wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:14 PM BST

PDB ID	:	4UI9
EMDB ID:	:	EMD-2924
Title	:	Atomic structure of the human Anaphase-Promoting Complex
Authors	:	Chang, L.; Zhang, Z.; Yang, J.; McLaughlin, S.H.; Barford, D.
Deposited on	:	2015-03-27
Resolution	:	3.60 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

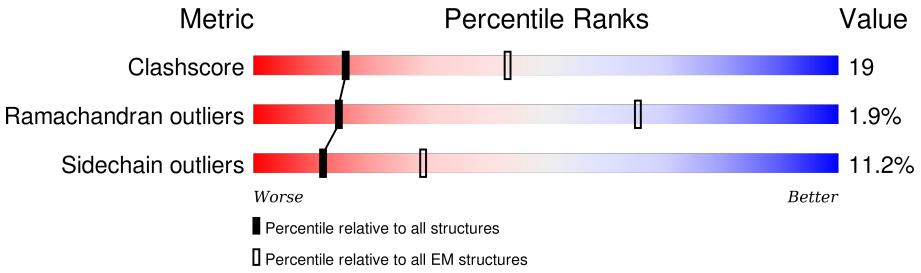
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1944	45% 25% • 26%
2	B	84	64% 25% 8% •
3	C	591	61% 24% • • 11%
3	P	591	58% 21% • 17%
4	D	121	33% 12% • 55%
5	E	110	35% 15% • 49%
6	F	824	43% 15% • 40%
6	H	824	42% 14% • 41%
7	G	85	25% • • 71%

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Mol	Chain	Length	Quality of chain
8	I	808	67% 21% • 10%
9	J	620	55% 21% 5% 19%
10	K	620	54% 22% • 20%
11	L	183	62% 32% 5% ••
12	M	74	45% 28% 7% 20%
13	N	822	40% 28% 7% • 23%
14	O	756	60% 25% 6% 9%
15	R	493	37% 32% 8% • 22%
16	S	447	14% 6% • 79%
17	T	21	71% 19% 10%
18	U	24	75% 25%
19	W	85	21% 7% • 71%
20	X	565	53% 29% • 14%
20	Y	565	56% 27% • 12%

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 66453 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ANAPHASE-PROMOTING COMPLEX SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1441	Total	C	N	O	S	0	0
			10947	7043	1853	1977	74		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	PHE	THR	CONFLICT	UNP Q9H1A4
A	940	ILE	THR	CONFLICT	UNP Q9H1A4
A	1059	GLU	ASP	CONFLICT	UNP Q9H1A4
A	1358	LEU	ILE	CONFLICT	UNP Q9H1A4
A	1637	LEU	THR	CONFLICT	UNP Q9H1A4
A	1880	PRO	LEU	CONFLICT	UNP Q9H1A4
A	1881	LEU	GLU	CONFLICT	UNP Q9H1A4

- Molecule 2 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	84	Total	C	N	O	S	1	0
			650	418	117	98	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	LEU	THR	CONFLICT	UNP Q9NYG5

- Molecule 3 is a protein called CELL DIVISION CYCLE PROTEIN 23 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	524	Total	C	N	O	S	0	0
			4305	2774	726	781	24		
3	P	491	Total	C	N	O	S	0	0
			4042	2611	678	729	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	161	LEU	LYS	CONFLICT	UNP Q9UJX2
P	161	LEU	LYS	CONFLICT	UNP Q9UJX2

- Molecule 4 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	55	Total	C	N	O	0	0
			437	277	73	87		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	5	TYR	PHE	CONFLICT	UNP P60006

- Molecule 5 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	56	Total	C	N	O	S	0	0
			450	290	74	85	1		

- Molecule 6 is a protein called CELL DIVISION CYCLE PROTEIN 27 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	498	Total	C	N	O	S	0	0
			3923	2514	664	719	26		
6	H	483	Total	C	N	O	S	0	0
			3853	2473	650	704	26		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	403	GLU	LYS	CONFLICT	UNP P30260
F	475	SER	ALA	CONFLICT	UNP P30260
F	484	SER	ALA	CONFLICT	UNP P30260
H	403	GLU	LYS	CONFLICT	UNP P30260
H	475	SER	ALA	CONFLICT	UNP P30260
H	484	SER	ALA	CONFLICT	UNP P30260

- Molecule 7 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	25	Total	C	N	O	S	0	0
			214	134	40	39	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	14	GLU	ASP	CONFLICT	UNP Q8NHZ8

- Molecule 8 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	730	Total	C	N	O	S	0	0
			5709	3660	950	1066	33		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	430	ASP	GLU	CONFLICT	UNP Q9UJX5

- Molecule 9 is a protein called CELL DIVISION CYCLE PROTEIN 16 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	504	Total	C	N	O	S	0	0
			4047	2602	685	735	25		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	225	ASN	ASP	CONFLICT	UNP Q13042
J	228	GLU	GLN	CONFLICT	UNP Q13042
J	229	LYS	GLU	CONFLICT	UNP Q13042

- Molecule 10 is a protein called CELL DIVISION CYCLE PROTEIN 16 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	493	Total	C	N	O	S	0	0
			3988	2565	673	726	24		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	228	GLU	GLN	CONFLICT	UNP Q13042

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Chain	Residue	Modelled	Actual	Comment	Reference
K	229	LYS	GLU	CONFLICT	UNP Q13042
K	265	LYS	ALA	CONFLICT	UNP Q13042

- Molecule 11 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	182	Total	C	N	O	S	0	0
			1435	898	263	268	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	.	-	GLU	DELETION	UNP Q9UM13

- Molecule 12 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	59	Total	C	N	O	S	0	0
			493	310	79	102	2		

- Molecule 13 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	631	Total	C	N	O	S	0	0
			4831	3064	877	868	22		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	410	ILE	LEU	CONFLICT	UNP Q9UJX6

- Molecule 14 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	685	Total	C	N	O	S	0	0
			5396	3439	939	991	27		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	42	SER	ASN	CONFLICT	UNP Q9UJX4

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Chain	Residue	Modelled	Actual	Comment	Reference
O	55	VAL	MET	CONFLICT	UNP Q9UJX4
O	63	GLN	LEU	CONFLICT	UNP Q9UJX4
O	75	VAL	LEU	CONFLICT	UNP Q9UJX4
O	79	LEU	TYR	CONFLICT	UNP Q9UJX4
O	164	SER	ASN	CONFLICT	UNP Q9UJX4
O	165	ASP	GLY	CONFLICT	UNP Q9UJX4
O	167	ASN	-	INSERTION	UNP Q9UJX4

- Molecule 15 is a protein called FIZZY-RELATED PROTEIN HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	387	Total	C	N	O	S	0	0
			3003	1895	541	557	10		

- Molecule 16 is a protein called F-BOX ONLY PROTEIN 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	94	Total	C	N	O	S	0	0
			648	396	119	124	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	323	ILE	THR	CONFLICT	UNP Q9UKT4
S	326	LYS	ALA	CONFLICT	UNP Q9UKT4

- Molecule 17 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	T	21	Total	C	N	O	0	0
			109	65	22	22		

- Molecule 18 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	U	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 19 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	25	Total	C	N	O	S	0	0
			213	133	40	39	1		

- Molecule 20 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	484	Total	C	N	O	S	0	0
			3770	2394	650	705	21		
20	Y	496	Total	C	N	O	S	0	0
			3865	2450	667	725	23		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	63	LEU	MET	CONFLICT	UNP Q9UJX3
X	142	LEU	MET	CONFLICT	UNP Q9UJX3
X	148	VAL	MET	CONFLICT	UNP Q9UJX3
X	466	ASN	ASP	CONFLICT	UNP Q9UJX3
X	472	GLU	ARG	CONFLICT	UNP Q9UJX3
Y	63	LEU	MET	CONFLICT	UNP Q9UJX3
Y	142	LEU	MET	CONFLICT	UNP Q9UJX3
Y	148	VAL	MET	CONFLICT	UNP Q9UJX3
Y	466	ASN	ASP	CONFLICT	UNP Q9UJX3
Y	472	GLU	ARG	CONFLICT	UNP Q9UJX3

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

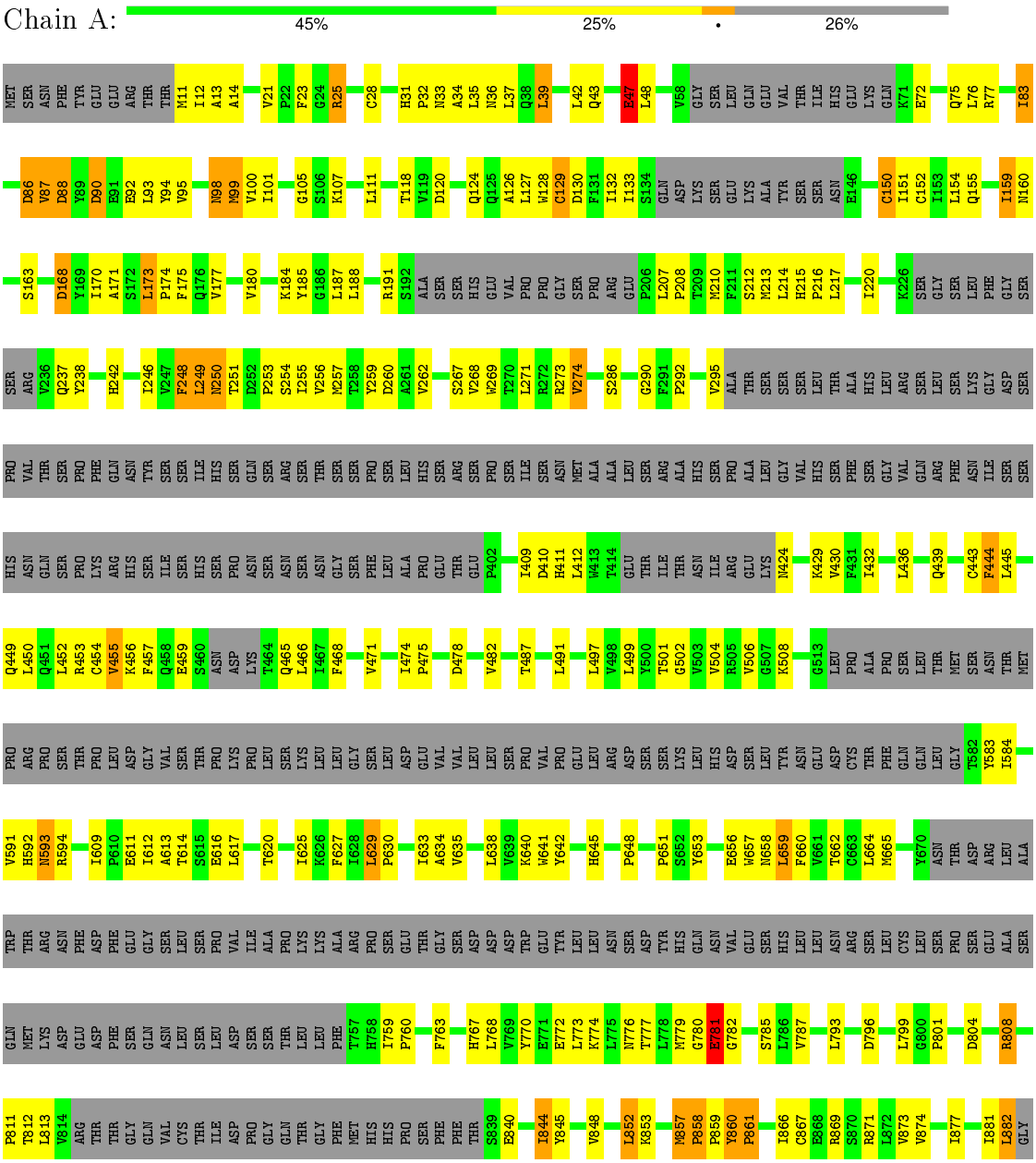
Mol	Chain	Residues	Atoms		AltConf
21	B	3	Total	Zn	0
			3	3	
21	S	2	Total	Zn	0
			2	2	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

- Molecule 1: ANAPHASE-PROMOTING COMPLEX SUBUNIT 1

Chain A:



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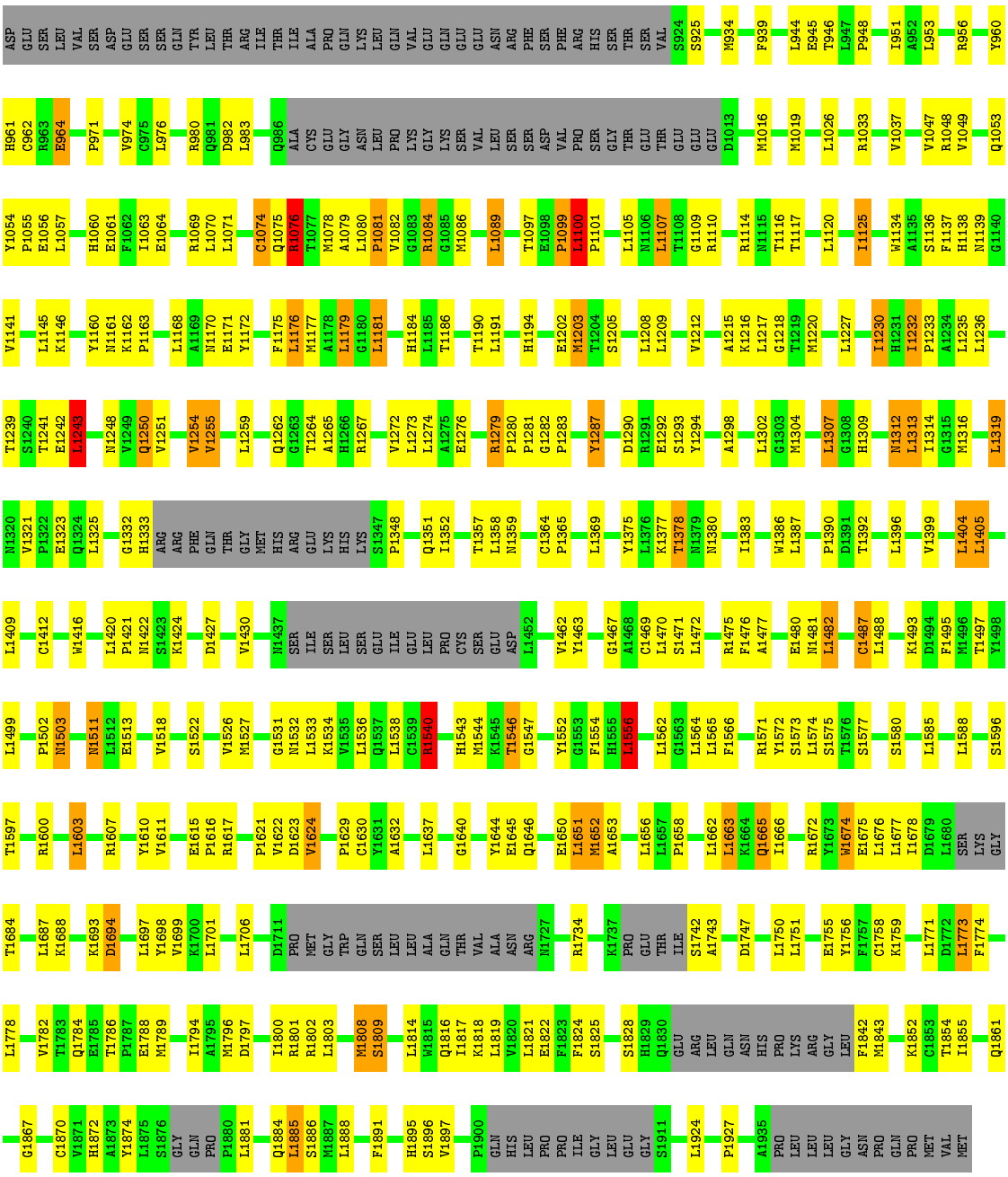
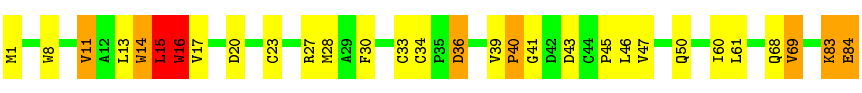


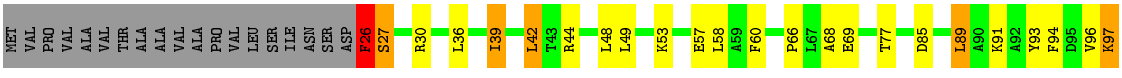
• Molecule 2: ANAPHASE-PROMOTING COMPLEX SUBUNIT 11

Chain B:



• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

Chain C:



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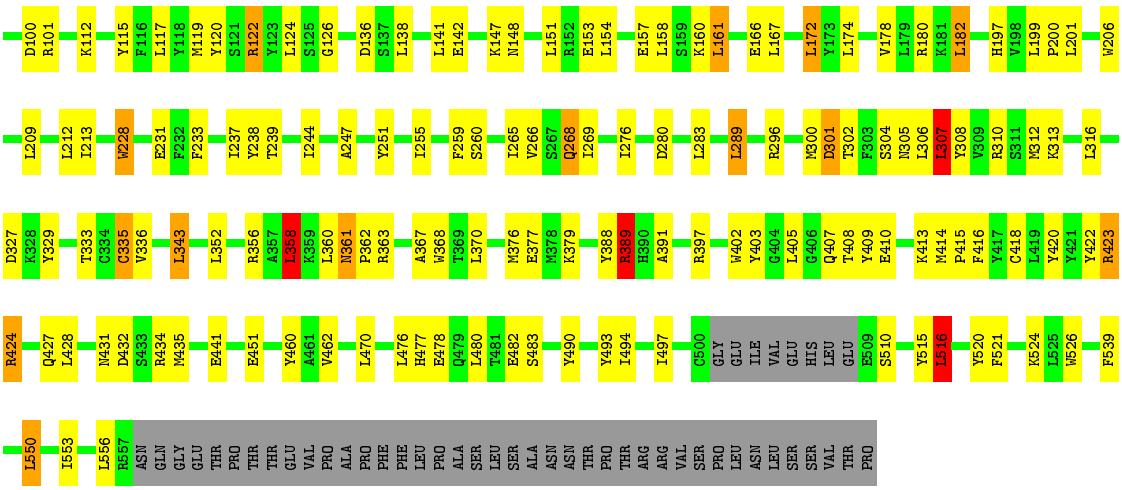
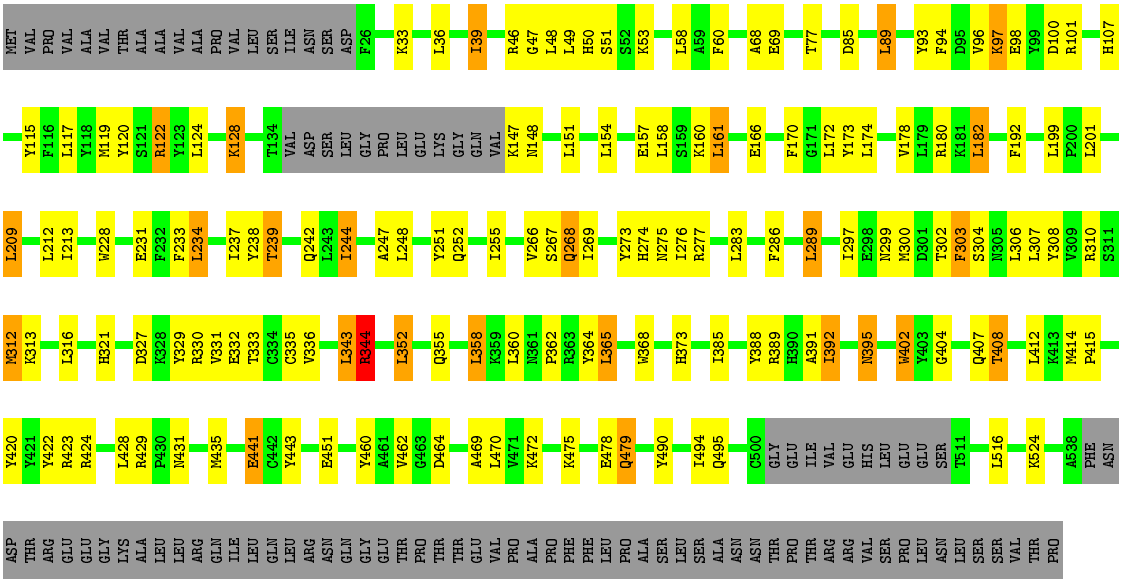


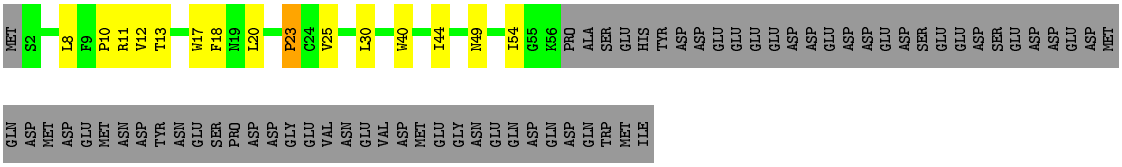
- Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

Chain P:



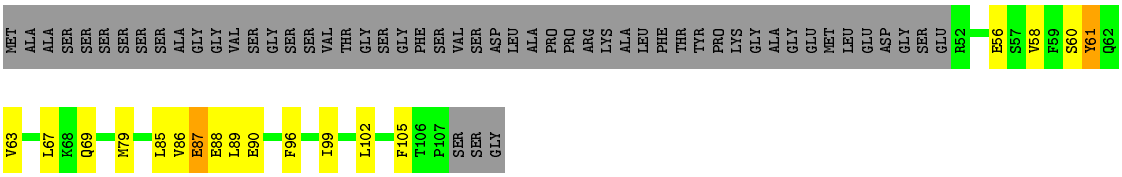
- Molecule 4: ANAPHASE-PROMOTING COMPLEX SUBUNIT 15

Chain D:



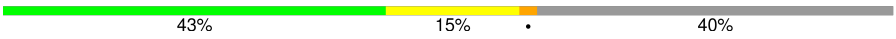
- Molecule 5: ANAPHASE-PROMOTING COMPLEX SUBUNIT 16

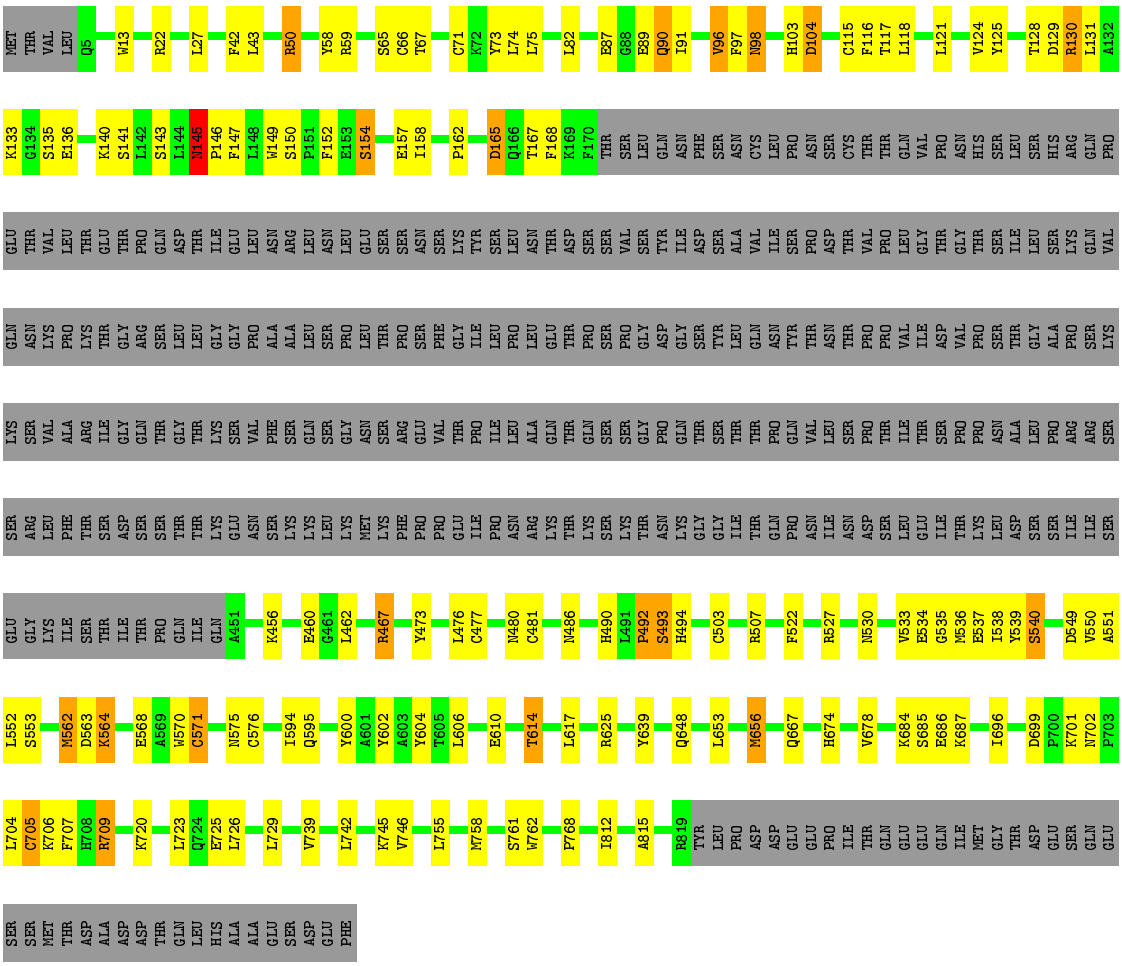
Chain E:



- Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

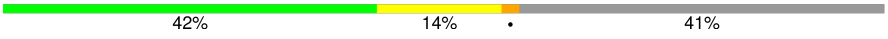
Chain F:

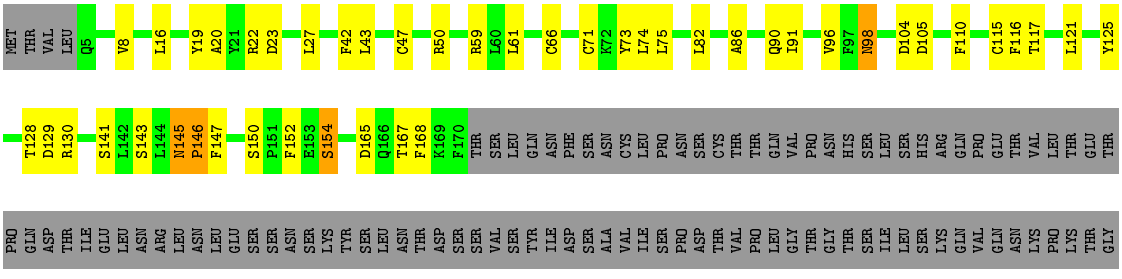


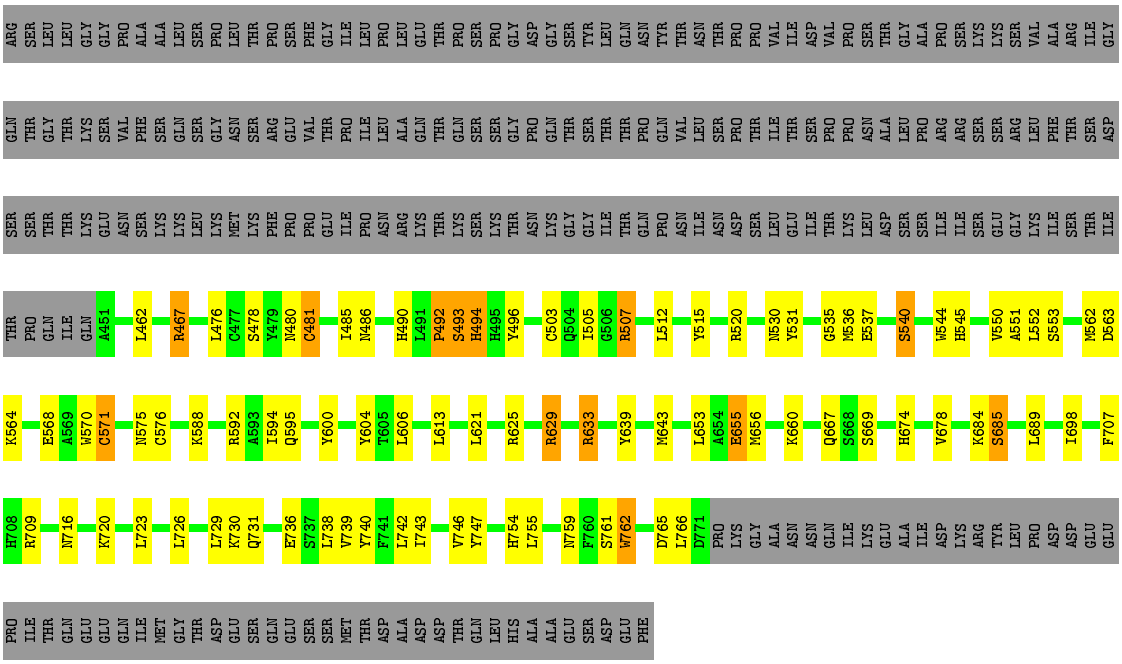


- Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

Chain H:

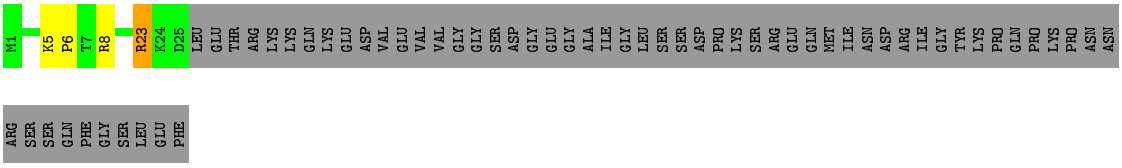






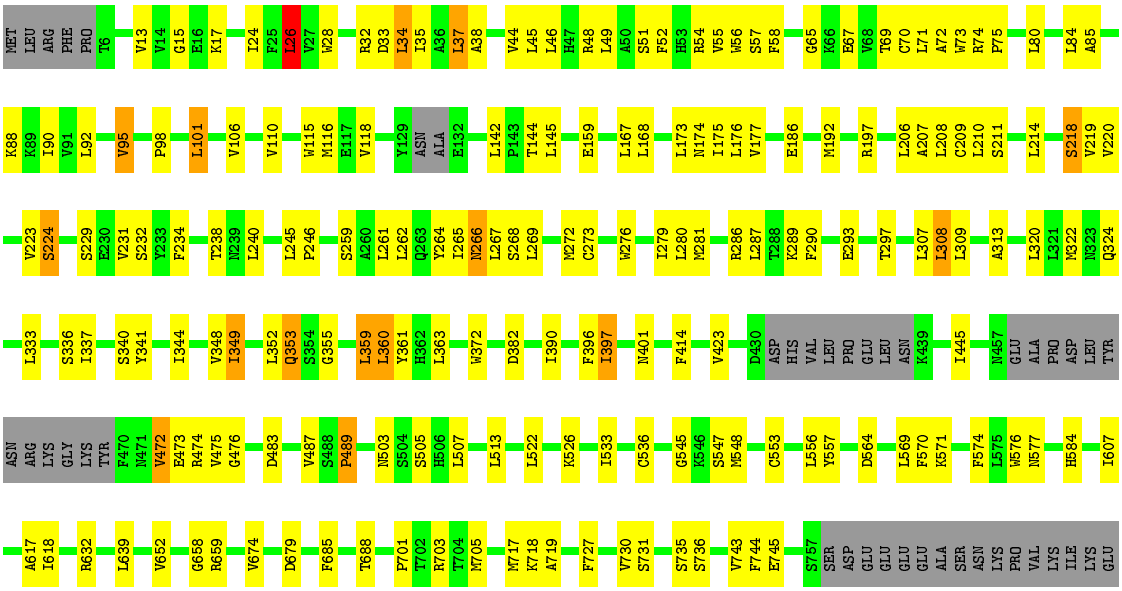
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

Chain G:



• Molecule 8: ANAPHASE-PROMOTING COMPLEX SUBUNIT 4

Chain I:



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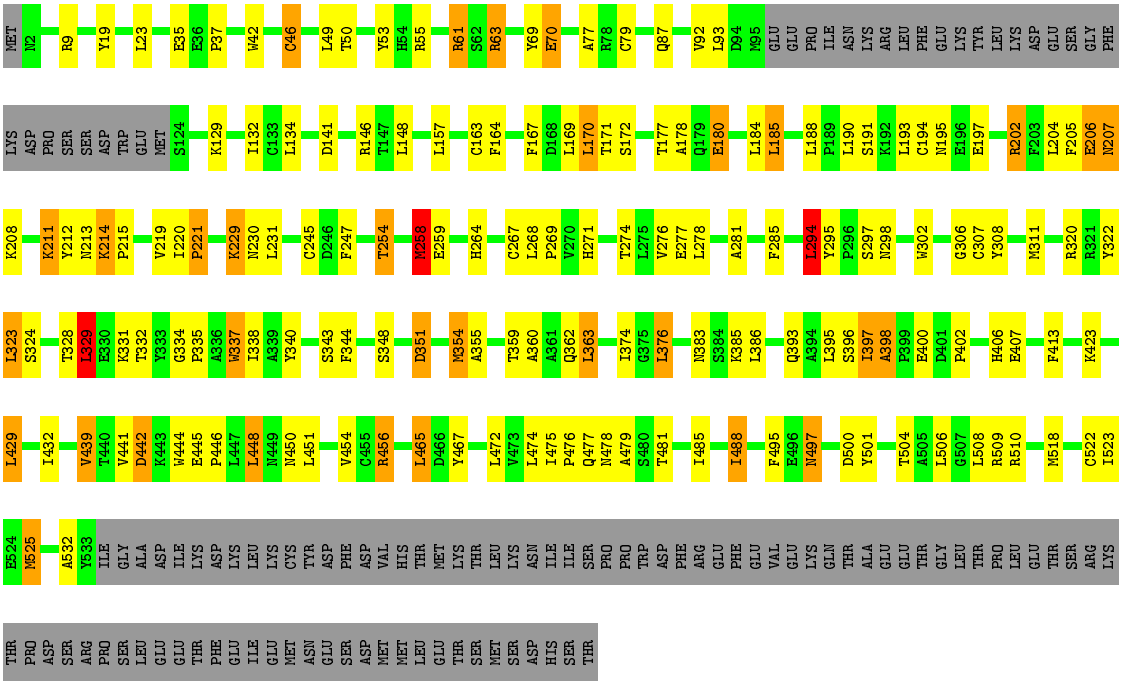
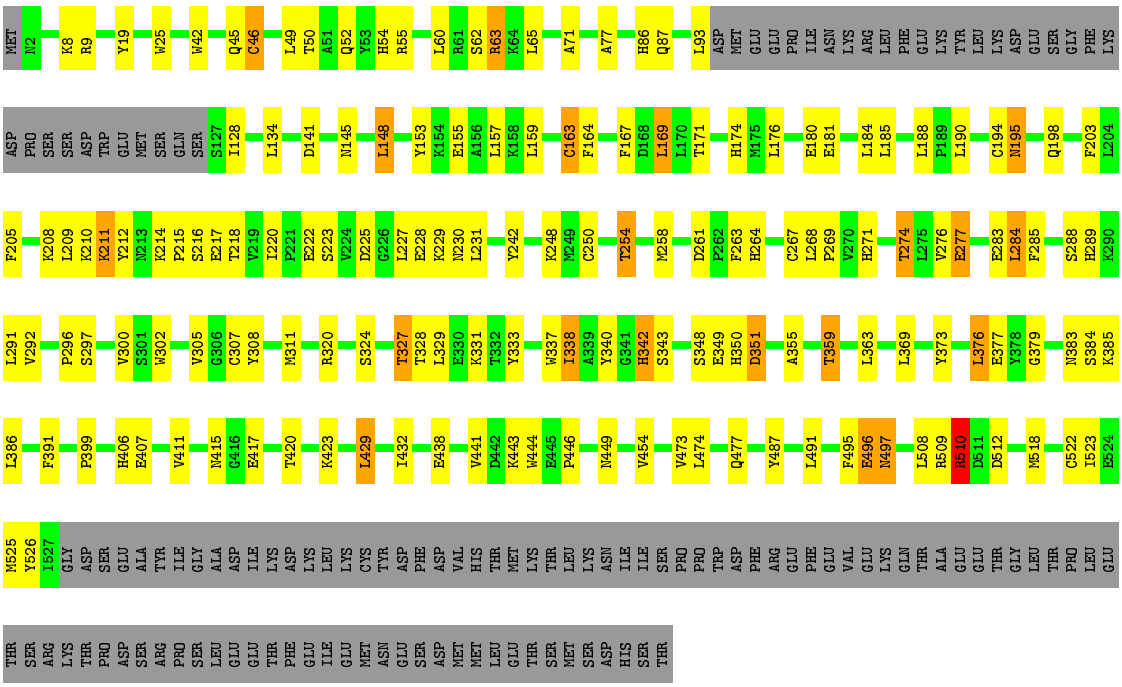
- Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

Chain J:



- Molecule 10: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

Chain K:



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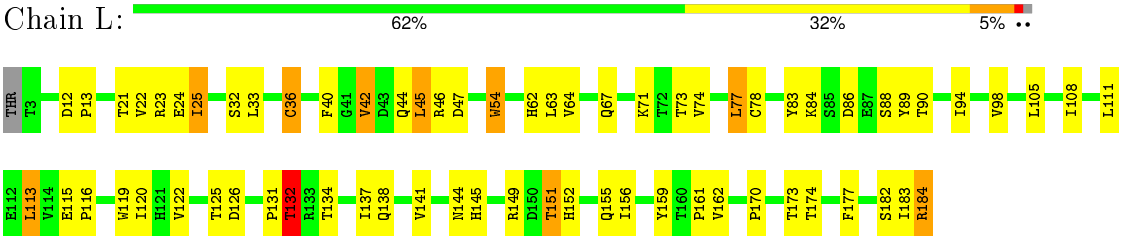
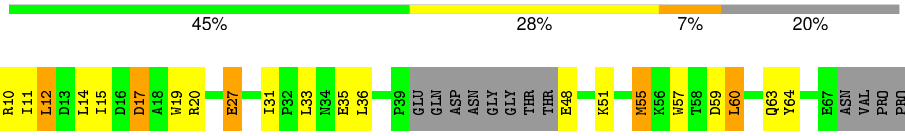
• Molecule 11: ANAPHASE-PROMOTING COMPLEX SUBUNIT 10

Chain L:



