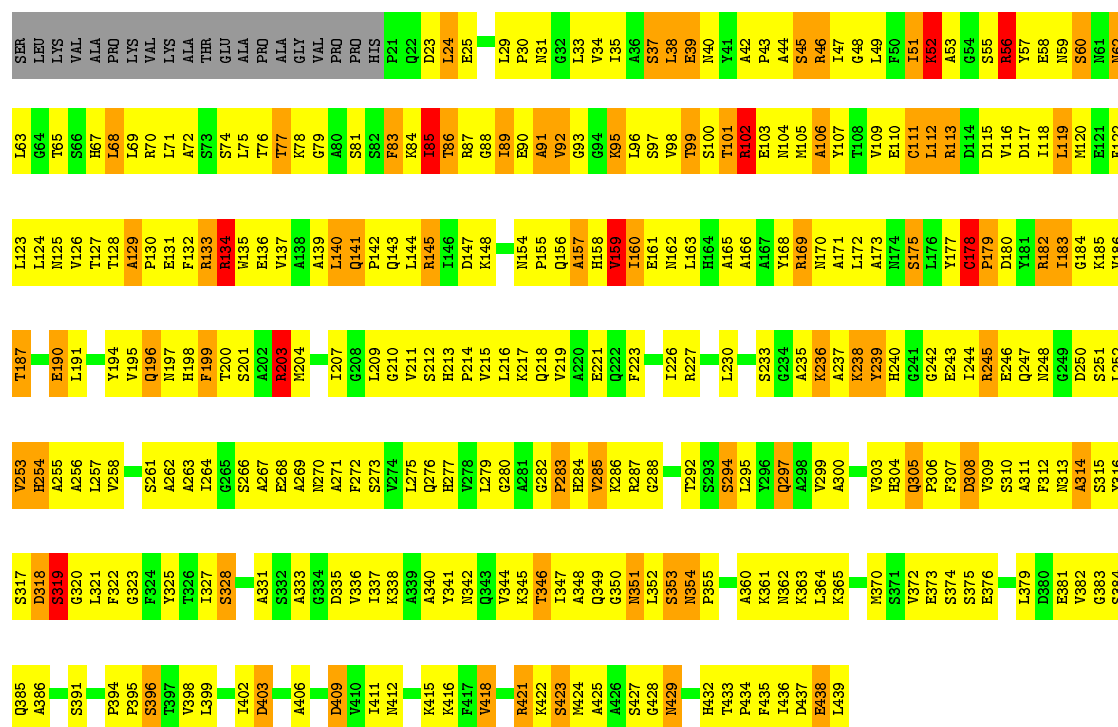
- Molecule 1: CYTOCHROME BC1 COMPLEX





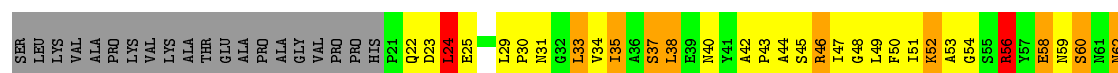
- Molecule 2: CYTOCHROME BC1 COMPLEX

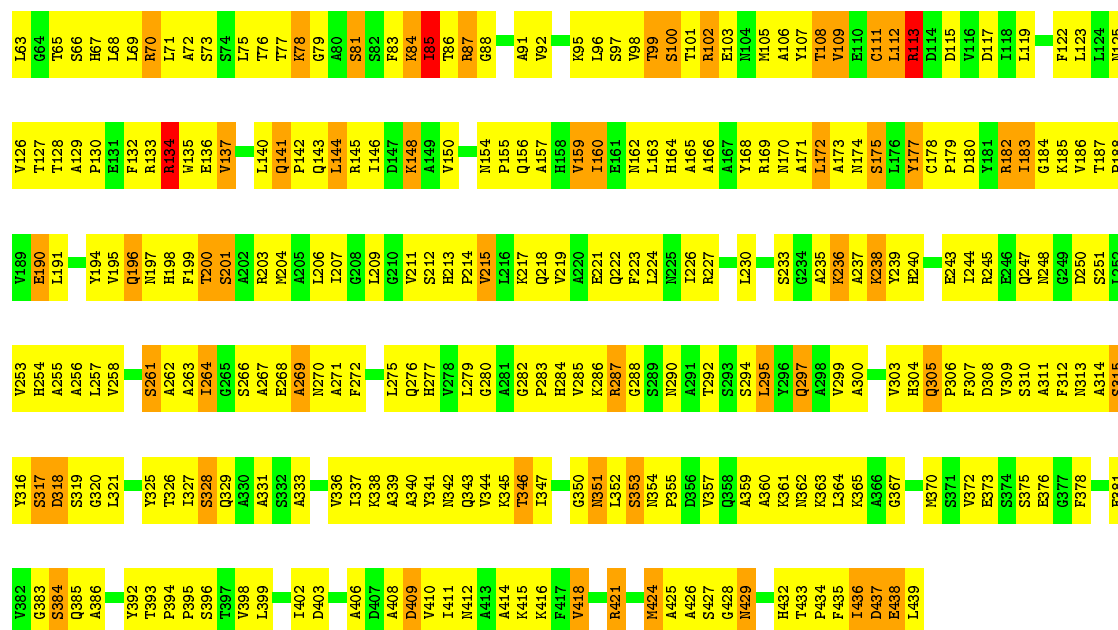
Chain B: 24% 54% 15% 5%



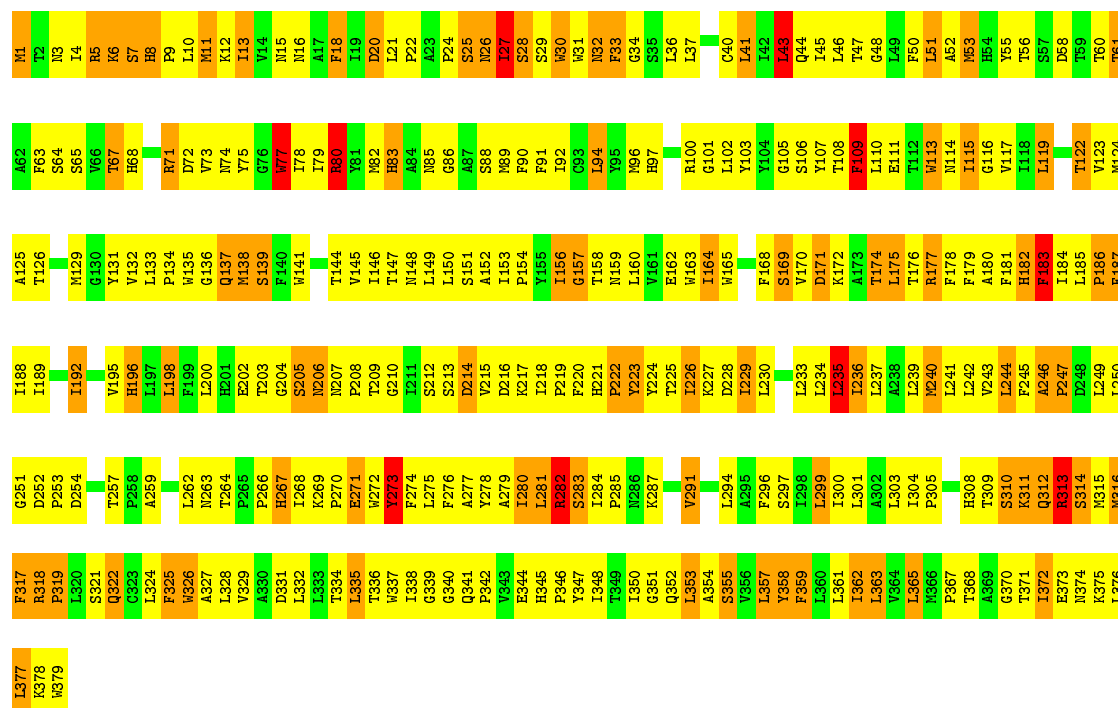
- Molecule 2: CYTOCHROME BC1 COMPLEX

Chain N: 26% 54% 14% • 5%

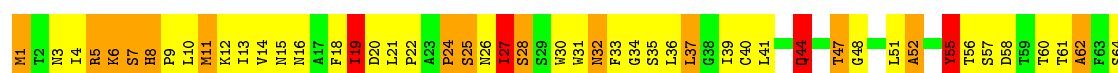


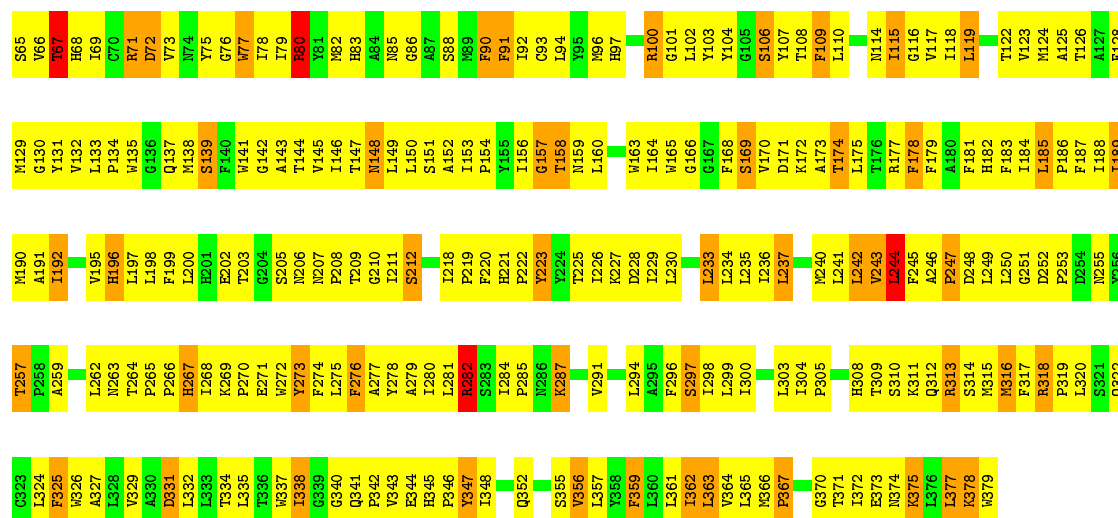


• Molecule 3: CYTOCHROME BC1 COMPLEX

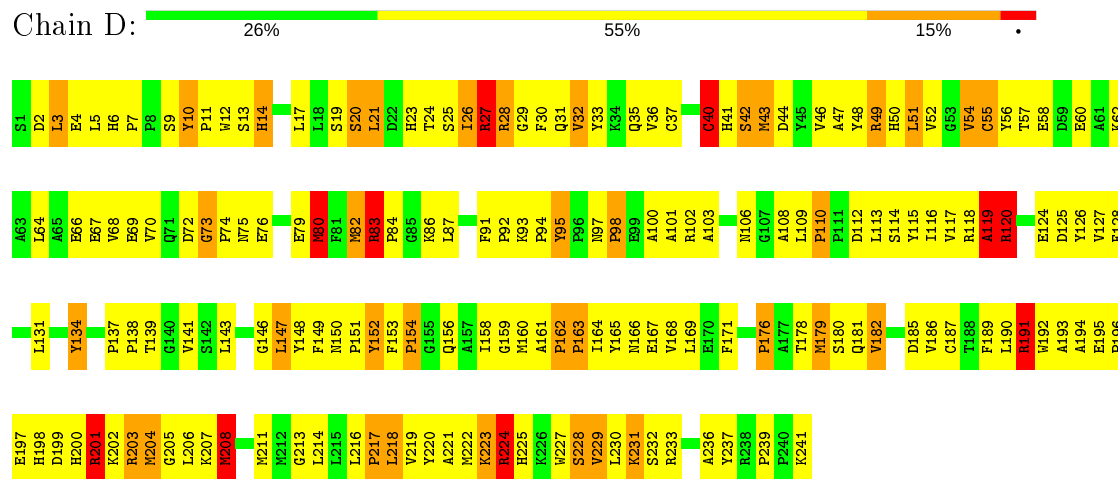


• Molecule 3: CYTOCHROME BC1 COMPLEX

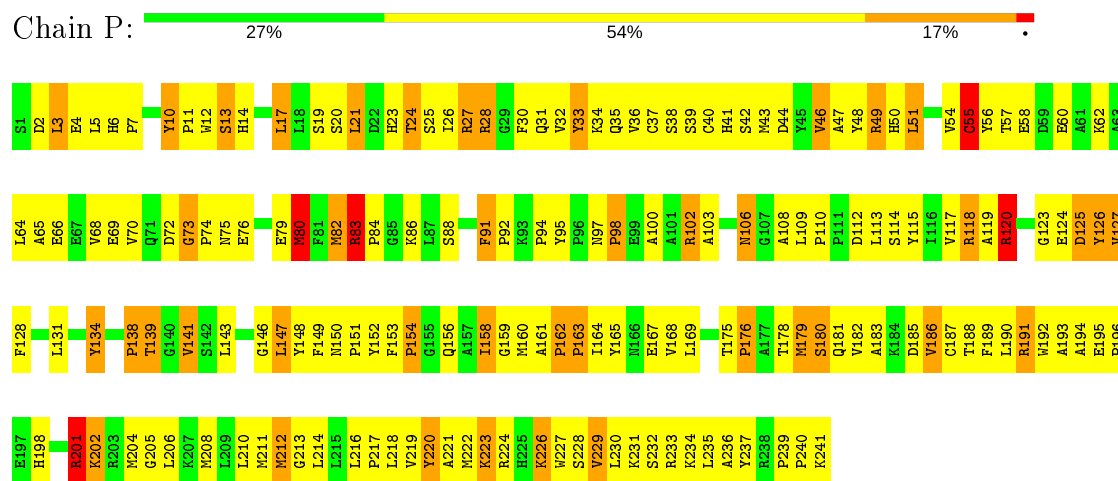




• Molecule 4: CYTOCHROME BC1 COMPLEX

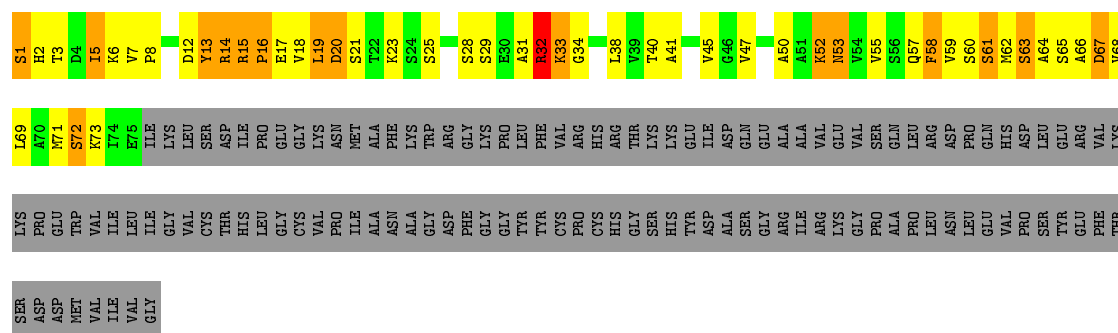


• Molecule 4: CYTOCHROME BC1 COMPLEX




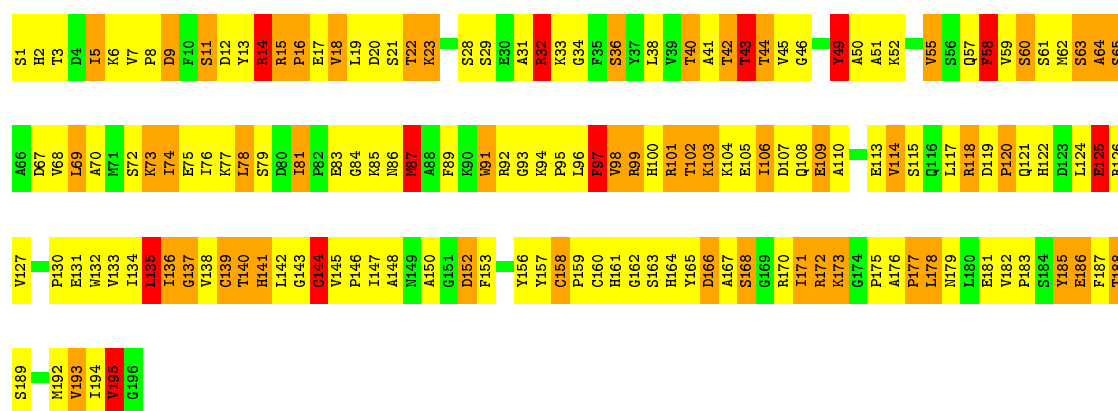
• Molecule 5: CYTOCHROME BC1 COMPLEX

Chain E: 



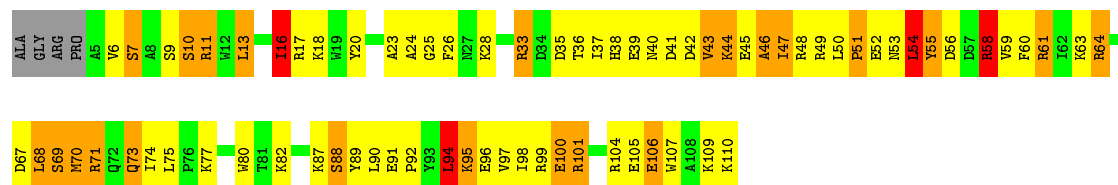
• Molecule 5: CYTOCHROME BC1 COMPLEX

Chain Q: 



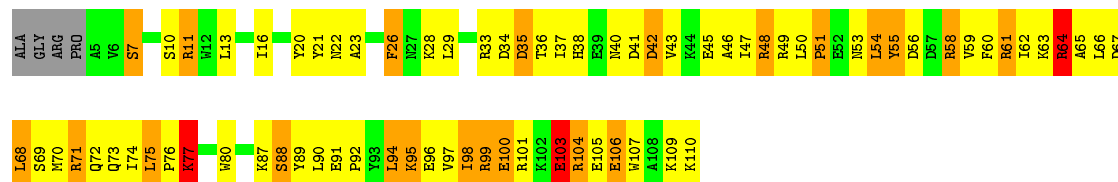
• Molecule 6: CYTOCHROME BC1 COMPLEX

Chain F: 



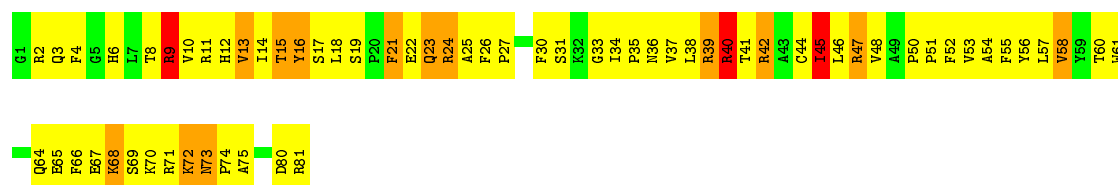
• Molecule 6: CYTOCHROME BC1 COMPLEX

Chain R: 

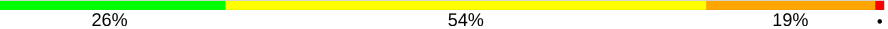


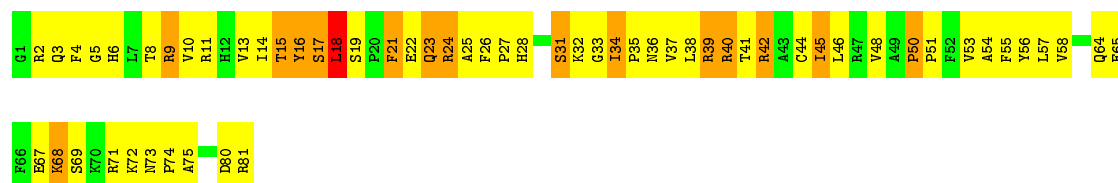
• Molecule 7: CYTOCHROME BC1 COMPLEX

Chain G: 



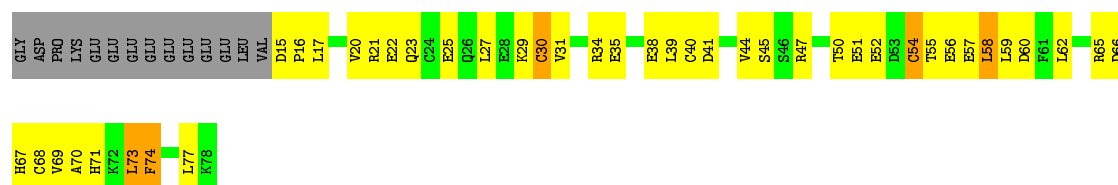
• Molecule 7: CYTOCHROME BC1 COMPLEX

Chain S: 



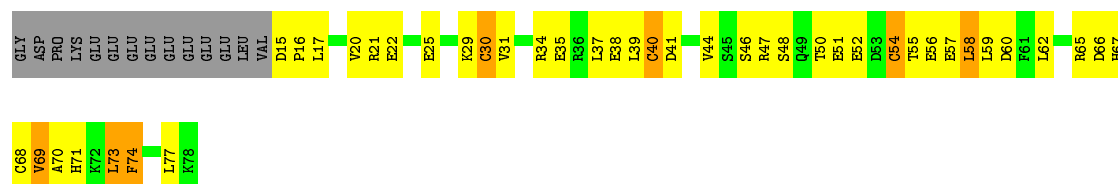
• Molecule 8: CYTOCHROME BC1 COMPLEX

Chain H: 



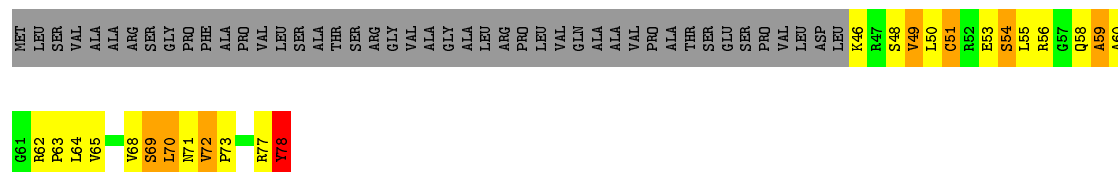
• Molecule 8: CYTOCHROME BC1 COMPLEX

Chain T: 



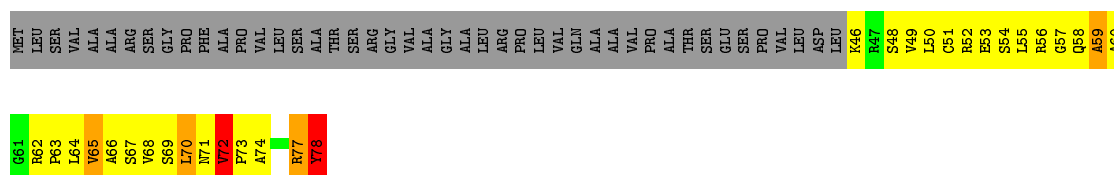
• Molecule 9: CYTOCHROME BC1 COMPLEX

Chain I: 



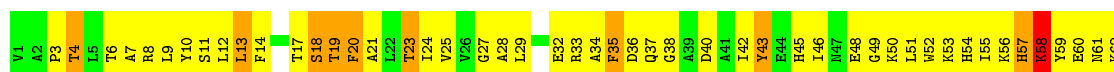
• Molecule 9: CYTOCHROME BC1 COMPLEX

Chain U: 



• Molecule 10: CYTOCHROME BC1 COMPLEX

Chain J: 



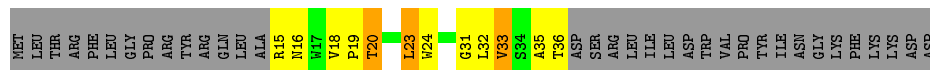
• Molecule 10: CYTOCHROME BC1 COMPLEX

Chain V: 



• Molecule 11: CYTOCHROME BC1 COMPLEX

Chain K: 



• Molecule 11: CYTOCHROME BC1 COMPLEX

Chain W: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	130.11Å 130.11Å 720.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	74.0 (20.00-3.00)	Depositor
R_{merge}	0.92	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.320 , 0.360	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31486	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A	0.60	2/3531 (0.1%)	1.58	43/4792 (0.9%)
1	M	0.63	3/3531 (0.1%)	1.61	58/4792 (1.2%)
2	B	0.51	0/3198	1.46	31/4336 (0.7%)
2	N	0.51	0/3198	1.33	11/4336 (0.3%)
3	C	0.71	2/3108 (0.1%)	1.73	63/4252 (1.5%)
3	O	0.69	3/3108 (0.1%)	1.62	51/4252 (1.2%)
4	D	0.55	0/1978	1.50	23/2684 (0.9%)
4	P	0.55	0/1978	1.40	24/2684 (0.9%)
5	E	0.60	0/574	1.63	7/775 (0.9%)
5	Q	0.61	0/1551	1.68	28/2097 (1.3%)
6	F	0.57	0/935	1.56	18/1253 (1.4%)
6	R	0.57	0/935	1.66	24/1253 (1.9%)
7	G	0.61	1/704 (0.1%)	1.41	9/951 (0.9%)
7	S	0.59	0/704	1.31	5/951 (0.5%)
8	H	0.41	0/529	1.12	0/708
8	T	0.39	0/529	1.06	0/708
9	I	0.48	0/250	1.31	2/335 (0.6%)
9	U	0.48	0/250	1.32	1/335 (0.3%)
10	J	0.51	0/525	1.31	5/707 (0.7%)
10	V	0.51	0/525	1.42	6/707 (0.8%)
11	K	0.42	0/163	1.01	0/225
11	W	0.46	0/163	1.18	0/225
All	All	0.59	11/31967 (0.0%)	1.52	409/43358 (0.9%)

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
1	A	0	13

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	3
2	B	0	9
2	N	0	5
3	C	0	14
3	O	0	6
4	D	0	5
4	P	0	4
5	E	0	1
5	Q	0	9
6	F	0	2
7	G	0	2
7	S	0	3
8	T	0	1
9	I	0	1
9	U	0	1
10	J	0	1
11	W	0	1
All	All	0	81

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	419	CYS	CB-SG	-7.17	1.70	1.82
1	M	253	VAL	C-O	6.79	1.36	1.23
1	A	104	LYS	CD-CE	6.57	1.67	1.51
1	M	169	GLY	N-CA	-6.53	1.36	1.46
3	O	106	SER	CB-OG	-6.43	1.33	1.42
7	G	16	TYR	CD2-CE2	-6.07	1.30	1.39
1	M	434	TYR	CG-CD2	-5.40	1.32	1.39
3	O	40	CYS	CB-SG	-5.30	1.73	1.81
3	C	75	TYR	CG-CD1	-5.09	1.32	1.39
3	C	183	PHE	CG-CD1	-5.08	1.31	1.38
3	O	37	LEU	C-N	-5.03	1.24	1.33

All (409) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	46	ARG	NE-CZ-NH2	-19.34	110.63	120.30
4	D	120	ARG	NE-CZ-NH2	-16.26	112.17	120.30
2	B	70	ARG	NE-CZ-NH2	16.26	128.43	120.30
1	A	419	CYS	CA-CB-SG	16.23	143.21	114.00
2	B	245	ARG	NE-CZ-NH2	14.98	127.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	253	VAL	O-C-N	-14.88	98.90	122.70
3	C	91	PHE	CB-CG-CD2	-14.45	110.69	120.80
1	A	434	TYR	CB-CG-CD1	13.93	129.36	121.00
3	O	199	PHE	CB-CG-CD2	13.38	130.16	120.80
2	B	133	ARG	NE-CZ-NH1	13.00	126.80	120.30
3	O	71	ARG	NE-CZ-NH1	-12.56	114.02	120.30
4	D	201	ARG	NE-CZ-NH1	-12.36	114.12	120.30
3	O	55	TYR	CB-CG-CD1	12.08	128.25	121.00
1	A	46	ARG	NE-CZ-NH2	-12.06	114.27	120.30
3	C	33	PHE	CG-CD2-CE2	11.88	133.87	120.80
1	M	398	ARG	NE-CZ-NH1	11.85	126.22	120.30
1	M	414	TYR	CB-CG-CD1	11.78	128.07	121.00
2	N	70	ARG	NE-CZ-NH2	-11.73	114.44	120.30
6	R	34	ASP	CB-CG-OD1	-11.72	107.75	118.30
1	M	344	ARG	NE-CZ-NH1	11.71	126.15	120.30
1	A	438	ARG	NE-CZ-NH2	11.69	126.14	120.30
2	B	70	ARG	NE-CZ-NH1	-11.34	114.63	120.30
1	A	244	ARG	NE-CZ-NH2	11.27	125.93	120.30
5	Q	14	ARG	NE-CZ-NH1	-11.26	114.67	120.30
5	Q	166	ASP	CB-CG-OD1	11.15	128.34	118.30
1	M	256	ALA	CB-CA-C	-11.09	93.47	110.10
3	C	313	ARG	NE-CZ-NH2	11.03	125.81	120.30
7	S	15	THR	CA-CB-CG2	-10.68	97.45	112.40
1	M	398	ARG	NE-CZ-NH2	-10.46	115.07	120.30
3	O	80	ARG	NE-CZ-NH1	-10.46	115.07	120.30
1	A	438	ARG	NE-CZ-NH1	-10.45	115.07	120.30
1	M	168	GLU	C-N-CA	10.45	144.24	122.30
10	V	26	VAL	CA-CB-CG1	10.38	126.47	110.90
1	M	414	TYR	CB-CG-CD2	-10.33	114.80	121.00
6	F	61	ARG	NE-CZ-NH2	10.29	125.45	120.30
6	F	58	ARG	NE-CZ-NH2	-10.27	115.17	120.30
1	A	24	ARG	NE-CZ-NH1	-10.25	115.18	120.30
3	C	187	PHE	CB-CG-CD2	-9.93	113.85	120.80
2	B	102	ARG	NE-CZ-NH2	9.88	125.24	120.30
2	N	56	ARG	CD-NE-CZ	9.77	137.28	123.60
5	Q	193	VAL	CG1-CB-CG2	9.74	126.49	110.90
3	C	131	TYR	CB-CG-CD1	-9.70	115.18	121.00
4	P	118	ARG	NE-CZ-NH2	-9.65	115.47	120.30
5	E	32	ARG	NE-CZ-NH1	-9.64	115.48	120.30
3	C	196	HIS	CA-CB-CG	9.63	129.97	113.60
2	B	102	ARG	NE-CZ-NH1	-9.60	115.50	120.30
3	C	183	PHE	CB-CG-CD1	9.55	127.49	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	199	PHE	CB-CG-CD2	-9.46	114.17	120.80
3	C	71	ARG	NE-CZ-NH1	-9.38	115.61	120.30
1	M	92	ARG	NE-CZ-NH1	9.36	124.98	120.30
6	R	26	PHE	CB-CG-CD2	9.31	127.32	120.80
3	O	196	HIS	CA-CB-CG	9.30	129.42	113.60
2	B	245	ARG	NE-CZ-NH1	-9.27	115.67	120.30
3	C	282	ARG	NE-CZ-NH1	-9.21	115.70	120.30
1	A	408	ARG	NE-CZ-NH2	-9.11	115.75	120.30
6	R	21	TYR	CB-CG-CD2	-8.96	115.62	121.00
1	A	434	TYR	CB-CG-CD2	-8.90	115.66	121.00
5	Q	55	VAL	CA-CB-CG1	8.72	123.98	110.90
6	R	58	ARG	NE-CZ-NH2	8.69	124.64	120.30
3	O	55	TYR	CB-CG-CD2	-8.61	115.83	121.00
6	R	64	ARG	NE-CZ-NH2	-8.58	116.01	120.30
6	R	77	LYS	CG-CD-CE	8.51	137.42	111.90
1	A	441	MET	CA-CB-CG	-8.41	99.00	113.30
3	C	33	PHE	CB-CG-CD1	8.41	126.69	120.80
5	Q	99	ARG	NE-CZ-NH2	8.39	124.49	120.30
3	O	104	TYR	CB-CG-CD1	8.38	126.03	121.00
3	C	359	PHE	CB-CG-CD1	8.35	126.64	120.80
2	B	199	PHE	CB-CG-CD1	8.33	126.63	120.80
3	C	171	ASP	CB-CG-OD1	8.29	125.77	118.30
1	M	253	VAL	CA-C-O	8.25	137.43	120.10
4	D	152	TYR	CB-CG-CD1	8.23	125.94	121.00
2	B	177	TYR	O-C-N	8.18	135.79	122.70
3	O	223	TYR	CB-CG-CD2	8.18	125.91	121.00
3	C	204	GLY	C-N-CA	8.14	142.06	121.70
2	B	56	ARG	CD-NE-CZ	8.10	134.95	123.60
3	O	185	LEU	CA-CB-CG	8.08	133.88	115.30
6	F	61	ARG	NE-CZ-NH1	-8.02	116.29	120.30
6	R	35	ASP	CB-CG-OD2	8.00	125.50	118.30
6	R	55	TYR	CB-CG-CD1	-7.96	116.22	121.00
10	V	31	PHE	CB-CG-CD2	-7.96	115.23	120.80
5	E	13	TYR	CB-CG-CD2	-7.94	116.23	121.00
3	C	131	TYR	CB-CG-CD2	7.91	125.75	121.00
1	A	343	MET	CA-CB-CG	-7.90	99.87	113.30
1	M	344	ARG	NE-CZ-NH2	-7.89	116.36	120.30
3	C	235	LEU	CB-CG-CD2	7.89	124.41	111.00
3	O	128	PHE	CB-CG-CD2	-7.88	115.28	120.80
5	E	13	TYR	CB-CG-CD1	7.88	125.73	121.00
10	V	31	PHE	CB-CG-CD1	7.85	126.29	120.80
1	M	342	TRP	CH2-CZ2-CE2	7.84	125.24	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	9	ARG	NE-CZ-NH1	-7.81	116.39	120.30
10	V	14	PHE	CB-CG-CD1	7.81	126.26	120.80
1	A	324	PHE	CB-CG-CD2	-7.75	115.38	120.80
1	A	436	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	A	235	ARG	NE-CZ-NH1	7.70	124.15	120.30
3	O	325	PHE	CG-CD2-CE2	7.70	129.27	120.80
1	A	395	TRP	NE1-CE2-CZ2	-7.65	121.98	130.40
2	B	319	SER	N-CA-CB	7.64	121.96	110.50
10	J	14	PHE	CB-CG-CD1	7.62	126.14	120.80
1	M	334	MET	O-C-N	-7.60	110.54	122.70
6	F	64	ARG	CD-NE-CZ	-7.59	112.98	123.60
3	O	19	ILE	O-C-N	-7.56	110.60	122.70
3	C	313	ARG	NE-CZ-NH1	-7.53	116.53	120.30
2	B	134	ARG	NE-CZ-NH1	-7.46	116.57	120.30
4	P	220	TYR	CB-CG-CD1	7.46	125.48	121.00
6	F	55	TYR	CB-CG-CD1	7.45	125.47	121.00
6	F	58	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	M	431	LEU	CB-CG-CD1	7.31	123.42	111.00
1	A	425	PHE	CB-CG-CD1	7.29	125.91	120.80
4	D	206	LEU	CB-CA-C	-7.29	96.34	110.20
1	M	307	PHE	CA-C-O	7.29	135.40	120.10
1	A	89	TYR	CB-CG-CD1	7.26	125.36	121.00
1	A	168	GLU	CA-C-O	7.25	135.32	120.10
3	C	80	ARG	NE-CZ-NH1	-7.24	116.68	120.30
3	O	44	GLN	C-N-CA	7.23	139.78	121.70
3	C	317	PHE	CB-CG-CD2	7.20	125.84	120.80
1	M	362	ARG	NE-CZ-NH1	-7.16	116.72	120.30
3	O	273	TYR	CB-CG-CD2	7.16	125.30	121.00
1	M	408	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	A	408	ARG	NH1-CZ-NH2	7.13	127.25	119.40
1	M	423	ALA	CB-CA-C	-7.12	99.42	110.10
1	M	419	CYS	CA-CB-SG	7.09	126.75	114.00
7	S	16	TYR	CG-CD1-CE1	7.08	126.97	121.30
3	C	214	ASP	CB-CG-OD2	7.04	124.64	118.30
2	B	147	ASP	CB-CG-OD2	7.04	124.64	118.30
3	C	273	TYR	CB-CG-CD2	7.04	125.22	121.00
6	R	61	ARG	NE-CZ-NH1	-7.04	116.78	120.30
4	P	125	ASP	CB-CG-OD2	7.02	124.62	118.30
4	P	28	ARG	NE-CZ-NH2	-7.01	116.79	120.30
6	R	21	TYR	CB-CG-CD1	7.00	125.20	121.00
1	M	70	ARG	NE-CZ-NH2	-6.98	116.81	120.30
5	Q	97	PHE	CB-CG-CD1	6.97	125.68	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	75	TYR	CB-CG-CD1	6.96	125.18	121.00
1	M	174	VAL	CA-CB-CG1	6.94	121.31	110.90
1	M	46	ARG	NH1-CZ-NH2	6.94	127.03	119.40
1	M	376	CYS	CA-CB-SG	-6.94	101.51	114.00
2	N	87	ARG	NE-CZ-NH1	-6.93	116.84	120.30
3	C	33	PHE	CZ-CE2-CD2	-6.91	111.81	120.10
4	D	208	MET	CA-CB-CG	6.89	125.02	113.30
3	O	47	THR	O-C-N	-6.87	111.52	123.20
3	O	325	PHE	CB-CG-CD2	6.82	125.57	120.80
6	R	55	TYR	CB-CG-CD2	6.80	125.08	121.00
1	A	415	PHE	O-C-N	-6.80	111.82	122.70
7	G	47	ARG	NE-CZ-NH2	-6.79	116.90	120.30
3	O	80	ARG	CD-NE-CZ	-6.79	114.09	123.60
1	M	417	ASP	CB-CG-OD2	-6.79	112.19	118.30
7	S	16	TYR	CB-CG-CD1	6.74	125.05	121.00
1	M	342	TRP	CD1-NE1-CE2	-6.74	102.93	109.00
3	C	75	TYR	CB-CG-CD2	-6.73	116.96	121.00
6	F	101	ARG	NE-CZ-NH1	-6.69	116.95	120.30
6	R	65	ALA	CA-C-O	6.69	134.15	120.10
3	C	55	TYR	CB-CG-CD2	6.68	125.01	121.00
3	C	41	LEU	N-CA-CB	6.68	123.75	110.40
1	M	319	LEU	CB-CG-CD2	6.65	122.31	111.00
5	Q	14	ARG	NE-CZ-NH2	6.65	123.63	120.30
3	O	276	PHE	CB-CG-CD1	-6.63	116.16	120.80
6	R	63	LYS	CB-CA-C	6.61	123.62	110.40
1	A	408	ARG	NE-CZ-NH1	-6.60	117.00	120.30
3	O	72	ASP	CB-CG-OD2	6.59	124.23	118.30
7	G	40	ARG	NE-CZ-NH2	-6.58	117.01	120.30
10	J	40	ASP	CB-CG-OD2	6.57	124.21	118.30
5	Q	15	ARG	NE-CZ-NH1	6.56	123.58	120.30
4	P	27	ARG	NE-CZ-NH1	6.56	123.58	120.30
4	P	235	LEU	CA-C-O	6.55	133.85	120.10
3	C	175	LEU	N-CA-CB	6.52	123.45	110.40
1	A	404	ALA	CB-CA-C	6.51	119.87	110.10
3	O	178	PHE	CB-CG-CD2	-6.51	116.24	120.80
3	C	180	ALA	N-CA-CB	6.49	119.18	110.10
2	N	177	TYR	CB-CG-CD1	-6.47	117.11	121.00
1	M	131	ARG	NE-CZ-NH2	-6.46	117.07	120.30
6	R	36	THR	CA-CB-CG2	6.46	121.44	112.40
4	D	120	ARG	NE-CZ-NH1	6.44	123.52	120.30
4	D	134	TYR	CB-CG-CD1	6.44	124.86	121.00
1	M	300	THR	CA-CB-CG2	-6.43	103.40	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	99	ARG	NE-CZ-NH1	-6.39	117.10	120.30
1	A	441	MET	CG-SD-CE	6.39	110.42	100.20
3	C	267	HIS	CA-CB-CG	-6.38	102.75	113.60
3	O	359	PHE	CB-CG-CD1	6.38	125.27	120.80
3	O	91	PHE	CB-CG-CD2	-6.38	116.34	120.80
1	M	421	ALA	CB-CA-C	6.36	119.64	110.10
1	M	435	ASN	OD1-CG-ND2	6.35	136.50	121.90
1	A	208	LEU	CA-CB-CG	6.34	129.88	115.30
1	A	190	TYR	CB-CG-CD2	6.33	124.80	121.00
3	O	242	LEU	CB-CA-C	-6.33	98.18	110.20
7	S	21	PHE	CB-CG-CD2	-6.32	116.38	120.80
3	C	246	ALA	N-CA-CB	-6.31	101.26	110.10
3	C	359	PHE	CB-CG-CD2	-6.31	116.39	120.80
6	R	42	ASP	CB-CG-OD1	6.30	123.97	118.30
7	S	21	PHE	CB-CG-CD1	6.30	125.21	120.80
2	B	177	TYR	CB-CG-CD1	6.30	124.78	121.00
3	O	276	PHE	CB-CG-CD2	6.30	125.21	120.80
3	O	40	CYS	CA-CB-SG	6.29	125.33	114.00
3	O	223	TYR	CZ-CE2-CD2	-6.24	114.18	119.80
4	P	118	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	97	TYR	CG-CD1-CE1	6.21	126.27	121.30
3	C	43	LEU	O-C-N	-6.19	112.79	122.70
3	C	325	PHE	CB-CG-CD1	-6.18	116.48	120.80
5	Q	91	TRP	CB-CG-CD1	-6.16	118.99	127.00
3	O	73	VAL	CG1-CB-CG2	-6.16	101.04	110.90
3	O	223	TYR	CB-CG-CD1	-6.16	117.31	121.00
3	O	331	ASP	CB-CG-OD2	6.16	123.84	118.30
2	N	188	PRO	O-C-N	-6.15	112.86	122.70
6	F	107	TRP	CD1-NE1-CE2	6.14	114.53	109.00
6	R	104	ARG	NE-CZ-NH1	-6.13	117.23	120.30
3	O	52	ALA	N-CA-CB	6.13	118.68	110.10
5	Q	91	TRP	CB-CG-CD2	6.13	134.57	126.60
6	F	71	ARG	NE-CZ-NH2	-6.11	117.25	120.30
3	O	223	TYR	CG-CD2-CE2	6.09	126.18	121.30
6	R	26	PHE	CG-CD2-CE2	6.09	127.50	120.80
1	M	112	LEU	CB-CG-CD2	-6.07	100.68	111.00
4	D	49	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	A	378	ASP	CB-CG-OD1	6.06	123.75	118.30
5	Q	97	PHE	CB-CG-CD2	-6.05	116.56	120.80
7	G	16	TYR	CZ-CE2-CD2	6.05	125.25	119.80
3	O	237	LEU	CB-CG-CD2	6.04	121.27	111.00
3	C	183	PHE	CB-CG-CD2	-6.04	116.57	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	83	PHE	CB-CG-CD1	-6.04	116.58	120.80
10	J	20	PHE	CZ-CE2-CD2	6.03	127.34	120.10
1	M	158	PHE	CB-CG-CD1	-6.03	116.58	120.80
1	M	24	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	M	89	TYR	CB-CG-CD1	6.02	124.61	121.00
5	E	14	ARG	CD-NE-CZ	-6.01	115.18	123.60
3	O	104	TYR	CB-CG-CD2	-6.01	117.39	121.00
6	F	73	GLN	CB-CA-C	6.00	122.40	110.40
6	F	33	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	168	GLU	O-C-N	-5.99	113.02	123.20
3	O	90	PHE	CB-CG-CD2	5.97	124.98	120.80
2	B	134	ARG	NE-CZ-NH2	5.97	123.28	120.30
2	N	157	ALA	N-CA-CB	5.96	118.45	110.10
3	C	115	ILE	C-N-CA	-5.96	109.78	122.30
3	C	205	SER	O-C-N	-5.95	113.18	122.70
2	B	179	PRO	N-CA-CB	5.95	110.44	103.30
1	A	251	ALA	CA-C-O	5.94	132.58	120.10
4	D	204	MET	CA-CB-CG	5.94	123.39	113.30
4	P	138	PRO	N-CD-CG	-5.93	94.30	103.20
7	G	16	TYR	CB-CG-CD2	5.93	124.56	121.00
1	M	236	PHE	CB-CG-CD1	5.92	124.95	120.80
10	J	14	PHE	CB-CG-CD2	-5.92	116.66	120.80
2	B	194	TYR	CB-CG-CD1	-5.91	117.45	121.00
3	O	267	HIS	CA-CB-CG	-5.91	103.55	113.60
2	B	308	ASP	CB-CG-OD2	5.90	123.61	118.30
5	Q	144	CYS	CA-CB-SG	5.90	124.62	114.00
5	Q	183	PRO	O-C-N	5.89	132.12	122.70
3	O	257	THR	N-CA-CB	5.89	121.49	110.30
10	V	39	ALA	O-C-N	5.88	132.11	122.70
3	O	199	PHE	CD1-CG-CD2	-5.88	110.66	118.30
3	C	18	PHE	CB-CG-CD1	5.87	124.91	120.80
4	D	182	VAL	CA-CB-CG1	5.87	119.70	110.90
1	M	325	VAL	CA-C-N	5.87	130.10	117.20
1	M	89	TYR	CA-CB-CG	5.86	124.53	113.40
4	P	134	TYR	CB-CG-CD1	5.85	124.51	121.00
3	C	358	TYR	CB-CG-CD1	-5.84	117.49	121.00
3	C	77	TRP	CD2-CE3-CZ3	-5.83	111.23	118.80
4	P	220	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	A	288	ALA	N-CA-CB	5.82	118.25	110.10
1	A	425	PHE	N-CA-CB	5.82	121.07	110.60
1	A	362	ARG	NE-CZ-NH2	5.80	123.20	120.30
4	D	28	ARG	NE-CZ-NH2	5.80	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	435	ASN	CB-CG-OD1	-5.80	110.00	121.60
2	N	287	ARG	NE-CZ-NH1	5.79	123.20	120.30
4	P	91	PHE	CZ-CE2-CD2	5.79	127.05	120.10
4	P	201	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	M	334	MET	N-CA-CB	-5.79	100.18	110.60
3	C	223	TYR	CB-CG-CD2	5.76	124.46	121.00
4	D	224	ARG	NE-CZ-NH1	5.76	123.18	120.30
4	P	55	CYS	CA-CB-SG	-5.76	103.64	114.00
1	M	137	GLU	OE1-CD-OE2	-5.75	116.39	123.30
3	C	357	LEU	CB-CG-CD2	5.75	120.77	111.00
4	D	14	HIS	CA-CB-CG	5.71	123.31	113.60
3	C	53	MET	CA-CB-CG	5.70	122.99	113.30
4	P	235	LEU	O-C-N	-5.68	113.61	122.70
5	Q	135	LEU	O-C-N	-5.67	113.62	122.70
2	B	314	ALA	N-CA-CB	-5.67	102.16	110.10
1	A	131	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	294	LEU	O-C-N	-5.66	113.64	122.70
4	D	119	ALA	CB-CA-C	-5.66	101.61	110.10
4	D	199	ASP	CB-CG-OD1	5.65	123.39	118.30
6	R	34	ASP	OD1-CG-OD2	5.64	134.02	123.30
5	Q	14	ARG	CD-NE-CZ	-5.63	115.72	123.60
2	B	178	CYS	O-C-N	5.62	131.78	121.10
3	C	122	THR	CA-CB-CG2	-5.61	104.54	112.40
2	N	66	SER	N-CA-CB	5.61	118.92	110.50
1	A	417	ASP	CB-CG-OD2	-5.60	113.26	118.30
3	C	187	PHE	CG-CD1-CE1	-5.60	114.64	120.80
3	C	303	LEU	N-CA-CB	5.59	121.58	110.40
2	B	203	ARG	NE-CZ-NH1	5.58	123.09	120.30
3	O	143	ALA	CB-CA-C	5.57	118.46	110.10
10	V	21	ALA	CB-CA-C	5.57	118.46	110.10
1	M	408	ARG	NH1-CZ-NH2	5.57	125.53	119.40
3	O	347	TYR	CB-CG-CD2	5.57	124.34	121.00
4	P	27	ARG	NE-CZ-NH2	-5.56	117.52	120.30
3	C	18	PHE	CB-CG-CD2	-5.54	116.92	120.80
4	D	201	ARG	CA-CB-CG	5.54	125.59	113.40
4	D	224	ARG	NE-CZ-NH2	-5.54	117.53	120.30
3	O	244	LEU	O-C-N	5.54	131.56	122.70
1	M	342	TRP	NE1-CE2-CD2	5.52	112.82	107.30
6	R	56	ASP	CB-CG-OD1	5.51	123.26	118.30
4	D	191	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	M	346	CYS	CA-CB-SG	5.50	123.89	114.00
1	M	442	PHE	CB-CG-CD1	5.48	124.64	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	109	PHE	CG-CD1-CE1	5.48	126.83	120.80
4	P	120	ARG	CD-NE-CZ	5.47	131.26	123.60
3	O	128	PHE	CB-CG-CD1	5.47	124.63	120.80
1	A	241	ILE	CA-CB-CG1	-5.47	100.61	111.00
4	P	49	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	M	92	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	341	GLN	O-C-N	5.45	131.42	122.70
5	Q	185	TYR	CB-CG-CD2	5.45	124.27	121.00
3	O	25	SER	N-CA-CB	-5.45	102.33	110.50
6	R	65	ALA	O-C-N	-5.45	113.99	122.70
6	R	71	ARG	NE-CZ-NH2	-5.44	117.58	120.30
6	R	103	GLU	OE1-CD-OE2	-5.44	116.77	123.30
4	D	201	ARG	NH1-CZ-NH2	5.42	125.36	119.40
6	F	94	LEU	CB-CG-CD1	5.41	120.19	111.00
3	O	72	ASP	CB-CG-OD1	-5.41	113.43	118.30
5	E	53	ASN	CB-CG-OD1	-5.39	110.81	121.60
2	B	254	HIS	CA-CB-CG	5.39	122.77	113.60
6	R	77	LYS	CD-CE-NZ	5.39	124.09	111.70
3	C	109	PHE	O-C-N	-5.39	114.08	122.70
6	F	59	VAL	CA-CB-CG1	-5.38	102.82	110.90
1	M	420	PRO	N-CA-CB	5.38	109.75	103.30
1	A	356	ARG	NE-CZ-NH1	-5.37	117.62	120.30
4	P	44	ASP	CB-CG-OD2	-5.35	113.48	118.30
3	C	206	ASN	CB-CG-OD1	-5.34	110.92	121.60
4	D	191	ARG	NE-CZ-NH1	-5.34	117.63	120.30
3	C	282	ARG	CD-NE-CZ	-5.33	116.13	123.60
5	Q	40	THR	CA-CB-CG2	5.33	119.86	112.40
1	M	217	SER	N-CA-CB	-5.32	102.52	110.50
3	O	67	THR	CA-CB-CG2	-5.32	104.95	112.40
7	G	21	PHE	CB-CG-CD1	-5.31	117.08	120.80
5	Q	193	VAL	CA-CB-CG2	-5.31	102.93	110.90
9	U	78	TYR	CA-CB-CG	5.30	123.48	113.40
6	F	54	LEU	CB-CG-CD1	5.30	120.01	111.00
5	Q	49	TYR	CB-CG-CD1	5.29	124.17	121.00
2	B	157	ALA	CB-CA-C	5.29	118.03	110.10
6	F	71	ARG	NE-CZ-NH1	5.28	122.94	120.30
5	Q	118	ARG	NE-CZ-NH1	-5.28	117.66	120.30
3	C	91	PHE	CD1-CG-CD2	5.27	125.15	118.30
3	O	131	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	M	131	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	N	113	ARG	NE-CZ-NH1	5.26	122.93	120.30
5	Q	5	ILE	CB-CA-C	-5.25	101.09	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	85	ILE	CB-CA-C	-5.25	101.10	111.60
4	D	40	CYS	CA-CB-SG	5.25	123.45	114.00
1	M	378	ASP	CB-CG-OD1	5.25	123.02	118.30
6	R	99	ARG	CD-NE-CZ	5.24	130.94	123.60
7	G	47	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	O	242	LEU	N-CA-CB	5.24	120.88	110.40
3	C	325	PHE	CB-CG-CD2	5.24	124.47	120.80
1	M	434	TYR	O-C-N	-5.24	114.32	122.70
7	G	13	VAL	O-C-N	-5.23	114.33	122.70
6	F	43	VAL	CA-C-O	5.21	131.05	120.10
3	C	195	VAL	CG1-CB-CG2	-5.21	102.56	110.90
3	C	196	HIS	O-C-N	5.21	131.03	122.70
3	C	183	PHE	CZ-CE2-CD2	5.20	126.34	120.10
5	E	14	ARG	NE-CZ-NH2	-5.20	117.70	120.30
3	O	325	PHE	CZ-CE2-CD2	-5.20	113.87	120.10
4	D	203	ARG	CD-NE-CZ	5.19	130.87	123.60
1	A	294	LEU	C-N-CA	5.19	134.67	121.70
1	M	325	VAL	O-C-N	-5.19	114.40	122.70
3	C	30	TRP	O-C-N	-5.18	114.41	122.70
1	M	421	ALA	N-CA-CB	-5.18	102.85	110.10
4	P	208	MET	CA-CB-CG	5.18	122.10	113.30
2	B	346	THR	CA-CB-OG1	5.17	119.86	109.00
4	P	191	ARG	NE-CZ-NH2	-5.17	117.72	120.30
5	Q	87	MET	CA-CB-CG	5.17	122.09	113.30
1	M	320	LEU	O-C-N	-5.17	114.42	123.20
5	Q	101	ARG	NE-CZ-NH2	-5.16	117.72	120.30
4	P	102	ARG	NE-CZ-NH1	-5.16	117.72	120.30
2	B	169	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	B	89	ILE	CA-CB-CG2	5.14	121.19	110.90
6	F	55	TYR	CB-CG-CD2	-5.13	117.92	121.00
2	B	92	VAL	O-C-N	-5.13	114.47	123.20
5	Q	58	PHE	CB-CG-CD1	5.13	124.39	120.80
3	O	93	CYS	N-CA-CB	5.12	119.83	110.60
1	M	408	ARG	NE-CZ-NH1	-5.12	117.74	120.30
7	G	13	VAL	CA-C-O	5.12	130.84	120.10
9	I	68	VAL	CB-CA-C	-5.12	101.68	111.40
3	C	13	ILE	CB-CA-C	-5.11	101.38	111.60
5	E	61	SER	CA-CB-OG	-5.11	97.41	111.20
3	C	13	ILE	CA-CB-CG1	5.10	120.69	111.00
1	M	438	ARG	CA-CB-CG	-5.10	102.18	113.40
1	A	420	PRO	N-CA-CB	5.10	109.42	103.30
2	N	134	ARG	NE-CZ-NH1	-5.09	117.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	70	ALA	CB-CA-C	-5.09	102.46	110.10
4	P	33	TYR	CB-CG-CD2	-5.09	117.95	121.00
2	B	102	ARG	CD-NE-CZ	-5.08	116.49	123.60
9	I	78	TYR	CA-CB-CG	5.08	123.05	113.40
3	C	51	LEU	CB-CG-CD1	5.08	119.64	111.00
4	P	212	MET	CA-CB-CG	5.08	121.93	113.30
3	C	113	TRP	O-C-N	-5.08	114.58	122.70
4	P	126	TYR	CB-CG-CD2	5.06	124.04	121.00
1	M	423	ALA	N-CA-CB	5.06	117.19	110.10
3	O	282	ARG	NE-CZ-NH1	-5.06	117.77	120.30
3	C	91	PHE	CZ-CE2-CD2	-5.06	114.03	120.10
3	C	182	HIS	CA-CB-CG	5.06	122.20	113.60
1	M	431	LEU	CB-CG-CD2	5.06	119.60	111.00
3	O	90	PHE	CB-CG-CD1	-5.06	117.26	120.80
5	Q	18	VAL	CB-CA-C	-5.05	101.80	111.40
10	J	19	THR	CA-CB-CG2	-5.05	105.33	112.40
1	A	349	ALA	CB-CA-C	5.04	117.67	110.10
1	A	419	CYS	N-CA-CB	5.04	119.68	110.60
6	F	54	LEU	CA-CB-CG	5.04	126.88	115.30
3	C	186	PRO	O-C-N	-5.03	114.65	122.70
2	N	172	LEU	CA-CB-CG	5.03	126.87	115.30
3	O	19	ILE	C-N-CA	5.03	134.28	121.70
4	D	134	TYR	CB-CG-CD2	-5.02	117.99	121.00
5	Q	32	ARG	CB-CA-C	5.02	120.44	110.40
1	A	89	TYR	CA-CB-CG	5.01	122.92	113.40
3	C	51	LEU	CB-CG-CD2	-5.01	102.48	111.00

There are no chirality outliers.

