Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 10:58 pm GMT

PDB ID	:	5A31
EMDB ID	:	EMD-2925
Title	:	Structure of the human APC-Cdh1-Hsl1-UbcH10 complex.
Authors	:	Chang, L.; Zhang, Z.; Yang, J.; Mclaughlin, S.H.; Barford, D.
Deposited on	:	2015-05-26
Resolution	:	4.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

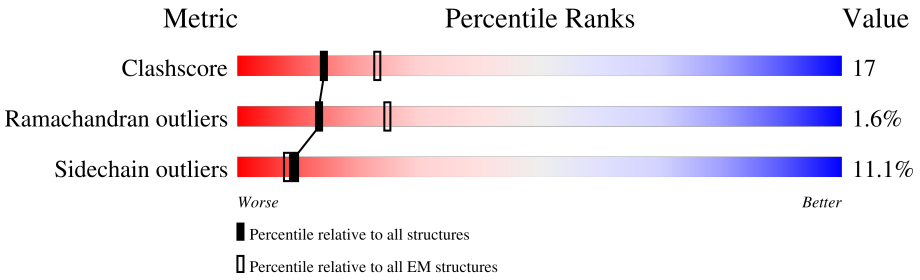
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1441	28% 61% 34% 5%
2	B	84	14% 51% 36% 8% 5%
3	C	597	23% 60% 23% • • 12%
3	P	597	11% 57% 21% • 18%
4	D	121	13% 32% 12% • 55%
5	E	110	13% 35% 15% • 49%
6	F	824	12% 44% 15% • 40%
6	H	824	13% 42% 14% • 41%

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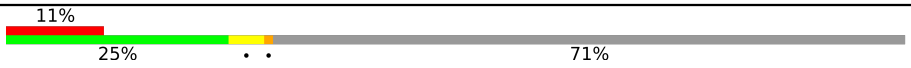
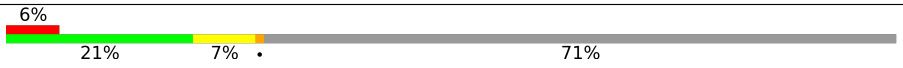
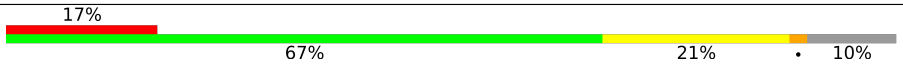
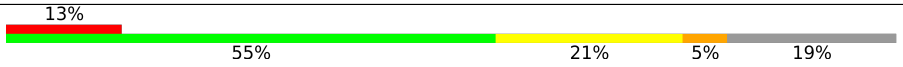
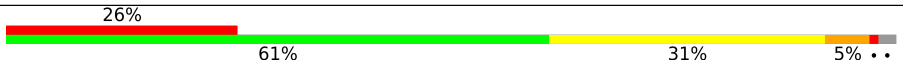
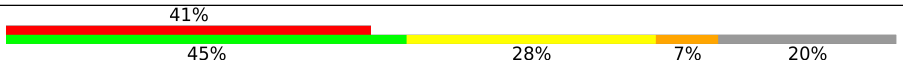
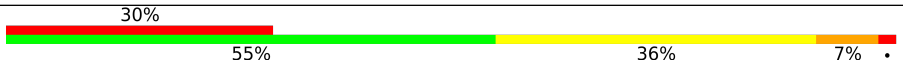
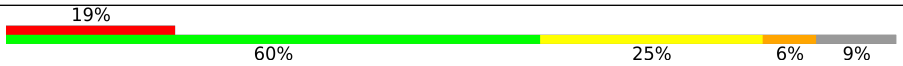
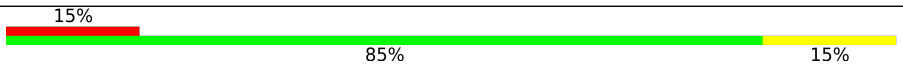
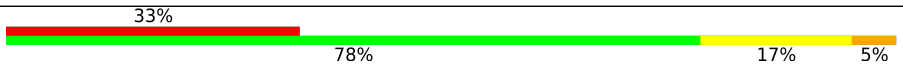
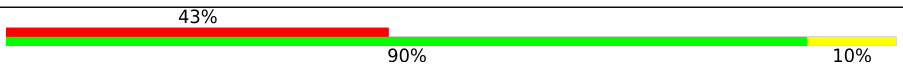
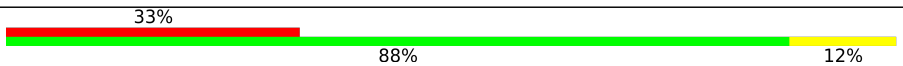
Mol	Chain	Length	Quality of chain
7	G	85	
7	W	85	
8	I	808	
9	J	620	
10	K	620	
11	L	185	
12	M	74	
13	N	703	
14	O	755	
15	Q	162	
16	R	386	
17	T	21	
18	U	24	
19	V	13	
20	X	599	
20	Y	599	

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 67685 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
			10950	7046	1853	1977	74		

- 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 are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	expression tag	UNP P60006
D	2	SER	-	expression tag	UNP P60006
D	3	THR	-	expression tag	UNP P60006
D	4	LEU	-	expression tag	UNP P60006
D	5	TYR	-	expression tag	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 ANAPHASE-PROMOTING COMPLEX SUBUNIT 3.

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 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	475	SER	ALA	conflict	UNP P30260
F	484	SER	ALA	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
			211	133	40	37	1		
7	W	25	Total	C	N	O	S	0	0
			213	133	40	39	1		

- 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 ANAPHASE-PROMOTING COMPLEX SUBUNIT 6.

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

There are 5 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
J	347	ALA	GLU	conflict	UNP Q13042
J	524	ALA	GLU	conflict	UNP Q13042

- Molecule 10 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 6.

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
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		

- 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	703	Total	C	N	O	S	0	0
			5400	3438	968	969	25		

- 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
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	LYS	conflict	UNP Q9UJX4

- Molecule 15 is a protein called FUSION PROTEIN - UBIQUITIN-CONJUGATING ENZYME E2 C, UBIQUITIN-CONJUGATING ENZYME E2 S.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	162	Total	C	N	O	S	1	0
			1227	789	204	229	5		

- Molecule 16 is a protein called THE ANAPHASE-PROMOTING COMPLEX CHAIN R.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	386	Total	C	N	O	S	0	0
			2990	1884	530	564	12		

- Molecule 17 is a protein called THE ANAPHASE-PROMOTING COMPLEX CHAIN T.

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

- Molecule 18 is a protein called THE ANAPHASE-PROMOTING COMPLEX CHAIN U.

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

- Molecule 19 is a protein called THE ANAPHASE-PROMOTING COMPLEX CHAIN V.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	V	13	Total 99	C 64	N 19	O 16	0	0

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

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

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

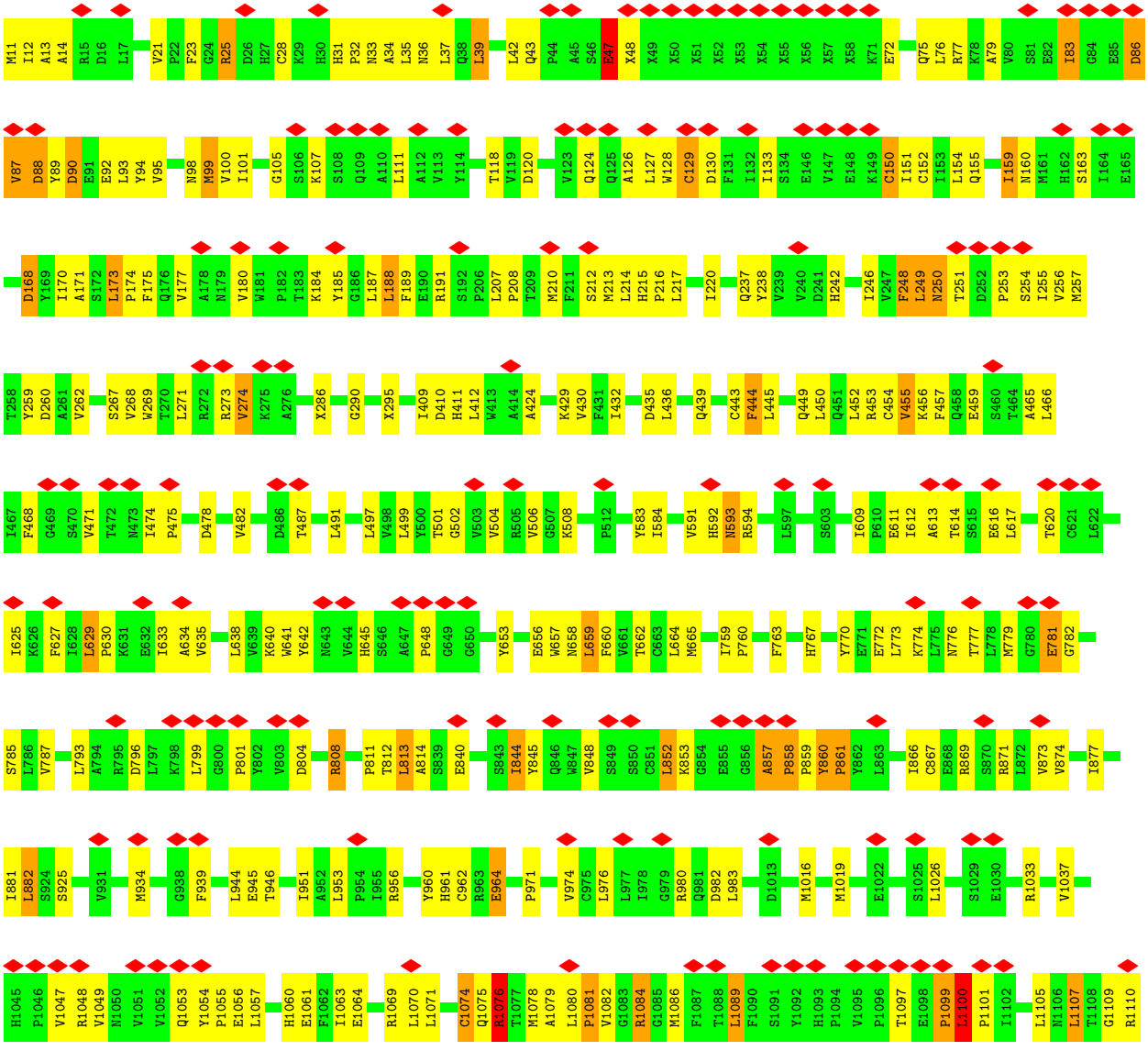
Mol	Chain	Residues	Atoms		AltConf
21	B	3	Total 3	Zn 3	0