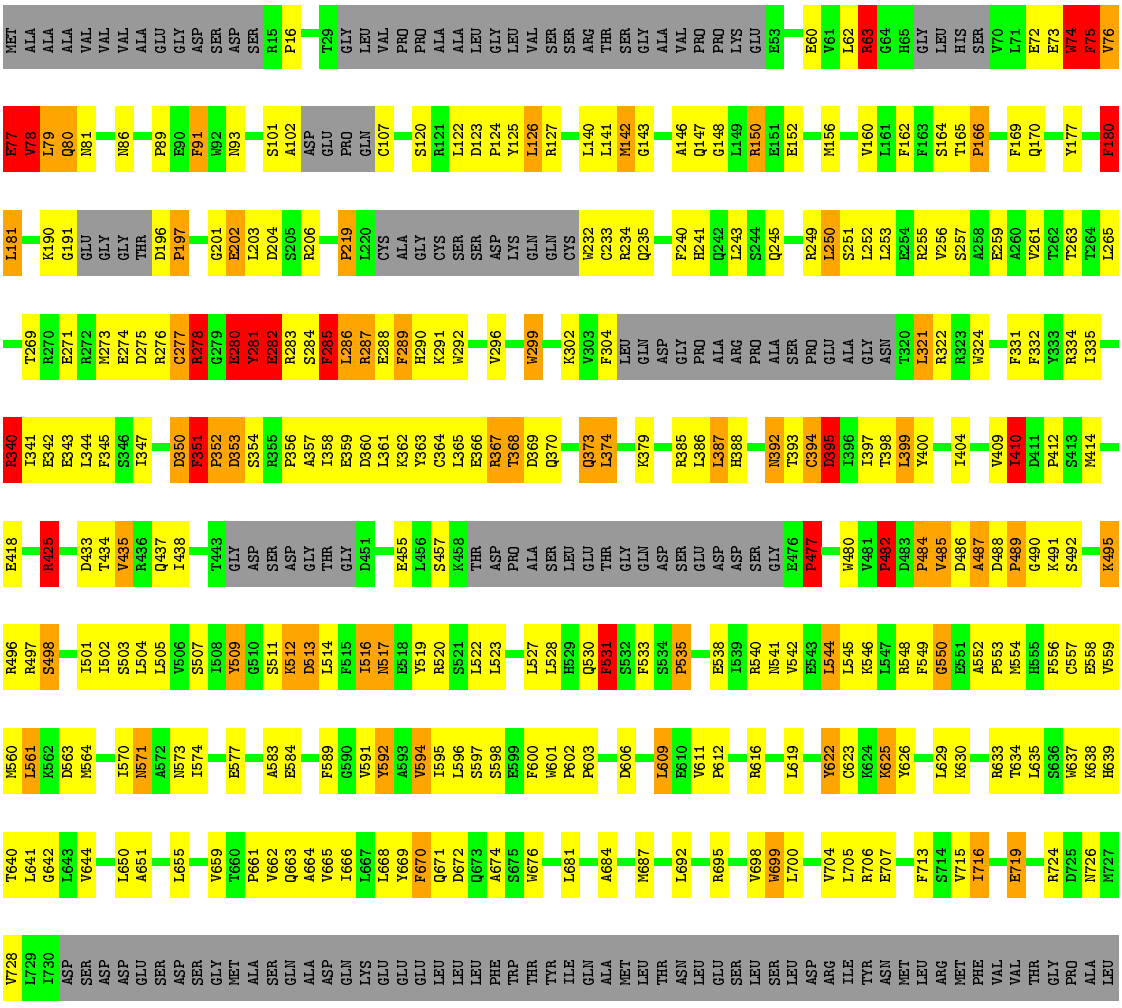
• Molecule 12: ANAPHASE-PROMOTING COMPLEX SUBUNIT 13

Chain M:



• Molecule 13: ANAPHASE-PROMOTING COMPLEX SUBUNIT 2

Chain N:



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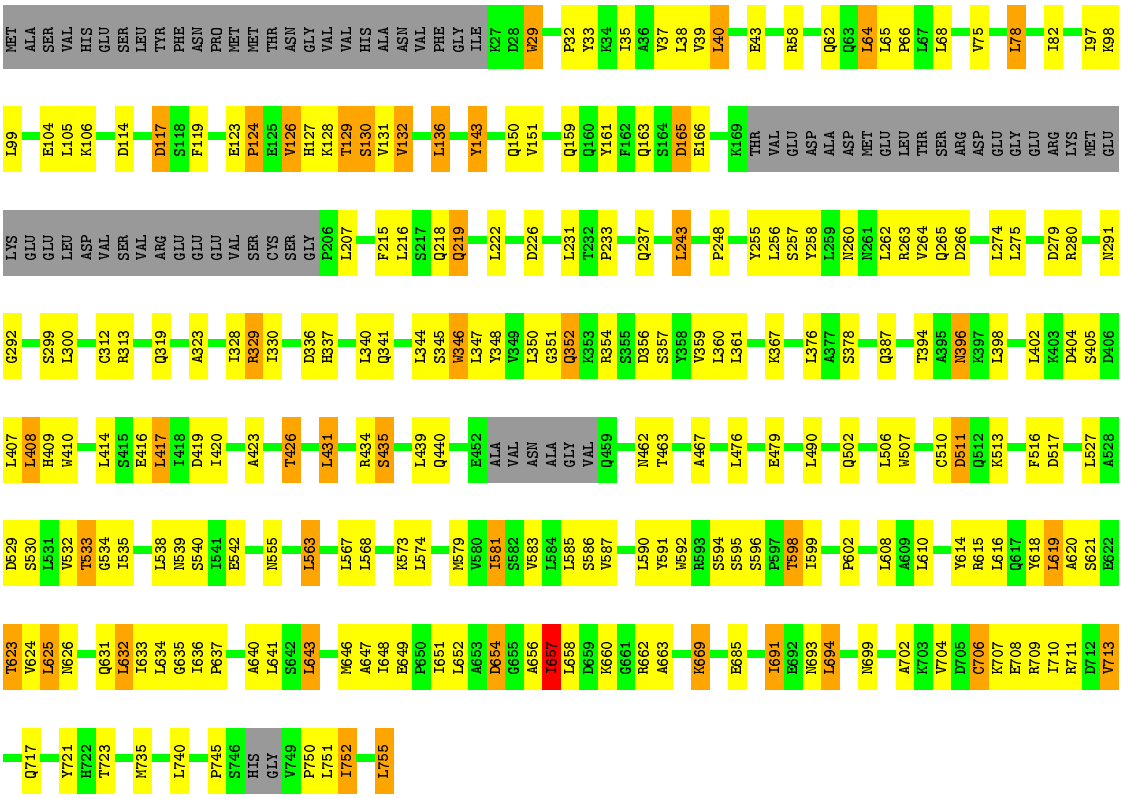
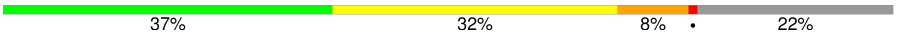
- Molecule 14: ANAPHASE-PROMOTING COMPLEX SUBUNIT 5

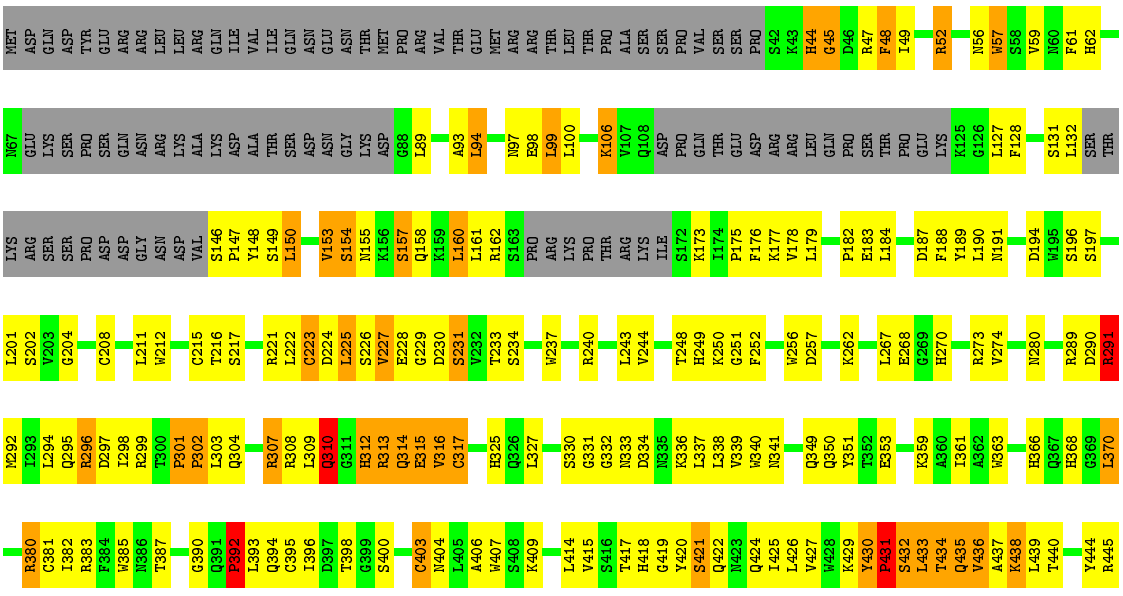
Chain O:



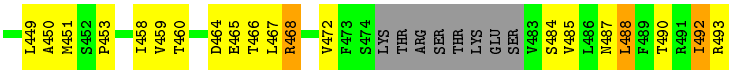
- Molecule 15: FIZZY-RELATED PROTEIN HOMOLOG

Chain R:



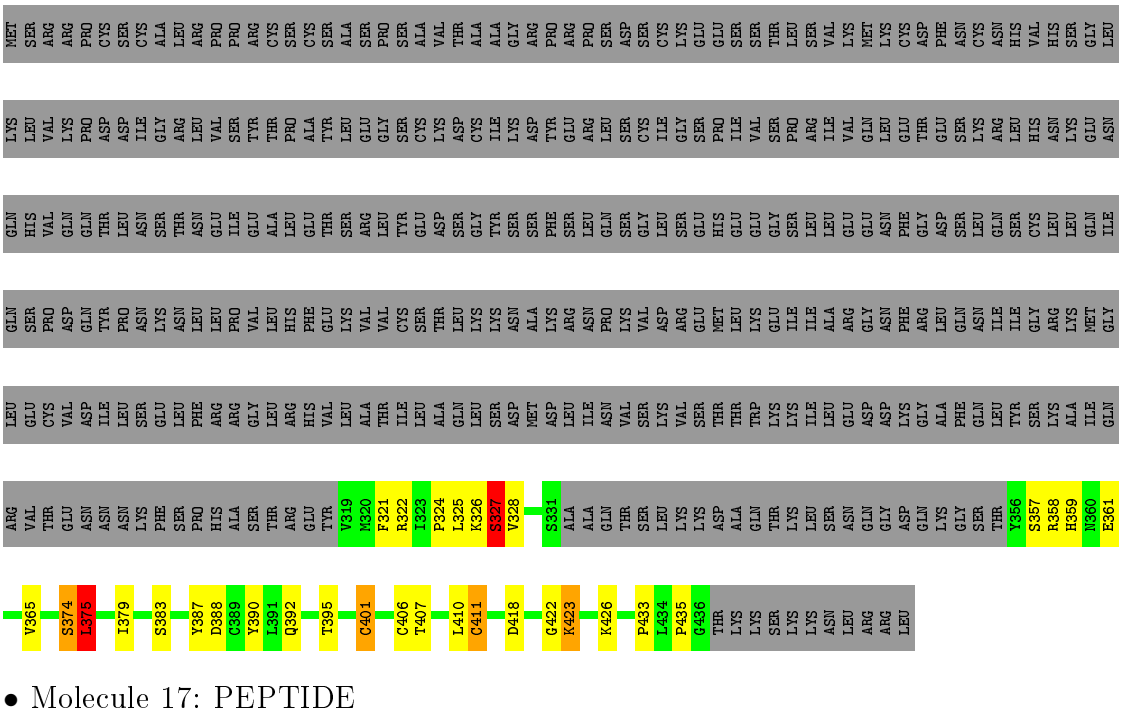


WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM



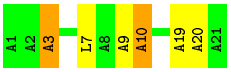
• Molecule 16: F-BOX ONLY PROTEIN 5

Chain S:



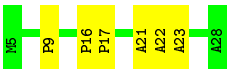
• Molecule 17: PEPTIDE

Chain T:



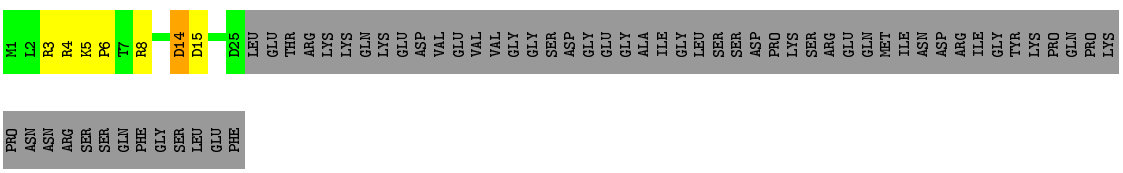
• Molecule 18: PEPTIDE

Chain U:



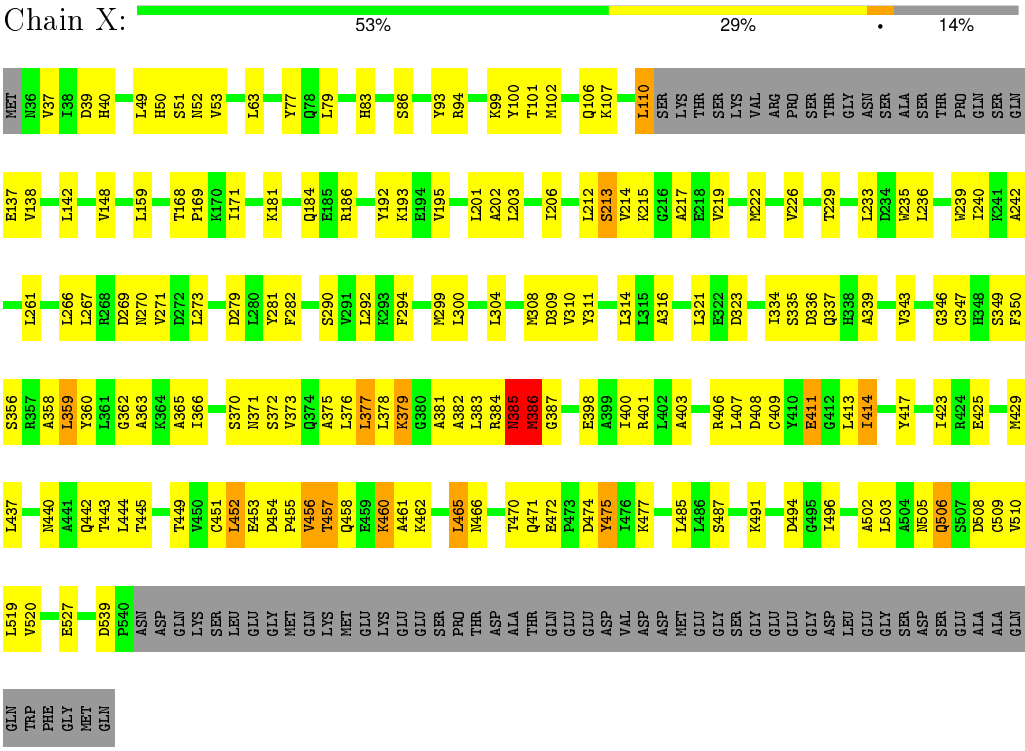
• Molecule 19: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

Chain W:



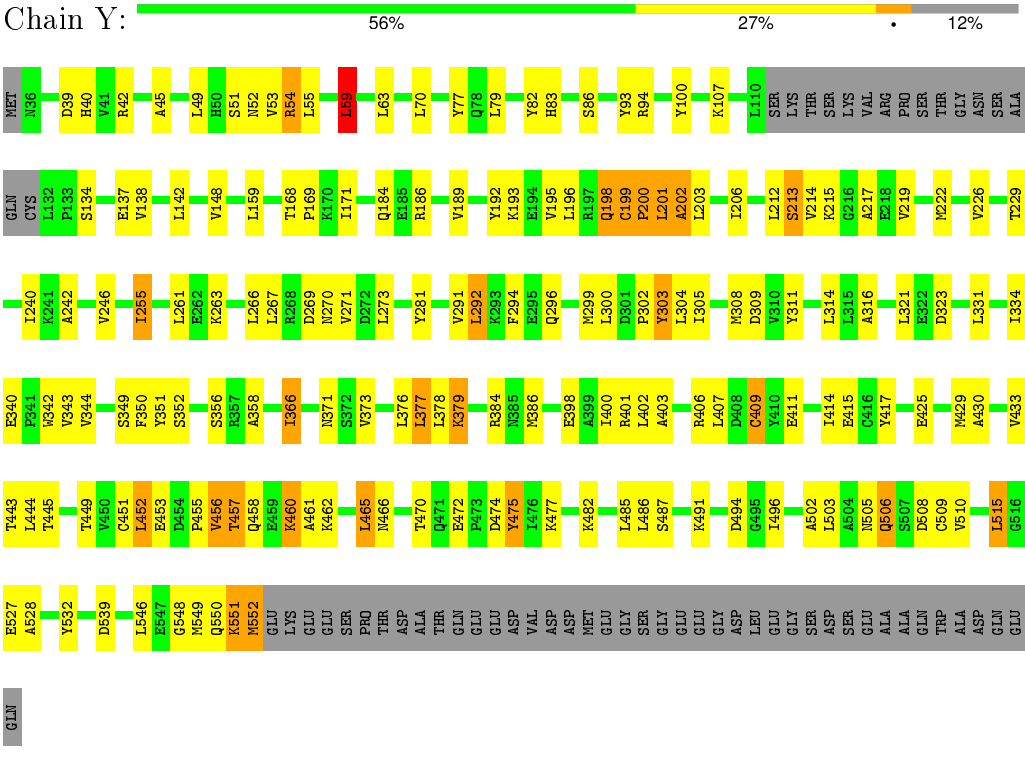
• Molecule 20: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

Chain X:



- Molecule 20: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

Chain Y:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	78000	Depositor
Image detector	FALCON II	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	0.75	0/11190	0.99	21/15238 (0.1%)
10	K	0.89	3/4086 (0.1%)	0.96	5/5532 (0.1%)
11	L	0.71	0/1468	0.96	5/1993 (0.3%)
12	M	0.73	0/502	1.05	1/680 (0.1%)
13	N	0.63	1/4913 (0.0%)	1.01	18/6650 (0.3%)
14	O	0.73	5/5494 (0.1%)	0.96	5/7425 (0.1%)
15	R	2.23	11/3068 (0.4%)	2.62	75/4162 (1.8%)
16	S	0.54	0/654	0.81	3/880 (0.3%)
17	T	1.02	0/108	1.11	0/149
18	U	0.91	0/119	1.10	3/165 (1.8%)
19	W	0.64	0/214	1.02	0/284
2	B	0.52	0/675	0.86	1/914 (0.1%)
20	X	0.60	4/3830 (0.1%)	0.84	6/5187 (0.1%)
20	Y	0.54	0/3925	0.85	4/5311 (0.1%)
3	C	0.75	1/4403 (0.0%)	0.95	9/5945 (0.2%)
3	P	0.70	1/4137 (0.0%)	0.92	3/5587 (0.1%)
4	D	0.71	0/447	0.98	1/612 (0.2%)
5	E	0.65	0/459	0.86	0/619
6	F	0.70	3/4013 (0.1%)	0.90	7/5428 (0.1%)
6	H	0.70	2/3943 (0.1%)	0.90	4/5329 (0.1%)
7	G	0.62	0/215	1.03	1/285 (0.4%)
8	I	0.58	0/5827	0.85	3/7899 (0.0%)
9	J	0.75	3/4146 (0.1%)	0.97	9/5615 (0.2%)
All	All	0.83	34/67836 (0.1%)	1.07	184/91889 (0.2%)

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	9
13	N	0	26
15	R	0	5
17	T	0	1
20	X	0	1
8	I	0	2
9	J	0	1
All	All	0	45

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	R	431	PRO	N-CD	53.78	2.23	1.47
15	R	392	PRO	N-CD	50.89	2.19	1.47
15	R	302	PRO	N-CD	48.99	2.16	1.47
15	R	301	PRO	N-CD	47.51	2.14	1.47
10	K	229	LYS	CB-CG	33.09	2.42	1.52
15	R	317	CYS	CB-SG	-23.44	1.42	1.82
15	R	403	CYS	CB-SG	-23.42	1.42	1.82
15	R	215	CYS	CB-SG	-23.42	1.42	1.82
15	R	395	CYS	CB-SG	-23.42	1.42	1.82
15	R	223	CYS	CB-SG	-23.41	1.42	1.82
15	R	208	CYS	CB-SG	-23.39	1.42	1.82
15	R	381	CYS	CB-SG	-23.39	1.42	1.82
20	X	385	ASN	N-CA	9.79	1.66	1.46
9	J	302	TRP	CB-CG	-9.02	1.34	1.50
20	X	355	TYR	CE1-CZ	8.81	1.50	1.38
9	J	337	TRP	CB-CG	-8.40	1.35	1.50
14	O	346	TRP	CB-CG	-7.91	1.36	1.50
6	F	570	TRP	CB-CG	-7.05	1.37	1.50
13	N	299	TRP	CE3-CZ3	-6.79	1.26	1.38
9	J	229	LYS	CB-CG	-6.55	1.34	1.52
3	P	402	TRP	CB-CG	-6.41	1.38	1.50
10	K	302	TRP	CB-CG	-6.38	1.38	1.50
3	C	402	TRP	CB-CG	-6.27	1.39	1.50
20	X	386	MET	N-CA	6.22	1.58	1.46
6	H	570	TRP	CB-CG	-6.12	1.39	1.50
14	O	507	TRP	CB-CG	-5.84	1.39	1.50
10	K	25	TRP	CB-CG	-5.74	1.40	1.50
14	O	592	TRP	CB-CG	-5.50	1.40	1.50
6	F	571	CYS	CB-SG	-5.33	1.73	1.81
20	X	355	TYR	CB-CG	5.26	1.59	1.51
6	H	544	TRP	CB-CG	-5.19	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	13	TRP	CB-CG	-5.08	1.41	1.50
14	O	29	TRP	CB-CG	-5.06	1.41	1.50
14	O	410	TRP	CB-CG	-5.03	1.41	1.50

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	R	431	PRO	O-C-N	-52.04	39.44	122.70
15	R	310	GLN	O-C-N	-29.51	73.03	123.20
15	R	240	ARG	NE-CZ-NH2	-25.22	107.69	120.30
15	R	307	ARG	NE-CZ-NH2	-25.20	107.70	120.30
15	R	313	ARG	NE-CZ-NH2	-25.18	107.71	120.30
15	R	221	ARG	NE-CZ-NH2	-25.17	107.71	120.30
15	R	313	ARG	NE-CZ-NH1	-25.17	107.71	120.30
15	R	468	ARG	NE-CZ-NH1	-25.15	107.73	120.30
15	R	291	ARG	NE-CZ-NH1	-25.14	107.73	120.30
15	R	308	ARG	NE-CZ-NH2	-25.14	107.73	120.30
15	R	296	ARG	NE-CZ-NH1	-25.14	107.73	120.30
15	R	308	ARG	NE-CZ-NH1	-25.13	107.73	120.30
15	R	291	ARG	NE-CZ-NH2	-25.11	107.75	120.30
15	R	380	ARG	NE-CZ-NH2	-25.10	107.75	120.30
15	R	383	ARG	NE-CZ-NH1	-25.10	107.75	120.30
15	R	468	ARG	NE-CZ-NH2	-25.09	107.76	120.30
15	R	296	ARG	NE-CZ-NH2	-25.08	107.76	120.30
15	R	383	ARG	NE-CZ-NH2	-25.06	107.77	120.30
15	R	380	ARG	NE-CZ-NH1	-25.05	107.77	120.30
15	R	307	ARG	NE-CZ-NH1	-25.03	107.78	120.30
15	R	221	ARG	NE-CZ-NH1	-25.02	107.79	120.30
15	R	240	ARG	NE-CZ-NH1	-24.95	107.82	120.30
15	R	434	THR	N-CA-CB	24.09	156.07	110.30
15	R	313	ARG	NH1-CZ-NH2	22.89	144.57	119.40
15	R	308	ARG	NH1-CZ-NH2	22.85	144.54	119.40
15	R	291	ARG	NH1-CZ-NH2	22.84	144.53	119.40
15	R	468	ARG	NH1-CZ-NH2	22.83	144.52	119.40
15	R	307	ARG	NH1-CZ-NH2	22.83	144.51	119.40
15	R	296	ARG	NH1-CZ-NH2	22.82	144.51	119.40
15	R	221	ARG	NH1-CZ-NH2	22.82	144.50	119.40
15	R	240	ARG	NH1-CZ-NH2	22.81	144.49	119.40
15	R	380	ARG	NH1-CZ-NH2	22.80	144.48	119.40
15	R	383	ARG	NH1-CZ-NH2	22.80	144.48	119.40
1	A	1540	ARG	NE-CZ-NH1	16.31	128.45	120.30
15	R	227	VAL	CB-CA-C	-15.17	82.58	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	R	430	TYR	C-N-CD	-14.70	88.26	120.60
15	R	316	VAL	CB-CA-C	-14.44	83.96	111.40
15	R	436	VAL	N-CA-CB	14.12	142.56	111.50
15	R	316	VAL	N-CA-CB	13.87	142.01	111.50
15	R	436	VAL	CB-CA-C	-13.79	85.19	111.40
15	R	227	VAL	N-CA-CB	13.59	141.40	111.50
10	K	229	LYS	CA-CB-CG	-13.30	84.15	113.40
15	R	434	THR	CB-CA-C	-12.29	78.42	111.60
15	R	432	SER	N-CA-CB	11.28	127.42	110.50
15	R	226	SER	N-CA-CB	11.19	127.28	110.50
20	X	379	LYS	CD-CE-NZ	10.60	136.08	111.70
13	N	489	PRO	N-CA-CB	10.41	115.79	103.30
13	N	425	ARG	NE-CZ-NH1	9.80	125.20	120.30
15	R	317	CYS	N-CA-CB	9.06	126.90	110.60
20	Y	379	LYS	CD-CE-NZ	8.99	132.39	111.70
10	K	229	LYS	CB-CG-CD	-8.37	89.84	111.60
15	R	431	PRO	N-CD-CG	-7.98	91.23	103.20
20	Y	59	LEU	CA-CB-CG	7.60	132.78	115.30
15	R	226	SER	CB-CA-C	-7.57	95.71	110.10
15	R	432	SER	CB-CA-C	-7.48	95.89	110.10
13	N	63	ARG	N-CA-C	7.46	131.15	111.00
15	R	392	PRO	CA-N-CD	-7.46	101.06	111.50
9	J	61	ARG	NE-CZ-NH1	7.44	124.02	120.30
15	R	431	PRO	CA-N-CD	-7.34	101.22	111.50
20	Y	54	ARG	NE-CZ-NH1	7.31	123.95	120.30
3	C	26	PHE	CB-CG-CD1	7.28	125.89	120.80
15	R	301	PRO	N-CD-CG	-7.26	92.32	103.20
11	L	132	THR	CB-CA-C	-7.24	92.04	111.60
15	R	302	PRO	CA-N-CD	-7.21	101.41	111.50
10	K	510	ARG	NE-CZ-NH1	7.15	123.88	120.30
6	F	768	PRO	N-CA-CB	7.11	111.83	103.30
1	A	665	MET	CG-SD-CE	7.09	111.55	100.20
3	C	26	PHE	CB-CG-CD2	-7.09	115.84	120.80
1	A	1540	ARG	NE-CZ-NH2	-7.04	116.78	120.30
20	X	110	LEU	CA-CB-CG	7.01	131.41	115.30
15	R	317	CYS	CB-CA-C	-6.97	96.45	110.40
15	R	435	GLN	N-CA-CB	6.84	122.91	110.60
20	X	366	ILE	CB-CA-C	-6.82	97.97	111.60
1	A	292	PRO	N-CA-CB	6.78	111.44	103.30
20	Y	366	ILE	CB-CA-C	-6.78	98.03	111.60
16	S	433	PRO	N-CA-CB	6.78	111.44	103.30
16	S	435	PRO	N-CA-CB	6.68	111.32	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	N	63	ARG	C-N-CA	6.65	136.27	122.30
15	R	392	PRO	N-CD-CG	-6.59	93.31	103.20
9	J	61	ARG	NE-CZ-NH2	-6.58	117.01	120.30
3	P	344	ARG	NE-CZ-NH2	-6.56	117.02	120.30
13	N	477	PRO	N-CA-CB	6.54	111.15	103.30
15	R	314	GLN	CB-CA-C	-6.53	97.35	110.40
15	R	302	PRO	N-CA-CB	6.52	111.12	103.30
18	U	16	PRO	N-CA-CB	6.47	111.06	103.30
9	J	294	LEU	CB-CG-CD2	6.44	121.95	111.00
1	A	1019	MET	CG-SD-CE	6.44	110.50	100.20
3	P	344	ARG	NE-CZ-NH1	6.42	123.51	120.30
3	C	516	LEU	CA-CB-CG	6.37	129.96	115.30
3	C	423	ARG	NE-CZ-NH1	6.35	123.48	120.30
3	C	424	ARG	NE-CZ-NH1	6.34	123.47	120.30
15	R	431	PRO	N-CA-CB	6.34	110.91	103.30
15	R	314	GLN	N-CA-CB	6.30	121.95	110.60
1	A	1084	ARG	NE-CZ-NH2	-6.30	117.15	120.30
8	I	223	VAL	CB-CA-C	-6.18	99.66	111.40
18	U	9	PRO	N-CA-CB	6.18	110.71	103.30
6	H	50	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	1203	MET	CG-SD-CE	-6.15	90.36	100.20
1	A	1927	PRO	N-CA-CB	6.12	110.64	103.30
15	R	302	PRO	N-CD-CG	-6.11	94.03	103.20
4	D	23	PRO	N-CA-CB	6.11	110.63	103.30
14	O	165	ASP	CB-CG-OD1	-6.11	112.80	118.30
1	A	1074	CYS	CA-CB-SG	-6.08	103.06	114.00
15	R	301	PRO	CA-N-CD	-6.07	103.00	111.50
15	R	313	ARG	CB-CA-C	-6.07	98.26	110.40
6	H	467	ARG	NE-CZ-NH1	6.05	123.33	120.30
15	R	301	PRO	N-CA-CB	6.04	110.55	103.30
15	R	45	GLY	N-CA-C	-6.03	98.03	113.10
2	B	40	PRO	N-CA-CB	6.02	110.53	103.30
6	F	625	ARG	NE-CZ-NH1	6.02	123.31	120.30
6	H	494	HIS	N-CA-CB	5.99	121.37	110.60
6	F	467	ARG	NE-CZ-NH1	5.97	123.29	120.30
6	F	625	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	882	LEU	CA-CB-CG	5.94	128.96	115.30
9	J	63	ARG	NE-CZ-NH1	5.93	123.26	120.30
15	R	313	ARG	N-CA-CB	5.91	121.23	110.60
14	O	165	ASP	CB-CG-OD2	5.86	123.58	118.30
16	S	324	PRO	N-CA-CB	5.85	110.32	103.30
15	R	435	GLN	CB-CA-C	-5.82	98.76	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	N	496	ARG	N-CA-C	5.79	126.63	111.00
15	R	52	ARG	CG-CD-NE	-5.79	99.65	111.80
13	N	16	PRO	N-CA-CB	5.78	110.24	103.30
15	R	225	LEU	N-CA-CB	5.76	121.92	110.40
3	C	358	LEU	CA-CB-CG	5.75	128.53	115.30
15	R	433	LEU	N-CA-CB	5.75	121.89	110.40
15	R	392	PRO	N-CA-CB	5.72	110.16	103.30
14	O	117	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	A	1255	VAL	CB-CA-C	-5.61	100.74	111.40
7	G	8	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	1267	ARG	NE-CZ-NH2	-5.59	117.51	120.30
13	N	180	PHE	CB-CG-CD1	5.58	124.71	120.80
1	A	1254	VAL	CB-CA-C	-5.57	100.82	111.40
15	R	312	HIS	N-CA-CB	5.56	120.61	110.60
1	A	1076	ARG	NE-CZ-NH2	-5.56	117.52	120.30
13	N	125	TYR	C-N-CA	5.55	135.58	121.70
13	N	395	ASP	N-CA-C	5.55	125.98	111.00
3	C	307	LEU	CA-CB-CG	5.52	127.99	115.30
13	N	482	PRO	N-CA-CB	5.48	109.88	103.30
13	N	219	PRO	N-CA-CB	5.47	109.86	103.30
9	J	329	LEU	CA-CB-CG	5.47	127.87	115.30
13	N	197	PRO	N-CA-CB	5.46	109.86	103.30
3	P	172	LEU	CA-CB-CG	5.46	127.85	115.30
13	N	509	TYR	N-CA-C	5.45	125.71	111.00
9	J	146	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	1556	LEU	CA-CB-CG	5.42	127.76	115.30
6	F	50	ARG	NE-CZ-NH2	-5.40	117.60	120.30
9	J	258	MET	CG-SD-CE	-5.40	91.57	100.20
6	H	507	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	1526	VAL	CB-CA-C	-5.37	101.20	111.40
12	M	19	TRP	CA-CB-CG	5.35	123.87	113.70
18	U	17	PRO	N-CA-CB	5.35	109.72	103.30
20	X	359	LEU	CB-CG-CD1	5.35	120.10	111.00
10	K	274	THR	CB-CA-C	-5.35	97.16	111.60
1	A	651	PRO	N-CA-CB	5.32	109.68	103.30
3	C	389	ARG	NE-CZ-NH2	-5.29	117.65	120.30
8	I	26	LEU	CA-CB-CG	5.29	127.47	115.30
6	F	130	ARG	NE-CZ-NH1	5.28	122.94	120.30
6	F	481	CYS	CA-CB-SG	-5.26	104.53	114.00
11	L	184	ARG	NE-CZ-NH1	5.25	122.93	120.30
13	N	340	ARG	NE-CZ-NH1	5.24	122.92	120.30
15	R	312	HIS	CB-CA-C	-5.23	99.95	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	ARG	NE-CZ-NH1	5.21	122.91	120.30
15	R	225	LEU	CB-CA-C	-5.20	100.32	110.20
15	R	421	SER	N-CA-CB	-5.20	102.70	110.50
1	A	1243	LEU	CA-CB-CG	5.19	127.23	115.30
15	R	433	LEU	CB-CA-C	-5.17	100.37	110.20
14	O	502	GLN	CB-CA-C	-5.17	100.05	110.40
20	X	385	ASN	N-CA-C	5.17	124.97	111.00
20	X	355	TYR	CA-CB-CG	5.17	123.22	113.40
13	N	425	ARG	NE-CZ-NH2	-5.16	117.72	120.30
11	L	42	VAL	CB-CA-C	-5.14	101.63	111.40
1	A	1540	ARG	CD-NE-CZ	5.14	130.79	123.60
11	L	132	THR	N-CA-CB	5.13	120.05	110.30
11	L	170	PRO	N-CA-CB	5.12	109.44	103.30
14	O	329	ARG	NE-CZ-NH1	5.08	122.84	120.30
10	K	320	ARG	CB-CA-C	5.08	120.56	110.40
15	R	315	GLU	N-CA-CB	5.08	119.74	110.60
13	N	285	PHE	N-CA-CB	5.05	119.69	110.60
8	I	659	ARG	N-CA-C	5.04	124.61	111.00
3	C	42	LEU	CB-CG-CD2	5.04	119.57	111.00
13	N	63	ARG	CA-C-N	5.04	126.27	116.20
1	A	1076	ARG	NE-CZ-NH1	5.02	122.81	120.30
9	J	362	GLN	CB-CA-C	-5.01	100.37	110.40
9	J	376	LEU	CB-CA-C	-5.00	100.69	110.20

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	MET	Peptide
1	A	124	GLN	Peptide
1	A	1282	GLY	Peptide
1	A	14	ALA	Peptide
1	A	1652	MET	Peptide
1	A	83	ILE	Peptide
1	A	840	GLU	Peptide
1	A	859	PRO	Peptide
1	A	86	ASP	Peptide
8	I	658	GLY	Peptide
8	I	727	PHE	Peptide
9	J	220	ILE	Peptide
13	N	147	GLN	Peptide
13	N	162	PHE	Peptide