All (81) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	GLN	Mainchain
1	A	122	LEU	Mainchain
1	A	196	VAL	Mainchain
1	A	210	ASP	Mainchain
1	A	239	SER	Mainchain
1	A	242	CYS	Mainchain
1	A	244	ARG	Mainchain
1	A	256	ALA	Mainchain
1	A	294	LEU	Mainchain
1	A	306	SER	Mainchain
1	A	345	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	383	LEU	Mainchain
1	A	53	ASN	Mainchain
2	B	106	ALA	Mainchain
2	B	159	VAL	Mainchain
2	B	178	CYS	Mainchain
2	B	239	TYR	Mainchain
2	B	285	VAL	Mainchain
2	B	335	ASP	Mainchain
2	B	353	SER	Mainchain
2	B	68	LEU	Mainchain
2	B	99	THR	Mainchain
3	C	134	PRO	Mainchain
3	C	164	ILE	Mainchain
3	C	20	ASP	Mainchain
3	C	21	LEU	Mainchain
3	C	222	PRO	Mainchain
3	C	235	LEU	Mainchain
3	C	281	LEU	Mainchain
3	C	322	GLN	Mainchain
3	C	326	TRP	Mainchain
3	C	335	LEU	Mainchain
3	C	355	SER	Mainchain
3	C	362	ILE	Mainchain
3	C	77	TRP	Mainchain
3	C	83	HIS	Mainchain
4	D	191	ARG	Mainchain
4	D	217	PRO	Mainchain
4	D	224	ARG	Mainchain
4	D	229	VAL	Mainchain
4	D	54	VAL	Mainchain
5	E	20	ASP	Mainchain
6	F	16	ILE	Mainchain
6	F	46	ALA	Mainchain
7	G	15	THR	Mainchain
7	G	73	ASN	Mainchain
9	I	69	SER	Mainchain
10	J	43	TYR	Mainchain
1	M	100	LYS	Mainchain
1	M	141	ASN	Mainchain
1	M	290	LEU	Mainchain
2	N	137	VAL	Mainchain
2	N	144	LEU	Mainchain

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Mol	Chain	Res	Type	Group
2	N	200	THR	Mainchain
2	N	290	ASN	Mainchain
2	N	353	SER	Mainchain
3	O	148	ASN	Mainchain
3	O	159	ASN	Mainchain
3	O	19	ILE	Mainchain
3	O	355	SER	Mainchain
3	O	55	TYR	Mainchain
3	O	77	TRP	Mainchain
4	P	202	LYS	Mainchain
4	P	229	VAL	Mainchain
4	P	24	THR	Mainchain
4	P	46	VAL	Mainchain
5	Q	125	GLU	Mainchain
5	Q	135	LEU	Mainchain
5	Q	186	GLU	Mainchain
5	Q	195	VAL	Mainchain
5	Q	32	ARG	Mainchain
5	Q	36	SER	Mainchain
5	Q	49	TYR	Mainchain
5	Q	9	ASP	Mainchain
5	Q	97	PHE	Mainchain
7	S	17	SER	Mainchain
7	S	18	LEU	Mainchain
7	S	34	ILE	Mainchain
8	T	40	CYS	Mainchain
9	U	72	VAL	Mainchain
11	W	24	TRP	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	465	0
1	M	3458	0	3355	458	0
2	B	3141	0	3123	402	0
2	N	3141	0	3123	408	1
3	C	3011	0	3076	456	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	3011	0	3076	415	0
4	D	1919	0	1868	297	0
4	P	1919	0	1868	284	0
5	E	566	0	564	65	0
5	Q	1518	0	1499	264	1
6	F	916	0	909	91	0
6	R	916	0	909	91	1
7	G	682	0	679	104	0
7	S	682	0	679	100	0
8	H	524	0	504	71	1
8	T	524	0	504	75	0
9	I	248	0	265	52	0
9	U	248	0	265	66	0
10	J	512	0	518	66	0
10	V	512	0	518	74	0
11	K	159	0	159	26	0
11	W	159	0	159	26	0
12	C	86	0	60	20	0
12	O	86	0	60	25	0
13	D	43	0	30	7	0
13	P	43	0	30	3	0
14	Q	4	0	0	0	0
All	All	31486	0	31156	3839	2

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 61.