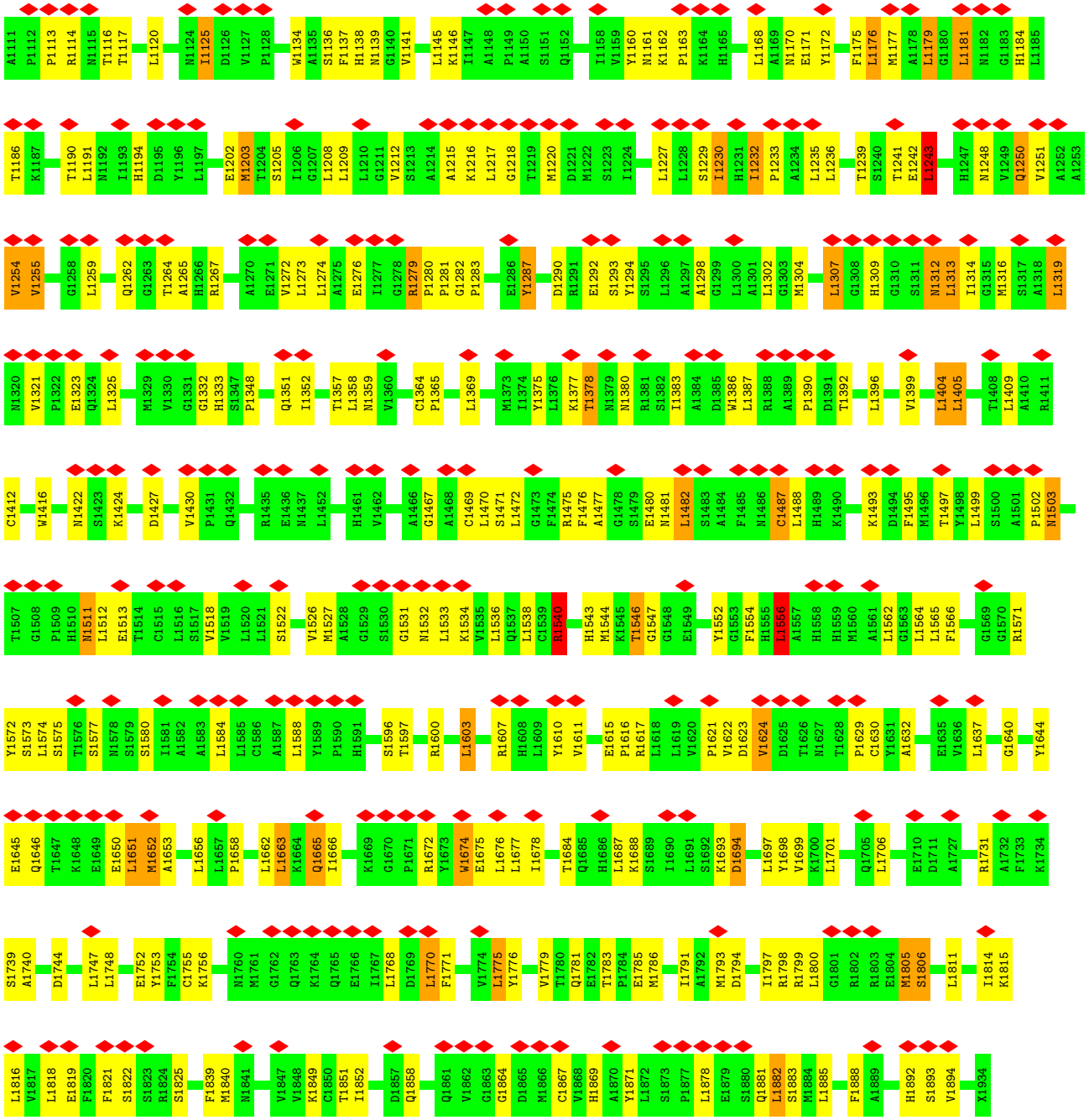
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

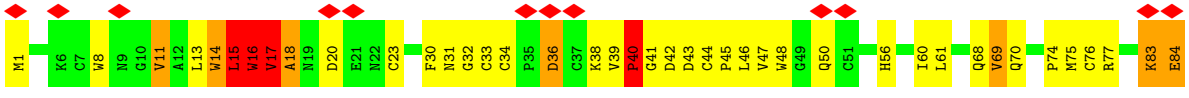
Chain A:





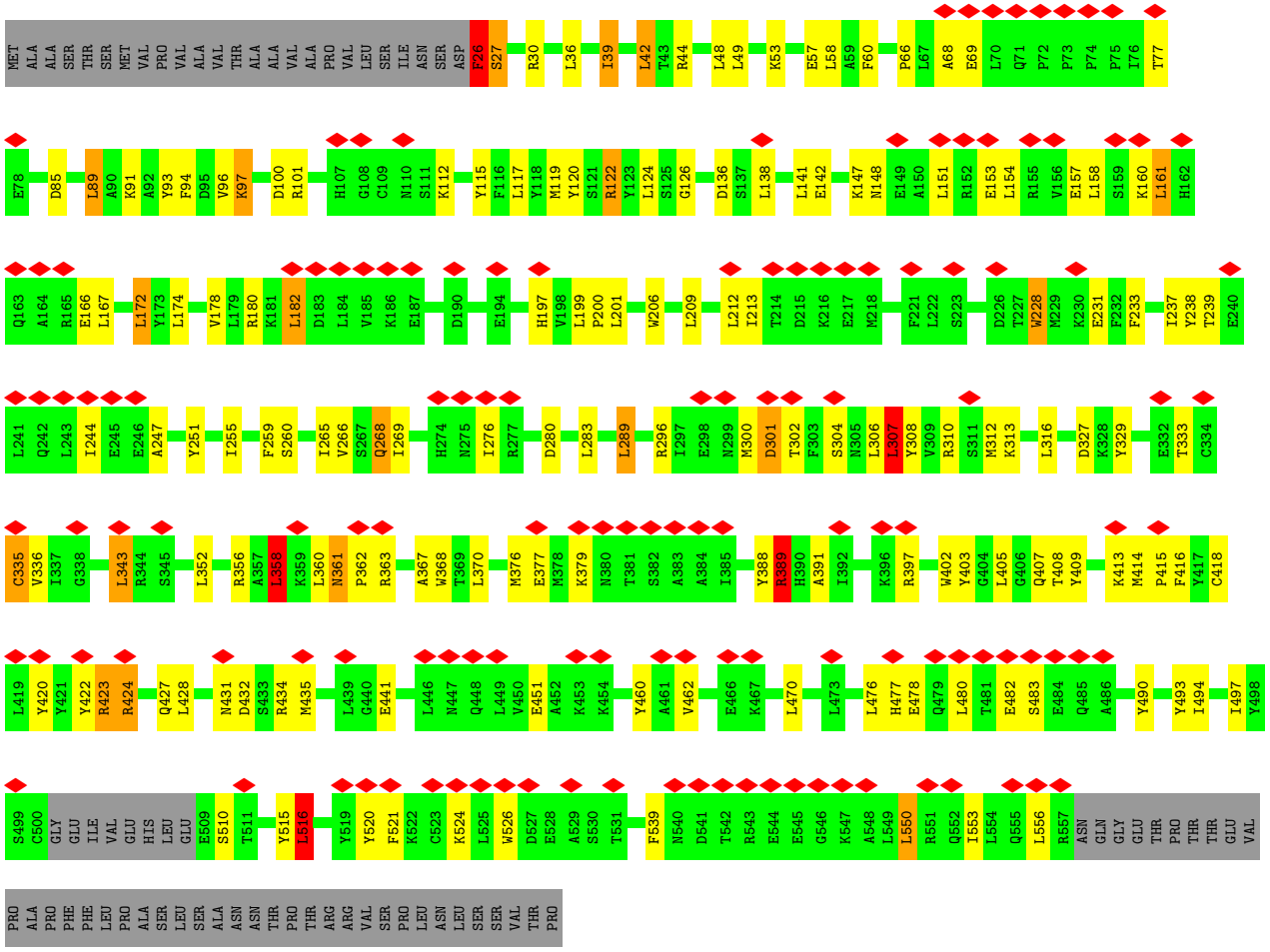
• Molecule 2: ANAPHASE-PROMOTING COMPLEX SUBUNIT 11

Chain B:



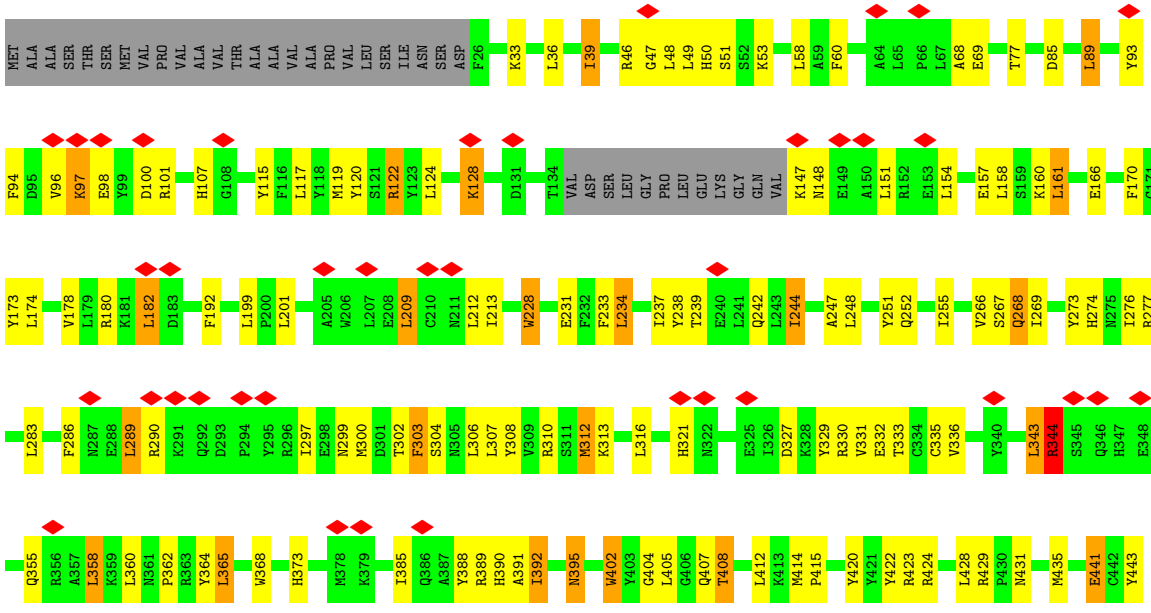
• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

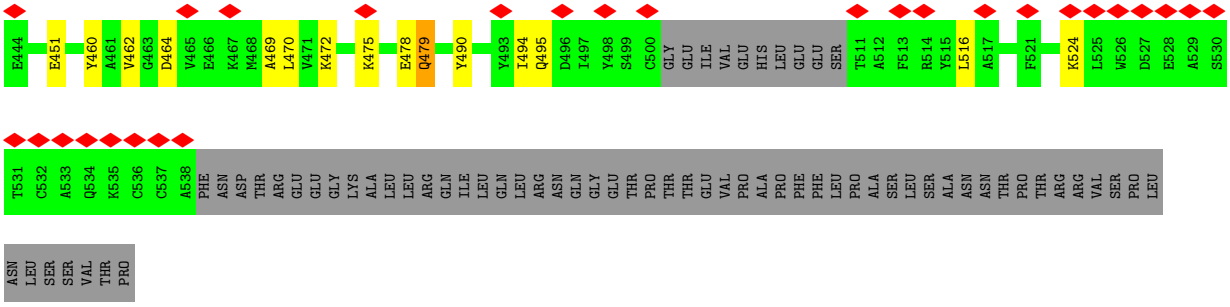
Chain C:



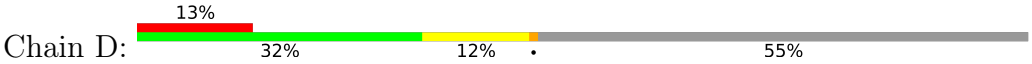
• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

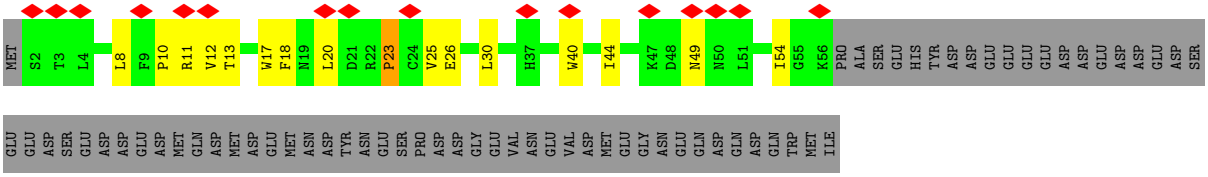
Chain P:



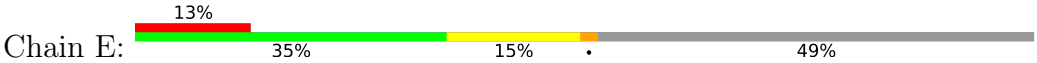


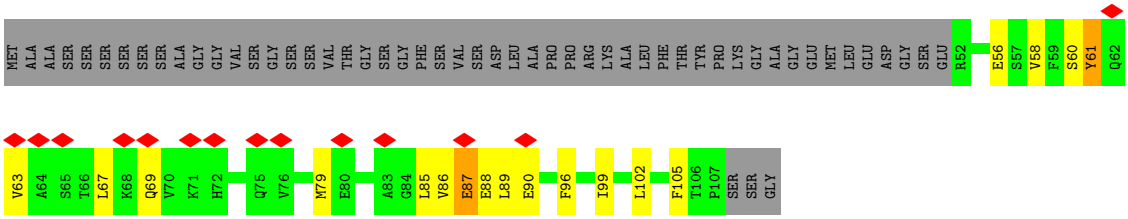
• Molecule 4: ANAPHASE-PROMOTING COMPLEX SUBUNIT 15



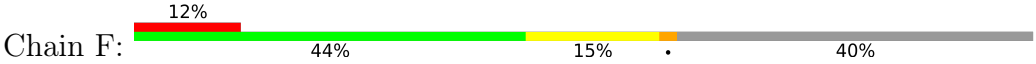


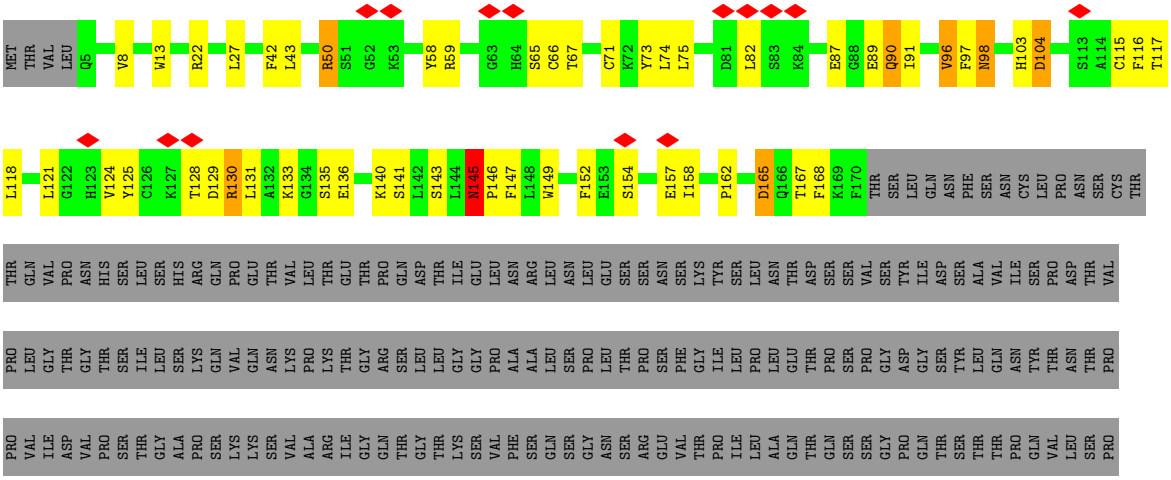
• Molecule 5: ANAPHASE-PROMOTING COMPLEX SUBUNIT 16

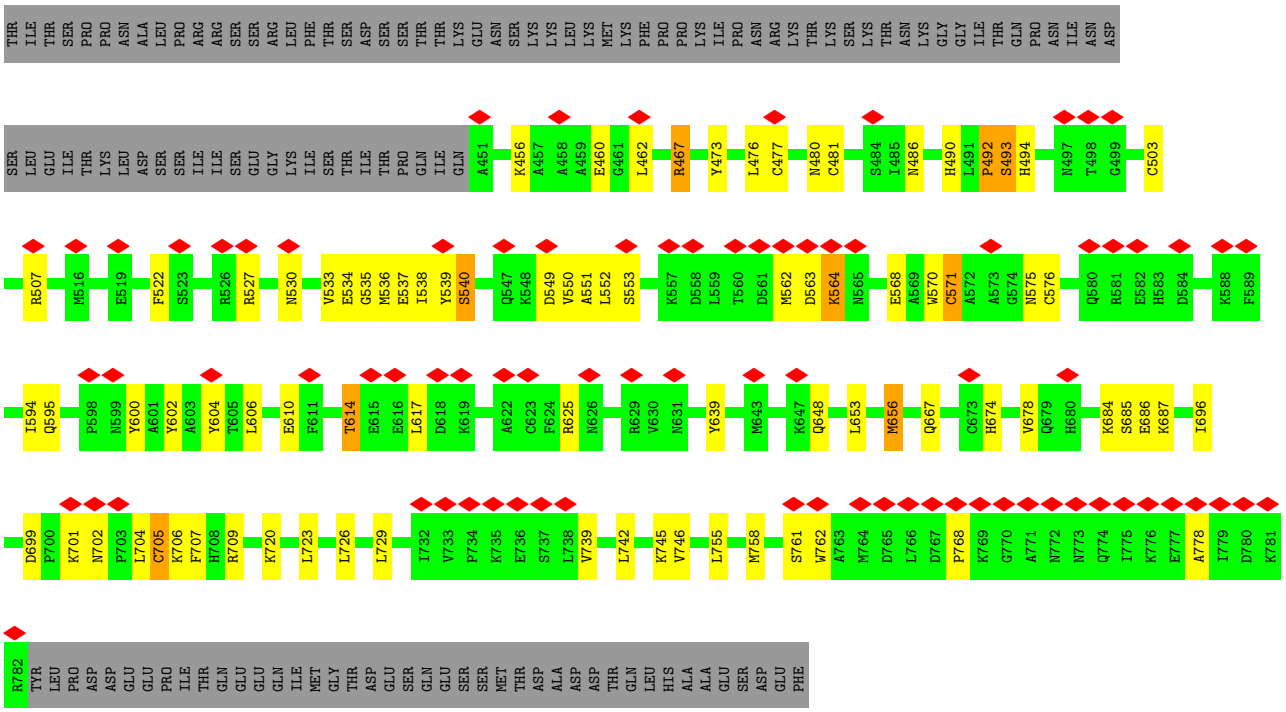




• Molecule 6: ANAPHASE-PROMOTING COMPLEX SUBUNIT 3

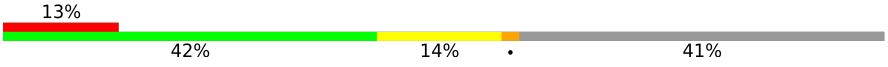


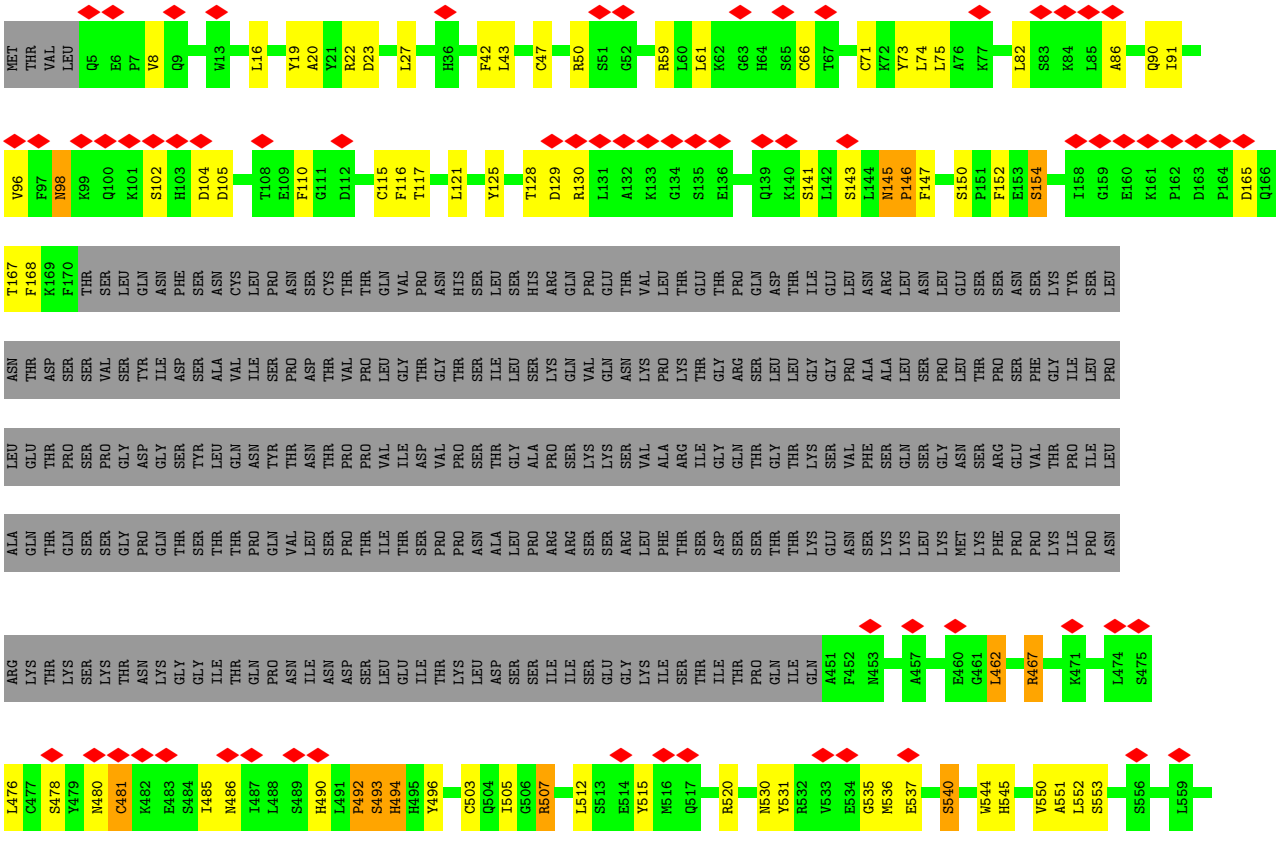


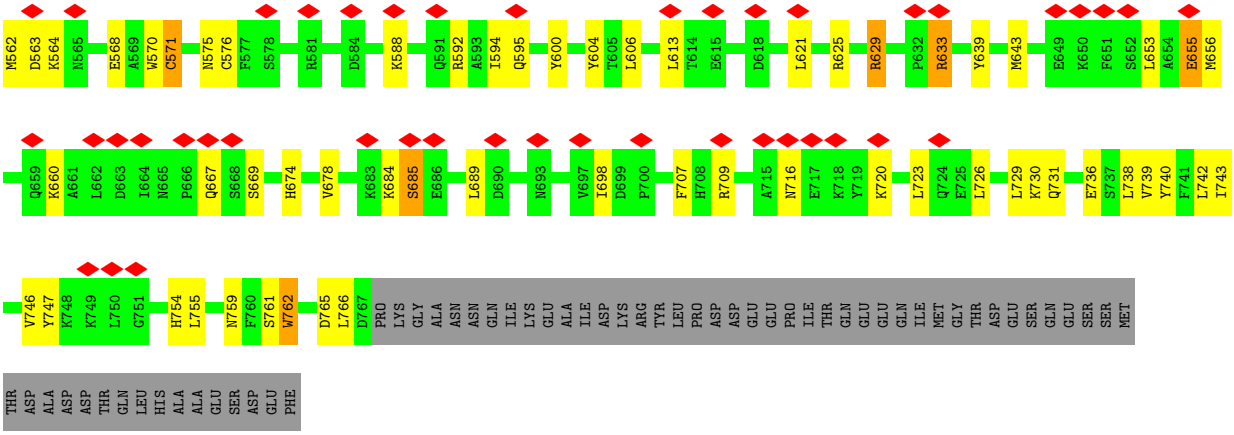


• Molecule 6: ANAPHASE-PROMOTING COMPLEX SUBUNIT 3

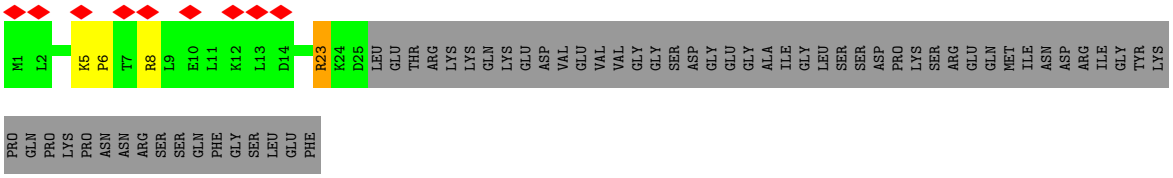
Chain H:



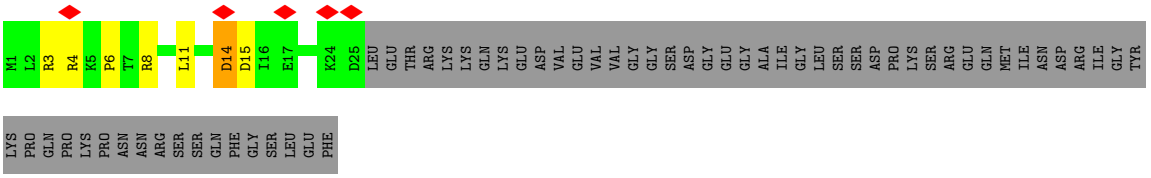




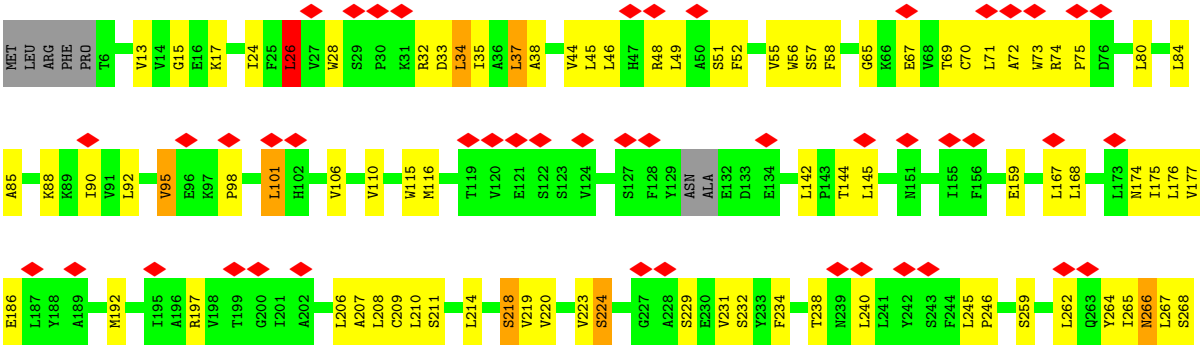
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

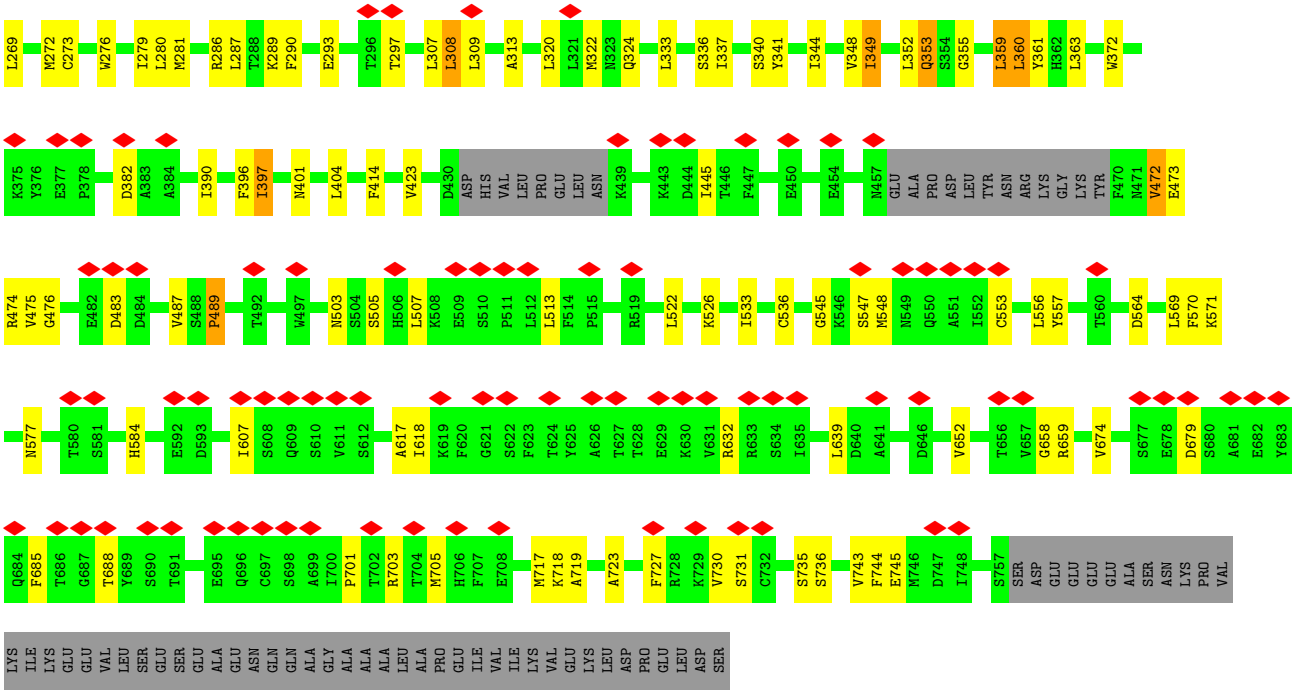


• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26



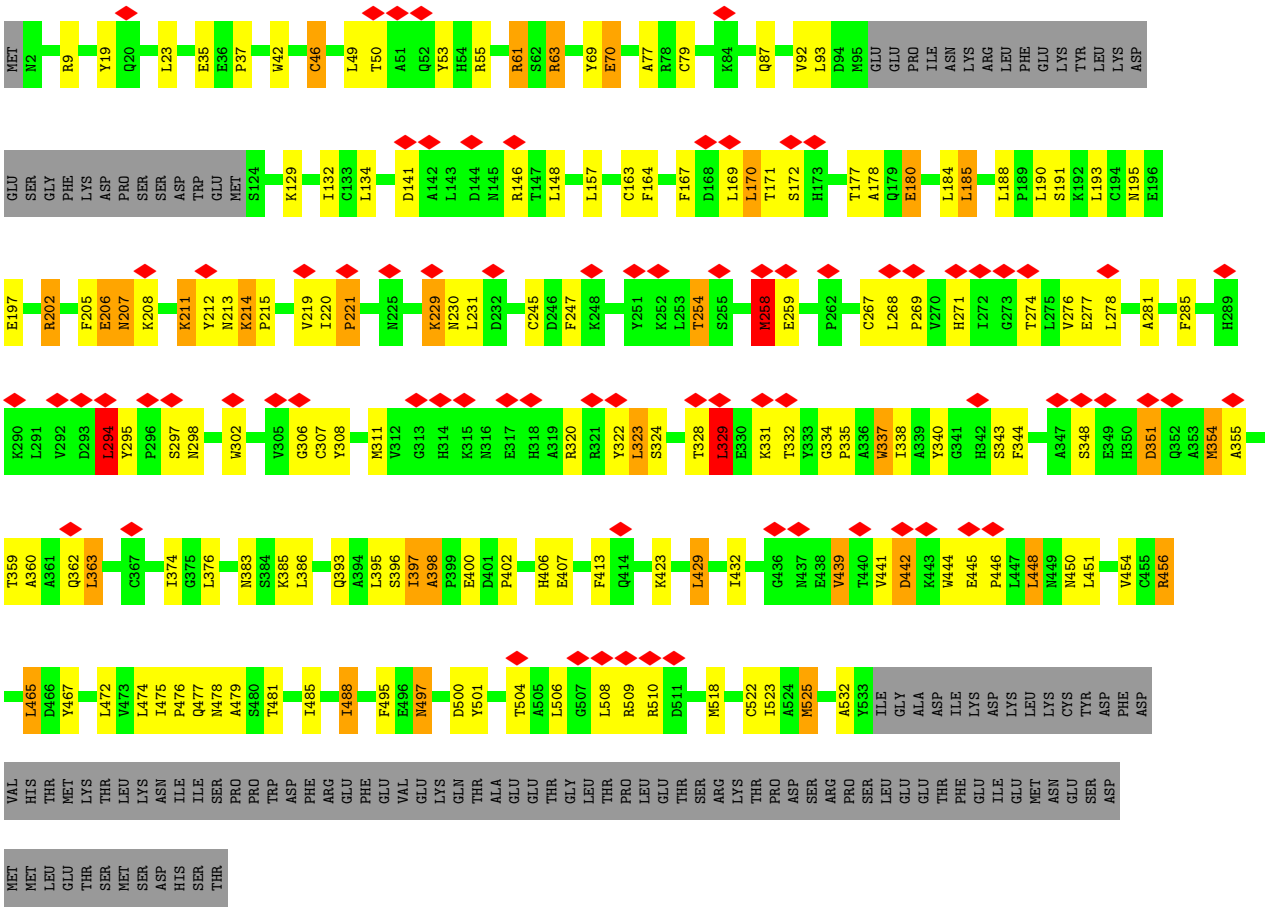
• Molecule 8: ANAPHASE-PROMOTING COMPLEX SUBUNIT 4