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Mol	Chain	Res	Type	Group
13	N	164	SER	Peptide
13	N	201	GLY	Peptide
13	N	280	GLU	Peptide
13	N	281	TYR	Peptide
13	N	282	GLU	Peptide
13	N	321	LEU	Peptide
13	N	351	PHE	Peptide
13	N	352	PRO	Peptide
13	N	353	ASP	Peptide
13	N	367	ARG	Peptide
13	N	387	LEU	Peptide
13	N	394	CYS	Peptide
13	N	395	ASP	Peptide
13	N	477	PRO	Peptide
13	N	482	PRO	Peptide
13	N	484	PRO	Peptide
13	N	485	VAL	Peptide
13	N	487	ALA	Peptide
13	N	495	LYS	Peptide
13	N	509	TYR	Peptide
13	N	62	LEU	Peptide
13	N	63	ARG	Peptide
13	N	77	GLU	Peptide
13	N	78	VAL	Peptide
15	R	131	SER	Peptide
15	R	310	GLN	Mainchain
15	R	431	PRO	Mainchain,Peptide
15	R	48	PHE	Peptide
17	T	3	ALA	Peptide
20	X	385	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10947	0	10690	367	0
2	B	650	0	600	33	0
3	C	4305	0	4273	121	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	4042	0	3998	137	0
4	D	437	0	396	14	0
5	E	450	0	435	12	0
6	F	3923	0	3813	95	0
6	H	3853	0	3788	95	0
7	G	214	0	222	2	0
8	I	5709	0	5597	124	0
9	J	4047	0	3956	138	0
10	K	3988	0	3917	126	0
11	L	1435	0	1382	69	0
12	M	493	0	469	28	0
13	N	4831	0	4527	292	0
14	O	5396	0	5425	160	0
15	R	3003	0	2951	432	0
16	S	648	0	543	31	0
17	T	109	0	107	9	0
18	U	120	0	80	1	0
19	W	213	0	220	8	0
20	X	3770	0	3829	254	0
20	Y	3865	0	3925	168	0
21	B	3	0	0	0	0
21	S	2	0	0	0	0
All	All	66453	0	65143	2494	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (2494) 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)
15:R:404:ASN:CB	15:R:449:LEU:HD21	1.22	1.60
15:R:404:ASN:HB2	15:R:449:LEU:CD2	1.35	1.53
15:R:292:MET:CE	15:R:309:LEU:HD21	1.42	1.47
20:X:358:ALA:HB3	20:X:382:ALA:CB	1.43	1.46
20:X:355:TYR:CD2	20:X:386:MET:N	1.83	1.46
15:R:189:TYR:HD1	15:R:316:VAL:N	1.00	1.44
13:N:180:PHE:CD1	13:N:299:TRP:CZ3	2.09	1.41
20:X:355:TYR:CD1	20:X:382:ALA:O	1.74	1.38
15:R:252:PHE:CE1	15:R:268:GLU:HG3	1.63	1.32
20:X:355:TYR:HA	20:X:382:ALA:O	1.30	1.30
15:R:223:CYS:SG	15:R:256:TRP:CE2	2.25	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:267:LEU:HB3	15:R:296:ARG:NH1	1.45	1.29
15:R:317:CYS:CB	15:R:331:GLY:O	1.79	1.28
13:N:180:PHE:CE1	13:N:299:TRP:CZ3	2.20	1.28
20:X:355:TYR:CA	20:X:382:ALA:O	1.83	1.27
11:L:40:PHE:HZ	15:R:176:PHE:CZ	1.51	1.27
11:L:40:PHE:CZ	15:R:176:PHE:CZ	2.22	1.26
15:R:310:GLN:HB2	15:R:340:TRP:CZ2	1.71	1.25
11:L:40:PHE:CZ	15:R:176:PHE:HZ	1.55	1.25
20:X:355:TYR:CB	20:X:382:ALA:O	1.85	1.24
15:R:394:GLN:NE2	15:R:432:SER:HB2	1.49	1.24
20:X:355:TYR:CD2	20:X:386:MET:CA	2.20	1.23
15:R:178:VAL:O	16:S:327:SER:O	1.57	1.22
15:R:189:TYR:CD1	15:R:316:VAL:N	1.79	1.22
13:N:180:PHE:CD1	13:N:299:TRP:CH2	2.28	1.22
20:X:355:TYR:CG	20:X:382:ALA:O	1.92	1.21
15:R:313:ARG:CB	15:R:333:ASN:H	1.53	1.21
15:R:316:VAL:HG22	15:R:317:CYS:N	1.34	1.21
15:R:290:ASP:O	15:R:291:ARG:HG2	1.05	1.21
20:X:355:TYR:HD1	20:X:382:ALA:C	1.44	1.20
15:R:252:PHE:HE1	15:R:268:GLU:CG	1.52	1.20
15:R:227:VAL:CG1	15:R:228:GLU:N	2.00	1.20
15:R:291:ARG:CD	15:R:312:HIS:ND1	2.04	1.20
15:R:290:ASP:O	15:R:291:ARG:CG	1.89	1.20
15:R:230:ASP:O	15:R:231:SER:O	1.57	1.19
20:Y:305:ILE:HG22	20:Y:340:GLU:OE1	1.39	1.18
20:X:350:PHE:CD1	20:X:382:ALA:N	2.11	1.18
15:R:227:VAL:O	15:R:230:ASP:OD1	1.61	1.18
13:N:78:VAL:O	13:N:81:ASN:N	1.77	1.17
20:X:355:TYR:CD2	20:X:387:GLY:N	2.12	1.16
15:R:404:ASN:HB3	15:R:449:LEU:HD21	1.20	1.15
15:R:327:LEU:HD23	15:R:341:ASN:HA	1.19	1.15
20:X:355:TYR:CE2	20:X:385:ASN:C	2.09	1.15
20:X:355:TYR:CG	20:X:386:MET:N	2.16	1.13
20:X:350:PHE:CE1	20:X:378:LEU:O	2.02	1.13
15:R:189:TYR:CD2	15:R:315:GLU:OE1	2.03	1.12
15:R:310:GLN:CB	15:R:340:TRP:HZ2	1.62	1.12
15:R:291:ARG:NE	15:R:312:HIS:ND1	1.97	1.11
15:R:292:MET:SD	15:R:309:LEU:CD2	1.03	1.11
20:X:355:TYR:HB2	20:X:386:MET:CB	1.80	1.11
20:X:355:TYR:HB2	20:X:386:MET:HB3	1.23	1.10
13:N:91:PHE:O	13:N:93:ASN:N	1.84	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:312:HIS:O	15:R:334:ASP:HB3	1.49	1.10
20:X:358:ALA:HB3	20:X:382:ALA:HB2	1.34	1.09
15:R:301:PRO:CD	15:R:301:PRO:N	2.14	1.09
20:X:358:ALA:HB3	20:X:382:ALA:HB3	1.12	1.09
15:R:313:ARG:HD3	15:R:332:GLY:HA2	1.30	1.09
15:R:316:VAL:CG2	15:R:317:CYS:H	1.66	1.08
15:R:223:CYS:SG	15:R:256:TRP:CZ2	2.42	1.08
20:X:347:CYS:HA	20:X:378:LEU:HD11	1.35	1.08
15:R:237:TRP:CZ3	15:R:244:VAL:CG2	2.36	1.08
15:R:225:LEU:CD1	15:R:230:ASP:O	2.01	1.08
20:X:355:TYR:HB3	20:X:383:LEU:HA	1.31	1.08
15:R:291:ARG:NE	15:R:312:HIS:CE1	2.23	1.07
13:N:180:PHE:CD1	13:N:299:TRP:HZ3	1.55	1.07
15:R:292:MET:SD	15:R:309:LEU:HD21	0.79	1.07
20:X:355:TYR:HD2	20:X:386:MET:C	1.59	1.06
15:R:302:PRO:N	15:R:302:PRO:CD	2.16	1.06
20:Y:42:ARG:HA	20:Y:82:TYR:CE2	1.91	1.06
20:X:350:PHE:CD1	20:X:381:ALA:C	2.29	1.05
15:R:429:LYS:O	15:R:433:LEU:O	1.75	1.05
3:C:301:ASP:OD1	3:C:335:CYS:SG	2.14	1.05
20:X:355:TYR:HD2	20:X:386:MET:CA	1.62	1.04
15:R:316:VAL:CG2	15:R:317:CYS:N	2.11	1.04
15:R:317:CYS:HB2	15:R:331:GLY:O	0.87	1.04
15:R:178:VAL:CG1	15:R:466:THR:HG23	1.87	1.04
15:R:227:VAL:HG12	15:R:228:GLU:N	1.38	1.04
15:R:404:ASN:HB2	15:R:449:LEU:HD23	1.40	1.03
20:X:358:ALA:CB	20:X:382:ALA:CB	2.36	1.03
15:R:392:PRO:N	15:R:392:PRO:CD	2.19	1.03
20:X:350:PHE:CE1	20:X:382:ALA:N	2.26	1.03
15:R:310:GLN:CG	15:R:340:TRP:HZ2	1.72	1.03
20:X:400:ILE:HD13	20:X:413:LEU:HD13	1.40	1.03
15:R:310:GLN:CB	15:R:340:TRP:CZ2	2.39	1.01
11:L:40:PHE:CE1	15:R:176:PHE:CE1	2.48	1.01
15:R:178:VAL:HG13	15:R:466:THR:HG23	1.42	1.01
15:R:292:MET:SD	15:R:309:LEU:CG	2.49	1.01
15:R:349:GLN:HB3	15:R:351:TYR:CE1	1.96	1.01
15:R:404:ASN:CB	15:R:449:LEU:CD2	2.09	1.00
20:X:355:TYR:CD1	20:X:382:ALA:C	2.28	1.00
20:X:355:TYR:CD2	20:X:385:ASN:C	2.26	1.00
13:N:120:SER:O	13:N:124:PRO:HD2	1.61	1.00
15:R:366:HIS:CE1	15:R:409:LYS:O	2.14	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:305:ILE:CG2	20:Y:340:GLU:OE1	2.10	1.00
20:X:343:VAL:O	20:X:378:LEU:HD21	1.63	0.99
20:X:347:CYS:CA	20:X:378:LEU:HD11	1.93	0.99
15:R:434:THR:OG1	15:R:435:GLN:N	1.67	0.98
15:R:252:PHE:CE1	15:R:268:GLU:CG	2.34	0.98
15:R:292:MET:CE	15:R:309:LEU:CD2	2.18	0.98
20:Y:373:VAL:HG11	20:Y:403:ALA:HB2	1.46	0.98
20:X:355:TYR:HD2	20:X:387:GLY:N	1.56	0.98
15:R:338:LEU:HD23	15:R:340:TRP:CZ2	1.97	0.98
15:R:431:PRO:N	15:R:431:PRO:CD	2.23	0.98
14:O:222:LEU:O	14:O:226:ASP:O	1.81	0.98
15:R:310:GLN:CG	15:R:340:TRP:CZ2	2.41	0.97
15:R:313:ARG:HB2	15:R:333:ASN:CB	1.94	0.97
15:R:313:ARG:CB	15:R:333:ASN:N	2.25	0.97
13:N:343:GLU:O	13:N:347:ILE:N	1.97	0.97
15:R:189:TYR:CE2	15:R:315:GLU:OE1	2.14	0.97
20:X:363:ALA:HB2	20:X:379:LYS:NZ	1.80	0.96
15:R:327:LEU:HD13	15:R:387:THR:HG21	1.47	0.96
20:Y:42:ARG:HA	20:Y:82:TYR:HE2	1.22	0.96
20:X:363:ALA:HB2	20:X:379:LYS:HZ2	1.27	0.96
6:H:537:GLU:OE2	6:H:568:GLU:OE1	1.82	0.96
15:R:252:PHE:CD1	15:R:268:GLU:HG3	2.01	0.95
20:X:350:PHE:CZ	20:X:381:ALA:HB3	2.00	0.95
20:X:359:LEU:HD12	20:X:383:LEU:HD11	1.49	0.95
15:R:237:TRP:CE3	15:R:244:VAL:HG22	2.02	0.95
14:O:219:GLN:HE22	14:O:231:LEU:HD13	1.30	0.94
15:R:313:ARG:HB2	15:R:333:ASN:H	1.29	0.94
15:R:229:GLY:O	15:R:249:HIS:HB3	1.67	0.94
15:R:313:ARG:CZ	15:R:317:CYS:SG	2.56	0.94
13:N:180:PHE:HD1	13:N:299:TRP:HZ3	1.09	0.94
11:L:40:PHE:HE1	15:R:176:PHE:HE1	1.12	0.93
15:R:227:VAL:HG12	15:R:228:GLU:CA	1.98	0.93
15:R:382:ILE:HD12	15:R:396:ILE:HD11	1.51	0.93
15:R:292:MET:SD	15:R:307:ARG:NH2	2.41	0.93
8:I:349:ILE:HD11	14:O:407:LEU:HD13	1.48	0.93
15:R:327:LEU:CD2	15:R:341:ASN:HA	1.99	0.92
20:Y:491:LYS:O	20:Y:494:ASP:OD1	1.87	0.92
15:R:237:TRP:CZ3	15:R:244:VAL:HG23	2.02	0.92
15:R:178:VAL:HG13	15:R:466:THR:CG2	2.00	0.92
11:L:126:ASP:HB2	11:L:132:THR:CA	1.98	0.92
15:R:223:CYS:SG	15:R:256:TRP:NE1	2.43	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:313:ARG:CD	15:R:317:CYS:HB3	1.97	0.91
15:R:313:ARG:HB3	15:R:333:ASN:N	1.84	0.91
11:L:40:PHE:HE1	15:R:176:PHE:CE1	1.85	0.91
9:J:445:GLU:HG2	9:J:446:PRO:HD3	1.49	0.91
15:R:267:LEU:CB	15:R:296:ARG:NH1	2.34	0.91
20:X:491:LYS:O	20:X:494:ASP:OD1	1.87	0.91
20:X:355:TYR:CE2	20:X:387:GLY:N	2.39	0.91
15:R:459:VAL:CG2	15:R:467:LEU:HD11	2.01	0.91
13:N:395:ASP:OD1	13:N:398:THR:N	2.05	0.90
20:X:358:ALA:CB	20:X:382:ALA:HB2	2.01	0.90
15:R:327:LEU:HD13	15:R:387:THR:CG2	2.02	0.90
14:O:291:ASN:O	14:O:336:ASP:HB2	1.70	0.90
20:X:350:PHE:CE2	20:X:381:ALA:HB3	2.06	0.90
13:N:180:PHE:HD1	13:N:299:TRP:CZ3	1.82	0.90
15:R:450:ALA:O	15:R:459:VAL:HG12	1.72	0.90
15:R:313:ARG:HB3	15:R:333:ASN:H	1.34	0.90
20:X:350:PHE:HD1	20:X:382:ALA:N	1.61	0.90
15:R:252:PHE:HE1	15:R:268:GLU:HG2	1.36	0.90
20:Y:452:LEU:CD2	20:Y:457:THR:O	2.20	0.89
10:K:250:CYS:SG	10:K:274:THR:CG2	2.60	0.89
15:R:429:LYS:HB3	15:R:433:LEU:HD23	1.55	0.89
20:X:355:TYR:HA	20:X:382:ALA:C	1.92	0.89
15:R:177:LYS:HE3	15:R:179:LEU:HD21	1.55	0.89
20:X:350:PHE:CZ	20:X:378:LEU:O	2.26	0.88
20:X:452:LEU:CD2	20:X:457:THR:O	2.20	0.88
13:N:511:SER:O	13:N:512:LYS:HG3	1.74	0.88
10:K:214:LYS:O	10:K:216:SER:N	2.07	0.88
15:R:310:GLN:HB2	15:R:340:TRP:CH2	2.08	0.88
13:N:393:THR:O	13:N:395:ASP:HB3	1.73	0.88
20:Y:196:LEU:O	20:Y:200:PRO:HA	1.74	0.88
15:R:429:LYS:CB	15:R:433:LEU:HD23	2.04	0.87
15:R:267:LEU:HB3	15:R:296:ARG:HH12	1.31	0.87
15:R:465:GLU:OE1	16:S:322:ARG:NH1	2.08	0.87
20:X:350:PHE:CE1	20:X:381:ALA:CA	2.57	0.87
15:R:313:ARG:HB2	15:R:333:ASN:HB3	1.55	0.86
15:R:227:VAL:CG1	15:R:229:GLY:H	1.88	0.86
15:R:351:TYR:OH	15:R:390:GLY:CA	2.24	0.86
1:A:1097:THR:HG23	14:O:340:LEU:HB3	1.57	0.86
11:L:40:PHE:CE1	15:R:176:PHE:CZ	2.64	0.85
20:X:355:TYR:CD2	20:X:386:MET:C	2.41	0.85
13:N:120:SER:O	13:N:124:PRO:CD	2.24	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:292:MET:SD	15:R:309:LEU:HD23	1.44	0.85
13:N:60:GLU:O	13:N:63:ARG:CB	2.24	0.85
20:Y:452:LEU:HD22	20:Y:461:ALA:N	1.91	0.85
20:X:452:LEU:HD22	20:X:461:ALA:N	1.90	0.85
15:R:313:ARG:HB2	15:R:333:ASN:N	1.91	0.85
13:N:538:GLU:HG2	13:N:561:LEU:HG	1.58	0.84
9:J:445:GLU:OE1	9:J:475:ILE:HG21	1.76	0.84
20:X:343:VAL:O	20:X:378:LEU:CD2	2.25	0.84
13:N:289:PHE:O	13:N:291:LYS:N	2.11	0.84
8:I:145:LEU:HD13	8:I:267:LEU:HD22	1.57	0.84
15:R:227:VAL:CG1	15:R:228:GLU:H	1.87	0.84
9:J:351:ASP:CG	15:R:393:LEU:CD2	2.45	0.84
6:H:537:GLU:CD	6:H:568:GLU:OE1	2.16	0.84
20:X:407:LEU:HD22	20:X:437:LEU:HD21	1.60	0.84
15:R:313:ARG:HD3	15:R:317:CYS:HB3	1.60	0.83
15:R:382:ILE:HG13	15:R:398:THR:CG2	2.09	0.83
15:R:227:VAL:HG12	15:R:229:GLY:H	1.42	0.83
15:R:437:ALA:O	15:R:438:LYS:HG3	1.79	0.83
13:N:609:LEU:HD21	13:N:662:VAL:HG12	1.58	0.83
9:J:451:LEU:HD12	9:J:467:TYR:CD2	2.13	0.83
20:X:452:LEU:HD23	20:X:457:THR:O	1.78	0.83
20:Y:503:LEU:O	20:Y:506:GLN:NE2	2.12	0.83
20:X:350:PHE:CE1	20:X:381:ALA:C	2.52	0.82
15:R:229:GLY:O	15:R:249:HIS:CD2	2.32	0.82
6:F:130:ARG:HG2	20:Y:506:GLN:NE2	1.93	0.82
20:Y:407:LEU:HD22	20:Y:437:LEU:HD21	1.60	0.82
20:X:359:LEU:HA	20:X:379:LYS:HG3	1.61	0.82
15:R:227:VAL:HG12	15:R:229:GLY:N	1.94	0.82
15:R:437:ALA:O	15:R:438:LYS:CB	2.28	0.82
11:L:126:ASP:HB2	11:L:132:THR:HA	1.59	0.82
15:R:404:ASN:HB2	15:R:449:LEU:HD21	0.83	0.82
15:R:291:ARG:HD3	15:R:312:HIS:ND1	1.95	0.82
9:J:254:THR:HG23	9:J:271:HIS:CD2	2.13	0.82
15:R:225:LEU:HD13	15:R:230:ASP:O	1.79	0.82
6:F:130:ARG:HG2	20:Y:506:GLN:HE21	1.43	0.82
16:S:374:SER:HB3	16:S:387:TYR:HB3	1.61	0.82
13:N:202:GLU:O	13:N:204:ASP:N	2.12	0.82
20:X:347:CYS:N	20:X:378:LEU:HD11	1.95	0.81
15:R:313:ARG:HD3	15:R:332:GLY:CA	2.10	0.81
1:A:1351:GLN:O	11:L:42:VAL:HG21	1.79	0.81
13:N:398:THR:HG21	16:S:426:LYS:CB	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:452:LEU:HD23	20:Y:457:THR:O	1.78	0.81
15:R:313:ARG:CD	15:R:332:GLY:HA2	2.10	0.81
1:A:1235:LEU:CD1	1:A:1272:VAL:HG21	2.10	0.81
11:L:83:TYR:CD2	11:L:115:GLU:HA	2.16	0.81
15:R:444:TYR:HD2	15:R:464:ASP:HB3	1.44	0.81
13:N:180:PHE:CD1	13:N:299:TRP:HH2	1.94	0.80
12:M:17:ASP:HA	12:M:20:ARG:HG2	1.61	0.80
13:N:180:PHE:CE1	13:N:299:TRP:CH2	2.63	0.80
20:Y:366:ILE:HD11	20:Y:379:LYS:HD2	1.63	0.80
20:X:359:LEU:HA	20:X:379:LYS:CG	2.11	0.80
20:X:350:PHE:HD1	20:X:382:ALA:CA	1.94	0.80
13:N:699:TRP:HB3	13:N:705:LEU:HD23	1.63	0.80
15:R:229:GLY:O	15:R:249:HIS:CB	2.30	0.79
15:R:349:GLN:CB	15:R:351:TYR:CE1	2.65	0.79
10:K:432:ILE:HD11	10:K:444:TRP:CD1	2.17	0.79
20:X:355:TYR:CD1	20:X:383:LEU:C	2.56	0.79
20:X:355:TYR:CG	20:X:383:LEU:O	2.35	0.79
6:F:653:LEU:HA	6:F:656:MET:SD	2.21	0.79
20:X:355:TYR:CD2	20:X:383:LEU:O	2.36	0.79
9:J:445:GLU:HG2	9:J:446:PRO:CD	2.11	0.79
20:X:355:TYR:HB3	20:X:383:LEU:CA	2.11	0.78
15:R:437:ALA:O	15:R:438:LYS:CG	2.32	0.78
9:J:351:ASP:CB	15:R:393:LEU:CD2	2.62	0.78
1:A:482:VAL:HG12	1:A:487:THR:O	1.83	0.78
15:R:297:ASP:O	15:R:303:LEU:CD2	2.30	0.78
1:A:1637:LEU:HD13	1:A:1665:GLN:HE21	1.49	0.78
8:I:224:SER:CB	8:I:229:SER:HA	2.13	0.78
20:X:503:LEU:O	20:X:506:GLN:NE2	2.17	0.78
20:X:350:PHE:CZ	20:X:378:LEU:HA	2.18	0.78
15:R:188:PHE:CE1	15:R:359:LYS:HD3	2.17	0.78
20:X:358:ALA:CB	20:X:382:ALA:HB3	2.06	0.78
15:R:351:TYR:OH	15:R:390:GLY:HA2	1.82	0.78
11:L:40:PHE:CE1	15:R:176:PHE:HE1	1.92	0.78
13:N:368:THR:OG1	13:N:369:ASP:HA	1.84	0.78
9:J:439:VAL:HG21	9:J:448:LEU:HD21	1.66	0.78
20:X:349:SER:HB2	20:X:358:ALA:HB2	1.66	0.77
20:Y:366:ILE:HD11	20:Y:379:LYS:CD	2.14	0.77
2:B:8:TRP:CD1	13:N:644:VAL:HG12	2.19	0.77
6:F:812:ILE:CB	15:R:368:HIS:NE2	2.48	0.77
10:K:62:SER:O	10:K:63:ARG:HG3	1.83	0.77
15:R:316:VAL:HG22	15:R:317:CYS:H	0.96	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:336:LYS:HD3	15:R:350:GLN:HE21	1.49	0.77
20:X:347:CYS:HA	20:X:378:LEU:CD1	2.13	0.77
20:X:355:TYR:CG	20:X:383:LEU:C	2.58	0.77
13:N:393:THR:O	13:N:395:ASP:CB	2.33	0.77
20:X:40:HIS:HB3	20:Y:201:LEU:HD11	1.66	0.77
15:R:431:PRO:HB2	15:R:432:SER:O	1.85	0.77
13:N:78:VAL:O	13:N:80:GLN:N	2.18	0.77
10:K:254:THR:HG23	10:K:271:HIS:CD2	2.20	0.77
1:A:1800:ILE:HG22	1:A:1855:ILE:HD11	1.66	0.77
15:R:466:THR:HG22	15:R:468:ARG:HG3	1.67	0.76
20:X:406:ARG:HB2	20:X:409:CYS:SG	2.25	0.76
9:J:285:PHE:HB2	9:J:308:TYR:CE1	2.20	0.76
3:P:233:PHE:CZ	3:P:237:ILE:CD1	2.67	0.76
9:J:219:VAL:HG12	9:J:221:PRO:HD3	1.68	0.76
3:C:251:TYR:HB3	3:C:269:ILE:HD11	1.67	0.76
11:L:126:ASP:N	11:L:132:THR:HG23	1.99	0.76
10:K:185:LEU:HD13	10:K:209:LEU:HD11	1.65	0.76
8:I:34:LEU:HD12	8:I:46:LEU:HD21	1.68	0.76
15:R:237:TRP:CZ3	15:R:244:VAL:HG22	2.15	0.76
6:F:89:GLU:OE1	6:F:130:ARG:NH2	2.18	0.76
9:J:35:GLU:OE2	9:J:63:ARG:NE	2.18	0.76
13:N:395:ASP:HB2	13:N:397:ILE:H	1.49	0.76
3:P:464:ASP:OD2	3:P:469:ALA:HB3	1.86	0.76
3:C:358:LEU:HD21	3:C:368:TRP:CD2	2.21	0.76
20:X:100:TYR:HB2	20:X:142:LEU:HD21	1.68	0.76
15:R:437:ALA:O	15:R:438:LYS:HB2	1.86	0.75
20:X:452:LEU:CD2	20:X:461:ALA:N	2.49	0.75
13:N:670:PHE:CE1	13:N:715:VAL:HB	2.21	0.75
14:O:414:LEU:CD1	14:O:417:LEU:HB2	2.16	0.75
10:K:285:PHE:HB2	10:K:308:TYR:CE1	2.21	0.75
11:L:33:LEU:HG	11:L:42:VAL:HG22	1.69	0.75
20:Y:406:ARG:HB2	20:Y:409:CYS:SG	2.26	0.75
15:R:394:GLN:HE21	15:R:432:SER:HB2	1.46	0.75
15:R:382:ILE:HG13	15:R:398:THR:HG23	1.69	0.75
3:P:358:LEU:O	3:P:362:PRO:HA	1.86	0.75
15:R:297:ASP:O	15:R:303:LEU:HD23	1.85	0.75
13:N:414:MET:SD	13:N:498:SER:N	2.60	0.75
20:Y:349:SER:HB2	20:Y:358:ALA:HB2	1.68	0.75
14:O:581:ILE:HD11	14:O:619:LEU:HB3	1.67	0.75
15:R:182:PRO:HB3	16:S:322:ARG:CB	2.16	0.75
20:Y:294:PHE:CD1	20:Y:311:TYR:CD1	2.74	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:362:GLY:HA3	20:X:379:LYS:HB2	1.69	0.74
13:N:180:PHE:HE1	13:N:299:TRP:CZ3	2.02	0.74
3:P:267:SER:OG	3:P:299:ASN:ND2	2.19	0.74
20:Y:452:LEU:CD2	20:Y:461:ALA:N	2.49	0.74
20:Y:452:LEU:HD21	20:Y:457:THR:O	1.87	0.74
20:Y:196:LEU:O	20:Y:200:PRO:CA	2.35	0.74
15:R:291:ARG:HE	15:R:312:HIS:CE1	2.05	0.74
15:R:233:THR:HG21	15:R:273:ARG:HG3	1.69	0.74
15:R:430:TYR:C	15:R:431:PRO:CD	2.56	0.74
1:A:1086:MET:HE1	1:A:1564:LEU:HD13	1.67	0.74
11:L:126:ASP:HB2	11:L:132:THR:N	2.01	0.74
11:L:45:LEU:O	11:L:155:GLN:OE1	2.04	0.74
20:X:452:LEU:HD21	20:X:457:THR:O	1.87	0.74
1:A:1235:LEU:HD11	1:A:1272:VAL:HG21	1.70	0.74
1:A:801:PRO:O	1:A:804:ASP:OD1	2.06	0.74
6:H:520:ARG:NH2	20:X:101:THR:OG1	2.20	0.73
3:C:493:TYR:CZ	3:C:497:ILE:HD11	2.23	0.73
14:O:539:ASN:HD22	14:O:542:GLU:CB	2.02	0.73
15:R:290:ASP:C	15:R:291:ARG:HG2	2.06	0.73
6:F:533:VAL:O	6:F:568:GLU:OE1	2.04	0.73
1:A:1279:ARG:NH1	1:A:1287:TYR:OH	2.21	0.73
9:J:351:ASP:OD2	15:R:393:LEU:CD2	2.36	0.73
9:J:351:ASP:OD2	15:R:393:LEU:HD22	1.89	0.73
6:H:655:GLU:OE2	6:H:684:LYS:NZ	2.22	0.73
20:X:350:PHE:HE1	20:X:382:ALA:H	1.34	0.73
14:O:32:PRO:O	14:O:35:ILE:HG22	1.87	0.73
13:N:395:ASP:HB2	13:N:397:ILE:N	2.03	0.73
3:P:402:TRP:CH2	3:P:424:ARG:HG2	2.23	0.73
1:A:1274:LEU:HD11	1:A:1321:VAL:HG12	1.71	0.73
8:I:279:ILE:CD1	8:I:337:ILE:HA	2.19	0.73
15:R:292:MET:SD	15:R:309:LEU:HD22	1.23	0.73
20:X:359:LEU:CA	20:X:379:LYS:HG3	2.18	0.73
3:C:96:VAL:HG21	3:P:53:LYS:HD3	1.70	0.73
1:A:1191:LEU:HD11	15:R:62:HIS:CB	2.19	0.73
9:J:351:ASP:CG	15:R:393:LEU:HD23	2.07	0.72
1:A:1784:GLN:HB2	1:A:1786:THR:HG22	1.71	0.72
1:A:1482:LEU:N	17:T:7:LEU:CB	2.52	0.72
15:R:291:ARG:HD2	15:R:312:HIS:ND1	2.02	0.72
15:R:211:LEU:HD11	15:R:222:LEU:HD22	1.70	0.72
16:S:374:SER:HB3	16:S:387:TYR:CB	2.19	0.72
1:A:207:LEU:HD12	1:A:208:PRO:HD3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:125:THR:HA	11:L:126:ASP:HB3	1.72	0.72
9:J:167:PHE:O	9:J:170:LEU:HD23	1.89	0.72
15:R:189:TYR:CD1	15:R:315:GLU:C	2.44	0.72
15:R:310:GLN:HG2	15:R:340:TRP:CZ2	2.25	0.72
13:N:528:LEU:HD11	13:N:641:LEU:HD13	1.72	0.72
15:R:313:ARG:HB2	15:R:333:ASN:CA	2.20	0.71
15:R:298:ILE:HA	15:R:303:LEU:HD22	1.71	0.71
15:R:459:VAL:HG21	15:R:467:LEU:HD11	1.72	0.71
3:P:233:PHE:CZ	3:P:237:ILE:HD12	2.24	0.71
14:O:414:LEU:HD12	14:O:417:LEU:HB2	1.73	0.71
9:J:211:LYS:O	9:J:212:TYR:CD2	2.43	0.71
9:J:215:PRO:HG3	9:J:402:PRO:HG2	1.72	0.71
13:N:676:TRP:O	13:N:713:PHE:HB2	1.89	0.71
15:R:313:ARG:NE	15:R:317:CYS:HB3	2.05	0.71
6:F:152:PHE:HE1	6:F:162:PRO:HG2	1.53	0.71
15:R:292:MET:HE1	15:R:309:LEU:HD21	1.65	0.71
20:Y:373:VAL:HG11	20:Y:403:ALA:CB	2.20	0.71
8:I:56:TRP:CE3	8:I:98:PRO:HB3	2.25	0.71
20:X:350:PHE:CE1	20:X:381:ALA:N	2.59	0.71
13:N:425:ARG:CZ	13:N:507:SER:HB2	2.20	0.71
20:Y:452:LEU:HD22	20:Y:460:LYS:C	2.11	0.71
15:R:229:GLY:O	15:R:249:HIS:CG	2.44	0.71
15:R:327:LEU:CD1	15:R:387:THR:HG21	2.20	0.71
15:R:351:TYR:HH	15:R:390:GLY:CA	2.03	0.71
14:O:539:ASN:HD22	14:O:542:GLU:HB2	1.56	0.71
8:I:307:LEU:HD13	8:I:313:ALA:HB2	1.71	0.71
10:K:210:LYS:O	10:K:212:TYR:N	2.23	0.71
8:I:279:ILE:HD11	8:I:337:ILE:HG23	1.72	0.71
9:J:441:VAL:HG21	9:J:444:TRP:HD1	1.55	0.71
20:X:452:LEU:HD22	20:X:460:LYS:C	2.11	0.71
20:X:359:LEU:HB2	20:X:383:LEU:HD21	1.73	0.70
1:A:1082:VAL:HG22	1:A:1138:HIS:CD2	2.25	0.70
20:Y:462:LYS:HG2	20:Y:485:LEU:HD13	1.73	0.70
14:O:490:LEU:HD13	14:O:511:ASP:HB2	1.73	0.70
3:P:233:PHE:CE1	3:P:237:ILE:HD11	2.26	0.70
3:C:358:LEU:O	3:C:362:PRO:HA	1.92	0.70
15:R:394:GLN:HE22	15:R:432:SER:HB2	1.54	0.70
1:A:1186:THR:HG23	1:A:1215:ALA:HB1	1.73	0.70
20:Y:474:ASP:OD1	20:Y:502:ALA:HA	1.91	0.70
13:N:341:ILE:O	13:N:344:LEU:HB3	1.92	0.70
15:R:484:SER:HB3	15:R:485:VAL:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:394:GLN:NE2	15:R:432:SER:CB	2.44	0.70
15:R:230:ASP:C	15:R:231:SER:O	2.30	0.70
9:J:351:ASP:HB3	15:R:393:LEU:HD21	1.73	0.70
6:F:705:CYS:SG	6:F:706:LYS:N	2.65	0.70
6:F:729:LEU:HD13	6:F:739:VAL:HG22	1.74	0.70
13:N:180:PHE:CG	13:N:299:TRP:HH2	2.09	0.69
3:C:358:LEU:HD13	3:C:367:ALA:HB3	1.74	0.69
13:N:435:VAL:HA	13:N:438:ILE:HD12	1.74	0.69
1:A:1033:ARG:NH1	1:A:1531:GLY:O	2.25	0.69
8:I:144:THR:HG21	8:I:159:GLU:HA	1.74	0.69
1:A:1470:LEU:HA	1:A:1522:SER:OG	1.92	0.69
20:X:359:LEU:HG	20:X:379:LYS:HE2	1.74	0.69
1:A:1191:LEU:HD11	15:R:62:HIS:HB2	1.73	0.69
2:B:39:VAL:CB	2:B:43:ASP:HB2	2.22	0.69
14:O:479:GLU:O	14:O:656:ALA:O	2.10	0.69
13:N:517:ASN:ND2	16:S:411:CYS:SG	2.65	0.69
11:L:78:CYS:SG	11:L:119:TRP:CE3	2.85	0.69
15:R:349:GLN:CB	15:R:351:TYR:HE1	2.06	0.69
11:L:44:GLN:HA	11:L:47:ASP:OD2	1.91	0.69
15:R:424:GLN:HG2	15:R:440:THR:HA	1.74	0.69
20:Y:294:PHE:CD1	20:Y:311:TYR:CE1	2.81	0.69
20:X:474:ASP:OD1	20:X:502:ALA:HA	1.92	0.69
11:L:105:LEU:HD12	11:L:138:GLN:OE1	1.92	0.69
3:C:352:LEU:HD21	3:C:356:ARG:CZ	2.23	0.69
15:R:459:VAL:CG2	15:R:467:LEU:CD1	2.71	0.69
15:R:188:PHE:CE2	15:R:359:LYS:HB2	2.28	0.69
15:R:189:TYR:CG	15:R:315:GLU:OE1	2.46	0.69
8:I:73:TRP:CZ2	8:I:80:LEU:HD22	2.28	0.69
1:A:1640:GLY:N	1:A:1645:GLU:O	2.26	0.69
3:P:252:GLN:O	3:P:255:ILE:HG22	1.93	0.69
15:R:435:GLN:HG3	15:R:436:VAL:N	2.08	0.68
20:X:400:ILE:HG21	20:X:413:LEU:HB2	1.73	0.68
11:L:94:ILE:HD12	11:L:113:LEU:HD11	1.75	0.68
1:A:612:ILE:O	1:A:641:TRP:CZ3	2.46	0.68
15:R:188:PHE:CZ	15:R:359:LYS:CD	2.77	0.68
20:X:434:TYR:HA	20:X:444:LEU:HD22	1.74	0.68
3:P:358:LEU:CD1	3:P:368:TRP:CE2	2.76	0.68
20:X:462:LYS:HG2	20:X:485:LEU:HD13	1.74	0.68
15:R:188:PHE:CZ	15:R:359:LYS:CB	2.77	0.68
15:R:290:ASP:O	15:R:291:ARG:CB	2.40	0.68
14:O:591:TYR:HA	14:O:594:SER:OG	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:596:LEU:HD13	13:N:601:TRP:CE2	2.28	0.68
20:X:359:LEU:HD12	20:X:383:LEU:CD1	2.23	0.68
9:J:254:THR:HG23	9:J:271:HIS:HD2	1.59	0.68
6:H:729:LEU:HD13	6:H:739:VAL:HG22	1.75	0.68
6:F:133:LYS:HA	6:F:136:GLU:OE1	1.94	0.68
15:R:194:ASP:O	15:R:201:LEU:HD12	1.93	0.67
10:K:174:HIS:HA	10:K:211:LYS:NZ	2.09	0.67
13:N:663:GLN:HE21	13:N:695:ARG:HG3	1.60	0.67
1:A:1076:ARG:HE	1:A:1543:HIS:CD2	2.12	0.67
15:R:406:ALA:C	15:R:414:LEU:HD12	2.14	0.67
15:R:201:LEU:CD2	15:R:467:LEU:HD21	2.24	0.67
13:N:519:TYR:CE1	13:N:523:LEU:HD21	2.30	0.67
6:H:73:TYR:CD1	6:H:117:THR:HG22	2.29	0.67
3:C:388:TYR:HB2	3:C:405:LEU:HD13	1.75	0.67
3:P:404:GLY:O	3:P:408:THR:HG22	1.93	0.67
15:R:225:LEU:HD11	15:R:230:ASP:O	1.94	0.67
15:R:382:ILE:CD1	15:R:398:THR:CG2	2.72	0.67
13:N:202:GLU:HB2	13:N:282:GLU:OE2	1.95	0.67
3:P:368:TRP:HB3	3:P:391:ALA:HB2	1.77	0.67
16:S:357:SER:O	16:S:359:HIS:N	2.28	0.67
14:O:467:ALA:HB1	14:O:506:LEU:HD11	1.76	0.67
20:Y:445:THR:O	20:Y:449:THR:HG23	1.95	0.67
16:S:387:TYR:CE1	16:S:407:THR:HG21	2.30	0.67
6:F:571:CYS:SG	6:F:606:LEU:HD12	2.35	0.67
20:X:316:ALA:HB1	20:X:351:TYR:CE1	2.30	0.67
15:R:225:LEU:CD1	15:R:230:ASP:C	2.63	0.67
20:Y:434:TYR:HA	20:Y:444:LEU:HD22	1.76	0.67
13:N:704:VAL:HG23	13:N:705:LEU:HD22	1.77	0.67
20:Y:407:LEU:CD2	20:Y:437:LEU:HD21	2.25	0.67
20:X:201:LEU:CD1	20:Y:40:HIS:HB3	2.25	0.67
15:R:57:TRP:HA	15:R:57:TRP:HE3	1.59	0.67
15:R:153:VAL:O	15:R:157:SER:OG	2.13	0.67
13:N:123:ASP:O	13:N:127:ARG:N	2.28	0.66
20:Y:215:LYS:O	20:Y:219:VAL:HG23	1.95	0.66
6:F:552:LEU:HG	6:F:576:CYS:SG	2.35	0.66
15:R:406:ALA:O	15:R:414:LEU:HD12	1.95	0.66
9:J:451:LEU:HD12	9:J:467:TYR:CE2	2.29	0.66
20:X:229:THR:HG21	20:X:233:LEU:HD12	1.77	0.66
13:N:577:GLU:HG2	13:N:583:ALA:HB2	1.77	0.66
20:X:355:TYR:CD1	20:X:384:ARG:N	2.62	0.66
1:A:1287:TYR:CD1	1:A:1287:TYR:O	2.48	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1481:ASN:HA	17:T:7:LEU:CB	2.25	0.66
6:H:552:LEU:HG	6:H:576:CYS:SG	2.35	0.66
15:R:237:TRP:CE3	15:R:244:VAL:CG2	2.68	0.66
3:C:136:ASP:O	14:O:150:GLN:NE2	2.28	0.66
6:F:73:TYR:CD1	6:F:117:THR:HG22	2.31	0.66
15:R:230:ASP:O	15:R:231:SER:C	2.31	0.66
15:R:380:ARG:NH2	15:R:420:TYR:HD2	1.93	0.66
6:H:571:CYS:SG	6:H:606:LEU:HD12	2.35	0.66
8:I:177:VAL:HG12	8:I:208:LEU:HD13	1.78	0.66
20:X:445:THR:O	20:X:449:THR:HG23	1.96	0.66
3:P:402:TRP:CZ3	3:P:424:ARG:HG2	2.31	0.66
9:J:476:PRO:HG2	3:P:182:LEU:HG	1.76	0.66
20:X:215:LYS:O	20:X:219:VAL:HG23	1.95	0.66
15:R:292:MET:CG	15:R:307:ARG:HH21	2.08	0.66
15:R:57:TRP:CE3	15:R:57:TRP:HA	2.30	0.66
15:R:173:LYS:HG2	15:R:439:LEU:CD2	2.26	0.66
20:Y:226:VAL:HG22	20:Y:236:LEU:HD23	1.77	0.66
15:R:307:ARG:HH21	15:R:309:LEU:HD21	1.59	0.66
2:B:14:TRP:HA	2:B:15:LEU:CG	2.26	0.66
15:R:382:ILE:HD12	15:R:396:ILE:CD1	2.24	0.66
3:C:460:TYR:CE1	3:C:470:LEU:HD11	2.31	0.66
8:I:186:GLU:OE2	8:I:197:ARG:NH1	2.29	0.66
15:R:315:GLU:H	15:R:333:ASN:CB	2.09	0.65
15:R:444:TYR:CD2	15:R:464:ASP:HB3	2.28	0.65
6:H:481:CYS:HB3	6:H:512:LEU:HD13	1.77	0.65
1:A:126:ALA:HA	1:A:152:CYS:O	1.97	0.65
1:A:1405:LEU:HD13	1:A:1467:GLY:CA	2.27	0.65
14:O:75:VAL:HG13	14:O:165:ASP:CB	2.25	0.65
7:G:6:PRO:HB3	9:J:406:HIS:CD2	2.32	0.65
15:R:337:LEU:HD13	15:R:361:ILE:CD1	2.26	0.65
20:X:294:PHE:CE2	20:X:311:TYR:HB2	2.32	0.65
15:R:188:PHE:CZ	15:R:359:LYS:HB3	2.31	0.65
15:R:178:VAL:CG1	15:R:466:THR:CG2	2.62	0.65
13:N:571:ASN:OD1	13:N:592:TYR:CD1	2.48	0.65
20:Y:229:THR:HG21	20:Y:233:LEU:HD12	1.77	0.65
20:X:294:PHE:CD1	20:X:311:TYR:CD1	2.85	0.65
8:I:265:ILE:HD11	8:I:396:PHE:CE2	2.32	0.65
13:N:699:TRP:CZ3	13:N:728:VAL:HG21	2.31	0.65
15:R:420:TYR:CE1	15:R:421:SER:HB3	2.32	0.65
15:R:182:PRO:HB3	16:S:322:ARG:HB3	1.77	0.65
6:F:537:GLU:OE1	6:F:602:TYR:HB3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:HIS:O	1:A:593:ASN:HB3	1.97	0.65
3:P:233:PHE:CZ	3:P:237:ILE:HD11	2.31	0.65
1:A:72:GLU:HG3	1:A:94:TYR:OH	1.97	0.65
20:X:271:VAL:CG1	20:X:304:LEU:HD21	2.27	0.65
11:L:74:VAL:HG21	11:L:137:ILE:HD11	1.77	0.65
20:X:353:LYS:HA	20:X:385:ASN:HB3	1.79	0.65
20:X:363:ALA:N	20:X:379:LYS:HD2	2.12	0.65
15:R:312:HIS:N	15:R:334:ASP:OD2	2.30	0.65
1:A:1191:LEU:HD21	15:R:62:HIS:CG	2.32	0.65
6:F:131:LEU:HD11	6:F:158:ILE:HG23	1.78	0.65
20:Y:271:VAL:CG1	20:Y:304:LEU:HD21	2.26	0.65
20:X:226:VAL:HG22	20:X:236:LEU:HD23	1.78	0.65
15:R:436:VAL:HG12	15:R:437:ALA:N	2.12	0.64
15:R:382:ILE:CG1	15:R:398:THR:CG2	2.74	0.64
14:O:581:ILE:HG22	14:O:610:LEU:HD23	1.78	0.64
1:A:1175:PHE:CZ	1:A:1179:LEU:HD21	2.33	0.64
15:R:225:LEU:HD13	15:R:230:ASP:C	2.17	0.64
15:R:382:ILE:HD11	15:R:398:THR:CG2	2.28	0.64
3:C:148:ASN:HB3	3:C:151:LEU:HG	1.79	0.64
1:A:1380:ASN:HD22	1:A:1383:ILE:HD12	1.61	0.64
15:R:230:ASP:HB3	15:R:250:LYS:CD	2.28	0.64
6:F:537:GLU:CD	6:F:600:TYR:OH	2.35	0.64
15:R:291:ARG:CZ	15:R:312:HIS:CE1	2.81	0.64
15:R:380:ARG:NH2	15:R:420:TYR:CD2	2.66	0.64
8:I:231:VAL:HG21	8:I:557:TYR:CZ	2.33	0.64
8:I:297:THR:O	14:O:58:ARG:NH2	2.30	0.64
13:N:181:LEU:HD22	13:N:299:TRP:CE2	2.33	0.64
11:L:108:ILE:HB	11:L:125:THR:O	1.97	0.64
15:R:187:ASP:HB3	15:R:190:LEU:HG	1.80	0.64
3:C:413:LYS:O	3:C:415:PRO:HD3	1.97	0.64
3:C:327:ASP:O	3:C:333:THR:HG21	1.98	0.64
3:C:259:PHE:HB3	3:C:265:ILE:HD12	1.79	0.64
1:A:1531:GLY:HA3	1:A:1566:PHE:CE1	2.33	0.64
10:K:384:SER:HB2	10:K:415:ASN:HD21	1.63	0.64
15:R:297:ASP:O	15:R:303:LEU:HD22	1.98	0.64
3:C:368:TRP:HB3	3:C:391:ALA:HB2	1.80	0.64
20:X:407:LEU:CD2	20:X:437:LEU:HD21	2.27	0.63
9:J:441:VAL:CG2	9:J:444:TRP:HD1	2.10	0.63
10:K:495:PHE:CZ	10:K:525:MET:HG2	2.33	0.63
15:R:225:LEU:HD13	15:R:230:ASP:CG	2.18	0.63
14:O:658:LEU:HD13	14:O:704:VAL:HG11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:279:ASP:OD1	20:X:310:VAL:HG21	1.98	0.63
13:N:563:ASP:C	13:N:564:MET:N	2.52	0.63
13:N:611:VAL:HG11	13:N:637:TRP:CH2	2.33	0.63
1:A:34:ALA:HB3	14:O:237:GLN:HE22	1.63	0.63
2:B:20:ASP:CB	2:B:30:PHE:HE2	2.11	0.63
13:N:281:TYR:CZ	13:N:357:ALA:HA	2.34	0.63
6:H:537:GLU:OE1	6:H:568:GLU:OE1	2.16	0.63
1:A:620:THR:HG23	1:A:866:ILE:CD1	2.29	0.63
11:L:78:CYS:SG	11:L:119:TRP:HE3	2.22	0.63
1:A:1773:LEU:HD23	1:A:1774:PHE:N	2.12	0.63
1:A:445:LEU:HD21	1:A:478:ASP:HA	1.80	0.63
4:D:54:ILE:HD12	3:P:389:ARG:NH2	2.14	0.63
15:R:280:ASN:HA	15:R:325:HIS:CE1	2.34	0.63
1:A:1312:ASN:O	1:A:1312:ASN:ND2	2.29	0.63
13:N:519:TYR:OH	13:N:541:ASN:HB3	1.98	0.63
6:F:130:ARG:CG	20:Y:506:GLN:HB2	2.29	0.63
2:B:14:TRP:HA	2:B:15:LEU:CB	2.29	0.63
20:X:373:VAL:HG11	20:X:403:ALA:HB2	1.81	0.63
15:R:280:ASN:HD21	15:R:325:HIS:HB3	1.64	0.63
13:N:281:TYR:CE2	13:N:356:PRO:HB2	2.34	0.63
3:C:36:LEU:HD21	3:C:58:LEU:HB2	1.80	0.63
15:R:188:PHE:CZ	15:R:359:LYS:HD3	2.33	0.62
3:P:327:ASP:O	3:P:333:THR:HG21	1.99	0.62
13:N:286:LEU:O	13:N:288:GLU:N	2.32	0.62
8:I:88:LYS:O	8:I:106:VAL:HG22	1.98	0.62
3:P:460:TYR:CE1	3:P:470:LEU:HD11	2.34	0.62
20:Y:532:TYR:CE2	20:Y:548:GLY:HA3	2.35	0.62
1:A:873:VAL:HG21	1:A:951:ILE:CG2	2.29	0.62
11:L:73:THR:HG22	11:L:131:PRO:HB2	1.80	0.62
13:N:418:GLU:OE2	13:N:495:LYS:O	2.18	0.62
15:R:189:TYR:HD1	15:R:316:VAL:CA	2.03	0.62
14:O:219:GLN:NE2	14:O:231:LEU:HD13	2.09	0.62
1:A:592:HIS:O	1:A:593:ASN:CB	2.47	0.62
11:L:86:ASP:HB3	11:L:89:TYR:HB2	1.80	0.62
8:I:209:CYS:SG	8:I:584:HIS:CE1	2.93	0.62
13:N:73:GLU:O	13:N:74:TRP:HB3	1.98	0.62
13:N:386:LEU:O	13:N:388:HIS:N	2.33	0.62
11:L:45:LEU:HD23	11:L:46:ARG:N	2.13	0.62
15:R:337:LEU:CD1	15:R:361:ILE:HD12	2.29	0.62
1:A:436:LEU:HG	1:A:501:THR:HG23	1.81	0.62
8:I:142:LEU:HD13	8:I:264:TYR:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:10:PRO:HG2	14:O:346:TRP:CZ2	2.34	0.62
13:N:249:ARG:HB3	13:N:250:LEU:HD23	1.82	0.62
1:A:617:LEU:HD11	1:A:782:GLY:HA2	1.81	0.62
20:X:355:TYR:HB2	20:X:386:MET:HB2	1.80	0.62
6:H:537:GLU:CD	6:H:600:TYR:OH	2.38	0.62
20:Y:294:PHE:CD1	20:Y:294:PHE:C	2.73	0.62
1:A:1220:MET:CG	1:A:1264:THR:HG21	2.30	0.62
3:P:286:PHE:HB3	3:P:303:PHE:CE2	2.35	0.62
6:H:726:LEU:HD21	6:H:742:LEU:HD22	1.81	0.62
20:X:430:ALA:CB	20:X:451:CYS:SG	2.88	0.62
15:R:484:SER:CB	15:R:485:VAL:HA	2.29	0.62
8:I:289:LYS:O	8:I:293:GLU:N	2.32	0.62
8:I:38:ALA:HB2	8:I:71:LEU:HD11	1.80	0.62
20:Y:316:ALA:HB1	20:Y:351:TYR:CE1	2.34	0.61
13:N:538:GLU:HG2	13:N:561:LEU:CG	2.28	0.61
1:A:1482:LEU:H	17:T:7:LEU:CB	2.13	0.61
5:E:61:TYR:CE1	20:X:360:TYR:CE2	2.89	0.61
6:F:726:LEU:HD21	6:F:742:LEU:HD22	1.81	0.61
6:F:684:LYS:HG2	6:F:687:LYS:HB2	1.82	0.61
20:X:350:PHE:CZ	20:X:378:LEU:C	2.73	0.61
15:R:366:HIS:HE1	15:R:409:LYS:O	1.78	0.61
10:K:250:CYS:SG	10:K:274:THR:HG22	2.40	0.61
9:J:294:LEU:HD12	10:K:54:HIS:CD2	2.35	0.61
3:C:233:PHE:CZ	3:C:237:ILE:HD12	2.35	0.61
6:H:730:LYS:HD3	6:H:740:TYR:HE1	1.65	0.61
9:J:281:ALA:HA	9:J:311:MET:CE	2.30	0.61
15:R:227:VAL:HG13	15:R:228:GLU:H	1.63	0.61
1:A:1191:LEU:HD21	15:R:62:HIS:ND1	2.15	0.61
6:F:146:PRO:HG3	6:F:167:THR:HA	1.82	0.61
1:A:1194:HIS:HB2	15:R:99:LEU:HD13	1.81	0.61
20:X:347:CYS:SG	20:X:378:LEU:HD13	2.41	0.61
20:X:400:ILE:HD13	20:X:413:LEU:CD1	2.25	0.61
13:N:274:GLU:OE2	13:N:278:ARG:NH2	2.32	0.61
15:R:188:PHE:CE1	15:R:359:LYS:CD	2.84	0.61
14:O:233:PRO:HA	14:O:263:ARG:HH21	1.66	0.61
1:A:869:ARG:NH2	1:A:946:THR:OG1	2.33	0.61
15:R:233:THR:OG1	15:R:274:VAL:O	2.07	0.61
15:R:291:ARG:HD2	15:R:312:HIS:HA	1.82	0.61
8:I:309:LEU:HD23	14:O:64:LEU:HD11	1.82	0.61
20:X:94:ARG:HG3	20:Y:334:ILE:O	2.00	0.61
20:X:350:PHE:CZ	20:X:381:ALA:CB	2.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:291:ARG:CD	15:R:312:HIS:CG	2.83	0.61
15:R:225:LEU:HD12	15:R:231:SER:C	2.21	0.60
15:R:382:ILE:HD11	15:R:398:THR:HG21	1.83	0.60
10:K:254:THR:HG23	10:K:271:HIS:HD2	1.66	0.60
14:O:417:LEU:HA	14:O:420:ILE:CG2	2.31	0.60
1:A:1624:VAL:HG22	1:A:1698:TYR:HD2	1.66	0.60
1:A:1054:TYR:O	1:A:1056:GLU:N	2.31	0.60
10:K:292:VAL:HG21	12:M:57:TRP:CB	2.31	0.60
1:A:43:GLN:NE2	3:C:142:GLU:O	2.34	0.60
20:X:350:PHE:CZ	20:X:378:LEU:CA	2.84	0.60
20:X:203:LEU:HD21	20:X:239:TRP:CH2	2.36	0.60
9:J:281:ALA:HA	9:J:311:MET:HE1	1.83	0.60
6:H:689:LEU:HD11	6:H:716:ASN:HD21	1.66	0.60
9:J:465:LEU:HA	9:J:488:ILE:CD1	2.32	0.60
9:J:258:MET:HE1	9:J:271:HIS:CG	2.36	0.60
3:P:267:SER:CB	3:P:299:ASN:HD21	2.14	0.60
15:R:337:LEU:HD13	15:R:361:ILE:HD12	1.82	0.60
6:H:130:ARG:HH12	10:K:473:VAL:HG22	1.66	0.60
1:A:1084:ARG:NH2	1:A:1139:ASN:OD1	2.31	0.60
13:N:281:TYR:CZ	13:N:284:SER:HB3	2.36	0.60
15:R:182:PRO:CB	16:S:322:ARG:CB	2.79	0.60
14:O:662:ARG:HD2	14:O:755:LEU:HD12	1.81	0.60
3:P:475:LYS:O	3:P:479:GLN:NE2	2.35	0.60
15:R:243:LEU:HD13	15:R:298:ILE:CD1	2.31	0.60
13:N:609:LEU:HD22	13:N:639:HIS:CD2	2.37	0.60
15:R:382:ILE:CG1	15:R:398:THR:HG21	2.31	0.60
20:X:94:ARG:CG	20:Y:334:ILE:O	2.49	0.60
1:A:1672:ARG:O	1:A:1701:LEU:HD12	2.00	0.60
15:R:363:TRP:CZ3	15:R:387:THR:OG1	2.54	0.60
1:A:873:VAL:HG21	1:A:951:ILE:HG21	1.84	0.60
1:A:956:ARG:NH1	1:A:1788:GLU:OE1	2.34	0.60
1:A:1621:PRO:HG3	1:A:1653:ALA:HB3	1.82	0.60
9:J:213:ASN:OD1	9:J:214:LYS:N	2.34	0.60
10:K:153:TYR:CE2	10:K:169:LEU:HD22	2.37	0.60
15:R:237:TRP:CH2	15:R:244:VAL:CG2	2.85	0.60
15:R:291:ARG:CZ	15:R:312:HIS:ND1	2.64	0.60
8:I:218:SER:OG	8:I:584:HIS:ND1	2.35	0.60
8:I:17:LYS:NZ	8:I:51:SER:O	2.34	0.60
1:A:629:LEU:HD11	1:A:634:ALA:HB2	1.82	0.60
3:C:414:MET:CE	14:O:300:LEU:HD13	2.30	0.60
13:N:75:PHE:CD1	13:N:79:LEU:HD23	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:521:PHE:CD1	3:C:553:ILE:HG22	2.37	0.60
6:F:115:CYS:SG	6:F:116:PHE:N	2.75	0.60
14:O:354:ARG:CD	14:O:573:LYS:O	2.50	0.60
2:B:41:GLY:O	2:B:45:PRO:HA	2.01	0.60
15:R:230:ASP:HB3	15:R:250:LYS:HD2	1.84	0.59
13:N:77:GLU:O	13:N:78:VAL:HG23	2.02	0.59
3:C:120:TYR:CE2	3:C:124:LEU:HD11	2.37	0.59
9:J:185:LEU:HD13	9:J:206:GLU:OE1	2.02	0.59
13:N:542:VAL:HG11	13:N:558:GLU:CD	2.23	0.59
20:Y:93:TYR:CE2	20:Y:148:VAL:HG11	2.37	0.59
20:Y:339:ALA:O	20:Y:343:VAL:HG23	2.02	0.59
13:N:609:LEU:CD2	13:N:662:VAL:HG12	2.31	0.59
1:A:1800:ILE:HG22	1:A:1855:ILE:CD1	2.32	0.59
20:X:100:TYR:HB2	20:X:142:LEU:CD2	2.30	0.59
1:A:617:LEU:HD11	1:A:782:GLY:CA	2.32	0.59
1:A:1251:VAL:HG12	1:A:1294:TYR:HA	1.83	0.59
15:R:188:PHE:HZ	15:R:359:LYS:HB3	1.67	0.59
15:R:380:ARG:HG2	15:R:400:SER:C	2.22	0.59
15:R:316:VAL:HG22	15:R:317:CYS:CA	2.27	0.59
15:R:317:CYS:HB3	15:R:332:GLY:HA2	1.85	0.59
15:R:349:GLN:HB3	15:R:351:TYR:CZ	2.38	0.59
20:X:407:LEU:HD13	20:X:443:THR:HG21	1.84	0.59
13:N:368:THR:CB	13:N:369:ASP:HA	2.31	0.59
3:P:355:GLN:HA	3:P:358:LEU:HD23	1.84	0.59
6:F:131:LEU:HD11	6:F:158:ILE:CG2	2.32	0.59
13:N:706:ARG:HB2	13:N:716:ILE:HD13	1.84	0.59
1:A:860:TYR:CG	1:A:861:PRO:HD2	2.38	0.59
1:A:1750:LEU:HD23	1:A:1782:VAL:HG22	1.85	0.59
20:X:93:TYR:CE2	20:X:148:VAL:HG11	2.36	0.59
20:X:339:ALA:O	20:X:343:VAL:HG23	2.02	0.59
20:X:350:PHE:CE1	20:X:381:ALA:HB3	2.37	0.59
15:R:211:LEU:HD22	15:R:237:TRP:CZ2	2.38	0.59
9:J:193:LEU:O	9:J:197:GLU:HB2	2.02	0.59
13:N:281:TYR:CE1	13:N:357:ALA:HA	2.37	0.59
11:L:77:LEU:HD12	11:L:78:CYS:N	2.17	0.59
2:B:14:TRP:HA	2:B:15:LEU:HG	1.85	0.59
3:P:385:ILE:HD11	3:P:412:LEU:HD11	1.85	0.59
1:A:811:PRO:HG3	1:A:1809:SER:O	2.03	0.59
14:O:351:GLY:O	14:O:352:GLN:HG3	2.02	0.59
1:A:1475:ARG:HG2	1:A:1476:PHE:CE1	2.38	0.59
20:X:359:LEU:HA	20:X:379:LYS:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:316:ALA:HB1	20:Y:351:TYR:CZ	2.38	0.59
13:N:619:LEU:HG	13:N:637:TRP:CZ2	2.37	0.59
3:C:93:TYR:OH	3:C:101:ARG:NH2	2.36	0.59
13:N:409:VAL:O	13:N:410:ILE:HG13	2.02	0.59
15:R:188:PHE:HE1	15:R:403:CYS:HG	1.51	0.59
6:F:707:PHE:HB2	6:F:729:LEU:HD11	1.85	0.59
14:O:657:ILE:HD11	14:O:704:VAL:HG23	1.83	0.59
14:O:105:LEU:HD11	14:O:151:VAL:CG1	2.33	0.59
3:P:120:TYR:CZ	3:P:124:LEU:HD11	2.38	0.59
6:H:115:CYS:SG	6:H:116:PHE:N	2.75	0.59
20:X:355:TYR:H	20:X:386:MET:HB2	1.68	0.59
20:Y:350:PHE:CZ	20:Y:378:LEU:HD12	2.38	0.59
9:J:35:GLU:OE2	9:J:63:ARG:NH2	2.35	0.59
14:O:635:GLY:O	14:O:637:PRO:HD3	2.03	0.59
13:N:670:PHE:CD1	13:N:715:VAL:HB	2.38	0.59
9:J:406:HIS:HE1	9:J:450:ASN:HD22	1.50	0.59
1:A:773:LEU:HD22	1:A:779:MET:HG3	1.85	0.59
15:R:310:GLN:HB2	15:R:340:TRP:HZ2	1.18	0.58
16:S:374:SER:O	16:S:375:LEU:O	2.20	0.58
9:J:523:ILE:HD11	3:P:420:TYR:CB	2.34	0.58
20:Y:462:LYS:HG2	20:Y:485:LEU:CD1	2.32	0.58
14:O:114:ASP:HA	14:O:117:ASP:OD1	2.03	0.58
14:O:119:PHE:CE1	14:O:136:LEU:HD11	2.37	0.58
1:A:454:CYS:O	1:A:471:VAL:HA	2.03	0.58
11:L:98:VAL:HB	11:L:134:THR:HG21	1.84	0.58
6:F:128:THR:HG21	6:F:130:ARG:NH1	2.18	0.58
3:C:493:TYR:CE2	3:C:497:ILE:HD11	2.38	0.58
1:A:1230:ILE:HG13	15:R:94:LEU:HD22	1.85	0.58
13:N:273:MET:HG2	13:N:277:CYS:SG	2.44	0.58
15:R:349:GLN:HB2	15:R:351:TYR:HE1	1.68	0.58
20:Y:452:LEU:HD21	20:Y:460:LYS:HB2	1.85	0.58
9:J:406:HIS:CE1	9:J:450:ASN:HD22	2.21	0.58
14:O:216:LEU:HD22	14:O:256:LEU:HD12	1.85	0.58
18:U:21:ALA:O	18:U:23:ALA:N	2.35	0.58
11:L:126:ASP:CB	11:L:132:THR:N	2.66	0.58
10:K:271:HIS:O	10:K:274:THR:OG1	2.20	0.58
6:F:696:ILE:HG12	6:F:705:CYS:SG	2.43	0.58
14:O:529:ASP:O	14:O:532:VAL:HG12	2.04	0.58
15:R:315:GLU:H	15:R:333:ASN:HB2	1.68	0.58
15:R:437:ALA:C	15:R:438:LYS:HG3	2.23	0.58
1:A:1086:MET:CE	1:A:1564:LEU:HD13	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:271:VAL:HG13	20:X:304:LEU:HD21	1.84	0.58
8:I:308:LEU:HD21	8:I:445:ILE:HG23	1.85	0.58
3:C:259:PHE:HB3	3:C:265:ILE:CD1	2.34	0.58
3:P:228:TRP:O	3:P:231:GLU:N	2.36	0.58
1:A:939:PHE:HZ	1:A:944:LEU:HD13	1.69	0.58
20:X:316:ALA:HB1	20:X:351:TYR:CZ	2.38	0.58
13:N:556:PHE:CZ	13:N:600:PHE:HA	2.38	0.58
13:N:560:MET:HA	13:N:560:MET:CE	2.34	0.58
6:H:685:SER:O	6:H:689:LEU:HD12	2.04	0.58
1:A:1546:THR:OG1	1:A:1547:GLY:N	2.35	0.58
1:A:1477:ALA:HB1	1:A:1574:LEU:CD1	2.33	0.58
3:P:39:ILE:HD12	3:P:201:LEU:HB2	1.86	0.58
15:R:202:SER:HA	15:R:211:LEU:HD23	1.86	0.58
3:P:392:ILE:CD1	3:P:402:TRP:CH2	2.86	0.58
3:C:93:TYR:CE1	3:P:53:LYS:HD2	2.39	0.58
2:B:15:LEU:HD22	13:N:634:THR:O	2.03	0.58
20:X:437:LEU:HB2	20:X:444:LEU:HD21	1.85	0.58
20:Y:219:VAL:HG22	20:Y:240:ILE:HG22	1.85	0.58
20:Y:271:VAL:HG13	20:Y:304:LEU:HD21	1.83	0.58
8:I:67:GLU:O	8:I:85:ALA:N	2.32	0.58
15:R:419:GLY:HA2	15:R:445:ARG:HB3	1.84	0.58
13:N:233:CYS:O	13:N:235:GLN:N	2.37	0.58
15:R:339:VAL:HG11	15:R:387:THR:HG23	1.86	0.58
15:R:433:LEU:HG	15:R:434:THR:N	2.17	0.58
11:L:89:TYR:O	11:L:151:THR:HG22	2.04	0.58
13:N:273:MET:CG	13:N:277:CYS:SG	2.91	0.58
5:E:89:LEU:O	6:H:592:ARG:NH2	2.37	0.58
1:A:1293:SER:HB3	1:A:1600:ARG:O	2.04	0.58
9:J:481:THR:O	9:J:485:ILE:HG12	2.04	0.58
1:A:1364:CYS:N	1:A:1365:PRO:HD2	2.19	0.58
13:N:177:TYR:CD2	13:N:261:VAL:HG12	2.39	0.58
15:R:175:PRO:HG3	15:R:468:ARG:NH1	2.18	0.57
3:C:358:LEU:HD21	3:C:368:TRP:CE2	2.39	0.57
3:P:392:ILE:HD11	3:P:402:TRP:CH2	2.37	0.57
11:L:144:ASN:ND2	11:L:151:THR:HG23	2.19	0.57
3:P:151:LEU:HD22	3:P:178:VAL:HG13	1.85	0.57
20:X:346:GLY:C	20:X:378:LEU:HD11	2.25	0.57
15:R:313:ARG:NH2	15:R:317:CYS:SG	2.77	0.57
13:N:284:SER:OG	13:N:285:PHE:HB2	2.03	0.57
13:N:395:ASP:OD2	13:N:397:ILE:HB	2.04	0.57
20:X:219:VAL:HG22	20:X:240:ILE:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:465:LEU:HA	9:J:488:ILE:HD12	1.85	0.57
13:N:455:GLU:CB	13:N:501:ILE:HD11	2.34	0.57
15:R:458:ILE:CG1	15:R:472:VAL:HG11	2.34	0.57
12:M:11:ILE:HG23	12:M:15:ILE:HD12	1.87	0.57
10:K:496:GLU:HB2	10:K:526:TYR:HE1	1.68	0.57
8:I:168:LEU:HD22	8:I:192:MET:SD	2.44	0.57
3:C:120:TYR:CZ	3:C:124:LEU:HD11	2.39	0.57
3:C:53:LYS:HD2	3:P:93:TYR:CE1	2.40	0.57
15:R:201:LEU:HD23	15:R:467:LEU:HD21	1.86	0.57
13:N:393:THR:CG2	13:N:434:THR:HG22	2.34	0.57
15:R:225:LEU:HD12	15:R:231:SER:CA	2.34	0.57
3:P:286:PHE:HB3	3:P:303:PHE:CD2	2.39	0.57
1:A:763:PHE:CD1	1:A:793:LEU:HD22	2.39	0.57
9:J:37:PRO:HB3	9:J:69:TYR:OH	2.04	0.57
6:F:168:PHE:CB	6:F:467:ARG:HD3	2.35	0.57
3:C:238:TYR:HB3	3:C:247:ALA:HB2	1.86	0.57
1:A:32:PRO:CD	14:O:264:VAL:HG11	2.34	0.57
1:A:1079:ALA:HB1	1:A:1556:LEU:HA	1.85	0.57
6:H:478:SER:HA	6:H:633:ARG:HH22	1.69	0.57
13:N:285:PHE:O	13:N:289:PHE:HD2	1.86	0.57
6:F:124:VAL:O	6:F:128:THR:OG1	2.14	0.57