All (3839) 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)
7:S:50:PRO:HB2	7:S:51:PRO:HD3	1.25	1.17
4:D:224:ARG:HB2	7:G:25:ALA:HB1	1.27	1.17
2:B:77:THR:HG22	2:B:130:PRO:HA	1.25	1.14
1:M:67:THR:HG23	1:M:70:ARG:H	1.13	1.14
1:M:426:GLY:CA	1:M:428:ILE:HG13	1.78	1.13
5:Q:15:ARG:HB2	5:Q:16:PRO:HD2	1.19	1.13
4:P:181:GLN:HG2	8:T:77:LEU:HD22	1.29	1.12
4:P:83:ARG:HB3	4:P:84:PRO:HD2	1.14	1.12
5:Q:114:VAL:HA	5:Q:117:LEU:HD12	1.24	1.11
1:A:428:ILE:HG22	1:A:431:LEU:HB2	1.29	1.11
7:G:72:LYS:HB3	7:G:75:ALA:HB2	1.20	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:MET:HG2	3:C:178:PHE:HD2	1.03	1.10
1:M:403:ASP:HB3	1:M:406:VAL:HG23	1.34	1.09
1:A:67:THR:HG23	1:A:70:ARG:H	0.94	1.09
9:I:72:VAL:HB	9:I:73:PRO:HD3	1.20	1.09
4:P:83:ARG:HB3	4:P:84:PRO:CD	1.81	1.09
3:O:206:ASN:HB2	3:O:313:ARG:NH2	1.68	1.08
5:Q:76:ILE:CG2	5:Q:194:ILE:HG12	1.84	1.07
1:M:428:ILE:HG21	1:M:431:LEU:HD22	1.35	1.07
3:C:206:ASN:HB2	3:C:313:ARG:NH2	1.70	1.07
2:B:429:ASN:HD21	2:N:60:SER:HB3	1.15	1.07
3:C:310:SER:HA	3:C:374:ASN:HD21	1.12	1.07
3:C:77:TRP:CZ3	3:C:78:ILE:HG23	1.88	1.07
2:B:60:SER:HB3	2:N:429:ASN:HD21	0.96	1.07
1:M:428:ILE:HG22	1:M:431:LEU:HB2	1.19	1.07
1:A:64:PHE:CE1	1:A:86:LEU:HG	1.90	1.06
2:N:305:GLN:HB2	2:N:306:PRO:HD3	1.34	1.06
3:O:310:SER:HA	3:O:374:ASN:HD21	1.21	1.05
9:I:72:VAL:HB	9:I:73:PRO:CD	1.86	1.05
5:Q:96:LEU:HD21	5:Q:195:VAL:HG21	1.38	1.05
3:O:26:ASN:HD21	3:O:207:ASN:HB2	1.15	1.04
2:B:283:PRO:HG3	9:I:55:LEU:HD22	1.39	1.04
4:D:83:ARG:HB3	4:D:84:PRO:CD	1.86	1.04
1:A:426:GLY:CA	1:A:428:ILE:HG13	1.87	1.04
4:D:181:GLN:HG2	8:H:77:LEU:HD22	1.39	1.04
1:M:18:GLN:HE21	1:M:22:GLY:HA2	1.22	1.04
2:B:165:ALA:HA	2:B:173:ALA:HB1	1.39	1.04
3:C:170:VAL:HG13	3:C:174:THR:HG21	1.34	1.04
9:U:70:LEU:HD21	9:U:73:PRO:HD2	1.40	1.04
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.39	1.03
2:N:200:THR:HG22	2:N:203:ARG:HD2	1.36	1.03
5:Q:75:GLU:O	5:Q:194:ILE:HA	1.57	1.03
2:B:60:SER:CB	2:N:429:ASN:HD21	1.72	1.03
3:C:10:LEU:HB2	3:O:202:GLU:OE2	1.59	1.03
1:M:24:ARG:HB2	1:M:196:VAL:HG22	1.37	1.02
5:Q:134:ILE:HD11	5:Q:185:TYR:CD2	1.94	1.02
3:C:129:MET:HG2	3:C:178:PHE:CD2	1.93	1.02
5:Q:109:GLU:HG2	5:Q:167:ALA:HB3	1.36	1.02
7:S:72:LYS:HB3	7:S:75:ALA:HB2	1.39	1.02
9:U:72:VAL:HB	9:U:73:PRO:HD3	1.36	1.02
2:B:95:LYS:HE3	9:I:70:LEU:HD22	1.41	1.02
3:C:206:ASN:HB2	3:C:313:ARG:HH21	1.24	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:HIS:HB3	3:C:222:PRO:HD3	1.42	1.02
3:C:202:GLU:OE2	3:O:10:LEU:HB2	1.59	1.02
10:J:18:SER:HB3	11:K:23:LEU:HD12	1.42	1.02
3:O:100:ARG:HH21	12:O:381:HEM:HBD1	1.23	1.02
1:M:143:THR:HG21	9:U:48:SER:H	1.24	1.01
3:C:16:ASN:ND2	3:C:20:ASP:OD2	1.94	1.01
1:A:18:GLN:HE21	1:A:22:GLY:HA2	1.19	1.01
1:M:428:ILE:HG22	1:M:431:LEU:CB	1.90	1.01
4:D:83:ARG:CB	4:D:84:PRO:HD2	1.90	1.00
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.39	1.00
3:C:100:ARG:HH21	12:C:381:HEM:HBD1	1.26	1.00
8:T:21:ARG:HB3	8:T:65:ARG:HH21	1.26	1.00
2:N:24:LEU:HG	2:N:38:LEU:HD11	1.43	1.00
3:C:26:ASN:HB2	6:F:69:SER:OG	1.62	1.00
2:N:166:ALA:HB2	2:N:244:ILE:HG13	1.39	1.00
3:O:345:HIS:HB3	3:O:346:PRO:HD3	1.42	1.00
4:D:83:ARG:HB3	4:D:84:PRO:HD2	1.00	1.00
4:D:118:ARG:HG3	4:D:194:ALA:HB1	1.44	0.99
4:D:74:PRO:HB2	4:D:79:GLU:HB2	1.43	0.99
4:P:224:ARG:HB2	7:S:25:ALA:HB1	1.40	0.99
1:A:24:ARG:HB2	1:A:196:VAL:HG22	1.43	0.99
1:M:64:PHE:CE1	1:M:86:LEU:HG	1.98	0.99
3:O:16:ASN:ND2	3:O:20:ASP:OD2	1.96	0.99
1:A:408:ARG:HH22	11:K:15:ARG:NE	1.61	0.99
3:C:174:THR:HG23	3:C:178:PHE:CE1	1.98	0.99
3:C:26:ASN:HD21	3:C:207:ASN:HB2	1.28	0.99
2:B:24:LEU:HG	2:B:38:LEU:HD11	1.42	0.99
6:R:28:LYS:HD2	6:R:74:ILE:HD11	1.42	0.99
2:B:67:HIS:HD2	2:B:144:LEU:HD22	1.27	0.98
2:B:24:LEU:HD12	2:B:24:LEU:H	1.23	0.98
2:B:429:ASN:HD21	2:N:60:SER:CB	1.74	0.98
1:M:408:ARG:HH22	11:W:15:ARG:NE	1.61	0.98
1:M:42:ASP:HB3	1:M:384:LEU:HD22	1.45	0.98
1:A:383:LEU:HD22	1:A:388:ARG:HA	1.45	0.98
6:F:50:LEU:HB2	6:F:55:TYR:HB2	1.45	0.98
3:O:77:TRP:CZ3	3:O:78:ILE:HG23	1.98	0.98
3:O:174:THR:HG23	3:O:178:PHE:HE2	1.25	0.98
3:O:106:SER:HB3	12:O:381:HEM:HBD2	1.46	0.98
4:P:158:ILE:CD1	4:P:160:MET:HB2	1.94	0.98
1:M:21:ASN:HB3	1:M:217:SER:HB3	1.46	0.97
1:A:67:THR:HG23	1:A:70:ARG:N	1.79	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:210:GLY:HA3	3:O:314:SER:HB2	1.46	0.97
5:Q:86:ASN:HB2	5:Q:99:ARG:HD2	1.45	0.97
1:A:304:CYS:HB3	1:A:334:MET:SD	2.04	0.97
2:B:200:THR:HG22	2:B:203:ARG:HD2	1.44	0.97
2:B:305:GLN:HB2	2:B:306:PRO:HD3	1.46	0.97
1:M:392:LEU:HA	1:M:395:TRP:CD1	2.00	0.97
6:F:51:PRO:HG2	6:F:54:LEU:HD23	1.44	0.96
3:C:264:THR:HG21	5:Q:144:CYS:HB3	1.44	0.96
13:P:242:HEC:HH2	13:P:242:HEC:HBC2	1.45	0.96
4:P:74:PRO:HB2	4:P:79:GLU:HB2	1.46	0.96
2:B:60:SER:HB3	2:N:429:ASN:ND2	1.81	0.96
9:I:70:LEU:HD21	9:I:73:PRO:HD2	1.48	0.96
8:H:50:THR:HG22	8:H:52:GLU:H	1.28	0.96
4:P:178:THR:HB	4:P:181:GLN:HG3	1.46	0.96
2:N:77:THR:HG22	2:N:130:PRO:HA	1.46	0.95
3:O:174:THR:HG23	3:O:178:PHE:CE2	2.00	0.95
7:S:31:SER:O	7:S:35:PRO:HD2	1.65	0.95
1:M:417:ASP:OD2	10:V:10:TYR:OH	1.82	0.95
1:A:133:VAL:HG12	1:A:134:ILE:HD13	1.48	0.95
2:B:304:HIS:CD2	2:B:306:PRO:HD2	2.01	0.95
2:N:29:LEU:HB3	2:N:30:PRO:HD2	1.48	0.95
2:N:283:PRO:HG3	9:U:55:LEU:HD22	1.47	0.95
7:G:36:ASN:HA	7:G:39:ARG:HD3	1.46	0.95
2:B:111:CYS:HB3	2:B:119:LEU:HD22	1.49	0.94
4:D:165:TYR:O	4:D:168:VAL:HG23	1.67	0.94
2:N:111:CYS:HB3	2:N:119:LEU:HD22	1.46	0.94
3:O:135:TRP:HH2	3:O:170:VAL:HG12	1.32	0.94
4:P:23:HIS:HA	4:P:26:ILE:HD12	1.49	0.94
1:A:67:THR:CG2	1:A:70:ARG:H	1.81	0.94
1:A:143:THR:HG21	9:I:48:SER:H	1.33	0.94
2:N:248:ASN:HB2	2:N:428:GLY:HA2	1.47	0.94
3:O:206:ASN:HB2	3:O:313:ARG:HH21	1.28	0.94
3:O:252:ASP:HB3	3:O:253:PRO:HD3	1.50	0.94
1:A:403:ASP:HB3	1:A:406:VAL:HG23	1.47	0.94
3:C:174:THR:HG23	3:C:178:PHE:HE1	1.31	0.93
4:P:158:ILE:HD13	4:P:160:MET:HB2	1.49	0.93
3:C:115:ILE:HG21	3:C:196:HIS:HB2	1.48	0.93
2:N:67:HIS:HD2	2:N:144:LEU:HD22	1.30	0.93
2:N:316:TYR:OH	9:U:64:LEU:HD23	1.67	0.93
1:A:61:HIS:CD2	1:A:134:ILE:HD11	2.03	0.93
1:M:61:HIS:NE2	1:M:134:ILE:HD11	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:132:PHE:CD2	2:N:191:LEU:HD13	2.04	0.93
3:O:108:THR:HB	3:O:313:ARG:HH11	1.31	0.93
2:B:159:VAL:HG12	2:B:160:ILE:HD13	1.48	0.93
3:C:310:SER:HB3	3:C:318:ARG:NH1	1.82	0.93
1:A:346:CYS:HB3	1:A:412:SER:OG	1.68	0.93
2:N:51:ILE:HG21	2:N:199:PHE:HA	1.48	0.93
2:N:207:ILE:HD11	2:N:383:GLY:HA2	1.49	0.93
2:B:77:THR:HG22	2:B:130:PRO:CA	1.99	0.92
3:C:179:PHE:HE2	3:O:179:PHE:HE2	1.05	0.92
7:G:9:ARG:NH2	7:G:11:ARG:HD2	1.83	0.92
1:M:61:HIS:CE1	1:M:134:ILE:HD11	2.04	0.92
1:A:69:ASN:O	1:A:71:PRO:HD3	1.70	0.92
1:M:91:THR:HG22	1:M:93:GLU:H	1.32	0.92
2:B:51:ILE:HG21	2:B:199:PHE:HA	1.49	0.92
5:Q:85:LYS:HG2	5:Q:86:ASN:H	1.33	0.92
9:U:72:VAL:HB	9:U:73:PRO:CD	1.98	0.92
1:A:91:THR:HG22	1:A:93:GLU:H	1.35	0.91
5:Q:15:ARG:HH21	5:Q:32:ARG:HG3	1.35	0.91
1:A:144:SER:O	1:A:148:VAL:HG23	1.69	0.91
3:C:240:MET:HA	3:C:243:VAL:HG12	1.49	0.91
3:O:26:ASN:ND2	3:O:207:ASN:HB2	1.85	0.91
1:A:392:LEU:HA	1:A:395:TRP:CD1	2.05	0.91
2:B:162:ASN:HD22	2:B:244:ILE:CG2	1.83	0.91
2:B:258:VAL:HG11	2:B:321:LEU:HB3	1.53	0.91
1:A:224:ASP:OD1	1:A:227:ALA:HB3	1.72	0.90
3:O:122:THR:HG22	3:O:189:ILE:HD11	1.51	0.90
5:Q:15:ARG:NH2	5:Q:32:ARG:HG3	1.87	0.90
4:D:74:PRO:HG2	4:D:82:MET:SD	2.10	0.90
1:M:408:ARG:HH12	11:W:15:ARG:HE	1.20	0.90
3:C:252:ASP:HB3	3:C:253:PRO:HD3	1.52	0.90
3:C:266:PRO:HB3	5:Q:160:CYS:HA	1.54	0.90
1:M:236:PHE:CE2	1:M:258:GLU:HB3	2.07	0.90
1:A:236:PHE:CE2	1:A:258:GLU:HB3	2.07	0.90
3:C:34:GLY:O	3:C:37:LEU:HB2	1.72	0.90
4:D:231:LYS:HD2	6:F:71:ARG:HG2	1.52	0.89
4:P:165:TYR:O	4:P:168:VAL:HG23	1.73	0.89
3:O:221:HIS:HB3	3:O:222:PRO:HD3	1.52	0.89
5:Q:109:GLU:CG	5:Q:167:ALA:HB3	2.01	0.89
2:B:342:ASN:O	2:B:345:LYS:HB2	1.72	0.89
2:B:385:GLN:HG2	9:I:62:ARG:HH12	1.35	0.89
5:Q:15:ARG:HB2	5:Q:16:PRO:CD	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.08	0.89
6:F:47:ILE:O	6:F:50:LEU:HG	1.72	0.89
1:A:417:ASP:OD2	10:J:10:TYR:OH	1.88	0.89
2:B:406:ALA:HB3	2:B:409:ASP:HB2	1.53	0.89
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.54	0.89
2:N:52:LYS:HB2	2:N:203:ARG:HB3	1.54	0.89
1:A:426:GLY:H	1:A:428:ILE:CG1	1.85	0.88
3:O:361:LEU:HD23	3:O:365:LEU:HD12	1.54	0.88
1:A:156:THR:HG23	1:A:239:SER:OG	1.73	0.88
1:A:408:ARG:HH12	11:K:15:ARG:HE	1.22	0.88
4:D:178:THR:OG1	4:D:181:GLN:NE2	2.05	0.88
1:A:408:ARG:NH1	11:K:15:ARG:HE	1.71	0.88
3:C:6:LYS:HE2	3:C:16:ASN:HD21	1.38	0.88
2:N:209:LEU:HD22	2:N:375:SER:HB2	1.56	0.88
3:C:170:VAL:HG13	3:C:174:THR:CG2	2.04	0.88
2:N:304:HIS:CD2	2:N:306:PRO:HD2	2.08	0.88
3:C:179:PHE:CE2	3:O:179:PHE:HE2	1.92	0.88
1:M:45:SER:HB3	1:M:92:ARG:HA	1.53	0.88
7:S:9:ARG:NH2	7:S:11:ARG:HD2	1.87	0.87
3:C:103:TYR:HA	3:C:315:MET:HE3	1.54	0.87
1:M:158:PHE:CE1	1:M:317:THR:HG21	2.08	0.87
8:H:73:LEU:HD23	8:H:74:PHE:N	1.89	0.87
7:S:50:PRO:HB2	7:S:51:PRO:CD	2.03	0.87
7:S:36:ASN:HA	7:S:39:ARG:HD3	1.57	0.87
5:E:15:ARG:HB2	5:E:16:PRO:HD2	1.57	0.86
3:O:108:THR:HB	3:O:313:ARG:NH1	1.89	0.86
1:A:64:PHE:HE1	1:A:86:LEU:HG	1.36	0.86
9:I:72:VAL:CB	9:I:73:PRO:HD3	2.05	0.86
1:M:383:LEU:HD22	1:M:388:ARG:HA	1.54	0.86
2:N:347:ILE:O	2:N:411:ILE:HG23	1.75	0.86
4:P:118:ARG:HG3	4:P:194:ALA:HB1	1.55	0.86
5:Q:118:ARG:HH11	5:Q:171:ILE:CG1	1.88	0.86
1:M:426:GLY:HA3	1:M:428:ILE:HG13	1.55	0.86
1:M:52:ASN:HB2	1:M:55:ALA:HB2	1.58	0.86
3:C:10:LEU:HD12	3:C:13:ILE:HD11	1.55	0.86
2:B:263:ALA:O	2:B:269:ALA:HB2	1.76	0.86
3:O:245:PHE:CD1	4:P:17:LEU:HD13	2.11	0.86
3:O:334:THR:O	3:O:338:ILE:HD13	1.75	0.86
2:N:305:GLN:HB2	2:N:306:PRO:CD	2.05	0.86
5:Q:114:VAL:HA	5:Q:117:LEU:CD1	2.06	0.86
1:A:260:PRO:HD3	1:A:414:TYR:CE1	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:PHE:HE2	3:O:179:PHE:CE2	1.92	0.85
3:C:185:LEU:HB3	3:C:186:PRO:HD3	1.55	0.85
10:J:58:LYS:HG2	10:J:59:TYR:H	1.41	0.85
2:N:123:LEU:O	2:N:127:THR:HG22	1.74	0.85
4:D:176:PRO:HB2	4:D:181:GLN:HE22	1.37	0.85
2:N:385:GLN:HG2	9:U:62:ARG:HH12	1.38	0.85
1:M:408:ARG:NH1	11:W:15:ARG:HE	1.73	0.85
5:Q:187:PHE:CD2	5:Q:193:VAL:HB	2.11	0.85
4:D:70:VAL:HG23	4:D:84:PRO:HD3	1.59	0.85
2:N:341:TYR:HE2	2:N:345:LYS:HE3	1.41	0.85
1:A:213:GLN:HB3	1:A:215:HIS:NE2	1.91	0.85
3:O:30:TRP:O	3:O:33:PHE:HD2	1.59	0.85
1:A:39:VAL:HG12	1:A:41:ILE:HD11	1.59	0.85
5:Q:134:ILE:HD11	5:Q:185:TYR:CG	2.12	0.85
7:S:34:ILE:HB	7:S:35:PRO:HD3	1.58	0.85
1:M:213:GLN:HB3	1:M:215:HIS:NE2	1.91	0.85
2:N:263:ALA:O	2:N:269:ALA:HB2	1.77	0.85
1:A:61:HIS:NE2	1:A:134:ILE:HD11	1.91	0.85
2:N:58:GLU:OE1	2:N:63:LEU:HA	1.77	0.85
5:Q:60:SER:HA	5:Q:63:SER:OG	1.75	0.85
2:B:57:TYR:O	2:B:233:SER:HB2	1.77	0.84
10:J:21:ALA:O	10:J:25:VAL:HG23	1.77	0.84
1:M:428:ILE:CG2	1:M:431:LEU:HD22	2.07	0.84
1:A:426:GLY:HA3	1:A:428:ILE:HG13	1.59	0.84
3:C:213:SER:O	3:C:216:ASP:N	2.10	0.84
1:M:378:ASP:O	1:M:382:SER:HB2	1.77	0.84
1:M:67:THR:HG23	1:M:70:ARG:N	1.92	0.84
7:G:73:ASN:N	7:G:74:PRO:HD2	1.91	0.84
6:R:37:ILE:HG12	6:R:43:VAL:HG21	1.59	0.84
1:M:106:LEU:HD22	1:M:203:LEU:HD22	1.58	0.84
1:A:106:LEU:HD22	1:A:203:LEU:HD22	1.60	0.84
2:B:286:LYS:HD3	2:B:287:ARG:NH1	1.92	0.84
5:E:15:ARG:CB	5:E:16:PRO:HD2	2.08	0.84
6:R:75:LEU:HD12	6:R:76:PRO:HD2	1.57	0.84
1:A:21:ASN:HB3	1:A:217:SER:CB	2.07	0.84
1:A:408:ARG:HH22	11:K:15:ARG:CZ	1.90	0.84
1:M:32:GLN:CG	1:M:33:PRO:HD2	2.08	0.83
1:M:40:TRP:CZ2	1:M:377:GLU:HA	2.13	0.83
2:B:213:HIS:N	2:B:214:PRO:HD2	1.91	0.83
2:B:198:HIS:HE1	2:B:233:SER:HB3	1.42	0.83
3:C:119:LEU:HG	12:C:381:HEM:CBB	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:70:LEU:CD2	9:I:73:PRO:HD2	2.07	0.83
1:A:84:ALA:HB2	1:A:101:ALA:HB2	1.59	0.83
2:B:198:HIS:CE1	2:B:233:SER:HB3	2.14	0.83
6:F:51:PRO:HD3	2:N:134:ARG:NH1	1.93	0.83
1:A:308:GLN:HG3	1:A:308:GLN:O	1.77	0.83
3:O:26:ASN:HD21	3:O:207:ASN:CB	1.90	0.83
3:O:234:LEU:HD23	4:P:216:LEU:HD21	1.59	0.83
5:Q:76:ILE:HG23	5:Q:194:ILE:HG12	1.60	0.83
10:J:18:SER:OG	11:K:23:LEU:HB2	1.77	0.83
1:M:445:ARG:O	1:M:446:PHE:HB2	1.79	0.83
1:M:67:THR:HG22	1:M:70:ARG:HB2	1.61	0.83
3:C:47:THR:HG21	3:C:83:HIS:HB2	1.61	0.82
3:O:234:LEU:CD2	4:P:216:LEU:HD21	2.08	0.82
1:A:145:MET:SD	1:A:248:LEU:HD12	2.18	0.82
4:D:178:THR:HB	4:D:181:GLN:HG3	1.60	0.82
1:A:241:ILE:HG13	7:G:16:TYR:CE1	2.15	0.82
1:M:383:LEU:HA	1:M:387:GLY:O	1.79	0.82
2:N:126:VAL:O	2:N:130:PRO:HG3	1.78	0.82
2:N:279:LEU:HB3	2:N:295:LEU:HD22	1.60	0.82
3:C:115:ILE:CG2	3:C:196:HIS:HB2	2.08	0.82
1:M:408:ARG:HH22	11:W:15:ARG:CZ	1.91	0.82
4:D:17:LEU:O	4:D:202:LYS:HD3	1.78	0.82
7:G:30:PHE:O	7:G:34:ILE:HG13	1.78	0.82
2:B:185:LYS:O	2:B:185:LYS:HG3	1.79	0.82
5:Q:91:TRP:HB3	5:Q:96:LEU:HB2	1.62	0.82
7:S:50:PRO:CB	7:S:51:PRO:HD3	2.09	0.82
7:S:72:LYS:CB	7:S:75:ALA:HB2	2.09	0.82
2:B:42:ALA:HB1	2:B:43:PRO:HD2	1.62	0.82
4:D:220:TYR:CE2	7:G:26:PHE:HE1	1.97	0.82
3:O:297:SER:O	3:O:300:ILE:HG22	1.79	0.82
4:P:41:HIS:CD2	4:P:113:LEU:HD11	2.15	0.82
6:F:6:VAL:HB	6:F:10:SER:HB2	1.60	0.82
2:B:207:ILE:HD11	2:B:383:GLY:HA2	1.62	0.82
1:A:53:ASN:OD1	1:A:165:GLN:HB2	1.80	0.81
3:C:27:ILE:HG22	3:C:27:ILE:O	1.79	0.81
3:C:341:GLN:HB3	3:C:347:TYR:CD2	2.15	0.81
4:P:176:PRO:HB2	4:P:181:GLN:HE22	1.44	0.81
5:Q:118:ARG:NH1	5:Q:171:ILE:HG13	1.95	0.81
2:B:394:PRO:O	2:B:398:VAL:HG23	1.80	0.81
4:P:10:TYR:HE1	8:T:73:LEU:HD21	1.46	0.81
1:M:224:ASP:OD1	1:M:227:ALA:HB3	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:106:SER:O	3:O:109:PHE:HD2	1.63	0.81
3:O:218:ILE:CG2	3:O:223:TYR:CD2	2.63	0.81
1:A:426:GLY:CA	1:A:428:ILE:CG1	2.59	0.81
2:N:331:ALA:HA	2:N:432:HIS:ND1	1.96	0.81
1:A:102:LEU:HB2	1:A:105:ASP:OD2	1.81	0.81
2:N:200:THR:CG2	2:N:203:ARG:HD2	2.10	0.81
2:N:56:ARG:NH2	2:N:318:ASP:OD1	2.12	0.81
5:Q:99:ARG:HD3	5:Q:156:TYR:OH	1.80	0.81
6:R:33:ARG:NH2	6:R:91:GLU:OE2	2.14	0.81
1:A:46:ARG:HH22	1:A:316:ASP:CG	1.83	0.81
8:T:21:ARG:HB3	8:T:65:ARG:NH2	1.95	0.81
3:C:51:LEU:HD21	3:C:79:ILE:HG22	1.63	0.81
7:S:9:ARG:HH21	7:S:11:ARG:HD2	1.44	0.81
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.63	0.81
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.61	0.81
12:O:380:HEM:HMC1	12:O:380:HEM:HBC2	1.61	0.81
10:J:58:LYS:HG2	10:J:59:TYR:N	1.96	0.81
3:O:185:LEU:HB3	3:O:186:PRO:HD3	1.61	0.81
1:A:155:ALA:HA	1:A:164:ALA:HB1	1.63	0.81
9:I:78:TYR:HD1	9:I:78:TYR:OXT	1.63	0.81
3:C:111:GLU:O	3:C:115:ILE:HD13	1.82	0.80
3:C:33:PHE:CE1	3:C:96:MET:HG3	2.16	0.80
4:P:220:TYR:CE2	7:S:26:PHE:HE1	1.98	0.80
1:A:379:ILE:HD12	1:A:390:ILE:HD12	1.62	0.80
3:C:169:SER:HB2	5:Q:93:GLY:HA3	1.64	0.80
1:A:426:GLY:N	1:A:428:ILE:CG1	2.45	0.80
2:B:305:GLN:HB2	2:B:306:PRO:CD	2.11	0.80
10:V:3:PRO:HG2	10:V:8:ARG:HG2	1.63	0.80
5:E:41:ALA:O	5:E:45:VAL:HG23	1.81	0.80
1:M:297:ILE:HG22	1:M:303:LEU:HD12	1.64	0.80
4:P:10:TYR:HE1	8:T:73:LEU:CD2	1.94	0.80
1:A:18:GLN:NE2	1:A:22:GLY:HA2	1.94	0.80
3:C:51:LEU:HD11	3:C:80:ARG:HA	1.62	0.80
4:D:50:HIS:HB3	4:D:54:VAL:HB	1.62	0.80
1:M:182:LEU:O	1:M:186:LEU:HD12	1.82	0.80
3:O:126:THR:OG1	3:O:185:LEU:HD23	1.82	0.80
4:P:220:TYR:HE2	7:S:26:PHE:HE1	1.29	0.80
3:C:218:ILE:CG2	3:C:223:TYR:CD2	2.65	0.80
10:V:58:LYS:HG2	10:V:59:TYR:N	1.97	0.80
4:D:3:LEU:HD11	7:G:71:ARG:HB2	1.64	0.80
3:O:102:LEU:HD21	3:O:304:ILE:CD1	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:50:THR:HG22	8:T:52:GLU:H	1.47	0.80
3:C:266:PRO:HA	5:Q:160:CYS:SG	2.21	0.80
3:O:135:TRP:CH2	3:O:170:VAL:HG12	2.17	0.80
4:P:50:HIS:HB3	4:P:54:VAL:HB	1.64	0.80
7:G:44:CYS:SG	7:G:48:VAL:HG21	2.22	0.79
1:A:42:ASP:HB3	1:A:384:LEU:HD22	1.62	0.79
2:B:169:ARG:NH2	2:N:438:GLU:OE2	2.14	0.79
2:N:24:LEU:H	2:N:24:LEU:HD12	1.47	0.79
3:C:310:SER:HB3	3:C:318:ARG:HH11	1.47	0.79
2:N:159:VAL:HG12	2:N:160:ILE:HD13	1.65	0.79
1:A:408:ARG:NH2	11:K:15:ARG:NE	2.28	0.79
2:B:209:LEU:HD22	2:B:375:SER:HB2	1.64	0.79
4:D:10:TYR:CZ	4:D:128:PHE:HE2	2.01	0.79
5:E:31:ALA:HB2	10:J:7:ALA:HB2	1.63	0.79
2:N:68:LEU:HD23	2:N:186:VAL:CG1	2.12	0.79
2:B:101:THR:HG23	2:B:104:ASN:H	1.48	0.79
3:C:106:SER:O	3:C:109:PHE:HD1	1.66	0.79
3:C:3:ASN:N	3:C:8:HIS:NE2	2.30	0.79
2:N:261:SER:OG	2:N:320:GLY:HA3	1.83	0.79
2:B:438:GLU:OE2	2:N:169:ARG:NH2	2.16	0.79
3:C:5:ARG:O	3:C:9:PRO:HD2	1.82	0.79
1:M:75:LEU:O	1:M:79:VAL:HG23	1.82	0.79
2:N:309:VAL:HG22	2:N:326:THR:HA	1.63	0.79
8:T:73:LEU:HD23	8:T:74:PHE:N	1.98	0.79
1:A:39:VAL:HG12	1:A:41:ILE:CD1	2.13	0.79
4:D:74:PRO:CB	4:D:79:GLU:HB2	2.13	0.79
1:A:86:LEU:HD13	1:A:99:ILE:HG12	1.64	0.79
4:D:220:TYR:HE2	7:G:26:PHE:HE1	1.31	0.79
3:C:264:THR:HG21	5:Q:144:CYS:CB	2.13	0.79
2:B:362:ASN:HA	2:B:365:LYS:HD3	1.65	0.79
7:G:31:SER:O	7:G:35:PRO:HD2	1.83	0.78
1:M:335:MET:HE2	1:M:339:GLN:HG3	1.63	0.78
6:R:51:PRO:HG2	6:R:54:LEU:CD2	2.12	0.78
1:M:39:VAL:HG12	1:M:41:ILE:HD11	1.65	0.78
4:P:178:THR:OG1	4:P:181:GLN:NE2	2.14	0.78
8:H:21:ARG:HB3	8:H:65:ARG:HH21	1.45	0.78
1:M:408:ARG:NH2	11:W:15:ARG:NE	2.30	0.78
1:M:260:PRO:HD3	1:M:414:TYR:CE1	2.17	0.78
3:O:1:MET:SD	3:O:7:SER:HB2	2.23	0.78
3:O:246:ALA:HB1	3:O:249:LEU:HB2	1.65	0.78
2:N:286:LYS:HD3	2:N:287:ARG:NH1	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ASN:HB3	1:A:217:SER:OG	1.84	0.78
2:B:347:ILE:O	2:B:411:ILE:HG23	1.83	0.78
4:P:115:TYR:HD1	4:P:119:ALA:HB2	1.47	0.78
4:P:198:HIS:NE2	4:P:202:LYS:NZ	2.31	0.78
1:M:262:TRP:CD2	1:M:385:THR:HG23	2.18	0.78
4:P:10:TYR:CZ	4:P:128:PHE:HE2	2.01	0.78
1:M:21:ASN:HB3	1:M:217:SER:CB	2.13	0.78
10:V:58:LYS:HG2	10:V:59:TYR:H	1.48	0.78
1:A:146:ARG:NH2	1:A:308:GLN:HE22	1.82	0.78
1:A:428:ILE:HG22	1:A:431:LEU:CB	2.12	0.78
2:N:29:LEU:HB3	2:N:30:PRO:CD	2.14	0.78
4:P:27:ARG:HH12	10:V:58:LYS:HG3	1.46	0.78
2:B:248:ASN:HB2	2:B:428:GLY:HA2	1.63	0.77
4:P:138:PRO:HG2	8:T:55:THR:OG1	1.82	0.77
7:G:9:ARG:HH21	7:G:11:ARG:HD2	1.49	0.77
4:D:228:SER:HB2	7:G:23:GLN:NE2	1.97	0.77
9:U:64:LEU:HG	9:U:65:VAL:HG23	1.65	0.77
6:F:28:LYS:CD	6:F:74:ILE:HD11	2.14	0.77
2:N:308:ASP:OD1	2:N:309:VAL:N	2.17	0.77
1:A:46:ARG:NH2	1:A:316:ASP:OD2	2.17	0.77
2:N:297:GLN:HA	2:N:297:GLN:OE1	1.83	0.77
1:M:92:ARG:HD2	1:M:163:LEU:HD12	1.65	0.77
1:A:386:TYR:H	1:A:386:TYR:HD1	1.32	0.77
5:Q:65:SER:OG	5:Q:67:ASP:HB3	1.85	0.77
4:P:181:GLN:HA	8:T:77:LEU:HD13	1.67	0.77
2:B:59:ASN:O	2:B:63:LEU:HG	1.84	0.77
3:O:129:MET:HG2	3:O:178:PHE:HD1	1.49	0.77
3:O:341:GLN:HB3	3:O:347:TYR:CD2	2.19	0.77
5:Q:114:VAL:CA	5:Q:117:LEU:HD12	2.12	0.77
1:A:45:SER:HB3	1:A:92:ARG:HA	1.66	0.77
2:B:297:GLN:OE1	2:B:297:GLN:HA	1.82	0.77
3:C:280:ILE:HD11	3:C:335:LEU:HD13	1.64	0.77
3:O:309:THR:CG2	3:O:370:GLY:HA3	2.14	0.77
1:A:249:PRO:O	1:A:250:LEU:HD23	1.85	0.77
4:D:14:HIS:HA	4:D:19:SER:HB3	1.66	0.77
2:N:341:TYR:CE2	2:N:345:LYS:HE3	2.19	0.77
2:B:331:ALA:HA	2:B:432:HIS:ND1	2.00	0.76
2:B:385:GLN:CG	9:I:62:ARG:HH12	1.96	0.76
4:D:182:VAL:O	4:D:186:VAL:HG23	1.84	0.76
1:M:331:ILE:HD11	1:M:427:PRO:O	1.85	0.76
3:O:3:ASN:N	3:O:8:HIS:NE2	2.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:28:LYS:CD	6:R:74:ILE:HD11	2.15	0.76
6:R:50:LEU:HB2	6:R:55:TYR:HB2	1.67	0.76
10:J:51:LEU:HD22	10:J:52:TRP:HZ3	1.50	0.76
1:M:102:LEU:HB2	1:M:105:ASP:OD2	1.85	0.76
2:N:200:THR:HG22	2:N:203:ARG:CD	2.15	0.76
3:O:170:VAL:HG13	3:O:174:THR:HG21	1.66	0.76
3:O:310:SER:OG	3:O:318:ARG:NH1	2.18	0.76
4:P:55:CYS:SG	10:V:52:TRP:HB2	2.25	0.76
6:R:73:GLN:NE2	7:S:32:LYS:NZ	2.33	0.76
2:N:49:LEU:HD11	2:N:204:MET:SD	2.26	0.76
3:C:26:ASN:ND2	3:C:207:ASN:HB2	1.99	0.76
3:C:310:SER:CB	3:C:318:ARG:HH11	1.99	0.76
1:M:386:TYR:HD1	1:M:386:TYR:H	1.33	0.76
3:O:177:ARG:O	3:O:181:PHE:HD2	1.69	0.76
3:C:187:PHE:CZ	3:O:184:ILE:HG13	2.20	0.76
4:D:229:VAL:HG12	4:D:233:ARG:HE	1.49	0.76
3:C:9:PRO:HG2	3:C:12:LYS:HB2	1.68	0.76
2:N:213:HIS:N	2:N:214:PRO:HD2	2.01	0.76
2:N:304:HIS:HD2	2:N:306:PRO:HD2	1.51	0.76
5:Q:157:TYR:HE2	5:Q:159:PRO:HA	1.51	0.76
5:Q:153:PHE:HE1	5:Q:173:LYS:HG3	1.50	0.76
3:C:338:ILE:N	3:C:338:ILE:HD12	1.99	0.76
3:C:47:THR:CG2	3:C:83:HIS:HB2	2.16	0.76
5:E:55:VAL:O	5:E:59:VAL:HG23	1.85	0.76
1:M:41:ILE:H	1:M:41:ILE:HD12	1.50	0.76
3:C:108:THR:HB	3:C:313:ARG:NH1	2.00	0.76
1:A:92:ARG:HD2	1:A:163:LEU:HD12	1.67	0.75
2:B:129:ALA:N	2:B:130:PRO:HD2	2.01	0.75
2:N:257:LEU:HD13	2:N:424:MET:HB2	1.68	0.75
2:N:314:ALA:CB	9:U:64:LEU:HD22	2.16	0.75
3:O:47:THR:CG2	3:O:83:HIS:HB2	2.16	0.75
4:P:143:LEU:HD22	4:P:147:LEU:O	1.86	0.75
5:Q:171:ILE:CD1	5:Q:176:ALA:HB3	2.16	0.75
7:S:15:THR:HG22	7:S:16:TYR:N	1.97	0.75
1:A:27:SER:HA	1:A:199:ALA:O	1.86	0.75
2:B:429:ASN:ND2	2:N:60:SER:HB3	1.98	0.75
5:Q:157:TYR:OH	5:Q:162:GLY:HA2	1.84	0.75
2:N:68:LEU:HD23	2:N:186:VAL:HG12	1.69	0.75
3:C:345:HIS:HB3	3:C:346:PRO:CD	2.17	0.75
9:U:72:VAL:CB	9:U:73:PRO:HD3	2.15	0.75
2:B:337:ILE:HG21	2:B:434:PRO:HG2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:127:VAL:HG12	4:D:187:CYS:SG	2.26	0.75
4:D:5:LEU:HB3	4:D:152:TYR:CD1	2.22	0.75
5:Q:118:ARG:HH11	5:Q:171:ILE:HG13	1.50	0.75
2:B:67:HIS:CD2	2:B:144:LEU:HD22	2.18	0.75
2:B:77:THR:CG2	2:B:130:PRO:HA	2.13	0.75
2:B:141:GLN:HB2	2:B:142:PRO:HD3	1.69	0.75
3:C:7:SER:HA	3:C:13:ILE:HG12	1.69	0.75
3:C:361:LEU:HD23	3:C:365:LEU:HD12	1.69	0.75
3:O:244:LEU:HD11	4:P:204:MET:HE2	1.67	0.75
1:A:236:PHE:HD2	1:A:258:GLU:HG2	1.52	0.74
2:B:207:ILE:HD12	2:B:382:VAL:HG12	1.69	0.74
5:Q:134:ILE:HD11	5:Q:185:TYR:CE2	2.21	0.74
2:B:148:LYS:HE2	2:B:180:ASP:OD1	1.85	0.74
2:N:217:LYS:HZ2	2:N:221:GLU:CD	1.91	0.74
3:C:210:GLY:HA3	3:C:314:SER:HB2	1.68	0.74
6:F:94:LEU:O	6:F:98:ILE:HG13	1.86	0.74
5:Q:77:LYS:HG3	5:Q:89:PHE:CE2	2.22	0.74
2:B:304:HIS:HD2	2:B:306:PRO:HD2	1.47	0.74
1:M:363:ASN:OD1	2:N:112:LEU:HD23	1.88	0.74
2:N:237:ALA:HB2	2:N:318:ASP:OD2	1.87	0.74
1:M:408:ARG:HH12	11:W:15:ARG:NE	1.85	0.74
2:B:328:SER:HB3	2:B:336:VAL:HG21	1.69	0.74
2:B:352:LEU:HB3	2:B:411:ILE:HD11	1.70	0.74
3:O:22:PRO:HG2	7:S:3:GLN:HB3	1.69	0.74
3:C:126:THR:OG1	3:C:185:LEU:HD23	1.87	0.74
6:F:28:LYS:HB3	6:F:74:ILE:HD11	1.69	0.74
8:H:15:ASP:N	8:H:16:PRO:HD2	2.03	0.74
4:D:11:PRO:O	8:H:74:PHE:CE2	2.41	0.74
1:M:18:GLN:NE2	1:M:22:GLY:HA2	2.01	0.74
1:M:32:GLN:HG3	1:M:33:PRO:HD2	1.67	0.74
1:M:53:ASN:OD1	1:M:165:GLN:HB2	1.87	0.74
1:A:236:PHE:CD2	1:A:258:GLU:HG2	2.22	0.74
1:A:75:LEU:O	1:A:79:VAL:HG23	1.88	0.74
5:Q:98:VAL:HA	5:Q:134:ILE:HG22	1.70	0.74
1:A:163:LEU:HD12	1:A:163:LEU:O	1.88	0.74
3:C:275:LEU:O	3:C:276:PHE:C	2.23	0.74
1:A:292:SER:O	1:A:295:ALA:HB3	1.88	0.74
1:A:72:GLY:O	1:A:73:ASN:OD1	2.04	0.74
3:O:206:ASN:CB	3:O:313:ARG:HH21	1.99	0.74
1:A:316:ASP:N	1:A:316:ASP:OD1	2.21	0.74
2:B:182:ARG:NH1	2:B:185:LYS:HG2	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:TRP:O	3:C:33:PHE:HD2	1.71	0.74
1:M:39:VAL:HG23	1:M:113:LEU:HD23	1.68	0.74
1:M:236:PHE:HE2	1:M:258:GLU:HB3	1.51	0.74
2:N:34:VAL:HG11	2:N:386:ALA:HB1	1.70	0.74
5:Q:55:VAL:O	5:Q:59:VAL:HG23	1.88	0.74
1:A:236:PHE:HE2	1:A:258:GLU:HB3	1.50	0.73
2:B:395:PRO:O	2:B:398:VAL:HB	1.88	0.73
1:M:24:ARG:CB	1:M:196:VAL:HG22	2.14	0.73
2:N:59:ASN:O	2:N:63:LEU:HG	1.87	0.73
3:O:122:THR:CG2	3:O:189:ILE:HD11	2.17	0.73
3:O:309:THR:HG21	3:O:370:GLY:HA3	1.70	0.73
1:A:171:SER:OG	1:A:172:GLU:N	2.19	0.73
3:C:26:ASN:HD21	3:C:207:ASN:CB	2.01	0.73
3:O:90:PHE:CE1	3:O:123:VAL:HG21	2.23	0.73
3:O:310:SER:CB	3:O:318:ARG:HH11	2.00	0.73
7:G:72:LYS:CB	7:G:75:ALA:HB2	2.09	0.73
2:N:385:GLN:CG	9:U:62:ARG:HH12	2.00	0.73
3:O:51:LEU:HD11	3:O:80:ARG:HA	1.69	0.73
1:A:274:ASN:HB3	1:A:309:THR:OG1	1.89	0.73
2:B:279:LEU:CD2	2:B:295:LEU:HD13	2.19	0.73
2:B:347:ILE:H	2:B:347:ILE:HD12	1.54	0.73
3:C:206:ASN:ND2	3:C:207:ASN:H	1.85	0.73
1:A:100:LYS:NZ	1:A:373:THR:OG1	2.18	0.73
1:A:84:ALA:CB	1:A:101:ALA:HB2	2.18	0.73
3:O:147:THR:HG21	3:O:165:TRP:NE1	2.03	0.73
3:O:184:ILE:O	3:O:188:ILE:HD12	1.88	0.73
2:N:95:LYS:HE3	9:U:70:LEU:HD22	1.70	0.73
5:Q:118:ARG:HD2	5:Q:171:ILE:HG12	1.70	0.73
1:M:426:GLY:N	1:M:428:ILE:HG13	2.03	0.73
4:P:10:TYR:CE1	8:T:73:LEU:HD21	2.23	0.73
5:Q:134:ILE:O	5:Q:135:LEU:HD23	1.89	0.73
2:B:251:SER:OG	2:B:252:LEU:N	2.22	0.72
2:B:283:PRO:HG3	9:I:55:LEU:CD2	2.18	0.72
2:B:56:ARG:NH2	2:B:318:ASP:OD1	2.22	0.72
3:C:169:SER:OG	3:C:170:VAL:N	2.18	0.72
3:C:252:ASP:HB3	3:C:253:PRO:CD	2.18	0.72
6:F:33:ARG:NH2	6:F:91:GLU:OE2	2.22	0.72
3:O:361:LEU:CD2	3:O:365:LEU:HD12	2.18	0.72
4:D:27:ARG:HH12	10:J:58:LYS:HG3	1.55	0.72
1:A:408:ARG:HH12	11:K:15:ARG:CG	2.02	0.72
5:Q:121:GLN:HB2	5:Q:170:ARG:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:ILE:HG13	3:O:187:PHE:CZ	2.23	0.72
4:D:41:HIS:CD2	4:D:113:LEU:HD11	2.24	0.72
1:A:408:ARG:HH12	11:K:15:ARG:NE	1.85	0.72
9:U:70:LEU:CD2	9:U:73:PRO:HD2	2.17	0.72
4:D:224:ARG:CB	7:G:25:ALA:HB1	2.14	0.72
3:O:280:ILE:HD13	3:O:335:LEU:HD22	1.72	0.72
1:A:273:ALA:HA	1:A:276:ILE:HD12	1.71	0.72
4:D:7:PRO:HG3	4:D:126:TYR:HA	1.71	0.72
9:I:78:TYR:OXT	9:I:78:TYR:CD1	2.43	0.72
2:N:305:GLN:CB	2:N:306:PRO:HD3	2.15	0.72
4:P:164:ILE:HD13	4:P:182:VAL:HG12	1.70	0.72
5:Q:15:ARG:CB	5:Q:16:PRO:HD2	2.06	0.72
1:A:41:ILE:H	1:A:41:ILE:HD12	1.54	0.72
1:M:8:LEU:O	1:M:11:VAL:HG23	1.90	0.72
1:M:262:TRP:CG	1:M:385:THR:HG23	2.24	0.72
1:A:41:ILE:HG13	1:A:195:MET:HE3	1.70	0.72
1:A:383:LEU:HA	1:A:387:GLY:O	1.88	0.72
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.20	0.72
3:C:110:LEU:HG	3:C:114:ASN:HD21	1.55	0.72
3:C:280:ILE:CD1	3:C:335:LEU:HD13	2.19	0.72
4:D:150:ASN:OD1	4:D:151:PRO:HD2	1.90	0.72
1:M:256:ALA:HA	1:M:320:LEU:O	1.89	0.72
5:E:19:LEU:HD12	5:E:19:LEU:O	1.90	0.72
9:I:70:LEU:HD12	9:I:71:ASN:N	2.04	0.72
1:A:408:ARG:CZ	11:K:15:ARG:HE	2.01	0.72
2:B:162:ASN:HD22	2:B:244:ILE:HG21	1.51	0.72
1:M:67:THR:CG2	1:M:70:ARG:HB2	2.20	0.72
5:Q:188:THR:N	5:Q:192:MET:O	2.21	0.72
2:B:162:ASN:O	2:B:244:ILE:HD12	1.89	0.71
1:M:329:MET:SD	7:S:5:GLY:HA3	2.31	0.71
7:S:15:THR:CG2	7:S:16:TYR:N	2.51	0.71
2:N:314:ALA:HB2	9:U:64:LEU:HD22	1.70	0.71
1:A:39:VAL:HG11	1:A:117:VAL:HG21	1.73	0.71
1:M:99:ILE:HG13	1:M:113:LEU:HD13	1.69	0.71
1:M:426:GLY:CA	1:M:428:ILE:CG1	2.64	0.71
3:C:122:THR:HG22	3:C:189:ILE:HD11	1.72	0.71
3:C:297:SER:O	3:C:300:ILE:HG22	1.90	0.71
12:C:380:HEM:HBC2	12:C:380:HEM:HMC1	1.73	0.71
10:J:49:GLY:HA2	10:J:54:HIS:CB	2.20	0.71
1:A:262:TRP:CD2	1:A:385:THR:HG23	2.24	0.71
2:N:67:HIS:CD2	2:N:144:LEU:HD22	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:46:ARG:HH12	2:N:376:GLU:HG3	1.55	0.71
2:N:24:LEU:CG	2:N:38:LEU:HD11	2.19	0.71
3:C:177:ARG:NH2	5:Q:62:MET:O	2.23	0.71
4:D:10:TYR:HE1	8:H:73:LEU:CD2	2.03	0.71
1:M:274:ASN:HB3	1:M:309:THR:OG1	1.91	0.71
2:N:277:HIS:NE2	2:N:364:LEU:HD13	2.05	0.71
5:Q:139:CYS:HB2	5:Q:165:TYR:HE2	1.54	0.71
11:W:18:VAL:HB	11:W:19:PRO:HD3	1.71	0.71
2:N:182:ARG:NH1	2:N:185:LYS:HG2	2.05	0.71
2:B:78:LYS:HB3	2:B:129:ALA:HB1	1.70	0.71
3:O:47:THR:HG21	3:O:83:HIS:HB2	1.73	0.71
4:P:74:PRO:CB	4:P:79:GLU:HB2	2.20	0.71
4:P:83:ARG:CB	4:P:84:PRO:CD	2.63	0.71
1:A:21:ASN:HB3	1:A:217:SER:HB3	1.73	0.71
2:B:384:SER:HB2	9:I:62:ARG:HG2	1.71	0.71
5:Q:121:GLN:O	5:Q:170:ARG:NH1	2.18	0.71
4:D:43:MET:HG2	4:D:46:VAL:HG23	1.70	0.71
5:E:15:ARG:HB2	5:E:16:PRO:CD	2.21	0.71
2:N:78:LYS:HB3	2:N:129:ALA:HB1	1.73	0.71
3:O:5:ARG:O	3:O:9:PRO:HD2	1.90	0.71
4:P:7:PRO:HG3	4:P:126:TYR:HA	1.73	0.71
4:P:74:PRO:HG2	4:P:82:MET:SD	2.30	0.71
1:A:233:PRO:HG2	5:E:23:LYS:CD	2.20	0.70
3:C:156:ILE:HG12	3:C:157:GLY:H	1.56	0.70
2:N:338:LYS:HG2	2:N:439:LEU:HD21	1.73	0.70
6:R:73:GLN:HE21	7:S:32:LYS:NZ	1.89	0.70
2:B:300:ALA:HA	2:B:307:PHE:CZ	2.26	0.70
4:D:102:ARG:HA	4:D:108:ALA:O	1.91	0.70
1:M:403:ASP:CB	1:M:406:VAL:HG23	2.19	0.70
1:M:45:SER:OG	1:M:92:ARG:HG3	1.91	0.70
4:D:94:PRO:HB2	4:D:95:TYR:CD1	2.27	0.70
5:E:13:TYR:O	7:G:23:GLN:HB3	1.91	0.70
3:O:27:ILE:O	3:O:27:ILE:HG22	1.92	0.70
5:Q:118:ARG:HH11	5:Q:171:ILE:HG12	1.55	0.70
1:A:60:GLU:OE2	1:A:88:ALA:O	2.09	0.70
1:M:255:ILE:HG13	1:M:422:VAL:HG22	1.71	0.70
2:N:100:SER:HB3	2:N:105:MET:HG3	1.74	0.70
2:B:140:LEU:O	2:B:141:GLN:C	2.30	0.70
3:C:18:PHE:O	3:C:220:PHE:CD2	2.44	0.70
1:M:365:LEU:HD21	1:M:395:TRP:CD1	2.27	0.70
2:N:165:ALA:HA	2:N:173:ALA:HB1	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:68:LEU:HD11	2:N:140:LEU:HD23	1.71	0.70
2:B:237:ALA:HB2	2:B:318:ASP:OD2	1.92	0.70
2:N:51:ILE:HD13	2:N:199:PHE:CG	2.26	0.70
4:P:11:PRO:O	8:T:74:PHE:CE2	2.45	0.70
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.74	0.70
3:C:147:THR:HG21	3:C:165:TRP:NE1	2.06	0.70
4:D:82:MET:SD	4:D:86:LYS:HD2	2.32	0.70
2:B:162:ASN:ND2	2:B:244:ILE:HG21	2.06	0.70
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.07	0.70
4:D:51:LEU:HA	4:D:56:TYR:O	1.91	0.70
3:O:237:LEU:HD13	4:P:212:MET:HG2	1.73	0.70
4:D:54:VAL:O	4:D:54:VAL:HG12	1.89	0.70
1:M:351:GLU:OE2	1:M:403:ASP:OD1	2.10	0.70
3:O:218:ILE:HD13	4:P:230:LEU:CD1	2.22	0.70
5:Q:185:TYR:HB3	5:Q:195:VAL:HG13	1.74	0.70
6:R:59:VAL:HG11	7:S:10:VAL:HG22	1.73	0.70
1:A:32:GLN:CG	1:A:33:PRO:HD2	2.22	0.70
3:O:100:ARG:NH2	12:O:381:HEM:HBD1	2.04	0.70
3:C:174:THR:CG2	3:C:178:PHE:HE1	2.03	0.69
1:M:21:ASN:CB	1:M:217:SER:HB3	2.22	0.69
3:O:129:MET:HG2	3:O:178:PHE:CD1	2.27	0.69
3:O:225:THR:O	3:O:229:ILE:HD12	1.92	0.69
5:Q:158:CYS:SG	5:Q:158:CYS:O	2.50	0.69
3:C:100:ARG:NH2	12:C:381:HEM:HBD1	2.05	0.69
7:G:34:ILE:CB	7:G:35:PRO:HD3	2.18	0.69
1:M:278:GLY:O	1:M:309:THR:HG23	1.93	0.69
4:P:158:ILE:HD11	4:P:160:MET:HB2	1.73	0.69
1:M:236:PHE:CD2	1:M:258:GLU:HG2	2.28	0.69
4:P:97:ASN:OD1	4:P:98:PRO:HD2	1.93	0.69
3:C:135:TRP:HH2	3:C:170:VAL:HG12	1.57	0.69
3:C:234:LEU:HD23	4:D:216:LEU:HD21	1.74	0.69
4:D:165:TYR:CZ	4:D:168:VAL:HG22	2.27	0.69
6:F:51:PRO:HD3	2:N:134:ARG:HH12	1.57	0.69
1:M:5:ALA:O	1:M:8:LEU:HB2	1.93	0.69
2:N:352:LEU:HB3	2:N:411:ILE:HD11	1.73	0.69
1:A:379:ILE:HD12	1:A:390:ILE:CD1	2.22	0.69
2:B:247:GLN:HE22	2:B:429:ASN:ND2	1.91	0.69
4:D:176:PRO:HB2	4:D:181:GLN:NE2	2.06	0.69
4:D:50:HIS:HB3	4:D:54:VAL:CB	2.22	0.69
3:C:79:ILE:HG12	5:E:58:PHE:HE1	1.57	0.69
1:M:426:GLY:HA2	1:M:428:ILE:HG13	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:212:SER:OG	2:N:215:VAL:HB	1.92	0.69
3:O:15:ASN:ND2	3:O:18:PHE:CE2	2.60	0.69
1:M:145:MET:SD	1:M:248:LEU:HD12	2.32	0.69
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.73	0.69
1:A:351:GLU:OE2	1:A:403:ASP:OD1	2.10	0.69
2:N:47:ILE:HG22	2:N:48:GLY:N	2.08	0.69
3:O:103:TYR:O	3:O:315:MET:HB2	1.93	0.69
5:Q:68:VAL:HG12	5:Q:69:LEU:N	2.08	0.69
1:A:341:GLN:OE1	1:A:344:ARG:NH1	2.25	0.69
1:A:426:GLY:HA2	1:A:428:ILE:N	2.08	0.69
2:B:129:ALA:N	2:B:130:PRO:CD	2.55	0.69
1:M:316:ASP:OD1	1:M:316:ASP:N	2.24	0.69
2:N:258:VAL:HG11	2:N:321:LEU:HB3	1.74	0.69
4:P:102:ARG:HA	4:P:108:ALA:O	1.92	0.69
4:P:5:LEU:HB3	4:P:152:TYR:CD1	2.28	0.69
1:M:304:CYS:HB3	1:M:334:MET:SD	2.33	0.69
3:O:252:ASP:HB3	3:O:253:PRO:CD	2.23	0.69
4:P:220:TYR:CE2	7:S:26:PHE:CE1	2.81	0.69
2:B:83:PHE:CE2	2:B:87:ARG:HG3	2.27	0.69
1:A:67:THR:HG22	1:A:70:ARG:HB2	1.75	0.69
2:B:34:VAL:HG11	2:B:386:ALA:HB1	1.74	0.69
3:C:132:VAL:HA	3:C:139:SER:HB3	1.74	0.69
7:G:73:ASN:N	7:G:74:PRO:CD	2.55	0.69
2:B:46:ARG:HH12	2:B:376:GLU:HG3	1.57	0.68
4:P:27:ARG:NH1	10:V:58:LYS:NZ	2.41	0.68
2:B:62:ASN:ND2	2:B:65:THR:OG1	2.26	0.68
3:C:310:SER:HA	3:C:374:ASN:ND2	1.97	0.68
3:C:244:LEU:HD23	4:D:205:GLY:HA2	1.76	0.68
4:D:97:ASN:OD1	4:D:98:PRO:HD2	1.92	0.68
4:P:10:TYR:CE1	8:T:73:LEU:CD2	2.75	0.68
9:I:53:GLU:O	9:I:55:LEU:HG	1.94	0.68
2:N:319:SER:OG	2:N:320:GLY:N	2.26	0.68
5:Q:114:VAL:HG12	5:Q:115:SER:N	2.08	0.68
1:A:162:PRO:O	1:A:165:GLN:HG2	1.93	0.68
2:N:264:ILE:CG2	2:N:317:SER:HA	2.23	0.68
3:O:119:LEU:HD23	12:O:381:HEM:C4B	2.28	0.68
1:A:244:ARG:HG2	7:G:10:VAL:HG12	1.74	0.68
1:A:408:ARG:NH1	11:K:15:ARG:CG	2.57	0.68
2:N:395:PRO:O	2:N:398:VAL:HB	1.94	0.68
5:Q:171:ILE:HG22	5:Q:179:ASN:OD1	1.92	0.68
7:S:2:ARG:HB2	7:S:6:HIS:HD2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:LEU:N	2:B:24:LEU:HD12	2.04	0.68
3:C:245:PHE:CD1	4:D:17:LEU:HD13	2.27	0.68
1:M:86:LEU:HD13	1:M:99:ILE:HG12	1.75	0.68
2:N:300:ALA:HA	2:N:307:PHE:CZ	2.28	0.68
5:Q:121:GLN:HB2	5:Q:170:ARG:CD	2.24	0.68
1:A:158:PHE:CE1	1:A:317:THR:HG21	2.28	0.68
1:M:245:GLU:OE1	1:M:248:LEU:HD23	1.92	0.68
1:M:389:ARG:O	1:M:390:ILE:HD13	1.94	0.68
3:O:79:ILE:HG12	5:Q:58:PHE:HE1	1.58	0.68
5:Q:83:GLU:HG3	5:Q:100:HIS:NE2	2.08	0.68
5:Q:34:GLY:HA2	10:V:10:TYR:HD1	1.57	0.68
1:M:39:VAL:HG12	1:M:41:ILE:CD1	2.23	0.68
2:N:148:LYS:HG3	2:N:177:TYR:HB3	1.76	0.68
3:O:156:ILE:HG13	3:O:157:GLY:H	1.58	0.68
1:A:350:THR:HB	1:A:353:GLU:CG	2.24	0.68
8:H:22:GLU:O	8:H:25:GLU:HG2	1.94	0.68
3:O:61:THR:O	3:O:62:ALA:C	2.29	0.68
3:O:72:ASP:OD1	4:P:49:ARG:NH1	2.25	0.68
2:B:135:TRP:CD2	6:R:49:ARG:HD3	2.29	0.68
2:B:308:ASP:OD1	2:B:309:VAL:N	2.26	0.68
4:D:134:TYR:HE2	4:D:163:PRO:HG2	1.58	0.68
5:E:53:ASN:OD1	5:E:53:ASN:N	2.27	0.68
5:Q:95:PRO:HG2	5:Q:145:VAL:HG22	1.74	0.68
6:R:51:PRO:HG2	6:R:54:LEU:HD22	1.74	0.68
1:A:286:GLY:O	1:A:287:GLY:C	2.33	0.67
3:C:174:THR:O	3:C:178:PHE:HD1	1.77	0.67
5:E:18:VAL:HG11	5:E:32:ARG:NH1	2.09	0.67
5:Q:171:ILE:HG23	5:Q:171:ILE:O	1.94	0.67
2:N:156:GLN:HE22	9:U:56:ARG:HD3	1.58	0.67
1:A:365:LEU:HD21	1:A:395:TRP:CD1	2.29	0.67
3:C:169:SER:CB	5:Q:93:GLY:HA3	2.24	0.67
8:H:73:LEU:HD21	8:H:74:PHE:HD1	1.58	0.67
1:M:4:TYR:CZ	1:M:8:LEU:HD11	2.28	0.67
2:N:191:LEU:O	2:N:195:VAL:HG23	1.94	0.67
10:V:22:LEU:O	10:V:26:VAL:HG23	1.93	0.67
2:B:257:LEU:HD13	2:B:424:MET:HB2	1.77	0.67
6:F:42:ASP:OD2	6:F:101:ARG:NH1	2.28	0.67
7:G:34:ILE:HB	7:G:35:PRO:CD	2.21	0.67
2:N:180:ASP:O	2:N:183:ILE:HD12	1.95	0.67
6:R:75:LEU:HD12	6:R:76:PRO:CD	2.23	0.67
4:P:233:ARG:HG3	7:S:17:SER:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:27:ARG:NH1	10:V:58:LYS:HZ2	1.92	0.67
1:A:80:GLU:O	1:A:83:GLY:N	2.26	0.67
2:B:348:ALA:HB1	2:B:415:LYS:HA	1.76	0.67
1:M:163:LEU:HD12	1:M:163:LEU:O	1.95	0.67
3:O:177:ARG:O	3:O:181:PHE:CD2	2.47	0.67
1:A:445:ARG:O	1:A:446:PHE:HB2	1.93	0.67
2:B:319:SER:OG	2:B:320:GLY:N	2.27	0.67
5:E:68:VAL:HG12	5:E:69:LEU:N	2.10	0.67
3:O:359:PHE:O	3:O:363:LEU:HB2	1.95	0.67
8:T:65:ARG:HG3	8:T:66:ASP:N	2.09	0.67
1:A:143:THR:HG23	1:A:143:THR:O	1.94	0.67
3:C:311:LYS:HD2	3:C:379:TRP:HB3	1.76	0.67
4:D:237:TYR:CE2	4:D:239:PRO:HG3	2.29	0.67
2:N:132:PHE:HB3	2:N:137:VAL:HG21	1.76	0.67
3:C:56:THR:HG21	3:O:58:ASP:OD2	1.94	0.67
8:T:22:GLU:O	8:T:25:GLU:HG2	1.95	0.67
1:A:151:ASN:ND2	5:E:2:HIS:NE2	2.42	0.67
1:A:408:ARG:NH1	11:K:15:ARG:HG2	2.08	0.67
2:N:394:PRO:O	2:N:398:VAL:HG23	1.94	0.67
3:O:267:HIS:NE2	3:O:269:LYS:HD3	2.10	0.67
3:C:22:PRO:HG2	7:G:3:GLN:HB3	1.76	0.67
4:D:75:ASN:ND2	4:D:80:MET:O	2.28	0.67
5:E:60:SER:HA	5:E:63:SER:OG	1.94	0.67
7:G:50:PRO:CB	7:G:51:PRO:HD3	2.24	0.67
1:M:236:PHE:CD2	1:M:258:GLU:HB3	2.30	0.67
7:S:51:PRO:O	7:S:54:ALA:HB3	1.94	0.67
1:A:426:GLY:N	1:A:428:ILE:HG13	2.06	0.67
4:D:241:LYS:HG2	4:D:241:LYS:OXT	1.95	0.67
2:N:248:ASN:HB2	2:N:428:GLY:CA	2.22	0.67
1:M:27:SER:HA	1:M:199:ALA:O	1.94	0.67
2:N:159:VAL:HG23	2:N:427:SER:OG	1.95	0.67
4:P:236:ALA:HB3	7:S:14:ILE:HB	1.75	0.67
4:P:138:PRO:HB3	8:T:55:THR:N	2.10	0.67
3:C:234:LEU:CD2	4:D:216:LEU:HD21	2.24	0.66
3:C:244:LEU:O	4:D:201:ARG:HD3	1.95	0.66
3:O:296:PHE:HD1	3:O:359:PHE:HE1	1.43	0.66
4:P:32:VAL:HG11	4:P:186:VAL:HG22	1.77	0.66
1:M:408:ARG:HH12	11:W:15:ARG:CG	2.07	0.66
1:A:324:PHE:CD1	1:A:334:MET:HG2	2.30	0.66
1:A:426:GLY:N	1:A:428:ILE:HG12	2.10	0.66
5:E:15:ARG:HH21	5:E:32:ARG:HB2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:15:ARG:HH21	5:Q:32:ARG:CG	2.08	0.66
1:M:405:ARG:O	1:M:409:GLU:HG3	1.95	0.66
2:N:209:LEU:CD2	2:N:375:SER:HB2	2.25	0.66
3:O:244:LEU:O	4:P:201:ARG:HD3	1.95	0.66
4:P:82:MET:SD	4:P:86:LYS:HD2	2.35	0.66
1:A:351:GLU:HA	1:A:404:ALA:HB2	1.77	0.66
2:B:109:VAL:HG22	2:B:119:LEU:HD23	1.77	0.66
6:F:28:LYS:CB	6:F:74:ILE:HD11	2.26	0.66
1:M:351:GLU:OE2	1:M:404:ALA:HB3	1.96	0.66
2:N:327:ILE:O	2:N:327:ILE:HG22	1.95	0.66
3:C:206:ASN:CB	3:C:313:ARG:HH21	2.05	0.66
3:C:332:LEU:HD21	3:C:358:TYR:HE1	1.60	0.66
7:G:2:ARG:HB2	7:G:6:HIS:HD2	1.59	0.66
2:N:71:LEU:HD13	2:N:143:GLN:HG3	1.78	0.66
3:O:26:ASN:ND2	3:O:208:PRO:HD2	2.11	0.66
3:O:22:PRO:CG	7:S:3:GLN:HB3	2.25	0.66
9:U:70:LEU:CD1	9:U:72:VAL:H	2.08	0.66
5:Q:109:GLU:CD	5:Q:167:ALA:HB3	2.15	0.66
7:S:73:ASN:N	7:S:74:PRO:CD	2.58	0.66
1:A:251:ALA:O	1:A:325:VAL:HA	1.95	0.66
2:B:279:LEU:HD22	2:B:295:LEU:HD13	1.76	0.66
2:B:253:VAL:HG23	2:B:427:SER:O	1.96	0.66
4:D:11:PRO:O	8:H:74:PHE:CZ	2.49	0.66
1:A:241:ILE:HG13	7:G:16:TYR:CD1	2.30	0.66
4:D:178:THR:HG23	8:H:15:ASP:N	2.11	0.66
5:Q:136:ILE:O	5:Q:136:ILE:HG22	1.93	0.66
1:A:106:LEU:N	1:A:107:PRO:HD2	2.11	0.66
1:A:236:PHE:CD2	1:A:258:GLU:HB3	2.31	0.66
3:C:32:ASN:HD21	3:C:228:ASP:HA	1.61	0.66
1:M:161:THR:HB	1:M:162:PRO:HD2	1.77	0.66
2:N:303:VAL:HG12	2:N:304:HIS:N	2.11	0.66
3:O:90:PHE:HE1	3:O:123:VAL:HG21	1.60	0.66
2:N:129:ALA:N	2:N:130:PRO:CD	2.58	0.66
3:O:8:HIS:HB3	3:O:9:PRO:HD3	1.76	0.66
4:P:158:ILE:HD13	4:P:160:MET:CB	2.22	0.66
2:B:354:ASN:N	2:B:355:PRO:HD2	2.11	0.66
3:C:108:THR:HB	3:C:313:ARG:HH11	1.59	0.66
2:N:436:ILE:HD12	2:N:437:ASP:OD1	1.96	0.66
2:N:98:VAL:HG22	2:N:107:TYR:CD2	2.31	0.66
5:Q:188:THR:OG1	5:Q:192:MET:HB2	1.96	0.66
10:V:9:LEU:HD12	10:V:13:LEU:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASN:OD1	1:A:170:PRO:HD3	1.95	0.65
3:C:183:PHE:CE1	3:O:183:PHE:CD1	2.84	0.65
3:O:122:THR:CG2	3:O:189:ILE:CD1	2.74	0.65
3:O:32:ASN:O	3:O:36:LEU:HG	1.95	0.65
5:Q:101:ARG:HD3	5:Q:133:VAL:HG11	1.76	0.65
1:A:198:ALA:O	1:A:199:ALA:HB2	1.95	0.65
4:D:236:ALA:HB3	7:G:14:ILE:HB	1.78	0.65
1:M:298:ALA:HA	1:M:303:LEU:HB2	1.77	0.65
2:N:247:GLN:HE22	2:N:429:ASN:ND2	1.95	0.65
4:P:54:VAL:HG12	4:P:54:VAL:O	1.96	0.65
3:O:200:LEU:O	3:O:200:LEU:HG	1.95	0.65
1:A:262:TRP:CG	1:A:385:THR:HG23	2.31	0.65
1:A:331:ILE:HD11	1:A:427:PRO:O	1.96	0.65
2:B:257:LEU:HD13	2:B:424:MET:HE2	1.78	0.65
3:C:174:THR:O	3:C:178:PHE:CD1	2.50	0.65
3:C:270:PRO:HB2	3:C:274:PHE:HB2	1.78	0.65
1:M:158:PHE:CZ	1:M:317:THR:HG21	2.31	0.65
2:N:134:ARG:HG2	2:N:135:TRP:N	2.11	0.65
4:P:50:HIS:HB3	4:P:54:VAL:CB	2.26	0.65
6:R:73:GLN:HA	7:S:39:ARG:HH21	1.62	0.65
1:M:45:SER:OG	1:M:92:ARG:CG	2.44	0.65
3:O:102:LEU:HD21	3:O:304:ILE:HD13	1.77	0.65
5:Q:1:SER:OG	5:Q:1:SER:CA	2.44	0.65
2:B:56:ARG:NH2	2:B:172:LEU:HD21	2.12	0.65
3:C:47:THR:HG21	3:C:83:HIS:CB	2.27	0.65
5:Q:89:PHE:HB2	5:Q:96:LEU:HB3	1.76	0.65
1:A:106:LEU:CD2	1:A:203:LEU:HD13	2.26	0.65
2:B:341:TYR:HE2	2:B:345:LYS:HE3	1.61	0.65
3:C:240:MET:O	3:C:244:LEU:HB2	1.96	0.65
6:F:75:LEU:O	6:F:80:TRP:NE1	2.30	0.65
4:D:229:VAL:HG22	7:G:18:LEU:O	1.97	0.65
1:M:236:PHE:HD2	1:M:258:GLU:HG2	1.60	0.65
1:M:279:HIS:HA	1:M:307:PHE:O	1.97	0.65
5:Q:102:THR:O	5:Q:106:ILE:HG13	1.96	0.65
6:R:96:GLU:O	6:R:97:VAL:C	2.32	0.65
1:M:408:ARG:CZ	11:W:15:ARG:HE	2.08	0.65
2:B:134:ARG:NH1	6:R:51:PRO:HD3	2.11	0.65
3:C:296:PHE:HD1	3:C:359:PHE:HE1	1.45	0.65
4:D:138:PRO:HB3	8:H:55:THR:N	2.12	0.65
2:N:56:ARG:NE	2:N:103:GLU:OE1	2.19	0.65
3:O:310:SER:CB	3:O:318:ARG:NH1	2.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:50:PRO:CB	7:S:51:PRO:CD	2.70	0.65
4:P:27:ARG:NH1	10:V:58:LYS:HG3	2.11	0.65
1:A:75:LEU:HD21	1:A:116:ILE:HG12	1.78	0.65
2:B:31:ASN:HB3	2:B:201:SER:HB3	1.78	0.65
3:O:102:LEU:HD21	3:O:304:ILE:HD12	1.78	0.65
3:O:44:GLN:OE1	3:O:83:HIS:ND1	2.30	0.65
6:R:75:LEU:O	6:R:80:TRP:NE1	2.27	0.65
4:D:178:THR:HG21	8:H:16:PRO:HG2	1.79	0.65
4:D:55:CYS:SG	10:J:55:ILE:HG22	2.37	0.65
3:C:78:ILE:HD11	5:E:57:GLN:NE2	2.12	0.65
6:F:96:GLU:OE1	6:F:99:ARG:HD2	1.98	0.65
4:D:10:TYR:HE1	8:H:73:LEU:HD21	1.60	0.65
9:I:70:LEU:CD1	9:I:72:VAL:H	2.09	0.65
10:J:12:LEU:HD23	10:J:13:LEU:HD21	1.79	0.65
4:P:164:ILE:HD11	4:P:186:VAL:HG21	1.79	0.65
4:P:51:LEU:HA	4:P:56:TYR:O	1.97	0.65
6:R:42:ASP:OD2	6:R:101:ARG:NH1	2.30	0.65
3:C:346:PRO:HG2	7:G:66:PHE:HD1	1.62	0.64
3:C:44:GLN:OE1	3:C:83:HIS:ND1	2.30	0.64
1:M:91:THR:CG2	1:M:92:ARG:N	2.60	0.64
3:O:122:THR:HG21	3:O:189:ILE:HG12	1.78	0.64
3:O:153:ILE:HG23	3:O:154:PRO:HD2	1.79	0.64
3:O:311:LYS:HD2	3:O:379:TRP:HB3	1.79	0.64
2:N:156:GLN:NE2	9:U:56:ARG:HD3	2.12	0.64
2:B:109:VAL:HG22	2:B:119:LEU:CD2	2.28	0.64
2:B:155:PRO:HB2	2:B:254:HIS:CE1	2.32	0.64
10:J:55:ILE:HG23	10:J:58:LYS:HE2	1.78	0.64
2:N:133:ARG:HD3	2:N:135:TRP:CZ2	2.32	0.64
2:N:352:LEU:O	2:N:352:LEU:HG	1.96	0.64
10:V:51:LEU:HB3	10:V:52:TRP:CZ3	2.32	0.64
1:A:41:ILE:HG13	1:A:195:MET:CE	2.27	0.64
1:A:297:ILE:HG22	1:A:303:LEU:HD12	1.80	0.64
3:C:243:VAL:HG13	3:C:244:LEU:HD13	1.77	0.64
4:D:32:VAL:HG21	4:D:186:VAL:HG22	1.79	0.64
3:O:345:HIS:HB3	3:O:346:PRO:CD	2.21	0.64
1:A:269:ALA:HB3	1:A:410:VAL:HG11	1.80	0.64
2:B:333:ALA:O	2:B:337:ILE:HD12	1.97	0.64
4:D:220:TYR:CE2	7:G:26:PHE:CE1	2.83	0.64
1:M:15:GLN:O	1:M:26:ALA:HA	1.98	0.64
1:A:346:CYS:CB	1:A:412:SER:OG	2.44	0.64
2:B:318:ASP:N	2:B:318:ASP:OD1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:434:PRO:HB3	2:B:438:GLU:HB3	1.80	0.64
3:C:338:ILE:N	3:C:338:ILE:CD1	2.61	0.64
3:C:78:ILE:HG21	4:D:204:MET:HE1	1.80	0.64
1:M:350:THR:HB	1:M:353:GLU:CG	2.28	0.64
3:O:218:ILE:HD13	4:P:230:LEU:HD11	1.78	0.64
3:O:102:LEU:HB3	3:O:325:PHE:HE1	1.62	0.64
4:P:26:ILE:HG22	4:P:54:VAL:HG13	1.78	0.64
2:N:384:SER:HB2	9:U:62:ARG:HG2	1.79	0.64
1:A:78:GLU:HG2	1:A:112:LEU:HD21	1.78	0.64
2:B:128:THR:HG23	2:B:226:ILE:HD11	1.80	0.64
1:A:358:LYS:HD2	1:A:402:VAL:CG1	2.28	0.64
1:M:91:THR:HG23	1:M:92:ARG:H	1.60	0.64
2:N:207:ILE:CD1	2:N:383:GLY:HA2	2.25	0.64
4:P:70:VAL:HG23	4:P:84:PRO:HD3	1.79	0.64
5:Q:63:SER:O	5:Q:64:ALA:HB2	1.98	0.64
1:M:408:ARG:NH1	11:W:15:ARG:CG	2.61	0.64
4:D:94:PRO:HB2	4:D:95:TYR:CE1	2.33	0.64
1:M:199:ALA:HB3	1:M:208:LEU:HD21	1.79	0.64
6:R:96:GLU:OE1	6:R:99:ARG:HD2	1.98	0.64
3:C:221:HIS:CB	3:C:222:PRO:HD3	2.22	0.64
5:E:62:MET:O	3:O:177:ARG:NH2	2.30	0.64
1:M:391:PRO:HB2	1:M:395:TRP:CZ2	2.32	0.64
1:M:38:GLY:HA3	1:M:40:TRP:HZ3	1.62	0.64
2:N:140:LEU:O	2:N:141:GLN:C	2.35	0.64
1:M:436:ARG:HE	3:O:222:PRO:HD3	1.62	0.64
6:R:43:VAL:HG22	6:R:94:LEU:HD21	1.80	0.64
3:C:309:THR:HG23	3:C:370:GLY:HA3	1.80	0.64
3:C:78:ILE:O	3:C:82:MET:HB2	1.98	0.64
1:M:404:ALA:O	1:M:408:ARG:HG3	1.98	0.64
5:Q:118:ARG:HB3	5:Q:171:ILE:HG23	1.80	0.64
1:A:224:ASP:O	1:A:227:ALA:N	2.31	0.63
1:A:32:GLN:HG3	1:A:33:PRO:HD2	1.80	0.63
3:C:119:LEU:HD13	3:C:192:ILE:HG22	1.80	0.63
3:C:329:VAL:HA	3:C:332:LEU:HD12	1.81	0.63
3:O:141:TRP:O	3:O:145:VAL:HG23	1.98	0.63
1:A:240:GLN:HG3	1:A:422:VAL:O	1.98	0.63
1:M:426:GLY:CA	1:M:428:ILE:N	2.61	0.63
3:C:183:PHE:CD1	3:O:183:PHE:CE1	2.86	0.63
3:O:79:ILE:HG12	5:Q:58:PHE:CE1	2.33	0.63
1:A:158:PHE:CB	1:A:164:ALA:HB2	2.29	0.63
1:A:333:ASP:O	1:A:337:VAL:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:MET:HA	3:C:243:VAL:CG1	2.24	0.63
1:M:352:SER:OG	1:M:353:GLU:N	2.31	0.63
4:P:127:VAL:HG12	4:P:187:CYS:SG	2.39	0.63
5:Q:126:ARG:NH2	5:Q:168:SER:O	2.23	0.63
5:Q:76:ILE:HG22	5:Q:193:VAL:C	2.19	0.63
8:T:67:HIS:CE1	8:T:71:HIS:HE2	2.16	0.63
1:A:158:PHE:HB2	1:A:164:ALA:HB2	1.79	0.63
3:O:207:ASN:HB2	3:O:208:PRO:HD2	1.80	0.63
4:P:120:ARG:HG2	4:P:120:ARG:HH11	1.62	0.63
4:P:50:HIS:HB3	4:P:54:VAL:CG2	2.28	0.63
1:A:38:GLY:HA3	1:A:40:TRP:HZ3	1.62	0.63
2:B:338:LYS:HD3	2:B:439:LEU:HD23	1.81	0.63
3:O:115:ILE:CG2	3:O:196:HIS:HB2	2.27	0.63
3:O:33:PHE:CE1	3:O:96:MET:HG3	2.34	0.63
5:Q:193:VAL:HG13	5:Q:193:VAL:O	1.97	0.63
6:R:28:LYS:HD2	6:R:74:ILE:CD1	2.24	0.63
10:V:35:PHE:O	10:V:36:ASP:C	2.37	0.63
1:A:24:ARG:CB	1:A:196:VAL:HG22	2.25	0.63
5:E:29:SER:HA	5:E:32:ARG:HD3	1.81	0.63
8:H:25:GLU:HA	8:H:30:CYS:SG	2.39	0.63
8:H:67:HIS:CE1	8:H:71:HIS:HE2	2.16	0.63
2:B:384:SER:CB	9:I:62:ARG:HG2	2.29	0.63
1:M:162:PRO:O	1:M:165:GLN:HG2	1.99	0.63
1:M:39:VAL:HG11	1:M:117:VAL:HG21	1.81	0.63
2:N:56:ARG:NH2	2:N:172:LEU:HD21	2.14	0.63
4:P:62:LYS:O	4:P:66:GLU:HG3	1.99	0.63
6:R:73:GLN:HE21	7:S:32:LYS:CE	2.12	0.63
1:A:308:GLN:CG	1:A:308:GLN:O	2.46	0.63
1:A:385:THR:HG22	1:A:386:TYR:N	2.12	0.63
1:A:436:ARG:HE	3:C:222:PRO:CG	2.12	0.63
10:J:36:ASP:O	10:J:37:GLN:C	2.35	0.63
3:O:137:GLN:OE1	3:O:259:ALA:HA	1.99	0.63
3:O:207:ASN:OD1	3:O:210:GLY:N	2.26	0.63
5:Q:78:LEU:HD23	5:Q:79:SER:H	1.64	0.63
5:Q:91:TRP:O	5:Q:92:ARG:HB2	1.97	0.63
7:S:34:ILE:HB	7:S:35:PRO:CD	2.27	0.63
10:V:51:LEU:HD22	10:V:52:TRP:HZ3	1.64	0.63
2:B:347:ILE:N	2:B:347:ILE:HD12	2.13	0.63
3:C:106:SER:HB3	12:C:381:HEM:HBD2	1.81	0.63
1:M:408:ARG:NH1	11:W:15:ARG:HG2	2.13	0.63
1:M:426:GLY:N	1:M:428:ILE:CG1	2.60	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:80:GLU:O	1:M:83:GLY:N	2.28	0.63
3:O:304:ILE:N	3:O:305:PRO:HD2	2.14	0.63
3:O:8:HIS:CB	3:O:9:PRO:HD3	2.29	0.63
5:Q:76:ILE:HD12	5:Q:192:MET:CE	2.28	0.63
7:S:71:ARG:HH21	8:T:60:ASP:CG	2.02	0.63
2:B:200:THR:CG2	2:B:203:ARG:HD2	2.23	0.63
2:B:341:TYR:CE2	2:B:345:LYS:HE3	2.34	0.63
3:C:183:PHE:CD1	3:C:183:PHE:O	2.52	0.63
3:C:116:GLY:HA3	12:C:381:HEM:C3C	2.34	0.63
4:D:10:TYR:O	4:D:12:TRP:CD1	2.51	0.63
3:C:311:LYS:O	6:F:38:HIS:HB2	1.98	0.63
1:M:144:SER:O	1:M:148:VAL:HG23	1.99	0.63
1:M:373:THR:HB	1:M:374:PRO:HD3	1.81	0.63
2:N:83:PHE:CE2	2:N:87:ARG:HG3	2.34	0.63
4:P:229:VAL:HG12	4:P:233:ARG:HE	1.63	0.63
2:B:156:GLN:NE2	9:I:56:ARG:HD3	2.14	0.62
3:C:170:VAL:O	3:C:170:VAL:HG12	1.97	0.62
3:C:15:ASN:ND2	3:C:18:PHE:CE1	2.67	0.62
3:C:25:SER:HA	3:C:218:ILE:CD1	2.29	0.62
3:C:372:ILE:O	3:C:375:LYS:N	2.32	0.62
1:M:72:GLY:O	1:M:73:ASN:OD1	2.17	0.62
2:N:129:ALA:N	2:N:130:PRO:HD3	2.14	0.62
2:N:195:VAL:HG13	2:N:199:PHE:CD2	2.34	0.62
3:O:30:TRP:O	3:O:33:PHE:CD2	2.47	0.62
4:P:231:LYS:HD2	6:R:71:ARG:HG2	1.81	0.62
1:A:64:PHE:CE2	1:A:88:ALA:HB2	2.33	0.62
2:B:303:VAL:HG12	2:B:304:HIS:N	2.14	0.62
3:C:296:PHE:CD1	3:C:359:PHE:HE1	2.17	0.62
3:C:230:LEU:HD12	4:D:219:VAL:HG12	1.80	0.62
1:M:155:ALA:HA	1:M:164:ALA:HB1	1.80	0.62
4:P:75:ASN:ND2	4:P:80:MET:O	2.32	0.62
1:A:91:THR:CG2	1:A:92:ARG:N	2.62	0.62
2:B:47:ILE:HD12	2:B:120:MET:SD	2.40	0.62
2:B:200:THR:HG22	2:B:203:ARG:CD	2.25	0.62
3:C:72:ASP:OD1	4:D:49:ARG:NH1	2.28	0.62
4:D:50:HIS:HB3	4:D:54:VAL:CG2	2.29	0.62
1:M:403:ASP:OD1	1:M:404:ALA:N	2.32	0.62
3:O:160:LEU:HD11	3:O:164:ILE:HD11	1.80	0.62
5:Q:76:ILE:HG23	5:Q:194:ILE:CG1	2.29	0.62
1:A:403:ASP:OD1	1:A:404:ALA:N	2.33	0.62
1:A:417:ASP:O	1:A:417:ASP:OD1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:THR:O	2:B:190:GLU:HB2	1.99	0.62
2:B:58:GLU:HB2	2:B:63:LEU:HD23	1.82	0.62
3:C:163:TRP:O	3:C:177:ARG:NH1	2.32	0.62
4:D:165:TYR:CE1	4:D:168:VAL:HG22	2.34	0.62
1:M:46:ARG:HH22	1:M:316:ASP:CG	2.02	0.62
1:A:342:TRP:O	1:A:343:MET:C	2.38	0.62
1:A:426:GLY:HA2	1:A:427:PRO:C	2.19	0.62
2:B:247:GLN:NE2	2:B:429:ASN:HA	2.14	0.62
2:B:385:GLN:HG2	9:I:62:ARG:NH1	2.10	0.62
2:B:59:ASN:OD1	2:B:60:SER:N	2.32	0.62
4:D:233:ARG:HG3	7:G:17:SER:HB2	1.79	0.62
1:M:151:ASN:ND2	5:Q:2:HIS:NE2	2.46	0.62
1:M:385:THR:HG22	1:M:386:TYR:N	2.14	0.62
2:N:279:LEU:HD22	2:N:344:VAL:HG22	1.79	0.62
2:N:255:ALA:HB2	2:N:426:ALA:HB2	1.81	0.62
3:O:119:LEU:HD13	3:O:192:ILE:HG22	1.80	0.62
3:O:28:SER:HB3	3:O:30:TRP:HD1	1.63	0.62
4:P:13:SER:O	4:P:19:SER:HB3	1.99	0.62
5:Q:85:LYS:HG2	5:Q:86:ASN:N	2.11	0.62
4:P:3:LEU:HD11	7:S:71:ARG:HB2	1.81	0.62
1:A:43:ALA:CB	1:A:189:HIS:HB3	2.30	0.62
1:M:45:SER:CB	1:M:167:VAL:HG22	2.29	0.62
1:M:309:THR:HA	1:M:322:ALA:HA	1.81	0.62
1:M:358:LYS:HE3	1:M:402:VAL:HB	1.82	0.62
3:O:52:ALA:HB2	12:O:380:HEM:HMD1	1.81	0.62
2:B:169:ARG:CZ	2:N:438:GLU:OE2	2.47	0.62
3:C:207:ASN:ND2	3:C:209:THR:OG1	2.32	0.62
3:C:345:HIS:HB3	3:C:346:PRO:HD3	1.79	0.62
10:J:3:PRO:HG2	10:J:8:ARG:HG2	1.81	0.62
2:N:37:SER:OG	2:N:213:HIS:HB2	2.00	0.62
2:N:385:GLN:HG2	9:U:62:ARG:NH1	2.13	0.62
4:P:27:ARG:HH11	10:V:58:LYS:NZ	1.98	0.62
5:Q:76:ILE:HG22	5:Q:194:ILE:HG12	1.79	0.62
8:T:34:ARG:O	8:T:38:GLU:HG2	1.99	0.62
10:V:51:LEU:HB3	10:V:52:TRP:CE3	2.35	0.62
1:A:280:TYR:O	1:A:306:SER:HA	2.00	0.62
2:B:123:LEU:O	2:B:127:THR:HG22	2.00	0.62
2:B:352:LEU:HB3	2:B:411:ILE:CD1	2.29	0.62
4:D:27:ARG:NH2	4:D:60:GLU:OE2	2.33	0.62
1:M:134:ILE:HG21	1:M:174:VAL:HG21	1.81	0.62
1:M:53:ASN:OD1	1:M:170:PRO:HD3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:79:GLU:OE1	4:P:82:MET:HG3	1.98	0.62
9:U:78:TYR:OXT	9:U:78:TYR:HD1	1.83	0.62
4:D:236:ALA:O	7:G:14:ILE:N	2.28	0.62
2:N:352:LEU:HD21	2:N:357:VAL:HG23	1.82	0.62
3:O:331:ASP:O	3:O:334:THR:HB	2.00	0.62
5:Q:157:TYR:CE2	5:Q:159:PRO:HA	2.33	0.62
1:M:91:THR:CG2	1:M:93:GLU:H	2.10	0.62
3:O:115:ILE:HG21	3:O:196:HIS:HB2	1.81	0.62
6:R:73:GLN:HG2	7:S:36:ASN:HD21	1.65	0.62
1:A:327:ASP:OD1	1:A:328:HIS:N	2.32	0.61
2:B:434:PRO:HB2	2:B:439:LEU:HD11	1.81	0.61
2:B:95:LYS:HE3	9:I:70:LEU:CD2	2.24	0.61
1:M:143:THR:O	1:M:143:THR:HG23	1.98	0.61
1:M:37:VAL:HG13	1:M:199:ALA:HB2	1.82	0.61
5:Q:141:HIS:NE2	5:Q:175:PRO:HB2	2.15	0.61
11:W:26:ALA:O	11:W:30:VAL:HG23	2.00	0.61
1:A:204:GLU:HG2	1:A:206:ARG:HB3	1.80	0.61
2:B:337:ILE:CG2	2:B:434:PRO:HG2	2.30	0.61
2:B:58:GLU:OE1	2:B:63:LEU:HA	2.00	0.61
3:C:153:ILE:HG23	3:C:154:PRO:HD2	1.82	0.61
3:C:119:LEU:HD13	3:C:192:ILE:CG2	2.29	0.61
1:M:365:LEU:HG	1:M:365:LEU:O	1.99	0.61
2:N:352:LEU:HB3	2:N:411:ILE:CD1	2.29	0.61
9:U:62:ARG:N	9:U:63:PRO:HD2	2.15	0.61
1:A:61:HIS:NE2	1:A:134:ILE:CD1	2.62	0.61
1:A:236:PHE:HD2	1:A:258:GLU:CG	2.12	0.61
2:B:163:LEU:HD22	2:B:256:ALA:CB	2.29	0.61
1:A:370:ASP:OD1	2:B:375:SER:HB3	1.99	0.61
4:D:72:ASP:O	4:D:73:GLY:O	2.18	0.61
3:O:8:HIS:CB	3:O:9:PRO:CD	2.78	0.61
4:P:68:VAL:HG12	4:P:92:PRO:HG2	1.82	0.61
5:Q:13:TYR:O	7:S:23:GLN:HB3	2.01	0.61
5:Q:188:THR:OG1	5:Q:189:SER:N	2.33	0.61
2:B:101:THR:OG1	2:B:102:ARG:N	2.32	0.61
2:B:435:PHE:HB2	2:B:438:GLU:OE1	2.00	0.61
4:D:10:TYR:CE1	8:H:73:LEU:CD2	2.84	0.61
3:O:7:SER:HA	3:O:13:ILE:HG12	1.81	0.61
5:Q:187:PHE:CE2	5:Q:193:VAL:HB	2.34	0.61
1:A:343:MET:HE1	1:A:416:TYR:CD2	2.36	0.61
1:A:5:ALA:O	1:A:8:LEU:HB2	2.00	0.61
1:A:92:ARG:HD2	1:A:163:LEU:CD1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:GLN:HE22	9:I:56:ARG:HD3	1.65	0.61
2:B:209:LEU:CD2	2:B:375:SER:HB2	2.30	0.61
3:C:156:ILE:O	3:C:157:GLY:C	2.39	0.61
3:C:315:MET:HA	3:C:318:ARG:HG3	1.82	0.61
4:D:28:ARG:HD2	4:D:185:ASP:OD2	2.01	0.61
3:C:313:ARG:HB3	6:F:38:HIS:CD2	2.35	0.61
2:N:283:PRO:HG3	9:U:55:LEU:CD2	2.24	0.61
2:B:299:VAL:O	2:B:303:VAL:HG23	2.01	0.61
1:A:433:ASP:HB2	3:C:219:PRO:HG2	1.82	0.61
4:P:27:ARG:NH2	4:P:60:GLU:OE2	2.34	0.61
5:Q:45:VAL:HG23	10:V:24:ILE:HA	1.83	0.61
1:A:145:MET:SD	1:A:248:LEU:CD1	2.86	0.61
3:C:109:PHE:O	3:C:110:LEU:C	2.36	0.61
3:C:146:ILE:O	3:C:149:LEU:HB3	2.00	0.61
3:C:122:THR:HG23	3:C:185:LEU:HD11	1.83	0.61
4:D:168:VAL:O	4:D:169:LEU:HD23	2.01	0.61
13:D:242:HEC:HMC1	13:D:242:HEC:HBC3	1.82	0.61
2:N:95:LYS:CE	9:U:70:LEU:HD22	2.29	0.61
3:O:242:LEU:HD21	3:O:250:LEU:HD22	1.83	0.61
4:P:138:PRO:HG2	8:T:55:THR:CB	2.30	0.61
1:A:336:PHE:HE2	1:A:446:PHE:HD2	1.47	0.61
2:B:47:ILE:HG22	2:B:48:GLY:N	2.15	0.61
10:J:51:LEU:HB3	10:J:52:TRP:CZ3	2.36	0.61
1:M:86:LEU:HB3	2:N:285:VAL:HG22	1.81	0.61
1:M:91:THR:HG23	1:M:92:ARG:N	2.16	0.61
2:N:203:ARG:NE	2:N:230:LEU:HD23	2.15	0.61
3:O:126:THR:HG21	12:O:380:HEM:C3B	2.36	0.61
3:O:4:ILE:HG22	3:O:4:ILE:O	2.00	0.61
4:D:57:THR:HG22	4:D:58:GLU:H	1.65	0.61
10:J:34:ALA:O	10:J:35:PHE:C	2.38	0.61
2:N:412:ASN:O	2:N:415:LYS:HB2	2.00	0.61
5:Q:117:LEU:O	5:Q:118:ARG:C	2.39	0.61
5:Q:118:ARG:HH22	5:Q:173:LYS:HA	1.66	0.61
10:V:55:ILE:HG23	10:V:58:LYS:HE2	1.82	0.61
3:C:18:PHE:O	3:C:220:PHE:HD2	1.84	0.61
3:C:267:HIS:NE2	3:C:269:LYS:HD3	2.15	0.61
6:F:106:GLU:HA	6:F:109:LYS:NZ	2.16	0.61
1:M:64:PHE:CE1	1:M:86:LEU:CG	2.81	0.61
3:O:156:ILE:O	3:O:157:GLY:C	2.39	0.61
8:T:37:LEU:HD21	8:T:58:LEU:HA	1.83	0.61
1:A:244:ARG:CZ	7:G:10:VAL:HB	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:134:TYR:HE2	4:P:163:PRO:HG2	1.66	0.60
4:P:32:VAL:HG11	4:P:186:VAL:CG2	2.31	0.60
5:Q:104:LYS:O	5:Q:104:LYS:HG2	2.01	0.60
1:A:413:LYS:HB2	1:A:414:TYR:CD2	2.36	0.60
8:H:40:CYS:HB2	8:H:57:GLU:HG2	1.83	0.60
4:P:214:LEU:O	4:P:218:LEU:HG	2.01	0.60
5:Q:29:SER:HA	5:Q:32:ARG:HD3	1.83	0.60
6:R:73:GLN:NE2	7:S:32:LYS:HZ1	1.98	0.60
4:P:11:PRO:O	8:T:74:PHE:CZ	2.54	0.60
1:A:182:LEU:O	1:A:186:LEU:HD12	2.01	0.60
2:B:140:LEU:HD12	2:B:143:GLN:HB3	1.83	0.60
3:C:207:ASN:OD1	3:C:210:GLY:N	2.32	0.60
3:C:26:ASN:O	3:C:27:ILE:HG13	2.01	0.60
1:A:233:PRO:HG2	5:E:23:LYS:HD2	1.84	0.60
6:F:28:LYS:HD3	6:F:74:ILE:HD11	1.84	0.60
7:G:71:ARG:O	8:H:56:GLU:OE2	2.20	0.60
2:N:354:ASN:N	2:N:355:PRO:HD2	2.16	0.60
4:P:176:PRO:HB2	4:P:181:GLN:NE2	2.14	0.60
5:Q:85:LYS:CG	5:Q:86:ASN:H	2.12	0.60
9:U:53:GLU:O	9:U:55:LEU:HG	2.00	0.60
1:A:80:GLU:O	1:A:82:MET:N	2.34	0.60
1:A:86:LEU:HD13	1:A:99:ILE:CG1	2.31	0.60
3:C:218:ILE:HG22	3:C:223:TYR:CD2	2.35	0.60
1:M:366:VAL:HG12	1:M:367:SER:N	2.16	0.60
1:M:354:VAL:CG1	1:M:407:VAL:HG21	2.31	0.60
1:M:64:PHE:CE2	1:M:88:ALA:HB2	2.36	0.60
3:O:132:VAL:HA	3:O:139:SER:HB3	1.81	0.60
3:O:196:HIS:HE1	12:O:381:HEM:C1D	2.19	0.60
5:Q:118:ARG:NH1	5:Q:171:ILE:CG1	2.57	0.60
1:A:154:HIS:O	1:A:158:PHE:HB2	2.00	0.60
3:C:327:ALA:O	3:C:331:ASP:N	2.32	0.60
8:H:73:LEU:HD21	8:H:74:PHE:CD1	2.35	0.60
1:M:4:TYR:CE2	1:M:396:GLU:HG3	2.36	0.60
2:N:362:ASN:HA	2:N:365:LYS:HD3	1.82	0.60
2:N:384:SER:CB	9:U:62:ARG:HG2	2.32	0.60
7:S:71:ARG:O	8:T:56:GLU:OE2	2.19	0.60
8:T:15:ASP:HB2	8:T:16:PRO:HD3	1.83	0.60
1:A:408:ARG:CZ	11:K:15:ARG:NE	2.63	0.60
2:B:258:VAL:CG1	2:B:321:LEU:HB3	2.29	0.60
9:I:62:ARG:HB3	9:I:63:PRO:HD3	1.83	0.60
1:M:146:ARG:NH2	1:M:308:GLN:HE22	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:206:LEU:HD13	2:N:224:LEU:HD11	1.84	0.60
2:N:34:VAL:HG11	2:N:386:ALA:CB	2.32	0.60
1:A:351:GLU:OE2	1:A:404:ALA:HB3	2.00	0.60
4:D:164:ILE:HD11	13:D:242:HEC:HBB2	1.83	0.60
4:D:30:PHE:HD1	4:D:189:PHE:CE1	2.19	0.60
2:N:183:ILE:HG22	2:N:184:GLY:N	2.16	0.60
5:Q:101:ARG:HD3	5:Q:133:VAL:CG1	2.31	0.60
5:Q:153:PHE:CE1	5:Q:173:LYS:HG3	2.34	0.60
7:S:54:ALA:O	7:S:58:VAL:HG23	2.01	0.60
4:D:165:TYR:CE2	4:D:168:VAL:HG22	2.37	0.60
4:D:57:THR:HG22	4:D:58:GLU:N	2.17	0.60
2:B:86:THR:HG23	9:I:71:ASN:HD21	1.66	0.60
1:M:184:GLU:O	1:M:188:ARG:HG3	2.02	0.60
1:M:6:GLN:O	1:M:7:ALA:C	2.39	0.60
1:M:233:PRO:HG2	5:Q:23:LYS:CD	2.32	0.60
7:S:2:ARG:HB2	7:S:6:HIS:CD2	2.37	0.60
3:C:239:LEU:HD12	3:C:239:LEU:O	2.02	0.60
3:C:28:SER:HB3	3:C:30:TRP:HD1	1.67	0.60
9:I:62:ARG:N	9:I:63:PRO:HD2	2.16	0.60
3:O:244:LEU:HD23	4:P:205:GLY:HA2	1.83	0.60
4:P:72:ASP:O	4:P:73:GLY:O	2.20	0.60
5:Q:12:ASP:O	7:S:24:ARG:NH2	2.32	0.60
1:M:46:ARG:NH2	1:M:316:ASP:OD2	2.34	0.60
3:O:348:ILE:O	3:O:352:GLN:HG3	2.02	0.60
4:P:42:SER:O	4:P:112:ASP:OD1	2.20	0.60
5:Q:103:LYS:HA	5:Q:106:ILE:HD12	1.82	0.60
5:Q:121:GLN:HB3	5:Q:126:ARG:HD3	1.83	0.60
5:Q:164:HIS:H	5:Q:173:LYS:HB2	1.67	0.60
8:T:73:LEU:O	8:T:73:LEU:HG	2.02	0.60
10:V:20:PHE:O	10:V:23:THR:HB	2.02	0.60
2:B:196:GLN:HG2	2:B:197:ASN:OD1	2.02	0.59
3:C:301:LEU:O	3:C:304:ILE:HD12	2.02	0.59
3:C:52:ALA:HB2	12:C:380:HEM:HMD2	1.83	0.59
1:M:236:PHE:HD2	1:M:258:GLU:CG	2.15	0.59
1:M:426:GLY:HA2	1:M:428:ILE:N	2.17	0.59
3:C:264:THR:CG2	5:Q:144:CYS:HB3	2.25	0.59
10:V:51:LEU:H	10:V:54:HIS:HD2	1.49	0.59
1:A:64:PHE:HE1	1:A:86:LEU:CG	2.12	0.59
3:C:10:LEU:HD12	3:C:13:ILE:CD1	2.28	0.59
3:C:27:ILE:CG2	3:C:27:ILE:O	2.46	0.59
13:D:242:HEC:HBB3	13:D:242:HEC:HMB1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:96:GLU:OE2	6:F:99:ARG:NH1	2.34	0.59
9:I:58:GLN:HA	9:I:78:TYR:CD2	2.37	0.59
1:M:312:ILE:HB	1:M:319:LEU:HB2	1.83	0.59
2:N:100:SER:HB3	2:N:105:MET:CG	2.32	0.59
2:N:269:ALA:O	2:N:272:PHE:N	2.35	0.59
3:O:110:LEU:HG	3:O:114:ASN:HD21	1.67	0.59
3:O:296:PHE:CD1	3:O:359:PHE:HE1	2.19	0.59
4:P:36:VAL:HG23	4:P:169:LEU:HD11	1.84	0.59
4:P:237:TYR:CD2	4:P:239:PRO:HD3	2.36	0.59
9:U:58:GLN:HA	9:U:78:TYR:CD2	2.37	0.59
10:V:9:LEU:HD12	10:V:13:LEU:CD1	2.32	0.59
10:V:18:SER:HB3	11:W:23:LEU:HD12	1.84	0.59
5:E:33:LYS:HB3	7:G:21:PHE:CE2	2.38	0.59
5:Q:121:GLN:HG3	5:Q:179:ASN:HD22	1.67	0.59
10:V:45:HIS:O	10:V:48:GLU:HG2	2.02	0.59
1:A:106:LEU:HD22	1:A:203:LEU:CD2	2.31	0.59
2:B:248:ASN:HB2	2:B:428:GLY:CA	2.33	0.59
3:C:22:PRO:CG	7:G:3:GLN:HB3	2.31	0.59
4:D:40:CYS:HB3	4:D:95:TYR:OH	2.02	0.59
9:I:58:GLN:O	9:I:59:ALA:HB2	2.01	0.59
1:M:343:MET:HE1	1:M:416:TYR:CD2	2.38	0.59
3:O:163:TRP:O	3:O:177:ARG:NH1	2.34	0.59