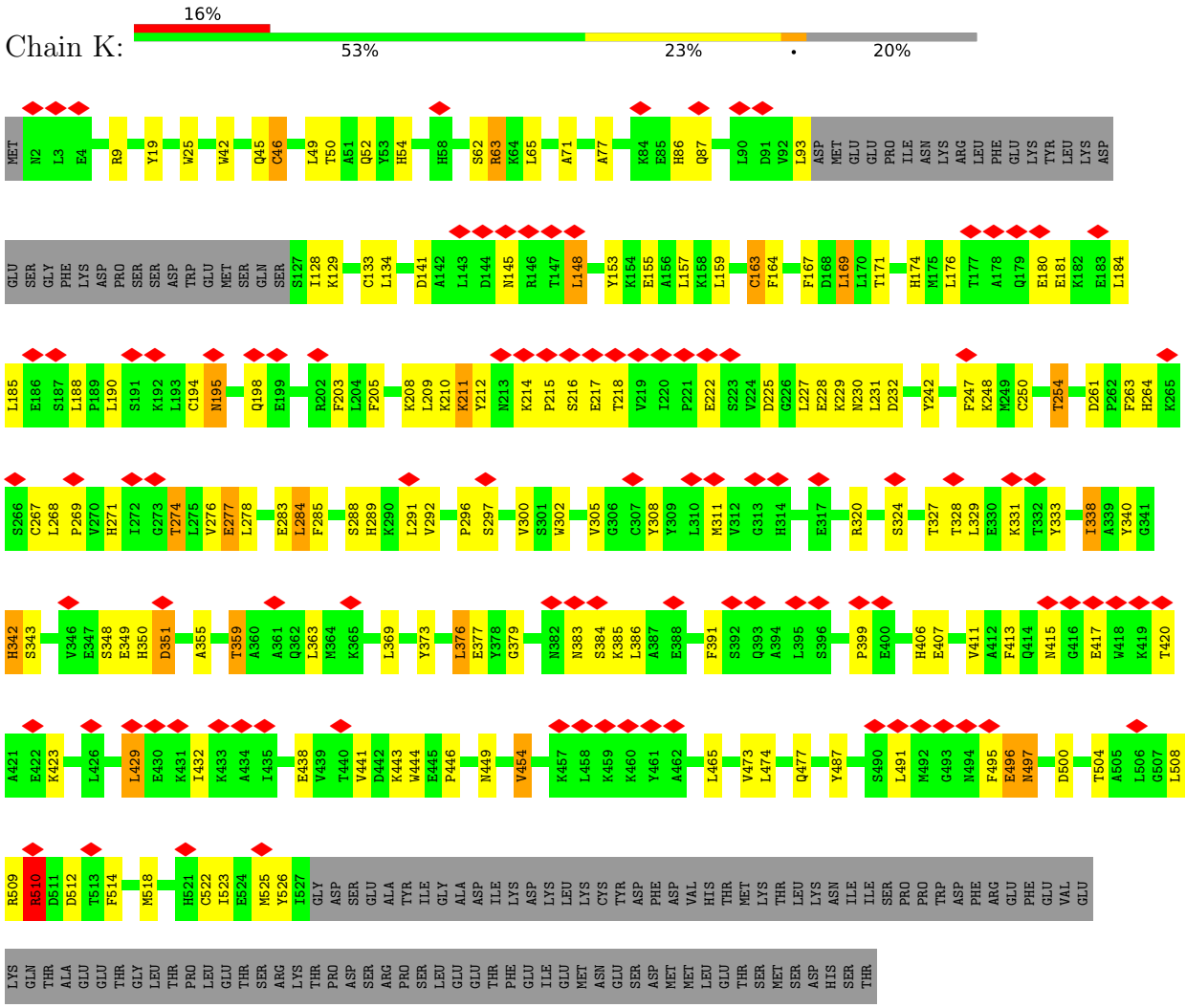
• Molecule 9: ANAPHASE-PROMOTING COMPLEX SUBUNIT 6

Chain J:



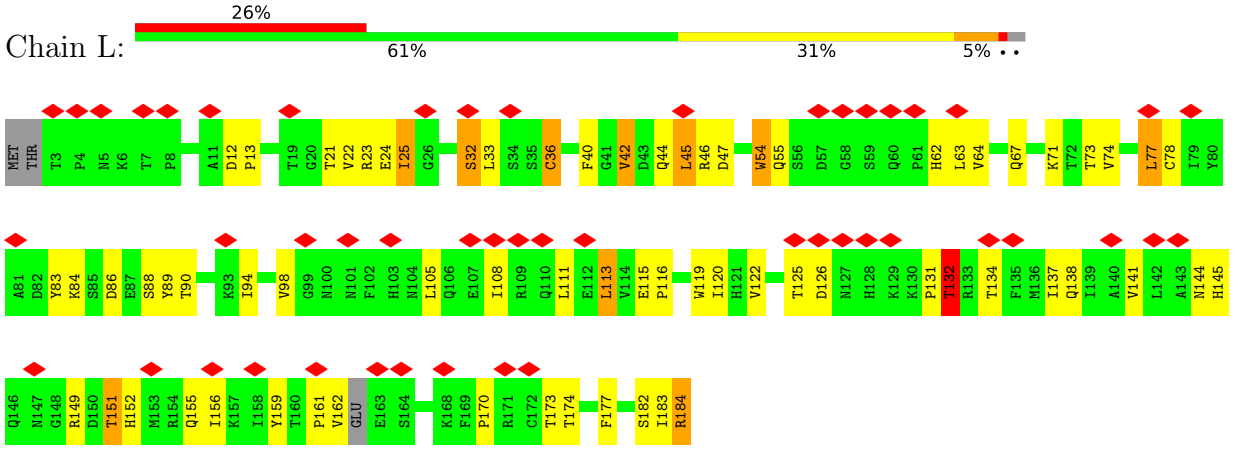
• Molecule 10: ANAPHASE-PROMOTING COMPLEX SUBUNIT 6

Chain K:



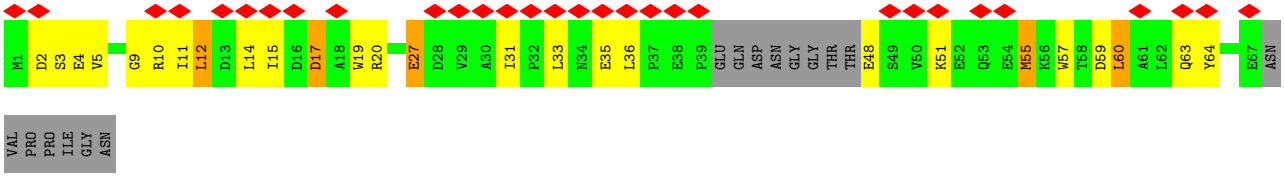
• Molecule 11: ANAPHASE-PROMOTING COMPLEX SUBUNIT 10

Chain L:



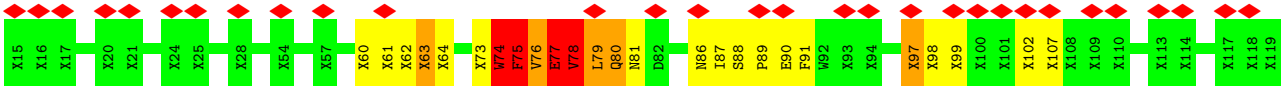
• Molecule 12: ANAPHASE-PROMOTING COMPLEX SUBUNIT 13

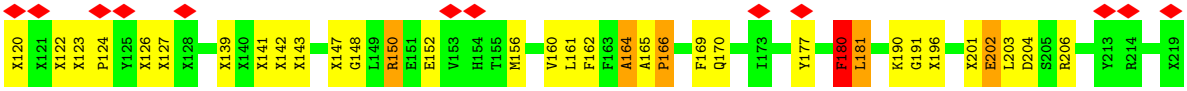
Chain M:

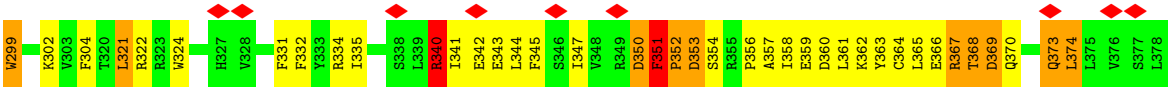


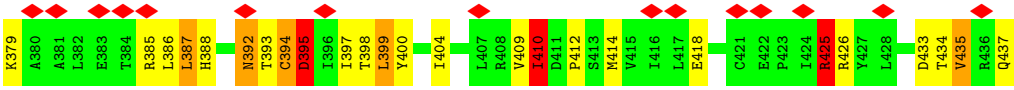
• Molecule 13: ANAPHASE-PROMOTING COMPLEX SUBUNIT 2

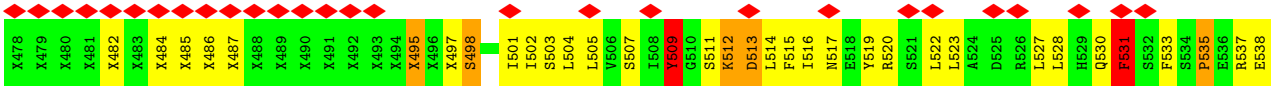
Chain N:

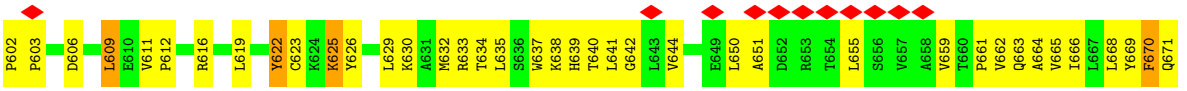


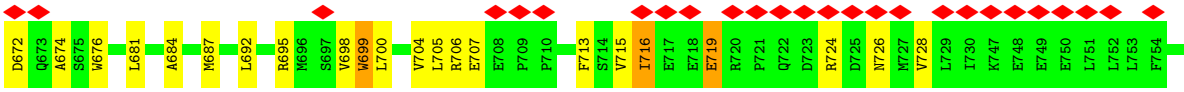






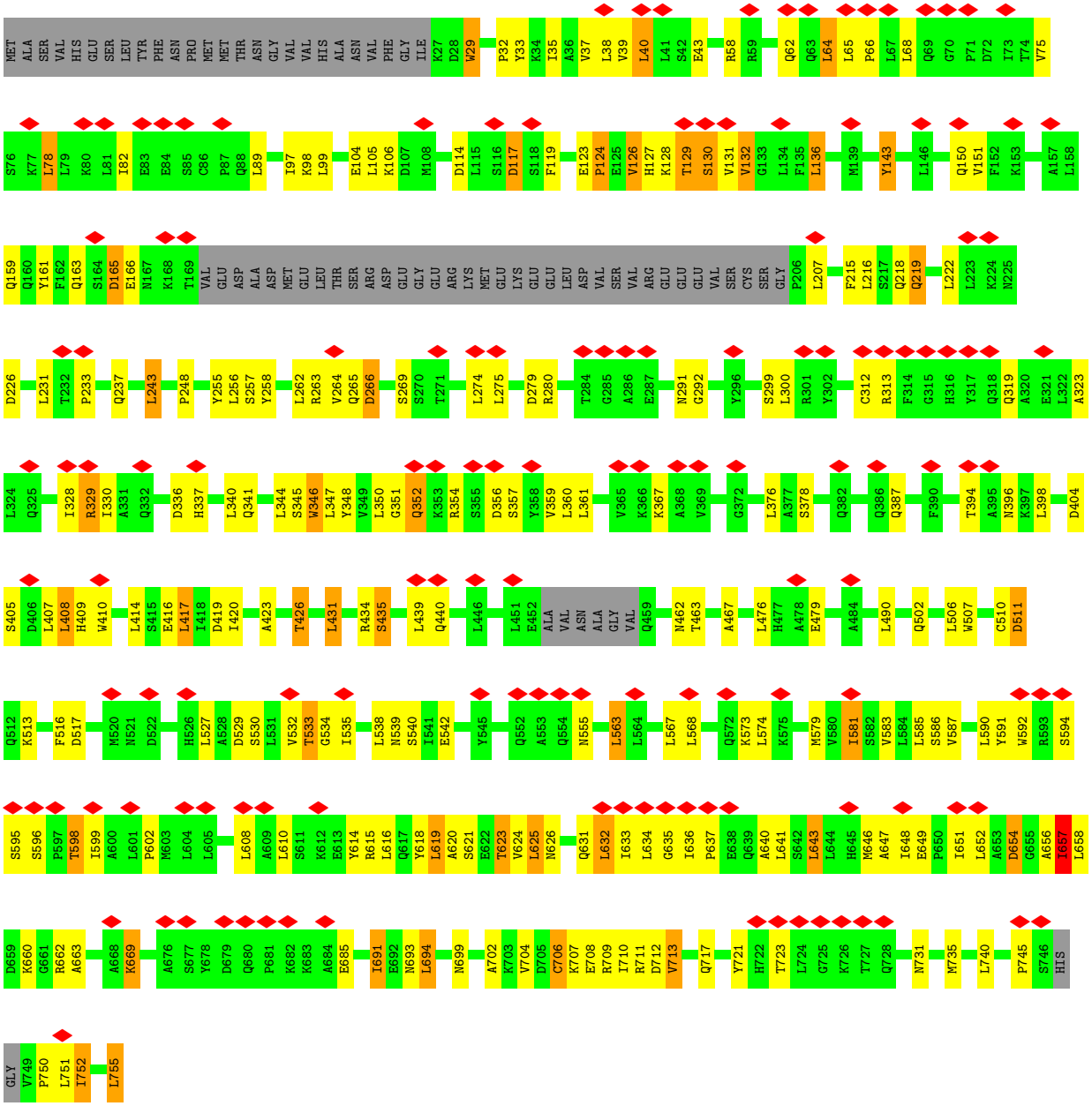






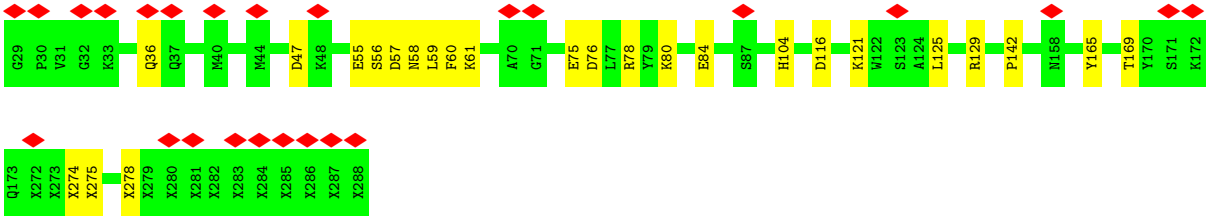
• Molecule 14: ANAPHASE-PROMOTING COMPLEX SUBUNIT 5

Chain O:



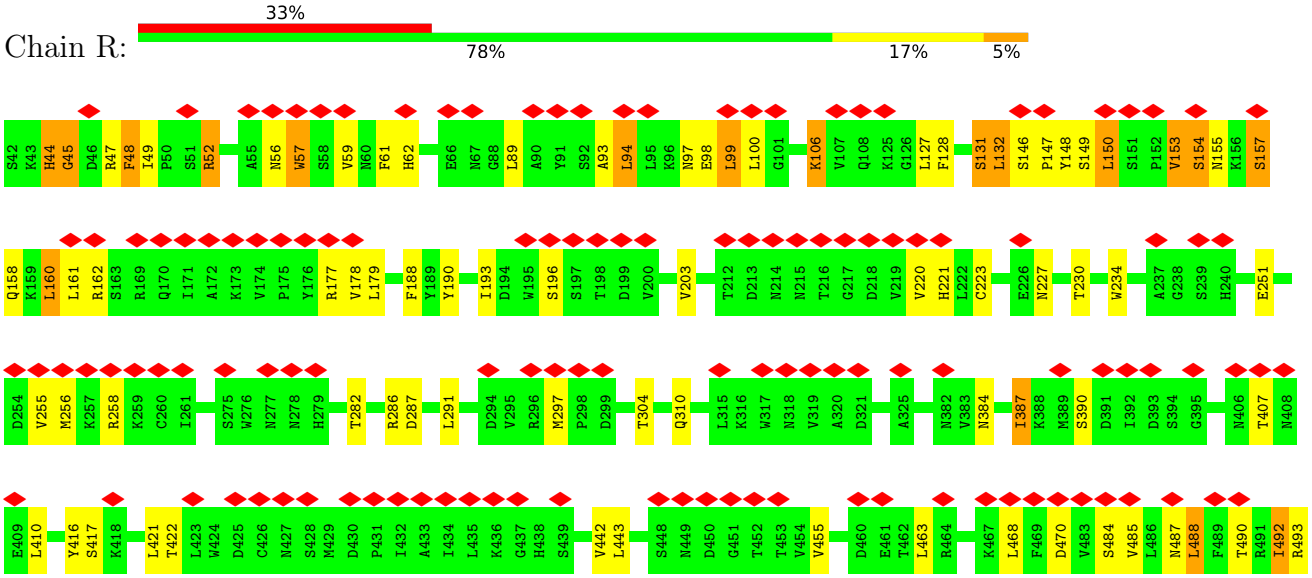
• Molecule 15: FUSION PROTEIN - UBIQUITIN-CONJUGATING ENZYME E2 C, UBIQUIT IN-CONJUGATING ENZYME E2 S

Chain Q:



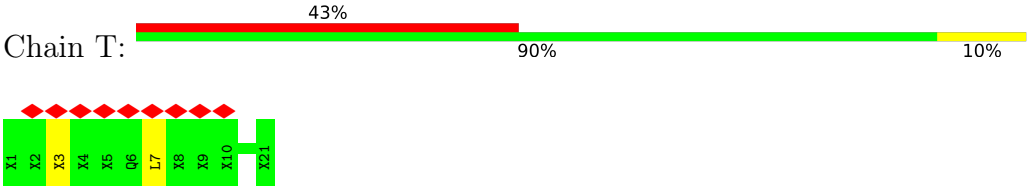
• Molecule 16: THE ANAPHASE-PROMOTING COMPLEX CHAIN R

Chain R:



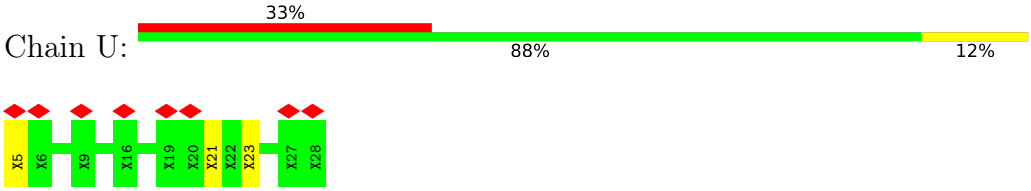
• Molecule 17: THE ANAPHASE-PROMOTING COMPLEX CHAIN T

Chain T:



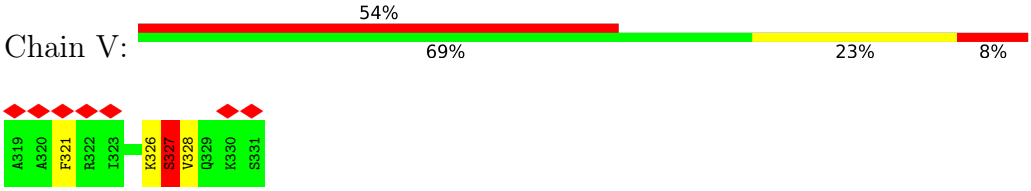
• Molecule 18: THE ANAPHASE-PROMOTING COMPLEX CHAIN U

Chain U:



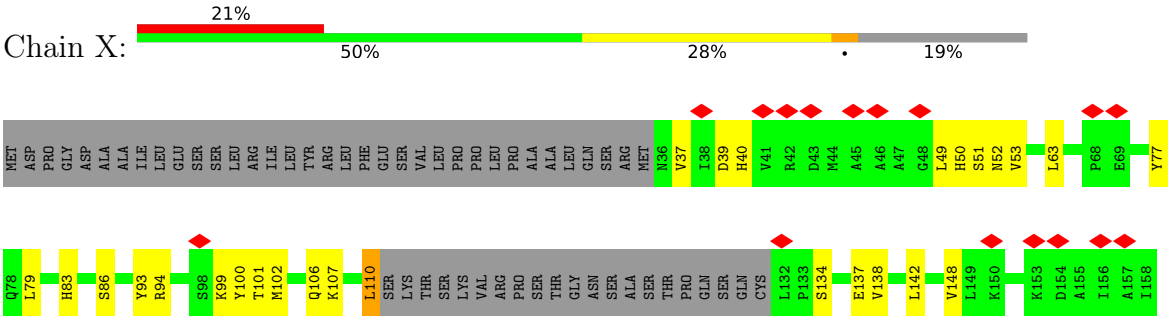
• Molecule 19: THE ANAPHASE-PROMOTING COMPLEX CHAIN V

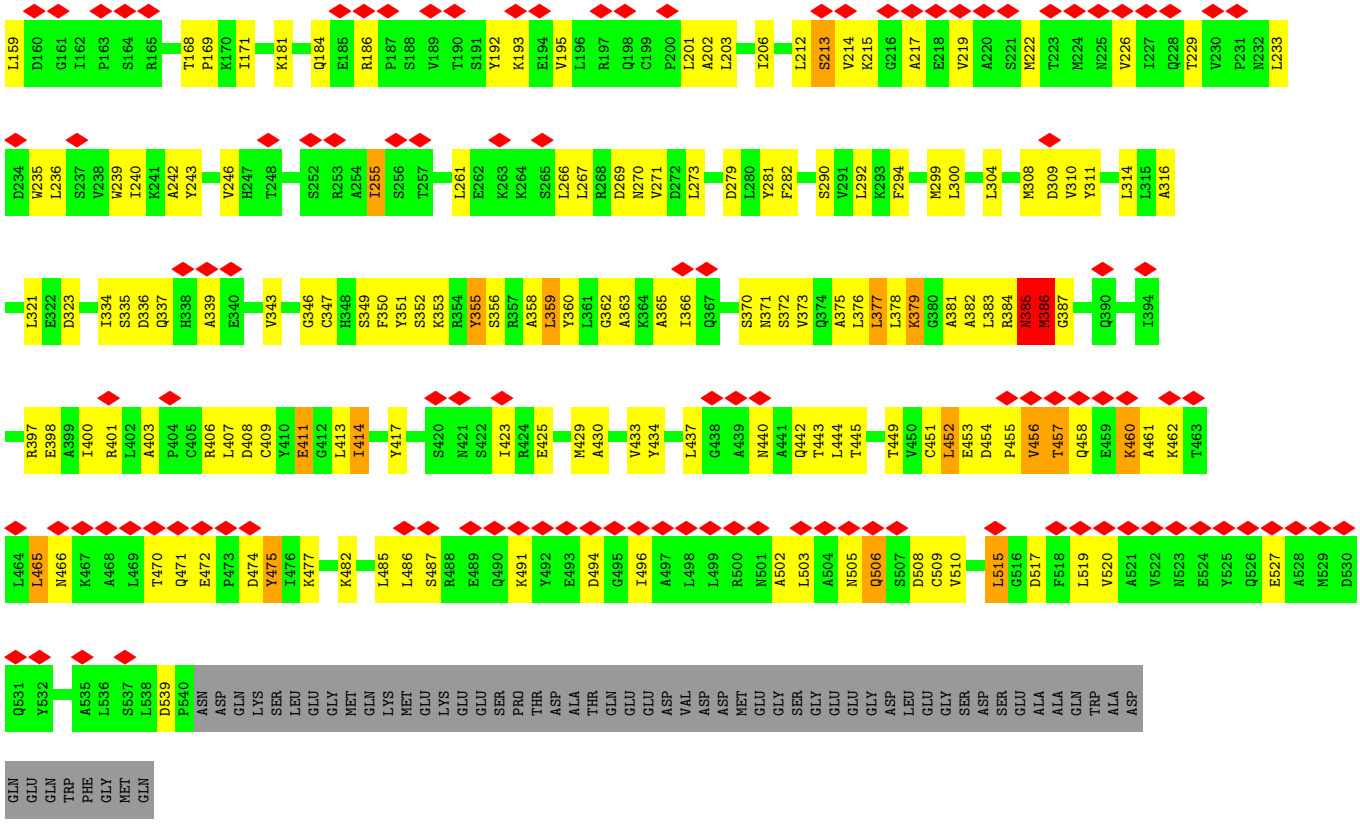
Chain V:



• Molecule 20: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

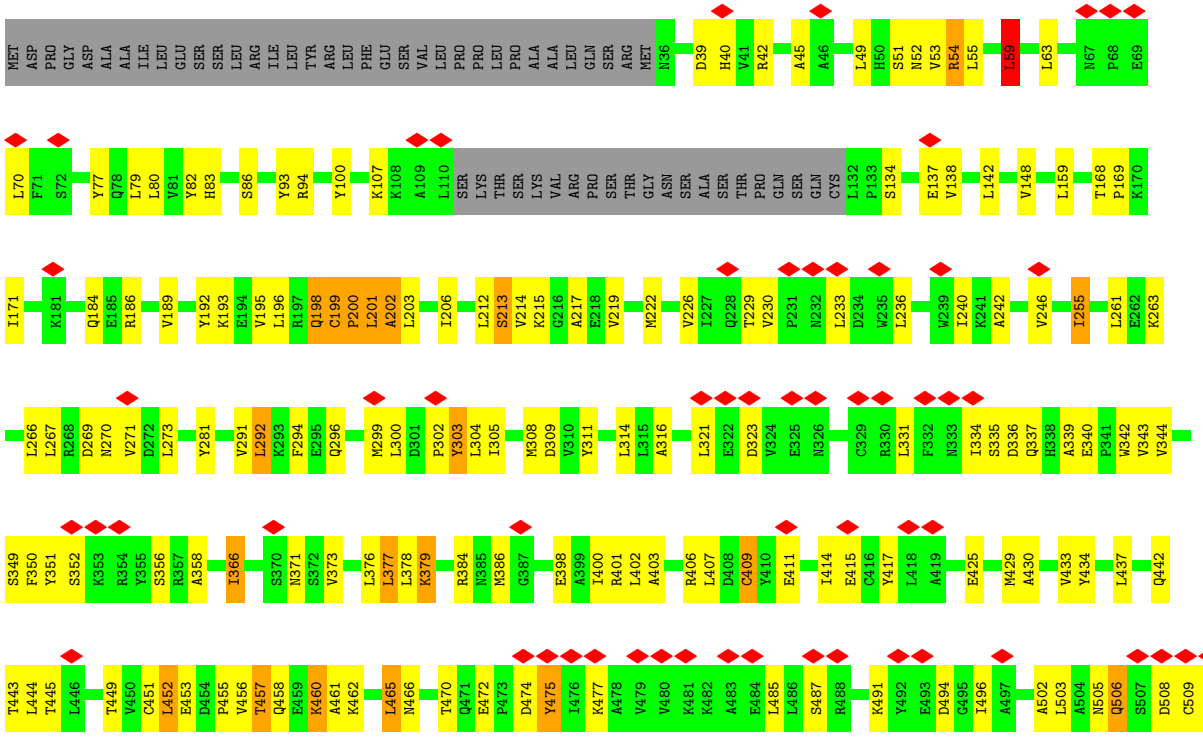
Chain X:

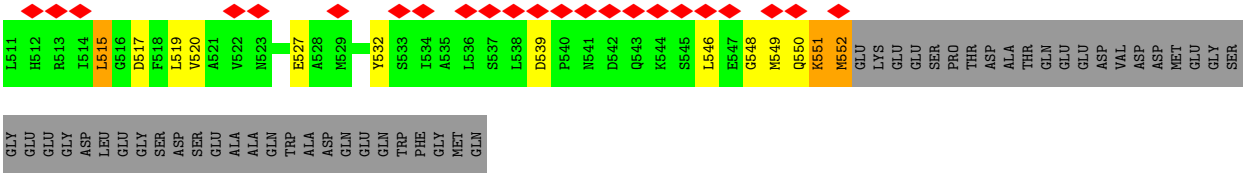




• Molecule 20: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

Chain Y:




L511 H512 R513 I514 L515 G516 D517 F518 L519 V520 A521 V522 N523 E527 A528 M529 Y532 S533 I534 A535 L536 S537 L538 D539 P540 N541 D542 Q543 K544 S545 L546 E547 G548 M549 Q550 K551 M552 GLU LYS GLU GLU SER PRO THR ASP ALA THR GLN GLU GLU ASP VAL ASP ASP MET GLU GLY SER
GLY GLU GLU GLY ASP LEU GLU GLY SER ASP SER GLU ALA ALA GLN TRP ALA ASP GLN GLU GLN TRP PHE GLY MET GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19939	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	16	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	78000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.397	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	354.0, 354.0, 354.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.77, 1.77, 1.77	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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.75	0/10949	1.00	18/14903 (0.1%)
2	B	0.52	0/675	0.85	1/914 (0.1%)
3	C	0.75	1/4403 (0.0%)	0.96	9/5945 (0.2%)
3	P	0.70	2/4137 (0.0%)	0.92	4/5587 (0.1%)
4	D	0.70	0/447	0.98	1/612 (0.2%)
5	E	0.66	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	0.63	0/212	1.03	1/281 (0.4%)
7	W	0.65	0/214	1.01	0/284
8	I	0.58	0/5827	0.85	3/7899 (0.0%)
9	J	0.75	3/4146 (0.1%)	0.97	8/5615 (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	0.60	1/4885 (0.0%)	0.96	8/6596 (0.1%)
14	O	0.73	5/5494 (0.1%)	0.97	5/7425 (0.1%)
15	Q	0.59	0/1174	0.69	0/1601
16	R	0.61	0/3052	0.85	2/4139 (0.0%)
17	T	0.84	0/13	0.99	0/16
19	V	0.65	0/99	0.91	0/130
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%)
All	All	0.70	24/67953 (0.0%)	0.93	92/92026 (0.1%)

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
8	I	0	2
9	J	0	1
13	N	0	28
16	R	0	2
17	T	0	1
20	X	0	1
All	All	0	44

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	229	LYS	CB-CG	33.03	2.41	1.52
20	X	385	ASN	N-CA	9.74	1.65	1.46
9	J	302	TRP	CB-CG	-9.04	1.33	1.50
20	X	355	TYR	CE1-CZ	8.78	1.50	1.38
9	J	337	TRP	CB-CG	-8.44	1.35	1.50
14	O	346	TRP	CB-CG	-7.91	1.36	1.50
6	F	570	TRP	CB-CG	-7.09	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	-6.42	1.38	1.50
10	K	302	TRP	CB-CG	-6.33	1.38	1.50
3	C	402	TRP	CB-CG	-6.25	1.39	1.50
20	X	386	MET	N-CA	6.23	1.58	1.46
6	H	570	TRP	CB-CG	-6.17	1.39	1.50
14	O	507	TRP	CB-CG	-5.86	1.39	1.50
10	K	25	TRP	CB-CG	-5.74	1.40	1.50
14	O	592	TRP	CB-CG	-5.45	1.40	1.50
6	F	571	CYS	CB-SG	-5.32	1.73	1.81
20	X	355	TYR	CB-CG	5.23	1.59	1.51
6	H	544	TRP	CB-CG	-5.22	1.40	1.50
6	F	13	TRP	CB-CG	-5.06	1.41	1.50
14	O	29	TRP	CB-CG	-5.03	1.41	1.50
14	O	410	TRP	CB-CG	-5.02	1.41	1.50
3	P	228	TRP	CB-CG	-5.01	1.41	1.50

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1540	ARG	NE-CZ-NH1	16.30	128.45	120.30
10	K	229	LYS	CA-CB-CG	-13.30	84.15	113.40
20	X	379	LYS	CD-CE-NZ	10.58	136.04	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	N	425	ARG	NE-CZ-NH1	9.72	125.16	120.30
20	Y	379	LYS	CD-CE-NZ	9.03	132.47	111.70
10	K	229	LYS	CB-CG-CD	-8.37	89.84	111.60
20	Y	59	LEU	CA-CB-CG	7.62	132.83	115.30
9	J	61	ARG	NE-CZ-NH1	7.50	124.05	120.30
20	Y	54	ARG	NE-CZ-NH1	7.33	123.97	120.30
11	L	132	THR	CB-CA-C	-7.26	91.99	111.60
3	C	26	PHE	CB-CG-CD1	7.22	125.85	120.80
10	K	510	ARG	NE-CZ-NH1	7.11	123.86	120.30
3	C	26	PHE	CB-CG-CD2	-7.10	115.83	120.80
6	F	768	PRO	N-CA-CB	7.09	111.81	103.30
1	A	665	MET	CG-SD-CE	7.07	111.52	100.20
20	X	110	LEU	CA-CB-CG	7.05	131.51	115.30
1	A	1540	ARG	NE-CZ-NH2	-6.95	116.83	120.30
20	X	366	ILE	CB-CA-C	-6.77	98.06	111.60
9	J	61	ARG	NE-CZ-NH2	-6.76	116.92	120.30
20	Y	366	ILE	CB-CA-C	-6.76	98.08	111.60
13	N	816	ARG	NE-CZ-NH1	-6.53	117.03	120.30
3	C	423	ARG	NE-CZ-NH1	6.50	123.55	120.30
9	J	294	LEU	CB-CG-CD2	6.46	121.98	111.00
1	A	1019	MET	CG-SD-CE	6.45	110.52	100.20
3	C	424	ARG	NE-CZ-NH1	6.39	123.50	120.30
3	P	344	ARG	NE-CZ-NH2	-6.39	117.11	120.30
3	C	516	LEU	CA-CB-CG	6.37	129.94	115.30
3	P	344	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	1203	MET	CG-SD-CE	-6.16	90.34	100.20
14	O	165	ASP	CB-CG-OD1	-6.16	112.76	118.30
6	H	50	ARG	NE-CZ-NH2	-6.15	117.22	120.30
4	D	23	PRO	N-CA-CB	6.14	110.67	103.30
6	F	625	ARG	NE-CZ-NH1	6.14	123.37	120.30
8	I	223	VAL	CB-CA-C	-6.13	99.75	111.40
6	H	467	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	1074	CYS	CA-CB-SG	-6.07	103.07	114.00
1	A	1084	ARG	NE-CZ-NH2	-6.05	117.28	120.30
6	F	467	ARG	NE-CZ-NH1	6.05	123.32	120.30
2	B	40	PRO	N-CA-CB	6.02	110.52	103.30
6	H	494	HIS	N-CA-CB	6.02	121.43	110.60
16	R	45	GLY	N-CA-C	-6.01	98.07	113.10
9	J	63	ARG	NE-CZ-NH1	5.98	123.29	120.30
6	F	625	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	882	LEU	CA-CB-CG	5.94	128.97	115.30
14	O	165	ASP	CB-CG-OD2	5.89	123.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	R	52	ARG	CG-CD-NE	-5.79	99.64	111.80
3	C	358	LEU	CA-CB-CG	5.77	128.57	115.30
14	O	117	ASP	CB-CG-OD1	-5.74	113.14	118.30
1	A	1076	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	1255	VAL	CB-CA-C	-5.60	100.77	111.40
1	A	1254	VAL	CB-CA-C	-5.59	100.78	111.40
13	N	395	ASP	N-CA-C	5.57	126.03	111.00
1	A	1267	ARG	NE-CZ-NH2	-5.53	117.53	120.30
3	C	307	LEU	CA-CB-CG	5.53	128.01	115.30
9	J	329	LEU	CA-CB-CG	5.45	127.84	115.30
13	N	509	TYR	N-CA-C	5.45	125.72	111.00
13	N	180	PHE	CB-CG-CD1	5.45	124.61	120.80
3	P	172	LEU	CA-CB-CG	5.45	127.83	115.30
1	A	1556	LEU	CA-CB-CG	5.43	127.78	115.30
7	G	8	ARG	NE-CZ-NH1	5.42	123.01	120.30
9	J	258	MET	CG-SD-CE	-5.40	91.56	100.20
20	X	359	LEU	CB-CG-CD1	5.38	120.14	111.00
11	L	184	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	1526	VAL	CB-CA-C	-5.36	101.22	111.40
6	F	50	ARG	NE-CZ-NH2	-5.36	117.62	120.30
10	K	274	THR	CB-CA-C	-5.34	97.17	111.60
9	J	146	ARG	NE-CZ-NH1	5.33	122.97	120.30
12	M	19	TRP	CA-CB-CG	5.32	123.81	113.70
8	I	26	LEU	CA-CB-CG	5.29	127.47	115.30
3	C	389	ARG	NE-CZ-NH2	-5.26	117.67	120.30
6	F	481	CYS	CA-CB-SG	-5.25	104.54	114.00
6	H	507	ARG	NE-CZ-NH1	5.22	122.91	120.30
13	N	340	ARG	NE-CZ-NH1	5.22	122.91	120.30
6	F	130	ARG	NE-CZ-NH1	5.20	122.90	120.30
14	O	502	GLN	CB-CA-C	-5.19	100.03	110.40
13	N	425	ARG	NE-CZ-NH2	-5.18	117.71	120.30
20	X	385	ASN	N-CA-C	5.17	124.96	111.00
1	A	1540	ARG	CD-NE-CZ	5.17	130.84	123.60
11	L	132	THR	N-CA-CB	5.17	120.12	110.30
11	L	170	PRO	N-CA-CB	5.16	109.49	103.30
1	A	1243	LEU	CA-CB-CG	5.16	127.16	115.30
20	X	355	TYR	CA-CB-CG	5.15	123.19	113.40
11	L	42	VAL	CB-CA-C	-5.13	101.65	111.40
3	C	42	LEU	CB-CG-CD2	5.09	119.66	111.00
1	A	25	ARG	NE-CZ-NH1	5.09	122.84	120.30
14	O	329	ARG	NE-CZ-NH1	5.08	122.84	120.30
10	K	320	ARG	CB-CA-C	5.04	120.49	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	290	ARG	NE-CZ-NH1	5.04	122.82	120.30
13	N	285	PHE	N-CA-CB	5.04	119.66	110.60
9	J	362	GLN	CB-CA-C	-5.02	100.36	110.40
1	A	1076	ARG	NE-CZ-NH1	5.02	122.81	120.30
8	I	659	ARG	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (44) 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	UNK	Peptide
13	N	162	PHE	Peptide
13	N	164	ALA	Peptide
13	N	201	UNK	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	369	ASP	Peptide
13	N	387	LEU	Peptide
13	N	394	CYS	Peptide
13	N	395	ASP	Peptide
13	N	477	UNK	Peptide
13	N	482	UNK	Peptide
13	N	484	UNK	Peptide
13	N	485	UNK	Peptide