10:K:284:LEU:HD13	10:K:308:TYR:HB2	1.86	0.57
20:X:462:LYS:HG2	20:X:485:LEU:CD1	2.33	0.57
20:X:423:ILE:HG22	20:X:454:ASP:OD1	2.05	0.57
20:X:83:HIS:O	20:X:86:SER:OG	2.20	0.57
2:B:1:MET:CE	13:N:650:LEU:HD22	2.34	0.57
15:R:313:ARG:NE	15:R:317:CYS:CB	2.68	0.57
3:P:36:LEU:HD21	3:P:58:LEU:HB2	1.86	0.57
1:A:1162:LYS:HG3	1:A:1163:PRO:CD	2.35	0.57
1:A:1220:MET:HG2	1:A:1264:THR:HG21	1.86	0.57
9:J:55:ARG:HH11	10:K:264:HIS:HA	1.69	0.57
13:N:531:PHE:O	13:N:533:PHE:HA	2.04	0.57
3:P:389:ARG:O	3:P:392:ILE:HG23	2.05	0.57
8:I:276:TRP:CH2	8:I:280:LEU:HD22	2.40	0.57
10:K:292:VAL:HG21	12:M:57:TRP:HB2	1.87	0.57
14:O:378:SER:HB2	14:O:408:LEU:HD11	1.87	0.57
3:C:416:PHE:CE2	14:O:323:ALA:HB2	2.40	0.57
15:R:426:LEU:HG	15:R:438:LYS:HG2	1.87	0.57
20:X:100:TYR:HD1	20:X:138:VAL:HG13	1.69	0.57
6:H:128:THR:HG21	6:H:130:ARG:NH1	2.20	0.57
3:P:120:TYR:CE2	3:P:124:LEU:HD11	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:449:ASN:HD22	19:W:8:ARG:NH1	2.02	0.57
1:A:1377:LYS:HG2	1:A:1416:TRP:CG	2.40	0.57
6:H:761:SER:O	6:H:765:ASP:HB2	2.05	0.57
9:J:351:ASP:CG	15:R:393:LEU:HD22	2.25	0.56
9:J:351:ASP:OD2	15:R:393:LEU:HD23	2.04	0.56
13:N:704:VAL:HA	13:N:719:GLU:CD	2.26	0.56
13:N:202:GLU:OE2	13:N:283:ARG:HB2	2.05	0.56
3:C:151:LEU:HD22	3:C:178:VAL:HG13	1.86	0.56
20:X:365:ALA:HB3	20:X:375:ALA:HB1	1.88	0.56
1:A:443:CYS:HB3	1:A:452:LEU:HD12	1.87	0.56
14:O:356:ASP:HA	14:O:357:SER:HB2	1.86	0.56
6:F:104:ASP:N	6:F:104:ASP:OD1	2.37	0.56
20:X:343:VAL:CG1	20:X:378:LEU:HD22	2.35	0.56
15:R:211:LEU:HD22	15:R:237:TRP:HZ2	1.69	0.56
15:R:227:VAL:HG12	15:R:228:GLU:C	2.26	0.56
13:N:60:GLU:C	13:N:63:ARG:CB	2.72	0.56
20:Y:437:LEU:HB2	20:Y:444:LEU:HD21	1.87	0.56
14:O:417:LEU:HA	14:O:420:ILE:HG22	1.85	0.56
6:H:707:PHE:HB2	6:H:729:LEU:HD11	1.87	0.56
20:X:294:PHE:CD1	20:X:294:PHE:C	2.79	0.56
10:K:305:VAL:HG22	12:M:57:TRP:CZ3	2.40	0.56
1:A:1674:TRP:CD1	1:A:1674:TRP:N	2.73	0.56
6:H:168:PHE:CB	6:H:467:ARG:HD3	2.35	0.56
6:H:515:TYR:HE2	6:H:545:HIS:CD2	2.23	0.56
14:O:620:ALA:O	14:O:624:VAL:HG23	2.05	0.56
15:R:363:TRP:HZ3	15:R:387:THR:OG1	1.89	0.56
13:N:202:GLU:HB2	13:N:282:GLU:CD	2.26	0.56
3:P:358:LEU:HD11	3:P:368:TRP:CZ2	2.40	0.56
13:N:395:ASP:OD1	13:N:398:THR:HG23	2.06	0.56
8:I:32:ARG:HD3	13:N:388:HIS:CE1	2.41	0.56
6:F:503:CYS:SG	6:F:535:GLY:HA3	2.45	0.56
14:O:243:LEU:O	14:O:243:LEU:HD12	2.05	0.56
20:X:449:THR:HG21	20:X:465:LEU:CA	2.36	0.56
20:X:100:TYR:CD1	20:X:138:VAL:HG13	2.40	0.56
2:B:33:CYS:HB3	2:B:39:VAL:O	2.06	0.56
1:A:1632:ALA:O	1:A:1653:ALA:HB2	2.05	0.56
6:H:145:ASN:HB2	6:H:146:PRO:O	2.06	0.56
13:N:281:TYR:CZ	13:N:357:ALA:N	2.73	0.56
15:R:267:LEU:CD1	15:R:296:ARG:HD3	2.36	0.56
13:N:278:ARG:HB3	13:N:343:GLU:OE2	2.04	0.56
13:N:560:MET:HA	13:N:560:MET:HE3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:330:SER:O	15:R:337:LEU:HD12	2.06	0.56
10:K:487:TYR:OH	19:W:15:ASP:O	2.23	0.56
20:X:452:LEU:HD21	20:X:460:LYS:HB2	1.86	0.56
13:N:520:ARG:HD2	13:N:556:PHE:CD1	2.40	0.56
10:K:441:VAL:HG13	10:K:474:LEU:HD22	1.87	0.56
6:H:20:ALA:O	6:H:23:ASP:OD1	2.24	0.56
15:R:429:LYS:CD	15:R:433:LEU:HD23	2.36	0.56
10:K:432:ILE:CD1	10:K:444:TRP:CG	2.89	0.56
1:A:1885:LEU:HD23	1:A:1886:SER:N	2.21	0.56
15:R:294:LEU:HD22	15:R:304:GLN:NE2	2.21	0.56
6:F:145:ASN:HB2	6:F:146:PRO:C	2.26	0.56
15:R:154:SER:O	15:R:158:GLN:HG2	2.06	0.56
1:A:213:MET:CE	1:A:216:PRO:HA	2.36	0.56
9:J:441:VAL:O	9:J:442:ASP:HB3	2.06	0.55
20:Y:219:VAL:HG22	20:Y:240:ILE:CG2	2.37	0.55
1:A:95:VAL:HG13	1:A:100:VAL:HG22	1.88	0.55
6:H:639:TYR:CE2	11:L:183:ILE:HG22	2.41	0.55
13:N:281:TYR:CE1	13:N:357:ALA:CA	2.90	0.55
9:J:351:ASP:CB	15:R:393:LEU:HD22	2.37	0.55
1:A:1086:MET:CE	1:A:1564:LEU:CD1	2.84	0.55
9:J:476:PRO:HB3	3:P:182:LEU:HB3	1.86	0.55
20:Y:100:TYR:HD1	20:Y:138:VAL:HG13	1.72	0.55
2:B:47:VAL:HG21	2:B:60:ILE:HG21	1.88	0.55
6:F:152:PHE:CE1	6:F:162:PRO:HG2	2.38	0.55
1:A:1037:VAL:HG21	1:A:1566:PHE:CE2	2.40	0.55
1:A:620:THR:HG23	1:A:866:ILE:HD13	1.87	0.55
3:C:233:PHE:CZ	3:C:237:ILE:CD1	2.89	0.55
1:A:154:LEU:HD21	1:A:177:VAL:HG11	1.88	0.55
3:P:233:PHE:CE1	3:P:237:ILE:CD1	2.90	0.55
20:X:494:ASP:OD1	20:X:494:ASP:N	2.40	0.55
13:N:141:LEU:O	13:N:143:GLY:N	2.39	0.55
3:P:238:TYR:HB3	3:P:247:ALA:HB2	1.88	0.55
1:A:1421:PRO:CD	17:T:3:ALA:HB1	2.37	0.55
1:A:99:MET:HB3	1:A:118:THR:HG22	1.88	0.55
20:X:350:PHE:HA	20:X:382:ALA:HA	1.89	0.55
13:N:281:TYR:OH	13:N:357:ALA:HA	2.07	0.55
20:Y:449:THR:HG21	20:Y:465:LEU:CA	2.37	0.55
20:Y:196:LEU:O	20:Y:200:PRO:HB3	2.07	0.55
8:I:56:TRP:CD2	8:I:98:PRO:HB3	2.41	0.55
20:Y:294:PHE:CE2	20:Y:311:TYR:HB2	2.41	0.55
20:X:359:LEU:HB2	20:X:383:LEU:CD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:351:TYR:HH	15:R:390:GLY:HA3	1.70	0.55
8:I:262:LEU:HA	8:I:265:ILE:HG22	1.89	0.55
14:O:64:LEU:C	14:O:64:LEU:HD12	2.27	0.55
10:K:153:TYR:CZ	10:K:169:LEU:HD22	2.41	0.55
13:N:257:SER:O	13:N:261:VAL:HG13	2.06	0.55
14:O:123:GLU:N	14:O:124:PRO:HA	2.22	0.55
3:P:283:LEU:HD21	3:P:312:MET:HE3	1.88	0.55
9:J:451:LEU:CD1	9:J:467:TYR:CE2	2.90	0.55
20:X:203:LEU:HD22	20:Y:55:LEU:HB3	1.89	0.55
1:A:87:VAL:HG12	1:A:88:ASP:N	2.22	0.55
9:J:190:LEU:HD13	9:J:202:ARG:HD3	1.88	0.55
5:E:96:PHE:HB2	6:H:595:GLN:HE21	1.71	0.55
20:X:350:PHE:CE1	20:X:381:ALA:CB	2.90	0.55
13:N:74:TRP:CH2	13:N:77:GLU:HB2	2.42	0.55
16:S:374:SER:CB	16:S:387:TYR:O	2.55	0.55
13:N:425:ARG:HH11	13:N:425:ARG:HG2	1.72	0.55
20:X:423:ILE:HA	20:X:454:ASP:OD2	2.07	0.55
8:I:507:LEU:HD22	8:I:513:LEU:HD11	1.89	0.55
9:J:445:GLU:HA	9:J:474:LEU:HD23	1.89	0.55
13:N:386:LEU:HD12	13:N:387:LEU:N	2.22	0.55
1:A:1241:THR:OG1	1:A:1243:LEU:HD22	2.06	0.55
8:I:24:ILE:O	8:I:569:LEU:HD22	2.06	0.55
1:A:1624:VAL:HG22	1:A:1698:TYR:CD2	2.41	0.55
1:A:1870:CYS:HB3	1:A:1884:GLN:CD	2.28	0.55
8:I:115:TRP:CE3	8:I:176:LEU:HD22	2.41	0.55
13:N:191:GLY:O	13:N:196:ASP:N	2.40	0.55
8:I:56:TRP:HZ3	8:I:58:PHE:HB2	1.70	0.54
1:A:616:GLU:O	1:A:620:THR:OG1	2.20	0.54
1:A:1248:ASN:O	1:A:1251:VAL:HG22	2.07	0.54
6:H:762:TRP:HA	6:H:765:ASP:HB3	1.89	0.54
3:C:39:ILE:HD12	3:C:201:LEU:HB2	1.88	0.54
1:A:457:PHE:HB3	1:A:468:PHE:CD2	2.42	0.54
14:O:648:ILE:CD1	14:O:663:ALA:HB1	2.37	0.54
15:R:227:VAL:HG11	15:R:229:GLY:H	1.69	0.54
9:J:258:MET:HE2	9:J:271:HIS:CD2	2.42	0.54
11:L:144:ASN:CG	11:L:151:THR:HG23	2.28	0.54
9:J:37:PRO:HB3	9:J:69:TYR:CE2	2.42	0.54
13:N:190:LYS:O	13:N:196:ASP:N	2.41	0.54
10:K:248:LYS:N	10:K:438:GLU:OE2	2.41	0.54
8:I:290:PHE:CE1	8:I:320:LEU:HD22	2.42	0.54
13:N:347:ILE:HG21	13:N:358:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:149:TRP:CZ3	6:F:152:PHE:HD2	2.25	0.54
8:I:15:GLY:O	8:I:743:VAL:N	2.37	0.54
8:I:214:LEU:O	8:I:238:THR:OG1	2.26	0.54
1:A:150:CYS:HB3	1:A:163:SER:HA	1.89	0.54
1:A:1802:ARG:HD3	1:A:1808:MET:HB3	1.88	0.54
6:H:503:CYS:SG	6:H:535:GLY:HA3	2.47	0.54
14:O:691:ILE:HD13	14:O:721:TYR:CE1	2.41	0.54
20:X:355:TYR:CB	20:X:383:LEU:HA	2.22	0.54
9:J:35:GLU:CD	9:J:63:ARG:HE	2.11	0.54
3:C:368:TRP:CB	3:C:391:ALA:HB2	2.37	0.54
14:O:114:ASP:O	14:O:117:ASP:OD1	2.26	0.54
13:N:650:LEU:HD12	13:N:651:ALA:N	2.22	0.54
1:A:1099:PRO:O	1:A:1161:ASN:ND2	2.39	0.54
8:I:341:TYR:CE1	8:I:475:VAL:HG21	2.42	0.54
13:N:523:LEU:HD22	13:N:538:GLU:OE1	2.07	0.54
14:O:354:ARG:HD3	14:O:574:LEU:HA	1.89	0.54
3:C:60:PHE:HA	3:P:85:ASP:CG	2.27	0.54
6:H:639:TYR:CD2	11:L:183:ILE:HG22	2.43	0.54
10:K:406:HIS:CE1	19:W:6:PRO:HB3	2.42	0.54
3:C:228:TRP:O	3:C:231:GLU:N	2.39	0.54
13:N:350:ASP:CB	13:N:351:PHE:HA	2.37	0.54
13:N:281:TYR:CE1	13:N:357:ALA:HB2	2.42	0.54
15:R:243:LEU:HD13	15:R:298:ILE:HD12	1.90	0.54
10:K:250:CYS:SG	10:K:274:THR:HG21	2.47	0.54
20:X:40:HIS:HB3	20:Y:201:LEU:CD1	2.36	0.54
20:Y:294:PHE:CE1	20:Y:311:TYR:CG	2.96	0.54
20:X:192:TYR:HA	20:X:195:VAL:HG22	1.89	0.54
9:J:322:TYR:HE1	12:M:36:LEU:HD11	1.72	0.54
14:O:435:SER:HB3	14:O:654:ASP:HB2	1.88	0.54
15:R:189:TYR:HA	15:R:316:VAL:HB	1.89	0.54
15:R:310:GLN:HG2	15:R:340:TRP:HZ2	1.58	0.54
15:R:182:PRO:O	15:R:183:GLU:HB2	2.07	0.54
2:B:23:CYS:HA	2:B:30:PHE:CZ	2.43	0.54
1:A:982:ASP:OD1	1:A:983:LEU:N	2.40	0.54
1:A:1658:PRO:HG2	1:A:1663:LEU:HD13	1.90	0.54
10:K:429:LEU:HA	10:K:432:ILE:HG22	1.90	0.54
3:P:420:TYR:OH	3:P:424:ARG:HD3	2.08	0.54
10:K:46:CYS:O	10:K:50:THR:OG1	2.22	0.54
6:H:621:LEU:O	6:H:625:ARG:HG3	2.08	0.54
10:K:432:ILE:HD11	10:K:444:TRP:CG	2.43	0.54
3:P:402:TRP:CZ2	3:P:424:ARG:HG2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:LEU:HD12	3:P:60:PHE:CG	2.42	0.54
6:H:146:PRO:HG3	6:H:167:THR:HA	1.89	0.54
1:A:1137:PHE:O	1:A:1141:VAL:HG23	2.07	0.54
10:K:296:PRO:HB2	12:M:55:MET:HG3	1.89	0.54
1:A:1540:ARG:CZ	13:N:486:ASP:O	2.56	0.54
20:Y:192:TYR:HA	20:Y:195:VAL:HG22	1.89	0.54
3:C:276:ILE:O	3:C:276:ILE:HG22	2.08	0.54
13:N:289:PHE:HA	13:N:292:TRP:HB3	1.90	0.54
13:N:180:PHE:CE1	13:N:299:TRP:HZ3	1.89	0.54
20:X:219:VAL:HG22	20:X:240:ILE:CG2	2.37	0.54
13:N:513:ASP:OD1	13:N:514:LEU:HD22	2.08	0.54
9:J:332:THR:HA	9:J:363:LEU:HD21	1.90	0.54
3:P:251:TYR:OH	3:P:268:GLN:HG3	2.08	0.54
13:N:345:PHE:CD1	13:N:385:ARG:CZ	2.91	0.54
15:R:351:TYR:OH	15:R:390:GLY:HA3	2.06	0.53
3:C:550:LEU:O	3:C:553:ILE:HG12	2.08	0.53
1:A:1290:ASP:OD2	1:A:1600:ARG:HA	2.08	0.53
1:A:129:CYS:SG	1:A:130:ASP:N	2.81	0.53
9:J:19:TYR:CD1	9:J:49:LEU:HD13	2.43	0.53
12:M:4:GLU:HG2	3:P:50:HIS:CE1	2.44	0.53
8:I:45:LEU:HG	8:I:57:SER:HA	1.89	0.53
10:K:19:TYR:CD1	10:K:49:LEU:HD13	2.42	0.53
10:K:369:LEU:HD21	19:W:3:ARG:HG2	1.89	0.53
13:N:165:THR:N	13:N:166:PRO:HA	2.23	0.53
1:A:1677:LEU:HD12	1:A:1678:ILE:N	2.24	0.53
15:R:314:GLN:N	15:R:333:ASN:HB3	2.23	0.53
13:N:414:MET:SD	13:N:498:SER:CA	2.96	0.53
1:A:860:TYR:CD2	1:A:861:PRO:HD2	2.43	0.53
6:H:743:ILE:CG2	6:H:759:ASN:HD21	2.21	0.53
9:J:46:CYS:O	9:J:50:THR:OG1	2.22	0.53
15:R:407:TRP:HA	15:R:414:LEU:HD12	1.90	0.53
6:F:89:GLU:OE2	6:F:125:TYR:HE1	1.91	0.53
13:N:86:ASN:C	13:N:89:PRO:HD2	2.29	0.53
3:P:304:SER:HB2	3:P:336:VAL:HG22	1.91	0.53
10:K:176:LEU:HD12	10:K:181:GLU:HG2	1.91	0.53
13:N:574:ILE:HD12	13:N:625:LYS:HG2	1.89	0.53
3:C:304:SER:HB2	3:C:336:VAL:HG22	1.89	0.53
14:O:348:TYR:CE1	14:O:361:LEU:HD11	2.44	0.53
13:N:344:LEU:HA	13:N:347:ILE:HB	1.90	0.53
3:C:251:TYR:CB	3:C:269:ILE:HD11	2.38	0.53
15:R:420:TYR:CZ	15:R:421:SER:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:537:GLU:CD	6:F:600:TYR:HH	2.10	0.53
14:O:652:LEU:HD23	14:O:660:LYS:HG3	1.90	0.53
8:I:142:LEU:HD13	8:I:264:TYR:CE2	2.43	0.53
20:Y:100:TYR:CD1	20:Y:138:VAL:HG13	2.42	0.53
10:K:190:LEU:O	10:K:198:GLN:NE2	2.42	0.53
1:A:1304:MET:O	1:A:1307:LEU:HB2	2.09	0.53
8:I:65:GLY:H	8:I:84:LEU:HG	1.74	0.53
13:N:364:CYS:O	13:N:367:ARG:O	2.26	0.53
14:O:710:ILE:O	14:O:711:ARG:C	2.47	0.53
1:A:857:MET:CB	1:A:858:PRO:HD3	2.38	0.53
6:F:755:LEU:HD13	9:J:393:GLN:HE22	1.74	0.53
8:I:26:LEU:HB3	8:I:37:LEU:HB3	1.91	0.53
3:P:431:ASN:HA	3:P:462:VAL:HG21	1.89	0.53
14:O:439:LEU:HG	14:O:476:LEU:HD13	1.90	0.53
4:D:13:THR:HG22	14:O:255:TYR:HE2	1.73	0.53
20:Y:309:ASP:HB2	20:Y:340:GLU:HG2	1.90	0.53
15:R:382:ILE:CD1	15:R:398:THR:HG21	2.38	0.53
1:A:612:ILE:O	1:A:641:TRP:CH2	2.62	0.53
1:A:237:GLN:HG3	1:A:238:TYR:N	2.24	0.53
1:A:1818:LYS:NZ	1:A:1896:SER:OG	2.29	0.53
14:O:431:LEU:HD12	14:O:431:LEU:O	2.08	0.53
15:R:385:TRP:CZ3	15:R:392:PRO:HB3	2.44	0.53
9:J:211:LYS:O	9:J:212:TYR:CG	2.62	0.53
14:O:467:ALA:CB	14:O:506:LEU:HD11	2.39	0.53
9:J:383:ASN:HB3	9:J:386:LEU:HD13	1.91	0.53
20:Y:551:LYS:HD3	20:Y:552:MET:N	2.24	0.53
20:X:350:PHE:CD2	20:X:381:ALA:HB3	2.43	0.53
1:A:1470:LEU:HD23	1:A:1470:LEU:C	2.28	0.53
6:H:540:SER:OG	6:H:575:ASN:ND2	2.30	0.53
15:R:313:ARG:NE	15:R:317:CYS:SG	2.81	0.53
15:R:182:PRO:CB	16:S:322:ARG:HB3	2.38	0.53
13:N:527:LEU:HD11	13:N:561:LEU:HD22	1.90	0.53
16:S:374:SER:HB3	16:S:387:TYR:CA	2.38	0.53
6:F:699:ASP:HB2	6:F:702:ASN:HD21	1.74	0.53
1:A:1227:LEU:O	1:A:1230:ILE:HG22	2.09	0.53
9:J:276:VAL:HA	9:J:311:MET:SD	2.49	0.53
3:C:307:LEU:CD2	3:C:316:LEU:HD13	2.39	0.53
1:A:269:TRP:HB3	1:A:409:ILE:HG23	1.90	0.53
6:F:704:LEU:HD21	15:R:488:LEU:HB3	1.90	0.53
20:X:350:PHE:HB2	20:X:351:TYR:CD1	2.44	0.52
15:R:189:TYR:CB	15:R:316:VAL:H	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:494:ILE:HA	3:C:497:ILE:HD12	1.91	0.52
13:N:501:ILE:O	13:N:505:LEU:HG	2.09	0.52
1:A:1794:ILE:HB	14:O:598:THR:HG21	1.90	0.52
14:O:596:SER:OG	14:O:599:ILE:HD12	2.08	0.52
6:F:686:GLU:N	6:F:686:GLU:OE1	2.42	0.52
15:R:291:ARG:HD2	15:R:312:HIS:CG	2.43	0.52
8:I:24:ILE:HG22	8:I:38:ALA:O	2.09	0.52
13:N:273:MET:HG3	13:N:277:CYS:SG	2.50	0.52
9:J:55:ARG:NH1	10:K:264:HIS:HA	2.25	0.52
9:J:53:TYR:O	9:J:79:CYS:SG	2.67	0.52
1:A:1064:GLU:HA	1:A:1125:ILE:HD11	1.89	0.52
1:A:1789:MET:CE	1:A:1789:MET:HA	2.38	0.52
15:R:310:GLN:O	15:R:338:LEU:HD21	2.09	0.52
10:K:185:LEU:HD21	10:K:205:PHE:CB	2.39	0.52
9:J:37:PRO:HB3	9:J:69:TYR:CZ	2.45	0.52
20:Y:159:LEU:HD22	20:Y:171:ILE:HG23	1.91	0.52
3:C:422:TYR:OH	15:R:52:ARG:NH2	2.42	0.52
3:C:516:LEU:HD22	3:C:520:TYR:CE2	2.45	0.52
14:O:258:TYR:CE1	14:O:262:LEU:HD22	2.44	0.52
14:O:462:ASN:O	14:O:463:THR:OG1	2.27	0.52
20:Y:350:PHE:HB2	20:Y:351:TYR:CD1	2.45	0.52
10:K:174:HIS:CE1	10:K:211:LYS:HD2	2.44	0.52
13:N:321:LEU:HD22	13:N:324:TRP:CD2	2.45	0.52
1:A:1412:CYS:HB2	1:A:1471:SER:OG	2.09	0.52
9:J:277:GLU:OE1	9:J:278:LEU:HD23	2.09	0.52
3:P:251:TYR:HB3	3:P:269:ILE:HD11	1.91	0.52
3:C:199:LEU:HD23	3:C:199:LEU:O	2.10	0.52
3:P:244:ILE:C	3:P:244:ILE:HD12	2.29	0.52
8:I:353:GLN:HE21	8:I:353:GLN:HA	1.74	0.52
11:L:40:PHE:HA	11:L:44:GLN:OE1	2.10	0.52
15:R:230:ASP:HA	15:R:249:HIS:HB3	1.91	0.52
13:N:394:CYS:O	13:N:395:ASP:CG	2.47	0.52
13:N:392:ASN:O	13:N:395:ASP:HA	2.10	0.52
20:Y:302:PRO:HG2	20:Y:303:TYR:CE2	2.45	0.52
1:A:956:ARG:CZ	1:A:1788:GLU:OE1	2.58	0.52
15:R:458:ILE:HG12	15:R:472:VAL:HG21	1.92	0.52
9:J:397:ILE:HG22	9:J:398:ALA:N	2.25	0.52
13:N:540:ARG:O	13:N:544:LEU:HD22	2.09	0.52
3:C:361:ASN:HB3	3:C:363:ARG:N	2.25	0.52
15:R:296:ARG:HA	15:R:303:LEU:O	2.10	0.52
15:R:179:LEU:HD13	16:S:325:LEU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:351:ASP:CB	15:R:393:LEU:HD21	2.32	0.52
2:B:1:MET:HE2	13:N:650:LEU:HD22	1.92	0.52
3:C:431:ASN:HA	3:C:462:VAL:HG21	1.91	0.52
20:X:282:PHE:HD1	20:X:314:LEU:HD21	1.74	0.52
3:P:407:GLN:HA	3:P:422:TYR:OH	2.10	0.52
20:Y:214:VAL:HG12	20:Y:217:ALA:HB3	1.91	0.52
15:R:182:PRO:HB3	16:S:322:ARG:CG	2.39	0.52
9:J:35:GLU:OE2	9:J:63:ARG:CZ	2.58	0.52
15:R:155:ASN:O	15:R:158:GLN:HB2	2.10	0.52
1:A:1540:ARG:NH1	13:N:486:ASP:O	2.42	0.52
14:O:348:TYR:CZ	14:O:361:LEU:HD11	2.45	0.52
15:R:44:HIS:CG	15:R:45:GLY:N	2.78	0.52
3:C:409:TYR:HB2	3:C:418:CYS:HB3	1.92	0.52
20:X:159:LEU:HD22	20:X:171:ILE:HG23	1.92	0.52
3:P:199:LEU:HD23	3:P:199:LEU:O	2.09	0.52
6:H:537:GLU:OE2	6:H:600:TYR:CZ	2.62	0.52
13:N:368:THR:HG1	13:N:369:ASP:HA	1.72	0.52
14:O:490:LEU:HD13	14:O:511:ASP:CB	2.40	0.52
1:A:612:ILE:O	1:A:641:TRP:HZ3	1.92	0.52
4:D:40:TRP:CZ2	4:D:44:ILE:HD11	2.44	0.52
6:H:486:ASN:O	6:H:490:HIS:CD2	2.63	0.52
1:A:174:PRO:HG2	1:A:175:PHE:CD2	2.45	0.52
10:K:62:SER:O	10:K:63:ARG:CG	2.56	0.51
1:A:1241:THR:HG22	15:R:161:LEU:HD22	1.90	0.51
6:H:689:LEU:HD11	6:H:716:ASN:ND2	2.25	0.51
1:A:980:ARG:NH2	1:A:1674:TRP:O	2.43	0.51
1:A:852:LEU:HD11	1:A:1822:GLU:HB3	1.92	0.51
8:I:74:ARG:HD2	8:I:174:ASN:HD22	1.75	0.51
13:N:281:TYR:CE1	13:N:284:SER:HB3	2.45	0.51
13:N:180:PHE:CG	13:N:299:TRP:CH2	2.85	0.51
13:N:611:VAL:HG23	13:N:616:ARG:HG2	1.93	0.51
3:P:388:TYR:O	3:P:392:ILE:HG22	2.10	0.51
1:A:504:VAL:HG11	1:A:635:VAL:HG13	1.90	0.51
1:A:77:ARG:HD3	1:A:128:TRP:CE3	2.45	0.51
3:C:370:LEU:HD22	15:R:47:ARG:CZ	2.40	0.51
6:H:669:SER:HA	6:H:698:ILE:HD11	1.92	0.51
13:N:156:MET:O	13:N:160:VAL:HG23	2.10	0.51
1:A:848:VAL:HG22	1:A:877:ILE:CD1	2.40	0.51
1:A:1274:LEU:HD21	1:A:1325:LEU:CD1	2.41	0.51
1:A:1230:ILE:HD11	15:R:94:LEU:HB3	1.92	0.51
2:B:20:ASP:O	2:B:30:PHE:CD2	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:264:TYR:O	8:I:268:SER:OG	2.22	0.51
15:R:458:ILE:HG12	15:R:472:VAL:HG11	1.92	0.51
14:O:431:LEU:HD11	14:O:616:LEU:HD22	1.92	0.51
6:H:492:PRO:O	6:H:493:SER:CB	2.59	0.51
6:H:653:LEU:HD22	10:K:523:ILE:HG21	1.91	0.51
11:L:40:PHE:HZ	15:R:176:PHE:HZ	0.76	0.51
13:N:425:ARG:NE	13:N:507:SER:HB2	2.25	0.51
11:L:89:TYR:CE1	11:L:152:HIS:CE1	2.98	0.51
14:O:119:PHE:CZ	14:O:136:LEU:HD11	2.45	0.51
1:A:1218:GLY:N	1:A:1259:LEU:O	2.44	0.51
10:K:250:CYS:SG	10:K:274:THR:HG23	2.50	0.51
13:N:386:LEU:C	13:N:388:HIS:HB3	2.31	0.51
1:A:801:PRO:C	1:A:804:ASP:OD1	2.49	0.51
14:O:539:ASN:HD22	14:O:542:GLU:HB3	1.74	0.51
1:A:1079:ALA:HB1	1:A:1556:LEU:CA	2.40	0.51
9:J:55:ARG:NH1	10:K:261:ASP:OD2	2.44	0.51
8:I:115:TRP:CZ3	8:I:176:LEU:HD22	2.46	0.51
15:R:291:ARG:CD	15:R:312:HIS:HA	2.41	0.51
13:N:75:PHE:O	13:N:78:VAL:N	2.43	0.51
13:N:663:GLN:HB3	13:N:699:TRP:CZ2	2.45	0.51
3:P:358:LEU:CD1	3:P:368:TRP:CD2	2.94	0.51
13:N:574:ILE:HD13	13:N:622:TYR:CE1	2.46	0.51
3:C:296:ARG:HA	3:P:101:ARG:NH1	2.26	0.51
12:M:2:ASP:OD1	12:M:3:SER:N	2.42	0.51
20:X:214:VAL:HG12	20:X:217:ALA:HB3	1.91	0.51
9:J:355:ALA:O	9:J:359:THR:HG23	2.10	0.51
20:Y:494:ASP:OD1	20:Y:494:ASP:N	2.40	0.51
13:N:662:VAL:CG2	13:N:695:ARG:HG2	2.41	0.51
6:F:130:ARG:HG2	20:Y:506:GLN:HB2	1.93	0.51
11:L:33:LEU:CG	11:L:42:VAL:HG22	2.41	0.51
8:I:344:ILE:O	8:I:348:VAL:HG23	2.11	0.51
2:B:36:ASP:OD1	2:B:36:ASP:N	2.43	0.51
20:X:358:ALA:O	20:X:379:LYS:HA	2.11	0.51
13:N:123:ASP:CB	13:N:250:LEU:HD11	2.41	0.51
20:Y:196:LEU:O	20:Y:200:PRO:CB	2.59	0.51
1:A:207:LEU:HD12	1:A:208:PRO:CD	2.39	0.51
13:N:681:LEU:HD23	13:N:692:LEU:HD11	1.93	0.51
9:J:495:PHE:CZ	9:J:525:MET:SD	3.04	0.51
20:X:267:LEU:CD1	20:Y:59:LEU:HD13	2.41	0.51
13:N:559:VAL:HG11	13:N:600:PHE:CZ	2.46	0.51
3:P:355:GLN:HA	3:P:358:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:LEU:HD23	1:A:1191:LEU:C	2.31	0.51
14:O:652:LEU:O	14:O:660:LYS:HD2	2.11	0.51
10:K:443:LYS:O	10:K:446:PRO:HD2	2.11	0.51
8:I:674:VAL:O	8:I:703:ARG:NH1	2.44	0.51
3:C:206:TRP:O	3:C:209:LEU:HB2	2.10	0.51
20:Y:376:LEU:HD21	20:Y:398:GLU:HG3	1.93	0.51
6:H:736:GLU:OE1	11:L:173:THR:O	2.28	0.51
11:L:40:PHE:CZ	15:R:176:PHE:CE1	2.80	0.51
1:A:1086:MET:HE1	1:A:1564:LEU:CD1	2.37	0.51
3:C:126:GLY:C	3:C:148:ASN:OD1	2.50	0.51
5:E:61:TYR:CE1	20:X:360:TYR:CZ	2.98	0.51
1:A:629:LEU:HD12	1:A:629:LEU:C	2.31	0.51
15:R:270:HIS:CE1	15:R:294:LEU:HG	2.45	0.51
1:A:1265:ALA:HB2	1:A:1309:HIS:CD2	2.46	0.51
3:P:276:ILE:HG22	3:P:277:ARG:H	1.76	0.51
8:I:414:PHE:HZ	8:I:472:VAL:HG13	1.76	0.51
20:X:355:TYR:CB	20:X:386:MET:CB	2.72	0.50
3:P:276:ILE:HG22	3:P:277:ARG:N	2.25	0.50
1:A:1572:TYR:CE1	1:A:1616:PRO:HB3	2.46	0.50
13:N:670:PHE:CE2	13:N:705:LEU:HD11	2.46	0.50
2:B:15:LEU:HD21	13:N:635:LEU:HA	1.94	0.50
3:P:303:PHE:CD1	3:P:303:PHE:C	2.84	0.50
20:Y:509:CYS:SG	20:Y:510:VAL:N	2.85	0.50
1:A:1427:ASP:O	1:A:1430:VAL:HG12	2.11	0.50
20:Y:199:CYS:HB2	20:Y:200:PRO:C	2.31	0.50
10:K:62:SER:C	10:K:63:ARG:CG	2.80	0.50
10:K:276:VAL:HA	10:K:311:MET:HE1	1.93	0.50
15:R:422:GLN:O	15:R:424:GLN:HG3	2.10	0.50
1:A:1250:GLN:O	1:A:1254:VAL:HG23	2.10	0.50
20:X:449:THR:HG22	20:X:461:ALA:O	2.12	0.50
3:P:368:TRP:CB	3:P:391:ALA:HB2	2.41	0.50
14:O:513:LYS:HG2	14:O:542:GLU:OE2	2.12	0.50
6:F:702:ASN:HB2	6:F:705:CYS:SG	2.51	0.50
2:B:39:VAL:CB	2:B:43:ASP:CB	2.89	0.50
1:A:1405:LEU:HD13	1:A:1467:GLY:HA2	1.93	0.50
1:A:174:PRO:HA	1:A:295:VAL:O	2.12	0.50
3:P:332:GLU:OE1	3:P:332:GLU:N	2.45	0.50
15:R:431:PRO:HB2	15:R:432:SER:C	2.31	0.50
15:R:466:THR:CG2	15:R:468:ARG:HG3	2.39	0.50
13:N:395:ASP:CG	13:N:398:THR:N	2.63	0.50
20:Y:449:THR:HG22	20:Y:461:ALA:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:47:ARG:O	15:R:48:PHE:CD1	2.65	0.50
1:A:1254:VAL:HG11	1:A:1298:ALA:HA	1.94	0.50
15:R:252:PHE:CE1	15:R:268:GLU:HG2	2.27	0.50
8:I:52:PHE:CD1	8:I:743:VAL:HG21	2.46	0.50
9:J:397:ILE:O	9:J:398:ALA:C	2.50	0.50
20:X:509:CYS:SG	20:X:510:VAL:N	2.84	0.50
14:O:78:LEU:O	14:O:78:LEU:HD12	2.11	0.50
1:A:1651:LEU:HD12	1:A:1651:LEU:N	2.25	0.50
1:A:641:TRP:CZ2	1:A:645:HIS:HB2	2.47	0.50
15:R:57:TRP:CE3	15:R:57:TRP:CA	2.95	0.50
1:A:1236:LEU:HD12	15:R:161:LEU:HD11	1.92	0.50
13:N:286:LEU:HG	13:N:360:ASP:OD2	2.11	0.50
3:P:234:LEU:HD22	3:P:238:TYR:CE2	2.47	0.50
3:P:283:LEU:HD21	3:P:312:MET:CE	2.42	0.50
3:P:251:TYR:OH	3:P:268:GLN:CG	2.60	0.50
1:A:1891:PHE:CE2	1:A:1895:HIS:CD2	3.00	0.50
12:M:12:LEU:HD13	3:P:360:LEU:CD2	2.42	0.50
1:A:170:ILE:HG21	3:C:427:GLN:HB2	1.94	0.50
6:F:75:LEU:HG	6:F:91:ILE:HD13	1.93	0.50
13:N:73:GLU:O	13:N:74:TRP:CB	2.59	0.50
13:N:74:TRP:CZ2	13:N:77:GLU:HB2	2.46	0.50
11:L:63:LEU:HD22	11:L:138:GLN:HE21	1.76	0.50
15:R:280:ASN:ND2	15:R:325:HIS:HB3	2.27	0.50
6:F:146:PRO:CG	6:F:167:THR:HA	2.40	0.50
1:A:42:LEU:HD23	3:C:142:GLU:HG2	1.93	0.50
1:A:852:LEU:HD12	1:A:852:LEU:C	2.32	0.50
3:P:365:LEU:HB3	3:P:395:ASN:HD21	1.77	0.50
10:K:509:ARG:HG3	10:K:512:ASP:HB2	1.93	0.50
11:L:125:THR:HA	11:L:126:ASP:O	2.12	0.50
13:N:563:ASP:OD2	13:N:597:SER:HB3	2.12	0.50
20:Y:515:LEU:HD23	20:Y:519:LEU:HG	1.94	0.50
13:N:644:VAL:HG21	13:N:664:ALA:CB	2.42	0.50
10:K:185:LEU:CD1	10:K:209:LEU:HD11	2.39	0.50
8:I:46:LEU:HD22	8:I:56:TRP:HE1	1.77	0.50
10:K:292:VAL:HG21	12:M:57:TRP:HB3	1.93	0.50
14:O:354:ARG:HD2	14:O:573:LYS:O	2.11	0.50
6:F:617:LEU:HD11	6:F:648:GLN:HG3	1.93	0.50
1:A:1615:GLU:OE2	1:A:1617:ARG:HD3	2.12	0.50
1:A:1089:LEU:HD11	1:A:1611:VAL:HG23	1.94	0.50
1:A:1469:CYS:O	1:A:1472:LEU:HB3	2.11	0.50
3:C:167:LEU:HD23	3:C:172:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:350:PHE:HZ	20:X:378:LEU:HA	1.73	0.49
20:X:363:ALA:CB	20:X:379:LYS:NZ	2.66	0.49
20:X:515:LEU:HD23	20:X:519:LEU:HG	1.94	0.49
1:A:1243:LEU:HD23	1:A:1243:LEU:O	2.12	0.49
8:I:286:ARG:NH1	8:I:324:GLN:HB3	2.27	0.49
13:N:304:PHE:CD1	13:N:324:TRP:CH2	3.00	0.49
20:Y:442:GLN:HG2	20:Y:472:GLU:HB2	1.94	0.49
15:R:310:GLN:CB	15:R:340:TRP:CH2	2.83	0.49
3:C:251:TYR:OH	3:C:268:GLN:HG3	2.12	0.49
1:A:1533:LEU:HD12	1:A:1534:LYS:N	2.26	0.49
9:J:334:GLY:N	9:J:335:PRO:CD	2.75	0.49
8:I:240:LEU:HD22	8:I:547:SER:CB	2.42	0.49
3:P:117:LEU:O	3:P:117:LEU:HD23	2.12	0.49
15:R:327:LEU:CD1	15:R:387:THR:CG2	2.83	0.49
13:N:141:LEU:O	13:N:142:MET:C	2.49	0.49
1:A:1262:GLN:HE21	1:A:1307:LEU:HD22	1.77	0.49
8:I:65:GLY:HA3	8:I:84:LEU:HB3	1.94	0.49
9:J:393:GLN:O	9:J:396:SER:HB3	2.11	0.49
14:O:40:LEU:HD22	14:O:82:ILE:HD12	1.94	0.49
1:A:260:ASP:OD1	1:A:262:VAL:HG22	2.12	0.49
3:P:122:ARG:HG2	3:P:154:LEU:HD11	1.92	0.49
15:R:425:ILE:HD11	15:R:460:THR:HG21	1.94	0.49
15:R:149:SER:O	15:R:150:LEU:HG	2.12	0.49
15:R:429:LYS:CD	15:R:433:LEU:CD2	2.91	0.49
13:N:597:SER:HG	13:N:600:PHE:HB2	1.77	0.49
1:A:1470:LEU:HD12	1:A:1518:VAL:HG13	1.95	0.49
6:H:128:THR:HG21	6:H:130:ARG:HH12	1.77	0.49
20:X:359:LEU:HB2	20:X:383:LEU:CG	2.43	0.49
15:R:327:LEU:HD13	15:R:387:THR:HG22	1.92	0.49
15:R:436:VAL:CG1	15:R:437:ALA:N	2.75	0.49
8:I:279:ILE:HD13	8:I:340:SER:HB2	1.95	0.49
6:H:481:CYS:CB	6:H:512:LEU:HD13	2.42	0.49
3:C:329:TYR:HB3	12:M:15:ILE:HD11	1.95	0.49
6:F:639:TYR:CD1	15:R:492:ILE:HG21	2.47	0.49
20:X:376:LEU:HD21	20:X:398:GLU:HG3	1.95	0.49
1:A:184:LYS:O	1:A:185:TYR:HB2	2.13	0.49
14:O:621:SER:HB3	14:O:651:ILE:HG12	1.94	0.49
1:A:1511:ASN:HD22	1:A:1511:ASN:N	2.11	0.49
13:N:519:TYR:HE1	13:N:523:LEU:HD21	1.76	0.49
20:Y:294:PHE:CG	20:Y:311:TYR:CD1	3.01	0.49
8:I:279:ILE:HD11	8:I:337:ILE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:ILE:HG22	1:A:642:TYR:HD2	1.78	0.49
2:B:15:LEU:HD11	13:N:635:LEU:HD12	1.93	0.49
13:N:501:ILE:HD12	13:N:501:ILE:H	1.77	0.49
15:R:188:PHE:CZ	15:R:359:LYS:HD2	2.48	0.49
15:R:267:LEU:HD13	15:R:296:ARG:HD3	1.95	0.49
13:N:74:TRP:CG	13:N:75:PHE:N	2.79	0.49
8:I:197:ARG:O	8:I:545:GLY:HA3	2.13	0.49
3:P:234:LEU:CD2	3:P:238:TYR:CZ	2.96	0.49
1:A:175:PHE:CD1	1:A:191:ARG:HG3	2.48	0.49
1:A:1469:CYS:HB2	1:A:1488:LEU:HD22	1.95	0.49
1:A:659:LEU:HD12	1:A:660:PHE:N	2.27	0.49
15:R:216:THR:O	15:R:217:SER:HB2	2.13	0.49
15:R:225:LEU:HB3	15:R:230:ASP:OD2	2.13	0.49
13:N:611:VAL:HG11	13:N:637:TRP:CZ2	2.47	0.49
3:P:358:LEU:HD11	3:P:368:TRP:CE2	2.47	0.49
3:P:303:PHE:C	3:P:303:PHE:HD1	2.16	0.49
13:N:253:LEU:O	13:N:257:SER:OG	2.18	0.49
14:O:264:VAL:O	14:O:265:GLN:HB2	2.13	0.49
13:N:165:THR:O	13:N:169:PHE:HB3	2.12	0.49
20:Y:425:GLU:O	20:Y:429:MET:HE2	2.13	0.49
11:L:62:HIS:NE2	11:L:149:ARG:O	2.42	0.49
9:J:77:ALA:CB	9:J:93:LEU:HD11	2.43	0.49
13:N:485:VAL:CB	13:N:487:ALA:HB2	2.42	0.49
20:X:266:LEU:HB3	20:Y:63:LEU:HD22	1.95	0.49
15:R:292:MET:SD	15:R:309:LEU:CD1	3.01	0.49
14:O:292:GLY:HA3	14:O:336:ASP:CB	2.43	0.49
13:N:556:PHE:CE1	13:N:600:PHE:HA	2.48	0.49
14:O:513:LYS:CE	14:O:542:GLU:OE2	2.61	0.49
9:J:429:LEU:HA	9:J:432:ILE:HG22	1.94	0.49
14:O:136:LEU:HD12	14:O:136:LEU:C	2.33	0.49
9:J:354:MET:HA	9:J:354:MET:CE	2.43	0.49
1:A:881:ILE:O	1:A:882:LEU:HG	2.12	0.49
10:K:324:SER:O	10:K:328:THR:HG23	2.12	0.49
15:R:189:TYR:O	15:R:316:VAL:HB	2.13	0.49
13:N:281:TYR:CZ	13:N:357:ALA:CA	2.96	0.49
15:R:233:THR:HG21	15:R:273:ARG:CG	2.40	0.49
9:J:258:MET:CE	9:J:271:HIS:CG	2.96	0.49
3:P:358:LEU:O	3:P:362:PRO:CA	2.58	0.49
1:A:1274:LEU:CD1	1:A:1321:VAL:HG12	2.39	0.49
13:N:669:TYR:CE1	13:N:684:ALA:HB1	2.48	0.49
10:K:384:SER:HB3	10:K:415:ASN:OD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:10:ARG:HD3	12:M:14:LEU:HD12	1.95	0.49
3:P:307:LEU:HD12	3:P:312:MET:HG3	1.95	0.49
1:A:1755:GLU:HB2	1:A:1756:TYR:HD1	1.78	0.49
15:R:382:ILE:HG13	15:R:398:THR:HG21	1.87	0.48
9:J:258:MET:CE	9:J:271:HIS:CD2	2.96	0.48
8:I:73:TRP:CD2	8:I:80:LEU:HD13	2.48	0.48
14:O:65:LEU:HB3	14:O:66:PRO:HD3	1.95	0.48
12:M:31:ILE:HG22	12:M:33:LEU:HD22	1.95	0.48
1:A:1316:MET:O	1:A:1319:LEU:O	2.30	0.48
3:C:122:ARG:HG2	3:C:154:LEU:HD11	1.94	0.48
3:P:494:ILE:HD13	3:P:516:LEU:HD13	1.95	0.48
1:A:1622:VAL:HA	1:A:1629:PRO:HA	1.95	0.48
1:A:268:VAL:HG12	1:A:412:LEU:HD21	1.94	0.48
1:A:1100:LEU:HB3	1:A:1101:PRO:CA	2.43	0.48
15:R:435:GLN:CG	15:R:436:VAL:N	2.65	0.48
13:N:659:VAL:HG23	13:N:728:VAL:HG23	1.94	0.48
20:Y:294:PHE:HZ	20:Y:308:MET:SD	2.35	0.48
10:K:297:SER:O	10:K:329:LEU:HD21	2.12	0.48
1:A:1803:LEU:HD11	1:A:1814:LEU:HD21	1.95	0.48
9:J:268:LEU:N	9:J:269:PRO:HD2	2.28	0.48
3:C:117:LEU:HD23	3:C:117:LEU:O	2.12	0.48
14:O:632:LEU:HD12	14:O:632:LEU:C	2.33	0.48
20:X:343:VAL:HG12	20:X:378:LEU:HD22	1.95	0.48
20:X:452:LEU:CD2	20:X:460:LYS:HB2	2.44	0.48
13:N:669:TYR:CZ	13:N:684:ALA:HB1	2.48	0.48
3:C:233:PHE:CE1	3:C:237:ILE:HD11	2.49	0.48
13:N:542:VAL:HG11	13:N:558:GLU:CG	2.43	0.48
3:C:60:PHE:HA	3:P:85:ASP:OD2	2.13	0.48
20:Y:384:ARG:HH22	20:Y:415:GLU:HB3	1.77	0.48
3:P:209:LEU:O	3:P:213:ILE:HG12	2.13	0.48
20:X:442:GLN:HG2	20:X:472:GLU:HB2	1.95	0.48
14:O:631:GLN:HE22	14:O:643:LEU:HD13	1.78	0.48
15:R:307:ARG:NH2	15:R:309:LEU:HD21	2.27	0.48
15:R:222:LEU:HG	15:R:223:CYS:SG	2.53	0.48
15:R:382:ILE:CD1	15:R:398:THR:HG22	2.42	0.48
14:O:513:LYS:HE3	14:O:542:GLU:OE2	2.13	0.48
13:N:560:MET:SD	13:N:601:TRP:CD1	3.07	0.48
14:O:657:ILE:HA	14:O:660:LYS:CB	2.43	0.48
13:N:363:TYR:OH	13:N:367:ARG:CZ	2.62	0.48
5:E:102:LEU:HD13	6:H:594:ILE:HG22	1.94	0.48
13:N:331:PHE:CZ	13:N:335:ILE:HD11	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:655:LEU:HD11	13:N:726:ASN:HB2	1.94	0.48
6:H:747:TYR:CZ	6:H:755:LEU:HD23	2.48	0.48
20:X:350:PHE:O	20:X:385:ASN:OD1	2.30	0.48
13:N:202:GLU:OE1	13:N:202:GLU:O	2.30	0.48
8:I:46:LEU:HD22	8:I:56:TRP:NE1	2.28	0.48
1:A:804:ASP:OD1	1:A:804:ASP:N	2.46	0.48
8:I:72:ALA:O	8:I:80:LEU:HD12	2.14	0.48
1:A:504:VAL:HG11	1:A:635:VAL:CG1	2.43	0.48
1:A:776:ASN:HD22	1:A:779:MET:HG2	1.79	0.48
1:A:808:ARG:NH2	1:A:1897:VAL:O	2.46	0.48
15:R:403:CYS:O	15:R:404:ASN:CG	2.51	0.48
13:N:281:TYR:HE2	13:N:356:PRO:HB2	1.77	0.48
15:R:433:LEU:HG	15:R:434:THR:O	2.14	0.48
20:Y:452:LEU:CD2	20:Y:460:LYS:HB2	2.43	0.48
8:I:73:TRP:CH2	8:I:80:LEU:HD22	2.48	0.48
8:I:209:CYS:SG	8:I:577:ASN:HB2	2.54	0.48
8:I:679:ASP:OD1	8:I:703:ARG:NH2	2.46	0.48
8:I:207:ALA:HB3	8:I:220:VAL:HB	1.95	0.48
9:J:320:ARG:HD3	9:J:344:PHE:CZ	2.48	0.48
9:J:324:SER:O	9:J:328:THR:HG23	2.13	0.48
3:C:141:LEU:HD12	3:C:141:LEU:O	2.13	0.48
15:R:417:THR:OG1	15:R:449:LEU:HD23	2.13	0.48
20:X:350:PHE:HZ	20:X:378:LEU:CA	2.26	0.48
20:Y:303:TYR:O	20:Y:304:LEU:HD23	2.14	0.48
8:I:209:CYS:HG	8:I:584:HIS:CE1	2.31	0.48
14:O:669:LYS:NZ	14:O:755:LEU:O	2.47	0.48
1:A:1884:GLN:NE2	1:A:1888:LEU:HD12	2.29	0.48
8:I:116:MET:HE1	8:I:211:SER:O	2.13	0.48
1:A:1172:TYR:CZ	1:A:1176:LEU:HD23	2.48	0.48
2:B:11:VAL:HG13	13:N:642:GLY:HA2	1.96	0.48
20:Y:466:ASN:O	20:Y:470:THR:HG23	2.14	0.48
6:F:492:PRO:O	6:F:493:SER:CB	2.60	0.48
20:X:52:ASN:HD22	20:Y:202:ALA:HB1	1.78	0.48
5:E:87:GLU:N	5:E:87:GLU:OE1	2.47	0.48
15:R:316:VAL:HG22	15:R:317:CYS:O	2.13	0.48
13:N:269:THR:HG23	13:N:292:TRP:CZ3	2.49	0.48
9:J:351:ASP:N	9:J:351:ASP:OD1	2.44	0.48
10:K:181:GLU:HB3	10:K:209:LEU:HD13	1.96	0.48
8:I:56:TRP:CE3	8:I:98:PRO:CB	2.96	0.48
9:J:523:ILE:HD11	3:P:420:TYR:CG	2.49	0.48
9:J:167:PHE:O	9:J:171:THR:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:231:VAL:HG11	8:I:556:LEU:HD12	1.96	0.48
3:C:477:HIS:HD2	3:C:482:GLU:OE1	1.96	0.48
15:R:237:TRP:CD2	15:R:244:VAL:HG22	2.47	0.48
15:R:201:LEU:HD21	15:R:467:LEU:HD21	1.93	0.48
20:X:452:LEU:HD23	20:X:461:ALA:HB2	1.96	0.48
15:R:182:PRO:HG3	16:S:322:ARG:HB3	1.95	0.48
13:N:520:ARG:CG	13:N:557:CYS:SG	3.02	0.48
2:B:23:CYS:HA	2:B:30:PHE:CE1	2.48	0.48
1:A:951:ILE:HD13	1:A:1819:LEU:HD13	1.96	0.48
8:I:289:LYS:HD2	8:I:324:GLN:HE22	1.79	0.48
2:B:83:LYS:O	2:B:84:GLU:HB2	2.13	0.48
1:A:1796:MET:HA	1:A:1817:ILE:HD11	1.95	0.48
1:A:772:GLU:HG3	1:A:867:CYS:HA	1.96	0.48
6:F:118:LEU:CD2	6:F:140:LYS:HB3	2.44	0.48
10:K:230:ASN:OD1	10:K:231:LEU:N	2.46	0.48
15:R:398:THR:HB	15:R:418:HIS:CE1	2.49	0.48
8:I:262:LEU:HD11	8:I:533:ILE:HG21	1.96	0.48
1:A:72:GLU:CG	1:A:94:TYR:OH	2.60	0.48
9:J:191:SER:O	9:J:193:LEU:HG	2.13	0.48
13:N:275:ASP:OD1	13:N:276:ARG:N	2.47	0.48
11:L:21:THR:O	11:L:162:VAL:HG12	2.14	0.48
1:A:23:PHE:HB2	1:A:111:LEU:HD22	1.96	0.48
10:K:167:PHE:O	10:K:171:THR:HG22	2.13	0.48
10:K:417:GLU:HB2	10:K:420:THR:OG1	2.13	0.48
1:A:1078:MET:HB2	1:A:1552:TYR:CE1	2.49	0.48
13:N:662:VAL:HB	13:N:687:MET:SD	2.54	0.47
20:Y:407:LEU:HD13	20:Y:443:THR:HG21	1.96	0.47
1:A:1405:LEU:CD1	1:A:1467:GLY:HA2	2.44	0.47
20:X:93:TYR:CZ	20:X:148:VAL:HG11	2.48	0.47
1:A:154:LEU:HD13	1:A:159:ILE:HG13	1.95	0.47
20:Y:255:ILE:HD11	20:Y:281:TYR:OH	2.14	0.47
8:I:730:VAL:HG22	8:I:731:SER:N	2.29	0.47
3:C:266:VAL:HG12	3:C:289:LEU:HD23	1.96	0.47
6:F:550:VAL:HG21	10:K:289:HIS:CG	2.49	0.47
20:Y:270:ASN:HB2	20:Y:273:LEU:CB	2.44	0.47
3:P:331:VAL:HG11	3:P:364:TYR:CD2	2.49	0.47
14:O:625:LEU:HD12	14:O:625:LEU:C	2.35	0.47
6:F:534:GLU:HA	6:F:568:GLU:OE1	2.14	0.47
3:P:424:ARG:HG3	3:P:424:ARG:NH1	2.30	0.47
1:A:501:THR:HB	1:A:504:VAL:HG22	1.95	0.47
6:H:145:ASN:CB	6:H:146:PRO:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:MET:HE1	1:A:216:PRO:HA	1.96	0.47
6:H:621:LEU:HD13	6:H:625:ARG:HH22	1.79	0.47
15:R:48:PHE:O	15:R:49:ILE:HG13	2.15	0.47
2:B:13:LEU:HD21	13:N:638:LYS:HD2	1.96	0.47
1:A:273:ARG:O	1:A:274:VAL:HG23	2.14	0.47
20:Y:294:PHE:CE1	20:Y:311:TYR:CD1	3.03	0.47
9:J:441:VAL:O	9:J:442:ASP:CB	2.62	0.47
9:J:456:ARG:CG	9:J:488:ILE:HG22	2.44	0.47
1:A:1621:PRO:HG2	1:A:1630:CYS:O	2.15	0.47
3:C:238:TYR:CB	3:C:247:ALA:HB2	2.44	0.47
20:X:365:ALA:CB	20:X:375:ALA:HB1	2.44	0.47
1:A:154:LEU:HD13	1:A:159:ILE:CG1	2.44	0.47
3:P:234:LEU:CD2	3:P:238:TYR:CE2	2.97	0.47
14:O:599:ILE:O	14:O:602:PRO:HD2	2.14	0.47
3:P:478:GLU:CD	3:P:490:TYR:OH	2.53	0.47
1:A:1742:SER:N	1:A:1743:ALA:HB3	2.28	0.47
6:H:629:ARG:NE	10:K:508:LEU:HD21	2.30	0.47
20:X:359:LEU:CG	20:X:379:LYS:HE2	2.43	0.47
15:R:189:TYR:CA	15:R:316:VAL:HB	2.44	0.47
15:R:224:ASP:C	15:R:224:ASP:OD1	2.52	0.47
13:N:574:ILE:HA	13:N:625:LYS:HE2	1.96	0.47
14:O:405:SER:O	14:O:409:HIS:CD2	2.67	0.47
3:C:209:LEU:O	3:C:213:ILE:HG12	2.14	0.47
8:I:49:LEU:HD13	8:I:730:VAL:HG21	1.95	0.47
1:A:250:ASN:OD1	1:A:432:ILE:HD12	2.13	0.47
14:O:39:VAL:HG11	14:O:97:ILE:HG13	1.96	0.47
14:O:341:GLN:HB3	14:O:376:LEU:HD23	1.95	0.47
12:M:5:VAL:HG13	12:M:5:VAL:O	2.14	0.47
1:A:1656:LEU:HD12	1:A:1656:LEU:H	1.78	0.47
20:Y:45:ALA:HB3	20:Y:82:TYR:CE2	2.50	0.47
15:R:435:GLN:NE2	15:R:437:ALA:HB2	2.30	0.47
15:R:459:VAL:HG22	15:R:467:LEU:CD1	2.43	0.47
9:J:178:ALA:HB1	9:J:213:ASN:HD22	1.78	0.47
13:N:501:ILE:HD13	13:N:548:ARG:NH2	2.28	0.47
6:F:96:VAL:HG12	6:F:97:PHE:CD1	2.50	0.47
15:R:184:LEU:CD1	15:R:204:GLY:O	2.62	0.47
20:Y:546:LEU:HD11	20:Y:550:GLN:HE21	1.79	0.47
16:S:361:GLU:O	16:S:365:VAL:HG23	2.14	0.47
1:A:1114:ARG:HB2	1:A:1116:THR:HG23	1.97	0.47
14:O:159:GLN:O	14:O:163:GLN:HG2	2.15	0.47
3:P:441:GLU:HG3	3:P:472:LYS:NZ	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:355:TYR:CE2	20:X:385:ASN:O	2.62	0.47
8:I:349:ILE:HD12	14:O:407:LEU:HA	1.96	0.47
3:C:96:VAL:N	3:C:97:LYS:HA	2.29	0.47
20:X:430:ALA:HB2	20:X:451:CYS:SG	2.55	0.47
3:C:53:LYS:HD3	3:P:96:VAL:HG21	1.96	0.47
14:O:624:VAL:HG11	14:O:647:ALA:HB2	1.96	0.47
20:X:466:ASN:O	20:X:470:THR:HG23	2.14	0.47
6:F:723:LEU:HG	6:F:746:VAL:HG11	1.97	0.47
20:X:359:LEU:CB	20:X:383:LEU:HD21	2.42	0.47
13:N:425:ARG:NH1	13:N:507:SER:HB2	2.28	0.47
20:X:294:PHE:HZ	20:X:308:MET:SD	2.37	0.47
13:N:286:LEU:O	13:N:287:ARG:C	2.52	0.47
15:R:99:LEU:O	15:R:100:LEU:HD23	2.15	0.47
1:A:1421:PRO:HD2	17:T:3:ALA:HB1	1.97	0.47
1:A:174:PRO:O	1:A:295:VAL:C	2.53	0.47
6:F:550:VAL:HG21	10:K:289:HIS:CB	2.44	0.47
3:P:331:VAL:CG1	3:P:364:TYR:CD2	2.97	0.47
6:H:75:LEU:HG	6:H:91:ILE:HD13	1.96	0.47
3:C:308:TYR:CE1	3:C:343:LEU:HG	2.50	0.47
15:R:415:VAL:HG22	15:R:427:VAL:HG22	1.97	0.47
1:A:767:HIS:O	1:A:770:TYR:HB3	2.15	0.47
15:R:189:TYR:HA	15:R:316:VAL:CB	2.45	0.47
13:N:296:VAL:O	13:N:299:TRP:HB3	2.14	0.47
15:R:230:ASP:HB3	15:R:250:LYS:CG	2.45	0.47
13:N:666:ILE:HG12	13:N:681:LEU:HD21	1.97	0.47
8:I:231:VAL:HG21	8:I:557:TYR:CE1	2.49	0.47
2:B:20:ASP:CB	2:B:30:PHE:CE2	2.94	0.47
20:X:451:CYS:O	20:X:455:PRO:HD2	2.15	0.47
20:X:267:LEU:HD11	20:Y:59:LEU:HD13	1.97	0.47
6:F:456:LYS:CB	6:F:460:GLU:OE2	2.62	0.47
4:D:17:TRP:CD1	4:D:17:TRP:C	2.87	0.47
10:K:277:GLU:OE1	10:K:277:GLU:HA	2.15	0.47
13:N:150:ARG:HE	13:N:150:ARG:N	2.13	0.47
15:R:56:ASN:OD1	15:R:56:ASN:N	2.45	0.47
15:R:313:ARG:CD	15:R:333:ASN:H	2.28	0.47
15:R:224:ASP:OD1	15:R:225:LEU:O	2.33	0.47
13:N:527:LEU:HD22	13:N:564:MET:HG3	1.96	0.47
3:P:358:LEU:HD12	3:P:368:TRP:CE2	2.50	0.47
14:O:619:LEU:O	14:O:623:THR:HG22	2.14	0.47
1:A:1313:LEU:HD13	1:A:1316:MET:CG	2.44	0.47
3:P:308:TYR:CE1	3:P:343:LEU:HG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:GLN:C	1:A:466:LEU:HD12	2.35	0.47
1:A:90:ASP:HB3	1:A:591:VAL:HG21	1.96	0.47
13:N:611:VAL:HG12	13:N:639:HIS:CE1	2.50	0.47
6:H:726:LEU:HD11	6:H:742:LEU:HD22	1.97	0.47
1:A:629:LEU:HD22	1:A:633:ILE:HG22	1.97	0.47
5:E:86:VAL:HG13	6:H:588:LYS:HD3	1.97	0.47
10:K:350:HIS:ND1	10:K:377:GLU:OE1	2.48	0.47
1:A:1070:LEU:HD23	1:A:1120:LEU:HG	1.96	0.47
6:H:150:SER:O	6:H:154:SER:OG	2.29	0.47
3:P:242:GLN:HE21	3:P:429:ARG:HA	1.79	0.47
10:K:77:ALA:CB	10:K:93:LEU:HD11	2.45	0.47
1:A:1842:PHE:CD1	1:A:1843:MET:HG3	2.49	0.47
9:J:497:ASN:N	9:J:497:ASN:OD1	2.48	0.47
20:X:37:VAL:N	20:Y:230:VAL:HG21	2.30	0.46
20:Y:400:ILE:HG13	20:Y:401:ARG:N	2.30	0.46
20:X:270:ASN:HB2	20:X:273:LEU:CB	2.45	0.46
20:X:355:TYR:CA	20:X:382:ALA:C	2.63	0.46
13:N:75:PHE:O	13:N:76:VAL:C	2.53	0.46
13:N:556:PHE:CG	13:N:600:PHE:HD1	2.32	0.46
11:L:33:LEU:HD13	11:L:54:TRP:CD2	2.49	0.46
3:C:93:TYR:CD1	3:P:53:LYS:HD2	2.50	0.46
20:X:458:GLN:O	20:X:462:LYS:HG3	2.15	0.46
6:H:481:CYS:SG	6:H:512:LEU:HB2	2.55	0.46
1:A:184:LYS:N	1:A:251:THR:HG22	2.30	0.46
6:H:594:ILE:HD11	6:H:604:TYR:HA	1.96	0.46
1:A:1114:ARG:HD3	16:S:401:CYS:O	2.16	0.46
10:K:268:LEU:N	10:K:269:PRO:HD2	2.30	0.46
20:Y:451:CYS:O	20:Y:455:PRO:HD2	2.15	0.46
3:P:392:ILE:HD12	3:P:402:TRP:CH2	2.50	0.46
13:N:528:LEU:CD1	13:N:641:LEU:HD13	2.45	0.46
10:K:495:PHE:CE1	10:K:525:MET:HG2	2.50	0.46
14:O:657:ILE:CG1	14:O:704:VAL:HG23	2.45	0.46
1:A:1421:PRO:HD3	17:T:3:ALA:HB1	1.98	0.46
14:O:126:VAL:HG13	14:O:132:VAL:HG12	1.98	0.46
3:P:68:ALA:O	3:P:69:GLU:CB	2.64	0.46
15:R:313:ARG:CG	15:R:333:ASN:H	2.24	0.46
20:Y:452:LEU:HD23	20:Y:461:ALA:HB2	1.96	0.46
6:F:130:ARG:HD3	20:Y:506:GLN:HB2	1.97	0.46
2:B:27:ARG:HB2	16:S:375:LEU:HD23	1.97	0.46
10:K:185:LEU:HD21	10:K:205:PHE:HB3	1.98	0.46
3:C:89:LEU:HD21	3:C:93:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1531:GLY:HA2	1:A:1565:LEU:HB3	1.98	0.46
2:B:15:LEU:O	2:B:17:VAL:HG23	2.15	0.46
6:H:86:ALA:HA	10:K:473:VAL:CG1	2.44	0.46
8:I:69:THR:HG23	8:I:85:ALA:HB2	1.98	0.46
1:A:255:ILE:HA	1:A:269:TRP:O	2.16	0.46
20:Y:376:LEU:HD11	20:Y:398:GLU:OE2	2.16	0.46
3:P:274:HIS:O	3:P:276:ILE:O	2.32	0.46
10:K:217:GLU:O	10:K:218:THR:OG1	2.20	0.46
20:Y:212:LEU:O	20:Y:213:SER:CB	2.63	0.46
20:X:363:ALA:HB2	20:X:379:LYS:CE	2.43	0.46
15:R:316:VAL:HG22	15:R:317:CYS:C	2.36	0.46
1:A:1637:LEU:CD1	1:A:1665:GLN:HE21	2.21	0.46
3:P:392:ILE:CD1	3:P:402:TRP:CZ2	2.99	0.46
2:B:20:ASP:O	2:B:30:PHE:HD2	1.98	0.46
8:I:289:LYS:O	8:I:293:GLU:CB	2.63	0.46
3:P:307:LEU:HD23	3:P:316:LEU:HD23	1.96	0.46
1:A:269:TRP:CZ3	1:A:411:HIS:HB2	2.51	0.46
20:X:376:LEU:HD11	20:X:398:GLU:OE2	2.15	0.46
1:A:1078:MET:SD	1:A:1078:MET:N	2.88	0.46
14:O:694:LEU:HD13	14:O:713:VAL:HG22	1.98	0.46
1:A:21:VAL:HG23	1:A:25:ARG:NH2	2.30	0.46
3:C:255:ILE:HG12	3:C:260:SER:HA	1.97	0.46
20:X:212:LEU:O	20:X:213:SER:CB	2.63	0.46
9:J:180:GLU:O	9:J:184:LEU:N	2.36	0.46
10:K:351:ASP:N	10:K:351:ASP:OD1	2.42	0.46
6:H:152:PHE:CD1	6:H:152:PHE:C	2.88	0.46
6:F:653:LEU:O	6:F:656:MET:HG2	2.16	0.46
1:A:845:TYR:CD1	1:A:951:ILE:HD11	2.51	0.46
4:D:10:PRO:HG2	14:O:346:TRP:CE2	2.50	0.46
1:A:170:ILE:HG22	1:A:171:ALA:O	2.15	0.46
3:C:478:GLU:CD	3:C:490:TYR:OH	2.54	0.46
13:N:400:TYR:CZ	13:N:404:ILE:HD11	2.50	0.46
8:I:219:VAL:N	8:I:234:PHE:O	2.47	0.46
3:P:344:ARG:CZ	3:P:344:ARG:HB3	2.46	0.46
20:X:355:TYR:CB	20:X:383:LEU:CA	2.88	0.46
15:R:370:LEU:HD13	15:R:407:TRP:CH2	2.50	0.46
15:R:225:LEU:HD21	15:R:248:THR:CG2	2.45	0.46
6:F:699:ASP:HB3	6:F:702:ASN:OD1	2.16	0.46
6:F:145:ASN:OD1	6:F:145:ASN:N	2.48	0.46
15:R:458:ILE:HG12	15:R:472:VAL:CG2	2.46	0.46
4:D:12:VAL:O	4:D:13:THR:OG1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:LEU:HD12	1:A:853:LYS:N	2.30	0.46
1:A:1897:VAL:O	1:A:1897:VAL:HG23	2.16	0.46
6:F:723:LEU:CD2	6:F:746:VAL:HG11	2.45	0.46
13:N:400:TYR:CE1	13:N:404:ILE:HD11	2.51	0.46
8:I:206:LEU:HD22	8:I:570:PHE:CG	2.50	0.46
13:N:148:GLY:HA3	13:N:152:GLU:OE2	2.15	0.46
20:Y:83:HIS:O	20:Y:86:SER:OG	2.20	0.46
6:F:462:LEU:HD23	6:H:8:VAL:HG21	1.98	0.46
3:C:420:TYR:CD2	14:O:275:LEU:HD23	2.51	0.46
8:I:607:ILE:HD12	8:I:607:ILE:H	1.81	0.46
14:O:527:LEU:O	14:O:527:LEU:HD12	2.15	0.46
15:R:230:ASP:HB3	15:R:250:LYS:HG3	1.97	0.46
13:N:619:LEU:HG	13:N:637:TRP:CH2	2.50	0.46
4:D:8:LEU:HD23	14:O:420:ILE:HD11	1.97	0.46
20:Y:458:GLN:O	20:Y:462:LYS:HG3	2.15	0.46