5:Q:78:LEU:HD23	5:Q:79:SER:N	2.17	0.59
9:U:70:LEU:HD12	9:U:71:ASN:N	2.16	0.59
2:B:256:ALA:O	2:B:424:MET:HG3	2.01	0.59
3:C:137:GLN:OE1	3:C:259:ALA:HA	2.02	0.59
3:C:296:PHE:O	3:C:300:ILE:HB	2.02	0.59
2:N:255:ALA:HA	2:N:425:ALA:O	2.01	0.59
4:P:50:HIS:O	4:P:51:LEU:C	2.40	0.59
7:S:25:ALA:O	7:S:27:PRO:HD3	2.02	0.59
1:A:36:THR:OG1	1:A:372:THR:HG22	2.03	0.59
2:B:203:ARG:CZ	2:B:230:LEU:HD23	2.32	0.59
2:B:438:GLU:OE2	2:N:169:ARG:CZ	2.51	0.59
3:C:221:HIS:HB3	3:C:222:PRO:CD	2.27	0.59
3:C:312:GLN:HE22	3:C:317:PHE:HB2	1.67	0.59
1:M:106:LEU:N	1:M:107:PRO:HD2	2.17	0.59
3:O:221:HIS:HB3	3:O:222:PRO:CD	2.29	0.59
5:Q:97:PHE:CE1	5:Q:137:GLY:HA3	2.37	0.59
1:A:32:GLN:HG2	1:A:33:PRO:CD	2.33	0.59
4:D:26:ILE:HG22	4:D:54:VAL:HG13	1.84	0.59
7:G:2:ARG:HB2	7:G:6:HIS:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:408:ARG:NH2	11:W:15:ARG:CZ	2.65	0.59
2:N:69:LEU:HD21	2:N:199:PHE:CZ	2.37	0.59
3:O:32:ASN:HD21	3:O:228:ASP:HA	1.67	0.59
1:A:373:THR:HB	1:A:374:PRO:HD3	1.84	0.59
1:A:4:TYR:CE2	1:A:396:GLU:HG3	2.38	0.59
3:C:160:LEU:HD12	3:C:160:LEU:O	2.03	0.59
3:C:377:LEU:HB3	6:F:33:ARG:HD2	1.85	0.59
2:N:264:ILE:HG21	2:N:317:SER:HA	1.85	0.59
3:O:270:PRO:HB2	3:O:274:PHE:HB2	1.85	0.59
7:S:25:ALA:C	7:S:27:PRO:HD3	2.23	0.59
8:T:58:LEU:HD11	8:T:62:LEU:CD1	2.32	0.59
1:A:428:ILE:HG21	1:A:431:LEU:HD22	1.83	0.59
1:A:48:GLU:OE1	1:A:53:ASN:O	2.20	0.59
2:B:132:PHE:HB3	2:B:137:VAL:HG21	1.85	0.59
3:C:359:PHE:O	3:C:363:LEU:HB2	2.03	0.59
3:O:153:ILE:N	3:O:153:ILE:HD12	2.18	0.59
3:O:377:LEU:O	3:O:378:LYS:HB3	2.03	0.59
5:Q:69:LEU:HG	5:Q:69:LEU:O	2.02	0.59
1:A:11:VAL:HG13	1:A:12:PRO:HD2	1.84	0.59
1:A:268:VAL:O	1:A:272:VAL:HG23	2.03	0.59
1:A:350:THR:HB	1:A:353:GLU:HG3	1.84	0.59
1:A:426:GLY:HA2	1:A:428:ILE:HG13	1.84	0.59
2:B:98:VAL:HG22	2:B:107:TYR:CD2	2.37	0.59
3:C:103:TYR:HA	3:C:315:MET:CE	2.32	0.59
3:C:213:SER:O	3:C:215:VAL:N	2.36	0.59
4:D:23:HIS:CD2	10:J:51:LEU:HA	2.37	0.59
2:N:203:ARG:CZ	2:N:230:LEU:HD23	2.33	0.59
2:N:264:ILE:HD12	2:N:315:SER:O	2.03	0.59
3:O:1:MET:SD	3:O:4:ILE:HB	2.43	0.59
3:O:92:ILE:O	3:O:96:MET:HG2	2.02	0.59
1:A:15:GLN:O	1:A:26:ALA:HA	2.03	0.58
1:A:426:GLY:HA2	1:A:428:ILE:CG1	2.32	0.58
4:D:178:THR:CB	4:D:181:GLN:HG3	2.32	0.58
1:M:272:VAL:HG21	1:M:402:VAL:HG21	1.85	0.58
1:M:341:GLN:OE1	1:M:344:ARG:HD3	2.03	0.58
1:M:91:THR:HG22	1:M:94:HIS:H	1.67	0.58
5:Q:147:ILE:N	5:Q:157:TYR:O	2.36	0.58
1:M:239:SER:HB2	7:S:18:LEU:HD23	1.84	0.58
1:A:343:MET:HE3	1:A:416:TYR:HD2	1.68	0.58
3:C:115:ILE:CD1	3:C:115:ILE:N	2.66	0.58
9:I:58:GLN:HG2	9:I:78:TYR:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:397:SER:O	1:M:400:ALA:HB3	2.03	0.58
3:O:310:SER:HB3	3:O:318:ARG:NH1	2.18	0.58
3:O:68:HIS:NE2	5:Q:67:ASP:HB2	2.18	0.58
5:Q:101:ARG:HA	5:Q:105:GLU:OE1	2.02	0.58
1:A:338:LEU:O	1:A:341:GLN:N	2.35	0.58
2:B:42:ALA:CB	2:B:43:PRO:HD2	2.28	0.58
3:C:8:HIS:CB	3:C:9:PRO:CD	2.81	0.58
1:M:18:GLN:HG2	1:M:19:LEU:O	2.04	0.58
1:M:43:ALA:CB	1:M:189:HIS:HB3	2.32	0.58
3:O:78:ILE:O	3:O:82:MET:HB2	2.02	0.58
4:P:161:ALA:HB1	4:P:162:PRO:HD2	1.86	0.58
5:Q:76:ILE:HA	5:Q:193:VAL:O	2.03	0.58
4:P:139:THR:HB	8:T:44:VAL:HB	1.83	0.58
5:Q:40:THR:HG22	10:V:20:PHE:HZ	1.67	0.58
2:B:162:ASN:HB3	2:B:244:ILE:HG21	1.84	0.58
4:D:138:PRO:HG2	8:H:55:THR:OG1	2.04	0.58
4:D:27:ARG:O	4:D:28:ARG:C	2.41	0.58
8:H:65:ARG:CG	8:H:66:ASP:N	2.66	0.58
3:O:240:MET:HA	3:O:243:VAL:HG12	1.86	0.58
4:P:120:ARG:HH11	4:P:120:ARG:CG	2.16	0.58
4:P:46:VAL:HG12	4:P:47:ALA:O	2.02	0.58
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.85	0.58
1:A:317:THR:HG22	1:A:318:GLY:H	1.67	0.58
2:B:134:ARG:HH12	6:R:51:PRO:HD3	1.69	0.58
3:O:240:MET:O	3:O:244:LEU:HB2	2.04	0.58
4:P:23:HIS:CD2	10:V:51:LEU:HA	2.38	0.58
6:R:73:GLN:HE21	7:S:32:LYS:HZ1	1.52	0.58
8:T:73:LEU:HD21	8:T:74:PHE:HD1	1.68	0.58
1:A:120:CYS:O	1:A:122:LEU:HG	2.04	0.58
1:A:436:ARG:HE	3:C:222:PRO:HD3	1.68	0.58
3:C:4:ILE:O	3:C:4:ILE:HG22	2.02	0.58
3:C:79:ILE:HG12	5:E:58:PHE:CE1	2.35	0.58
1:M:428:ILE:HG22	1:M:431:LEU:CG	2.32	0.58
2:N:109:VAL:O	2:N:109:VAL:HG13	2.04	0.58
2:N:328:SER:HB3	2:N:336:VAL:HG21	1.86	0.58
5:Q:188:THR:CG2	5:Q:194:ILE:HG13	2.34	0.58
9:U:62:ARG:HB3	9:U:63:PRO:HD3	1.84	0.58
1:A:426:GLY:CA	1:A:428:ILE:N	2.66	0.58
4:D:32:VAL:HG11	4:D:182:VAL:HG13	1.84	0.58
4:D:43:MET:HG2	4:D:46:VAL:CG2	2.33	0.58
4:D:138:PRO:CB	8:H:55:THR:N	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:275:LEU:HD22	2:N:414:ALA:HB2	1.85	0.58
3:O:129:MET:CG	3:O:178:PHE:HD1	2.14	0.58
1:M:233:PRO:HG2	5:Q:23:LYS:NZ	2.19	0.58
1:A:343:MET:CE	1:A:416:TYR:HD2	2.17	0.58
2:B:169:ARG:HG2	2:N:435:PHE:CE1	2.39	0.58
5:E:34:GLY:HA2	10:J:10:TYR:HD2	1.67	0.58
2:N:299:VAL:HG13	2:N:303:VAL:HG21	1.86	0.58
2:N:304:HIS:CG	2:N:305:GLN:H	2.22	0.58
6:R:58:ARG:HG2	6:R:58:ARG:HH11	1.68	0.58
6:R:28:LYS:CB	6:R:74:ILE:HD11	2.34	0.58
8:T:25:GLU:HA	8:T:30:CYS:SG	2.44	0.58
2:B:238:LYS:HE3	2:B:239:TYR:O	2.04	0.58
2:B:72:ALA:O	2:B:75:LEU:HG	2.04	0.58
1:M:350:THR:HB	1:M:353:GLU:HG3	1.85	0.58
1:M:354:VAL:HG13	1:M:407:VAL:HG21	1.86	0.58
1:A:156:THR:OG1	1:A:241:ILE:HB	2.03	0.58
1:A:417:ASP:OD1	5:E:33:LYS:HD2	2.04	0.58
2:B:111:CYS:HB3	2:B:119:LEU:CD2	2.29	0.58
2:B:239:TYR:OH	2:B:421:ARG:O	2.19	0.58
3:C:51:LEU:HD21	3:C:79:ILE:CG2	2.33	0.58
4:D:10:TYR:CE1	8:H:73:LEU:HD21	2.37	0.58
4:D:138:PRO:O	4:D:139:THR:C	2.40	0.58
4:D:21:LEU:HD11	4:D:192:TRP:HB2	1.84	0.58
7:G:44:CYS:SG	7:G:48:VAL:CG2	2.91	0.58
10:J:38:GLY:O	10:J:42:ILE:HG13	2.04	0.58
3:O:218:ILE:HG23	3:O:219:PRO:HD2	1.86	0.58
4:P:158:ILE:HG12	4:P:159:GLY:N	2.19	0.58
4:P:240:PRO:CD	4:P:241:LYS:H	2.16	0.58
6:R:28:LYS:HB3	6:R:74:ILE:HD11	1.86	0.58
10:V:29:LEU:HD13	11:W:34:SER:HB2	1.84	0.58
1:A:346:CYS:HB3	1:A:412:SER:HG	1.69	0.57
3:C:309:THR:HG21	3:C:367:PRO:O	2.03	0.57
8:H:35:GLU:O	8:H:39:LEU:HG	2.04	0.57
2:N:76:THR:HG21	2:N:133:ARG:NH2	2.18	0.57
2:N:148:LYS:HD2	2:N:178:CYS:O	2.04	0.57
2:N:79:GLY:HA3	2:N:125:ASN:HD21	1.69	0.57
3:O:211:ILE:HG21	6:R:62:ILE:HD13	1.86	0.57
7:S:68:LYS:O	7:S:72:LYS:N	2.31	0.57
2:B:99:THR:O	2:B:106:ALA:N	2.37	0.57
5:E:33:LYS:HA	7:G:21:PHE:CE2	2.38	0.57
1:M:317:THR:HG22	1:M:318:GLY:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:262:ALA:HB2	2:N:272:PHE:HE2	1.69	0.57
3:O:206:ASN:CB	3:O:313:ARG:NH2	2.55	0.57
2:B:49:LEU:HD21	2:B:204:MET:SD	2.44	0.57
3:C:240:MET:CA	3:C:243:VAL:HG12	2.28	0.57
3:C:67:THR:O	3:C:71:ARG:HG3	2.04	0.57
1:M:240:GLN:HG3	1:M:422:VAL:O	2.05	0.57
1:M:268:VAL:O	1:M:272:VAL:HG23	2.04	0.57
1:M:308:GLN:O	1:M:308:GLN:HG3	2.02	0.57
3:O:165:TRP:HA	3:O:174:THR:OG1	2.04	0.57
5:Q:87:MET:HG2	5:Q:89:PHE:CE1	2.40	0.57
4:P:138:PRO:CB	8:T:55:THR:N	2.67	0.57
1:M:408:ARG:NH1	11:W:15:ARG:NE	2.47	0.57
1:A:311:ASN:OD1	1:A:320:LEU:CD2	2.52	0.57
8:H:34:ARG:O	8:H:38:GLU:HG2	2.05	0.57
1:M:45:SER:HB3	1:M:167:VAL:HG22	1.86	0.57
1:M:342:TRP:O	1:M:345:LEU:HB2	2.04	0.57
1:M:351:GLU:HA	1:M:404:ALA:HB2	1.85	0.57
1:M:434:TYR:HA	1:M:437:ILE:HD12	1.87	0.57
1:M:55:ALA:O	1:M:56:GLY:C	2.43	0.57
2:N:146:ILE:O	2:N:150:VAL:HG13	2.03	0.57
3:O:67:THR:O	3:O:71:ARG:HG3	2.04	0.57
2:N:97:SER:OG	9:U:70:LEU:HB2	2.04	0.57
1:A:272:VAL:HG21	1:A:402:VAL:HG21	1.87	0.57
3:C:332:LEU:HD21	3:C:358:TYR:CE1	2.38	0.57
5:E:29:SER:CB	5:E:32:ARG:HD3	2.35	0.57
4:D:3:LEU:HD22	7:G:70:LYS:NZ	2.19	0.57
1:M:270:LEU:O	1:M:273:ALA:HB3	2.04	0.57
2:N:206:LEU:HD13	2:N:224:LEU:CD1	2.34	0.57
4:P:178:THR:CB	4:P:181:GLN:HG3	2.28	0.57
5:Q:153:PHE:CE1	5:Q:172:ARG:HB2	2.39	0.57
1:A:151:ASN:O	1:A:152:TYR:C	2.43	0.57
3:O:15:ASN:O	3:O:18:PHE:HD2	1.87	0.57
3:O:28:SER:HB3	3:O:30:TRP:CD1	2.39	0.57
5:Q:114:VAL:O	5:Q:117:LEU:HB2	2.04	0.57
1:A:394:GLU:O	1:A:397:SER:N	2.38	0.57
1:A:408:ARG:NH1	11:K:15:ARG:NE	2.45	0.57
2:B:111:CYS:CB	2:B:119:LEU:HD22	2.28	0.57
2:B:155:PRO:O	2:B:156:GLN:C	2.43	0.57
2:B:59:ASN:CG	2:B:60:SER:H	2.07	0.57
2:B:68:LEU:HD11	2:B:140:LEU:HD23	1.86	0.57
3:C:163:TRP:CZ2	5:Q:62:MET:HE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:79:GLU:OE1	4:D:82:MET:HG3	2.03	0.57
1:A:136:GLN:HE21	9:I:50:LEU:HB3	1.70	0.57
10:J:32:GLU:CG	10:J:33:ARG:N	2.67	0.57
3:O:169:SER:OG	3:O:170:VAL:N	2.37	0.57
3:O:320:LEU:HB2	3:O:373:GLU:OE2	2.04	0.57
4:P:117:VAL:HG11	4:P:191:ARG:HH11	1.70	0.57
10:V:13:LEU:O	10:V:19:THR:OG1	2.17	0.57
1:A:25:VAL:HG21	1:A:209:LEU:HD12	1.87	0.57
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.86	0.57
3:C:28:SER:HB3	3:C:30:TRP:CD1	2.40	0.57
4:D:115:TYR:HD2	4:D:119:ALA:HB2	1.69	0.57
1:M:134:ILE:HA	1:M:137:GLU:HG3	1.87	0.57
1:M:338:LEU:O	1:M:341:GLN:N	2.38	0.57
1:M:51:LYS:O	1:M:53:ASN:N	2.38	0.57
2:N:79:GLY:CA	2:N:125:ASN:HD21	2.17	0.57
1:M:417:ASP:OD1	5:Q:33:LYS:HD2	2.05	0.57
6:R:51:PRO:HG2	6:R:54:LEU:HD23	1.84	0.57
2:B:247:GLN:HG3	2:B:248:ASN:N	2.18	0.57
3:C:218:ILE:HG22	3:C:219:PRO:N	2.20	0.57
4:P:10:TYR:O	4:P:12:TRP:CD1	2.58	0.57
5:Q:121:GLN:HG3	5:Q:179:ASN:ND2	2.20	0.57
5:Q:185:TYR:HA	5:Q:194:ILE:O	2.04	0.57
1:A:436:ARG:HE	3:C:222:PRO:CD	2.18	0.57
3:C:71:ARG:NH2	4:D:193:ALA:O	2.38	0.57
4:D:204:MET:O	4:D:205:GLY:C	2.42	0.57
4:D:35:GLN:HB2	4:D:169:LEU:CD1	2.35	0.57
6:F:39:GLU:HB3	6:F:44:LYS:HE2	1.87	0.57
8:H:58:LEU:HD11	8:H:62:LEU:CD1	2.34	0.57
4:D:27:ARG:NH1	10:J:58:LYS:HG3	2.18	0.57
1:M:408:ARG:CZ	11:W:15:ARG:NE	2.67	0.57
1:M:64:PHE:HE1	1:M:86:LEU:HG	1.61	0.57
2:N:304:HIS:CG	2:N:305:GLN:N	2.72	0.57
2:N:352:LEU:HD12	2:N:353:SER:N	2.20	0.57
3:O:313:ARG:HB3	6:R:38:HIS:CD2	2.40	0.57
8:T:21:ARG:CB	8:T:65:ARG:HH21	2.09	0.57
1:A:86:LEU:HD13	1:A:99:ILE:CD1	2.35	0.56
2:B:47:ILE:CD1	2:B:120:MET:SD	2.93	0.56
2:B:52:LYS:HB2	2:B:203:ARG:CB	2.25	0.56
4:D:100:ALA:O	4:D:103:ALA:N	2.37	0.56
4:D:50:HIS:HE1	4:D:91:PHE:HZ	1.53	0.56
2:N:217:LYS:O	2:N:221:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:155:PRO:HB2	2:N:254:HIS:CE1	2.40	0.56
3:O:26:ASN:HD22	3:O:208:PRO:HD2	1.70	0.56
3:O:88:SER:HA	3:O:272:TRP:HZ2	1.70	0.56
6:R:47:ILE:O	6:R:50:LEU:HG	2.04	0.56
3:C:225:THR:O	3:C:229:ILE:HD12	2.05	0.56
5:E:31:ALA:HB1	10:J:6:THR:OG1	2.05	0.56
8:H:21:ARG:HB3	8:H:65:ARG:NH2	2.17	0.56
7:G:71:ARG:HH21	8:H:60:ASP:CG	2.07	0.56
1:A:408:ARG:NH2	11:K:15:ARG:CZ	2.64	0.56
1:M:32:GLN:HG2	1:M:33:PRO:HD2	1.85	0.56
2:N:141:GLN:HE22	2:N:186:VAL:HB	1.70	0.56
2:N:303:VAL:CG1	2:N:304:HIS:N	2.67	0.56
2:N:280:GLY:HA2	2:N:311:ALA:HB3	1.85	0.56
3:O:172:LYS:O	3:O:173:ALA:C	2.41	0.56
3:O:18:PHE:O	3:O:220:PHE:CD2	2.58	0.56
1:A:338:LEU:O	1:A:339:GLN:C	2.41	0.56
2:B:203:ARG:NE	2:B:230:LEU:HD23	2.20	0.56
3:C:135:TRP:HH2	3:C:170:VAL:O	1.89	0.56
6:F:42:ASP:O	6:F:43:VAL:C	2.43	0.56
4:D:139:THR:HB	8:H:44:VAL:HB	1.87	0.56
1:M:245:GLU:O	1:M:247:GLY:N	2.39	0.56
1:M:349:ALA:HB3	1:M:408:ARG:CG	2.35	0.56
1:M:438:ARG:HG3	1:M:438:ARG:HH11	1.70	0.56
12:O:380:HEM:CMC	12:O:380:HEM:HBC2	2.35	0.56
2:B:277:HIS:CD2	2:B:364:LEU:HD13	2.40	0.56
5:E:72:SER:O	5:E:73:LYS:HG2	2.05	0.56
1:M:33:PRO:O	1:M:103:SER:N	2.34	0.56
1:M:64:PHE:HA	1:M:75:LEU:CD2	2.35	0.56
2:N:141:GLN:HB2	2:N:142:PRO:HD3	1.86	0.56
2:N:294:SER:HB3	2:N:343:GLN:HE21	1.70	0.56
7:G:25:ALA:C	7:G:27:PRO:HD3	2.26	0.56
10:J:60:GLU:O	10:J:60:GLU:HG3	2.06	0.56
1:M:270:LEU:O	1:M:273:ALA:N	2.38	0.56
2:N:154:ASN:O	2:N:155:PRO:C	2.43	0.56
3:O:300:ILE:O	3:O:300:ILE:HG12	2.05	0.56
4:P:182:VAL:O	4:P:186:VAL:HG23	2.06	0.56
4:D:150:ASN:OD1	4:D:151:PRO:CD	2.53	0.56
2:N:68:LEU:HD23	2:N:186:VAL:HG11	1.87	0.56
2:N:435:PHE:HB2	2:N:438:GLU:OE1	2.05	0.56
3:O:309:THR:HG23	3:O:370:GLY:HA3	1.86	0.56
4:P:21:LEU:HD11	4:P:192:TRP:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:118:ARG:HB3	5:Q:171:ILE:CG2	2.36	0.56
1:A:248:LEU:N	1:A:248:LEU:HD23	2.19	0.56
1:A:30:SER:N	1:A:201:GLY:O	2.38	0.56
1:A:395:TRP:O	1:A:396:GLU:C	2.43	0.56
3:C:300:ILE:CD1	3:C:362:ILE:HG21	2.36	0.56
2:N:198:HIS:HE1	2:N:233:SER:OG	1.89	0.56
2:N:342:ASN:O	2:N:345:LYS:HB2	2.06	0.56
3:O:170:VAL:HG13	3:O:174:THR:CG2	2.34	0.56
1:A:143:THR:HG21	9:I:48:SER:N	2.14	0.56
1:A:309:THR:HA	1:A:322:ALA:HA	1.86	0.56
1:A:425:PHE:O	1:A:426:GLY:O	2.23	0.56
3:C:192:ILE:HD13	3:C:192:ILE:N	2.21	0.56
3:C:51:LEU:CD2	3:C:79:ILE:HG22	2.34	0.56
1:M:32:GLN:HG2	1:M:33:PRO:CD	2.35	0.56
1:M:426:GLY:HA3	1:M:428:ILE:H	1.71	0.56
3:O:108:THR:CB	3:O:313:ARG:HH11	2.12	0.56
4:P:180:SER:HB3	8:T:17:LEU:HB2	1.88	0.56
10:V:47:ASN:HB3	10:V:50:LYS:HD2	1.88	0.56
1:A:6:GLN:O	1:A:7:ALA:C	2.41	0.56
3:C:218:ILE:HG21	3:C:223:TYR:CD2	2.38	0.56
4:D:69:GLU:O	4:D:73:GLY:HA3	2.05	0.56
2:N:168:TYR:HB2	2:N:173:ALA:HB2	1.88	0.56
3:O:24:PRO:HG2	3:O:205:SER:O	2.06	0.56
3:O:218:ILE:CG2	3:O:223:TYR:HD2	2.19	0.56
3:O:149:LEU:HD21	3:O:281:LEU:HD22	1.86	0.56
7:S:31:SER:O	7:S:35:PRO:CD	2.47	0.56
1:A:278:GLY:O	1:A:309:THR:HG23	2.05	0.56
1:A:394:GLU:O	1:A:395:TRP:C	2.44	0.56
2:B:264:ILE:CG2	2:B:317:SER:HA	2.36	0.56
3:C:264:THR:O	3:C:266:PRO:HD3	2.06	0.56
6:F:106:GLU:HA	6:F:109:LYS:HZ3	1.70	0.56
6:F:74:ILE:HD13	6:F:80:TRP:CZ2	2.40	0.56
3:O:315:MET:HA	3:O:318:ARG:HG3	1.87	0.56
3:O:310:SER:HB3	3:O:318:ARG:HH11	1.69	0.56
4:P:83:ARG:CB	4:P:84:PRO:HD2	2.09	0.56
1:M:233:PRO:HG2	5:Q:23:LYS:CE	2.36	0.56
1:A:5:ALA:O	1:A:6:GLN:C	2.43	0.56
3:C:115:ILE:N	3:C:115:ILE:HD12	2.21	0.56
3:C:338:ILE:H	3:C:338:ILE:CD1	2.19	0.56
3:C:353:LEU:N	3:C:353:LEU:HD23	2.21	0.56
4:D:181:GLN:HA	8:H:77:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:69:GLU:HA	4:D:73:GLY:HA2	1.88	0.56
6:F:50:LEU:CB	6:F:55:TYR:HB2	2.29	0.56
6:F:91:GLU:HB2	6:F:92:PRO:HD3	1.86	0.56
1:M:266:ASP:O	1:M:270:LEU:HG	2.06	0.56
4:P:128:PHE:HB2	4:P:187:CYS:SG	2.46	0.56
4:P:138:PRO:O	4:P:141:VAL:HB	2.06	0.56
7:S:73:ASN:HD22	8:T:56:GLU:CD	2.08	0.56
9:U:58:GLN:HG2	9:U:78:TYR:CD2	2.40	0.56
2:B:160:ILE:HD11	2:B:325:TYR:CE2	2.40	0.55
2:B:185:LYS:O	2:B:185:LYS:CG	2.54	0.55
3:C:102:LEU:HB3	3:C:325:PHE:HE1	1.71	0.55
4:D:229:VAL:O	4:D:233:ARG:HG3	2.05	0.55
5:E:45:VAL:HG13	10:J:28:ALA:N	2.21	0.55
1:M:249:PRO:O	1:M:250:LEU:HD23	2.07	0.55
5:Q:142:LEU:HD12	5:Q:161:HIS:HE1	1.71	0.55
8:T:15:ASP:HB2	8:T:16:PRO:CD	2.37	0.55
1:A:162:PRO:O	1:A:165:GLN:NE2	2.38	0.55
1:A:426:GLY:H	1:A:428:ILE:HG13	1.63	0.55
2:B:90:GLU:O	2:B:91:ALA:C	2.44	0.55
3:C:25:SER:O	3:C:26:ASN:C	2.45	0.55
3:C:310:SER:HB3	3:C:318:ARG:HH12	1.71	0.55
6:F:101:ARG:HG2	6:F:105:GLU:OE2	2.06	0.55
1:M:134:ILE:CG2	1:M:174:VAL:HG21	2.35	0.55
1:M:111:GLU:HG2	1:M:213:GLN:HE22	1.71	0.55
1:M:331:ILE:CD1	1:M:427:PRO:O	2.55	0.55
6:F:49:ARG:HD3	2:N:135:TRP:CD2	2.41	0.55
2:N:159:VAL:HG12	2:N:160:ILE:N	2.21	0.55
2:N:187:THR:O	2:N:190:GLU:HB2	2.05	0.55
1:M:136:GLN:HE21	9:U:50:LEU:HB3	1.70	0.55
2:N:308:ASP:OD2	9:U:55:LEU:HA	2.06	0.55
1:A:343:MET:O	1:A:344:ARG:C	2.41	0.55
1:A:39:VAL:CG1	1:A:41:ILE:HD11	2.36	0.55
2:B:100:SER:HB3	2:B:105:MET:HG3	1.89	0.55
1:M:413:LYS:HB2	1:M:414:TYR:CD2	2.42	0.55
3:O:148:ASN:O	3:O:151:SER:OG	2.24	0.55
3:O:171:ASP:O	3:O:172:LYS:C	2.44	0.55
3:O:34:GLY:O	3:O:37:LEU:HB2	2.05	0.55
5:Q:140:THR:HG21	5:Q:178:LEU:HB2	1.88	0.55
7:S:33:GLY:O	7:S:37:VAL:N	2.35	0.55
1:A:385:THR:CG2	1:A:386:TYR:CD1	2.89	0.55
1:A:343:MET:CE	1:A:416:TYR:CD2	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:MET:HG2	3:C:274:PHE:HE1	1.71	0.55
4:D:229:VAL:CG1	4:D:233:ARG:HE	2.18	0.55
1:M:112:LEU:O	1:M:116:ILE:HG13	2.07	0.55
1:M:161:THR:CB	1:M:162:PRO:HD2	2.34	0.55
2:N:92:VAL:O	2:N:92:VAL:HG12	2.06	0.55
3:O:296:PHE:O	3:O:300:ILE:HB	2.05	0.55
4:P:139:THR:HG21	8:T:41:ASP:O	2.06	0.55
3:O:234:LEU:HD21	4:P:216:LEU:HD21	1.85	0.55
5:Q:187:PHE:HA	5:Q:193:VAL:HA	1.88	0.55
8:T:40:CYS:HB2	8:T:57:GLU:HG2	1.89	0.55
1:A:146:ARG:CZ	1:A:308:GLN:HE22	2.19	0.55
1:A:386:TYR:N	1:A:386:TYR:CD1	2.72	0.55
2:B:273:SER:O	2:B:276:GLN:HB3	2.06	0.55
3:C:378:LYS:HD3	6:F:33:ARG:HH12	1.72	0.55
6:F:73:GLN:HA	7:G:39:ARG:HH21	1.71	0.55
1:M:46:ARG:NH1	1:M:316:ASP:OD1	2.40	0.55
5:Q:102:THR:OG1	5:Q:105:GLU:HB2	2.06	0.55
1:A:39:VAL:CG2	1:A:197:LEU:HD22	2.37	0.55
2:B:261:SER:OG	2:B:262:ALA:N	2.39	0.55
2:B:276:GLN:O	2:B:280:GLY:N	2.40	0.55
3:C:71:ARG:HE	4:D:196:PRO:HG3	1.72	0.55
1:M:224:ASP:O	1:M:227:ALA:N	2.39	0.55
3:O:122:THR:HG22	3:O:189:ILE:CD1	2.27	0.55
4:P:69:GLU:HG3	4:P:84:PRO:HA	1.89	0.55
5:Q:150:ALA:HB3	5:Q:157:TYR:CB	2.36	0.55
5:Q:76:ILE:O	5:Q:77:LYS:HG2	2.06	0.55
7:S:34:ILE:CB	7:S:35:PRO:HD3	2.33	0.55
1:A:33:PRO:O	1:A:103:SER:N	2.36	0.55
1:A:342:TRP:O	1:A:345:LEU:N	2.40	0.55
1:A:255:ILE:HG13	1:A:422:VAL:CG2	2.37	0.55
2:B:280:GLY:HA2	2:B:311:ALA:HB3	1.88	0.55
1:A:142:ASP:OD1	5:E:2:HIS:ND1	2.36	0.55
6:F:10:SER:OG	6:F:13:LEU:HD11	2.07	0.55
7:G:68:LYS:O	7:G:72:LYS:N	2.34	0.55
7:G:73:ASN:HD22	8:H:56:GLU:CD	2.10	0.55
10:J:12:LEU:HD23	10:J:13:LEU:CD2	2.36	0.55
2:N:257:LEU:HD13	2:N:424:MET:HE2	1.88	0.55
2:N:264:ILE:HB	2:N:316:TYR:O	2.06	0.55
3:O:132:VAL:HA	3:O:139:SER:CB	2.36	0.55
1:A:173:ASN:O	1:A:177:LEU:HB2	2.07	0.55
1:A:256:ALA:HA	1:A:320:LEU:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLU:O	1:A:352:SER:C	2.42	0.55
1:A:397:SER:O	1:A:400:ALA:HB3	2.07	0.55
2:B:55:SER:OG	2:B:102:ARG:HG2	2.06	0.55
3:C:312:GLN:O	3:C:314:SER:N	2.40	0.55
3:C:41:LEU:O	3:C:45:ILE:HG13	2.06	0.55
4:D:219:VAL:HA	4:D:222:MET:HG3	1.88	0.55
4:D:50:HIS:O	4:D:54:VAL:N	2.28	0.55
1:M:363:ASN:CG	2:N:112:LEU:HD23	2.27	0.55
2:N:88:GLY:O	2:N:91:ALA:HB3	2.07	0.55
3:O:147:THR:O	3:O:150:LEU:HB2	2.07	0.55
3:O:275:LEU:O	3:O:276:PHE:C	2.45	0.55
4:P:149:PHE:HZ	8:T:55:THR:HG23	1.72	0.55
4:P:219:VAL:HA	4:P:222:MET:HG3	1.89	0.55
5:Q:188:THR:HG21	5:Q:194:ILE:HD11	1.87	0.55
1:A:317:THR:HG22	1:A:318:GLY:N	2.21	0.55
3:C:25:SER:HA	3:C:218:ILE:HD12	1.89	0.55
3:C:137:GLN:HB2	3:C:257:THR:OG1	2.07	0.55
4:D:11:PRO:HB2	8:H:74:PHE:CG	2.41	0.55
3:C:72:ASP:HB3	5:E:67:ASP:H	1.71	0.55
10:J:51:LEU:HB3	10:J:52:TRP:CE3	2.42	0.55
3:O:265:PRO:O	3:O:268:ILE:HG13	2.07	0.55
3:O:345:HIS:CB	3:O:346:PRO:HD3	2.26	0.55
3:O:44:GLN:HE22	3:O:86:GLY:HA3	1.70	0.55
1:A:241:ILE:HG23	1:A:241:ILE:O	2.07	0.55
2:B:102:ARG:HH12	2:B:175:SER:HA	1.71	0.55
2:B:203:ARG:NH2	2:B:230:LEU:HD23	2.22	0.55
2:B:262:ALA:HB2	2:B:272:PHE:HE2	1.72	0.55
2:B:33:LEU:HB2	2:B:204:MET:O	2.07	0.55
3:C:182:HIS:O	3:C:186:PRO:HD2	2.06	0.55
3:C:244:LEU:HD11	4:D:204:MET:CE	2.37	0.55
4:D:164:ILE:HD11	13:D:242:HEC:CBB	2.37	0.55
4:D:21:LEU:CD1	4:D:192:TRP:HB2	2.36	0.55
4:D:213:GLY:O	4:D:217:PRO:HG3	2.07	0.55
5:E:29:SER:CA	5:E:32:ARG:HD3	2.37	0.55
1:M:240:GLN:HA	1:M:422:VAL:O	2.06	0.55
2:N:62:ASN:O	2:N:62:ASN:ND2	2.40	0.55
4:P:216:LEU:N	4:P:217:PRO:HD2	2.22	0.55
5:Q:118:ARG:HH22	5:Q:173:LYS:CA	2.20	0.55
8:T:70:ALA:HA	8:T:73:LEU:HD22	1.89	0.55
9:U:58:GLN:HG2	9:U:78:TYR:HD2	1.72	0.55
2:N:213:HIS:N	2:N:214:PRO:CD	2.69	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:GLU:OE1	2:B:175:SER:HB2	2.07	0.54
3:C:61:THR:O	3:C:64:SER:N	2.41	0.54
5:E:15:ARG:NH2	5:E:32:ARG:HG3	2.22	0.54
6:F:35:ASP:OD2	6:F:61:ARG:HD2	2.07	0.54
6:F:96:GLU:O	6:F:97:VAL:C	2.45	0.54
8:H:21:ARG:CB	8:H:65:ARG:HH21	2.17	0.54
2:N:258:VAL:HG12	2:N:321:LEU:HD22	1.89	0.54
2:N:33:LEU:HD23	2:N:33:LEU:O	2.07	0.54
3:O:185:LEU:HB3	3:O:186:PRO:CD	2.35	0.54
3:O:219:PRO:HB2	3:O:222:PRO:HD2	1.89	0.54
1:A:334:MET:CE	1:A:334:MET:HA	2.37	0.54
2:B:303:VAL:CG1	2:B:304:HIS:N	2.70	0.54
2:B:86:THR:CG2	9:I:71:ASN:HD21	2.19	0.54
1:M:241:ILE:HG13	7:S:16:TYR:CE2	2.43	0.54
6:R:51:PRO:HG2	6:R:54:LEU:HB2	1.89	0.54
9:U:62:ARG:H	9:U:63:PRO:HD2	1.71	0.54
1:A:272:VAL:HG13	1:A:358:LYS:HA	1.88	0.54
3:C:215:VAL:O	6:F:63:LYS:NZ	2.37	0.54
7:G:73:ASN:H	7:G:74:PRO:HD2	1.67	0.54
1:M:279:HIS:ND1	1:M:284:TYR:OH	2.39	0.54
6:F:51:PRO:CD	2:N:134:ARG:NH1	2.68	0.54
3:O:133:LEU:HB2	3:O:134:PRO:HD3	1.90	0.54
3:O:206:ASN:ND2	3:O:207:ASN:H	2.04	0.54
4:P:7:PRO:CB	4:P:125:ASP:HB3	2.37	0.54
4:P:160:MET:HE3	4:P:163:PRO:HG3	1.89	0.54
4:P:4:GLU:HG3	4:P:6:HIS:CE1	2.42	0.54
4:P:94:PRO:HB2	4:P:95:TYR:CE1	2.42	0.54
1:A:61:HIS:CB	1:A:130:GLU:HG3	2.37	0.54
1:A:62:LEU:O	1:A:63:ALA:C	2.46	0.54
2:B:132:PHE:CD2	2:B:191:LEU:HD13	2.43	0.54
2:B:217:LYS:O	2:B:218:GLN:C	2.45	0.54
2:N:318:ASP:N	2:N:318:ASP:OD1	2.39	0.54
2:N:408:ALA:O	2:N:411:ILE:N	2.40	0.54
2:N:95:LYS:HE3	2:N:97:SER:OG	2.08	0.54
3:O:119:LEU:HD13	3:O:192:ILE:CG2	2.37	0.54
3:O:234:LEU:HD21	4:P:216:LEU:CD2	2.37	0.54
1:A:109:ALA:O	1:A:112:LEU:N	2.40	0.54
3:C:106:SER:O	3:C:109:PHE:CD1	2.54	0.54
3:C:15:ASN:O	3:C:18:PHE:HD1	1.90	0.54
3:C:1:MET:SD	3:C:4:ILE:HB	2.48	0.54
3:C:218:ILE:HG22	3:C:223:TYR:HD2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:TRP:HA	3:C:33:PHE:HE2	1.73	0.54
4:D:211:MET:HA	4:D:211:MET:HE3	1.90	0.54
10:J:32:GLU:HG2	10:J:33:ARG:N	2.22	0.54
3:O:207:ASN:ND2	3:O:209:THR:OG1	2.41	0.54
3:O:37:LEU:HD11	3:O:97:HIS:CG	2.43	0.54
6:R:7:SER:HA	6:R:11:ARG:HE	1.73	0.54
8:T:35:GLU:O	8:T:39:LEU:HG	2.07	0.54
3:C:309:THR:CG2	3:C:370:GLY:HA3	2.38	0.54
4:D:33:TYR:HA	4:D:37:CYS:HB2	1.89	0.54
4:D:4:GLU:HG3	4:D:6:HIS:CE1	2.43	0.54
4:D:74:PRO:O	4:D:79:GLU:N	2.36	0.54
1:M:143:THR:HG21	9:U:48:SER:N	2.08	0.54
1:M:256:ALA:HB3	1:M:421:ALA:HB3	1.89	0.54
1:M:61:HIS:CB	1:M:130:GLU:HG3	2.38	0.54
1:A:112:LEU:O	1:A:116:ILE:HD12	2.07	0.54
1:A:18:GLN:HG2	1:A:19:LEU:O	2.07	0.54
2:B:62:ASN:O	2:B:62:ASN:ND2	2.41	0.54
2:B:90:GLU:O	2:B:92:VAL:N	2.41	0.54
1:A:436:ARG:HE	3:C:222:PRO:HG3	1.73	0.54
3:C:348:ILE:O	3:C:352:GLN:HG3	2.08	0.54
4:D:74:PRO:HG2	4:D:82:MET:HB3	1.89	0.54
3:C:68:HIS:NE2	5:E:67:ASP:HB2	2.22	0.54
7:G:33:GLY:O	7:G:37:VAL:N	2.36	0.54
1:M:191:LYS:NZ	1:M:220:SER:OG	2.41	0.54
4:P:168:VAL:O	4:P:169:LEU:HD23	2.08	0.54
6:R:106:GLU:OE1	6:R:109:LYS:HE2	2.06	0.54
6:R:91:GLU:N	6:R:92:PRO:HD2	2.22	0.54
1:A:236:PHE:CD2	1:A:258:GLU:CB	2.91	0.54
1:A:93:GLU:O	1:A:94:HIS:ND1	2.40	0.54
1:A:61:HIS:CD2	2:B:287:ARG:HD3	2.43	0.54
3:C:135:TRP:CH2	3:C:170:VAL:HG12	2.41	0.54
3:C:88:SER:HA	3:C:272:TRP:HZ2	1.73	0.54
5:E:63:SER:O	5:E:64:ALA:HB2	2.08	0.54
10:J:45:HIS:O	10:J:48:GLU:HG2	2.08	0.54
1:M:317:THR:HG22	1:M:318:GLY:H	1.73	0.54
1:M:335:MET:CE	1:M:339:GLN:HG3	2.35	0.54
2:N:280:GLY:HA2	2:N:311:ALA:CB	2.38	0.54
3:O:245:PHE:CG	4:P:17:LEU:HD13	2.43	0.54
4:P:50:HIS:O	4:P:54:VAL:N	2.32	0.54
5:Q:136:ILE:CG2	5:Q:136:ILE:O	2.55	0.54
5:Q:77:LYS:HG3	5:Q:89:PHE:HE2	1.68	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:SER:CB	2:B:105:MET:HG3	2.37	0.54
2:B:160:ILE:CD1	2:B:325:TYR:HE2	2.21	0.54
3:C:88:SER:HB3	3:C:250:LEU:CD2	2.38	0.54
3:C:310:SER:CB	3:C:318:ARG:NH1	2.58	0.54
4:D:131:LEU:CD2	4:D:163:PRO:HB3	2.38	0.54
4:D:51:LEU:HD22	4:D:58:GLU:HA	1.89	0.54
7:G:15:THR:O	7:G:15:THR:HG22	2.07	0.54
1:M:53:ASN:HB3	1:M:170:PRO:HD2	1.89	0.54
1:M:324:PHE:CD1	1:M:334:MET:HG2	2.42	0.54
3:O:76:GLY:HA2	3:O:79:ILE:HD12	1.90	0.54
4:P:7:PRO:HG3	4:P:126:TYR:CA	2.36	0.54
4:P:3:LEU:HD21	7:S:71:ARG:HA	1.90	0.54
4:P:50:HIS:HE1	4:P:91:PHE:HZ	1.54	0.54
3:O:377:LEU:HB3	6:R:33:ARG:HD2	1.88	0.54
1:A:252:HIS:CD2	1:A:325:VAL:CG2	2.92	0.53
1:A:32:GLN:CG	1:A:33:PRO:CD	2.86	0.53
3:C:133:LEU:HD21	3:C:179:PHE:HA	1.88	0.53
1:M:22:GLY:O	1:M:24:ARG:HG2	2.08	0.53
1:M:236:PHE:CD2	1:M:258:GLU:CB	2.91	0.53
3:O:174:THR:O	3:O:178:PHE:CD2	2.62	0.53
4:P:82:MET:HE2	4:P:86:LYS:NZ	2.23	0.53
5:Q:150:ALA:HB3	5:Q:157:TYR:HB3	1.91	0.53
4:P:237:TYR:HD1	7:S:13:VAL:HG22	1.73	0.53
10:V:34:ALA:O	10:V:35:PHE:C	2.45	0.53
1:A:11:VAL:CG1	1:A:12:PRO:HD2	2.39	0.53
2:B:140:LEU:HD12	2:B:143:GLN:CB	2.38	0.53
2:B:266:SER:O	2:B:269:ALA:HB3	2.07	0.53
2:B:305:GLN:CB	2:B:306:PRO:HD3	2.31	0.53
3:C:148:ASN:O	3:C:151:SER:OG	2.26	0.53
8:H:73:LEU:O	8:H:73:LEU:HG	2.08	0.53
9:I:58:GLN:HG2	9:I:78:TYR:HD2	1.72	0.53
2:N:262:ALA:HB2	2:N:268:GLU:HB3	1.90	0.53
2:N:255:ALA:HB2	2:N:426:ALA:CB	2.37	0.53
5:Q:171:ILE:HD12	5:Q:176:ALA:HB3	1.90	0.53
5:Q:78:LEU:HD21	5:Q:132:TRP:CZ2	2.43	0.53
5:Q:89:PHE:O	5:Q:96:LEU:N	2.23	0.53
4:P:138:PRO:HB3	8:T:55:THR:HA	1.90	0.53
1:A:334:MET:HA	1:A:334:MET:HE3	1.90	0.53
1:A:418:GLN:O	1:A:420:PRO:HD3	2.08	0.53
2:B:79:GLY:H	2:B:125:ASN:ND2	2.07	0.53
6:F:45:GLU:O	6:F:49:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:7:SER:HA	6:F:11:ARG:HE	1.73	0.53
10:J:52:TRP:CE3	10:J:52:TRP:N	2.76	0.53
2:N:168:TYR:HD2	2:N:238:LYS:O	1.92	0.53
3:C:58:ASP:OD2	3:O:56:THR:HG21	2.08	0.53
4:P:42:SER:HB3	4:P:94:PRO:HD2	1.89	0.53
10:V:49:GLY:HA2	10:V:54:HIS:CB	2.39	0.53
1:A:239:SER:OG	1:A:240:GLN:N	2.40	0.53
2:B:191:LEU:O	2:B:195:VAL:HG23	2.09	0.53
2:B:163:LEU:HD22	2:B:256:ALA:HB1	1.90	0.53
2:B:396:SER:O	2:B:399:LEU:HB2	2.08	0.53
3:C:219:PRO:CB	3:C:222:PRO:HD2	2.39	0.53
4:D:149:PHE:HZ	8:H:55:THR:HG23	1.74	0.53
8:H:65:ARG:HG3	8:H:66:ASP:N	2.23	0.53
1:M:106:LEU:HD22	1:M:203:LEU:CD2	2.35	0.53
2:N:264:ILE:HG22	2:N:317:SER:HA	1.88	0.53
3:O:170:VAL:HG12	3:O:170:VAL:O	2.08	0.53
8:T:73:LEU:HD21	8:T:74:PHE:CD1	2.43	0.53
3:C:141:TRP:HB3	3:C:268:ILE:HD13	1.90	0.53
10:J:57:HIS:O	10:J:58:LYS:C	2.46	0.53
1:M:88:ALA:O	2:N:286:LYS:HE2	2.08	0.53
2:N:372:VAL:O	2:N:372:VAL:HG12	2.08	0.53
5:Q:139:CYS:HB2	5:Q:165:TYR:CE2	2.39	0.53
5:Q:34:GLY:CA	10:V:10:TYR:HD1	2.22	0.53
1:A:134:ILE:HA	1:A:137:GLU:HG3	1.91	0.53
1:A:55:ALA:O	1:A:58:PHE:N	2.35	0.53
2:B:286:LYS:O	2:B:287:ARG:HB2	2.09	0.53
3:C:377:LEU:O	3:C:378:LYS:HB3	2.09	0.53
3:C:88:SER:CB	3:C:250:LEU:HD23	2.37	0.53
4:D:138:PRO:HG2	8:H:55:THR:CB	2.38	0.53
3:O:124:MET:HE1	3:O:298:ILE:HG21	1.89	0.53
3:O:6:LYS:HE2	3:O:16:ASN:HD21	1.74	0.53
5:Q:139:CYS:O	5:Q:143:GLY:HA2	2.08	0.53
1:A:111:GLU:HG2	1:A:213:GLN:HE22	1.73	0.53
3:C:103:TYR:O	3:C:315:MET:CB	2.57	0.53
5:E:31:ALA:O	5:E:34:GLY:N	2.42	0.53
6:F:96:GLU:OE1	6:F:96:GLU:HA	2.09	0.53
1:M:277:ILE:CG2	1:M:294:LEU:HD12	2.39	0.53
1:M:392:LEU:O	1:M:392:LEU:HG	2.09	0.53
2:N:164:HIS:O	2:N:173:ALA:HA	2.09	0.53
2:B:435:PHE:CE1	2:N:169:ARG:HG2	2.44	0.53
2:N:25:GLU:O	2:N:213:HIS:CE1	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:285:VAL:HG12	2:N:288:GLY:HA3	1.91	0.53
3:O:218:ILE:HG21	3:O:223:TYR:CD2	2.43	0.53
3:O:7:SER:O	3:O:8:HIS:O	2.26	0.53
2:B:160:ILE:HD11	2:B:325:TYR:HE2	1.74	0.53
2:B:69:LEU:HD21	2:B:199:PHE:CZ	2.44	0.53
2:B:92:VAL:HG12	2:B:92:VAL:O	2.08	0.53
5:E:52:LYS:NZ	10:J:32:GLU:OE1	2.40	0.53
1:M:411:CYS:O	1:M:415:PHE:HD1	1.92	0.53
3:O:174:THR:O	3:O:178:PHE:HD2	1.90	0.53
4:P:48:TYR:OH	4:P:68:VAL:HG11	2.08	0.53
8:T:62:LEU:O	8:T:65:ARG:HG2	2.09	0.53
10:V:18:SER:HB3	11:W:23:LEU:HB2	1.90	0.53
1:A:260:PRO:HD3	1:A:414:TYR:CD1	2.44	0.53
1:A:335:MET:HE2	1:A:339:GLN:HG3	1.90	0.53
1:A:53:ASN:HB3	1:A:170:PRO:HD2	1.91	0.53
2:B:279:LEU:HD22	2:B:344:VAL:HG22	1.91	0.53
3:C:183:PHE:CE1	3:C:187:PHE:CE2	2.96	0.53
4:D:48:TYR:OH	4:D:68:VAL:HG11	2.09	0.53
7:G:25:ALA:O	7:G:27:PRO:HD3	2.09	0.53
1:M:428:ILE:CG2	1:M:431:LEU:CD2	2.85	0.53
2:N:262:ALA:HB3	2:N:269:ALA:N	2.24	0.53
3:O:200:LEU:HD13	12:O:381:HEM:HAD2	1.90	0.53
3:O:275:LEU:O	3:O:278:TYR:N	2.42	0.53
4:P:237:TYR:CE2	4:P:239:PRO:HG3	2.44	0.53
5:Q:95:PRO:HG2	5:Q:145:VAL:CG2	2.38	0.53
6:R:49:ARG:NH2	6:R:100:GLU:OE2	2.37	0.53
5:Q:45:VAL:CG2	10:V:24:ILE:HA	2.39	0.53
10:V:4:THR:HG22	10:V:6:THR:OG1	2.09	0.53
1:A:143:THR:CG2	1:A:143:THR:O	2.56	0.53
1:A:106:LEU:HD21	1:A:203:LEU:HD13	1.89	0.53
3:C:24:PRO:O	3:C:224:TYR:OH	2.20	0.53
3:C:119:LEU:HD23	12:C:381:HEM:C4B	2.44	0.53
4:D:10:TYR:CZ	4:D:128:PHE:CE2	2.92	0.53
5:E:2:HIS:O	5:E:5:ILE:HG12	2.09	0.53
2:N:59:ASN:CG	2:N:60:SER:H	2.11	0.53
3:O:218:ILE:HG23	3:O:223:TYR:CD2	2.43	0.53
6:R:73:GLN:HE21	7:S:32:LYS:HE3	1.74	0.53
1:A:166:SER:CB	5:E:3:THR:HG22	2.39	0.52
1:A:67:THR:OG1	1:A:119:ASN:HB2	2.09	0.52
2:B:141:GLN:OE1	2:B:183:ILE:O	2.27	0.52
6:F:28:LYS:HD2	6:F:74:ILE:HD11	1.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:244:ARG:CZ	7:S:10:VAL:HB	2.38	0.52
2:N:277:HIS:CD2	2:N:364:LEU:HD13	2.43	0.52
4:P:26:ILE:O	4:P:27:ARG:C	2.47	0.52
4:P:51:LEU:HD22	4:P:58:GLU:HA	1.90	0.52
2:B:304:HIS:CG	2:B:305:GLN:N	2.76	0.52
3:C:135:TRP:CH2	3:C:170:VAL:O	2.62	0.52
9:I:58:GLN:HB3	9:I:78:TYR:HB2	1.91	0.52
2:N:47:ILE:CG2	2:N:48:GLY:N	2.72	0.52
4:P:120:ARG:HG2	4:P:120:ARG:NH1	2.24	0.52
4:P:27:ARG:NH1	10:V:58:LYS:CE	2.72	0.52
10:V:57:HIS:O	10:V:58:LYS:C	2.46	0.52
1:A:40:TRP:CZ2	1:A:377:GLU:CA	2.89	0.52
1:A:91:THR:HG23	1:A:92:ARG:H	1.74	0.52
4:D:68:VAL:HG12	4:D:92:PRO:HG2	1.91	0.52
4:D:79:GLU:HB3	4:D:82:MET:HB2	1.91	0.52
8:H:73:LEU:CD2	8:H:74:PHE:HD1	2.21	0.52
1:M:426:GLY:HA3	1:M:428:ILE:N	2.24	0.52
1:M:336:PHE:HE2	1:M:446:PHE:HD2	1.55	0.52
1:M:53:ASN:HB3	1:M:170:PRO:CD	2.39	0.52
3:O:244:LEU:HD11	4:P:204:MET:CE	2.37	0.52
3:O:327:ALA:O	3:O:331:ASP:N	2.35	0.52
4:P:55:CYS:SG	10:V:52:TRP:CB	2.97	0.52
1:A:397:SER:OG	1:A:398:ARG:N	2.41	0.52
2:B:77:THR:HG22	2:B:130:PRO:N	2.24	0.52
3:C:103:TYR:O	3:C:315:MET:HB2	2.10	0.52
3:C:26:ASN:ND2	3:C:26:ASN:C	2.63	0.52
1:M:152:TYR:O	1:M:153:LEU:C	2.47	0.52
3:O:52:ALA:HB2	12:O:380:HEM:CMD	2.40	0.52
3:O:71:ARG:NH2	4:P:193:ALA:O	2.42	0.52
4:P:69:GLU:O	4:P:73:GLY:HA3	2.09	0.52
5:Q:135:LEU:HD22	5:Q:182:VAL:HG22	1.92	0.52
4:P:138:PRO:HB3	8:T:55:THR:CA	2.40	0.52
2:B:97:SER:OG	9:I:70:LEU:HB2	2.10	0.52
3:C:368:THR:O	3:C:371:THR:HB	2.10	0.52
1:M:241:ILE:CD1	7:S:16:TYR:CE2	2.92	0.52
2:N:24:LEU:N	2:N:24:LEU:HD12	2.21	0.52
4:P:11:PRO:HB2	8:T:74:PHE:CG	2.44	0.52
4:P:237:TYR:CE2	4:P:239:PRO:HD3	2.44	0.52
1:A:134:ILE:HD13	1:A:134:ILE:N	2.23	0.52
1:A:381:ARG:HA	1:A:384:LEU:HD12	1.91	0.52
2:B:135:TRP:CD1	2:B:136:GLU:HG3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:GLU:O	2:B:213:HIS:CE1	2.63	0.52
2:B:340:ALA:O	2:B:344:VAL:HG23	2.08	0.52
2:B:347:ILE:H	2:B:347:ILE:CD1	2.21	0.52
2:B:383:GLY:O	2:B:386:ALA:HB3	2.10	0.52
2:B:60:SER:CB	2:N:429:ASN:ND2	2.53	0.52
3:C:184:ILE:O	3:C:188:ILE:HD12	2.10	0.52
3:C:80:ARG:HD3	3:C:80:ARG:O	2.09	0.52
3:C:92:ILE:O	3:C:96:MET:HG2	2.10	0.52
4:D:113:LEU:O	4:D:114:SER:C	2.48	0.52
4:D:164:ILE:HG21	4:D:182:VAL:HG12	1.92	0.52
4:D:228:SER:HB2	7:G:23:GLN:HE21	1.74	0.52
6:F:25:GLY:O	6:F:28:LYS:HG3	2.09	0.52
6:F:75:LEU:C	6:F:80:TRP:HE1	2.12	0.52
9:I:53:GLU:O	9:I:54:SER:C	2.47	0.52
10:J:49:GLY:HA2	10:J:54:HIS:HB3	1.92	0.52
1:M:29:GLN:HG3	1:M:203:LEU:O	2.09	0.52
1:M:25:VAL:HG21	1:M:209:LEU:CD1	2.39	0.52
1:M:386:TYR:N	1:M:386:TYR:CD1	2.75	0.52
1:M:67:THR:CG2	1:M:70:ARG:H	2.03	0.52
2:N:67:HIS:CE1	2:N:177:TYR:HD1	2.28	0.52
2:N:258:VAL:CG1	2:N:321:LEU:HD22	2.40	0.52
5:Q:20:ASP:O	5:Q:21:SER:C	2.46	0.52
1:A:426:GLY:H	1:A:428:ILE:CD1	2.22	0.52
1:A:85:HIS:HA	2:B:284:HIS:O	2.09	0.52
2:B:308:ASP:OD2	9:I:55:LEU:HA	2.09	0.52
1:A:34:THR:HB	2:B:373:GLU:OE1	2.09	0.52
2:B:85:ILE:O	2:B:89:ILE:HG13	2.10	0.52
3:C:183:PHE:CD1	3:O:183:PHE:CD1	2.97	0.52
3:C:88:SER:O	3:C:89:MET:C	2.47	0.52
4:D:64:LEU:O	4:D:68:VAL:HG23	2.09	0.52
5:E:18:VAL:HG11	5:E:32:ARG:HH11	1.73	0.52
1:M:394:GLU:O	1:M:395:TRP:C	2.47	0.52
2:N:279:LEU:CD2	2:N:344:VAL:HG22	2.40	0.52
8:T:65:ARG:CG	8:T:66:ASP:N	2.72	0.52
2:B:352:LEU:HD23	2:B:411:ILE:HD11	1.92	0.52
3:C:312:GLN:NE2	3:C:317:PHE:HB2	2.25	0.52
4:D:50:HIS:O	4:D:51:LEU:C	2.48	0.52
1:M:106:LEU:HB3	1:M:107:PRO:HD3	1.90	0.52
1:M:270:LEU:O	1:M:271:GLN:C	2.47	0.52
1:M:392:LEU:HA	1:M:395:TRP:NE1	2.25	0.52
2:N:304:HIS:CD2	2:N:305:GLN:N	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:435:PHE:H	2:N:438:GLU:HB2	1.74	0.52
3:O:117:VAL:N	12:O:381:HEM:HBC2	2.25	0.52
3:O:153:ILE:H	3:O:153:ILE:HD12	1.74	0.52
5:Q:81:ILE:HD12	5:Q:81:ILE:H	1.75	0.52
8:T:58:LEU:O	8:T:58:LEU:HD12	2.10	0.52
1:A:329:MET:HA	1:A:430:GLN:OE1	2.10	0.52
2:B:375:SER:OG	2:B:376:GLU:N	2.42	0.52
2:B:89:ILE:O	2:B:90:GLU:C	2.47	0.52
3:C:282:ARG:O	3:C:284:ILE:N	2.43	0.52
4:D:82:MET:HE2	4:D:86:LYS:NZ	2.25	0.52
7:G:80:ASP:O	7:G:81:ARG:HB2	2.10	0.52
1:M:204:GLU:HG2	1:M:206:ARG:HB3	1.90	0.52
3:O:107:TYR:OH	3:O:308:HIS:ND1	2.09	0.52
1:A:279:HIS:CE1	1:A:284:TYR:OH	2.63	0.52
1:A:326:CYS:SG	1:A:331:ILE:HA	2.50	0.52
3:C:153:ILE:HD12	3:C:153:ILE:N	2.25	0.52
3:C:90:PHE:CE1	3:C:123:VAL:HG21	2.44	0.52
2:B:316:TYR:OH	9:I:64:LEU:HD23	2.09	0.52
5:E:38:LEU:HD13	10:J:9:LEU:HD23	1.92	0.52
1:M:292:SER:O	1:M:295:ALA:HB3	2.09	0.52
2:N:393:THR:HG22	2:N:394:PRO:O	2.10	0.52
3:O:246:ALA:N	3:O:247:PRO:CD	2.73	0.52
7:S:67:GLU:O	7:S:71:ARG:HB3	2.10	0.52
2:B:148:LYS:HD2	2:B:178:CYS:O	2.10	0.51
2:B:162:ASN:HB3	2:B:244:ILE:CG2	2.40	0.51
2:B:268:GLU:O	2:B:271:ALA:HB3	2.10	0.51
2:B:34:VAL:HG11	2:B:386:ALA:CB	2.40	0.51
2:B:381:GLU:O	2:B:384:SER:OG	2.24	0.51
4:D:46:VAL:HG12	4:D:47:ALA:O	2.10	0.51
10:J:56:LYS:HE2	10:J:60:GLU:OE1	2.09	0.51
1:M:25:VAL:HG21	1:M:209:LEU:HD13	1.91	0.51
1:M:111:GLU:HG2	1:M:213:GLN:NE2	2.25	0.51
1:M:262:TRP:CE3	1:M:385:THR:CG2	2.93	0.51
3:O:106:SER:O	3:O:109:PHE:CD2	2.54	0.51
3:O:30:TRP:HA	3:O:33:PHE:HE2	1.75	0.51
3:O:196:HIS:CE1	12:O:381:HEM:C1D	2.97	0.51
4:P:43:MET:HA	4:P:112:ASP:OD1	2.10	0.51
4:P:11:PRO:HG2	8:T:74:PHE:HB2	1.92	0.51
4:P:7:PRO:HB2	4:P:125:ASP:HB3	1.93	0.51
4:P:195:GLU:HG3	4:P:198:HIS:HB2	1.92	0.51
5:Q:114:VAL:CG1	5:Q:115:SER:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:119:ASP:OD1	5:Q:120:PRO:HD2	2.09	0.51
5:Q:86:ASN:HD21	5:Q:97:PHE:HD2	1.54	0.51
6:R:35:ASP:OD1	6:R:89:TYR:OH	2.22	0.51
1:A:37:VAL:HG13	1:A:199:ALA:CB	2.40	0.51
2:B:237:ALA:HB2	2:B:318:ASP:CG	2.31	0.51
3:C:301:LEU:HA	3:C:304:ILE:HD12	1.91	0.51
4:D:26:ILE:HG21	4:D:54:VAL:HG22	1.92	0.51
4:D:62:LYS:O	4:D:66:GLU:HG3	2.10	0.51
6:F:7:SER:O	6:F:11:ARG:HD2	2.10	0.51
4:D:139:THR:HG21	8:H:41:ASP:O	2.09	0.51
10:J:51:LEU:H	10:J:54:HIS:HD2	1.57	0.51
2:N:102:ARG:HH12	2:N:175:SER:HA	1.75	0.51
3:O:200:LEU:HD13	12:O:381:HEM:CAD	2.40	0.51
4:P:113:LEU:O	4:P:114:SER:C	2.46	0.51
4:P:69:GLU:HA	4:P:73:GLY:HA2	1.93	0.51
5:Q:102:THR:H	5:Q:105:GLU:HB2	1.74	0.51
5:Q:119:ASP:HB3	5:Q:179:ASN:ND2	2.26	0.51
6:R:96:GLU:OE2	6:R:99:ARG:NH1	2.43	0.51
1:A:19:LEU:HB2	1:A:23:LEU:HB3	1.92	0.51
2:B:166:ALA:HB2	2:B:244:ILE:CD1	2.40	0.51
3:C:171:ASP:O	3:C:172:LYS:C	2.47	0.51
3:C:177:ARG:O	3:C:181:PHE:HD2	1.93	0.51
3:C:221:HIS:HA	3:C:225:THR:HG23	1.92	0.51
3:C:372:ILE:O	3:C:373:GLU:C	2.46	0.51
1:M:134:ILE:HD13	1:M:137:GLU:HG3	1.91	0.51
3:O:19:ILE:HG23	3:O:221:HIS:HB2	1.92	0.51
3:O:47:THR:HG22	3:O:83:HIS:HB2	1.91	0.51
1:A:200:ALA:HB2	1:A:375:VAL:HG12	1.92	0.51
2:B:115:ASP:HA	2:B:118:ILE:HD12	1.92	0.51
4:D:10:TYR:HD1	8:H:74:PHE:CE1	2.28	0.51
4:D:224:ARG:O	4:D:225:HIS:C	2.47	0.51
4:D:233:ARG:HG3	7:G:17:SER:CB	2.40	0.51
1:M:106:LEU:HB3	1:M:107:PRO:CD	2.40	0.51
1:M:19:LEU:HD13	1:M:214:LYS:HG2	1.92	0.51
2:N:262:ALA:HB3	2:N:269:ALA:HA	1.91	0.51
2:N:275:LEU:HB2	2:N:410:VAL:HG13	1.92	0.51
3:O:304:ILE:N	3:O:305:PRO:CD	2.73	0.51
4:P:181:GLN:HG2	8:T:77:LEU:CD2	2.21	0.51
5:Q:51:ALA:O	5:Q:55:VAL:HG23	2.11	0.51
1:A:111:GLU:HG2	1:A:213:GLN:NE2	2.25	0.51
1:A:113:LEU:HA	1:A:116:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ILE:CD1	1:A:427:PRO:O	2.58	0.51
1:A:55:ALA:O	1:A:56:GLY:C	2.48	0.51
2:B:213:HIS:N	2:B:214:PRO:CD	2.66	0.51
2:B:304:HIS:CG	2:B:305:GLN:H	2.29	0.51
2:B:350:GLY:HA2	2:B:411:ILE:HG21	1.92	0.51
1:A:236:PHE:HB2	5:E:25:SER:HB2	1.93	0.51
11:K:32:LEU:O	11:K:33:VAL:C	2.46	0.51
1:M:277:ILE:HB	1:M:309:THR:HG21	1.91	0.51
2:N:141:GLN:OE1	2:N:183:ILE:O	2.28	0.51
2:N:247:GLN:NE2	2:N:429:ASN:HA	2.25	0.51
3:O:10:LEU:HD12	3:O:13:ILE:HD11	1.92	0.51
1:A:426:GLY:H	1:A:428:ILE:HG12	1.66	0.51
2:B:261:SER:HB3	2:B:321:LEU:N	2.25	0.51
2:B:275:LEU:HD11	2:B:279:LEU:CD1	2.41	0.51
2:B:280:GLY:HA2	2:B:311:ALA:CB	2.40	0.51
2:B:88:GLY:O	2:B:91:ALA:HB3	2.11	0.51
3:C:26:ASN:HB2	6:F:69:SER:HG	1.70	0.51
3:C:300:ILE:HD13	3:C:362:ILE:HG21	1.92	0.51
4:D:143:LEU:HD22	4:D:147:LEU:O	2.09	0.51
4:D:228:SER:HB2	7:G:23:GLN:HE22	1.71	0.51
5:E:15:ARG:HH21	5:E:32:ARG:HG3	1.74	0.51
10:J:49:GLY:HA2	10:J:54:HIS:HB2	1.91	0.51
1:M:162:PRO:O	1:M:165:GLN:NE2	2.42	0.51
2:N:185:LYS:O	2:N:185:LYS:HG3	2.11	0.51
2:N:198:HIS:CE1	2:N:233:SER:HB3	2.45	0.51
2:N:406:ALA:HB3	2:N:409:ASP:HB2	1.92	0.51
3:O:210:GLY:CA	3:O:314:SER:HB2	2.31	0.51
4:P:48:TYR:CD2	4:P:65:ALA:HB2	2.46	0.51
5:Q:152:ASP:N	5:Q:164:HIS:ND1	2.59	0.51
2:B:166:ALA:HB2	2:B:244:ILE:CG1	2.39	0.51
3:C:147:THR:O	3:C:150:LEU:HB2	2.11	0.51
4:D:120:ARG:CG	4:D:120:ARG:HH11	2.24	0.51
5:E:47:VAL:O	5:E:50:ALA:HB3	2.10	0.51
8:H:70:ALA:HA	8:H:73:LEU:HD22	1.92	0.51
1:M:40:TRP:HZ2	1:M:377:GLU:HB2	1.75	0.51
2:N:247:GLN:HG3	2:N:248:ASN:N	2.24	0.51
2:N:257:LEU:CD1	2:N:424:MET:HB2	2.40	0.51
4:P:30:PHE:HD1	4:P:189:PHE:CE1	2.29	0.51
6:R:37:ILE:HG23	6:R:37:ILE:O	2.11	0.51
6:R:58:ARG:HG2	6:R:58:ARG:NH1	2.25	0.51
7:S:80:ASP:O	7:S:81:ARG:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:408:ARG:O	1:M:412:SER:OG	2.28	0.51
2:N:206:LEU:CD1	2:N:224:LEU:HD11	2.41	0.51
2:N:198:HIS:HE1	2:N:233:SER:CB	2.23	0.51
3:O:357:LEU:O	3:O:361:LEU:HG	2.11	0.51
3:O:361:LEU:HD23	3:O:365:LEU:CD1	2.36	0.51
4:P:165:TYR:H	4:P:168:VAL:CG2	2.24	0.51
5:Q:45:VAL:HG22	10:V:28:ALA:N	2.26	0.51
1:A:211:LEU:HD12	1:A:211:LEU:O	2.11	0.51
3:C:105:GLY:HA2	3:C:107:TYR:CD1	2.46	0.51
4:D:229:VAL:HG12	4:D:233:ARG:NE	2.22	0.51
7:G:33:GLY:O	7:G:37:VAL:HB	2.11	0.51
1:M:161:THR:HB	1:M:162:PRO:CD	2.41	0.51
2:N:209:LEU:O	2:N:209:LEU:HG	2.09	0.51
2:N:262:ALA:CB	2:N:268:GLU:HB3	2.41	0.51
2:N:303:VAL:CG1	2:N:304:HIS:H	2.24	0.51
2:B:429:ASN:ND2	2:N:60:SER:CB	2.59	0.51
3:O:27:ILE:CG2	3:O:27:ILE:O	2.58	0.51
3:O:344:GLU:O	3:O:348:ILE:HG13	2.11	0.51
9:U:78:TYR:OXT	9:U:78:TYR:CD1	2.64	0.51
1:A:63:ALA:HB2	1:A:97:TYR:HE2	1.76	0.51
2:B:79:GLY:HA3	2:B:125:ASN:HD21	1.75	0.51
3:C:240:MET:SD	3:C:243:VAL:HG11	2.51	0.51
3:C:251:GLY:O	3:C:252:ASP:C	2.50	0.51
5:E:20:ASP:O	5:E:21:SER:C	2.49	0.51
3:O:196:HIS:CE1	12:O:381:HEM:ND	2.78	0.51
3:O:218:ILE:HD13	4:P:230:LEU:HD13	1.91	0.51
4:P:168:VAL:HG12	4:P:169:LEU:HD23	1.93	0.51
1:A:124:ASP:O	1:A:128:GLU:HG2	2.11	0.50
1:A:34:THR:CB	2:B:373:GLU:OE1	2.59	0.50
2:B:38:LEU:O	2:B:40:ASN:N	2.45	0.50
3:C:106:SER:CB	12:C:381:HEM:HBD2	2.41	0.50
4:D:2:ASP:HB3	4:D:156:GLN:NE2	2.26	0.50
6:F:13:LEU:O	6:F:16:ILE:N	2.42	0.50
6:F:96:GLU:O	6:F:99:ARG:N	2.44	0.50
1:M:329:MET:HA	1:M:430:GLN:OE1	2.11	0.50
3:O:166:GLY:HA3	3:O:177:ARG:NH2	2.26	0.50
3:O:174:THR:CG2	3:O:178:PHE:HE2	2.12	0.50
3:O:371:THR:O	3:O:372:ILE:C	2.49	0.50
3:O:200:LEU:CD1	12:O:381:HEM:HAD2	2.40	0.50
4:P:14:HIS:HA	4:P:19:SER:HB3	1.93	0.50
4:P:224:ARG:NH2	7:S:27:PRO:HD2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:58:GLN:O	9:U:59:ALA:HB2	2.11	0.50
1:A:106:LEU:HB3	1:A:107:PRO:CD	2.41	0.50
1:A:433:ASP:CB	3:C:219:PRO:HG2	2.40	0.50
1:A:49:SER:N	1:A:52:ASN:OD1	2.35	0.50
2:B:197:ASN:HB2	2:B:198:HIS:CD2	2.46	0.50
3:C:164:ILE:O	3:C:177:ARG:NH1	2.42	0.50
3:C:331:ASP:OD1	3:C:354:ALA:HB1	2.11	0.50
3:C:37:LEU:HD21	3:C:94:LEU:HD13	1.93	0.50
2:N:350:GLY:HA2	2:N:411:ILE:HG21	1.93	0.50
3:O:147:THR:HG21	3:O:165:TRP:CD1	2.46	0.50
5:Q:119:ASP:HB3	5:Q:179:ASN:HD21	1.76	0.50
4:P:10:TYR:HD1	8:T:74:PHE:CE1	2.29	0.50
1:A:26:ALA:O	1:A:27:SER:HB3	2.11	0.50
1:A:291:SER:HB3	2:B:87:ARG:HD3	1.93	0.50
1:A:347:THR:O	11:K:16:ASN:ND2	2.43	0.50
1:A:378:ASP:O	1:A:382:SER:HB2	2.11	0.50
1:A:41:ILE:HD12	1:A:41:ILE:N	2.24	0.50
3:C:344:GLU:O	3:C:348:ILE:HG13	2.11	0.50
4:D:134:TYR:HE2	4:D:163:PRO:CG	2.24	0.50
4:D:30:PHE:CE1	4:D:50:HIS:CE1	2.99	0.50
4:D:79:GLU:O	4:D:80:MET:C	2.49	0.50
8:H:27:LEU:O	8:H:30:CYS:N	2.38	0.50
3:O:142:GLY:O	3:O:146:ILE:HG12	2.12	0.50
3:O:160:LEU:O	3:O:164:ILE:HD12	2.11	0.50
3:O:164:ILE:O	3:O:177:ARG:NH1	2.44	0.50
3:O:191:ALA:O	3:O:195:VAL:HG23	2.12	0.50
3:O:378:LYS:HD3	3:O:378:LYS:O	2.11	0.50
1:A:106:LEU:HD22	1:A:203:LEU:HD13	1.93	0.50
1:A:37:VAL:HG13	1:A:199:ALA:HB2	1.93	0.50
2:B:178:CYS:SG	2:B:179:PRO:HD2	2.51	0.50
3:C:122:THR:HG21	3:C:189:ILE:CG1	2.42	0.50
4:D:138:PRO:CB	8:H:55:THR:CA	2.90	0.50
1:M:82:MET:SD	1:M:105:ASP:HB3	2.51	0.50
1:M:30:SER:N	1:M:201:GLY:O	2.44	0.50
3:O:152:ALA:N	3:O:287:LYS:NZ	2.59	0.50
3:O:242:LEU:HD21	3:O:250:LEU:CD2	2.41	0.50
5:Q:32:ARG:HH12	7:S:22:GLU:CD	2.15	0.50
1:A:279:HIS:ND1	1:A:284:TYR:OH	2.42	0.50
1:A:48:GLU:HB3	1:A:52:ASN:O	2.10	0.50
3:C:183:PHE:HD1	3:C:183:PHE:O	1.94	0.50
3:C:373:GLU:HB3	6:F:20:TYR:OH	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:LEU:HD13	12:C:381:HEM:HAD2	1.93	0.50
4:D:32:VAL:HG11	4:D:186:VAL:CG2	2.41	0.50
1:M:327:ASP:OD1	1:M:328:HIS:N	2.44	0.50
2:N:109:VAL:HG22	2:N:119:LEU:CD2	2.41	0.50
2:N:133:ARG:O	2:N:134:ARG:C	2.49	0.50
3:O:317:PHE:CD1	6:R:26:PHE:HB3	2.47	0.50
4:P:134:TYR:HE2	4:P:163:PRO:CG	2.25	0.50
4:P:232:SER:CB	7:S:23:GLN:OE1	2.59	0.50
7:S:27:PRO:O	7:S:28:HIS:C	2.48	0.50
10:V:32:GLU:CG	10:V:33:ARG:N	2.74	0.50
4:P:23:HIS:CD2	10:V:50:LYS:O	2.65	0.50
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.94	0.50
3:C:107:TYR:OH	3:C:308:HIS:ND1	2.09	0.50
4:D:102:ARG:HG2	4:D:109:LEU:HB2	1.93	0.50
4:D:160:MET:HE2	4:D:163:PRO:HG3	1.94	0.50
1:M:370:ASP:OD1	2:N:375:SER:HB3	2.12	0.50
2:B:429:ASN:ND2	2:N:60:SER:OG	2.45	0.50
3:O:152:ALA:HB2	3:O:287:LYS:NZ	2.26	0.50
4:P:146:GLY:O	4:P:148:TYR:CD1	2.65	0.50
4:P:72:ASP:OD1	4:P:76:GLU:OE1	2.29	0.50
5:Q:18:VAL:HG11	5:Q:32:ARG:NH1	2.27	0.50
6:R:10:SER:HA	6:R:13:LEU:CD1	2.42	0.50
6:R:98:ILE:O	6:R:99:ARG:C	2.48	0.50
2:B:275:LEU:O	2:B:275:LEU:HD12	2.12	0.50
2:B:412:ASN:O	2:B:415:LYS:HB2	2.11	0.50
3:C:100:ARG:NH2	12:C:381:HEM:O2A	2.44	0.50
4:D:7:PRO:HB2	4:D:125:ASP:HB3	1.92	0.50
4:D:42:SER:O	4:D:112:ASP:OD1	2.29	0.50
4:D:72:ASP:OD1	4:D:76:GLU:OE1	2.30	0.50
10:J:52:TRP:HE3	10:J:52:TRP:H	1.57	0.50
1:M:334:MET:O	1:M:335:MET:C	2.48	0.50
2:N:359:ALA:O	2:N:360:ALA:C	2.50	0.50
9:U:70:LEU:HD21	9:U:73:PRO:CD	2.26	0.50
2:B:200:THR:OG1	2:B:201:SER:N	2.44	0.50
2:B:372:VAL:O	2:B:372:VAL:HG12	2.11	0.50
3:C:26:ASN:ND2	3:C:208:PRO:HD2	2.27	0.50
4:D:230:LEU:O	4:D:233:ARG:HB2	2.12	0.50
8:H:73:LEU:HD23	8:H:73:LEU:C	2.31	0.50
10:J:4:THR:HG22	10:J:6:THR:H	1.77	0.50
2:N:261:SER:HB3	2:N:321:LEU:N	2.26	0.50
2:N:304:HIS:CD2	2:N:305:GLN:H	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:47:ILE:HG22	2:N:48:GLY:H	1.76	0.50
5:Q:109:GLU:HG2	5:Q:167:ALA:CB	2.25	0.50
8:T:50:THR:HG22	8:T:51:GLU:N	2.25	0.50
1:A:22:GLY:O	1:A:24:ARG:HG2	2.12	0.50
1:A:252:HIS:CD2	1:A:325:VAL:HG22	2.47	0.50
1:A:272:VAL:O	1:A:275:ALA:HB3	2.12	0.50
1:A:64:PHE:HE2	1:A:88:ALA:HB2	1.75	0.50
2:B:132:PHE:HB3	2:B:137:VAL:CG2	2.42	0.50
4:D:13:SER:O	4:D:19:SER:HB3	2.11	0.50
4:D:138:PRO:O	4:D:141:VAL:HB	2.12	0.50
4:D:161:ALA:O	4:D:163:PRO:N	2.45	0.50
1:A:142:ASP:OD2	5:E:1:SER:HB3	2.11	0.50
3:C:74:ASN:O	5:E:61:SER:HA	2.12	0.50
9:I:62:ARG:H	9:I:63:PRO:HD2	1.76	0.50
9:I:62:ARG:N	9:I:63:PRO:CD	2.75	0.50
1:M:291:SER:HB3	2:N:87:ARG:HD3	1.94	0.50
1:M:92:ARG:HD2	1:M:163:LEU:CD1	2.37	0.50
2:N:130:PRO:HB2	2:N:132:PHE:CE1	2.46	0.50
2:N:159:VAL:CG1	2:N:160:ILE:HD13	2.40	0.50
3:O:21:LEU:HD12	3:O:22:PRO:HD2	1.94	0.50
4:P:138:PRO:O	4:P:139:THR:C	2.50	0.50
4:P:213:GLY:O	4:P:217:PRO:HG3	2.11	0.50
5:Q:142:LEU:HD12	5:Q:161:HIS:CE1	2.46	0.50
9:U:58:GLN:HB3	9:U:78:TYR:HB2	1.92	0.50
2:N:97:SER:HA	9:U:70:LEU:HB2	1.94	0.50
1:A:395:TRP:O	1:A:398:ARG:N	2.45	0.49
2:B:45:SER:HB2	2:B:210:GLY:HA3	1.93	0.49
2:B:255:ALA:HA	2:B:425:ALA:O	2.12	0.49
3:C:280:ILE:N	3:C:280:ILE:HD13	2.27	0.49
3:C:77:TRP:CE3	3:C:78:ILE:HG23	2.44	0.49
4:D:33:TYR:O	4:D:37:CYS:HB2	2.12	0.49
7:G:54:ALA:O	7:G:58:VAL:HG23	2.12	0.49
1:M:294:LEU:CD2	1:M:337:VAL:HG12	2.41	0.49
2:N:76:THR:HG21	2:N:133:ARG:CZ	2.42	0.49
3:O:130:GLY:O	12:O:380:HEM:HAA1	2.11	0.49
3:O:274:PHE:O	3:O:275:LEU:C	2.47	0.49
4:P:100:ALA:O	4:P:103:ALA:N	2.45	0.49
10:V:60:GLU:O	10:V:60:GLU:HG3	2.11	0.49
11:W:18:VAL:CB	11:W:19:PRO:HD3	2.41	0.49
1:A:236:PHE:CD2	1:A:258:GLU:CG	2.92	0.49
1:A:335:MET:CE	1:A:339:GLN:HG3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:HB2	1:A:189:HIS:HB3	1.94	0.49
1:A:64:PHE:HA	1:A:75:LEU:CD2	2.42	0.49
2:B:247:GLN:NE2	2:B:429:ASN:ND2	2.59	0.49
2:B:279:LEU:HD23	2:B:295:LEU:HD13	1.94	0.49
3:C:85:ASN:O	3:C:86:GLY:C	2.50	0.49
4:D:27:ARG:NH1	10:J:58:LYS:HE3	2.26	0.49
8:H:66:ASP:O	8:H:67:HIS:C	2.50	0.49
1:M:124:ASP:O	1:M:128:GLU:HG2	2.11	0.49
1:M:55:ALA:O	1:M:58:PHE:N	2.39	0.49
2:N:196:GLN:HG2	2:N:197:ASN:OD1	2.12	0.49
4:P:146:GLY:O	4:P:148:TYR:N	2.42	0.49
4:P:79:GLU:HB3	4:P:82:MET:HB2	1.93	0.49
7:S:48:VAL:O	7:S:51:PRO:HD2	2.12	0.49
4:P:138:PRO:CB	8:T:55:THR:CA	2.90	0.49
9:U:53:GLU:O	9:U:54:SER:C	2.51	0.49
1:A:286:GLY:O	1:A:287:GLY:O	2.30	0.49
2:B:258:VAL:CG1	2:B:321:LEU:HD22	2.42	0.49
3:C:337:TRP:O	3:C:338:ILE:C	2.48	0.49
4:D:26:ILE:HG22	4:D:27:ARG:N	2.27	0.49
1:M:64:PHE:HE1	1:M:86:LEU:CG	2.22	0.49
2:N:227:ARG:HD2	2:N:227:ARG:N	2.27	0.49
7:S:71:ARG:O	7:S:73:ASN:N	2.46	0.49
1:A:408:ARG:HH12	11:K:15:ARG:CD	2.25	0.49
2:B:299:VAL:HG13	2:B:303:VAL:HG21	1.94	0.49
6:F:55:TYR:C	6:F:55:TYR:CD1	2.86	0.49
1:M:120:CYS:O	1:M:122:LEU:HG	2.12	0.49
1:M:349:ALA:O	1:M:408:ARG:NH2	2.45	0.49
2:N:276:GLN:O	2:N:280:GLY:N	2.40	0.49
2:N:68:LEU:CD1	2:N:140:LEU:HD23	2.39	0.49
4:P:82:MET:HE2	4:P:86:LYS:HZ2	1.77	0.49
5:Q:118:ARG:HH12	5:Q:173:LYS:N	2.11	0.49
1:A:15:GLN:O	1:A:205:HIS:CE1	2.66	0.49
1:A:403:ASP:CB	1:A:406:VAL:HG23	2.33	0.49
3:C:175:LEU:O	3:C:175:LEU:HG	2.11	0.49
3:C:46:LEU:O	3:C:50:PHE:HD1	1.94	0.49
4:D:116:ILE:HD11	4:D:120:ARG:HH11	1.78	0.49
4:D:224:ARG:NH2	7:G:27:PRO:HD2	2.28	0.49
6:F:51:PRO:CD	2:N:134:ARG:HH12	2.24	0.49
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.38	0.49
7:G:64:GLN:O	7:G:65:GLU:C	2.50	0.49
1:M:307:PHE:HA	1:M:323:HIS:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:283:PRO:HG3	9:U:55:LEU:HB3	1.95	0.49
2:N:340:ALA:O	2:N:344:VAL:HG23	2.12	0.49
2:N:255:ALA:CB	2:N:426:ALA:HB2	2.42	0.49
3:O:109:PHE:O	3:O:110:LEU:C	2.49	0.49
3:O:51:LEU:HD21	3:O:79:ILE:HG22	1.95	0.49
4:P:35:GLN:HB2	4:P:169:LEU:CD1	2.42	0.49
4:P:2:ASP:HB3	4:P:156:GLN:NE2	2.27	0.49
5:Q:76:ILE:HG22	5:Q:193:VAL:O	2.12	0.49
3:C:115:ILE:O	3:C:116:GLY:C	2.46	0.49
4:D:161:ALA:HB1	4:D:162:PRO:HD2	1.93	0.49
4:D:237:TYR:HB2	6:F:60:PHE:CE1	2.47	0.49
1:M:349:ALA:HB3	1:M:408:ARG:HE	1.78	0.49
2:N:155:PRO:O	2:N:156:GLN:C	2.49	0.49
6:R:75:LEU:CD1	6:R:76:PRO:HD2	2.36	0.49
2:N:308:ASP:OD2	9:U:54:SER:O	2.29	0.49
9:U:62:ARG:N	9:U:63:PRO:CD	2.75	0.49
1:A:37:VAL:CG1	1:A:199:ALA:HB2	2.43	0.49
1:A:385:THR:HB	1:A:386:TYR:CD1	2.48	0.49
2:B:79:GLY:CA	2:B:125:ASN:HD21	2.25	0.49
2:B:207:ILE:CD1	2:B:383:GLY:HA2	2.37	0.49
2:B:352:LEU:HD23	2:B:411:ILE:CD1	2.43	0.49
3:C:269:LYS:CD	3:C:340:GLY:HA2	2.43	0.49
3:C:276:PHE:HE2	3:C:297:SER:OG	1.95	0.49
3:C:103:TYR:OH	3:C:322:GLN:HG3	2.12	0.49
4:D:217:PRO:HG2	4:D:218:LEU:H	1.78	0.49
8:H:40:CYS:O	8:H:44:VAL:HG23	2.12	0.49
5:Q:38:LEU:O	5:Q:42:THR:OG1	2.30	0.49
5:Q:75:GLU:O	5:Q:194:ILE:CA	2.47	0.49
4:P:10:TYR:CE1	8:T:73:LEU:HD22	2.47	0.49
1:A:171:SER:O	1:A:174:VAL:HB	2.13	0.49
2:B:348:ALA:HB3	2:B:418:VAL:HG21	1.94	0.49
4:D:139:THR:CG2	8:H:44:VAL:HB	2.43	0.49
4:D:158:ILE:HG13	13:D:242:HEC:HBD2	1.95	0.49
1:M:106:LEU:O	1:M:107:PRO:C	2.51	0.49
2:N:111:CYS:CB	2:N:119:LEU:HD22	2.31	0.49
3:O:372:ILE:O	3:O:375:LYS:N	2.45	0.49
4:D:138:PRO:HB3	8:H:55:THR:HA	1.94	0.49
3:O:284:ILE:CG2	3:O:285:PRO:HD2	2.43	0.49
3:O:329:VAL:HA	3:O:332:LEU:HD12	1.94	0.49
4:P:233:ARG:HG3	7:S:17:SER:CB	2.42	0.49
5:Q:193:VAL:CG1	5:Q:193:VAL:O	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ALA:HB3	1:A:408:ARG:HG2	1.95	0.49
2:B:141:GLN:HA	2:B:141:GLN:OE1	2.13	0.49
2:B:141:GLN:CB	2:B:142:PRO:HD3	2.41	0.49
3:C:185:LEU:HB3	3:C:186:PRO:CD	2.36	0.49
3:C:43:LEU:O	3:C:44:GLN:C	2.51	0.49
6:F:45:GLU:O	6:F:46:ALA:O	2.31	0.49
1:M:256:ALA:CA	1:M:320:LEU:O	2.59	0.49
1:M:39:VAL:CG1	1:M:41:ILE:HD11	2.40	0.49
1:M:436:ARG:HE	3:O:222:PRO:CD	2.26	0.49
1:M:62:LEU:HB3	1:M:122:LEU:HD22	1.94	0.49
2:N:129:ALA:H	2:N:130:PRO:HD3	1.76	0.49
2:N:217:LYS:O	2:N:218:GLN:C	2.51	0.49
5:Q:188:THR:HG21	5:Q:194:ILE:CD1	2.43	0.49
7:S:56:TYR:HD1	7:S:57:LEU:HD23	1.78	0.49
1:A:158:PHE:O	1:A:164:ALA:HB2	2.12	0.48
1:A:261:GLY:HA2	1:A:314:TYR:O	2.13	0.48
1:A:89:TYR:C	1:A:89:TYR:CD1	2.85	0.48
2:B:187:THR:HG23	2:B:190:GLU:OE1	2.13	0.48
3:C:357:LEU:O	3:C:361:LEU:HG	2.13	0.48
3:C:88:SER:HB3	3:C:250:LEU:HD21	1.95	0.48
4:D:138:PRO:HB3	8:H:55:THR:CA	2.43	0.48
4:D:178:THR:O	4:D:179:MET:C	2.50	0.48
4:D:237:TYR:CD2	4:D:239:PRO:HD3	2.48	0.48
6:F:73:GLN:HG2	7:G:36:ASN:HD21	1.78	0.48
1:M:379:ILE:O	1:M:383:LEU:HG	2.13	0.48
3:O:150:LEU:O	3:O:153:ILE:HD13	2.13	0.48
5:E:72:SER:HB2	3:O:168:PHE:CE2	2.48	0.48
4:P:117:VAL:CG1	4:P:191:ARG:HH11	2.25	0.48
1:A:39:VAL:HG23	1:A:113:LEU:HD23	1.95	0.48
2:B:303:VAL:CG1	2:B:304:HIS:H	2.26	0.48
2:B:207:ILE:CG2	2:B:379:LEU:HD12	2.43	0.48
3:C:210:GLY:HA3	3:C:314:SER:CB	2.41	0.48
1:A:433:ASP:CG	3:C:223:TYR:HH	2.14	0.48
3:C:338:ILE:HA	3:C:341:GLN:CG	2.43	0.48
3:C:341:GLN:O	3:C:342:PRO:C	2.52	0.48
6:F:40:ASN:CG	6:F:41:ASP:H	2.16	0.48
1:M:213:GLN:CB	1:M:215:HIS:NE2	2.70	0.48
1:M:243:HIS:CD2	1:M:425:PHE:CE1	3.01	0.48
1:M:262:TRP:CE3	1:M:385:THR:HG21	2.48	0.48
1:M:426:GLY:HA2	1:M:428:ILE:CG1	2.37	0.48
2:N:24:LEU:HD13	2:N:392:TYR:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:262:ALA:HB2	2:N:272:PHE:CE2	2.49	0.48
2:N:294:SER:O	2:N:295:LEU:C	2.51	0.48
1:M:4:TYR:CE1	2:N:43:PRO:HB3	2.48	0.48
2:N:72:ALA:HB2	2:N:140:LEU:CD2	2.43	0.48
4:P:79:GLU:O	4:P:80:MET:C	2.52	0.48
5:Q:50:ALA:O	5:Q:51:ALA:C	2.49	0.48
3:O:26:ASN:HA	6:R:70:MET:HA	1.94	0.48
8:T:66:ASP:O	8:T:67:HIS:C	2.49	0.48
5:Q:33:LYS:HB2	10:V:10:TYR:CE1	2.48	0.48
1:A:156:THR:HG23	1:A:239:SER:HG	1.76	0.48
2:B:130:PRO:HB2	2:B:132:PHE:CE1	2.48	0.48
2:B:213:HIS:HD2	2:B:213:HIS:O	1.96	0.48
2:B:76:THR:HG21	2:B:133:ARG:NH2	2.29	0.48
4:D:153:PHE:O	4:D:156:GLN:N	2.35	0.48
4:D:224:ARG:HH21	7:G:27:PRO:HD2	1.78	0.48
2:N:132:PHE:HD2	2:N:191:LEU:HD13	1.67	0.48
2:N:367:GLY:HA2	2:N:370:MET:HE2	1.94	0.48
3:O:192:ILE:N	3:O:192:ILE:HD13	2.28	0.48
3:O:221:HIS:N	3:O:222:PRO:HD2	2.28	0.48
3:O:126:THR:HG21	12:O:380:HEM:CAB	2.43	0.48
6:R:45:GLU:O	6:R:49:ARG:HG3	2.14	0.48
3:C:119:LEU:HG	12:C:381:HEM:HBB2	1.90	0.48
2:N:111:CYS:HB3	2:N:119:LEU:CD2	2.32	0.48
2:N:24:LEU:HD13	2:N:392:TYR:HD2	1.78	0.48
2:N:381:GLU:HA	2:N:381:GLU:OE1	2.13	0.48
2:N:92:VAL:O	2:N:92:VAL:CG1	2.60	0.48
3:O:147:THR:CG2	3:O:165:TRP:NE1	2.75	0.48
3:O:251:GLY:O	3:O:252:ASP:C	2.51	0.48
3:O:28:SER:CB	3:O:30:TRP:HD1	2.26	0.48
3:O:296:PHE:O	3:O:297:SER:C	2.52	0.48
3:O:300:ILE:HD13	3:O:362:ILE:HG21	1.95	0.48
4:P:224:ARG:HH21	7:S:27:PRO:HD2	1.79	0.48
1:A:239:SER:HB2	7:G:18:LEU:HD23	1.95	0.48
2:B:126:VAL:HG12	2:B:126:VAL:O	2.11	0.48
13:D:242:HEC:HBD1	13:D:242:HEC:HHA	1.95	0.48
4:D:3:LEU:HD21	7:G:71:ARG:HA	1.95	0.48
4:D:69:GLU:HG3	4:D:84:PRO:HA	1.94	0.48
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.58	0.48
5:E:12:ASP:O	7:G:24:ARG:NH2	2.35	0.48
5:E:15:ARG:HH21	5:E:32:ARG:CB	2.24	0.48
6:F:16:ILE:O	6:F:17:ARG:C	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:100:LYS:HD2	1:M:373:THR:OG1	2.13	0.48
1:M:392:LEU:HA	1:M:395:TRP:HD1	1.72	0.48
1:M:53:ASN:ND2	1:M:165:GLN:HG3	2.29	0.48
3:O:122:THR:CG2	3:O:189:ILE:HG12	2.44	0.48
5:Q:141:HIS:HE2	5:Q:175:PRO:HB2	1.78	0.48
5:Q:87:MET:HG2	5:Q:89:PHE:HE1	1.78	0.48
10:V:38:GLY:O	10:V:42:ILE:HG13	2.14	0.48
1:A:43:ALA:HB1	1:A:189:HIS:HB3	1.94	0.48
1:A:84:ALA:HB2	1:A:101:ALA:CB	2.37	0.48
4:D:102:ARG:HE	4:D:109:LEU:HB2	1.78	0.48
4:D:165:TYR:H	4:D:168:VAL:CG2	2.26	0.48
4:D:241:LYS:HE3	6:F:53:ASN:HB3	1.96	0.48
5:E:40:THR:HG22	10:J:20:PHE:HZ	1.79	0.48
8:H:62:LEU:O	8:H:65:ARG:HG2	2.14	0.48
4:D:23:HIS:NE2	10:J:51:LEU:HA	2.29	0.48
1:M:290:LEU:HD13	1:M:295:ALA:HB1	1.95	0.48
1:M:80:GLU:O	1:M:82:MET:N	2.46	0.48
2:N:312:PHE:HD1	9:U:58:GLN:O	1.97	0.48
3:O:115:ILE:HD13	3:O:115:ILE:N	2.27	0.48
8:T:15:ASP:CB	8:T:16:PRO:CD	2.91	0.48
2:B:183:ILE:HG22	2:B:184:GLY:N	2.28	0.48
2:B:207:ILE:HG22	2:B:379:LEU:HD12	1.95	0.48
3:C:277:ALA:O	3:C:278:TYR:C	2.52	0.48
4:D:82:MET:CG	4:D:86:LYS:HZ2	2.26	0.48
6:F:35:ASP:OD1	6:F:89:TYR:OH	2.21	0.48
9:I:60:ALA:HB3	9:I:63:PRO:O	2.12	0.48
11:K:19:PRO:O	11:K:23:LEU:HG	2.14	0.48
1:M:255:ILE:O	1:M:321:GLY:HA3	2.14	0.48
1:M:34:THR:HB	2:N:373:GLU:OE1	2.14	0.48
3:O:107:TYR:HE1	3:O:305:PRO:HA	1.78	0.48
3:O:130:GLY:HA3	3:O:182:HIS:CE1	2.49	0.48
4:P:10:TYR:CZ	4:P:128:PHE:CE2	2.92	0.48
4:P:168:VAL:HG12	4:P:169:LEU:CD2	2.42	0.48
5:Q:122:HIS:ND1	5:Q:124:LEU:HB2	2.29	0.48
5:Q:158:CYS:SG	5:Q:160:CYS:HB2	2.54	0.48
6:R:7:SER:O	6:R:11:ARG:HD2	2.13	0.48
9:U:51:CYS:SG	9:U:53:GLU:HB3	2.52	0.48
2:B:198:HIS:HE1	2:B:233:SER:CB	2.19	0.48
2:B:52:LYS:CB	2:B:203:ARG:HB3	2.28	0.48
3:C:236:ILE:O	3:C:237:LEU:C	2.48	0.48
3:C:361:LEU:CD2	3:C:365:LEU:HD12	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:GLN:HE22	3:C:86:GLY:HA3	1.78	0.48
4:D:131:LEU:HD22	4:D:163:PRO:HB3	1.95	0.48
3:C:26:ASN:N	6:F:70:MET:HB2	2.29	0.48
8:H:50:THR:HG22	8:H:51:GLU:N	2.29	0.48
9:I:70:LEU:HG	9:I:72:VAL:H	1.78	0.48
4:P:27:ARG:O	4:P:28:ARG:C	2.52	0.48
4:P:220:TYR:CD2	7:S:26:PHE:CE1	3.02	0.48
10:V:32:GLU:HG2	10:V:33:ARG:N	2.29	0.48
10:V:61:ASN:O	10:V:62:LYS:HB2	2.13	0.48
1:A:84:ALA:HB1	1:A:100:LYS:O	2.14	0.48
1:A:277:ILE:CG2	1:A:294:LEU:HD12	2.44	0.48
2:B:47:ILE:CG2	2:B:48:GLY:N	2.77	0.48
3:C:147:THR:HG21	3:C:165:TRP:CD1	2.48	0.48
3:C:284:ILE:CG2	3:C:285:PRO:HD2	2.44	0.48
4:D:20:SER:OG	4:D:21:LEU:N	2.46	0.48
4:D:83:ARG:CB	4:D:84:PRO:CD	2.66	0.48
3:C:215:VAL:O	6:F:63:LYS:CE	2.62	0.48
10:J:13:LEU:O	10:J:19:THR:OG1	2.16	0.48
1:M:280:TYR:O	1:M:306:SER:HA	2.14	0.48
2:N:128:THR:HG23	2:N:226:ILE:HD11	1.96	0.48
2:N:250:ASP:OD1	2:N:251:SER:N	2.47	0.48
3:O:122:THR:HB	3:O:189:ILE:HD13	1.95	0.48
3:O:252:ASP:CB	3:O:253:PRO:HD3	2.34	0.48
4:P:106:ASN:HD22	4:P:106:ASN:C	2.17	0.48
5:Q:103:LYS:HA	5:Q:106:ILE:CD1	2.43	0.48
5:Q:134:ILE:HD11	5:Q:185:TYR:CD1	2.48	0.48
5:Q:46:GLY:O	5:Q:49:TYR:HB3	2.14	0.48
1:A:61:HIS:CE1	1:A:134:ILE:HD11	2.49	0.48
2:B:276:GLN:OE1	2:B:313:ASN:HB3	2.14	0.48
2:B:99:THR:O	2:B:99:THR:HG22	2.14	0.48
3:C:192:ILE:CD1	3:C:192:ILE:N	2.77	0.48
4:D:32:VAL:CB	4:D:186:VAL:HG22	2.43	0.48
4:D:82:MET:CE	4:D:86:LYS:HZ2	2.25	0.48
6:F:67:ASP:HA	6:F:70:MET:HE2	1.96	0.48
1:M:436:ARG:HE	3:O:222:PRO:HG3	1.79	0.48
2:N:254:HIS:O	2:N:426:ALA:HA	2.13	0.48
2:N:262:ALA:HB3	2:N:269:ALA:CA	2.44	0.48
2:N:360:ALA:O	2:N:363:LYS:N	2.47	0.48
3:O:47:THR:HG21	3:O:83:HIS:CB	2.43	0.48
13:P:242:HEC:CHD	13:P:242:HEC:HBC2	2.26	0.48
4:P:49:ARG:HG3	4:P:49:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:121:GLN:CG	5:Q:179:ASN:ND2	2.77	0.48
5:Q:9:ASP:OD1	5:Q:11:SER:OG	2.30	0.48
1:A:131:ARG:NH2	1:A:177:LEU:O	2.47	0.47
1:A:315:ALA:HB3	1:A:316:ASP:OD1	2.13	0.47
1:A:260:PRO:HG3	1:A:414:TYR:CZ	2.49	0.47
2:B:76:THR:HG21	2:B:133:ARG:CZ	2.44	0.47
2:B:140:LEU:O	2:B:142:PRO:N	2.47	0.47
2:B:141:GLN:HE22	2:B:186:VAL:HB	1.79	0.47
2:B:381:GLU:HA	2:B:381:GLU:OE1	2.13	0.47
1:M:385:THR:CG2	1:M:386:TYR:CD1	2.96	0.47
3:O:269:LYS:HA	3:O:270:PRO:HD3	1.74	0.47
5:Q:102:THR:O	5:Q:105:GLU:N	2.46	0.47
8:T:68:CYS:O	8:T:69:VAL:C	2.51	0.47
1:A:64:PHE:HE2	1:A:88:ALA:CB	2.27	0.47
2:B:162:ASN:ND2	2:B:244:ILE:CG2	2.61	0.47
3:C:334:THR:HG1	7:G:55:PHE:HD1	1.63	0.47
4:D:117:VAL:CG1	4:D:191:ARG:HH11	2.27	0.47
4:D:7:PRO:CB	4:D:125:ASP:HB3	2.43	0.47
8:H:15:ASP:N	8:H:16:PRO:CD	2.73	0.47
1:M:406:VAL:O	1:M:410:VAL:HG23	2.13	0.47
2:N:299:VAL:O	2:N:303:VAL:HG23	2.14	0.47
3:O:119:LEU:CD1	3:O:192:ILE:HG22	2.45	0.47
4:P:153:PHE:O	4:P:156:GLN:N	2.36	0.47
3:O:233:LEU:CD2	4:P:219:VAL:HG21	2.44	0.47
4:P:220:TYR:HE2	7:S:26:PHE:CE1	2.19	0.47
5:Q:163:SER:HA	5:Q:173:LYS:O	2.14	0.47
5:Q:18:VAL:HG21	7:S:22:GLU:OE1	2.14	0.47
10:V:52:TRP:CE3	10:V:52:TRP:N	2.82	0.47
2:B:235:ALA:O	2:B:236:LYS:CB	2.62	0.47
2:B:360:ALA:O	2:B:363:LYS:HB2	2.14	0.47
2:B:83:PHE:CZ	2:B:87:ARG:HG3	2.49	0.47
3:C:345:HIS:N	3:C:346:PRO:HD2	2.29	0.47
4:D:76:GLU:OE2	4:D:93:LYS:O	2.33	0.47
7:G:34:ILE:O	7:G:38:LEU:HG	2.14	0.47
2:B:252:LEU:HD11	9:I:49:VAL:HB	1.95	0.47
10:J:35:PHE:O	10:J:36:ASP:C	2.50	0.47
1:M:431:LEU:HD12	1:M:432:PRO:HD2	1.94	0.47
3:O:218:ILE:HG23	3:O:223:TYR:CE2	2.48	0.47