14:O:75:VAL:HG13	14:O:165:ASP:CG	2.36	0.46
10:K:19:TYR:CE1	10:K:49:LEU:HD13	2.51	0.46
3:C:409:TYR:CB	3:C:418:CYS:HB3	2.45	0.46
6:H:492:PRO:O	6:H:493:SER:HB3	2.16	0.46
3:P:441:GLU:HG3	3:P:472:LYS:CE	2.45	0.46
20:Y:269:ASP:HB3	20:Y:300:LEU:HD21	1.98	0.46
13:N:280:GLU:O	13:N:354:SER:HA	2.16	0.46
11:L:33:LEU:CD2	11:L:64:VAL:HG13	2.46	0.46
1:A:1279:ARG:HG2	1:A:1280:PRO:HD2	1.98	0.46
3:C:352:LEU:C	3:C:352:LEU:HD23	2.35	0.46
1:A:776:ASN:O	1:A:777:THR:HB	2.16	0.46
1:A:1364:CYS:N	1:A:1365:PRO:CD	2.78	0.46
8:I:52:PHE:HD1	8:I:743:VAL:HG21	1.81	0.46
9:J:247:PHE:CZ	9:J:277:GLU:HG3	2.51	0.46
20:X:261:LEU:HD22	20:X:267:LEU:HD23	1.97	0.46
3:P:47:GLY:O	3:P:49:LEU:HD12	2.15	0.46
1:A:1057:LEU:HA	1:A:1061:GLU:OE1	2.16	0.46
20:X:255:ILE:HD11	20:X:281:TYR:OH	2.16	0.46
9:J:230:ASN:OD1	9:J:231:LEU:N	2.48	0.46
6:F:65:SER:N	20:Y:296:GLN:HE22	2.14	0.46
10:K:376:LEU:HG	10:K:407:GLU:OE1	2.16	0.46
1:A:1242:GLU:HG3	1:A:1242:GLU:O	2.16	0.46
13:N:292:TRP:CZ3	13:N:296:VAL:HG21	2.51	0.46
15:R:225:LEU:HD12	15:R:230:ASP:O	2.04	0.46
15:R:382:ILE:HD11	15:R:398:THR:HG22	1.98	0.46
20:Y:496:ILE:HD13	20:Y:519:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:676:TRP:CZ3	13:N:684:ALA:HB2	2.51	0.46
20:Y:222:MET:O	20:Y:226:VAL:HG23	2.16	0.46
6:H:730:LYS:HD3	6:H:740:TYR:CE1	2.46	0.46
1:A:1181:LEU:HB3	1:A:1611:VAL:HG11	1.97	0.46
20:X:517:ASP:O	20:X:520:VAL:HG22	2.16	0.46
1:A:1049:VAL:HG23	1:A:1069:ARG:HG2	1.97	0.46
10:K:300:VAL:HG12	10:K:333:TYR:OH	2.15	0.46
15:R:229:GLY:O	15:R:249:HIS:HD2	1.93	0.45
20:X:400:ILE:HG13	20:X:401:ARG:N	2.31	0.45
11:L:98:VAL:CG1	11:L:108:ILE:HD13	2.45	0.45
1:A:95:VAL:HG13	1:A:100:VAL:CG2	2.46	0.45
6:F:726:LEU:HD11	6:F:742:LEU:HD22	1.98	0.45
9:J:295:TYR:OH	10:K:54:HIS:HB2	2.17	0.45
5:E:67:LEU:HD22	20:Y:342:TRP:HH2	1.81	0.45
3:C:180:ARG:HG3	3:C:212:LEU:HD21	1.98	0.45
14:O:706:CYS:HB3	14:O:709:ARG:HB3	1.97	0.45
1:A:286:SER:O	1:A:290:GLY:N	2.42	0.45
15:R:339:VAL:CG1	15:R:387:THR:HG23	2.45	0.45
13:N:519:TYR:CD2	13:N:554:MET:SD	3.09	0.45
3:C:36:LEU:HD21	3:C:58:LEU:CB	2.44	0.45
1:A:42:LEU:HD23	3:C:142:GLU:CG	2.46	0.45
20:Y:93:TYR:CZ	20:Y:148:VAL:HG11	2.50	0.45
9:J:485:ILE:HD12	9:J:501:TYR:CE1	2.51	0.45
9:J:478:ASN:OD1	9:J:479:ALA:N	2.49	0.45
1:A:259:TYR:OH	1:A:424:ASN:O	2.17	0.45
12:M:9:GLY:HA3	3:P:329:TYR:CG	2.52	0.45
20:X:425:GLU:O	20:X:429:MET:HE2	2.17	0.45
1:A:47:GLU:OE1	1:A:48:LEU:N	2.39	0.45
3:C:526:TRP:HE1	3:C:556:LEU:HD23	1.79	0.45
3:C:48:LEU:HD23	3:C:48:LEU:N	2.31	0.45
13:N:245:GLN:O	13:N:249:ARG:HG3	2.17	0.45
20:Y:506:GLN:HG3	20:Y:508:ASP:OD1	2.17	0.45
14:O:105:LEU:HD11	14:O:151:VAL:HG12	1.99	0.45
9:J:247:PHE:HB3	9:J:278:LEU:HD21	1.97	0.45
10:K:373:TYR:CE1	19:W:4:ARG:HG2	2.52	0.45
20:X:336:ASP:OD1	20:X:337:GLN:N	2.36	0.45
6:F:674:HIS:O	6:F:678:VAL:HG23	2.16	0.45
14:O:33:TYR:CE2	14:O:37:VAL:HG21	2.51	0.45
11:L:125:THR:CA	11:L:126:ASP:HB3	2.44	0.45
6:F:130:ARG:HH11	20:Y:506:GLN:HB3	1.81	0.45
9:J:271:HIS:O	9:J:274:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:294:PHE:CZ	20:Y:311:TYR:CG	3.05	0.45
15:R:458:ILE:HG12	15:R:472:VAL:CG1	2.47	0.45
1:A:32:PRO:O	1:A:33:ASN:HB3	2.16	0.45
9:J:397:ILE:HG22	9:J:398:ALA:H	1.81	0.45
3:P:119:MET:HG2	3:P:158:LEU:HD21	1.98	0.45
3:C:153:GLU:O	3:C:157:GLU:HG2	2.17	0.45
1:A:658:ASN:O	1:A:662:THR:HG23	2.17	0.45
13:N:659:VAL:HG22	13:N:663:GLN:HB2	1.98	0.45
20:Y:519:LEU:HD13	20:Y:527:GLU:CB	2.46	0.45
16:S:374:SER:OG	16:S:387:TYR:O	2.33	0.45
15:R:458:ILE:HG13	15:R:472:VAL:HG11	1.98	0.45
9:J:322:TYR:CE1	12:M:31:ILE:HD13	2.52	0.45
10:K:349:GLU:OE1	15:R:150:LEU:HD22	2.17	0.45
12:M:9:GLY:HA3	3:P:329:TYR:CB	2.46	0.45
16:S:379:ILE:HG21	16:S:410:LEU:HB3	1.99	0.45
20:Y:517:ASP:O	20:Y:520:VAL:HG22	2.16	0.45
1:A:1480:GLU:HA	1:A:1527:MET:HB3	1.98	0.45
10:K:383:ASN:HB3	10:K:386:LEU:HD13	1.99	0.45
15:R:146:SER:N	15:R:147:PRO:HD3	2.32	0.45
3:P:128:LYS:HA	3:P:128:LYS:HE3	1.98	0.45
15:R:292:MET:HG3	15:R:307:ARG:NH2	2.32	0.45
15:R:407:TRP:HA	15:R:414:LEU:CD1	2.47	0.45
15:R:353:GLU:HG3	15:R:385:TRP:HH2	1.82	0.45
2:B:8:TRP:HD1	13:N:644:VAL:HG12	1.72	0.45
20:X:294:PHE:CE1	20:X:311:TYR:CG	3.05	0.45
6:F:537:GLU:OE1	6:F:600:TYR:CE2	2.70	0.45
20:Y:100:TYR:HB2	20:Y:142:LEU:HD13	1.99	0.45
6:F:755:LEU:HA	6:F:755:LEU:HD12	1.87	0.45
8:I:26:LEU:CB	8:I:37:LEU:HB3	2.46	0.45
10:K:509:ARG:HG3	10:K:509:ARG:O	2.16	0.45
20:X:168:THR:HB	20:X:169:PRO:HD2	1.98	0.45
8:I:245:LEU:HB3	8:I:246:PRO:HD3	1.97	0.45
1:A:1821:LEU:HD21	1:A:1852:LYS:HB2	1.99	0.45
20:Y:77:TYR:CE1	20:Y:107:LYS:HB2	2.51	0.45
3:C:30:ARG:O	3:C:30:ARG:HG3	2.16	0.45
13:N:285:PHE:O	13:N:289:PHE:CD2	2.69	0.45
15:R:406:ALA:C	15:R:414:LEU:CD1	2.82	0.45
15:R:233:THR:HG21	15:R:249:HIS:HA	1.99	0.45
13:N:522:LEU:HD13	13:N:523:LEU:HD23	1.99	0.45
1:A:1232:ILE:HD11	1:A:1235:LEU:HD22	1.98	0.45
20:X:506:GLN:HG3	20:X:508:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:386:LEU:HD21	13:N:399:LEU:HD22	1.99	0.45
6:F:553:SER:HA	6:F:576:CYS:SG	2.57	0.45
9:J:294:LEU:HD12	10:K:54:HIS:NE2	2.31	0.45
1:A:1420:LEU:HG	17:T:3:ALA:HB2	1.99	0.45
13:N:570:ILE:HA	13:N:573:ASN:ND2	2.32	0.45
15:R:191:ASN:O	15:R:234:SER:HA	2.17	0.45
20:X:77:TYR:CE1	20:X:107:LYS:HB2	2.52	0.45
15:R:202:SER:HB2	15:R:211:LEU:CD2	2.47	0.45
20:X:519:LEU:HD13	20:X:527:GLU:CB	2.47	0.45
20:X:496:ILE:HD13	20:X:519:LEU:HD23	1.99	0.45
13:N:560:MET:HE1	13:N:601:TRP:CD1	2.52	0.45
8:I:70:CYS:C	8:I:71:LEU:HD12	2.37	0.45
15:R:251:GLY:O	15:R:270:HIS:HB2	2.17	0.45
7:G:23:ARG:CG	9:J:525:MET:HE1	2.47	0.45
9:J:354:MET:HE1	9:J:374:ILE:HA	1.97	0.45
1:A:1313:LEU:HD13	1:A:1316:MET:HB2	1.99	0.45
1:A:430:VAL:HG12	1:A:444:PHE:HA	1.98	0.45
9:J:297:SER:O	9:J:329:LEU:HD11	2.17	0.45
1:A:1160:TYR:OH	14:O:337:HIS:ND1	2.44	0.45
20:Y:261:LEU:HD22	20:Y:267:LEU:HD23	1.99	0.45
6:H:723:LEU:CD2	6:H:746:VAL:HG11	2.45	0.45
1:A:1205:SER:O	1:A:1209:LEU:HG	2.17	0.45
3:P:266:VAL:HG12	3:P:289:LEU:HD23	1.98	0.45
13:N:292:TRP:CH2	13:N:296:VAL:HG21	2.52	0.45
14:O:292:GLY:HA3	14:O:336:ASP:HB3	1.99	0.45
13:N:386:LEU:O	13:N:388:HIS:HB3	2.16	0.45
15:R:94:LEU:CD1	15:R:161:LEU:HD21	2.46	0.45
1:A:1276:GLU:HB3	1:A:1294:TYR:HE1	1.82	0.45
14:O:532:VAL:HA	14:O:535:ILE:HD12	1.98	0.45
1:A:939:PHE:CZ	1:A:944:LEU:HB2	2.52	0.45
3:P:238:TYR:CB	3:P:247:ALA:HB2	2.47	0.45
3:P:251:TYR:CZ	3:P:268:GLN:HG3	2.52	0.45
14:O:631:GLN:OE1	14:O:640:ALA:HA	2.17	0.45
6:H:754:HIS:CE1	6:H:755:LEU:HD13	2.52	0.45
3:C:480:LEU:O	3:C:482:GLU:N	2.49	0.45
3:C:478:GLU:OE2	3:C:490:TYR:OH	2.35	0.45
6:H:723:LEU:HG	6:H:746:VAL:HG11	1.99	0.45
3:P:180:ARG:HG3	3:P:212:LEU:HD21	1.99	0.45
14:O:699:ASN:O	14:O:702:ALA:HB3	2.17	0.45
10:K:145:ASN:HB3	10:K:148:LEU:HB2	1.99	0.45
3:P:48:LEU:HD23	3:P:48:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:403:TYR:C	3:C:403:TYR:CD1	2.90	0.45
20:X:350:PHE:HD1	20:X:382:ALA:HA	1.79	0.45
15:R:267:LEU:HB3	15:R:296:ARG:HH11	1.65	0.45
15:R:230:ASP:HA	15:R:250:LYS:HG3	1.99	0.45
13:N:512:LYS:HG2	13:N:549:PHE:CZ	2.52	0.45
4:D:54:ILE:HG12	9:J:506:LEU:HD23	1.99	0.45
6:F:149:TRP:CZ3	6:F:152:PHE:CD2	3.05	0.45
8:I:73:TRP:CG	8:I:80:LEU:HD13	2.52	0.45
6:H:707:PHE:CD1	6:H:707:PHE:C	2.91	0.45
1:A:1236:LEU:HD12	15:R:161:LEU:CD1	2.47	0.45
13:N:501:ILE:HD12	13:N:501:ILE:N	2.32	0.45
20:X:235:TRP:CZ2	20:Y:59:LEU:HD11	2.53	0.45
9:J:376:LEU:CD2	9:J:407:GLU:HG2	2.46	0.45
11:L:111:LEU:HD11	11:L:122:VAL:HG22	1.99	0.45
13:N:552:ALA:HB3	13:N:553:PRO:HD3	1.98	0.45
8:I:639:LEU:HB2	8:I:652:VAL:HG12	1.98	0.45
8:I:13:VAL:HG22	8:I:744:PHE:CE2	2.52	0.45
11:L:98:VAL:HG11	11:L:108:ILE:HD13	1.98	0.44
20:Y:503:LEU:HD12	20:Y:515:LEU:HD13	1.98	0.44
20:X:100:TYR:CB	20:X:142:LEU:HD21	2.42	0.44
10:K:276:VAL:HA	10:K:311:MET:CE	2.47	0.44
20:Y:349:SER:CB	20:Y:358:ALA:HB2	2.45	0.44
1:A:1236:LEU:CB	15:R:153:VAL:HG21	2.47	0.44
20:X:271:VAL:CG1	20:X:304:LEU:CD2	2.95	0.44
14:O:114:ASP:CA	14:O:117:ASP:OD1	2.64	0.44
9:J:322:TYR:CZ	12:M:31:ILE:HD13	2.52	0.44
6:F:492:PRO:O	6:F:493:SER:HB3	2.16	0.44
9:J:413:PHE:CD1	9:J:454:VAL:HG12	2.53	0.44
20:X:491:LYS:C	20:X:494:ASP:OD1	2.54	0.44
15:R:467:LEU:HD23	16:S:325:LEU:HD22	1.99	0.44
1:A:1274:LEU:HG	1:A:1302:LEU:HD11	1.99	0.44
20:Y:474:ASP:OD2	20:Y:505:ASN:ND2	2.51	0.44
9:J:281:ALA:CA	9:J:311:MET:CE	2.93	0.44
3:C:360:LEU:HD23	12:M:14:LEU:HD13	2.00	0.44
1:A:93:LEU:HB2	1:A:128:TRP:CH2	2.52	0.44
1:A:1469:CYS:HB2	1:A:1488:LEU:CD2	2.47	0.44
13:N:655:LEU:HA	13:N:724:ARG:O	2.17	0.44
1:A:249:LEU:HD12	1:A:250:ASN:N	2.31	0.44
8:I:360:LEU:HD21	8:I:390:ILE:HG23	1.98	0.44
20:Y:336:ASP:OD1	20:Y:337:GLN:N	2.41	0.44
8:I:617:ALA:O	8:I:618:ILE:HD13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:359:VAL:HG13	14:O:360:LEU:HD12	1.99	0.44
1:A:1675:GLU:CG	1:A:1676:LEU:N	2.80	0.44
15:R:106:LYS:HE3	15:R:106:LYS:HA	2.00	0.44
13:N:76:VAL:O	13:N:80:GLN:HB3	2.17	0.44
13:N:120:SER:O	13:N:124:PRO:HD3	2.13	0.44
1:A:1191:LEU:HD12	15:R:59:VAL:HA	1.99	0.44
1:A:1233:PRO:HA	1:A:1236:LEU:CD2	2.47	0.44
9:J:185:LEU:HD11	9:J:205:PHE:HB2	1.99	0.44
13:N:276:ARG:O	13:N:277:CYS:C	2.55	0.44
12:M:11:ILE:HG23	12:M:15:ILE:CD1	2.47	0.44
6:H:761:SER:O	6:H:765:ASP:CB	2.64	0.44
6:F:540:SER:OG	6:F:575:ASN:ND2	2.33	0.44
1:A:1399:VAL:HG11	1:A:1404:LEU:HG	1.99	0.44
10:K:42:TRP:CE3	10:K:42:TRP:HA	2.51	0.44
10:K:497:ASN:N	10:K:497:ASN:OD1	2.51	0.44
13:N:180:PHE:CE2	13:N:240:PHE:HB3	2.51	0.44
8:I:32:ARG:CD	13:N:388:HIS:CE1	3.00	0.44
10:K:284:LEU:HD12	10:K:311:MET:CE	2.48	0.44
1:A:1477:ALA:HB1	1:A:1574:LEU:HD12	2.00	0.44
20:Y:417:TYR:CD2	20:Y:429:MET:CE	3.01	0.44
14:O:706:CYS:O	14:O:708:GLU:N	2.50	0.44
6:F:594:ILE:HD11	6:F:604:TYR:HA	1.97	0.44
1:A:1047:VAL:O	1:A:1109:GLY:HA2	2.17	0.44
13:N:122:LEU:O	13:N:126:LEU:CB	2.65	0.44
1:A:39:LEU:HD12	14:O:248:PRO:HB3	1.99	0.44
13:N:102:ALA:HA	13:N:107:CYS:C	2.37	0.44
13:N:520:ARG:HG3	13:N:557:CYS:SG	2.58	0.44
6:F:533:VAL:HB	6:F:562:MET:HE1	2.00	0.44
13:N:681:LEU:HD22	13:N:713:PHE:CZ	2.52	0.44
14:O:652:LEU:HA	14:O:660:LYS:HG3	2.00	0.44
6:F:726:LEU:HD11	6:F:742:LEU:CD2	2.47	0.44
6:H:656:MET:O	6:H:660:LYS:HG3	2.18	0.44
14:O:127:HIS:O	14:O:128:LYS:HB3	2.17	0.44
1:A:1134:TRP:CD2	1:A:1203:MET:HE1	2.52	0.44
20:X:355:TYR:HD1	20:X:382:ALA:O	1.26	0.44
13:N:425:ARG:HG2	13:N:425:ARG:NH1	2.32	0.44
11:L:113:LEU:HB3	11:L:116:PRO:HG3	2.00	0.44
1:A:1276:GLU:CD	1:A:1294:TYR:HH	2.21	0.44
1:A:793:LEU:HD23	1:A:793:LEU:C	2.37	0.44
12:M:12:LEU:HD13	3:P:360:LEU:HD23	1.99	0.44
15:R:429:LYS:HD3	15:R:433:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:437:LEU:HD22	20:Y:444:LEU:CD2	2.47	0.44
14:O:416:GLU:O	14:O:420:ILE:HG22	2.18	0.44
20:X:474:ASP:OD2	20:X:505:ASN:ND2	2.50	0.44
6:H:110:PHE:CD2	6:H:117:THR:HG21	2.52	0.44
20:Y:271:VAL:CG1	20:Y:304:LEU:CD2	2.96	0.44
20:X:222:MET:O	20:X:226:VAL:HG23	2.18	0.44
10:K:288:SER:HB3	12:M:57:TRP:CZ3	2.53	0.44
14:O:669:LYS:HE3	14:O:751:LEU:HD13	1.99	0.44
3:C:60:PHE:CG	3:P:89:LEU:HD12	2.53	0.44
6:H:486:ASN:O	6:H:490:HIS:HD2	2.01	0.44
14:O:643:LEU:C	14:O:643:LEU:HD23	2.38	0.44
3:P:441:GLU:HG3	3:P:472:LYS:HZ1	1.81	0.44
1:A:759:ILE:N	1:A:760:PRO:HD2	2.32	0.44
13:N:75:PHE:CG	13:N:79:LEU:HD23	2.53	0.44
9:J:445:GLU:CG	9:J:446:PRO:HD3	2.33	0.44
4:D:8:LEU:CD2	14:O:420:ILE:HD11	2.47	0.44
14:O:467:ALA:HB1	14:O:506:LEU:CD1	2.47	0.44
20:X:294:PHE:CD1	20:X:311:TYR:CE1	3.06	0.44
1:A:1623:ASP:O	1:A:1624:VAL:HB	2.18	0.44
8:I:167:LEU:HD12	8:I:168:LEU:N	2.32	0.44
20:X:281:TYR:HB3	20:X:290:SER:OG	2.18	0.44
3:C:119:MET:HG2	3:C:158:LEU:HD21	2.00	0.44
6:F:758:MET:O	6:F:762:TRP:CD1	2.70	0.44
5:E:105:PHE:HD1	10:K:510:ARG:HD3	1.83	0.44
1:A:1699:VAL:HG23	1:A:1699:VAL:O	2.18	0.44
1:A:1053:GLN:OE1	1:A:1053:GLN:N	2.51	0.44
14:O:143:TYR:CD1	14:O:143:TYR:C	2.91	0.44
15:R:316:VAL:HG13	15:R:316:VAL:O	2.12	0.44
16:S:375:LEU:HD22	16:S:375:LEU:N	2.33	0.44
6:H:726:LEU:HD11	6:H:742:LEU:CD2	2.48	0.44
9:J:281:ALA:CA	9:J:311:MET:HE1	2.48	0.44
8:I:101:LEU:HD21	8:I:168:LEU:HD11	2.00	0.44
6:H:545:HIS:HE1	11:L:182:SER:O	2.01	0.44
14:O:631:GLN:HB2	14:O:640:ALA:HB2	2.00	0.44
20:X:417:TYR:CD2	20:X:429:MET:CE	3.01	0.44
1:A:1502:PRO:O	1:A:1503:ASN:CB	2.65	0.44
14:O:129:THR:O	14:O:130:SER:CB	2.64	0.44
1:A:254:SER:OG	1:A:271:LEU:HB2	2.18	0.44
6:F:42:PHE:HB2	6:F:71:CYS:SG	2.57	0.44
3:C:483:SER:HA	3:C:515:TYR:OH	2.18	0.44
9:J:337:TRP:HB3	9:J:360:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:338:ILE:HG23	10:K:342:HIS:CE1	2.53	0.44
13:N:511:SER:O	13:N:512:LYS:CG	2.55	0.43
8:I:224:SER:HB3	8:I:229:SER:HA	1.98	0.43
20:X:503:LEU:HD12	20:X:515:LEU:HD13	1.99	0.43
6:H:553:SER:HA	6:H:576:CYS:SG	2.58	0.43
9:J:19:TYR:CE1	9:J:49:LEU:HD13	2.53	0.43
5:E:67:LEU:HD22	20:Y:342:TRP:CH2	2.53	0.43
1:A:39:LEU:CD1	14:O:248:PRO:HB3	2.47	0.43
6:F:58:TYR:OH	6:F:87:GLU:OE1	2.35	0.43
20:X:355:TYR:CB	20:X:382:ALA:C	2.78	0.43
20:Y:343:VAL:HG13	20:Y:378:LEU:HD22	2.00	0.43
13:N:75:PHE:O	13:N:77:GLU:C	2.57	0.43
20:X:452:LEU:HB3	20:X:461:ALA:HB2	2.00	0.43
20:X:201:LEU:O	20:X:203:LEU:N	2.52	0.43
1:A:1134:TRP:CE2	1:A:1203:MET:HE2	2.53	0.43
20:X:181:LYS:HE3	20:X:370:SER:HB2	2.00	0.43
6:F:67:THR:HG21	20:Y:263:LYS:HD3	2.00	0.43
14:O:215:PHE:C	14:O:215:PHE:CD1	2.90	0.43
20:X:350:PHE:HE1	20:X:378:LEU:O	1.86	0.43
20:Y:45:ALA:HB2	20:Y:82:TYR:CD2	2.52	0.43
11:L:108:ILE:HD12	11:L:125:THR:O	2.19	0.43
3:P:389:ARG:HA	3:P:392:ILE:CG2	2.48	0.43
14:O:75:VAL:HG13	14:O:165:ASP:HB2	2.00	0.43
11:L:141:VAL:HG11	11:L:151:THR:HG21	2.00	0.43
1:A:625:ILE:O	1:A:629:LEU:HG	2.17	0.43
6:H:592:ARG:HA	6:H:592:ARG:HD3	1.80	0.43
10:K:509:ARG:CG	10:K:512:ASP:HB2	2.48	0.43
1:A:659:LEU:HD12	1:A:659:LEU:C	2.38	0.43
1:A:961:HIS:ND1	1:A:964:GLU:OE2	2.51	0.43
6:H:531:TYR:O	6:H:562:MET:CE	2.66	0.43
10:K:163:CYS:SG	10:K:163:CYS:O	2.77	0.43
15:R:429:LYS:HB2	15:R:433:LEU:HD23	1.97	0.43
20:Y:491:LYS:C	20:Y:494:ASP:OD1	2.54	0.43
15:R:182:PRO:CB	16:S:322:ARG:HB2	2.48	0.43
20:X:437:LEU:HD22	20:X:444:LEU:CD2	2.49	0.43
15:R:400:SER:OG	15:R:422:GLN:CG	2.67	0.43
15:R:94:LEU:O	15:R:98:GLU:HG2	2.18	0.43
20:Y:549:MET:O	20:Y:552:MET:HG3	2.19	0.43
1:A:1265:ALA:HB2	1:A:1309:HIS:HD2	1.84	0.43
1:A:256:VAL:O	1:A:268:VAL:HA	2.17	0.43
13:N:655:LEU:HD12	13:N:724:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:747:TYR:CE2	6:H:755:LEU:HD23	2.53	0.43
8:I:116:MET:SD	8:I:210:LEU:HG	2.58	0.43
20:Y:475:TYR:CE1	20:Y:477:LYS:HB2	2.53	0.43
19:W:14:ASP:OD1	19:W:14:ASP:N	2.52	0.43
15:R:404:ASN:HB3	15:R:449:LEU:CD2	2.15	0.43
6:F:128:THR:O	6:F:129:ASP:CB	2.66	0.43
1:A:1239:THR:HG23	1:A:1241:THR:HG23	2.01	0.43
15:R:94:LEU:HD11	15:R:161:LEU:HD21	2.00	0.43
3:P:36:LEU:HD21	3:P:58:LEU:CB	2.48	0.43
15:R:146:SER:N	15:R:147:PRO:CD	2.81	0.43
3:P:297:ILE:HG21	3:P:330:ARG:NH1	2.34	0.43
14:O:583:VAL:O	14:O:587:VAL:HG23	2.19	0.43
1:A:1060:HIS:O	1:A:1063:ILE:HG22	2.19	0.43
14:O:312:CYS:SG	14:O:350:LEU:HD21	2.58	0.43
15:R:160:LEU:O	15:R:160:LEU:HD12	2.18	0.43
20:X:309:ASP:OD1	20:X:343:VAL:HG11	2.19	0.43
20:X:203:LEU:HA	20:X:206:ILE:HD12	1.99	0.43
20:X:229:THR:CG2	20:X:233:LEU:HD12	2.47	0.43
14:O:64:LEU:HD12	14:O:65:LEU:N	2.33	0.43
20:Y:334:ILE:HG13	20:Y:335:SER:N	2.34	0.43
10:K:153:TYR:CE1	10:K:169:LEU:HD13	2.53	0.43
15:R:270:HIS:CD2	15:R:294:LEU:HD12	2.53	0.43
15:R:295:GLN:O	15:R:304:GLN:HA	2.18	0.43
1:A:213:MET:HE2	1:A:216:PRO:HA	2.00	0.43
6:H:639:TYR:CZ	6:H:643:MET:SD	3.12	0.43
15:R:48:PHE:O	15:R:49:ILE:CG1	2.67	0.43
13:N:612:PRO:HB3	13:N:665:VAL:HG23	2.00	0.43
1:A:1080:LEU:HB2	1:A:1081:PRO:HD3	1.99	0.43
1:A:1758:CYS:O	1:A:1771:LEU:HD21	2.18	0.43
8:I:266:ASN:HA	8:I:526:LYS:NZ	2.33	0.43
13:N:589:PHE:O	13:N:591:VAL:HG13	2.18	0.43
20:X:347:CYS:N	20:X:378:LEU:HD21	2.34	0.43
20:X:355:TYR:HD1	20:X:382:ALA:CA	2.26	0.43
15:R:196:SER:HB3	15:R:237:TRP:CD2	2.54	0.43
1:A:1191:LEU:HD21	15:R:62:HIS:CE1	2.53	0.43
14:O:114:ASP:C	14:O:117:ASP:OD1	2.56	0.43
13:N:304:PHE:CD1	13:N:324:TRP:HH2	2.37	0.43
1:A:173:LEU:HA	1:A:174:PRO:HD2	1.88	0.43
6:F:118:LEU:HD21	6:F:140:LYS:HB3	2.01	0.43
9:J:129:LYS:O	9:J:132:ILE:HG22	2.19	0.43
15:R:431:PRO:CB	15:R:432:SER:C	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:78:VAL:O	13:N:80:GLN:C	2.50	0.43
20:X:449:THR:HG21	20:X:465:LEU:HA	2.01	0.43
13:N:559:VAL:HG11	13:N:600:PHE:CE1	2.54	0.43
11:L:13:PRO:HG3	11:L:78:CYS:SG	2.59	0.43
1:A:1624:VAL:HG22	1:A:1698:TYR:HB3	2.01	0.43
9:J:214:LYS:HD2	9:J:400:GLU:OE2	2.19	0.43
3:C:521:PHE:HD1	3:C:553:ILE:HG22	1.82	0.43
1:A:944:LEU:HD12	1:A:944:LEU:O	2.17	0.43
10:K:496:GLU:HB2	10:K:526:TYR:CE1	2.51	0.43
3:C:416:PHE:CD2	14:O:323:ALA:HB2	2.53	0.43
10:K:487:TYR:CE2	10:K:491:LEU:HD11	2.54	0.43
10:K:355:ALA:O	10:K:359:THR:HG22	2.19	0.43
6:F:745:LYS:NZ	6:F:815:ALA:HB1	2.34	0.43
13:N:241:HIS:CE1	13:N:302:LYS:HE2	2.54	0.43
5:E:60:SER:O	5:E:63:VAL:HG12	2.19	0.43
1:A:1375:TYR:HB3	1:A:1378:THR:CG2	2.49	0.43
8:I:32:ARG:HB2	8:I:34:LEU:CD2	2.49	0.43
8:I:276:TRP:CE2	8:I:476:GLY:HA2	2.54	0.43
10:K:208:LYS:O	10:K:211:LYS:HG2	2.19	0.43
3:C:414:MET:HG2	14:O:330:ILE:HD11	2.01	0.43
14:O:516:PHE:HB2	14:O:535:ILE:HD11	1.99	0.43
13:N:502:ILE:HA	13:N:505:LEU:HD12	2.00	0.43
3:C:306:LEU:HD12	3:C:307:LEU:N	2.34	0.43
1:A:105:GLY:O	1:A:111:LEU:HG	2.19	0.43
4:D:18:PHE:CE1	4:D:20:LEU:HD11	2.53	0.43
6:H:496:TYR:CE1	6:H:505:ILE:HD11	2.54	0.43
1:A:1074:CYS:SG	1:A:1107:LEU:CB	3.07	0.43
20:X:99:LYS:HD3	20:X:102:MET:CE	2.49	0.43
3:P:248:LEU:HD21	3:P:273:TYR:CZ	2.53	0.43
20:Y:168:THR:HB	20:Y:169:PRO:HD2	1.99	0.43
6:F:50:ARG:HE	6:H:19:TYR:HE1	1.66	0.43
14:O:534:GLY:O	14:O:538:LEU:HD12	2.18	0.43
20:X:359:LEU:HB2	20:X:383:LEU:HG	2.01	0.43
13:N:181:LEU:HD22	13:N:299:TRP:NE1	2.34	0.43
20:Y:452:LEU:HB3	20:Y:461:ALA:HB2	2.00	0.43
20:X:452:LEU:HG	20:X:457:THR:OG1	2.19	0.43
10:K:185:LEU:HD13	10:K:209:LEU:CD1	2.41	0.43
20:X:100:TYR:CB	20:X:142:LEU:CD2	2.96	0.43
1:A:1640:GLY:HA2	1:A:1644:TYR:CE1	2.54	0.43
1:A:844:ILE:HD11	1:A:873:VAL:HG13	2.01	0.43
1:A:1621:PRO:HG3	1:A:1653:ALA:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:VAL:HB	1:A:471:VAL:HG12	2.00	0.43
14:O:216:LEU:HD22	14:O:256:LEU:CD1	2.49	0.43
6:H:762:TRP:O	6:H:766:LEU:N	2.50	0.43
13:N:345:PHE:C	13:N:345:PHE:CD1	2.91	0.43
9:J:177:THR:HG22	9:J:180:GLU:HG2	2.01	0.43
20:X:417:TYR:CD2	20:X:429:MET:HE3	2.54	0.43
8:I:717:MET:HG3	8:I:719:ALA:HB2	2.00	0.43
6:F:98:ASN:N	6:F:98:ASN:OD1	2.52	0.43
10:K:8:LYS:HD2	10:K:8:LYS:HA	1.90	0.43
20:X:359:LEU:CD1	20:X:383:LEU:HD11	2.34	0.42
13:N:354:SER:O	13:N:357:ALA:HB3	2.19	0.42
13:N:76:VAL:O	13:N:78:VAL:N	2.52	0.42
9:J:445:GLU:CA	9:J:474:LEU:HD23	2.48	0.42
6:F:639:TYR:C	6:F:639:TYR:CD1	2.93	0.42
14:O:33:TYR:HA	14:O:161:TYR:OH	2.18	0.42
11:L:22:VAL:HG12	11:L:161:PRO:HA	2.01	0.42
15:R:487:ASN:OD1	15:R:490:THR:HG23	2.17	0.42
10:K:222:GLU:O	10:K:225:ASP:O	2.36	0.42
20:X:242:ALA:O	20:X:246:VAL:HG23	2.19	0.42
1:A:627:PHE:C	1:A:627:PHE:CD1	2.92	0.42
13:N:265:LEU:C	13:N:265:LEU:HD23	2.40	0.42
13:N:434:THR:O	13:N:437:GLN:N	2.52	0.42
16:S:392:GLN:C	16:S:407:THR:HG22	2.39	0.42
8:I:32:ARG:HB2	8:I:34:LEU:HD22	2.02	0.42
6:F:563:ASP:OD1	6:F:564:LYS:O	2.37	0.42
4:D:54:ILE:HD12	3:P:389:ARG:CZ	2.49	0.42
8:I:90:ILE:HD12	8:I:106:VAL:HG11	2.02	0.42
13:N:409:VAL:O	13:N:410:ILE:CG1	2.66	0.42
3:C:407:GLN:HA	3:C:422:TYR:OH	2.18	0.42
1:A:174:PRO:HD2	1:A:220:ILE:HD12	2.02	0.42
1:A:1487:CYS:SG	1:A:1488:LEU:N	2.92	0.42
1:A:591:VAL:O	1:A:591:VAL:HG23	2.18	0.42
6:H:550:VAL:HG13	6:H:551:ALA:N	2.34	0.42
9:J:42:TRP:HA	9:J:42:TRP:CE3	2.53	0.42
1:A:246:ILE:HG23	1:A:246:ILE:O	2.19	0.42
14:O:402:LEU:HD23	14:O:402:LEU:HA	1.90	0.42
20:X:350:PHE:HZ	20:X:377:LEU:O	2.01	0.42
20:X:359:LEU:C	20:X:379:LYS:HG3	2.26	0.42
15:R:225:LEU:HD21	15:R:248:THR:HG21	2.01	0.42
20:Y:373:VAL:HG12	20:Y:402:LEU:HB2	2.01	0.42
13:N:414:MET:SD	13:N:498:SER:HA	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:73:TRP:CZ3	8:I:95:VAL:HG21	2.54	0.42
20:X:414:ILE:HD11	20:X:451:CYS:SG	2.60	0.42
14:O:751:LEU:HD12	14:O:752:ILE:N	2.34	0.42
12:M:10:ARG:HD2	12:M:11:ILE:HD12	2.00	0.42
3:P:306:LEU:HD12	3:P:307:LEU:N	2.35	0.42
15:R:492:ILE:HA	15:R:492:ILE:HD13	1.84	0.42
11:L:24:GLU:HG2	11:L:159:TYR:CE1	2.53	0.42
11:L:88:SER:HA	11:L:145:HIS:O	2.19	0.42
8:I:48:ARG:HG3	8:I:55:VAL:CG2	2.50	0.42
3:C:389:ARG:NE	14:O:279:ASP:OD2	2.39	0.42
15:R:93:ALA:O	15:R:97:ASN:OD1	2.37	0.42
1:A:1369:LEU:HA	1:A:1369:LEU:HD23	1.85	0.42
13:N:520:ARG:HD2	13:N:556:PHE:HD1	1.80	0.42
11:L:77:LEU:C	11:L:77:LEU:HD12	2.38	0.42
20:X:294:PHE:CE2	20:X:311:TYR:CB	3.00	0.42
1:A:593:ASN:OD1	1:A:609:ILE:O	2.37	0.42
10:K:406:HIS:ND1	19:W:6:PRO:HB3	2.35	0.42
20:Y:552:MET:SD	20:Y:552:MET:C	2.97	0.42
20:Y:430:ALA:HA	20:Y:433:VAL:HG12	2.01	0.42
1:A:215:HIS:CD2	1:A:217:LEU:H	2.36	0.42
17:T:9:ALA:O	17:T:10:ALA:HB3	2.19	0.42
2:B:16:TRP:CD1	2:B:46:LEU:HG	2.54	0.42
1:A:168:ASP:N	1:A:168:ASP:OD1	2.51	0.42
13:N:386:LEU:HD12	13:N:387:LEU:HG	2.01	0.42
1:A:1621:PRO:HA	1:A:1697:LEU:O	2.19	0.42
1:A:1803:LEU:CD1	1:A:1814:LEU:HD21	2.49	0.42
2:B:13:LEU:HD22	13:N:598:SER:HA	2.01	0.42
10:K:203:PHE:HE1	10:K:218:THR:HB	1.85	0.42
8:I:397:ILE:HD12	14:O:440:GLN:HG3	2.01	0.42
1:A:12:ILE:HD11	1:A:506:VAL:HG12	2.01	0.42
10:K:71:ALA:HA	10:K:128:ILE:HD13	2.02	0.42
10:K:220:ILE:O	10:K:223:SER:OG	2.32	0.42
6:F:90:GLN:OE1	20:Y:292:LEU:HG	2.20	0.42
1:A:1495:PHE:O	1:A:1499:LEU:HD13	2.19	0.42
15:R:237:TRP:CH2	15:R:244:VAL:HG21	2.54	0.42
13:N:393:THR:HG21	13:N:434:THR:HG22	2.01	0.42
11:L:45:LEU:HD23	11:L:45:LEU:C	2.39	0.42
13:N:571:ASN:HA	13:N:574:ILE:HG22	2.01	0.42
9:J:465:LEU:CA	9:J:488:ILE:HD12	2.49	0.42
6:H:128:THR:O	6:H:129:ASP:CB	2.67	0.42
1:A:1332:GLY:O	1:A:1358:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:CYS:SG	1:A:101:ILE:HD12	2.60	0.42
15:R:230:ASP:OD1	15:R:230:ASP:C	2.56	0.42
15:R:227:VAL:CG2	15:R:250:LYS:NZ	2.83	0.42
13:N:395:ASP:OD1	13:N:398:THR:CB	2.68	0.42
13:N:597:SER:OG	13:N:600:PHE:HB2	2.20	0.42
3:C:358:LEU:O	3:C:362:PRO:CA	2.64	0.42
1:A:1190:THR:HG23	1:A:1191:LEU:N	2.35	0.42
1:A:1481:ASN:OD1	1:A:1482:LEU:N	2.53	0.42
11:L:113:LEU:HD13	11:L:120:ILE:CD1	2.50	0.42
6:H:481:CYS:O	6:H:485:ILE:HG12	2.20	0.42
1:A:1532:ASN:O	1:A:1533:LEU:C	2.58	0.42
2:B:11:VAL:HB	13:N:594:VAL:CG1	2.50	0.42
1:A:1552:TYR:CE2	1:A:1596:SER:HA	2.55	0.42
20:Y:242:ALA:O	20:Y:246:VAL:HG23	2.20	0.42
10:K:180:GLU:O	10:K:184:LEU:N	2.40	0.42
13:N:340:ARG:CB	13:N:361:LEU:HD13	2.49	0.42
6:F:157:GLU:HA	6:F:477:CYS:SG	2.60	0.42
15:R:493:ARG:C	15:R:493:ARG:HD3	2.40	0.42
13:N:393:THR:HG23	13:N:434:THR:HG22	2.02	0.42
20:Y:452:LEU:HG	20:Y:457:THR:OG1	2.19	0.42
13:N:556:PHE:CG	13:N:600:PHE:CD1	3.08	0.42
2:B:28:MET:CE	16:S:375:LEU:O	2.67	0.42
11:L:25:ILE:HD11	11:L:74:VAL:HG12	2.02	0.42
3:C:53:LYS:HD2	3:P:93:TYR:CD1	2.55	0.42
13:N:533:PHE:C	13:N:535:PRO:HD3	2.40	0.42
3:C:410:GLU:OE1	15:R:52:ARG:NH2	2.50	0.42
10:K:227:LEU:O	10:K:230:ASN:N	2.52	0.42
3:P:242:GLN:NE2	3:P:429:ARG:HA	2.33	0.42
20:Y:53:VAL:HG23	20:Y:86:SER:HB3	2.02	0.42
14:O:127:HIS:O	14:O:128:LYS:CB	2.68	0.42
20:Y:169:PRO:HG3	20:Y:198:GLN:OE1	2.20	0.42
20:X:440:ASN:HA	20:X:471:GLN:HE22	1.84	0.42
1:A:1333:HIS:HB2	1:A:1357:THR:HA	2.01	0.42
9:J:477:GLN:O	9:J:508:LEU:HD13	2.19	0.42
2:B:68:GLN:HA	2:B:69:VAL:C	2.39	0.42
13:N:516:ILE:HA	13:N:516:ILE:HD12	1.89	0.42
20:X:362:GLY:C	20:X:379:LYS:HD2	2.41	0.42
15:R:310:GLN:HG2	15:R:338:LEU:HB2	1.75	0.42
15:R:225:LEU:HD12	15:R:230:ASP:C	2.41	0.42
13:N:394:CYS:C	13:N:395:ASP:CG	2.76	0.42
20:Y:437:LEU:HB2	20:Y:444:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:174:HIS:CE1	10:K:211:LYS:CD	3.03	0.42
1:A:32:PRO:HD2	14:O:264:VAL:HG11	2.01	0.42
8:I:44:VAL:C	8:I:45:LEU:HD12	2.40	0.42
1:A:174:PRO:O	1:A:295:VAL:O	2.38	0.42
10:K:167:PHE:CE2	10:K:171:THR:HG21	2.55	0.42
8:I:618:ILE:HG23	8:I:705:MET:HE2	2.01	0.42
1:A:961:HIS:HA	1:A:964:GLU:HG3	2.02	0.42
14:O:538:LEU:H	14:O:538:LEU:HD12	1.85	0.42
14:O:394:THR:HA	14:O:615:ARG:NH1	2.35	0.42
10:K:379:GLY:HA3	10:K:411:VAL:HG22	2.01	0.42
9:J:61:ARG:NH1	9:J:92:VAL:HG22	2.35	0.42
14:O:423:ALA:O	14:O:426:THR:HG23	2.19	0.42
20:Y:291:VAL:CG2	20:Y:314:LEU:HD13	2.50	0.42
14:O:530:SER:O	14:O:533:THR:HG22	2.19	0.42
3:C:26:PHE:O	3:C:27:SER:CB	2.67	0.42
6:H:98:ASN:OD1	6:H:98:ASN:N	2.53	0.42
20:Y:52:ASN:N	20:Y:52:ASN:OD1	2.52	0.42
11:L:44:GLN:HA	11:L:47:ASP:CG	2.41	0.42
10:K:432:ILE:CD1	10:K:444:TRP:CD1	2.95	0.42
1:A:487:THR:OG1	1:A:499:LEU:HD11	2.20	0.42
10:K:185:LEU:HD21	10:K:205:PHE:HB2	2.00	0.42
20:X:294:PHE:CZ	20:X:311:TYR:CG	3.08	0.42
1:A:1632:ALA:O	1:A:1653:ALA:CB	2.68	0.42
20:X:50:HIS:HA	20:X:53:VAL:HG22	2.02	0.42
6:H:515:TYR:CE2	6:H:545:HIS:CD2	3.06	0.42
4:D:17:TRP:O	4:D:18:PHE:HB3	2.20	0.42
13:N:602:PRO:N	13:N:603:PRO:HD2	2.34	0.42
13:N:259:GLU:O	13:N:263:THR:HG23	2.20	0.42
1:A:1513:GLU:HB2	1:A:1554:PHE:CE2	2.55	0.42
13:N:359:GLU:O	13:N:362:LYS:HB3	2.20	0.42
20:Y:203:LEU:HA	20:Y:206:ILE:HD12	2.01	0.42
1:A:1208:LEU:O	1:A:1212:VAL:HG23	2.20	0.42
15:R:188:PHE:HE1	15:R:403:CYS:SG	2.43	0.41
15:R:182:PRO:CG	16:S:322:ARG:HB3	2.50	0.41
13:N:619:LEU:O	13:N:619:LEU:HD13	2.20	0.41
20:Y:496:ILE:CD1	20:Y:519:LEU:HD23	2.50	0.41
13:N:560:MET:CE	13:N:601:TRP:CD1	3.03	0.41
6:H:707:PHE:CZ	6:H:738:LEU:HD21	2.55	0.41
14:O:657:ILE:HA	14:O:660:LYS:HB2	2.00	0.41
13:N:273:MET:HE3	13:N:332:PHE:CE1	2.54	0.41
14:O:378:SER:OG	14:O:409:HIS:CD2	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASP:O	1:A:594:ARG:NH2	2.53	0.41
3:P:192:PHE:CB	3:P:209:LEU:HD13	2.50	0.41
6:H:747:TYR:CD2	6:H:755:LEU:HB3	2.55	0.41
8:I:719:ALA:HA	8:I:735:SER:HA	2.01	0.41
6:H:42:PHE:HB2	6:H:71:CYS:SG	2.60	0.41
6:H:121:LEU:HG	6:H:125:TYR:CE1	2.54	0.41
20:X:269:ASP:HB3	20:X:300:LEU:HD21	2.01	0.41
6:H:104:ASP:OD1	6:H:105:ASP:N	2.53	0.41
20:Y:134:SER:N	20:Y:137:GLU:OE1	2.53	0.41
3:C:510:SER:HB3	3:C:539:PHE:HB2	2.01	0.41
9:J:306:GLY:HA3	9:J:323:LEU:HD13	2.02	0.41
20:X:334:ILE:HG13	20:X:335:SER:N	2.35	0.41
8:I:261:LEU:HA	8:I:261:LEU:HD23	1.90	0.41
15:R:189:TYR:C	15:R:316:VAL:HB	2.41	0.41
20:Y:309:ASP:OD1	20:Y:343:VAL:HG11	2.20	0.41
13:N:545:LEU:O	13:N:549:PHE:N	2.51	0.41
8:I:224:SER:HB2	8:I:229:SER:HA	1.99	0.41
20:X:294:PHE:CE1	20:X:311:TYR:CD1	3.08	0.41
8:I:231:VAL:CG1	8:I:556:LEU:HD12	2.50	0.41
3:C:413:LYS:O	3:C:415:PRO:CD	2.65	0.41
11:L:89:TYR:CD1	11:L:152:HIS:CE1	3.08	0.41
1:A:1888:LEU:O	1:A:1888:LEU:HD23	2.19	0.41
1:A:409:ILE:CG2	1:A:410:ASP:N	2.83	0.41
3:C:115:TYR:OH	3:C:161:LEU:CD1	2.68	0.41
10:K:263:PHE:CD1	10:K:291:LEU:HD21	2.56	0.41
9:J:500:ASP:O	9:J:504:THR:HG23	2.20	0.41
8:I:685:PHE:HA	8:I:701:PRO:HD3	2.02	0.41
1:A:13:ALA:HB3	1:A:648:PRO:HB3	2.01	0.41
1:A:1575:SER:O	1:A:1580:SER:OG	2.17	0.41
1:A:98:ASN:N	1:A:98:ASN:OD1	2.53	0.41
13:N:699:TRP:CB	13:N:705:LEU:HD23	2.42	0.41
1:A:1351:GLN:CG	11:L:36:CYS:HB3	2.50	0.41
3:P:233:PHE:CE2	3:P:237:ILE:HD12	2.53	0.41
3:P:402:TRP:CE3	3:P:424:ARG:HG2	2.55	0.41
3:P:96:VAL:N	3:P:97:LYS:HA	2.36	0.41
3:C:409:TYR:HB2	3:C:418:CYS:CB	2.50	0.41
1:A:248:PHE:C	1:A:248:PHE:CD1	2.93	0.41
1:A:248:PHE:CB	1:A:430:VAL:HG22	2.49	0.41
3:P:308:TYR:CD1	3:P:343:LEU:HG	2.54	0.41
6:H:674:HIS:O	6:H:678:VAL:HG23	2.20	0.41
1:A:1281:PRO:HB3	1:A:1352:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:546:LYS:HA	13:N:550:GLY:HA2	2.03	0.41
20:X:134:SER:N	20:X:137:GLU:OE1	2.53	0.41
1:A:1110:ARG:HG2	1:A:1117:THR:HG22	2.02	0.41
10:K:155:GLU:O	10:K:159:LEU:HD13	2.19	0.41
14:O:396:ASN:OD1	14:O:396:ASN:N	2.53	0.41
20:X:316:ALA:HB1	20:X:351:TYR:CD1	2.56	0.41
13:N:350:ASP:HB3	13:N:351:PHE:HA	2.02	0.41
13:N:351:PHE:HB2	13:N:354:SER:OG	2.21	0.41
15:R:256:TRP:CE3	15:R:262:LYS:C	2.94	0.41
15:R:227:VAL:HG23	15:R:250:LYS:HZ2	1.85	0.41
15:R:212:TRP:HB2	16:S:325:LEU:HD13	2.02	0.41
20:X:437:LEU:HB2	20:X:444:LEU:HD11	2.02	0.41
1:A:94:TYR:O	1:A:100:VAL:HA	2.19	0.41
14:O:751:LEU:C	14:O:751:LEU:HD12	2.40	0.41
3:P:94:PHE:O	3:P:97:LYS:HB2	2.21	0.41
14:O:356:ASP:HA	14:O:357:SER:CB	2.50	0.41
3:P:115:TYR:OH	3:P:161:LEU:CD1	2.68	0.41
1:A:1390:PRO:HG3	1:A:1396:LEU:HD23	2.02	0.41
12:M:60:LEU:N	12:M:60:LEU:HD23	2.35	0.41
15:R:175:PRO:HG3	15:R:468:ARG:HH11	1.85	0.41
20:Y:321:LEU:HD21	20:Y:351:TYR:CB	2.51	0.41
6:F:89:GLU:CD	6:F:130:ARG:NH2	2.72	0.41
9:J:167:PHE:HA	9:J:170:LEU:CD2	2.51	0.41
1:A:1531:GLY:HA3	1:A:1566:PHE:CZ	2.54	0.41
1:A:1236:LEU:HB3	15:R:153:VAL:HG21	2.02	0.41
8:I:209:CYS:SG	8:I:584:HIS:ND1	2.87	0.41
10:K:305:VAL:HG22	12:M:57:TRP:CE3	2.56	0.41
3:P:283:LEU:HD13	3:P:306:LEU:HD11	2.02	0.41
14:O:711:ARG:HA	14:O:740:LEU:HD12	2.03	0.41
3:P:478:GLU:OE2	3:P:490:TYR:OH	2.38	0.41
1:A:248:PHE:CG	1:A:249:LEU:N	2.88	0.41
3:C:161:LEU:HD23	3:C:166:GLU:HB2	2.03	0.41
14:O:68:LEU:HD23	14:O:131:VAL:HG12	2.02	0.41
20:X:63:LEU:HD22	20:Y:266:LEU:HB3	2.02	0.41
13:N:342:GLU:OE1	13:N:342:GLU:HA	2.20	0.41
3:P:352:LEU:C	3:P:352:LEU:HD23	2.41	0.41
15:R:243:LEU:CD1	15:R:298:ILE:CD1	2.99	0.41
10:K:63:ARG:HB2	10:K:65:LEU:HD13	2.03	0.41
11:L:46:ARG:NH1	11:L:156:ILE:O	2.54	0.41
3:C:94:PHE:O	3:C:97:LYS:HB2	2.21	0.41
3:C:151:LEU:HB3	3:C:182:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:657:ILE:HG22	14:O:660:LYS:HE2	2.02	0.41
14:O:657:ILE:CD1	14:O:704:VAL:HG23	2.49	0.41
11:L:86:ASP:HB2	11:L:90:THR:OG1	2.21	0.41
20:X:430:ALA:HA	20:X:433:VAL:HG12	2.01	0.41
9:J:69:TYR:O	9:J:70:GLU:CB	2.68	0.41
1:A:1867:GLY:HA2	1:A:1870:CYS:SG	2.60	0.41
9:J:245:CYS:HA	9:J:247:PHE:CE1	2.55	0.41
20:X:52:ASN:OD1	20:X:52:ASN:N	2.54	0.41
3:C:85:ASP:OD2	3:P:33:LYS:NZ	2.52	0.41
3:P:170:PHE:O	3:P:173:TYR:HB3	2.19	0.41
15:R:429:LYS:HD3	15:R:433:LEU:CD2	2.50	0.41
13:N:556:PHE:CD1	13:N:600:PHE:HD1	2.39	0.41
9:J:308:TYR:OH	12:M:27:GLU:O	2.24	0.41
20:Y:349:SER:HA	20:Y:352:SER:OG	2.21	0.41
20:Y:294:PHE:CE1	20:Y:311:TYR:CD2	3.08	0.41
15:R:420:TYR:HA	15:R:421:SER:HA	1.62	0.41
1:A:1276:GLU:CD	1:A:1294:TYR:OH	2.58	0.41
3:C:60:PHE:HA	3:P:85:ASP:OD1	2.21	0.41
19:W:5:LYS:HA	19:W:6:PRO:HD3	1.95	0.41
3:C:305:ASN:HD22	15:R:47:ARG:HG3	1.86	0.41
20:X:243:TYR:O	20:X:246:VAL:HB	2.21	0.41
6:F:150:SER:O	6:F:154:SER:OG	2.38	0.41
13:N:700:LEU:HD13	13:N:707:GLU:HG3	2.02	0.41
13:N:630:LYS:HB3	13:N:633:ARG:HD2	2.02	0.41
20:X:408:ASP:O	20:X:411:GLU:HG2	2.21	0.41
1:A:1571:ARG:NH1	1:A:1694:ASP:O	2.54	0.41
15:R:314:GLN:H	15:R:333:ASN:HB3	1.84	0.41
15:R:243:LEU:HD23	15:R:257:ASP:HA	2.03	0.41
15:R:225:LEU:HD13	15:R:230:ASP:CB	2.50	0.41
15:R:230:ASP:CB	15:R:250:LYS:HG3	2.51	0.41
10:K:258:MET:HG3	10:K:271:HIS:CD2	2.56	0.41
13:N:644:VAL:HG21	13:N:664:ALA:HB2	2.03	0.41
1:A:1405:LEU:C	1:A:1405:LEU:HD12	2.41	0.41
1:A:592:HIS:O	1:A:592:HIS:CD2	2.74	0.41
9:J:185:LEU:CD1	9:J:206:GLU:OE1	2.68	0.41
20:X:53:VAL:HG23	20:X:86:SER:HB3	2.02	0.41
8:I:175:ILE:HG22	8:I:176:LEU:N	2.35	0.41
6:H:621:LEU:HD13	6:H:625:ARG:NH2	2.36	0.41
3:C:304:SER:CB	3:C:336:VAL:HG22	2.51	0.41
12:M:2:ASP:CG	12:M:3:SER:N	2.74	0.41
8:I:272:MET:SD	8:I:348:VAL:HG22	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:320:ARG:HD3	9:J:344:PHE:CE1	2.55	0.41
1:A:1842:PHE:CE1	1:A:1843:MET:HG3	2.55	0.41
3:P:161:LEU:HD23	3:P:166:GLU:HB2	2.02	0.41
1:A:86:ASP:OD2	14:O:563:LEU:HD13	2.21	0.41
1:A:75:GLN:O	1:A:76:LEU:HD12	2.21	0.41
16:S:422:GLY:O	16:S:423:LYS:CB	2.68	0.41
1:A:257:MET:HA	1:A:267:SER:O	2.21	0.41
20:Y:186:ARG:HA	20:Y:189:VAL:HG12	2.03	0.41
20:Y:186:ARG:O	20:Y:189:VAL:HG12	2.21	0.41
8:I:28:TRP:HZ3	8:I:33:ASP:O	2.03	0.41
10:K:195:ASN:N	10:K:195:ASN:OD1	2.54	0.41
9:J:204:LEU:HA	9:J:204:LEU:HD23	1.95	0.41
20:X:321:LEU:HD21	20:X:351:TYR:CB	2.51	0.41
15:R:211:LEU:CD1	15:R:222:LEU:HD22	2.44	0.41
15:R:297:ASP:OD2	15:R:299:ARG:NH2	2.44	0.41
15:R:243:LEU:CD1	15:R:298:ILE:HD11	2.51	0.41
15:R:178:VAL:HG11	15:R:466:THR:HG23	1.91	0.41
15:R:230:ASP:OD1	15:R:231:SER:N	2.54	0.41
13:N:78:VAL:C	13:N:80:GLN:N	2.73	0.41
13:N:123:ASP:CB	13:N:124:PRO:HD3	2.50	0.41
20:X:496:ILE:CD1	20:X:519:LEU:HD23	2.51	0.41
8:I:276:TRP:CZ2	8:I:476:GLY:HA3	2.56	0.41
3:C:91:LYS:O	3:C:94:PHE:HB3	2.21	0.41
6:F:696:ILE:CG1	6:F:705:CYS:SG	3.09	0.41
9:J:476:PRO:HB2	3:P:148:ASN:HD21	1.85	0.41
6:H:146:PRO:CG	6:H:167:THR:HA	2.50	0.41
3:C:200:PRO:O	3:C:201:LEU:HB2	2.21	0.41
8:I:238:THR:HG22	8:I:548:MET:SD	2.61	0.41
13:N:367:ARG:NH2	17:T:20:ALA:HB3	2.36	0.41
4:D:40:TRP:CE2	4:D:44:ILE:HD11	2.55	0.41
1:A:174:PRO:CA	1:A:295:VAL:O	2.67	0.41
3:P:209:LEU:HD12	3:P:209:LEU:HA	1.96	0.41
3:C:477:HIS:CD2	3:C:482:GLU:OE1	2.73	0.41
5:E:67:LEU:HD13	20:Y:342:TRP:CZ3	2.56	0.41
3:C:68:ALA:O	3:C:69:GLU:CB	2.69	0.41
6:H:731:GLN:HE22	20:X:186:ARG:HG3	1.85	0.41
3:C:379:LYS:HG3	15:R:61:PHE:CE1	2.56	0.41
20:Y:482:LYS:O	20:Y:486:LEU:HD13	2.21	0.41
9:J:532:ALA:HB2	3:P:443:TYR:OH	2.20	0.41
13:N:668:LEU:O	13:N:671:GLN:HB3	2.21	0.41
1:A:1493:LYS:O	1:A:1497:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:LEU:HD23	1:A:768:LEU:HA	1.98	0.41
1:A:1585:LEU:HA	1:A:1585:LEU:HD23	1.93	0.41
1:A:971:PRO:HG2	1:A:974:VAL:HG23	2.01	0.41
1:A:155:GLN:HE22	1:A:160:ASN:ND2	2.19	0.41
20:X:475:TYR:CE1	20:X:477:LYS:HB2	2.56	0.41
8:I:355:GLY:O	8:I:359:LEU:HB2	2.20	0.41
8:I:359:LEU:O	8:I:363:LEU:HG	2.21	0.41
15:R:313:ARG:NH1	15:R:313:ARG:HG2	2.36	0.41
15:R:370:LEU:HD11	15:R:430:TYR:CZ	2.56	0.41
20:Y:449:THR:HG21	20:Y:465:LEU:HA	2.03	0.41
1:A:799:LEU:O	1:A:801:PRO:CD	2.69	0.41
6:F:562:MET:HG3	6:F:563:ASP:N	2.36	0.41
1:A:1274:LEU:HD23	1:A:1274:LEU:HA	1.87	0.41
2:B:33:CYS:CB	2:B:39:VAL:O	2.69	0.41
9:J:465:LEU:HG	9:J:488:ILE:HD11	2.01	0.41
9:J:193:LEU:O	9:J:194:CYS:HB2	2.21	0.41
15:R:451:MET:HG3	15:R:458:ILE:HD13	2.03	0.41
10:K:19:TYR:CD1	10:K:49:LEU:CD1	3.04	0.41
1:A:184:LYS:O	1:A:185:TYR:CB	2.67	0.41
6:H:531:TYR:O	6:H:562:MET:HE3	2.21	0.41
1:A:780:GLY:O	1:A:781:GLU:CB	2.69	0.41
6:F:522:PHE:CB	6:F:539:TYR:CD1	3.04	0.41
8:I:118:VAL:HG12	8:I:173:LEU:O	2.21	0.41
20:Y:331:LEU:HD12	20:Y:344:VAL:HG11	2.03	0.41
9:J:207:ASN:OD1	9:J:208:LYS:N	2.54	0.41
1:A:948:PRO:HB3	1:A:1816:GLN:CD	2.42	0.41
1:A:657:TRP:CD1	1:A:785:SER:OG	2.74	0.41
1:A:1145:LEU:HD23	1:A:1145:LEU:HA	1.67	0.41
20:X:456:VAL:O	20:X:456:VAL:HG12	2.21	0.41
1:A:1610:TYR:C	1:A:1610:TYR:CD2	2.95	0.41
13:N:344:LEU:HD22	13:N:374:LEU:HD21	2.03	0.40
6:F:130:ARG:CD	20:Y:506:GLN:HB2	2.50	0.40
13:N:368:THR:CG2	13:N:369:ASP:HA	2.52	0.40
10:K:284:LEU:HD11	10:K:307:CYS:SG	2.61	0.40
9:J:432:ILE:HD11	9:J:444:TRP:NE1	2.36	0.40
11:L:63:LEU:HD13	11:L:138:GLN:NE2	2.37	0.40
20:X:203:LEU:CD2	20:Y:55:LEU:HD23	2.50	0.40
14:O:233:PRO:HA	14:O:263:ARG:NH2	2.34	0.40
3:P:89:LEU:HD21	3:P:93:TYR:CE2	2.56	0.40
9:J:180:GLU:OE1	9:J:180:GLU:CA	2.70	0.40
3:C:478:GLU:OE2	3:C:490:TYR:CZ	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:248:LEU:HD21	3:P:273:TYR:CE1	2.56	0.40
10:K:391:PHE:CE2	10:K:411:VAL:HG21	2.56	0.40
1:A:132:ILE:HG22	1:A:133:ILE:N	2.36	0.40
1:A:613:ALA:O	1:A:614:THR:CB	2.69	0.40
1:A:1462:VAL:HG23	1:A:1463:TYR:N	2.36	0.40
6:F:486:ASN:O	6:F:490:HIS:ND1	2.51	0.40
13:N:370:GLN:HE21	13:N:373:GLN:HB3	1.86	0.40
6:H:16:LEU:HD21	6:H:47:CYS:SG	2.61	0.40
20:Y:377:LEU:HD12	20:Y:377:LEU:C	2.41	0.40
20:X:350:PHE:CE2	20:X:378:LEU:HD12	2.56	0.40
20:Y:309:ASP:HB2	20:Y:340:GLU:CG	2.51	0.40
13:N:75:PHE:CE1	13:N:79:LEU:HD23	2.56	0.40
13:N:639:HIS:CD2	13:N:661:PRO:HB2	2.56	0.40
13:N:663:GLN:HE22	13:N:698:VAL:CG1	2.33	0.40
13:N:574:ILE:HG13	13:N:625:LYS:HE2	2.03	0.40
9:J:332:THR:CA	9:J:363:LEU:HD21	2.52	0.40
8:I:65:GLY:O	8:I:84:LEU:HD12	2.21	0.40
3:C:283:LEU:HD13	3:C:306:LEU:HD11	2.03	0.40
1:A:273:ARG:O	1:A:274:VAL:CB	2.69	0.40
1:A:466:LEU:HD12	1:A:466:LEU:N	2.36	0.40
1:A:133:ILE:O	1:A:133:ILE:HD12	2.21	0.40
6:F:709:ARG:HD3	6:F:725:GLU:OE2	2.21	0.40
10:K:327:THR:OG1	10:K:337:TRP:CE2	2.72	0.40
20:Y:456:VAL:O	20:Y:456:VAL:HG12	2.22	0.40
10:K:242:TYR:C	10:K:242:TYR:CD1	2.94	0.40
13:N:281:TYR:CE1	13:N:357:ALA:CB	3.04	0.40
8:I:276:TRP:CD1	8:I:279:ILE:HG21	2.56	0.40
1:A:1230:ILE:CD1	15:R:94:LEU:HB3	2.52	0.40
1:A:1476:PHE:N	1:A:1476:PHE:CD1	2.89	0.40
1:A:1870:CYS:CB	1:A:1884:GLN:CD	2.90	0.40
1:A:1789:MET:HA	1:A:1789:MET:HE2	2.03	0.40
20:X:214:VAL:HG12	20:X:217:ALA:CB	2.51	0.40
14:O:587:VAL:O	14:O:590:LEU:HB2	2.21	0.40
13:N:340:ARG:HB2	13:N:361:LEU:HD13	2.04	0.40
3:C:66:PRO:HD2	3:C:68:ALA:O	2.21	0.40
6:F:610:GLU:O	6:F:614:THR:OG1	2.37	0.40
15:R:197:SER:HA	15:R:453:PRO:HB3	2.03	0.40
14:O:614:TYR:N	14:O:614:TYR:CD1	2.90	0.40
20:Y:321:LEU:HD21	20:Y:351:TYR:HB2	2.03	0.40
15:R:429:LYS:HD2	15:R:433:LEU:HD21	2.04	0.40
13:N:538:GLU:HG2	13:N:561:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:611:VAL:HG11	13:N:637:TRP:CZ3	2.56	0.40
13:N:666:ILE:CG2	13:N:681:LEU:HD21	2.52	0.40
14:O:658:LEU:HD12	14:O:658:LEU:HA	1.93	0.40
1:A:1162:LYS:HG3	1:A:1163:PRO:HD2	2.04	0.40
10:K:248:LYS:HB2	10:K:438:GLU:OE2	2.20	0.40
8:I:45:LEU:CD2	8:I:54:ARG:NH1	2.84	0.40
13:N:457:SER:HA	13:N:544:LEU:HD11	2.03	0.40
6:F:550:VAL:HG13	6:F:551:ALA:N	2.37	0.40
8:I:574:PHE:CE2	8:I:576:TRP:HB2	2.56	0.40
6:F:473:TYR:CD1	6:F:473:TYR:C	2.94	0.40
20:X:343:VAL:HG13	20:X:378:LEU:HD22	2.02	0.40
10:K:432:ILE:HD12	10:K:444:TRP:CD2	2.57	0.40
20:Y:229:THR:CG2	20:Y:233:LEU:HD12	2.46	0.40
10:K:384:SER:HB2	10:K:415:ASN:ND2	2.33	0.40
1:A:1773:LEU:HD21	1:A:1797:ASP:OD2	2.21	0.40
20:Y:528:ALA:O	20:Y:532:TYR:HD1	2.05	0.40
14:O:260:ASN:O	14:O:263:ARG:HB3	2.21	0.40
8:I:174:ASN:OD1	8:I:174:ASN:N	2.54	0.40
6:H:656:MET:SD	10:K:523:ILE:HD13	2.61	0.40
20:Y:270:ASN:HB2	20:Y:273:LEU:HB3	2.04	0.40
3:P:239:THR:O	3:P:275:ASN:ND2	2.50	0.40
9:J:264:HIS:HA	10:K:55:ARG:HH11	1.87	0.40
10:K:60:LEU:HD23	10:K:60:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1399/1944 (72%)	1260 (90%)	107 (8%)	32 (2%)	8 50
2	B	83/84 (99%)	72 (87%)	7 (8%)	4 (5%)	3 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	520/591 (88%)	495 (95%)	23 (4%)	2 (0%)	39	80
3	P	485/591 (82%)	460 (95%)	24 (5%)	1 (0%)	52	87
4	D	53/121 (44%)	46 (87%)	6 (11%)	1 (2%)	10	53
5	E	54/110 (49%)	54 (100%)	0	0	100	100
6	F	494/824 (60%)	477 (97%)	11 (2%)	6 (1%)	16	62
6	H	479/824 (58%)	462 (96%)	12 (2%)	5 (1%)	19	66
7	G	23/85 (27%)	23 (100%)	0	0	100	100
8	I	722/808 (89%)	690 (96%)	28 (4%)	4 (1%)	30	74
9	J	500/620 (81%)	467 (93%)	28 (6%)	5 (1%)	19	66
10	K	489/620 (79%)	458 (94%)	26 (5%)	5 (1%)	19	66
11	L	180/183 (98%)	170 (94%)	8 (4%)	2 (1%)	17	64
12	M	55/74 (74%)	46 (84%)	9 (16%)	0	100	100
13	N	609/822 (74%)	501 (82%)	50 (8%)	58 (10%)	1	12
14	O	677/756 (90%)	644 (95%)	25 (4%)	8 (1%)	16	62
15	R	375/493 (76%)	343 (92%)	25 (7%)	7 (2%)	10	53
16	S	88/447 (20%)	68 (77%)	15 (17%)	5 (6%)	2	25
17	T	19/21 (90%)	14 (74%)	3 (16%)	2 (10%)	1	10
18	U	22/24 (92%)	19 (86%)	2 (9%)	1 (4%)	3	31
19	W	23/85 (27%)	23 (100%)	0	0	100	100
20	X	480/565 (85%)	462 (96%)	15 (3%)	3 (1%)	30	74
20	Y	492/565 (87%)	471 (96%)	16 (3%)	5 (1%)	19	66
All	All	8321/11257 (74%)	7725 (93%)	440 (5%)	156 (2%)	14	53