4:P:10:TYR:HD1	8:T:74:PHE:CD1	2.32	0.47
4:P:43:MET:HE3	4:P:91:PHE:HE2	1.79	0.47
5:Q:122:HIS:HB3	5:Q:125:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:THR:CB	1:A:372:THR:HG22	2.44	0.47
1:A:51:LYS:O	1:A:53:ASN:N	2.46	0.47
2:B:139:ALA:O	2:B:142:PRO:HD2	2.14	0.47
3:C:108:THR:O	3:C:110:LEU:N	2.46	0.47
5:E:65:SER:OG	5:E:67:ASP:HB3	2.15	0.47
4:D:232:SER:CB	7:G:23:GLN:OE1	2.62	0.47
1:M:64:PHE:HA	1:M:75:LEU:HD23	1.96	0.47
2:N:163:LEU:HD22	2:N:256:ALA:CB	2.45	0.47
2:N:79:GLY:H	2:N:125:ASN:ND2	2.11	0.47
3:O:153:ILE:CG2	3:O:154:PRO:HD2	2.45	0.47
3:O:221:HIS:N	3:O:222:PRO:CD	2.77	0.47
3:O:234:LEU:CD2	4:P:216:LEU:CD2	2.87	0.47
4:P:66:GLU:O	4:P:69:GLU:HG2	2.13	0.47
5:Q:94:LYS:HD2	5:Q:138:VAL:HG21	1.97	0.47
1:A:260:PRO:CD	1:A:414:TYR:CE1	2.92	0.47
1:A:53:ASN:HD22	1:A:53:ASN:C	2.16	0.47
1:A:360:LEU:HD22	2:B:93:GLY:HA2	1.97	0.47
3:C:218:ILE:CG2	3:C:223:TYR:CE2	2.97	0.47
3:C:326:TRP:NE1	7:G:48:VAL:HG22	2.29	0.47
4:D:161:ALA:O	4:D:163:PRO:HD3	2.14	0.47
6:F:36:THR:O	6:F:36:THR:HG22	2.14	0.47
8:H:15:ASP:HB2	8:H:16:PRO:CD	2.45	0.47
1:M:5:ALA:O	1:M:6:GLN:C	2.53	0.47
3:O:322:GLN:HE21	3:O:326:TRP:HE1	1.62	0.47
3:O:269:LYS:CD	3:O:340:GLY:HA2	2.44	0.47
3:O:91:PHE:O	3:O:92:ILE:C	2.52	0.47
5:Q:122:HIS:ND1	5:Q:124:LEU:N	2.57	0.47
1:M:241:ILE:HG13	7:S:16:TYR:CD2	2.50	0.47
1:A:345:LEU:HA	1:A:345:LEU:HD23	1.68	0.47
1:A:405:ARG:O	1:A:409:GLU:HG3	2.15	0.47
2:B:37:SER:HB3	2:B:213:HIS:HB2	1.97	0.47
3:C:6:LYS:HG2	3:C:16:ASN:OD1	2.15	0.47
4:D:82:MET:SD	4:D:86:LYS:NZ	2.82	0.47
7:G:67:GLU:O	7:G:71:ARG:HB3	2.14	0.47
1:M:260:PRO:HG3	1:M:414:TYR:CZ	2.50	0.47
2:N:132:PHE:CE2	2:N:191:LEU:HD22	2.49	0.47
2:N:197:ASN:HB2	2:N:198:HIS:CD2	2.49	0.47
3:O:119:LEU:HD23	12:O:381:HEM:C3B	2.49	0.47
5:Q:29:SER:CA	5:Q:32:ARG:HD3	2.44	0.47
7:S:34:ILE:O	7:S:38:LEU:HG	2.14	0.47
1:A:53:ASN:CG	1:A:165:GLN:HB2	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:LEU:C	2:B:68:LEU:HD12	2.34	0.47
3:C:206:ASN:ND2	3:C:207:ASN:N	2.60	0.47
3:C:350:ILE:O	3:C:351:GLY:C	2.53	0.47
4:D:36:VAL:HG23	4:D:169:LEU:HD11	1.96	0.47
4:D:190:LEU:O	4:D:191:ARG:C	2.52	0.47
6:F:23:ALA:O	6:F:24:ALA:C	2.52	0.47
6:F:51:PRO:HG3	2:N:134:ARG:HH12	1.78	0.47
6:F:73:GLN:HA	7:G:39:ARG:NH2	2.28	0.47
11:K:18:VAL:HB	11:K:19:PRO:HD3	1.95	0.47
1:M:75:LEU:HD12	1:M:112:LEU:HD11	1.96	0.47
1:M:134:ILE:O	1:M:137:GLU:N	2.47	0.47
1:M:61:HIS:CD2	2:N:287:ARG:HD3	2.49	0.47
3:O:107:TYR:CE1	3:O:305:PRO:HA	2.50	0.47
3:O:9:PRO:HB2	3:O:12:LYS:HB2	1.96	0.47
3:O:276:PHE:CG	3:O:277:ALA:N	2.82	0.47
5:Q:105:GLU:O	5:Q:108:GLN:HB3	2.14	0.47
6:R:46:ALA:O	6:R:47:ILE:C	2.53	0.47
1:A:70:ARG:HB3	1:A:74:ALA:HB3	1.97	0.47
4:D:32:VAL:HG11	4:D:186:VAL:HG22	1.97	0.47
7:G:36:ASN:HA	7:G:39:ARG:CD	2.32	0.47
10:J:32:GLU:HG2	10:J:33:ARG:H	1.79	0.47
1:M:251:ALA:O	1:M:325:VAL:HA	2.14	0.47
3:O:26:ASN:ND2	3:O:26:ASN:O	2.48	0.47
3:O:341:GLN:NE2	3:O:341:GLN:HA	2.29	0.47
3:O:218:ILE:CD1	4:P:230:LEU:HD13	2.45	0.47
5:Q:127:VAL:CG1	5:Q:133:VAL:HG23	2.44	0.47
5:Q:141:HIS:HA	5:Q:177:PRO:HD3	1.96	0.47
10:V:56:LYS:HE2	10:V:60:GLU:OE1	2.15	0.47
1:A:312:ILE:HB	1:A:319:LEU:HB2	1.97	0.47
1:A:392:LEU:HA	1:A:395:TRP:NE1	2.30	0.47
1:A:85:HIS:CE1	2:B:284:HIS:ND1	2.82	0.47
3:C:334:THR:O	3:C:337:TRP:HB3	2.15	0.47
7:G:34:ILE:CB	7:G:35:PRO:CD	2.89	0.47
7:G:45:ILE:HA	7:G:45:ILE:HD12	1.67	0.47
1:M:33:PRO:O	1:M:103:SER:HB3	2.14	0.47
1:M:37:VAL:HG13	1:M:199:ALA:CB	2.45	0.47
3:O:137:GLN:HE22	3:O:263:ASN:HB3	1.80	0.47
5:Q:171:ILE:O	5:Q:171:ILE:CG2	2.62	0.47
6:R:73:GLN:NE2	7:S:32:LYS:HZ2	2.13	0.47
6:R:88:SER:O	6:R:92:PRO:HD2	2.15	0.47
8:T:40:CYS:O	8:T:44:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ARG:O	2:B:116:VAL:HG23	2.15	0.47
2:B:24:LEU:HG	2:B:38:LEU:CD1	2.31	0.47
2:B:207:ILE:HG22	2:B:379:LEU:CD1	2.44	0.47
3:C:26:ASN:ND2	3:C:26:ASN:O	2.48	0.47
3:C:373:GLU:HA	3:C:376:LEU:HD12	1.97	0.47
4:D:168:VAL:HG12	4:D:169:LEU:HD23	1.97	0.47
1:M:408:ARG:HH12	11:W:15:ARG:CD	2.28	0.47
2:N:279:LEU:CD2	2:N:295:LEU:HD13	2.45	0.47
4:P:131:LEU:HD22	4:P:163:PRO:HB2	1.96	0.47
4:P:64:LEU:O	4:P:68:VAL:HG23	2.15	0.47
5:Q:170:ARG:O	5:Q:172:ARG:HG2	2.15	0.47
3:O:313:ARG:CB	6:R:38:HIS:CD2	2.98	0.47
7:S:39:ARG:HA	7:S:42:ARG:HD2	1.96	0.47
1:A:67:THR:CG2	1:A:70:ARG:HB2	2.43	0.47
2:B:242:GLY:H	2:B:423:SER:HB3	1.80	0.47
3:C:280:ILE:H	3:C:280:ILE:HD13	1.80	0.47
3:C:310:SER:OG	3:C:311:LYS:N	2.48	0.47
4:D:30:PHE:O	4:D:31:GLN:C	2.53	0.47
4:D:50:HIS:CE1	4:D:91:PHE:HZ	2.31	0.47
10:J:61:ASN:O	10:J:62:LYS:HB2	2.15	0.47
1:M:361:LEU:HG	1:M:399:ILE:HD11	1.96	0.47
1:M:49:SER:N	1:M:52:ASN:OD1	2.41	0.47
1:M:34:THR:CB	2:N:373:GLU:OE1	2.62	0.47
2:N:396:SER:O	2:N:399:LEU:HB2	2.15	0.47
3:O:61:THR:O	3:O:64:SER:N	2.48	0.47
4:P:178:THR:HB	4:P:181:GLN:CG	2.32	0.47
4:P:220:TYR:O	4:P:221:ALA:C	2.53	0.47
5:Q:122:HIS:CE1	5:Q:124:LEU:HD12	2.50	0.47
5:Q:141:HIS:HB3	5:Q:142:LEU:H	1.49	0.47
5:Q:153:PHE:HE1	5:Q:173:LYS:CG	2.25	0.47
5:Q:15:ARG:HH21	5:Q:32:ARG:CB	2.27	0.47
10:V:4:THR:HG22	10:V:6:THR:H	1.79	0.47
1:A:106:LEU:N	1:A:107:PRO:CD	2.77	0.46
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.74	0.46
1:A:191:LYS:NZ	1:A:220:SER:OG	2.45	0.46
1:A:365:LEU:HG	1:A:365:LEU:O	2.15	0.46
2:B:145:ARG:HG3	2:B:183:ILE:HD13	1.97	0.46
3:C:165:TRP:HA	3:C:174:THR:OG1	2.15	0.46
3:C:252:ASP:CB	3:C:253:PRO:CD	2.88	0.46
3:C:297:SER:O	3:C:300:ILE:CG2	2.62	0.46
4:D:35:GLN:OE1	4:D:35:GLN:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:33:LYS:HA	7:G:21:PHE:CD2	2.50	0.46
6:F:104:ARG:O	6:F:105:GLU:C	2.53	0.46
1:M:151:ASN:O	1:M:152:TYR:C	2.53	0.46
1:M:279:HIS:CE1	1:M:284:TYR:HH	2.32	0.46
1:M:253:VAL:O	1:M:323:HIS:HA	2.16	0.46
1:M:51:LYS:C	1:M:53:ASN:H	2.19	0.46
1:M:46:ARG:HB3	1:M:92:ARG:O	2.15	0.46
2:N:38:LEU:HD13	2:N:378:PHE:CE2	2.50	0.46
4:P:30:PHE:CE1	4:P:50:HIS:CE1	3.03	0.46
1:A:52:ASN:HB2	1:A:55:ALA:HB2	1.96	0.46
2:B:159:VAL:HG12	2:B:160:ILE:N	2.30	0.46
2:B:300:ALA:HA	2:B:307:PHE:HZ	1.74	0.46
2:B:71:LEU:HD13	2:B:143:GLN:HG3	1.97	0.46
3:C:183:PHE:CD1	3:C:183:PHE:C	2.88	0.46
3:C:202:GLU:OE2	3:O:10:LEU:CB	2.48	0.46
3:C:31:TRP:CD2	3:C:100:ARG:HD2	2.50	0.46
4:D:195:GLU:O	4:D:195:GLU:HG3	2.15	0.46
1:M:252:HIS:O	1:M:424:GLY:HA2	2.16	0.46
3:O:276:PHE:O	3:O:277:ALA:C	2.52	0.46
3:O:26:ASN:O	3:O:27:ILE:HG13	2.14	0.46
4:P:146:GLY:O	4:P:148:TYR:HD1	1.97	0.46
1:A:60:GLU:OE1	1:A:90:SER:HB2	2.15	0.46
2:B:135:TRP:NE1	2:B:136:GLU:HG3	2.31	0.46
2:B:24:LEU:H	2:B:24:LEU:CD1	2.03	0.46
3:C:376:LEU:HD13	6:F:20:TYR:CD2	2.51	0.46
6:F:50:LEU:HA	6:F:51:PRO:HD2	1.74	0.46
7:G:11:ARG:HB3	7:G:12:HIS:CD2	2.50	0.46
10:J:55:ILE:O	10:J:58:LYS:HD2	2.14	0.46
1:M:28:GLU:OE1	1:M:375:VAL:HG11	2.15	0.46
1:M:45:SER:OG	1:M:92:ARG:HG2	2.15	0.46
1:M:61:HIS:HB3	1:M:130:GLU:HG3	1.97	0.46
2:N:346:THR:HG23	2:N:351:ASN:HB3	1.96	0.46
3:O:309:THR:HG23	3:O:310:SER:N	2.30	0.46
5:Q:114:VAL:O	5:Q:117:LEU:CB	2.63	0.46
5:Q:99:ARG:NH1	5:Q:156:TYR:CZ	2.83	0.46
10:V:21:ALA:O	10:V:22:LEU:C	2.53	0.46
1:A:120:CYS:HB2	1:A:122:LEU:HD21	1.96	0.46
1:A:39:VAL:CG1	1:A:195:MET:CE	2.94	0.46
3:C:125:ALA:O	3:C:126:THR:C	2.53	0.46
3:C:315:MET:O	3:C:318:ARG:N	2.35	0.46
5:E:7:VAL:HG13	7:G:16:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:39:VAL:HG13	1:M:195:MET:HE3	1.97	0.46
1:M:40:TRP:HZ2	1:M:377:GLU:CB	2.28	0.46
1:M:430:GLN:CG	1:M:430:GLN:O	2.63	0.46
2:N:286:LYS:O	2:N:287:ARG:HB2	2.14	0.46
3:O:152:ALA:HB2	3:O:287:LYS:HZ3	1.79	0.46
4:P:220:TYR:CD2	7:S:26:PHE:CZ	3.04	0.46
5:Q:133:VAL:O	5:Q:133:VAL:HG13	2.15	0.46
5:Q:42:THR:O	5:Q:45:VAL:N	2.45	0.46
8:T:73:LEU:CD2	8:T:74:PHE:HD1	2.28	0.46
10:V:36:ASP:O	10:V:37:GLN:C	2.52	0.46
1:A:184:GLU:O	1:A:188:ARG:HG3	2.16	0.46
1:A:21:ASN:CB	1:A:217:SER:CB	2.89	0.46
2:B:227:ARG:HD2	2:B:227:ARG:N	2.30	0.46
2:B:262:ALA:HB2	2:B:268:GLU:HB3	1.98	0.46
2:B:429:ASN:HD22	2:B:429:ASN:C	2.19	0.46
3:C:136:GLY:O	3:C:139:SER:N	2.49	0.46
3:C:149:LEU:O	3:C:291:VAL:HG21	2.15	0.46
3:C:269:LYS:HA	3:C:270:PRO:HD3	1.81	0.46
4:D:116:ILE:HD11	4:D:120:ARG:HG3	1.97	0.46
4:D:150:ASN:OD1	4:D:151:PRO:N	2.49	0.46
7:G:44:CYS:O	7:G:47:ARG:N	2.47	0.46
1:M:53:ASN:CG	1:M:165:GLN:HB2	2.35	0.46
1:M:236:PHE:HD2	1:M:258:GLU:CB	2.29	0.46
1:M:389:ARG:C	1:M:391:PRO:HD3	2.36	0.46
1:M:41:ILE:HD12	1:M:41:ILE:N	2.24	0.46
2:N:203:ARG:NH2	2:N:230:LEU:HD23	2.31	0.46
2:N:198:HIS:HE1	2:N:233:SER:HB3	1.81	0.46
4:P:91:PHE:HA	4:P:92:PRO:HD3	1.60	0.46
2:B:134:ARG:HE	2:B:134:ARG:HB3	1.54	0.46
3:C:132:VAL:HA	3:C:139:SER:CB	2.42	0.46
3:C:51:LEU:CD2	3:C:79:ILE:CG2	2.93	0.46
1:M:32:GLN:CG	1:M:33:PRO:CD	2.86	0.46
1:M:394:GLU:O	1:M:397:SER:N	2.49	0.46
1:M:243:HIS:O	1:M:425:PHE:HA	2.16	0.46
3:O:312:GLN:NE2	3:O:317:PHE:HB2	2.30	0.46
11:W:34:SER:OG	11:W:35:ALA:N	2.46	0.46
1:A:32:GLN:HG2	1:A:33:PRO:N	2.30	0.46
2:B:218:GLN:O	2:B:221:GLU:HB2	2.15	0.46
3:C:237:LEU:HD12	4:D:208:MET:HE3	1.97	0.46
4:D:138:PRO:CB	8:H:55:THR:HA	2.46	0.46
1:M:16:VAL:HG11	1:M:388:ARG:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:24:ARG:CG	1:M:196:VAL:HG22	2.45	0.46
1:M:246:ASP:HA	1:M:427:PRO:HD3	1.97	0.46
1:M:50:GLU:O	1:M:173:ASN:ND2	2.49	0.46
2:N:352:LEU:HD21	2:N:357:VAL:CG2	2.46	0.46
2:N:424:MET:HE3	2:N:424:MET:HB3	1.78	0.46
3:O:41:LEU:HD23	3:O:190:MET:HG3	1.96	0.46
5:Q:131:GLU:HG2	5:Q:132:TRP:CD1	2.51	0.46
6:R:64:ARG:O	6:R:68:LEU:HD12	2.16	0.46
1:A:277:ILE:HG22	1:A:294:LEU:HD12	1.96	0.46
1:A:324:PHE:CG	1:A:334:MET:HG2	2.50	0.46
2:B:262:ALA:HB3	2:B:269:ALA:N	2.31	0.46
3:C:15:ASN:ND2	3:C:18:PHE:HE1	2.12	0.46
3:C:40:CYS:HB3	3:C:90:PHE:HD2	1.81	0.46
2:B:308:ASP:OD2	9:I:54:SER:O	2.32	0.46
1:M:279:HIS:CE1	1:M:284:TYR:OH	2.68	0.46
2:N:141:GLN:CB	2:N:142:PRO:HD3	2.46	0.46
2:N:170:ASN:CG	2:N:171:ALA:N	2.69	0.46
2:N:35:ILE:HD11	2:N:213:HIS:CD2	2.50	0.46
2:N:345:LYS:HG2	2:N:418:VAL:CG1	2.46	0.46
3:O:44:GLN:OE1	3:O:83:HIS:CE1	2.69	0.46
5:Q:136:ILE:O	5:Q:138:VAL:N	2.49	0.46
5:Q:188:THR:HG21	5:Q:194:ILE:HG13	1.96	0.46
5:Q:43:THR:HG22	5:Q:44:THR:N	2.30	0.46
1:A:192:ALA:HA	1:A:194:ARG:N	2.31	0.46
1:A:379:ILE:CD1	1:A:390:ILE:HD12	2.41	0.46
1:A:415:PHE:O	1:A:441:MET:HE2	2.15	0.46
2:B:112:LEU:O	2:B:113:ARG:C	2.54	0.46
3:C:105:GLY:HA2	3:C:107:TYR:CE1	2.50	0.46
3:C:281:LEU:HD12	3:C:281:LEU:O	2.16	0.46
3:C:30:TRP:HA	3:C:33:PHE:CE2	2.51	0.46
5:E:71:MET:O	5:E:72:SER:C	2.54	0.46
1:M:57:TYR:HE2	1:M:134:ILE:HD12	1.80	0.46
1:M:192:ALA:HA	1:M:194:ARG:N	2.31	0.46
1:M:287:GLY:O	1:M:289:HIS:N	2.48	0.46
1:M:294:LEU:HD23	1:M:337:VAL:HG12	1.98	0.46
1:M:426:GLY:HA2	1:M:427:PRO:C	2.36	0.46
2:N:159:VAL:CG1	2:N:160:ILE:N	2.79	0.46
2:N:433:THR:HA	2:N:434:PRO:HD2	1.58	0.46
3:O:116:GLY:HA3	12:O:381:HEM:C3C	2.51	0.46
4:P:218:LEU:HA	4:P:218:LEU:HD23	1.73	0.46
5:Q:120:PRO:O	5:Q:121:GLN:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:186:GLU:O	5:Q:186:GLU:HG3	2.16	0.46
6:R:95:LYS:O	6:R:96:GLU:C	2.53	0.46
1:A:197:LEU:HD11	1:A:208:LEU:HD11	1.98	0.46
1:A:91:THR:HG22	1:A:92:ARG:N	2.31	0.46
2:B:84:LYS:HG3	2:B:122:PHE:HZ	1.80	0.46
2:B:299:VAL:CG1	2:B:303:VAL:HG21	2.46	0.46
3:C:246:ALA:N	3:C:247:PRO:HD3	2.31	0.46
3:C:108:THR:CB	3:C:313:ARG:HH11	2.27	0.46
3:C:61:THR:O	3:C:64:SER:HB3	2.16	0.46
4:D:10:TYR:CE1	8:H:73:LEU:HD22	2.51	0.46
4:D:5:LEU:HG	4:D:152:TYR:CE1	2.51	0.46
4:D:54:VAL:O	4:D:54:VAL:CG1	2.60	0.46
4:D:220:TYR:CD2	7:G:26:PHE:CE1	3.03	0.46
3:O:109:PHE:HD1	3:O:203:THR:HG1	1.60	0.46
4:P:241:LYS:NZ	6:R:53:ASN:HB2	2.31	0.46
7:S:73:ASN:N	7:S:74:PRO:HD2	2.31	0.46
10:V:52:TRP:H	10:V:52:TRP:HE3	1.62	0.46
10:V:55:ILE:CG2	10:V:58:LYS:HE2	2.46	0.46
1:A:39:VAL:HG22	1:A:197:LEU:HD22	1.98	0.45
1:A:358:LYS:HD2	1:A:402:VAL:HB	1.98	0.45
2:B:122:PHE:O	2:B:123:LEU:C	2.53	0.45
3:C:152:ALA:CA	3:C:287:LYS:HZ2	2.29	0.45
3:C:182:HIS:O	3:C:186:PRO:CD	2.64	0.45
3:C:312:GLN:O	3:C:313:ARG:C	2.53	0.45
4:D:153:PHE:O	4:D:154:PRO:C	2.54	0.45
5:E:15:ARG:HH21	5:E:32:ARG:CG	2.29	0.45
5:E:45:VAL:HG13	10:J:28:ALA:CA	2.46	0.45
6:F:10:SER:HA	6:F:13:LEU:CD1	2.45	0.45
7:G:48:VAL:O	7:G:51:PRO:HD2	2.16	0.45
1:M:3:THR:O	1:M:4:TYR:C	2.54	0.45
1:M:438:ARG:HG3	1:M:438:ARG:NH1	2.31	0.45
2:N:50:PHE:CE1	2:N:207:ILE:HG13	2.52	0.45
2:N:276:GLN:OE1	2:N:313:ASN:HB3	2.15	0.45
3:O:4:ILE:O	3:O:5:ARG:C	2.55	0.45
4:P:161:ALA:O	4:P:163:PRO:N	2.49	0.45
4:P:183:ALA:HA	4:P:186:VAL:HG23	1.97	0.45
4:P:240:PRO:CG	4:P:241:LYS:N	2.79	0.45
5:Q:51:ALA:O	5:Q:52:LYS:C	2.54	0.45
8:T:65:ARG:O	8:T:69:VAL:HG23	2.16	0.45
2:N:314:ALA:HB1	9:U:64:LEU:HD22	1.97	0.45
2:B:304:HIS:CD2	2:B:305:GLN:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:PHE:CE2	3:C:297:SER:OG	2.68	0.45
3:C:152:ALA:N	3:C:287:LYS:NZ	2.64	0.45
3:C:341:GLN:HA	3:C:341:GLN:NE2	2.31	0.45
4:D:109:LEU:HA	4:D:110:PRO:HD2	1.74	0.45
4:D:24:THR:O	4:D:25:SER:C	2.53	0.45
10:J:55:ILE:CG2	10:J:58:LYS:HE2	2.44	0.45
1:M:43:ALA:CB	1:M:189:HIS:CB	2.94	0.45
1:M:70:ARG:HB3	1:M:74:ALA:HB3	1.97	0.45
2:N:51:ILE:CG2	2:N:199:PHE:HA	2.33	0.45
3:O:218:ILE:CG2	3:O:219:PRO:HD2	2.46	0.45
3:O:280:ILE:HD13	3:O:335:LEU:CD2	2.44	0.45
4:P:115:TYR:O	4:P:119:ALA:N	2.47	0.45
4:P:24:THR:O	4:P:25:SER:C	2.54	0.45
5:Q:7:VAL:HG13	5:Q:8:PRO:HD2	1.98	0.45
6:R:75:LEU:C	6:R:80:TRP:HE1	2.17	0.45
1:A:17:SER:HB2	1:A:25:VAL:HB	1.99	0.45
1:A:289:HIS:O	1:A:290:LEU:C	2.55	0.45
1:A:341:GLN:OE1	1:A:344:ARG:HD3	2.16	0.45
2:B:285:VAL:HG12	2:B:288:GLY:HA3	1.98	0.45
3:C:90:PHE:CE1	3:C:123:VAL:HG11	2.52	0.45
3:C:200:LEU:O	3:C:200:LEU:HG	2.15	0.45
3:C:4:ILE:O	3:C:5:ARG:C	2.53	0.45
4:D:98:PRO:O	4:D:101:ALA:HB3	2.16	0.45
4:D:165:TYR:CD1	4:D:168:VAL:HG22	2.51	0.45
7:G:71:ARG:O	7:G:73:ASN:N	2.50	0.45
3:O:116:GLY:O	3:O:119:LEU:HB2	2.16	0.45
3:O:183:PHE:CE1	3:O:187:PHE:CE2	3.03	0.45
5:Q:29:SER:OG	5:Q:32:ARG:HD3	2.17	0.45
8:T:73:LEU:C	8:T:73:LEU:HD23	2.37	0.45
5:Q:40:THR:CG2	10:V:20:PHE:HZ	2.28	0.45
10:V:52:TRP:O	10:V:53:LYS:C	2.53	0.45
2:B:243:GLU:HA	2:B:424:MET:O	2.17	0.45
3:C:278:TYR:O	3:C:279:ALA:C	2.55	0.45
3:C:294:LEU:O	3:C:297:SER:HB3	2.17	0.45
4:D:7:PRO:HG3	4:D:126:TYR:CA	2.43	0.45
1:M:125:SER:O	1:M:129:LYS:HG3	2.16	0.45
4:P:227:TRP:CE3	4:P:230:LEU:HD12	2.51	0.45
5:Q:42:THR:O	5:Q:43:THR:C	2.53	0.45
6:R:7:SER:O	6:R:11:ARG:HB2	2.16	0.45
1:A:146:ARG:NH2	1:A:308:GLN:NE2	2.58	0.45
1:A:252:HIS:NE2	1:A:325:VAL:HG21	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:ARG:NH1	2:B:185:LYS:CG	2.77	0.45
2:B:42:ALA:HB1	2:B:43:PRO:CD	2.40	0.45
3:C:136:GLY:O	3:C:138:MET:N	2.49	0.45
4:D:233:ARG:CG	7:G:17:SER:CB	2.94	0.45
4:D:6:HIS:HA	4:D:7:PRO:HD3	1.80	0.45
1:M:131:ARG:O	1:M:132:ASP:C	2.53	0.45
1:M:277:ILE:HG22	1:M:294:LEU:HD12	1.99	0.45
1:M:64:PHE:CZ	1:M:88:ALA:HB2	2.51	0.45
2:N:239:TYR:HE2	2:N:421:ARG:HB3	1.81	0.45
2:N:62:ASN:HD21	2:N:65:THR:CB	2.28	0.45
3:O:10:LEU:O	3:O:13:ILE:HG13	2.17	0.45
4:P:26:ILE:HG21	4:P:54:VAL:HG22	1.98	0.45
4:P:65:ALA:O	4:P:69:GLU:OE2	2.35	0.45
4:P:74:PRO:O	4:P:79:GLU:N	2.42	0.45
1:M:233:PRO:HG2	5:Q:23:LYS:HD3	1.98	0.45
1:A:199:ALA:HB3	1:A:208:LEU:HD21	1.99	0.45
1:A:369:LEU:HD21	1:A:378:ASP:OD2	2.16	0.45
1:A:428:ILE:CG2	1:A:431:LEU:HD22	2.47	0.45
1:A:91:THR:HG22	1:A:93:GLU:N	2.18	0.45
2:B:160:ILE:HA	2:B:160:ILE:HD12	1.73	0.45
3:C:63:PHE:O	3:C:67:THR:OG1	2.33	0.45
1:M:11:VAL:CG1	1:M:12:PRO:HD2	2.46	0.45
2:N:135:TRP:CD1	2:N:136:GLU:HG3	2.52	0.45
3:O:85:ASN:O	3:O:86:GLY:C	2.53	0.45
4:P:50:HIS:CE1	4:P:91:PHE:HZ	2.33	0.45
5:Q:107:ASP:O	5:Q:108:GLN:C	2.55	0.45
6:R:73:GLN:HA	7:S:39:ARG:NH2	2.29	0.45
7:S:64:GLN:O	7:S:65:GLU:C	2.55	0.45
4:P:138:PRO:CB	8:T:55:THR:HA	2.46	0.45
1:A:236:PHE:HD2	1:A:258:GLU:CB	2.29	0.45
1:A:39:VAL:HG12	1:A:41:ILE:HD12	1.95	0.45
1:A:291:SER:OG	2:B:90:GLU:OE1	2.26	0.45
3:C:192:ILE:H	3:C:192:ILE:HD13	1.82	0.45
3:C:357:LEU:HG	3:C:361:LEU:HD11	1.98	0.45
4:D:23:HIS:CD2	10:J:50:LYS:O	2.70	0.45
4:D:74:PRO:CG	4:D:82:MET:HB3	2.46	0.45
3:C:378:LYS:NZ	6:F:91:GLU:OE1	2.48	0.45
7:G:50:PRO:CB	7:G:51:PRO:CD	2.92	0.45
1:A:417:ASP:CG	10:J:10:TYR:OH	2.55	0.45
1:M:236:PHE:CD2	1:M:258:GLU:CG	2.95	0.45
1:M:43:ALA:HB1	1:M:189:HIS:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:445:ARG:O	1:M:446:PHE:CB	2.55	0.45
2:N:156:GLN:OE1	9:U:58:GLN:NE2	2.39	0.45
2:N:68:LEU:HG	2:N:191:LEU:HD21	1.98	0.45
2:N:84:LYS:O	2:N:88:GLY:N	2.47	0.45
3:O:341:GLN:O	3:O:342:PRO:C	2.55	0.45
4:P:228:SER:HB2	7:S:23:GLN:NE2	2.32	0.45
5:Q:76:ILE:CG2	5:Q:194:ILE:CG1	2.74	0.45
8:T:59:LEU:HD23	8:T:59:LEU:HA	1.71	0.45
1:A:248:LEU:HA	1:A:249:PRO:HD3	1.59	0.45
1:A:255:ILE:HG13	1:A:422:VAL:HG22	1.98	0.45
1:A:64:PHE:CZ	1:A:88:ALA:HB2	2.51	0.45
2:B:170:ASN:CG	2:B:171:ALA:N	2.70	0.45
2:B:264:ILE:HG21	2:B:317:SER:HA	1.97	0.45
2:B:322:PHE:CD1	2:B:322:PHE:C	2.90	0.45
2:B:29:LEU:HD12	2:B:33:LEU:HD21	1.98	0.45
3:C:183:PHE:HZ	3:O:184:ILE:HB	1.82	0.45
9:I:51:CYS:SG	9:I:53:GLU:HB3	2.57	0.45
10:J:57:HIS:O	10:J:60:GLU:HG2	2.17	0.45
1:M:426:GLY:H	1:M:428:ILE:HD11	1.82	0.45
2:N:235:ALA:O	2:N:236:LYS:CB	2.65	0.45
3:O:337:TRP:O	3:O:341:GLN:HG2	2.17	0.45
3:O:373:GLU:O	3:O:377:LEU:HD12	2.16	0.45
4:P:102:ARG:O	4:P:106:ASN:N	2.49	0.45
4:P:23:HIS:NE2	10:V:51:LEU:HA	2.31	0.45
4:P:55:CYS:SG	10:V:52:TRP:HA	2.56	0.45
5:Q:81:ILE:HD11	5:Q:132:TRP:HH2	1.82	0.45
2:B:83:PHE:CZ	6:R:104:ARG:HG2	2.52	0.45
6:R:43:VAL:HG22	6:R:94:LEU:CD2	2.45	0.45
7:S:26:PHE:N	7:S:27:PRO:HD3	2.32	0.45
1:A:243:HIS:CD2	1:A:425:PHE:CE2	3.04	0.45
1:A:255:ILE:HD12	1:A:335:MET:CE	2.47	0.45
1:A:293:PRO:HA	1:A:296:SER:OG	2.17	0.45
1:A:53:ASN:ND2	1:A:53:ASN:C	2.69	0.45
2:B:160:ILE:N	2:B:160:ILE:HD13	2.31	0.45
4:D:138:PRO:HB3	8:H:54:CYS:C	2.37	0.45
4:D:180:SER:HB3	8:H:17:LEU:HB2	1.98	0.45
4:D:32:VAL:CG2	4:D:186:VAL:HG22	2.44	0.45
4:D:28:ARG:HB2	4:D:185:ASP:HB3	1.99	0.45
6:F:58:ARG:HH11	6:F:58:ARG:HG2	1.82	0.45
10:J:51:LEU:O	10:J:54:HIS:N	2.46	0.45
1:M:339:GLN:O	1:M:343:MET:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:207:ILE:CD1	2:N:383:GLY:CA	2.93	0.45
2:N:308:ASP:O	2:N:309:VAL:HG23	2.17	0.45
3:O:26:ASN:HB2	6:R:69:SER:OG	2.17	0.45
4:P:23:HIS:CD2	10:V:52:TRP:N	2.85	0.45
6:R:40:ASN:CG	6:R:41:ASP:H	2.20	0.45
11:W:23:LEU:HD23	11:W:23:LEU:N	2.32	0.45
1:A:332:ASP:O	1:A:332:ASP:OD1	2.34	0.45
2:B:211:VAL:HG12	2:B:212:SER:N	2.32	0.45
2:B:124:LEU:HD13	2:B:223:PHE:CG	2.52	0.45
1:M:43:ALA:HB2	1:M:189:HIS:HB3	1.99	0.45
1:M:14:THR:HG21	1:M:390:ILE:HG13	1.98	0.45
1:M:40:TRP:CZ2	1:M:377:GLU:CA	2.95	0.45
2:N:56:ARG:HH22	2:N:318:ASP:CG	2.18	0.45
3:O:90:PHE:CE1	3:O:123:VAL:HG11	2.52	0.45
3:O:364:VAL:O	3:O:367:PRO:HG2	2.17	0.45
3:O:55:TYR:CE2	3:O:56:THR:O	2.71	0.45
4:P:190:LEU:O	4:P:191:ARG:C	2.55	0.45
1:M:329:MET:HG3	7:S:2:ARG:HH11	1.82	0.45
10:V:49:GLY:HA2	10:V:54:HIS:HB3	1.98	0.45
1:A:33:PRO:O	1:A:103:SER:HB3	2.17	0.44
1:A:349:ALA:O	1:A:408:ARG:NH2	2.50	0.44
1:A:240:GLN:HE21	1:A:431:LEU:HD21	1.81	0.44
2:B:285:VAL:O	2:B:285:VAL:HG12	2.16	0.44
3:C:115:ILE:HG21	3:C:196:HIS:CB	2.33	0.44
6:F:37:ILE:CD1	6:F:43:VAL:HG22	2.47	0.44
1:M:381:ARG:HA	1:M:384:LEU:HD12	1.98	0.44
2:N:109:VAL:HG22	2:N:119:LEU:HD23	1.99	0.44
2:N:300:ALA:HA	2:N:307:PHE:HZ	1.77	0.44
2:N:338:LYS:O	2:N:341:TYR:N	2.50	0.44
2:N:53:ALA:HB2	2:N:198:HIS:HB3	1.99	0.44
3:O:264:THR:O	3:O:266:PRO:HD3	2.16	0.44
3:O:277:ALA:HB1	3:O:294:LEU:HD11	1.98	0.44
4:P:28:ARG:HD2	4:P:185:ASP:OD2	2.17	0.44
9:U:57:GLY:O	9:U:78:TYR:CE2	2.70	0.44
2:B:122:PHE:O	2:B:126:VAL:HG23	2.18	0.44
3:C:177:ARG:HG2	3:C:181:PHE:HE2	1.82	0.44
3:C:243:VAL:HG22	3:C:243:VAL:O	2.17	0.44
3:C:310:SER:OG	3:C:312:GLN:N	2.48	0.44
12:C:380:HEM:CMB	12:C:380:HEM:HBB2	2.48	0.44
4:D:26:ILE:O	4:D:27:ARG:C	2.56	0.44
3:C:26:ASN:CA	6:F:70:MET:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:68:CYS:O	8:H:69:VAL:C	2.55	0.44
11:K:31:GLY:O	11:K:35:ALA:N	2.46	0.44
1:M:272:VAL:HG13	1:M:358:LYS:HA	1.98	0.44
2:N:395:PRO:O	2:N:396:SER:C	2.52	0.44
3:O:185:LEU:N	3:O:186:PRO:CD	2.80	0.44
3:O:278:TYR:O	3:O:279:ALA:C	2.55	0.44
3:O:276:PHE:HE2	3:O:297:SER:OG	2.00	0.44
4:P:143:LEU:HD11	4:P:149:PHE:HB2	1.98	0.44
4:P:211:MET:O	4:P:214:LEU:N	2.41	0.44
4:P:237:TYR:HB2	6:R:60:PHE:CE1	2.53	0.44
6:R:28:LYS:HB3	6:R:74:ILE:CD1	2.47	0.44
10:V:52:TRP:CG	10:V:53:LYS:N	2.85	0.44
1:A:152:TYR:OH	1:A:243:HIS:CD2	2.70	0.44
1:A:349:ALA:HB3	1:A:408:ARG:CG	2.48	0.44
2:B:211:VAL:CG1	2:B:212:SER:N	2.81	0.44
2:B:264:ILE:HG22	2:B:317:SER:HA	1.99	0.44
3:C:110:LEU:HG	3:C:114:ASN:ND2	2.27	0.44
3:C:125:ALA:HB3	3:C:185:LEU:HD21	1.98	0.44
4:D:120:ARG:HH11	4:D:120:ARG:HG2	1.82	0.44
10:J:52:TRP:CG	10:J:53:LYS:N	2.86	0.44
1:M:366:VAL:HG11	2:N:44:ALA:HB2	1.99	0.44
1:M:430:GLN:HG2	1:M:430:GLN:O	2.16	0.44
2:N:53:ALA:O	2:N:105:MET:HB2	2.17	0.44
2:N:267:ALA:O	2:N:268:GLU:C	2.56	0.44
2:N:304:HIS:HD2	2:N:306:PRO:CD	2.28	0.44
2:N:51:ILE:HD13	2:N:199:PHE:CD2	2.53	0.44
3:O:303:LEU:HD23	3:O:303:LEU:HA	1.85	0.44
3:O:315:MET:O	3:O:318:ARG:N	2.40	0.44
3:O:352:GLN:O	3:O:356:VAL:HG23	2.17	0.44
3:O:64:SER:O	3:O:65:SER:C	2.55	0.44
3:O:327:ALA:HA	7:S:51:PRO:HB3	1.99	0.44
10:V:46:ILE:HG12	10:V:46:ILE:H	1.40	0.44
1:A:61:HIS:HB3	1:A:130:GLU:HG3	1.97	0.44
3:C:183:PHE:CE1	3:C:187:PHE:HE2	2.35	0.44
3:C:235:LEU:HG	3:C:236:ILE:N	2.32	0.44
3:C:47:THR:HG23	3:C:79:ILE:HG23	1.99	0.44
4:D:10:TYR:HD1	8:H:74:PHE:CD1	2.35	0.44
4:D:116:ILE:HA	4:D:116:ILE:HD12	1.69	0.44
1:M:19:LEU:HB2	1:M:23:LEU:HB3	1.99	0.44
1:M:286:GLY:O	1:M:287:GLY:C	2.56	0.44
1:M:287:GLY:O	1:M:290:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:324:PHE:CG	1:M:334:MET:HG2	2.52	0.44
2:N:112:LEU:O	2:N:113:ARG:C	2.54	0.44
1:M:433:ASP:CG	3:O:223:TYR:HH	2.17	0.44
3:O:48:GLY:HA3	12:O:380:HEM:C3C	2.52	0.44
4:P:138:PRO:HB3	8:T:54:CYS:C	2.37	0.44
4:P:165:TYR:CZ	4:P:168:VAL:HG22	2.53	0.44
5:Q:99:ARG:NH1	5:Q:148:ALA:HB1	2.32	0.44
7:S:40:ARG:O	7:S:44:CYS:SG	2.71	0.44
10:V:57:HIS:O	10:V:60:GLU:HG2	2.18	0.44
1:A:179:ARG:HG3	1:A:180:ALA:N	2.31	0.44
2:B:262:ALA:CB	2:B:268:GLU:HB3	2.47	0.44
3:C:28:SER:CB	3:C:30:TRP:HD1	2.28	0.44
3:C:336:THR:HG22	3:C:336:THR:O	2.18	0.44
4:D:167:GLU:O	4:D:167:GLU:HG2	2.17	0.44
4:D:165:TYR:CD2	4:D:168:VAL:HG22	2.52	0.44
4:D:233:ARG:CG	7:G:17:SER:HB3	2.48	0.44
5:E:7:VAL:HA	5:E:8:PRO:HD3	1.84	0.44
6:F:46:ALA:O	6:F:49:ARG:N	2.30	0.44
3:C:26:ASN:HA	6:F:70:MET:HA	1.98	0.44
8:H:69:VAL:O	8:H:73:LEU:HB3	2.18	0.44
1:M:349:ALA:O	1:M:408:ARG:CZ	2.65	0.44
2:N:182:ARG:O	2:N:185:LYS:HB3	2.17	0.44
2:N:286:LYS:HD3	2:N:287:ARG:HH12	1.80	0.44
3:O:41:LEU:HD12	12:O:380:HEM:HBB1	2.00	0.44
4:P:43:MET:HE3	4:P:91:PHE:CE2	2.53	0.44
7:S:73:ASN:ND2	8:T:56:GLU:OE2	2.38	0.44
2:N:316:TYR:HH	9:U:64:LEU:HD23	1.76	0.44
2:B:38:LEU:O	2:B:39:GLU:C	2.56	0.44
2:B:361:LYS:NZ	2:B:403:ASP:O	2.39	0.44
2:B:71:LEU:HD23	2:B:71:LEU:HA	1.72	0.44
3:C:245:PHE:CE1	4:D:17:LEU:HB3	2.53	0.44
3:C:242:LEU:HD21	3:C:250:LEU:HD22	1.99	0.44
4:D:168:VAL:HG12	4:D:169:LEU:CD2	2.47	0.44
4:D:67:GLU:O	4:D:70:VAL:HG12	2.17	0.44
6:F:106:GLU:OE1	6:F:109:LYS:HE2	2.17	0.44
1:M:64:PHE:HE1	1:M:86:LEU:CD1	2.31	0.44
3:O:334:THR:HG1	7:S:55:PHE:HD1	1.63	0.44
3:O:341:GLN:HE21	3:O:341:GLN:HA	1.82	0.44
3:O:227:LYS:HG2	4:P:223:LYS:HZ3	1.83	0.44
1:A:16:VAL:HG11	1:A:388:ARG:HB2	1.99	0.44
1:A:197:LEU:CD1	1:A:208:LEU:HD11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:LEU:O	2:B:143:GLN:N	2.40	0.44
2:B:294:SER:O	2:B:295:LEU:C	2.55	0.44
2:B:346:THR:O	2:B:349:GLN:N	2.39	0.44
3:C:113:TRP:O	3:C:117:VAL:HG23	2.17	0.44
3:C:271:GLU:OE2	3:C:273:TYR:OH	2.36	0.44
4:D:10:TYR:CE1	4:D:128:PHE:HE2	2.34	0.44
4:D:220:TYR:CD2	7:G:26:PHE:CZ	3.06	0.44
4:D:35:GLN:HB2	4:D:169:LEU:HD11	1.98	0.44
7:G:40:ARG:O	7:G:41:THR:C	2.55	0.44
1:M:38:GLY:HA3	1:M:40:TRP:CZ3	2.50	0.44
2:N:134:ARG:HE	2:N:134:ARG:HB3	1.49	0.44
1:M:85:HIS:HA	2:N:284:HIS:O	2.18	0.44
2:N:279:LEU:HD23	2:N:295:LEU:HD13	2.00	0.44
2:N:62:ASN:ND2	2:N:65:THR:CB	2.81	0.44
3:O:101:GLY:O	3:O:107:TYR:HD2	2.01	0.44
3:O:252:ASP:CB	3:O:253:PRO:CD	2.90	0.44
3:O:124:MET:HE1	3:O:298:ILE:HD13	1.99	0.44
3:O:310:SER:HA	3:O:374:ASN:ND2	2.07	0.44
5:Q:22:THR:O	5:Q:22:THR:OG1	2.34	0.44
4:P:27:ARG:NH1	10:V:58:LYS:HE3	2.33	0.44
3:C:157:GLY:O	3:C:160:LEU:N	2.51	0.44
3:C:170:VAL:CG1	3:C:174:THR:CG2	2.89	0.44
7:G:33:GLY:O	7:G:34:ILE:C	2.56	0.44
10:J:4:THR:HG22	10:J:6:THR:N	2.33	0.44
2:N:140:LEU:O	2:N:142:PRO:N	2.51	0.44
2:N:170:ASN:OD1	2:N:171:ALA:N	2.50	0.44
2:N:222:GLN:HB3	2:N:223:PHE:CD2	2.53	0.44
2:N:357:VAL:O	2:N:360:ALA:HB3	2.18	0.44
3:O:126:THR:CG2	12:O:380:HEM:C3B	3.01	0.44
3:O:80:ARG:HD2	3:O:80:ARG:HH11	1.33	0.44
5:Q:107:ASP:O	5:Q:110:ALA:N	2.51	0.44
6:R:103:GLU:O	6:R:104:ARG:C	2.55	0.44
1:A:89:TYR:C	1:A:89:TYR:HD1	2.21	0.44
2:B:338:LYS:HD3	2:B:439:LEU:CD2	2.46	0.44
3:C:282:ARG:O	3:C:283:SER:C	2.55	0.44
3:C:299:LEU:HA	3:C:299:LEU:HD22	1.79	0.44
3:C:30:TRP:O	3:C:33:PHE:CD2	2.61	0.44
3:C:32:ASN:O	3:C:36:LEU:HG	2.18	0.44
4:D:138:PRO:CG	8:H:55:THR:HA	2.48	0.44
4:D:161:ALA:O	4:D:163:PRO:CD	2.66	0.44
4:D:229:VAL:O	4:D:229:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:HIS:O	4:D:24:THR:C	2.55	0.44
4:D:31:GLN:HA	4:D:31:GLN:OE1	2.17	0.44
4:D:72:ASP:OD2	4:D:92:PRO:HB2	2.18	0.44
6:F:52:GLU:HG3	6:F:56:ASP:OD2	2.18	0.44
7:G:39:ARG:HA	7:G:42:ARG:HD2	2.00	0.44
10:J:18:SER:CB	11:K:23:LEU:HD12	2.30	0.44
4:P:26:ILE:CG2	4:P:54:VAL:HG13	2.47	0.44
3:O:373:GLU:HB3	6:R:20:TYR:OH	2.18	0.44
1:M:417:ASP:CG	10:V:10:TYR:OH	2.52	0.44
1:A:32:GLN:HE22	2:B:373:GLU:HA	1.83	0.43
1:A:426:GLY:CA	1:A:427:PRO:C	2.86	0.43
3:C:338:ILE:HA	3:C:341:GLN:HG3	1.99	0.43
7:G:44:CYS:O	7:G:45:ILE:C	2.57	0.43
7:G:80:ASP:CG	8:H:47:ARG:HH22	2.22	0.43
1:M:145:MET:CE	1:M:248:LEU:HD12	2.48	0.43
1:M:345:LEU:HA	1:M:345:LEU:HD23	1.69	0.43
2:N:99:THR:O	2:N:106:ALA:N	2.51	0.43
3:O:31:TRP:CD2	3:O:100:ARG:HD2	2.53	0.43
3:O:102:LEU:HA	3:O:102:LEU:HD23	1.67	0.43
3:O:160:LEU:HD12	3:O:160:LEU:O	2.18	0.43
4:P:161:ALA:O	4:P:163:PRO:HD3	2.18	0.43
5:Q:122:HIS:HB3	5:Q:125:GLU:CG	2.48	0.43
5:Q:186:GLU:O	5:Q:186:GLU:CG	2.66	0.43
9:U:70:LEU:CD2	9:U:73:PRO:CD	2.92	0.43
10:V:4:THR:CG2	10:V:6:THR:OG1	2.66	0.43
1:A:385:THR:HG22	1:A:386:TYR:CD1	2.52	0.43
1:A:433:ASP:O	1:A:434:TYR:C	2.56	0.43
2:B:275:LEU:HD11	2:B:279:LEU:HD12	1.99	0.43
3:C:153:ILE:HD12	3:C:153:ILE:H	1.82	0.43
3:C:122:THR:CG2	3:C:189:ILE:CG1	2.97	0.43
3:C:103:TYR:CE1	3:C:322:GLN:HG3	2.53	0.43
3:C:357:LEU:HD12	3:C:361:LEU:HG	2.00	0.43
6:F:88:SER:O	6:F:92:PRO:HD3	2.18	0.43
10:J:52:TRP:HE3	10:J:52:TRP:N	2.14	0.43
10:J:49:GLY:H	10:J:54:HIS:CD2	2.37	0.43
11:K:20:THR:HG23	11:K:24:TRP:HD1	1.83	0.43
1:M:211:LEU:HD12	1:M:211:LEU:O	2.18	0.43
1:M:8:LEU:HD11	1:M:396:GLU:HG3	2.00	0.43
1:M:4:TYR:O	1:M:5:ALA:C	2.56	0.43
2:N:271:ALA:O	2:N:272:PHE:C	2.57	0.43
3:C:53:MET:SD	3:O:181:PHE:CZ	3.10	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:208:PRO:O	3:O:314:SER:OG	2.30	0.43
3:O:107:TYR:OH	3:O:308:HIS:HB2	2.17	0.43
3:O:248:ASP:CG	4:P:118:ARG:HH21	2.22	0.43
4:P:178:THR:O	4:P:179:MET:C	2.55	0.43
5:Q:150:ALA:CB	5:Q:157:TYR:HB2	2.48	0.43
5:Q:121:GLN:O	5:Q:170:ARG:HD3	2.18	0.43
2:B:347:ILE:N	2:B:347:ILE:CD1	2.81	0.43
2:B:433:THR:HA	2:B:434:PRO:HD2	1.90	0.43
3:C:26:ASN:HD22	3:C:208:PRO:HD2	1.82	0.43
4:D:158:ILE:CG1	4:D:159:GLY:N	2.81	0.43
3:C:234:LEU:HD21	4:D:216:LEU:HD21	2.00	0.43
2:B:314:ALA:CB	9:I:64:LEU:HD22	2.48	0.43
1:A:347:THR:HA	11:K:16:ASN:HD22	1.84	0.43
1:M:292:SER:O	1:M:295:ALA:N	2.52	0.43
1:M:158:PHE:HE1	1:M:317:THR:HG21	1.72	0.43
1:M:157:ALA:HB2	1:M:421:ALA:HB1	1.99	0.43
1:M:89:TYR:C	1:M:89:TYR:CD1	2.90	0.43
2:N:237:ALA:HB2	2:N:318:ASP:CG	2.37	0.43
2:N:283:PRO:HG3	9:U:55:LEU:CG	2.49	0.43
2:N:81:SER:O	2:N:84:LYS:N	2.50	0.43
3:O:338:ILE:HA	3:O:341:GLN:HG3	1.99	0.43
4:P:33:TYR:O	4:P:37:CYS:N	2.41	0.43
4:P:34:LYS:O	4:P:34:LYS:HG2	2.18	0.43
4:P:94:PRO:HB2	4:P:95:TYR:CD1	2.53	0.43
5:Q:171:ILE:HB	5:Q:178:LEU:O	2.17	0.43
6:R:67:ASP:HA	6:R:70:MET:HE3	2.00	0.43
7:S:68:LYS:HD3	7:S:72:LYS:HE3	2.01	0.43
1:A:231:LEU:H	1:A:231:LEU:HG	1.67	0.43
2:B:341:TYR:O	2:B:342:ASN:C	2.57	0.43
2:B:24:LEU:CG	2:B:38:LEU:HD11	2.31	0.43
3:C:319:PRO:O	3:C:322:GLN:N	2.52	0.43
5:E:15:ARG:H	5:E:15:ARG:HG2	1.66	0.43
1:M:75:LEU:HD21	1:M:116:ILE:HG12	2.00	0.43
1:M:307:PHE:C	1:M:307:PHE:CD1	2.91	0.43
2:N:47:ILE:CG2	2:N:48:GLY:H	2.31	0.43
3:O:30:TRP:HA	3:O:33:PHE:CE2	2.52	0.43
1:A:296:SER:O	1:A:297:ILE:C	2.55	0.43
1:A:86:LEU:HD12	1:A:98:TYR:O	2.19	0.43
2:B:295:LEU:O	2:B:299:VAL:HG23	2.19	0.43
3:C:7:SER:O	3:C:8:HIS:O	2.36	0.43
4:D:116:ILE:CD1	4:D:120:ARG:HH11	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:10:TYR:CE1	4:D:128:PHE:CE2	3.07	0.43
2:N:372:VAL:O	2:N:372:VAL:CG1	2.67	0.43
3:O:227:LYS:CG	4:P:223:LYS:NZ	2.82	0.43
3:O:278:TYR:O	3:O:281:LEU:N	2.48	0.43
5:Q:76:ILE:HD12	5:Q:192:MET:HE3	2.00	0.43
6:R:50:LEU:HA	6:R:51:PRO:HD2	1.71	0.43
6:R:94:LEU:O	6:R:98:ILE:HG13	2.19	0.43
1:A:260:PRO:HG3	1:A:414:TYR:OH	2.19	0.43
1:A:29:GLN:HA	1:A:201:GLY:O	2.18	0.43
3:C:213:SER:O	3:C:214:ASP:C	2.56	0.43
3:C:107:TYR:CE2	3:C:305:PRO:HA	2.53	0.43
3:C:80:ARG:C	3:C:80:ARG:HD3	2.39	0.43
4:D:208:MET:HE2	4:D:208:MET:O	2.18	0.43
6:F:46:ALA:O	6:F:47:ILE:C	2.56	0.43
7:G:26:PHE:N	7:G:27:PRO:HD3	2.33	0.43
1:M:158:PHE:O	1:M:164:ALA:HB2	2.18	0.43
1:M:281:ASP:HB3	1:M:284:TYR:CD1	2.53	0.43
2:N:211:VAL:HG12	2:N:212:SER:N	2.34	0.43
3:O:123:VAL:CG1	3:O:123:VAL:O	2.65	0.43
3:O:183:PHE:CD1	3:O:183:PHE:O	2.72	0.43
5:Q:97:PHE:CD1	5:Q:137:GLY:HA3	2.54	0.43
1:A:213:GLN:HB3	1:A:215:HIS:CD2	2.53	0.43
2:B:110:GLU:O	2:B:111:CYS:HB3	2.18	0.43
3:C:147:THR:CG2	3:C:165:TRP:NE1	2.78	0.43
3:C:254:ASP:HB3	4:D:119:ALA:O	2.18	0.43
4:D:131:LEU:HD13	4:D:164:ILE:CD1	2.48	0.43
1:M:106:LEU:HA	1:M:109:ALA:HB3	2.01	0.43
1:M:184:GLU:O	1:M:185:TYR:C	2.56	0.43
1:M:73:ASN:O	1:M:77:LYS:CD	2.66	0.43
2:N:194:TYR:O	2:N:195:VAL:C	2.54	0.43
2:N:83:PHE:CZ	2:N:87:ARG:HG3	2.53	0.43
3:O:207:ASN:OD1	3:O:207:ASN:O	2.37	0.43
5:Q:49:TYR:O	5:Q:50:ALA:C	2.56	0.43
8:T:58:LEU:CD1	8:T:62:LEU:HG	2.48	0.43
1:A:426:GLY:CA	1:A:428:ILE:HG12	2.48	0.43
1:A:66:GLY:O	1:A:121:SER:N	2.50	0.43
2:B:68:LEU:O	2:B:71:LEU:N	2.50	0.43
3:C:196:HIS:HE1	12:C:381:HEM:C1D	2.37	0.43
3:C:200:LEU:HD13	12:C:381:HEM:CAD	2.49	0.43
3:C:8:HIS:HB2	3:C:9:PRO:HD2	2.00	0.43
4:D:93:LYS:O	4:D:94:PRO:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:68:LEU:HD11	6:F:75:LEU:HD13	2.01	0.43
1:M:149:VAL:CG1	1:M:150:PHE:N	2.81	0.43
1:M:297:ILE:HG22	1:M:303:LEU:CD1	2.43	0.43
1:M:385:THR:HB	1:M:386:TYR:CD1	2.53	0.43
1:M:91:THR:HG22	1:M:94:HIS:N	2.33	0.43
2:N:182:ARG:NH1	2:N:185:LYS:CG	2.79	0.43
2:N:213:HIS:O	2:N:213:HIS:HD2	2.02	0.43
2:N:258:VAL:HG21	2:N:312:PHE:HD2	1.82	0.43
2:N:160:ILE:HD11	2:N:325:TYR:CE2	2.53	0.43
2:N:47:ILE:HB	2:N:109:VAL:CG1	2.49	0.43
3:O:103:TYR:CE1	3:O:322:GLN:HG3	2.53	0.43
3:O:211:ILE:HG22	3:O:212:SER:N	2.34	0.43
3:O:235:LEU:O	3:O:235:LEU:HD12	2.19	0.43
4:P:131:LEU:HD22	4:P:163:PRO:CB	2.48	0.43
6:R:71:ARG:O	6:R:72:GLN:HB2	2.19	0.43
1:M:239:SER:CB	7:S:18:LEU:HD23	2.49	0.43
1:A:385:THR:HB	1:A:386:TYR:HD1	1.83	0.43
1:A:436:ARG:NE	3:C:222:PRO:HG3	2.33	0.43
3:C:328:LEU:O	3:C:329:VAL:C	2.56	0.43
4:D:221:ALA:O	4:D:222:MET:C	2.57	0.43
5:E:65:SER:O	5:E:66:ALA:C	2.55	0.43
6:F:49:ARG:NH2	6:F:100:GLU:OE2	2.47	0.43
1:M:152:TYR:OH	1:M:243:HIS:CD2	2.71	0.43
1:M:170:PRO:O	1:M:171:SER:C	2.55	0.43
1:M:226:ASP:O	1:M:228:VAL:N	2.51	0.43
2:N:163:LEU:HD22	2:N:256:ALA:HB1	2.01	0.43
2:N:269:ALA:O	2:N:270:ASN:C	2.57	0.43
1:M:4:TYR:CD1	2:N:43:PRO:HB3	2.53	0.43
2:N:84:LYS:O	2:N:85:ILE:C	2.56	0.43
3:O:56:THR:HG22	3:O:57:SER:N	2.34	0.43
4:P:131:LEU:CD2	4:P:163:PRO:HB3	2.48	0.43
4:P:165:TYR:CE1	4:P:168:VAL:HA	2.54	0.43
5:Q:119:ASP:OD1	5:Q:120:PRO:CD	2.67	0.43
1:A:168:GLU:HG3	1:A:168:GLU:H	1.63	0.43
3:C:243:VAL:HG13	3:C:244:LEU:CD1	2.48	0.43
3:C:37:LEU:CD1	3:C:97:HIS:CD2	3.01	0.43
3:C:71:ARG:HB3	4:D:49:ARG:HH22	1.84	0.43
4:D:7:PRO:HB2	4:D:125:ASP:CB	2.49	0.43
3:C:342:PRO:HG2	7:G:66:PHE:CZ	2.53	0.43
8:H:15:ASP:HB2	8:H:16:PRO:HD3	2.01	0.43
3:O:122:THR:HB	3:O:189:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:44:GLN:OE1	3:O:44:GLN:HA	2.19	0.43
4:P:102:ARG:HE	4:P:109:LEU:HB2	1.83	0.43
4:P:188:THR:O	4:P:189:PHE:C	2.55	0.43
4:P:226:LYS:HD3	4:P:226:LYS:HA	1.76	0.43
4:P:35:GLN:OE1	4:P:35:GLN:HA	2.18	0.43
6:R:48:ARG:HA	6:R:48:ARG:HD3	1.51	0.43
7:S:45:ILE:HA	7:S:45:ILE:HD12	1.88	0.43
1:A:154:HIS:HE1	1:A:314:TYR:OH	2.02	0.42
1:A:277:ILE:HB	1:A:309:THR:HG21	2.00	0.42
1:A:41:ILE:H	1:A:41:ILE:CD1	2.25	0.42
2:B:331:ALA:CA	2:B:432:HIS:ND1	2.79	0.42
3:C:90:PHE:CZ	3:C:123:VAL:HG21	2.54	0.42
3:C:239:LEU:O	3:C:243:VAL:HB	2.19	0.42
4:D:195:GLU:HA	4:D:196:PRO:HD2	1.80	0.42
5:E:32:ARG:HH12	7:G:22:GLU:CD	2.21	0.42
8:H:15:ASP:CB	8:H:16:PRO:CD	2.97	0.42
1:M:213:GLN:CB	1:M:215:HIS:CD2	3.02	0.42
1:M:428:ILE:CG2	1:M:431:LEU:CG	2.97	0.42
2:N:34:VAL:O	2:N:35:ILE:HG22	2.19	0.42
2:N:99:THR:OG1	9:U:68:VAL:HG13	2.19	0.42
10:V:4:THR:O	10:V:5:LEU:C	2.57	0.42
1:A:19:LEU:HD22	1:A:214:LYS:NZ	2.34	0.42
1:A:426:GLY:H	1:A:428:ILE:HD11	1.83	0.42
2:B:128:THR:C	2:B:130:PRO:HD2	2.39	0.42
2:B:158:HIS:ND1	2:B:246:GLU:OE1	2.52	0.42
2:B:262:ALA:HB2	2:B:272:PHE:CE2	2.53	0.42
2:B:46:ARG:NH1	2:B:376:GLU:HG3	2.30	0.42
3:C:163:TRP:CZ2	5:Q:62:MET:CE	3.02	0.42
3:C:373:GLU:O	3:C:377:LEU:HD12	2.18	0.42
3:C:8:HIS:O	3:C:9:PRO:C	2.57	0.42
7:G:56:TYR:O	7:G:57:LEU:C	2.56	0.42
9:I:64:LEU:HG	9:I:65:VAL:HG23	1.99	0.42
1:M:78:GLU:HG2	1:M:112:LEU:HD21	2.02	0.42
2:N:109:VAL:CG1	2:N:109:VAL:O	2.66	0.42
2:N:257:LEU:HA	2:N:257:LEU:HD12	1.67	0.42
3:O:183:PHE:CE1	3:O:187:PHE:HE2	2.37	0.42
3:O:230:LEU:O	3:O:230:LEU:HG	2.17	0.42
3:O:277:ALA:O	3:O:278:TYR:C	2.57	0.42
3:O:314:SER:OG	3:O:316:MET:HB3	2.19	0.42
3:O:338:ILE:HA	3:O:341:GLN:CG	2.49	0.42
3:O:47:THR:HG23	3:O:79:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:114:VAL:HG13	5:Q:120:PRO:HB3	2.01	0.42
5:Q:33:LYS:HA	7:S:21:PHE:CE1	2.55	0.42
6:R:37:ILE:CG1	6:R:43:VAL:HG21	2.40	0.42
4:P:139:THR:HB	8:T:54:CYS:SG	2.58	0.42
1:A:54:GLY:O	1:A:55:ALA:O	2.37	0.42
3:C:126:THR:HG21	12:C:380:HEM:C3B	2.53	0.42
3:C:92:ILE:HG12	3:C:272:TRP:CH2	2.54	0.42
3:C:107:TYR:HE2	3:C:305:PRO:HA	1.83	0.42
4:D:69:GLU:O	4:D:73:GLY:CA	2.67	0.42
6:F:87:LYS:HG3	6:F:89:TYR:HB3	2.00	0.42
7:G:52:PHE:O	7:G:53:VAL:C	2.54	0.42
8:H:22:GLU:O	8:H:23:GLN:C	2.57	0.42
1:M:136:GLN:HE21	9:U:50:LEU:HG	1.84	0.42
1:M:334:MET:HA	1:M:334:MET:CE	2.49	0.42
1:M:255:ILE:HD13	1:M:335:MET:HE1	2.00	0.42
1:M:262:TRP:CE3	1:M:385:THR:HG23	2.52	0.42
2:N:294:SER:O	2:N:297:GLN:N	2.53	0.42
4:P:240:PRO:CG	4:P:241:LYS:H	2.33	0.42
4:P:68:VAL:CG1	4:P:92:PRO:HG2	2.47	0.42
5:Q:114:VAL:O	5:Q:117:LEU:N	2.48	0.42
5:Q:141:HIS:CE1	5:Q:175:PRO:HG2	2.54	0.42
5:Q:29:SER:CB	5:Q:32:ARG:HD3	2.49	0.42
1:A:56:GLY:O	1:A:59:VAL:HB	2.19	0.42
1:A:62:LEU:HB3	1:A:122:LEU:HD22	2.02	0.42
2:B:79:GLY:H	2:B:125:ASN:HD22	1.67	0.42
3:C:13:ILE:HD13	3:C:13:ILE:HG21	1.83	0.42
3:C:206:ASN:CB	3:C:313:ARG:NH2	2.61	0.42
3:C:53:MET:SD	3:O:181:PHE:HZ	2.43	0.42
4:D:3:LEU:HD22	7:G:70:LYS:HZ3	1.84	0.42
4:D:41:HIS:CD2	13:D:242:HEC:NB	2.84	0.42
6:F:95:LYS:O	6:F:96:GLU:C	2.57	0.42
3:C:346:PRO:CG	7:G:66:PHE:HD1	2.28	0.42
1:M:153:LEU:CD2	1:M:319:LEU:HD13	2.48	0.42
1:M:64:PHE:HE2	1:M:88:ALA:HB2	1.81	0.42
2:N:162:ASN:ND2	2:N:244:ILE:HG21	2.33	0.42
2:N:308:ASP:C	2:N:308:ASP:OD1	2.57	0.42
2:N:338:LYS:O	2:N:339:ALA:C	2.58	0.42
3:O:234:LEU:O	3:O:237:LEU:HB3	2.19	0.42
1:M:446:PHE:HE2	3:O:6:LYS:HZ1	1.65	0.42
3:O:88:SER:HA	3:O:272:TRP:CZ2	2.53	0.42
4:P:230:LEU:O	4:P:233:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:185:TYR:HD2	5:Q:193:VAL:HG21	1.84	0.42
3:C:163:TRP:CD1	5:Q:63:SER:HA	2.55	0.42
2:B:135:TRP:CE2	6:R:49:ARG:HD3	2.53	0.42
3:O:211:ILE:CG2	6:R:62:ILE:HD13	2.50	0.42
5:Q:14:ARG:HA	7:S:23:GLN:HA	2.01	0.42
7:S:80:ASP:CG	8:T:47:ARG:HH22	2.22	0.42
1:A:106:LEU:O	1:A:107:PRO:C	2.56	0.42
1:A:134:ILE:O	1:A:137:GLU:N	2.53	0.42
1:A:227:ALA:O	1:A:229:PRO:HD3	2.19	0.42
1:A:328:HIS:NE2	1:A:329:MET:HG2	2.35	0.42
1:A:343:MET:HG2	1:A:343:MET:H	1.34	0.42
2:B:170:ASN:OD1	2:B:171:ALA:N	2.52	0.42
3:C:156:ILE:HG12	3:C:157:GLY:N	2.29	0.42
3:C:177:ARG:O	3:C:181:PHE:CD2	2.72	0.42
4:D:21:LEU:CD1	4:D:26:ILE:HD11	2.49	0.42
2:N:282:GLY:HA2	2:N:283:PRO:HD2	1.78	0.42
2:N:309:VAL:CG1	2:N:310:SER:N	2.82	0.42
2:N:312:PHE:CD1	9:U:58:GLN:O	2.73	0.42
3:O:14:VAL:HG12	3:O:14:VAL:O	2.20	0.42
4:P:7:PRO:HB3	4:P:125:ASP:HB3	2.01	0.42
4:P:175:THR:HA	4:P:176:PRO:HD2	1.71	0.42
4:P:5:LEU:HG	4:P:152:TYR:CE1	2.54	0.42
5:Q:118:ARG:HH11	5:Q:118:ARG:HD2	1.69	0.42
5:Q:73:LYS:O	5:Q:74:ILE:HD13	2.20	0.42
6:R:101:ARG:HG2	6:R:105:GLU:OE2	2.19	0.42
10:V:52:TRP:HE3	10:V:52:TRP:N	2.18	0.42
1:A:262:TRP:CE3	1:A:385:THR:CG2	3.02	0.42
1:A:61:HIS:HB2	1:A:130:GLU:HG3	2.00	0.42
3:C:25:SER:HA	3:C:218:ILE:HD11	1.98	0.42
4:D:25:SER:O	4:D:26:ILE:C	2.58	0.42
1:M:224:ASP:OD1	1:M:224:ASP:O	2.37	0.42
1:M:283:THR:OG1	9:U:74:ALA:HB3	2.20	0.42
1:M:395:TRP:O	1:M:396:GLU:C	2.57	0.42
1:M:67:THR:OG1	1:M:119:ASN:HB2	2.20	0.42
2:N:31:ASN:HB3	2:N:201:SER:CB	2.50	0.42
3:O:18:PHE:O	3:O:220:PHE:HD2	2.03	0.42
3:O:119:LEU:CD1	3:O:192:ILE:CG2	2.97	0.42
3:O:192:ILE:CD1	3:O:192:ILE:N	2.82	0.42
4:P:206:LEU:HG	4:P:210:LEU:HD11	2.02	0.42
4:P:31:GLN:O	4:P:32:VAL:C	2.56	0.42
5:Q:102:THR:H	5:Q:105:GLU:CB	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:150:ALA:CB	5:Q:157:TYR:CB	2.98	0.42
11:W:24:TRP:HA	11:W:24:TRP:CE3	2.55	0.42
2:B:134:ARG:HG2	2:B:135:TRP:N	2.35	0.42
2:B:283:PRO:HG3	9:I:55:LEU:CG	2.50	0.42
1:A:83:GLY:O	2:B:370:MET:HE1	2.19	0.42
2:B:348:ALA:CB	2:B:418:VAL:HG21	2.49	0.42
3:C:163:TRP:CE2	5:Q:62:MET:HE2	2.54	0.42
4:D:220:TYR:O	4:D:221:ALA:C	2.56	0.42
2:B:283:PRO:CG	9:I:55:LEU:HD13	2.50	0.42
1:M:252:HIS:CD2	1:M:325:VAL:HG22	2.53	0.42
1:M:349:ALA:HB3	1:M:408:ARG:NE	2.34	0.42
1:M:43:ALA:HB1	1:M:189:HIS:CB	2.50	0.42
1:M:63:ALA:HB2	1:M:97:TYR:HE2	1.84	0.42
2:N:303:VAL:HG12	2:N:304:HIS:H	1.84	0.42
2:N:360:ALA:O	2:N:361:LYS:C	2.58	0.42
2:N:396:SER:HA	2:N:399:LEU:HD12	2.02	0.42
3:O:196:HIS:HE1	12:O:381:HEM:CHD	2.32	0.42
3:O:25:SER:HA	3:O:218:ILE:HD12	2.02	0.42
3:O:284:ILE:HG23	3:O:285:PRO:HD2	2.02	0.42
3:O:378:LYS:CD	6:R:33:ARG:HH12	2.32	0.42
4:P:233:ARG:O	4:P:234:LYS:HE2	2.19	0.42
5:Q:145:VAL:HA	5:Q:146:PRO:HD3	1.75	0.42
5:Q:185:TYR:HB3	5:Q:195:VAL:HA	2.00	0.42
5:Q:20:ASP:O	5:Q:22:THR:N	2.52	0.42
5:Q:40:THR:HG22	10:V:20:PHE:CZ	2.51	0.42
4:P:178:THR:HG23	8:T:15:ASP:N	2.34	0.42
1:A:151:ASN:O	1:A:154:HIS:N	2.53	0.42
1:A:253:VAL:O	1:A:323:HIS:HA	2.20	0.42
1:A:311:ASN:OD1	1:A:320:LEU:HD23	2.18	0.42
2:B:68:LEU:HB2	2:B:144:LEU:HD21	2.02	0.42
2:B:258:VAL:HG11	2:B:321:LEU:HD22	2.00	0.42
2:B:279:LEU:CD2	2:B:344:VAL:HG22	2.49	0.42
4:D:223:LYS:NZ	4:D:227:TRP:CD1	2.86	0.42
4:D:55:CYS:SG	10:J:52:TRP:HB2	2.60	0.42
6:F:99:ARG:O	6:F:100:GLU:C	2.57	0.42
11:K:20:THR:HG23	11:K:24:TRP:CD1	2.54	0.42
1:M:61:HIS:HB2	1:M:130:GLU:HG3	2.02	0.42
1:M:19:LEU:CD1	1:M:214:LYS:HG2	2.48	0.42
1:M:152:TYR:CE2	1:M:243:HIS:HD2	2.38	0.42
2:N:129:ALA:O	2:N:130:PRO:C	2.58	0.42
2:N:135:TRP:NE1	2:N:136:GLU:HG3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:49:LEU:HD21	2:N:204:MET:SD	2.60	0.42
2:N:72:ALA:HB1	2:N:75:LEU:CD1	2.49	0.42
3:O:115:ILE:HG22	3:O:196:HIS:HB2	1.97	0.42
3:O:248:ASP:O	3:O:249:LEU:C	2.58	0.42
3:O:282:ARG:CZ	3:O:343:VAL:HG22	2.49	0.42
3:O:366:MET:N	3:O:367:PRO:HD2	2.33	0.42
4:P:167:GLU:O	4:P:167:GLU:HG2	2.20	0.42
3:O:244:LEU:O	4:P:201:ARG:HG2	2.20	0.42
4:P:240:PRO:HG2	4:P:241:LYS:N	2.34	0.42
4:P:43:MET:HB2	4:P:43:MET:HE2	1.74	0.42
4:P:58:GLU:O	4:P:62:LYS:HB2	2.19	0.42
2:B:83:PHE:CE1	6:R:104:ARG:HG2	2.54	0.42
9:U:66:ALA:O	9:U:77:ARG:HG3	2.20	0.42
1:A:224:ASP:OD1	1:A:224:ASP:O	2.38	0.42
1:A:280:TYR:HB3	1:A:307:PHE:CD2	2.55	0.42
1:A:33:PRO:O	1:A:103:SER:CB	2.67	0.42
1:A:361:LEU:O	1:A:361:LEU:HD12	2.19	0.42
1:A:8:LEU:HD11	1:A:396:GLU:HG3	2.02	0.42
2:B:239:TYR:OH	2:B:423:SER:OG	2.37	0.42
3:C:184:ILE:HG12	3:C:184:ILE:O	2.19	0.42
3:C:218:ILE:CG2	3:C:219:PRO:N	2.82	0.42
3:C:280:ILE:HA	3:C:355:SER:OG	2.20	0.42
3:C:3:ASN:HA	3:C:8:HIS:CD2	2.55	0.42
3:C:78:ILE:HG21	3:C:78:ILE:HD13	1.80	0.42
4:D:29:GLY:HA2	4:D:32:VAL:HG23	2.02	0.42
6:F:10:SER:HA	6:F:13:LEU:HG	2.01	0.42
6:F:43:VAL:O	6:F:44:LYS:C	2.57	0.42
6:F:64:ARG:O	6:F:68:LEU:HD12	2.20	0.42
7:G:36:ASN:O	7:G:37:VAL:C	2.56	0.42
1:M:130:GLU:O	1:M:131:ARG:C	2.57	0.42
1:M:297:ILE:CG2	1:M:303:LEU:HD12	2.43	0.42
2:N:343:GLN:O	2:N:343:GLN:HG3	2.20	0.42
2:N:243:GLU:HA	2:N:424:MET:O	2.20	0.42
4:P:195:GLU:HA	4:P:196:PRO:HD2	1.73	0.42
5:Q:147:ILE:O	5:Q:148:ALA:C	2.57	0.42
5:Q:13:TYR:O	7:S:24:ARG:HG3	2.20	0.42
9:U:64:LEU:CG	9:U:65:VAL:HG23	2.42	0.42
10:V:23:THR:O	10:V:24:ILE:C	2.58	0.42
1:A:314:TYR:HB2	1:A:317:THR:O	2.20	0.42
1:A:46:ARG:NH1	1:A:316:ASP:OD1	2.50	0.42
2:B:161:GLU:CD	2:B:175:SER:HB2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:116:ILE:CD1	4:D:120:ARG:HG3	2.49	0.42
4:D:171:PHE:HZ	4:D:182:VAL:HG22	1.85	0.42
6:F:94:LEU:O	6:F:94:LEU:HD12	2.20	0.42
1:M:100:LYS:HG2	2:N:370:MET:SD	2.59	0.42
1:M:31:SER:N	1:M:202:GLY:HA2	2.35	0.42
1:M:420:PRO:HG3	1:M:441:MET:SD	2.60	0.42
1:M:59:VAL:CG2	1:M:186:LEU:HD11	2.50	0.42
3:O:236:ILE:O	3:O:237:LEU:C	2.57	0.42
4:P:150:ASN:OD1	4:P:151:PRO:HD2	2.19	0.42
4:P:192:TRP:CE3	4:P:193:ALA:N	2.88	0.42
4:P:23:HIS:O	4:P:26:ILE:HB	2.20	0.42
4:P:50:HIS:HB3	4:P:54:VAL:HG21	2.01	0.42
6:R:22:ASN:O	6:R:23:ALA:C	2.57	0.42
11:W:24:TRP:O	11:W:25:GLY:C	2.59	0.42
1:A:146:ARG:HH21	1:A:308:GLN:HE22	1.62	0.41
1:A:46:ARG:NH2	1:A:316:ASP:OD1	2.52	0.41
2:B:51:ILE:CG2	2:B:199:PHE:HA	2.34	0.41
3:C:159:ASN:O	3:C:162:GLU:HB2	2.20	0.41
3:C:235:LEU:O	3:C:235:LEU:HD12	2.19	0.41
4:D:201:ARG:HD3	4:D:201:ARG:HH11	1.50	0.41
7:G:36:ASN:OD1	7:G:39:ARG:NE	2.52	0.41
7:G:3:GLN:OE1	7:G:3:GLN:HA	2.20	0.41
10:J:20:PHE:O	10:J:23:THR:HB	2.20	0.41
1:M:213:GLN:HB2	1:M:215:HIS:CD2	2.54	0.41
1:M:241:ILE:HG21	1:M:241:ILE:HD13	1.64	0.41
1:M:385:THR:HG22	1:M:386:TYR:CD1	2.55	0.41
2:N:33:LEU:HB2	2:N:204:MET:O	2.20	0.41
2:N:276:GLN:OE1	9:U:59:ALA:HB1	2.20	0.41
2:N:29:LEU:HG	2:N:33:LEU:CD2	2.50	0.41
2:N:362:ASN:O	2:N:363:LYS:C	2.57	0.41
2:N:435:PHE:N	2:N:438:GLU:HB2	2.35	0.41
4:P:165:TYR:CE2	4:P:168:VAL:HG22	2.55	0.41
6:R:87:LYS:HE2	6:R:89:TYR:HB3	2.01	0.41
7:S:33:GLY:O	7:S:37:VAL:HB	2.19	0.41
11:W:20:THR:HG23	11:W:24:TRP:HD1	1.85	0.41
1:A:252:HIS:O	1:A:424:GLY:HA2	2.20	0.41
1:A:5:ALA:O	1:A:6:GLN:O	2.38	0.41
2:B:312:PHE:N	2:B:323:GLY:O	2.47	0.41
3:C:300:ILE:HD11	3:C:362:ILE:CG2	2.50	0.41
3:C:36:LEU:HD22	3:C:235:LEU:HB2	2.02	0.41
4:D:214:LEU:O	4:D:218:LEU:HG	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:122:PHE:HD1	2:N:122:PHE:HA	1.74	0.41
3:O:244:LEU:HA	3:O:244:LEU:HD12	1.91	0.41
3:O:277:ALA:HB1	3:O:294:LEU:CD1	2.50	0.41
3:O:300:ILE:CD1	3:O:362:ILE:HG21	2.50	0.41
4:P:220:TYR:O	4:P:223:LYS:N	2.52	0.41
5:Q:109:GLU:OE2	5:Q:166:ASP:OD2	2.37	0.41
1:M:166:SER:HB2	5:Q:3:THR:HG22	2.02	0.41
5:Q:31:ALA:HB2	10:V:7:ALA:HB2	2.03	0.41
1:A:127:ILE:HA	1:A:127:ILE:HD13	1.88	0.41
1:A:184:GLU:O	1:A:185:TYR:C	2.59	0.41
1:A:64:PHE:HA	1:A:75:LEU:HD22	2.02	0.41
2:B:55:SER:OG	2:B:102:ARG:HA	2.20	0.41
2:B:270:ASN:O	2:B:271:ALA:C	2.59	0.41
4:D:137:PRO:HA	4:D:138:PRO:HD3	1.44	0.41
4:D:197:GLU:O	4:D:198:HIS:C	2.59	0.41
4:D:207:LYS:HB3	10:J:35:PHE:HE2	1.85	0.41
4:D:237:TYR:HE2	4:D:239:PRO:HG3	1.81	0.41
5:E:33:LYS:HA	7:G:21:PHE:HE2	1.82	0.41
6:F:75:LEU:HA	6:F:75:LEU:HD12	1.80	0.41
1:A:136:GLN:HE21	9:I:50:LEU:HG	1.84	0.41
1:M:369:LEU:HD21	1:M:378:ASP:OD2	2.20	0.41
3:O:207:ASN:CB	3:O:208:PRO:HD2	2.45	0.41
3:O:282:ARG:NH1	3:O:343:VAL:HG22	2.36	0.41
4:P:102:ARG:HG2	4:P:109:LEU:HB2	2.02	0.41
7:S:36:ASN:OD1	7:S:39:ARG:NE	2.53	0.41
4:P:139:THR:CG2	8:T:44:VAL:HB	2.50	0.41
1:A:260:PRO:HG3	1:A:414:TYR:CE1	2.55	0.41
2:B:250:ASP:OD1	2:B:251:SER:N	2.54	0.41
2:B:267:ALA:O	2:B:268:GLU:C	2.59	0.41
2:B:327:ILE:HG22	2:B:327:ILE:O	2.20	0.41
3:C:335:LEU:HA	3:C:335:LEU:HD23	1.70	0.41
9:I:62:ARG:HB3	9:I:63:PRO:CD	2.50	0.41
1:M:227:ALA:O	1:M:229:PRO:HD3	2.20	0.41
1:M:333:ASP:O	1:M:337:VAL:HG23	2.21	0.41
1:M:88:ALA:O	2:N:286:LYS:HD2	2.20	0.41
2:N:160:ILE:CD1	2:N:325:TYR:HE2	2.33	0.41
3:O:347:TYR:O	3:O:348:ILE:C	2.58	0.41
1:A:29:GLN:HG3	1:A:203:LEU:O	2.21	0.41
1:A:335:MET:O	1:A:335:MET:HE3	2.21	0.41
1:A:43:ALA:HB1	1:A:189:HIS:CB	2.51	0.41
2:B:72:ALA:HB2	2:B:140:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:ALA:O	2:B:272:PHE:C	2.58	0.41
2:B:312:PHE:HB3	2:B:323:GLY:O	2.20	0.41
1:A:34:THR:OG1	2:B:373:GLU:OE1	2.39	0.41
3:C:103:TYR:O	3:C:315:MET:HB3	2.20	0.41
3:C:163:TRP:CH2	5:Q:62:MET:HE1	2.56	0.41
3:C:219:PRO:HB2	3:C:222:PRO:HD2	2.03	0.41
4:D:146:GLY:O	4:D:148:TYR:HD1	2.04	0.41
3:C:317:PHE:CD1	6:F:26:PHE:HB3	2.55	0.41
8:H:50:THR:CG2	8:H:51:GLU:N	2.83	0.41
8:H:65:ARG:HG2	8:H:66:ASP:OD2	2.21	0.41
10:J:43:TYR:O	10:J:43:TYR:CG	2.73	0.41
1:M:257:VAL:O	1:M:320:LEU:HB2	2.20	0.41
1:M:329:MET:CA	1:M:329:MET:HE3	2.50	0.41
1:M:335:MET:HE1	1:M:338:LEU:HD23	2.02	0.41
2:N:201:SER:OG	2:N:226:ILE:N	2.51	0.41
2:N:223:PHE:O	2:N:224:LEU:HD23	2.21	0.41
2:N:255:ALA:HA	2:N:426:ALA:HA	2.02	0.41
2:N:264:ILE:HD12	2:N:315:SER:OG	2.20	0.41
2:N:333:ALA:O	2:N:337:ILE:HD12	2.20	0.41
3:C:198:LEU:HD22	3:O:11:MET:HG2	2.02	0.41
4:P:48:TYR:OH	4:P:68:VAL:HG21	2.21	0.41
5:Q:106:ILE:HG13	5:Q:106:ILE:H	1.78	0.41
5:Q:134:ILE:HG21	5:Q:134:ILE:HD13	1.76	0.41
1:A:48:GLU:HB2	1:A:53:ASN:HA	2.03	0.41
2:B:92:VAL:HG11	2:B:115:ASP:HB3	2.02	0.41
2:B:162:ASN:CB	2:B:244:ILE:HG21	2.50	0.41
2:B:282:GLY:HA2	2:B:283:PRO:HD2	1.77	0.41
3:C:101:GLY:HA2	3:C:106:SER:HB2	2.02	0.41
3:C:119:LEU:HD12	3:C:119:LEU:HA	1.85	0.41
3:C:145:VAL:HG12	3:C:145:VAL:O	2.20	0.41
4:D:146:GLY:O	4:D:148:TYR:CD1	2.73	0.41
4:D:165:TYR:CE1	4:D:168:VAL:HA	2.56	0.41
1:M:356:ARG:HG2	1:M:357:GLY:N	2.36	0.41
2:N:47:ILE:HB	2:N:109:VAL:HG12	2.02	0.41
3:O:242:LEU:HD12	3:O:242:LEU:HA	1.96	0.41
3:O:246:ALA:N	3:O:247:PRO:HD3	2.36	0.41
4:P:41:HIS:HD2	4:P:113:LEU:HD11	1.81	0.41
4:P:229:VAL:HG12	4:P:233:ARG:NE	2.32	0.41
5:Q:41:ALA:HA	10:V:24:ILE:HD11	2.03	0.41
1:A:136:GLN:NE2	9:I:50:LEU:HG	2.35	0.41
1:A:372:THR:O	1:A:373:THR:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ALA:HB3	1:A:421:ALA:HB3	2.02	0.41
2:B:163:LEU:HD21	2:B:258:VAL:HG21	2.03	0.41
3:C:11:MET:HG2	3:O:198:LEU:HD22	2.03	0.41
3:C:122:THR:HG21	3:C:189:ILE:HG12	2.03	0.41
3:C:257:THR:O	3:C:257:THR:OG1	2.38	0.41
3:C:263:ASN:OD1	3:C:264:THR:N	2.54	0.41
3:C:316:MET:HG2	3:C:317:PHE:CD1	2.54	0.41
4:D:43:MET:HA	4:D:112:ASP:OD1	2.20	0.41
4:D:211:MET:HA	4:D:211:MET:CE	2.49	0.41
4:D:44:ASP:OD1	4:D:93:LYS:HE3	2.20	0.41
1:M:262:TRP:CD2	1:M:385:THR:CG2	2.97	0.41
1:M:276:ILE:O	1:M:277:ILE:C	2.57	0.41
1:M:48:GLU:HB3	1:M:52:ASN:O	2.21	0.41
2:N:285:VAL:HG12	2:N:285:VAL:O	2.20	0.41
2:N:79:GLY:CA	2:N:125:ASN:ND2	2.83	0.41
3:O:10:LEU:HD12	3:O:13:ILE:CD1	2.50	0.41
3:O:149:LEU:O	3:O:291:VAL:HG21	2.21	0.41
3:O:125:ALA:HB3	3:O:185:LEU:HD21	2.03	0.41
3:O:337:TRP:NE1	3:O:341:GLN:OE1	2.54	0.41
5:Q:15:ARG:HH21	5:Q:32:ARG:HB2	1.85	0.41
5:Q:76:ILE:O	5:Q:77:LYS:CG	2.68	0.41
6:R:74:ILE:HG23	6:R:75:LEU:O	2.21	0.41
1:A:433:ASP:O	1:A:436:ARG:N	2.52	0.41
2:B:154:ASN:O	2:B:157:ALA:N	2.54	0.41
3:C:338:ILE:O	3:C:341:GLN:N	2.51	0.41
3:C:73:VAL:O	3:C:73:VAL:HG12	2.18	0.41
4:D:204:MET:O	4:D:207:LYS:N	2.53	0.41
4:D:57:THR:CG2	4:D:58:GLU:N	2.83	0.41
6:F:45:GLU:O	6:F:46:ALA:C	2.56	0.41
2:N:134:ARG:CG	2:N:135:TRP:N	2.81	0.41
2:N:38:LEU:O	2:N:40:ASN:N	2.54	0.41
3:O:133:LEU:HA	3:O:175:LEU:HD11	2.01	0.41
3:O:227:LYS:HG3	4:P:223:LYS:NZ	2.36	0.41
3:O:66:VAL:O	3:O:69:ILE:HB	2.21	0.41
4:P:28:ARG:HD2	4:P:28:ARG:HH11	1.75	0.41
5:Q:14:ARG:HB2	5:Q:15:ARG:H	1.70	0.41
5:Q:177:PRO:HB2	5:Q:178:LEU:HG	2.03	0.41
6:R:54:LEU:HA	6:R:54:LEU:HD12	1.95	0.41
4:P:139:THR:O	8:T:44:VAL:HG11	2.20	0.41
4:P:138:PRO:CG	8:T:55:THR:HA	2.50	0.41
7:S:71:ARG:NH2	8:T:60:ASP:OD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:95:LYS:HG3	9:U:70:LEU:HD13	2.02	0.41
3:C:341:GLN:OE1	3:C:347:TYR:CZ	2.74	0.41
3:C:1:MET:HG3	3:C:4:ILE:HB	2.03	0.41
3:C:227:LYS:HG3	4:D:223:LYS:HZ3	1.86	0.41
1:M:142:ASP:OD1	5:Q:2:HIS:ND1	2.45	0.41
1:M:156:THR:OG1	1:M:241:ILE:HB	2.21	0.41
1:M:37:VAL:CG1	1:M:199:ALA:HB2	2.51	0.41
1:M:271:GLN:O	1:M:272:VAL:C	2.59	0.41
2:N:200:THR:OG1	2:N:201:SER:N	2.53	0.41
2:N:22:GLN:HA	2:N:22:GLN:OE1	2.21	0.41
2:N:261:SER:HB3	2:N:321:LEU:C	2.42	0.41
3:O:156:ILE:HG13	3:O:157:GLY:N	2.29	0.41
3:O:160:LEU:CD1	3:O:164:ILE:HD11	2.51	0.41
4:P:14:HIS:HA	4:P:19:SER:CB	2.51	0.41
4:P:229:VAL:CG1	4:P:233:ARG:HE	2.32	0.41
6:R:35:ASP:OD2	6:R:61:ARG:HD2	2.20	0.41
1:M:241:ILE:HD11	7:S:16:TYR:CE2	2.55	0.41
6:R:74:ILE:H	7:S:39:ARG:NH2	2.19	0.41
9:U:70:LEU:HD11	9:U:72:VAL:H	1.85	0.41
10:V:55:ILE:HD13	10:V:55:ILE:HG21	1.90	0.41
1:A:241:ILE:O	1:A:241:ILE:CG2	2.69	0.41
1:A:358:LYS:HD2	1:A:402:VAL:HG12	2.03	0.41
1:A:75:LEU:O	1:A:79:VAL:CG2	2.63	0.41
1:A:86:LEU:CD1	1:A:99:ILE:HG12	2.44	0.41
2:B:55:SER:HG	2:B:102:ARG:HG2	1.85	0.41
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.44	0.41
2:B:216:LEU:O	2:B:217:LYS:C	2.58	0.41
1:A:366:VAL:HG11	2:B:44:ALA:HB2	2.01	0.41
3:C:109:PHE:HD2	3:C:203:THR:HG1	1.59	0.41
3:C:244:LEU:HD11	4:D:204:MET:HE3	2.03	0.41
3:C:48:GLY:HA3	12:C:380:HEM:C3C	2.56	0.41
3:C:97:HIS:HD2	12:C:381:HEM:C1C	2.39	0.41
1:A:244:ARG:NH1	7:G:10:VAL:HG21	2.35	0.41
4:D:139:THR:CB	8:H:44:VAL:HB	2.50	0.41
9:I:70:LEU:CG	9:I:72:VAL:H	2.34	0.41
4:D:27:ARG:NH1	10:J:58:LYS:CE	2.84	0.41
1:M:257:VAL:N	1:M:320:LEU:O	2.47	0.41
1:M:28:GLU:OE1	1:M:375:VAL:CG1	2.68	0.41
1:M:64:PHE:HE2	1:M:88:ALA:CB	2.34	0.41
5:Q:109:GLU:OE2	5:Q:166:ASP:HB2	2.21	0.41
5:Q:87:MET:O	5:Q:89:PHE:HD1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:62:ILE:O	6:R:66:LEU:HG	2.21	0.41
4:P:139:THR:CB	8:T:44:VAL:HB	2.49	0.41
8:T:58:LEU:HD11	8:T:62:LEU:HD12	2.03	0.41
1:A:266:ASP:OD1	1:A:266:ASP:N	2.54	0.41
1:A:277:ILE:HG12	1:A:277:ILE:H	1.53	0.41
2:B:211:VAL:HG11	2:B:216:LEU:HD13	2.02	0.41
2:B:262:ALA:HB3	2:B:269:ALA:HA	2.03	0.41
2:B:346:THR:HG23	2:B:351:ASN:HB3	2.03	0.41
2:B:57:TYR:HB3	2:B:198:HIS:CE1	2.55	0.41
3:C:152:ALA:HB2	3:C:287:LYS:NZ	2.36	0.41
1:M:158:PHE:HB2	1:M:164:ALA:HB2	2.02	0.41
1:M:53:ASN:CG	1:M:170:PRO:HD3	2.42	0.41
1:M:329:MET:HA	1:M:329:MET:CE	2.50	0.41
1:M:32:GLN:HG2	1:M:33:PRO:N	2.36	0.41
1:M:347:THR:HA	11:W:16:ASN:HD22	1.85	0.41
2:N:245:ARG:HH11	2:N:245:ARG:HD3	1.67	0.41
3:O:156:ILE:O	3:O:158:THR:N	2.54	0.41
3:O:276:PHE:CE2	3:O:297:SER:OG	2.74	0.41
3:O:75:TYR:CG	5:Q:57:GLN:HG2	2.56	0.41
4:P:120:ARG:HD2	13:P:242:HEC:CGA	2.50	0.41
4:P:138:PRO:CG	8:T:55:THR:OG1	2.61	0.41
9:U:62:ARG:HB3	9:U:63:PRO:CD	2.51	0.41
1:A:43:ALA:CB	1:A:189:HIS:CB	2.97	0.40
1:A:97:TYR:CD1	1:A:97:TYR:N	2.88	0.40
2:B:182:ARG:HD2	2:B:182:ARG:HH11	1.72	0.40
2:B:342:ASN:O	2:B:345:LYS:N	2.52	0.40
2:B:92:VAL:CG1	2:B:92:VAL:O	2.68	0.40
3:C:174:THR:HG23	3:C:178:PHE:CD1	2.52	0.40
8:H:62:LEU:HA	8:H:62:LEU:HD23	1.91	0.40
1:M:146:ARG:CZ	1:M:308:GLN:HE22	2.34	0.40
1:M:245:GLU:C	1:M:247:GLY:H	2.24	0.40
1:M:248:LEU:HA	1:M:249:PRO:HD3	1.78	0.40
2:N:97:SER:HB2	2:N:108:THR:CG2	2.52	0.40
2:N:309:VAL:CG2	2:N:326:THR:HG22	2.50	0.40
2:N:309:VAL:HG22	2:N:326:THR:HG22	2.03	0.40
2:N:70:ARG:HD2	9:U:69:SER:HB3	2.01	0.40
3:O:15:ASN:ND2	3:O:18:PHE:CD2	2.88	0.40
3:O:135:TRP:HH2	3:O:170:VAL:O	2.04	0.40
3:O:316:MET:CE	3:O:317:PHE:CE1	3.04	0.40
4:P:153:PHE:HA	4:P:154:PRO:HD2	1.87	0.40
4:P:21:LEU:CD1	4:P:192:TRP:HB2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:78:LEU:CD2	5:Q:132:TRP:CZ2	3.05	0.40
5:Q:7:VAL:HA	5:Q:8:PRO:HD2	1.77	0.40
6:R:10:SER:HA	6:R:13:LEU:HG	2.03	0.40
8:T:37:LEU:HD21	8:T:58:LEU:CA	2.49	0.40
10:V:42:ILE:O	10:V:46:ILE:HG12	2.22	0.40
1:A:270:LEU:O	1:A:273:ALA:HB3	2.21	0.40
2:B:53:ALA:HB2	2:B:198:HIS:HB3	2.03	0.40
2:B:264:ILE:HA	2:B:315:SER:OG	2.22	0.40
2:B:395:PRO:O	2:B:396:SER:C	2.59	0.40
3:C:264:THR:HG21	5:Q:144:CYS:SG	2.60	0.40
3:C:347:TYR:O	3:C:348:ILE:C	2.59	0.40
3:C:8:HIS:CB	3:C:9:PRO:HD2	2.51	0.40
4:D:143:LEU:HD11	4:D:149:PHE:HB2	2.03	0.40
4:D:150:ASN:OD1	4:D:150:ASN:C	2.59	0.40
4:D:187:CYS:O	4:D:190:LEU:N	2.55	0.40
3:C:317:PHE:O	6:F:24:ALA:CB	2.69	0.40
7:G:31:SER:O	7:G:35:PRO:CD	2.62	0.40
7:G:60:THR:O	7:G:61:TRP:C	2.59	0.40
4:D:149:PHE:CZ	8:H:55:THR:HG23	2.54	0.40
10:J:29:LEU:HD12	10:J:32:GLU:OE2	2.21	0.40
2:N:160:ILE:HG21	9:U:65:VAL:CG2	2.52	0.40
2:N:168:TYR:CZ	2:N:172:LEU:HD12	2.56	0.40
3:O:184:ILE:HG12	3:O:184:ILE:O	2.20	0.40
4:P:206:LEU:HG	4:P:210:LEU:CD1	2.52	0.40
4:P:206:LEU:O	4:P:210:LEU:HD12	2.22	0.40
4:P:57:THR:HB	4:P:60:GLU:H	1.86	0.40
6:R:91:GLU:O	6:R:95:LYS:HG3	2.21	0.40
1:M:130:GLU:OE2	9:U:52:ARG:NH2	2.54	0.40
10:V:2:ALA:HB1	10:V:3:PRO:HD2	2.03	0.40
1:A:257:VAL:N	1:A:320:LEU:O	2.48	0.40
2:B:213:HIS:CD2	2:B:213:HIS:O	2.74	0.40
2:B:304:HIS:CD2	2:B:305:GLN:H	2.40	0.40
2:B:360:ALA:O	2:B:361:LYS:C	2.60	0.40
3:C:168:PHE:CE2	5:Q:72:SER:HB2	2.56	0.40
3:C:226:ILE:HD13	3:C:226:ILE:N	2.35	0.40
12:C:380:HEM:CMB	12:C:380:HEM:CBB	2.99	0.40
3:C:200:LEU:CD1	12:C:381:HEM:HAD2	2.51	0.40
3:C:40:CYS:CB	3:C:90:PHE:HD2	2.34	0.40
5:E:5:ILE:HG13	5:E:5:ILE:H	1.71	0.40
11:K:24:TRP:CE3	11:K:24:TRP:HA	2.56	0.40
1:M:134:ILE:HG21	1:M:174:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:24:ARG:HH11	1:M:24:ARG:HD2	1.75	0.40
1:M:426:GLY:H	1:M:428:ILE:CG1	2.31	0.40
1:M:97:TYR:CD1	1:M:97:TYR:N	2.88	0.40
2:N:102:ARG:NH1	2:N:174:ASN:O	2.53	0.40
2:N:178:CYS:HA	2:N:179:PRO:HD3	1.63	0.40
2:N:54:GLY:HA3	2:N:102:ARG:O	2.20	0.40
3:O:211:ILE:CG2	3:O:212:SER:N	2.83	0.40
3:O:345:HIS:CB	3:O:346:PRO:CD	2.88	0.40
4:P:10:TYR:CE1	4:P:128:PHE:HE2	2.37	0.40
4:P:220:TYR:HD2	7:S:26:PHE:CZ	2.39	0.40
5:Q:181:GLU:HG2	5:Q:182:VAL:N	2.36	0.40
5:Q:62:MET:HE2	5:Q:62:MET:HB2	1.94	0.40
6:R:29:LEU:HD22	6:R:68:LEU:HB2	2.03	0.40
1:M:244:ARG:NH1	7:S:10:VAL:HB	2.36	0.40
7:S:44:CYS:O	7:S:45:ILE:C	2.59	0.40
1:A:39:VAL:HG13	1:A:195:MET:CE	2.51	0.40
2:B:154:ASN:O	2:B:155:PRO:C	2.60	0.40
2:B:68:LEU:O	2:B:68:LEU:HD12	2.21	0.40
3:C:149:LEU:HD21	3:C:281:LEU:HD22	2.04	0.40
4:D:165:TYR:HD1	4:D:166:ASN:O	2.04	0.40
4:D:200:HIS:O	4:D:203:ARG:HB3	2.20	0.40
4:D:237:TYR:HD1	7:G:13:VAL:HG22	1.85	0.40
5:E:34:GLY:CA	10:J:10:TYR:HD2	2.33	0.40
1:M:17:SER:HB2	1:M:25:VAL:HB	2.03	0.40
1:M:391:PRO:HB2	1:M:395:TRP:CE2	2.57	0.40
1:M:4:TYR:HE2	1:M:396:GLU:HG3	1.85	0.40
1:M:418:GLN:O	1:M:420:PRO:HD3	2.21	0.40
2:N:160:ILE:HD12	2:N:160:ILE:HA	1.93	0.40
2:N:180:ASP:HA	2:N:183:ILE:HD12	2.02	0.40
2:N:239:TYR:OH	2:N:421:ARG:O	2.29	0.40
2:N:42:ALA:HA	2:N:43:PRO:HD3	1.80	0.40
3:O:11:MET:O	3:O:14:VAL:HB	2.21	0.40
4:P:69:GLU:O	4:P:73:GLY:CA	2.70	0.40
5:Q:119:ASP:HA	5:Q:120:PRO:HD3	1.91	0.40
9:U:60:ALA:HB3	9:U:63:PRO:O	2.21	0.40
1:A:297:ILE:HG22	1:A:303:LEU:CD1	2.49	0.40
2:B:112:LEU:HD22	2:B:112:LEU:HA	1.79	0.40
2:B:168:TYR:HD2	2:B:238:LYS:O	2.04	0.40
2:B:56:ARG:HH21	2:B:103:GLU:CD	2.25	0.40
3:C:276:PHE:HE2	3:C:297:SER:HG	1.63	0.40
3:C:68:HIS:NE2	5:E:67:ASP:CB	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:50:HIS:HB3	4:D:54:VAL:HG21	2.01	0.40
4:D:5:LEU:HG	4:D:152:TYR:HE1	1.86	0.40
10:J:27:GLY:O	10:J:28:ALA:C	2.59	0.40
1:M:289:HIS:O	2:N:87:ARG:NE	2.54	0.40
1:M:343:MET:CE	1:M:416:TYR:CD2	3.03	0.40
2:N:92:VAL:HG11	2:N:115:ASP:CB	2.51	0.40
2:N:275:LEU:O	2:N:276:GLN:C	2.60	0.40
2:N:275:LEU:HD11	2:N:279:LEU:HD11	2.03	0.40
3:O:170:VAL:CG1	3:O:170:VAL:O	2.68	0.40
3:O:272:TRP:CE2	3:O:273:TYR:HD1	2.39	0.40
3:O:51:LEU:HD12	12:O:380:HEM:O1D	2.21	0.40
5:Q:138:VAL:O	5:Q:139:CYS:C	2.59	0.40
5:Q:29:SER:O	5:Q:33:LYS:HG3	2.22	0.40
5:Q:87:MET:O	5:Q:98:VAL:HG22	2.21	0.40
7:S:50:PRO:O	7:S:53:VAL:HB	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:412:ASN:ND2	5:Q:122:HIS:NE2[6_554]	2.01	0.19
8:H:41:ASP:OD1	6:R:77:LYS:NZ[5_565]	2.19	0.01

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	A	444/446 (100%)	355 (80%)	66 (15%)	23 (5%)	2	12
1	M	444/446 (100%)	370 (83%)	54 (12%)	20 (4%)	2	14
2	B	417/439 (95%)	341 (82%)	67 (16%)	9 (2%)	6	31
2	N	417/439 (95%)	344 (82%)	62 (15%)	11 (3%)	5	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	377/379 (100%)	303 (80%)	60 (16%)	14 (4%)	3	19
3	O	377/379 (100%)	317 (84%)	49 (13%)	11 (3%)	4	24
4	D	239/241 (99%)	188 (79%)	36 (15%)	15 (6%)	1	7
4	P	239/241 (99%)	195 (82%)	32 (13%)	12 (5%)	2	12
5	E	73/196 (37%)	57 (78%)	14 (19%)	2 (3%)	5	26
5	Q	194/196 (99%)	148 (76%)	35 (18%)	11 (6%)	1	10
6	F	104/110 (94%)	89 (86%)	12 (12%)	3 (3%)	4	24
6	R	104/110 (94%)	86 (83%)	16 (15%)	2 (2%)	8	36
7	G	79/81 (98%)	63 (80%)	13 (16%)	3 (4%)	3	18
7	S	79/81 (98%)	60 (76%)	16 (20%)	3 (4%)	3	18
8	H	62/78 (80%)	52 (84%)	10 (16%)	0	100	100
8	T	62/78 (80%)	51 (82%)	10 (16%)	1 (2%)	9	40
9	I	31/78 (40%)	19 (61%)	10 (32%)	2 (6%)	1	7
9	U	31/78 (40%)	17 (55%)	11 (36%)	3 (10%)	0	2
10	J	60/62 (97%)	41 (68%)	13 (22%)	6 (10%)	0	2
10	V	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	6
11	K	20/56 (36%)	17 (85%)	2 (10%)	1 (5%)	2	12
11	W	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	0	2
All	All	3933/4332 (91%)	3172 (81%)	603 (15%)	158 (4%)	3	17