All (156) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	VAL
1	A	630	PRO
1	A	857	MET
1	A	860	TYR
1	A	1125	ILE
2	B	15	LEU
6	F	147	PHE
6	F	493	SER
6	H	493	SER

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Mol	Chain	Res	Type
8	I	489	PRO
8	I	503	ASN
9	J	221	PRO
10	K	211	LYS
10	K	215	PRO
13	N	63	ARG
13	N	74	TRP
13	N	75	PHE
13	N	78	VAL
13	N	79	LEU
13	N	101	SER
13	N	126	LEU
13	N	140	LEU
13	N	142	MET
13	N	203	LEU
13	N	234	ARG
13	N	252	LEU
13	N	280	GLU
13	N	285	PHE
13	N	286	LEU
13	N	287	ARG
13	N	290	HIS
13	N	395	ASP
13	N	410	ILE
13	N	412	PRO
13	N	477	PRO
13	N	484	PRO
13	N	488	ASP
13	N	489	PRO
13	N	492	SER
13	N	497	ARG
13	N	530	GLN
13	N	606	ASP
13	N	674	ALA
13	N	716	ILE
15	R	153	VAL
15	R	231	SER
15	R	431	PRO
15	R	438	LYS
16	S	328	VAL
16	S	423	LYS
18	U	22	ALA