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASP
1	A	426	GLY
1	A	427	PRO
2	B	141	GLN
2	B	183	ILE
2	B	305	GLN
3	C	8	HIS
3	C	27	ILE
3	C	109	PHE
4	D	51	LEU
4	D	73	GLY
4	D	98	PRO
9	I	72	VAL

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Mol	Chain	Res	Type
1	M	55	ALA
1	M	427	PRO
2	N	141	GLN
2	N	183	ILE
2	N	351	ASN
3	O	8	HIS
3	O	27	ILE
3	O	157	GLY
4	P	51	LEU
4	P	73	GLY
5	Q	114	VAL
5	Q	141	HIS
9	U	72	VAL
10	V	58	LYS
1	A	55	ALA
1	A	56	GLY
1	A	72	GLY
1	A	80	GLU
1	A	81	SER
1	A	227	ALA
1	A	287	GLY
1	A	288	ALA
1	A	342	TRP
2	B	236	LYS
2	B	351	ASN
3	C	28	SER
3	C	137	GLN
3	C	157	GLY
3	C	313	ARG
4	D	119	ALA
4	D	154	PRO
7	G	68	LYS
10	J	58	LYS
1	M	52	ASN
1	M	72	GLY
1	M	227	ALA
1	M	246	ASP
1	M	282	CYS
1	M	385	THR
2	N	236	LYS
5	Q	137	GLY
9	U	59	ALA