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Mol	Chain	Res	Type
20	X	213	SER
20	Y	201	LEU
20	Y	213	SER
1	A	1099	PRO
1	A	1307	LEU
1	A	1314	ILE
1	A	1924	LEU
3	C	27	SER
6	F	103	HIS
6	F	165	ASP
6	H	147	PHE
9	J	70	GLU
10	K	228	GLU
13	N	72	GLU
13	N	219	PRO
13	N	278	ARG
13	N	350	ASP
13	N	353	ASP
13	N	482	PRO
13	N	512	LYS
13	N	595	ILE
13	N	672	ASP
16	S	375	LEU
20	X	456	VAL
20	Y	202	ALA
20	Y	456	VAL
1	A	87	VAL
1	A	1100	LEU
1	A	1287	TYR
1	A	1577	SER
1	A	1603	LEU
2	B	16	TRP
8	I	483	ASP
8	I	487	VAL
9	J	442	ASP
11	L	71	LYS
11	L	174	THR
13	N	91	PHE
13	N	480	TRP
13	N	491	LYS
13	N	531	PHE
13	N	550	GLY

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Mol	Chain	Res	Type
13	N	629	LEU
14	O	126	VAL
14	O	555	ASN
14	O	707	LYS
3	P	415	PRO
15	R	154	SER
16	S	327	SER
16	S	358	ARG
17	T	19	ALA
20	X	202	ALA
1	A	653	TYR
1	A	781	GLU
1	A	1055	PRO
1	A	1283	PRO
1	A	1422	ASN
1	A	1503	ASN
4	D	23	PRO
6	F	145	ASN
6	H	145	ASN
13	N	76	VAL
13	N	146	ALA
13	N	277	CYS
13	N	289	PHE
13	N	352	PRO
13	N	368	THR
13	N	719	GLU
14	O	540	SER
1	A	47	GLU
1	A	253	PRO
1	A	502	GLY
1	A	593	ASN
1	A	813	LEU
1	A	858	PRO
2	B	69	VAL
6	F	96	VAL
10	K	86	HIS
13	N	77	GLU
15	R	291	ARG
1	A	1624	VAL
1	A	1825	SER
3	C	228	TRP
6	H	96	VAL