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Mol	Chain	Res	Type
10	V	23	THR
10	V	24	ILE
1	A	52	ASN
1	A	352	SER
1	A	385	THR
1	A	395	TRP
2	B	91	ALA
3	C	283	SER
3	C	319	PRO
4	D	27	ARG
4	D	162	PRO
4	D	218	LEU
5	E	16	PRO
5	E	72	SER
9	I	59	ALA
10	J	23	THR
10	J	35	PHE
1	M	81	SER
1	M	107	PRO
1	M	426	GLY
2	N	24	LEU
2	N	305	GLN
3	O	28	SER
3	O	62	ALA
3	O	316	MET
3	O	319	PRO
4	P	80	MET
4	P	162	PRO
5	Q	64	ALA
5	Q	177	PRO
7	S	68	LYS
10	V	57	HIS
11	W	33	VAL
1	A	107	PRO
1	A	246	ASP
1	A	391	PRO
3	C	236	ILE
3	C	365	LEU
4	D	80	MET
4	D	147	LEU
6	F	95	LYS
10	J	4	THR

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Mol	Chain	Res	Type
10	J	57	HIS
1	M	6	GLN
1	M	109	ALA
2	N	269	ALA
2	N	409	ASP
3	O	24	PRO
3	O	109	PHE
4	P	147	LEU
5	Q	130	PRO
6	R	95	LYS
1	A	6	GLN
1	A	152	TYR
2	B	39	GLU
3	C	316	MET
7	G	72	LYS
1	M	338	LEU
1	M	391	PRO
3	O	247	PRO
3	O	255	ASN
4	P	83	ARG
4	P	98	PRO
4	P	110	PRO
4	P	154	PRO
5	Q	16	PRO
5	Q	69	LEU
5	Q	188	THR
7	S	50	PRO
11	W	34	SER
1	A	33	PRO
2	B	52	LYS
4	D	110	PRO
4	D	163	PRO
4	D	176	PRO
7	G	45	ILE
1	M	185	TYR
2	N	52	LYS
4	P	176	PRO
5	Q	43	THR
2	B	129	ALA
6	F	51	PRO
1	M	56	GLY
1	M	293	PRO

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Mol	Chain	Res	Type
3	C	339	GLY
4	D	83	ARG
2	N	85	ILE
2	N	109	VAL
4	P	123	GLY
8	T	69	VAL
10	J	24	ILE
5	Q	84	GLY
6	R	51	PRO
7	S	45	ILE
1	A	260	PRO
4	D	26	ILE
11	K	33	VAL
4	P	163	PRO
9	U	65	VAL
3	C	372	ILE
6	F	47	ILE
1	M	71	PRO
1	M	193	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	A	370/370 (100%)	289 (78%)	81 (22%)	1	5
1	M	370/370 (100%)	286 (77%)	84 (23%)	1	4
2	B	328/343 (96%)	259 (79%)	69 (21%)	1	5
2	N	328/343 (96%)	262 (80%)	66 (20%)	1	6
3	C	327/327 (100%)	269 (82%)	58 (18%)	2	9
3	O	327/327 (100%)	276 (84%)	51 (16%)	2	13
4	D	206/206 (100%)	179 (87%)	27 (13%)	4	18
4	P	206/206 (100%)	179 (87%)	27 (13%)	4	18
5	E	65/168 (39%)	51 (78%)	14 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Q	167/168 (99%)	123 (74%)	44 (26%)	0	2
6	F	96/98 (98%)	74 (77%)	22 (23%)	1	4
6	R	96/98 (98%)	78 (81%)	18 (19%)	1	8
7	G	71/71 (100%)	58 (82%)	13 (18%)	1	9
7	S	71/71 (100%)	57 (80%)	14 (20%)	1	7
8	H	61/74 (82%)	51 (84%)	10 (16%)	2	11
8	T	61/74 (82%)	51 (84%)	10 (16%)	2	11
9	I	27/60 (45%)	19 (70%)	8 (30%)	0	1
9	U	27/60 (45%)	20 (74%)	7 (26%)	0	2
10	J	52/52 (100%)	46 (88%)	6 (12%)	5	24
10	V	52/52 (100%)	43 (83%)	9 (17%)	2	10
11	K	15/46 (33%)	12 (80%)	3 (20%)	1	7
11	W	15/46 (33%)	11 (73%)	4 (27%)	0	2
All	All	3338/3630 (92%)	2693 (81%)	645 (19%)	1	8

All (645) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	24	ARG
1	A	31	SER
1	A	35	CYS
1	A	37	VAL
1	A	42	ASP
1	A	46	ARG
1	A	48	GLU
1	A	49	SER
1	A	53	ASN
1	A	58	PHE
1	A	68	LYS
1	A	70	ARG
1	A	79	VAL
1	A	89	TYR
1	A	90	SER
1	A	97	TYR
1	A	99	ILE
1	A	102	LEU

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Mol	Chain	Res	Type
1	A	108	LYS
1	A	112	LEU
1	A	120	CYS
1	A	125	SER
1	A	127	ILE
1	A	130	GLU
1	A	131	ARG
1	A	133	VAL
1	A	143	THR
1	A	149	VAL
1	A	163	LEU
1	A	174	VAL
1	A	175	ARG
1	A	177	LEU
1	A	178	SER
1	A	179	ARG
1	A	183	THR
1	A	187	SER
1	A	191	LYS
1	A	195	MET
1	A	197	LEU
1	A	208	LEU
1	A	211	LEU
1	A	213	GLN
1	A	216	PHE
1	A	222	THR
1	A	225	GLU
1	A	231	LEU
1	A	239	SER
1	A	241	ILE
1	A	243	HIS
1	A	245	GLU
1	A	246	ASP
1	A	255	ILE
1	A	266	ASP
1	A	272	VAL
1	A	277	ILE
1	A	296	SER
1	A	302	LYS
1	A	307	PHE
1	A	316	ASP
1	A	330	SER

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Mol	Chain	Res	Type
1	A	334	MET
1	A	337	VAL
1	A	341	GLN
1	A	344	ARG
1	A	346	CYS
1	A	351	GLU
1	A	352	SER
1	A	353	GLU
1	A	356	ARG
1	A	358	LYS
1	A	360	LEU
1	A	367	SER
1	A	370	ASP
1	A	379	ILE
1	A	384	LEU
1	A	386	TYR
1	A	398	ARG
1	A	413	LYS
1	A	428	ILE
1	A	441	MET
2	B	23	ASP
2	B	24	LEU
2	B	35	ILE
2	B	37	SER
2	B	38	LEU
2	B	45	SER
2	B	46	ARG
2	B	51	ILE
2	B	52	LYS
2	B	56	ARG
2	B	60	SER
2	B	62	ASN
2	B	74	SER
2	B	77	THR
2	B	81	SER
2	B	85	ILE
2	B	86	THR
2	B	95	LYS
2	B	96	LEU
2	B	101	THR
2	B	102	ARG
2	B	111	CYS

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Mol	Chain	Res	Type
2	B	112	LEU
2	B	113	ARG
2	B	117	ASP
2	B	119	LEU
2	B	131	GLU
2	B	134	ARG
2	B	140	LEU
2	B	145	ARG
2	B	159	VAL
2	B	160	ILE
2	B	175	SER
2	B	182	ARG
2	B	187	THR
2	B	190	GLU
2	B	196	GLN
2	B	203	ARG
2	B	215	VAL
2	B	219	VAL
2	B	238	LYS
2	B	240	HIS
2	B	245	ARG
2	B	253	VAL
2	B	283	PRO
2	B	292	THR
2	B	294	SER
2	B	297	GLN
2	B	310	SER
2	B	318	ASP
2	B	319	SER
2	B	328	SER
2	B	353	SER
2	B	354	ASN
2	B	374	SER
2	B	391	SER
2	B	396	SER
2	B	402	ILE
2	B	403	ASP
2	B	409	ASP
2	B	416	LYS
2	B	418	VAL
2	B	421	ARG
2	B	422	LYS

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Mol	Chain	Res	Type
2	B	423	SER
2	B	429	ASN
2	B	436	ILE
2	B	437	ASP
2	B	438	GLU
3	C	1	MET
3	C	5	ARG
3	C	6	LYS
3	C	7	SER
3	C	11	MET
3	C	25	SER
3	C	26	ASN
3	C	27	ILE
3	C	29	SER
3	C	32	ASN
3	C	43	LEU
3	C	60	THR
3	C	61	THR
3	C	65	SER
3	C	67	THR
3	C	80	ARG
3	C	94	LEU
3	C	119	LEU
3	C	138	MET
3	C	139	SER
3	C	144	THR
3	C	156	ILE
3	C	158	THR
3	C	169	SER
3	C	174	THR
3	C	176	THR
3	C	177	ARG
3	C	183	PHE
3	C	192	ILE
3	C	198	LEU
3	C	205	SER
3	C	212	SER
3	C	217	LYS
3	C	226	ILE
3	C	229	ILE
3	C	233	LEU
3	C	240	MET

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Mol	Chain	Res	Type
3	C	241	LEU
3	C	244	LEU
3	C	247	PRO
3	C	262	LEU
3	C	271	GLU
3	C	273	TYR
3	C	280	ILE
3	C	282	ARG
3	C	291	VAL
3	C	299	LEU
3	C	310	SER
3	C	311	LYS
3	C	312	GLN
3	C	313	ARG
3	C	314	SER
3	C	318	ARG
3	C	321	SER
3	C	324	LEU
3	C	353	LEU
3	C	363	LEU
3	C	377	LEU
4	D	3	LEU
4	D	9	SER
4	D	10	TYR
4	D	20	SER
4	D	21	LEU
4	D	27	ARG
4	D	32	VAL
4	D	40	CYS
4	D	42	SER
4	D	43	MET
4	D	52	VAL
4	D	55	CYS
4	D	80	MET
4	D	82	MET
4	D	83	ARG
4	D	87	LEU
4	D	95	TYR
4	D	106	ASN
4	D	120	ARG
4	D	124	GLU
4	D	179	MET

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Mol	Chain	Res	Type
4	D	201	ARG
4	D	208	MET
4	D	223	LYS
4	D	224	ARG
4	D	228	SER
4	D	231	LYS
5	E	1	SER
5	E	5	ILE
5	E	6	LYS
5	E	14	ARG
5	E	15	ARG
5	E	17	GLU
5	E	19	LEU
5	E	28	SER
5	E	32	ARG
5	E	33	LYS
5	E	52	LYS
5	E	58	PHE
5	E	63	SER
5	E	67	ASP
6	F	7	SER
6	F	9	SER
6	F	10	SER
6	F	11	ARG
6	F	13	LEU
6	F	16	ILE
6	F	18	LYS
6	F	44	LYS
6	F	48	ARG
6	F	54	LEU
6	F	58	ARG
6	F	68	LEU
6	F	69	SER
6	F	70	MET
6	F	77	LYS
6	F	82	LYS
6	F	88	SER
6	F	90	LEU
6	F	94	LEU
6	F	100	GLU
6	F	106	GLU
6	F	110	LYS

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Mol	Chain	Res	Type
7	G	4	PHE
7	G	8	THR
7	G	9	ARG
7	G	19	SER
7	G	23	GLN
7	G	24	ARG
7	G	39	ARG
7	G	40	ARG
7	G	42	ARG
7	G	45	ILE
7	G	46	LEU
7	G	58	VAL
7	G	69	SER
8	H	20	VAL
8	H	29	LYS
8	H	30	CYS
8	H	31	VAL
8	H	45	SER
8	H	54	CYS
8	H	58	LEU
8	H	59	LEU
8	H	73	LEU
8	H	74	PHE
9	I	46	LYS
9	I	49	VAL
9	I	51	CYS
9	I	54	SER
9	I	69	SER
9	I	70	LEU
9	I	77	ARG
9	I	78	TYR
10	J	11	SER
10	J	13	LEU
10	J	17	THR
10	J	18	SER
10	J	46	ILE
10	J	58	LYS
11	K	20	THR
11	K	23	LEU
11	K	36	THR
1	M	13	GLU
1	M	24	ARG

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Mol	Chain	Res	Type
1	M	31	SER
1	M	37	VAL
1	M	42	ASP
1	M	45	SER
1	M	46	ARG
1	M	48	GLU
1	M	51	LYS
1	M	53	ASN
1	M	58	PHE
1	M	70	ARG
1	M	82	MET
1	M	86	LEU
1	M	89	TYR
1	M	91	THR
1	M	92	ARG
1	M	97	TYR
1	M	99	ILE
1	M	100	LYS
1	M	108	LYS
1	M	112	LEU
1	M	125	SER
1	M	127	ILE
1	M	130	GLU
1	M	131	ARG
1	M	137	GLU
1	M	138	LEU
1	M	143	THR
1	M	149	VAL
1	M	156	THR
1	M	159	GLN
1	M	163	LEU
1	M	175	ARG
1	M	176	LYS
1	M	177	LEU
1	M	179	ARG
1	M	186	LEU
1	M	187	SER
1	M	191	LYS
1	M	195	MET
1	M	197	LEU
1	M	208	LEU
1	M	211	LEU

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Mol	Chain	Res	Type
1	M	213	GLN
1	M	216	PHE
1	M	222	THR
1	M	225	GLU
1	M	231	LEU
1	M	232	SER
1	M	243	HIS
1	M	245	GLU
1	M	246	ASP
1	M	248	LEU
1	M	257	VAL
1	M	266	ASP
1	M	277	ILE
1	M	302	LYS
1	M	307	PHE
1	M	309	THR
1	M	316	ASP
1	M	319	LEU
1	M	329	MET
1	M	330	SER
1	M	334	MET
1	M	341	GLN
1	M	344	ARG
1	M	346	CYS
1	M	347	THR
1	M	351	GLU
1	M	353	GLU
1	M	356	ARG
1	M	358	LYS
1	M	360	LEU
1	M	370	ASP
1	M	379	ILE
1	M	382	SER
1	M	384	LEU
1	M	386	TYR
1	M	412	SER
1	M	413	LYS
1	M	419	CYS
1	M	428	ILE
1	M	441	MET
2	N	23	ASP
2	N	24	LEU

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Mol	Chain	Res	Type
2	N	33	LEU
2	N	35	ILE
2	N	37	SER
2	N	38	LEU
2	N	45	SER
2	N	46	ARG
2	N	56	ARG
2	N	58	GLU
2	N	60	SER
2	N	62	ASN
2	N	73	SER
2	N	78	LYS
2	N	81	SER
2	N	84	LYS
2	N	85	ILE
2	N	86	THR
2	N	96	LEU
2	N	99	THR
2	N	100	SER
2	N	101	THR
2	N	102	ARG
2	N	108	THR
2	N	111	CYS
2	N	112	LEU
2	N	113	ARG
2	N	117	ASP
2	N	134	ARG
2	N	145	ARG
2	N	148	LYS
2	N	159	VAL
2	N	160	ILE
2	N	175	SER
2	N	182	ARG
2	N	190	GLU
2	N	196	GLN
2	N	201	SER
2	N	215	VAL
2	N	219	VAL
2	N	238	LYS
2	N	240	HIS
2	N	253	VAL
2	N	261	SER

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Mol	Chain	Res	Type
2	N	264	ILE
2	N	266	SER
2	N	292	THR
2	N	295	LEU
2	N	297	GLN
2	N	315	SER
2	N	317	SER
2	N	318	ASP
2	N	328	SER
2	N	329	GLN
2	N	346	THR
2	N	384	SER
2	N	402	ILE
2	N	403	ASP
2	N	416	LYS
2	N	418	VAL
2	N	421	ARG
2	N	424	MET
2	N	429	ASN
2	N	436	ILE
2	N	437	ASP
2	N	438	GLU
3	O	1	MET
3	O	5	ARG
3	O	6	LYS
3	O	7	SER
3	O	11	MET
3	O	27	ILE
3	O	32	ASN
3	O	35	SER
3	O	39	ILE
3	O	44	GLN
3	O	60	THR
3	O	67	THR
3	O	80	ARG
3	O	94	LEU
3	O	100	ARG
3	O	115	ILE
3	O	118	ILE
3	O	119	LEU
3	O	138	MET
3	O	139	SER

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Mol	Chain	Res	Type
3	O	144	THR
3	O	158	THR
3	O	169	SER
3	O	174	THR
3	O	189	ILE
3	O	192	ILE
3	O	197	LEU
3	O	212	SER
3	O	226	ILE
3	O	233	LEU
3	O	241	LEU
3	O	243	VAL
3	O	244	LEU
3	O	257	THR
3	O	262	LEU
3	O	271	GLU
3	O	282	ARG
3	O	287	LYS
3	O	297	SER
3	O	299	LEU
3	O	313	ARG
3	O	318	ARG
3	O	324	LEU
3	O	338	ILE
3	O	356	VAL
3	O	362	ILE
3	O	363	LEU
3	O	367	PRO
3	O	375	LYS
3	O	377	LEU
3	O	378	LYS
4	P	3	LEU
4	P	10	TYR
4	P	13	SER
4	P	17	LEU
4	P	20	SER
4	P	21	LEU
4	P	38	SER
4	P	39	SER
4	P	40	CYS
4	P	55	CYS
4	P	80	MET

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Mol	Chain	Res	Type
4	P	82	MET
4	P	83	ARG
4	P	88	SER
4	P	106	ASN
4	P	120	ARG
4	P	124	GLU
4	P	127	VAL
4	P	139	THR
4	P	141	VAL
4	P	158	ILE
4	P	179	MET
4	P	180	SER
4	P	186	VAL
4	P	201	ARG
4	P	223	LYS
4	P	226	LYS
5	Q	5	ILE
5	Q	6	LYS
5	Q	11	SER
5	Q	14	ARG
5	Q	17	GLU
5	Q	19	LEU
5	Q	22	THR
5	Q	23	LYS
5	Q	28	SER
5	Q	32	ARG
5	Q	36	SER
5	Q	42	THR
5	Q	43	THR
5	Q	44	THR
5	Q	58	PHE
5	Q	60	SER
5	Q	61	SER
5	Q	63	SER
5	Q	65	SER
5	Q	73	LYS
5	Q	74	ILE
5	Q	78	LEU
5	Q	81	ILE
5	Q	87	MET
5	Q	98	VAL
5	Q	102	THR

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Mol	Chain	Res	Type
5	Q	103	LYS
5	Q	106	ILE
5	Q	109	GLU
5	Q	113	GLU
5	Q	120	PRO
5	Q	125	GLU
5	Q	136	ILE
5	Q	139	CYS
5	Q	140	THR
5	Q	144	CYS
5	Q	152	ASP
5	Q	158	CYS
5	Q	168	SER
5	Q	171	ILE
5	Q	172	ARG
5	Q	173	LYS
5	Q	178	LEU
5	Q	195	VAL
6	R	7	SER
6	R	11	ARG
6	R	16	ILE
6	R	48	ARG
6	R	54	LEU
6	R	64	ARG
6	R	68	LEU
6	R	75	LEU
6	R	77	LYS
6	R	88	SER
6	R	90	LEU
6	R	94	LEU
6	R	98	ILE
6	R	100	GLU
6	R	103	GLU
6	R	106	GLU
6	R	107	TRP
6	R	110	LYS
7	S	4	PHE
7	S	8	THR
7	S	9	ARG
7	S	18	LEU
7	S	19	SER
7	S	23	GLN

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Mol	Chain	Res	Type
7	S	24	ARG
7	S	31	SER
7	S	39	ARG
7	S	40	ARG
7	S	41	THR
7	S	42	ARG
7	S	46	LEU
7	S	69	SER
8	T	20	VAL
8	T	29	LYS
8	T	30	CYS
8	T	31	VAL
8	T	46	SER
8	T	48	SER
8	T	54	CYS
8	T	58	LEU
8	T	73	LEU
8	T	74	PHE
9	U	46	LYS
9	U	49	VAL
9	U	67	SER
9	U	70	LEU
9	U	72	VAL
9	U	77	ARG
9	U	78	TYR
10	V	9	LEU
10	V	12	LEU
10	V	13	LEU
10	V	15	ARG
10	V	16	ARG
10	V	18	SER
10	V	46	ILE
10	V	53	LYS
10	V	58	LYS
11	W	20	THR
11	W	23	LEU
11	W	34	SER
11	W	36	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	32	GLN
1	A	73	ASN
1	A	85	HIS
1	A	136	GLN
1	A	151	ASN
1	A	154	HIS
1	A	189	HIS
1	A	240	GLN
1	A	243	HIS
1	A	252	HIS
1	A	308	GLN
1	A	323	HIS
1	A	435	ASN
2	B	62	ASN
2	B	67	HIS
2	B	125	ASN
2	B	162	ASN
2	B	164	HIS
2	B	198	HIS
2	B	247	GLN
2	B	304	HIS
2	B	429	ASN
3	C	15	ASN
3	C	26	ASN
3	C	32	ASN
3	C	114	ASN
3	C	201	HIS
3	C	206	ASN
3	C	312	GLN
3	C	374	ASN
4	D	6	HIS
4	D	50	HIS
4	D	106	ASN
4	D	181	GLN
4	D	200	HIS
4	D	225	HIS
6	F	22	ASN
6	F	27	ASN
6	F	38	HIS
7	G	6	HIS
7	G	73	ASN
9	I	71	ASN

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Mol	Chain	Res	Type
10	J	54	HIS
1	M	18	GLN
1	M	32	GLN
1	M	85	HIS
1	M	136	GLN
1	M	151	ASN
1	M	154	HIS
1	M	159	GLN
1	M	173	ASN
1	M	189	HIS
1	M	213	GLN
1	M	240	GLN
1	M	243	HIS
1	M	308	GLN
1	M	323	HIS
1	M	435	ASN
2	N	62	ASN
2	N	67	HIS
2	N	125	ASN
2	N	141	GLN
2	N	164	HIS
2	N	198	HIS
2	N	247	GLN
2	N	304	HIS
2	N	429	ASN
3	O	15	ASN
3	O	26	ASN
3	O	32	ASN
3	O	114	ASN
3	O	206	ASN
3	O	374	ASN
4	P	6	HIS
4	P	50	HIS
4	P	75	ASN
4	P	106	ASN
4	P	181	GLN
4	P	225	HIS
5	Q	121	GLN
6	R	38	HIS
6	R	73	GLN
7	S	6	HIS
10	V	54	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 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$
12	HEM	O	380	3	27,50,50	2.09	6 (22%)	17,82,82	3.26	9 (52%)
13	HEC	D	242	4	26,50,50	2.40	4 (15%)	18,82,82	2.19	9 (50%)
14	FES	Q	197	5	0,4,4	0.00	-	-		
12	HEM	O	381	3	27,50,50	2.01	5 (18%)	17,82,82	2.46	9 (52%)
12	HEM	C	381	3	27,50,50	1.74	6 (22%)	17,82,82	3.07	6 (35%)
13	HEC	P	242	4	26,50,50	2.43	5 (19%)	18,82,82	2.09	8 (44%)
12	HEM	C	380	3	27,50,50	2.08	4 (14%)	17,82,82	2.67	6 (35%)

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
12	HEM	O	380	3	-	0/6/54/54	-
13	HEC	D	242	4	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FES	Q	197	5	-	-	0/1/1/1
12	HEM	O	381	3	-	0/6/54/54	-
12	HEM	C	381	3	-	0/6/54/54	-
13	HEC	P	242	4	-	2/6/54/54	-
12	HEM	C	380	3	-	0/6/54/54	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	242	HEC	C3C-C2C	-7.16	1.33	1.40
13	D	242	HEC	C3B-C2B	-7.05	1.33	1.40
13	P	242	HEC	C3B-C2B	-6.84	1.33	1.40
12	C	380	HEM	C3B-C2B	-6.72	1.31	1.40
13	D	242	HEC	C3C-C2C	-6.59	1.33	1.40
12	O	381	HEM	C3C-C2C	-5.08	1.33	1.40
12	O	380	HEM	C3C-C2C	-4.84	1.33	1.40
12	O	380	HEM	C3B-C2B	-4.60	1.34	1.40
12	O	381	HEM	C3B-C2B	-4.41	1.34	1.40
12	C	380	HEM	C3B-CAB	4.22	1.56	1.47
12	C	380	HEM	C3C-C2C	-4.17	1.34	1.40
12	C	381	HEM	C3B-C2B	-4.17	1.34	1.40
12	O	380	HEM	C3B-CAB	4.16	1.56	1.47
12	O	381	HEM	C1A-NA	3.99	1.44	1.36
13	D	242	HEC	CBB-CAB	-3.68	1.35	1.49
13	P	242	HEC	CBC-CAC	-3.62	1.35	1.49
13	D	242	HEC	CBC-CAC	-3.49	1.36	1.49
13	P	242	HEC	CBB-CAB	-3.44	1.36	1.49
12	O	381	HEM	C3C-CAC	3.34	1.54	1.47
12	O	380	HEM	C1B-C2B	3.31	1.50	1.42
12	O	380	HEM	C3C-CAC	3.18	1.54	1.47
12	C	381	HEM	C4A-CHB	-3.06	1.32	1.41
12	C	381	HEM	C1C-C2C	3.00	1.49	1.42
12	C	380	HEM	C3C-CAC	2.97	1.53	1.47
12	C	381	HEM	C3C-C2C	-2.95	1.36	1.40
12	O	381	HEM	C3B-CAB	2.69	1.53	1.47
12	C	381	HEM	C3B-CAB	2.57	1.53	1.47
12	O	380	HEM	C4B-NB	2.18	1.40	1.36
12	C	381	HEM	CAD-C3D	2.09	1.55	1.52
13	P	242	HEC	CAD-C3D	2.07	1.55	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	380	HEM	CBD-CAD-C3D	7.22	125.78	112.48
12	O	380	HEM	CMA-C3A-C4A	-6.86	117.92	128.46
12	C	381	HEM	CAA-CBA-CGA	6.65	123.83	112.67
12	C	381	HEM	CMA-C3A-C4A	-5.41	120.16	128.46
12	O	380	HEM	CMB-C2B-C3B	5.16	134.33	124.68
12	O	380	HEM	CMD-C2D-C1D	-5.00	120.78	128.46
12	C	381	HEM	CAD-CBD-CGD	4.78	120.70	112.67
12	O	381	HEM	CMD-C2D-C1D	-4.43	121.66	128.46
12	C	380	HEM	CMA-C3A-C4A	-4.40	121.71	128.46
12	O	381	HEM	CMC-C2C-C3C	4.27	132.67	124.68
12	O	380	HEM	CMA-C3A-C2A	4.07	132.61	124.94
12	C	381	HEM	CMC-C2C-C3C	4.05	132.26	124.68
12	C	380	HEM	CMB-C2B-C3B	3.95	132.07	124.68
12	C	381	HEM	CBD-CAD-C3D	3.94	119.75	112.48
13	D	242	HEC	CMD-C2D-C1D	-3.94	122.40	128.46
12	O	380	HEM	CBD-CAD-C3D	3.78	119.45	112.48
13	P	242	HEC	CAD-CBD-CGD	3.64	118.77	112.67
12	C	381	HEM	CMA-C3A-C2A	3.55	131.64	124.94
13	P	242	HEC	CMD-C2D-C1D	-3.47	123.13	128.46
12	O	380	HEM	C4A-C3A-C2A	3.44	109.39	107.00
12	O	380	HEM	CAA-CBA-CGA	3.44	118.44	112.67
13	D	242	HEC	CMB-C2B-C1B	-3.43	123.19	128.46
12	O	380	HEM	CMD-C2D-C3D	3.34	131.24	124.94
12	O	381	HEM	CAA-CBA-CGA	3.17	117.99	112.67
12	O	381	HEM	CMA-C3A-C4A	-3.16	123.61	128.46
13	D	242	HEC	CBD-CAD-C3D	3.02	118.06	112.49
12	O	381	HEM	CMD-C2D-C3D	3.00	130.59	124.94
13	P	242	HEC	CMA-C3A-C2A	2.99	130.58	124.94
12	O	381	HEM	CBD-CAD-C3D	2.87	117.76	112.48
13	P	242	HEC	CBD-CAD-C3D	2.86	117.77	112.49
12	O	381	HEM	C4A-C3A-C2A	2.81	108.95	107.00
13	P	242	HEC	CMB-C2B-C1B	-2.66	124.38	128.46
12	C	380	HEM	CMA-C3A-C2A	2.66	129.95	124.94
13	D	242	HEC	CMB-C2B-C3B	2.61	128.89	125.82
13	D	242	HEC	C4C-C3C-C2C	2.58	109.14	106.35
12	O	381	HEM	CAD-CBD-CGD	2.52	116.90	112.67
13	P	242	HEC	CBA-CAA-C2A	2.50	117.09	112.48
12	O	380	HEM	CBA-CAA-C2A	2.48	117.07	112.49
13	D	242	HEC	CMD-C2D-C3D	2.26	129.21	124.94
13	D	242	HEC	CMA-C3A-C2A	2.26	129.21	124.94
12	C	380	HEM	CAD-CBD-CGD	2.25	116.45	112.67
13	P	242	HEC	CMD-C2D-C3D	2.20	129.09	124.94
12	O	381	HEM	CBA-CAA-C2A	2.15	116.46	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	242	HEC	C4C-C3C-C2C	2.10	108.62	106.35
12	C	380	HEM	CAA-CBA-CGA	2.08	116.16	112.67
13	D	242	HEC	CMC-C2C-C1C	-2.06	125.29	128.46
13	D	242	HEC	CAD-CBD-CGD	2.01	116.04	112.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

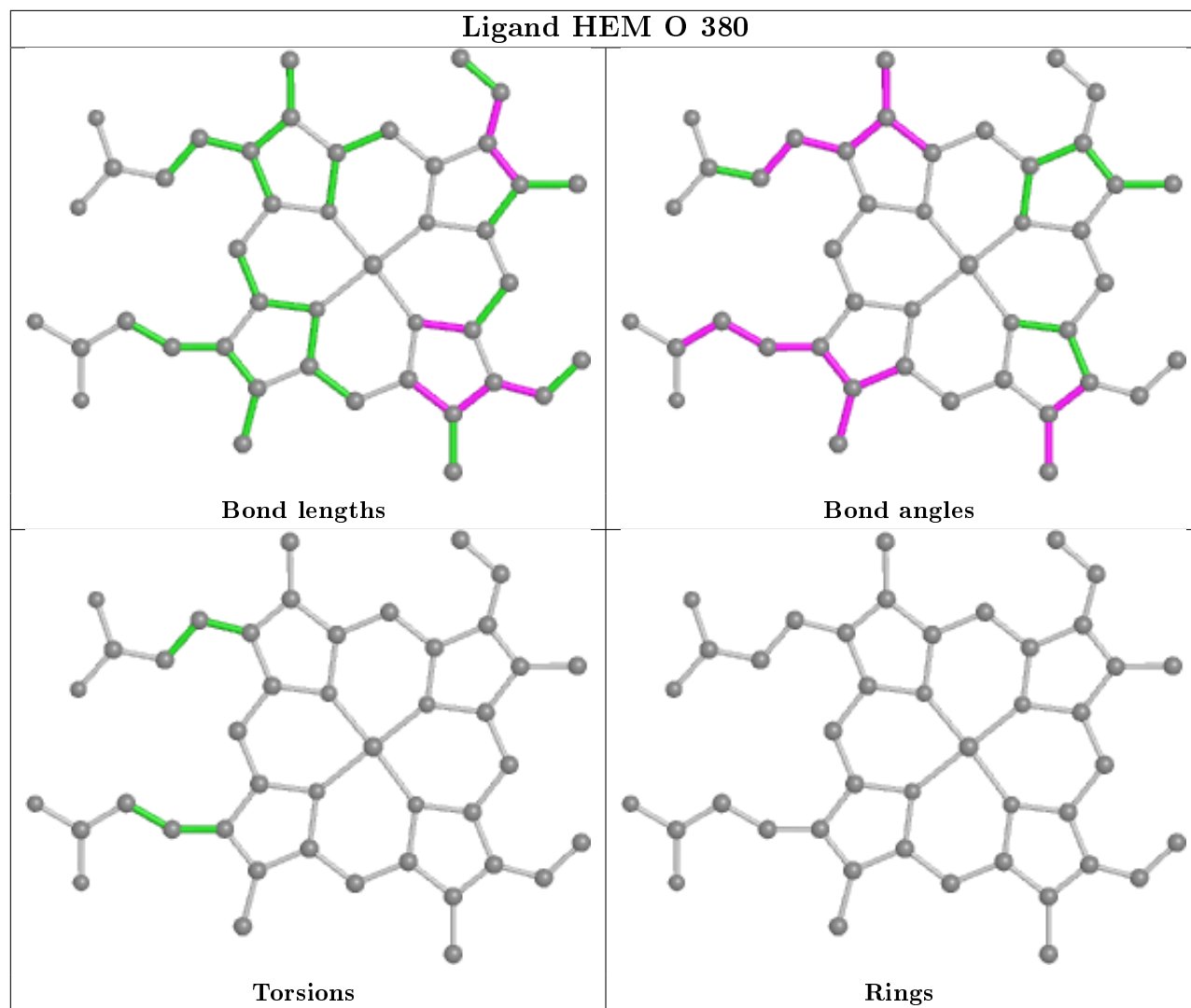
Mol	Chain	Res	Type	Atoms
13	P	242	HEC	C1A-C2A-CAA-CBA
13	P	242	HEC	C3A-C2A-CAA-CBA

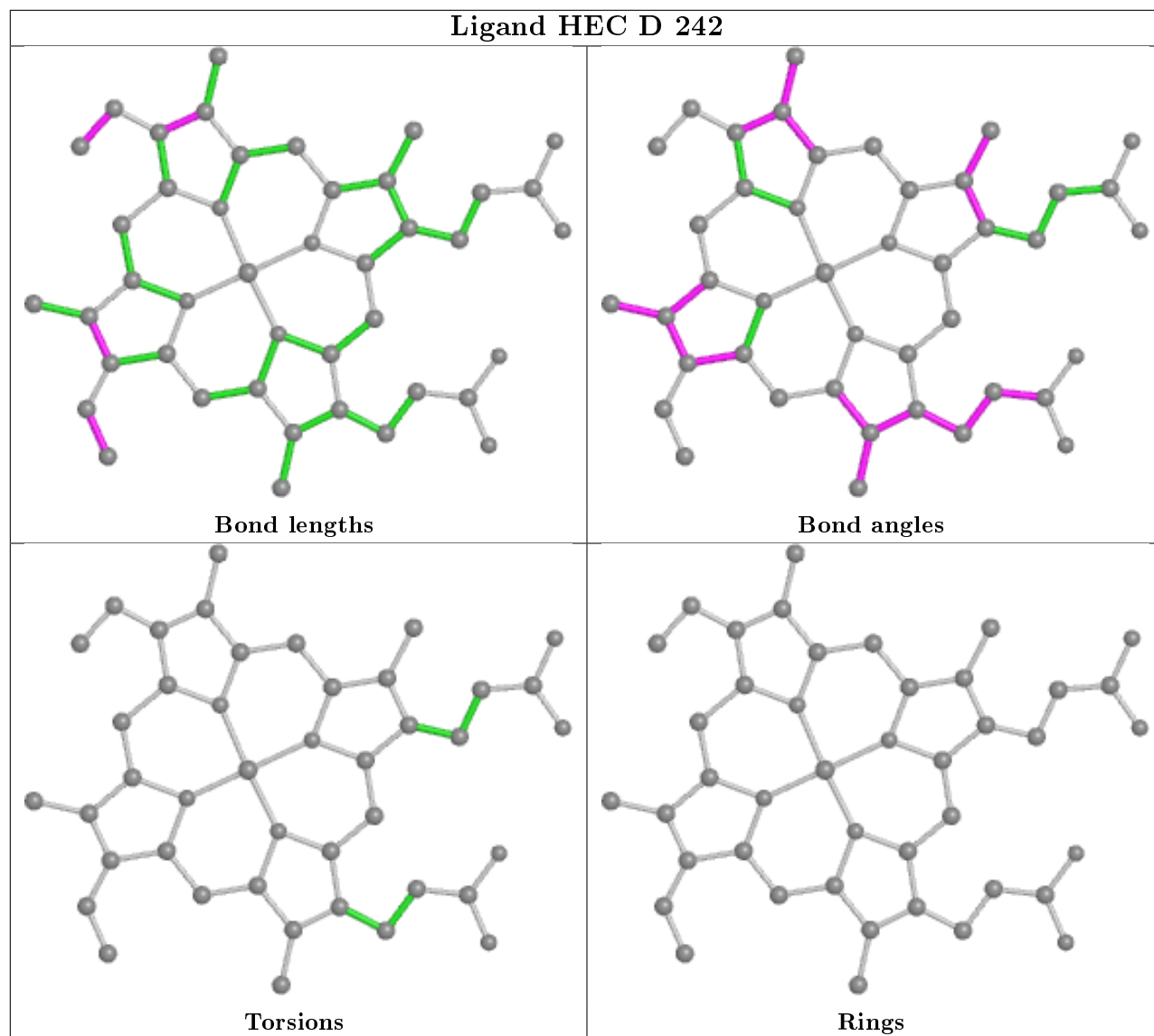
There are no ring outliers.

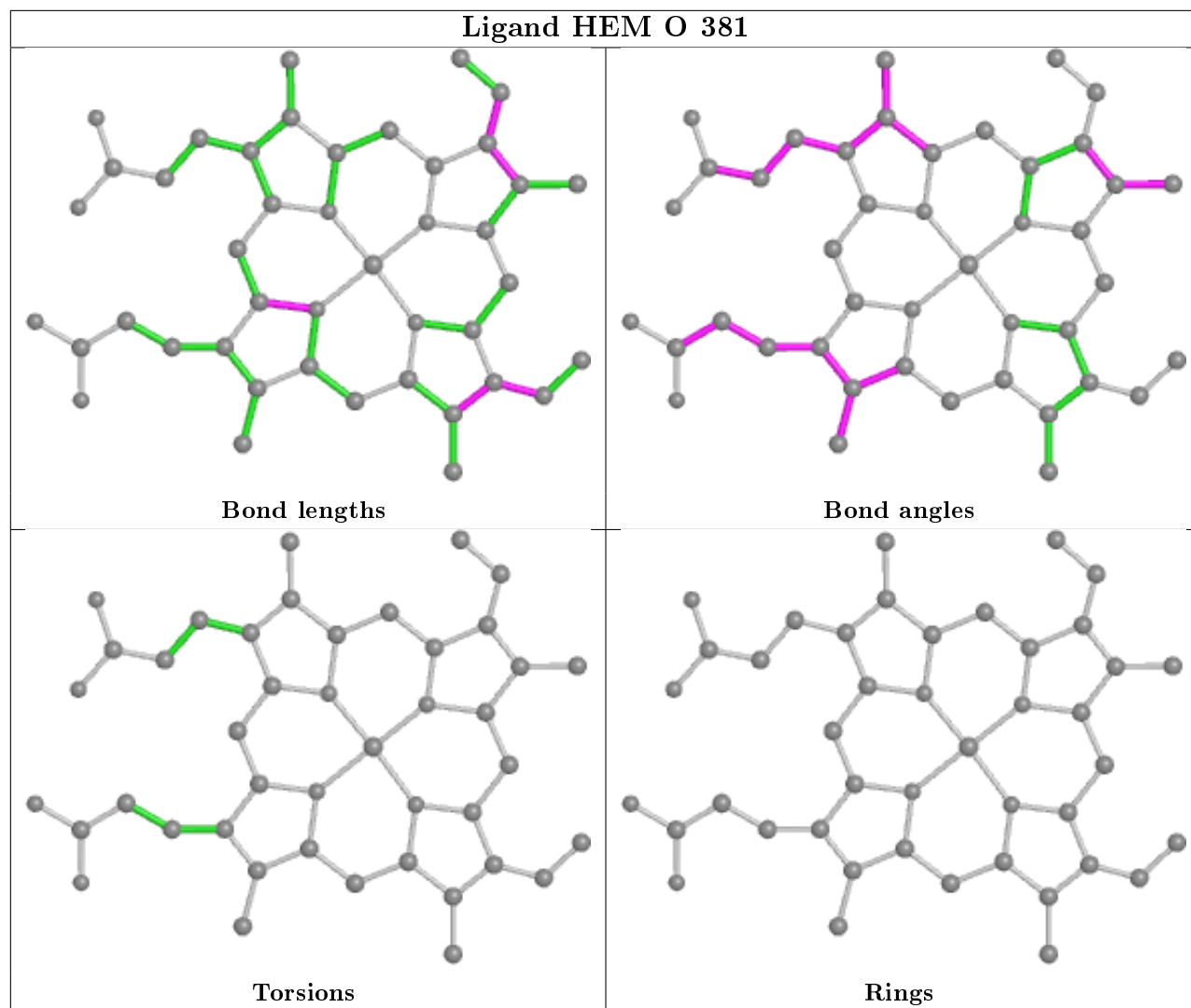
6 monomers are involved in 55 short contacts:

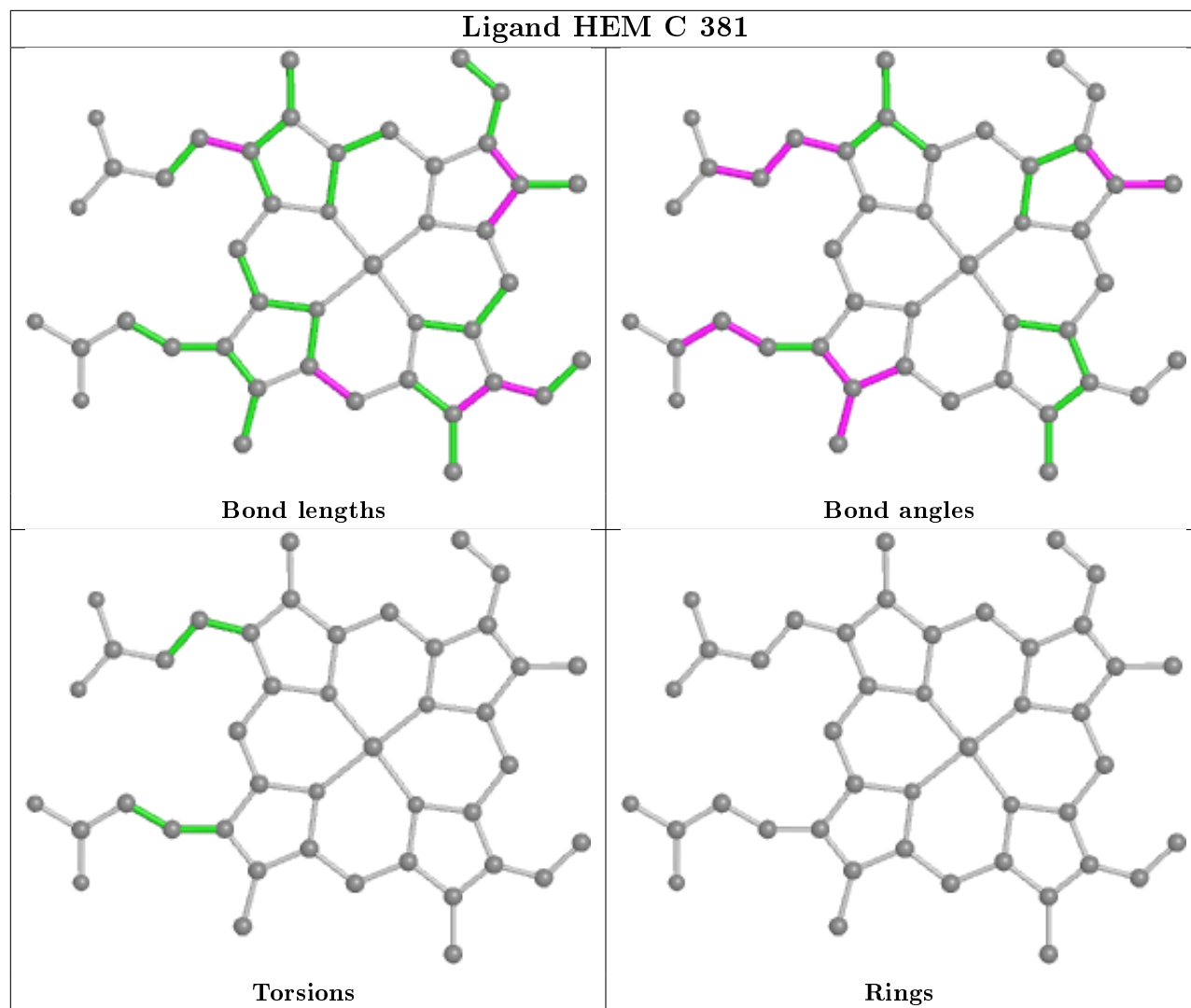
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	O	380	HEM	11	0
13	D	242	HEC	7	0
12	O	381	HEM	14	0
12	C	381	HEM	14	0
13	P	242	HEC	3	0
12	C	380	HEM	6	0

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.

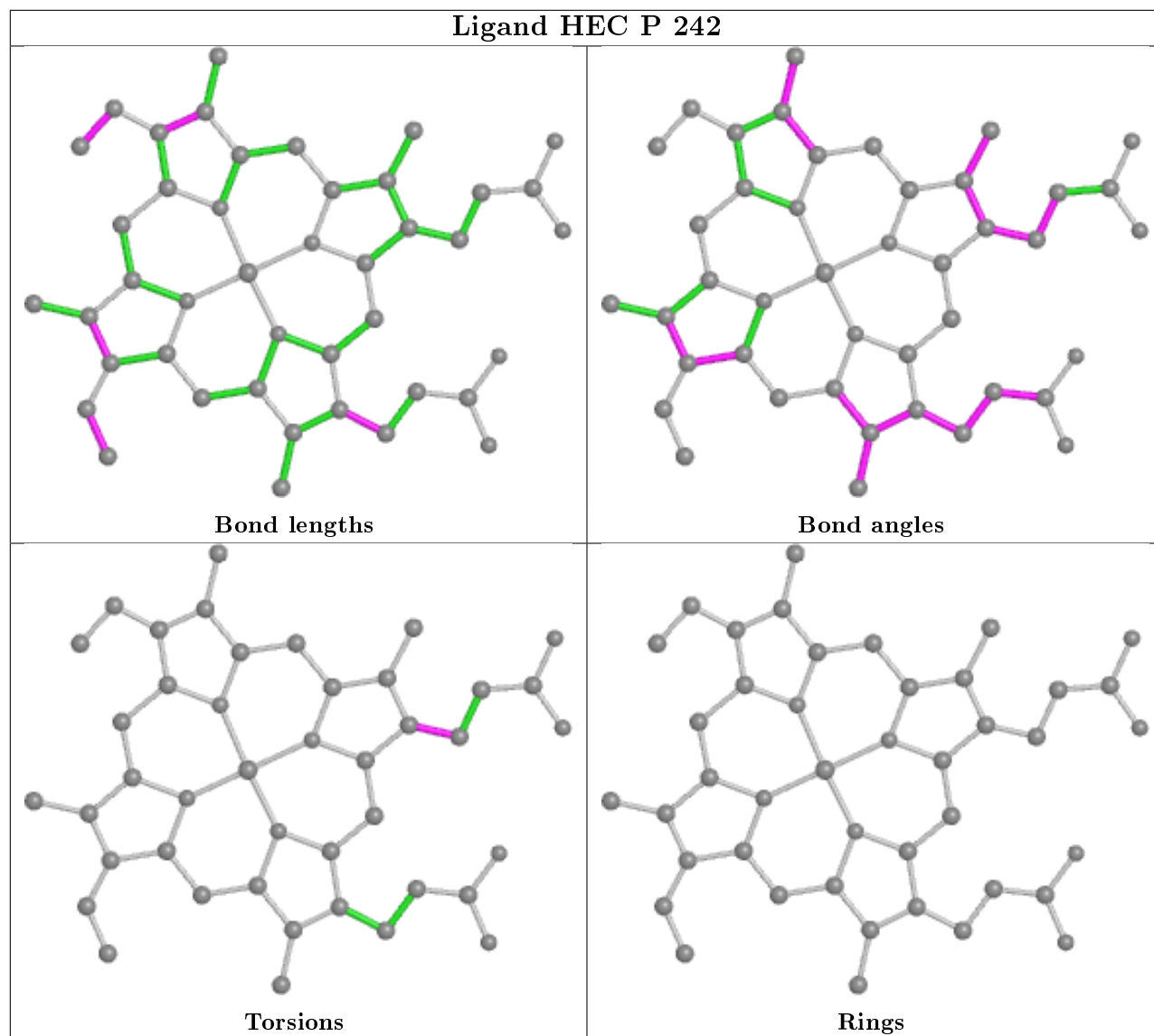


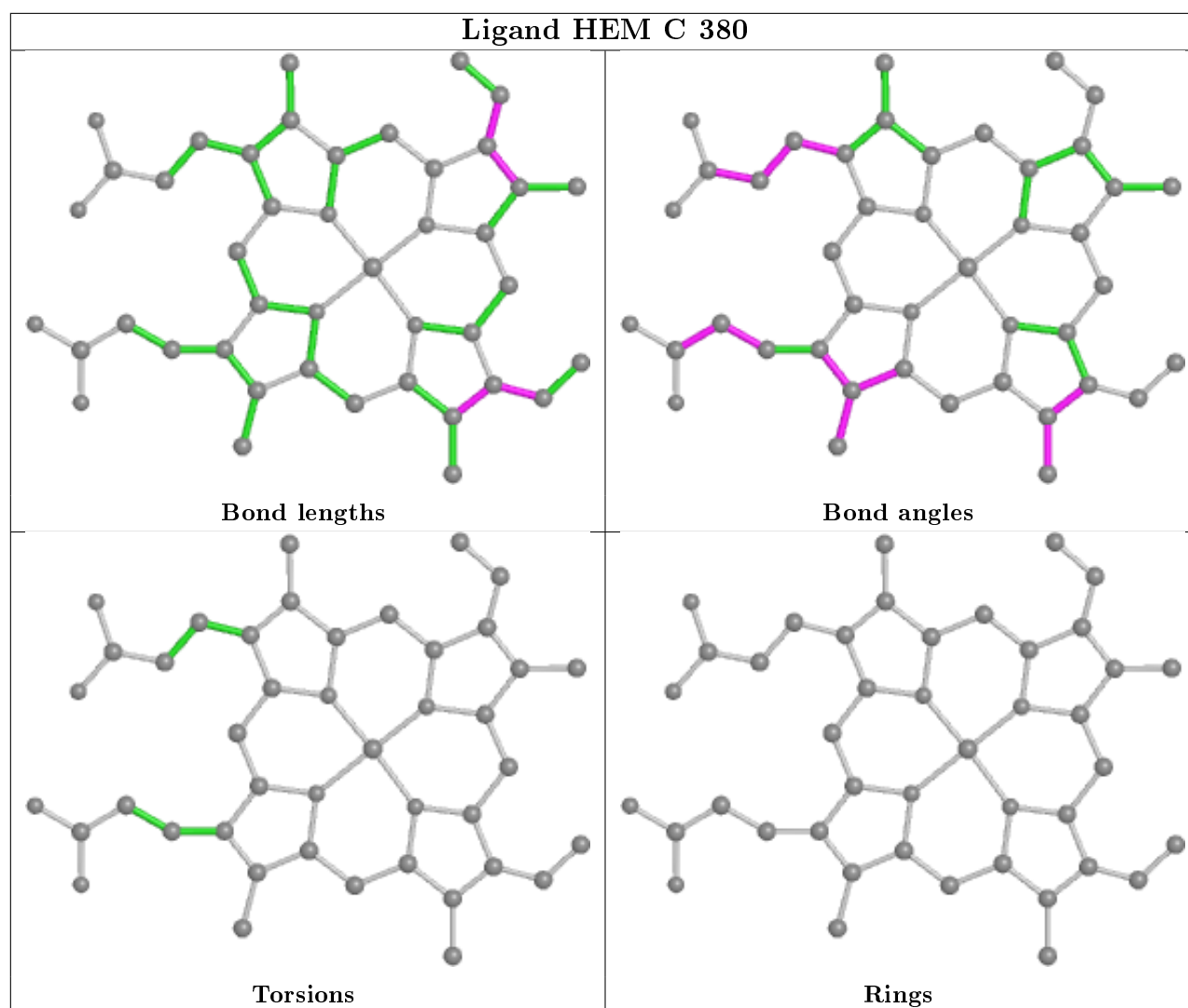






Ligand HEC P 242





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.