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Mol	Chain	Res	Type
9	J	398	ALA
13	N	197	PRO
13	N	282	GLU
13	N	490	GLY
17	T	10	ALA
9	J	397	ILE
15	R	392	PRO
2	B	40	PRO
14	O	657	ILE
1	A	83	ILE
1	A	861	PRO
14	O	750	PRO
1	A	475	PRO
1	A	1348	PRO
10	K	399	PRO
13	N	535	PRO
14	O	745	PRO
6	H	146	PRO
20	Y	200	PRO
13	N	166	PRO
14	O	124	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1150/1720 (67%)	988 (86%)	162 (14%)	4 28
2	B	65/75 (87%)	55 (85%)	10 (15%)	3 23
3	C	452/516 (88%)	399 (88%)	53 (12%)	7 35
3	P	422/516 (82%)	373 (88%)	49 (12%)	7 36
4	D	46/115 (40%)	42 (91%)	4 (9%)	13 51
5	E	47/89 (53%)	37 (79%)	10 (21%)	1 10
6	F	407/729 (56%)	367 (90%)	40 (10%)	10 44
6	H	408/729 (56%)	372 (91%)	36 (9%)	12 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	G	23/77 (30%)	21 (91%)	2 (9%)	13 51
8	I	620/730 (85%)	572 (92%)	48 (8%)	16 56
9	J	424/548 (77%)	368 (87%)	56 (13%)	5 30
10	K	423/549 (77%)	381 (90%)	42 (10%)	10 44
11	L	155/168 (92%)	140 (90%)	15 (10%)	10 45
12	M	55/67 (82%)	44 (80%)	11 (20%)	1 11
13	N	459/724 (63%)	403 (88%)	56 (12%)	6 32
14	O	578/652 (89%)	491 (85%)	87 (15%)	3 24
15	R	324/428 (76%)	306 (94%)	18 (6%)	26 68
16	S	56/404 (14%)	43 (77%)	13 (23%)	1 7
17	T	1/2 (50%)	1 (100%)	0	100 100
19	W	23/77 (30%)	22 (96%)	1 (4%)	35 75
20	X	407/484 (84%)	378 (93%)	29 (7%)	18 59
20	Y	418/484 (86%)	382 (91%)	36 (9%)	13 51
All	All	6963/9883 (70%)	6185 (89%)	778 (11%)	12 38

All (778) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	35	LEU
1	A	36	ASN
1	A	37	LEU
1	A	39	LEU
1	A	47	GLU
1	A	88	ASP
1	A	90	ASP
1	A	92	GLU
1	A	98	ASN
1	A	99	MET
1	A	107	LYS
1	A	120	ASP
1	A	127	LEU
1	A	129	CYS
1	A	150	CYS
1	A	151	ILE
1	A	159	ILE

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Mol	Chain	Res	Type
1	A	168	ASP
1	A	173	LEU
1	A	180	VAL
1	A	187	LEU
1	A	188	LEU
1	A	210	MET
1	A	212	SER
1	A	214	LEU
1	A	242	HIS
1	A	248	PHE
1	A	249	LEU
1	A	250	ASN
1	A	429	LYS
1	A	439	GLN
1	A	444	PHE
1	A	449	GLN
1	A	450	LEU
1	A	453	ARG
1	A	455	VAL
1	A	456	LYS
1	A	459	GLU
1	A	474	ILE
1	A	491	LEU
1	A	497	LEU
1	A	508	LYS
1	A	583	TYR
1	A	584	ILE
1	A	611	GLU
1	A	629	LEU
1	A	638	LEU
1	A	640	LYS
1	A	656	GLU
1	A	659	LEU
1	A	664	LEU
1	A	774	LYS
1	A	781	GLU
1	A	787	VAL
1	A	796	ASP
1	A	808	ARG
1	A	812	THR
1	A	844	ILE
1	A	852	LEU

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Mol	Chain	Res	Type
1	A	871	ARG
1	A	874	VAL
1	A	925	SER
1	A	934	MET
1	A	945	GLU
1	A	953	LEU
1	A	960	TYR
1	A	962	CYS
1	A	964	GLU
1	A	976	LEU
1	A	1016	MET
1	A	1026	LEU
1	A	1048	ARG
1	A	1071	LEU
1	A	1075	GLN
1	A	1076	ARG
1	A	1081	PRO
1	A	1089	LEU
1	A	1100	LEU
1	A	1105	LEU
1	A	1107	LEU
1	A	1136	SER
1	A	1146	LYS
1	A	1168	LEU
1	A	1170	ASN
1	A	1171	GLU
1	A	1176	LEU
1	A	1177	MET
1	A	1179	LEU
1	A	1181	LEU
1	A	1184	HIS
1	A	1202	GLU
1	A	1216	LYS
1	A	1217	LEU
1	A	1230	ILE
1	A	1232	ILE
1	A	1243	LEU
1	A	1250	GLN
1	A	1255	VAL
1	A	1273	LEU
1	A	1279	ARG
1	A	1292	GLU

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Mol	Chain	Res	Type
1	A	1312	ASN
1	A	1313	LEU
1	A	1319	LEU
1	A	1323	GLU
1	A	1359	ASN
1	A	1378	THR
1	A	1386	TRP
1	A	1387	LEU
1	A	1392	THR
1	A	1404	LEU
1	A	1405	LEU
1	A	1409	LEU
1	A	1424	LYS
1	A	1482	LEU
1	A	1487	CYS
1	A	1511	ASN
1	A	1536	LEU
1	A	1538	LEU
1	A	1540	ARG
1	A	1544	MET
1	A	1546	THR
1	A	1556	LEU
1	A	1562	LEU
1	A	1573	SER
1	A	1588	LEU
1	A	1597	THR
1	A	1603	LEU
1	A	1607	ARG
1	A	1646	GLN
1	A	1650	GLU
1	A	1651	LEU
1	A	1652	MET
1	A	1662	LEU
1	A	1663	LEU
1	A	1665	GLN
1	A	1666	ILE
1	A	1674	TRP
1	A	1684	THR
1	A	1687	LEU
1	A	1688	LYS
1	A	1693	LYS
1	A	1694	ASP

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Mol	Chain	Res	Type
1	A	1706	LEU
1	A	1734	ARG
1	A	1747	ASP
1	A	1751	LEU
1	A	1759	LYS
1	A	1773	LEU
1	A	1778	LEU
1	A	1801	ARG
1	A	1808	MET
1	A	1809	SER
1	A	1824	PHE
1	A	1828	SER
1	A	1854	THR
1	A	1861	GLN
1	A	1872	HIS
1	A	1874	TYR
1	A	1881	LEU
1	A	1885	LEU
2	B	11	VAL
2	B	14	TRP
2	B	15	LEU
2	B	16	TRP
2	B	34	CYS
2	B	36	ASP
2	B	50	GLN
2	B	61	LEU
2	B	83	LYS
2	B	84	GLU
3	C	26	PHE
3	C	39	ILE
3	C	42	LEU
3	C	44	ARG
3	C	49	LEU
3	C	57	GLU
3	C	77	THR
3	C	89	LEU
3	C	97	LYS
3	C	100	ASP
3	C	112	LYS
3	C	122	ARG
3	C	138	LEU
3	C	147	LYS

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Mol	Chain	Res	Type
3	C	160	LYS
3	C	161	LEU
3	C	172	LEU
3	C	174	LEU
3	C	182	LEU
3	C	197	HIS
3	C	239	THR
3	C	244	ILE
3	C	268	GLN
3	C	280	ASP
3	C	289	LEU
3	C	300	MET
3	C	301	ASP
3	C	302	THR
3	C	307	LEU
3	C	310	ARG
3	C	312	MET
3	C	313	LYS
3	C	335	CYS
3	C	343	LEU
3	C	358	LEU
3	C	361	ASN
3	C	376	MET
3	C	377	GLU
3	C	389	ARG
3	C	397	ARG
3	C	408	THR
3	C	423	ARG
3	C	424	ARG
3	C	428	LEU
3	C	432	ASP
3	C	434	ARG
3	C	435	MET
3	C	441	GLU
3	C	451	GLU
3	C	476	LEU
3	C	516	LEU
3	C	524	LYS
3	C	550	LEU
4	D	11	ARG
4	D	25	VAL
4	D	30	LEU

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Mol	Chain	Res	Type
4	D	49	ASN
5	E	56	GLU
5	E	58	VAL
5	E	61	TYR
5	E	69	GLN
5	E	79	MET
5	E	85	LEU
5	E	87	GLU
5	E	88	GLU
5	E	90	GLU
5	E	99	ILE
6	F	22	ARG
6	F	27	LEU
6	F	43	LEU
6	F	59	ARG
6	F	66	CYS
6	F	74	LEU
6	F	82	LEU
6	F	90	GLN
6	F	98	ASN
6	F	104	ASP
6	F	121	LEU
6	F	135	SER
6	F	141	SER
6	F	143	SER
6	F	145	ASN
6	F	154	SER
6	F	165	ASP
6	F	476	LEU
6	F	480	ASN
6	F	492	PRO
6	F	494	HIS
6	F	507	ARG
6	F	527	ARG
6	F	530	ASN
6	F	536	MET
6	F	538	ILE
6	F	540	SER
6	F	549	ASP
6	F	562	MET
6	F	564	LYS
6	F	595	GLN

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Mol	Chain	Res	Type
6	F	614	THR
6	F	656	MET
6	F	667	GLN
6	F	685	SER
6	F	701	LYS
6	F	705	CYS
6	F	709	ARG
6	F	720	LYS
6	F	761	SER
7	G	5	LYS
7	G	23	ARG
6	H	22	ARG
6	H	27	LEU
6	H	43	LEU
6	H	59	ARG
6	H	61	LEU
6	H	66	CYS
6	H	74	LEU
6	H	82	LEU
6	H	90	GLN
6	H	98	ASN
6	H	141	SER
6	H	143	SER
6	H	154	SER
6	H	165	ASP
6	H	462	LEU
6	H	476	LEU
6	H	480	ASN
6	H	481	CYS
6	H	492	PRO
6	H	494	HIS
6	H	507	ARG
6	H	530	ASN
6	H	536	MET
6	H	540	SER
6	H	563	ASP
6	H	564	LYS
6	H	571	CYS
6	H	613	LEU
6	H	629	ARG
6	H	633	ARG
6	H	655	GLU

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Mol	Chain	Res	Type
6	H	667	GLN
6	H	685	SER
6	H	709	ARG
6	H	720	LYS
6	H	762	TRP
8	I	26	LEU
8	I	34	LEU
8	I	35	ILE
8	I	37	LEU
8	I	75	PRO
8	I	92	LEU
8	I	95	VAL
8	I	101	LEU
8	I	110	VAL
8	I	218	SER
8	I	224	SER
8	I	232	SER
8	I	259	SER
8	I	266	ASN
8	I	269	LEU
8	I	273	CYS
8	I	281	MET
8	I	287	LEU
8	I	308	LEU
8	I	322	MET
8	I	333	LEU
8	I	336	SER
8	I	349	ILE
8	I	352	LEU
8	I	353	GLN
8	I	359	LEU
8	I	360	LEU
8	I	361	TYR
8	I	372	TRP
8	I	382	ASP
8	I	397	ILE
8	I	401	ASN
8	I	423	VAL
8	I	472	VAL
8	I	473	GLU
8	I	474	ARG
8	I	489	PRO

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Mol	Chain	Res	Type
8	I	505	SER
8	I	522	LEU
8	I	536	CYS
8	I	553	CYS
8	I	564	ASP
8	I	571	LYS
8	I	632	ARG
8	I	688	THR
8	I	718	LYS
8	I	736	SER
8	I	745	GLU
9	J	9	ARG
9	J	23	LEU
9	J	46	CYS
9	J	87	GLN
9	J	134	LEU
9	J	141	ASP
9	J	148	LEU
9	J	157	LEU
9	J	163	CYS
9	J	164	PHE
9	J	169	LEU
9	J	170	LEU
9	J	172	SER
9	J	180	GLU
9	J	185	LEU
9	J	188	LEU
9	J	195	ASN
9	J	202	ARG
9	J	206	GLU
9	J	207	ASN
9	J	211	LYS
9	J	214	LYS
9	J	229	LYS
9	J	254	THR
9	J	258	MET
9	J	259	GLU
9	J	267	CYS
9	J	294	LEU
9	J	298	ASN
9	J	307	CYS
9	J	323	LEU

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Mol	Chain	Res	Type
9	J	329	LEU
9	J	331	LYS
9	J	338	ILE
9	J	340	TYR
9	J	343	SER
9	J	348	SER
9	J	351	ASP
9	J	354	MET
9	J	363	LEU
9	J	385	LYS
9	J	395	LEU
9	J	423	LYS
9	J	429	LEU
9	J	439	VAL
9	J	448	LEU
9	J	456	ARG
9	J	465	LEU
9	J	472	LEU
9	J	488	ILE
9	J	497	ASN
9	J	509	ARG
9	J	510	ARG
9	J	518	MET
9	J	522	CYS
9	J	525	MET
10	K	9	ARG
10	K	45	GLN
10	K	46	CYS
10	K	52	GLN
10	K	63	ARG
10	K	87	GLN
10	K	134	LEU
10	K	141	ASP
10	K	148	LEU
10	K	157	LEU
10	K	163	CYS
10	K	164	PHE
10	K	169	LEU
10	K	188	LEU
10	K	194	CYS
10	K	195	ASN
10	K	254	THR

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Mol	Chain	Res	Type
10	K	267	CYS
10	K	277	GLU
10	K	283	GLU
10	K	284	LEU
10	K	327	THR
10	K	331	LYS
10	K	338	ILE
10	K	340	TYR
10	K	342	HIS
10	K	343	SER
10	K	348	SER
10	K	351	ASP
10	K	359	THR
10	K	363	LEU
10	K	376	LEU
10	K	385	LYS
10	K	423	LYS
10	K	429	LEU
10	K	454	VAL
10	K	477	GLN
10	K	496	GLU
10	K	497	ASN
10	K	510	ARG
10	K	518	MET
10	K	522	CYS
11	L	12	ASP
11	L	23	ARG
11	L	25	ILE
11	L	32	SER
11	L	36	CYS
11	L	45	LEU
11	L	54	TRP
11	L	67	GLN
11	L	77	LEU
11	L	84	LYS
11	L	113	LEU
11	L	132	THR
11	L	151	THR
11	L	177	PHE
11	L	184	ARG
12	M	12	LEU
12	M	17	ASP

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Mol	Chain	Res	Type
12	M	27	GLU
12	M	35	GLU
12	M	48	GLU
12	M	51	LYS
12	M	55	MET
12	M	59	ASP
12	M	60	LEU
12	M	63	GLN
12	M	64	TYR
13	N	74	TRP
13	N	75	PHE
13	N	77	GLU
13	N	80	GLN
13	N	150	ARG
13	N	170	GLN
13	N	180	PHE
13	N	181	LEU
13	N	202	GLU
13	N	206	ARG
13	N	232	TRP
13	N	243	LEU
13	N	250	LEU
13	N	251	SER
13	N	255	ARG
13	N	256	VAL
13	N	271	GLU
13	N	278	ARG
13	N	281	TYR
13	N	285	PHE
13	N	322	ARG
13	N	334	ARG
13	N	340	ARG
13	N	351	PHE
13	N	365	LEU
13	N	366	GLU
13	N	373	GLN
13	N	374	LEU
13	N	379	LYS
13	N	392	ASN
13	N	399	LEU
13	N	410	ILE
13	N	425	ARG

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Mol	Chain	Res	Type
13	N	433	ASP
13	N	435	VAL
13	N	498	SER
13	N	503	SER
13	N	504	LEU
13	N	513	ASP
13	N	516	ILE
13	N	517	ASN
13	N	531	PHE
13	N	544	LEU
13	N	561	LEU
13	N	571	ASN
13	N	584	GLU
13	N	592	TYR
13	N	594	VAL
13	N	609	LEU
13	N	622	TYR
13	N	623	CYS
13	N	625	LYS
13	N	626	TYR
13	N	640	THR
13	N	670	PHE
13	N	699	TRP
14	O	29	TRP
14	O	38	LEU
14	O	40	LEU
14	O	43	GLU
14	O	62	GLN
14	O	64	LEU
14	O	78	LEU
14	O	98	LYS
14	O	99	LEU
14	O	104	GLU
14	O	106	LYS
14	O	129	THR
14	O	130	SER
14	O	132	VAL
14	O	136	LEU
14	O	143	TYR
14	O	166	GLU
14	O	207	LEU
14	O	218	GLN

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Mol	Chain	Res	Type
14	O	219	GLN
14	O	243	LEU
14	O	257	SER
14	O	266	ASP
14	O	274	LEU
14	O	280	ARG
14	O	299	SER
14	O	313	ARG
14	O	319	GLN
14	O	328	ILE
14	O	329	ARG
14	O	344	LEU
14	O	345	SER
14	O	347	LEU
14	O	352	GLN
14	O	367	LYS
14	O	387	GLN
14	O	396	ASN
14	O	398	LEU
14	O	404	ASP
14	O	408	LEU
14	O	417	LEU
14	O	419	ASP
14	O	426	THR
14	O	431	LEU
14	O	434	ARG
14	O	435	SER
14	O	510	CYS
14	O	511	ASP
14	O	517	ASP
14	O	533	THR
14	O	563	LEU
14	O	567	LEU
14	O	568	LEU
14	O	579	MET
14	O	581	ILE
14	O	585	LEU
14	O	586	SER
14	O	595	SER
14	O	598	THR
14	O	608	LEU
14	O	618	TYR

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Mol	Chain	Res	Type
14	O	619	LEU
14	O	623	THR
14	O	625	LEU
14	O	626	ASN
14	O	632	LEU
14	O	633	ILE
14	O	634	LEU
14	O	636	ILE
14	O	641	LEU
14	O	643	LEU
14	O	646	MET
14	O	649	GLU
14	O	654	ASP
14	O	657	ILE
14	O	669	LYS
14	O	685	GLU
14	O	691	ILE
14	O	693	ASN
14	O	694	LEU
14	O	706	CYS
14	O	713	VAL
14	O	717	GLN
14	O	723	THR
14	O	735	MET
14	O	752	ILE
14	O	755	LEU
3	P	39	ILE
3	P	46	ARG
3	P	51	SER
3	P	77	THR
3	P	89	LEU
3	P	97	LYS
3	P	98	GLU
3	P	100	ASP
3	P	107	HIS
3	P	122	ARG
3	P	128	LYS
3	P	147	LYS
3	P	157	GLU
3	P	160	LYS
3	P	161	LEU
3	P	174	LEU

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Mol	Chain	Res	Type
3	P	182	LEU
3	P	209	LEU
3	P	234	LEU
3	P	239	THR
3	P	244	ILE
3	P	268	GLN
3	P	289	LEU
3	P	300	MET
3	P	302	THR
3	P	303	PHE
3	P	310	ARG
3	P	312	MET
3	P	313	LYS
3	P	321	HIS
3	P	335	CYS
3	P	343	LEU
3	P	344	ARG
3	P	352	LEU
3	P	358	LEU
3	P	365	LEU
3	P	373	HIS
3	P	392	ILE
3	P	395	ASN
3	P	408	THR
3	P	414	MET
3	P	423	ARG
3	P	428	LEU
3	P	435	MET
3	P	441	GLU
3	P	451	GLU
3	P	479	GLN
3	P	495	GLN
3	P	524	LYS
15	R	44	HIS
15	R	57	TRP
15	R	89	LEU
15	R	94	LEU
15	R	99	LEU
15	R	106	LYS
15	R	127	LEU
15	R	128	PHE
15	R	132	LEU

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Mol	Chain	Res	Type
15	R	148	TYR
15	R	150	LEU
15	R	157	SER
15	R	160	LEU
15	R	162	ARG
15	R	289	ARG
15	R	370	LEU
15	R	488	LEU
15	R	492	ILE
16	S	321	PHE
16	S	326	LYS
16	S	327	SER
16	S	374	SER
16	S	375	LEU
16	S	383	SER
16	S	388	ASP
16	S	390	TYR
16	S	395	THR
16	S	401	CYS
16	S	406	CYS
16	S	411	CYS
16	S	418	ASP
19	W	14	ASP
20	X	39	ASP
20	X	49	LEU
20	X	51	SER
20	X	79	LEU
20	X	106	GLN
20	X	110	LEU
20	X	184	GLN
20	X	193	LYS
20	X	255	ILE
20	X	292	LEU
20	X	299	MET
20	X	323	ASP
20	X	356	SER
20	X	371	ASN
20	X	372	SER
20	X	377	LEU
20	X	386	MET
20	X	411	GLU
20	X	414	ILE

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Mol	Chain	Res	Type
20	X	452	LEU
20	X	453	GLU
20	X	457	THR
20	X	460	LYS
20	X	465	LEU
20	X	475	TYR
20	X	487	SER
20	X	506	GLN
20	X	515	LEU
20	X	539	ASP
20	Y	39	ASP
20	Y	49	LEU
20	Y	51	SER
20	Y	54	ARG
20	Y	59	LEU
20	Y	70	LEU
20	Y	79	LEU
20	Y	94	ARG
20	Y	184	GLN
20	Y	193	LYS
20	Y	198	GLN
20	Y	199	CYS
20	Y	255	ILE
20	Y	292	LEU
20	Y	299	MET
20	Y	303	TYR
20	Y	323	ASP
20	Y	356	SER
20	Y	371	ASN
20	Y	377	LEU
20	Y	386	MET
20	Y	409	CYS
20	Y	411	GLU
20	Y	414	ILE
20	Y	452	LEU
20	Y	453	GLU
20	Y	457	THR
20	Y	460	LYS
20	Y	465	LEU
20	Y	475	TYR
20	Y	487	SER
20	Y	506	GLN

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Mol	Chain	Res	Type
20	Y	515	LEU
20	Y	539	ASP
20	Y	551	LYS
20	Y	552	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	36	ASN
1	A	38	GLN
1	A	160	ASN
1	A	176	GLN
1	A	179	ASN
1	A	215	HIS
1	A	593	ASN
1	A	619	GLN
1	A	792	GLN
1	A	846	GLN
1	A	1021	HIS
1	A	1060	HIS
1	A	1138	HIS
1	A	1165	HIS
1	A	1170	ASN
1	A	1309	HIS
1	A	1359	ASN
1	A	1380	ASN
1	A	1511	ASN
1	A	1543	HIS
1	A	1559	HIS
1	A	1604	GLN
1	A	1646	GLN
1	A	1665	GLN
1	A	1798	GLN
1	A	1816	GLN
1	A	1895	HIS
2	B	9	ASN
2	B	50	GLN
3	C	71	GLN
3	C	145	GLN
3	C	236	HIS
3	C	287	ASN

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Mol	Chain	Res	Type
3	C	299	ASN
3	C	305	ASN
3	C	321	HIS
3	C	373	HIS
3	C	518	GLN
4	D	49	ASN
5	E	75	GLN
6	F	64	HIS
6	F	634	HIS
6	F	636	ASN
6	H	14	GLN
6	H	90	GLN
6	H	480	ASN
6	H	545	HIS
6	H	595	GLN
6	H	634	HIS
6	H	648	GLN
6	H	657	HIS
6	H	667	GLN
6	H	702	ASN
6	H	716	ASN
6	H	754	HIS
6	H	759	ASN
8	I	235	GLN
8	I	266	ASN
8	I	323	ASN
8	I	353	GLN
8	I	374	GLN
8	I	523	HIS
8	I	535	GLN
8	I	740	HIS
9	J	16	GLN
9	J	18	GLN
9	J	58	HIS
9	J	271	HIS
9	J	316	ASN
9	J	342	HIS
9	J	382	ASN
9	J	393	GLN
9	J	406	HIS
9	J	477	GLN
10	K	17	GLN

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Mol	Chain	Res	Type
10	K	18	GLN
10	K	20	GLN
10	K	45	GLN
10	K	271	HIS
10	K	352	GLN
10	K	449	ASN
11	L	49	ASN
11	L	146	GLN
11	L	152	HIS
13	N	266	HIS
13	N	370	GLN
13	N	388	HIS
13	N	517	ASN
13	N	571	ASN
13	N	639	HIS
13	N	663	GLN
13	N	671	GLN
14	O	62	GLN
14	O	91	ASN
14	O	138	HIS
14	O	219	GLN
14	O	242	ASN
14	O	247	ASN
14	O	318	GLN
14	O	319	GLN
14	O	363	HIS
14	O	387	GLN
14	O	424	GLN
14	O	441	GLN
14	O	449	ASN
14	O	462	ASN
14	O	472	HIS
14	O	539	ASN
14	O	552	GLN
14	O	556	GLN
14	O	671	GLN
14	O	693	ASN
14	O	717	GLN
3	P	50	HIS
3	P	71	GLN
3	P	236	HIS
3	P	249	GLN

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Mol	Chain	Res	Type
3	P	287	ASN
3	P	299	ASN
3	P	305	ASN
3	P	321	HIS
3	P	339	ASN
3	P	355	GLN
3	P	361	ASN
15	R	60	ASN
15	R	249	HIS
15	R	350	GLN
15	R	366	HIS
15	R	435	GLN
20	X	106	GLN
20	X	151	GLN
20	X	337	GLN
20	X	371	ASN
20	X	471	GLN
20	X	506	GLN
20	Y	296	GLN
20	Y	337	GLN
20	Y	371	ASN
20	Y	432	ASN
20	Y	506	GLN
20	Y	541	ASN

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

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.