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Mol	Chain	Res	Type	Group
13	N	487	UNK	Peptide
13	N	495	UNK	Peptide
13	N	509	TYR	Peptide
13	N	62	UNK	Peptide
13	N	63	UNK	Peptide
13	N	77	GLU	Peptide
13	N	78	VAL	Peptide
13	N	97	UNK	Peptide
16	R	131	SER	Peptide
16	R	48	PHE	Peptide
17	T	3	UNK	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	10950	0	10677	405	0
2	B	650	0	598	120	0
3	C	4305	0	4273	122	0
3	P	4042	0	3998	138	0
4	D	437	0	396	14	0
5	E	450	0	435	12	0
6	F	3923	0	3813	90	0
6	H	3853	0	3788	99	0
7	G	211	0	220	2	0
7	W	213	0	220	8	0
8	I	5709	0	5597	123	0
9	J	4047	0	3962	126	0
10	K	3988	0	3917	124	0
11	L	1435	0	1382	61	0
12	M	493	0	469	28	0
13	N	5400	0	4967	426	0
14	O	5396	0	5425	162	0
15	Q	1227	0	1128	27	0
16	R	2990	0	2913	62	0
17	T	109	0	32	3	0
18	U	120	0	27	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	V	99	0	111	1	0
20	X	3770	0	3829	254	0
20	Y	3865	0	3925	159	0
21	B	3	0	0	0	0
All	All	67685	0	66102	2317	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 17.

All (2317) 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)
13:N:435:VAL:CG1	13:N:515:PHE:CE2	1.81	1.63
1:A:1114:ARG:HE	13:N:779:MET:CG	1.13	1.57
2:B:14:TRP:CH2	2:B:41:GLY:N	1.73	1.54
13:N:502:ILE:CG1	13:N:548:ARG:HH12	1.21	1.50
1:A:1116:THR:CG2	13:N:779:MET:CE	1.87	1.49
1:A:1116:THR:HG23	13:N:779:MET:CE	1.38	1.48
20:X:358:ALA:HB3	20:X:382:ALA:CB	1.44	1.47
20:X:355:TYR:CD2	20:X:386:MET:N	1.83	1.47
13:N:502:ILE:HG13	13:N:548:ARG:NH1	1.19	1.45
13:N:435:VAL:HG13	13:N:515:PHE:CZ	1.50	1.44
2:B:38:LYS:CB	13:N:562:LYS:NZ	1.80	1.43
13:N:91:PHE:CE2	13:N:161:LEU:HD13	1.55	1.40
13:N:180:PHE:CD1	13:N:299:TRP:CZ3	2.09	1.40
13:N:435:VAL:HG13	13:N:515:PHE:CE2	1.42	1.40
20:X:355:TYR:CD1	20:X:382:ALA:O	1.74	1.40
13:N:527:LEU:HD13	13:N:564:MET:SD	1.61	1.40
1:A:1114:ARG:NE	13:N:779:MET:CG	1.79	1.38
13:N:513:ASP:HB3	13:N:789:GLU:CB	1.54	1.37
1:A:1114:ARG:NE	13:N:779:MET:HG3	1.34	1.37
2:B:17:VAL:CG1	2:B:30:PHE:HB2	1.56	1.34
2:B:16:TRP:CZ2	2:B:45:PRO:HA	1.61	1.33
13:N:502:ILE:CG1	13:N:548:ARG:NH1	1.82	1.31
13:N:180:PHE:CE1	13:N:299:TRP:CZ3	2.20	1.29
1:A:1116:THR:CG2	13:N:779:MET:HE2	1.52	1.28
1:A:1116:THR:CG2	13:N:779:MET:HE1	1.55	1.27
2:B:16:TRP:CE3	2:B:41:GLY:HA3	1.71	1.26
20:X:355:TYR:CA	20:X:382:ALA:O	1.83	1.26
20:X:355:TYR:CB	20:X:382:ALA:O	1.85	1.24
20:X:355:TYR:HA	20:X:382:ALA:O	1.29	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:355:TYR:CD2	20:X:386:MET:CA	2.20	1.23
1:A:1114:ARG:CG	13:N:779:MET:HG2	1.68	1.23
13:N:180:PHE:CD1	13:N:299:TRP:CH2	2.28	1.22
2:B:74:PRO:O	15:Q:125:LEU:CD1	1.89	1.21
20:X:355:TYR:CG	20:X:382:ALA:O	1.92	1.21
20:X:355:TYR:HD1	20:X:382:ALA:C	1.45	1.20
20:Y:305:ILE:HG22	20:Y:340:GLU:OE1	1.39	1.20
2:B:16:TRP:O	2:B:17:VAL:HG13	1.41	1.19
20:X:350:PHE:CD1	20:X:382:ALA:N	2.11	1.19
13:N:527:LEU:HD13	13:N:564:MET:CG	1.71	1.18
2:B:74:PRO:O	15:Q:125:LEU:HD11	1.42	1.18
2:B:75:MET:HA	15:Q:125:LEU:HD11	1.20	1.18
2:B:38:LYS:CB	13:N:562:LYS:HZ1	1.44	1.17
20:X:355:TYR:CD2	20:X:387:GLY:N	2.12	1.17
13:N:78:VAL:O	13:N:81:ASN:N	1.77	1.16
20:X:355:TYR:HB2	20:X:386:MET:HB3	1.23	1.15
20:X:355:TYR:CG	20:X:386:MET:N	2.16	1.14
2:B:15:LEU:O	2:B:17:VAL:HG22	1.48	1.13
13:N:435:VAL:HG12	13:N:515:PHE:CE2	1.78	1.13
1:A:1114:ARG:HB3	13:N:779:MET:CE	1.79	1.13
2:B:16:TRP:HZ2	2:B:45:PRO:CA	1.60	1.13
13:N:511:SER:CB	13:N:789:GLU:CB	2.26	1.12
20:X:350:PHE:CE1	20:X:378:LEU:O	2.02	1.12
2:B:42:ASP:CA	13:N:630:LYS:CG	2.07	1.12
20:X:355:TYR:CE2	20:X:385:ASN:C	2.09	1.12
1:A:1114:ARG:HB3	13:N:779:MET:HE3	1.15	1.11
2:B:75:MET:HA	15:Q:125:LEU:CD1	1.78	1.11
13:N:513:ASP:CB	13:N:789:GLU:CB	2.28	1.10
20:X:355:TYR:HB2	20:X:386:MET:CB	1.80	1.10
1:A:1114:ARG:HG3	13:N:779:MET:HG2	1.22	1.10
2:B:16:TRP:CD2	2:B:41:GLY:HA3	1.86	1.10
2:B:42:ASP:HA	13:N:630:LYS:CG	1.75	1.09
20:X:358:ALA:HB3	20:X:382:ALA:HB3	1.12	1.09
20:X:355:TYR:CD2	20:X:385:ASN:C	2.26	1.08
20:X:355:TYR:HB3	20:X:383:LEU:HA	1.31	1.08
20:X:358:ALA:HB3	20:X:382:ALA:HB2	1.34	1.08
2:B:17:VAL:HG12	2:B:30:PHE:HB2	1.21	1.06
2:B:75:MET:CA	15:Q:125:LEU:HD11	1.84	1.06
3:C:301:ASP:OD1	3:C:335:CYS:SG	2.14	1.05
20:X:347:CYS:HA	20:X:378:LEU:HD11	1.35	1.05
20:X:350:PHE:CD1	20:X:381:ALA:C	2.29	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:355:TYR:HD2	20:X:386:MET:C	1.59	1.05
13:N:91:PHE:CE2	13:N:161:LEU:CD1	2.39	1.04
13:N:91:PHE:CD2	13:N:161:LEU:HD13	1.92	1.04
13:N:97:UNK:O	13:N:99:UNK:CB	2.05	1.04
20:X:350:PHE:CE1	20:X:382:ALA:N	2.26	1.04
1:A:1114:ARG:CD	13:N:779:MET:HG2	1.88	1.03
2:B:74:PRO:O	15:Q:125:LEU:CG	2.06	1.03
13:N:435:VAL:CG1	13:N:515:PHE:CD2	2.40	1.03
20:Y:42:ARG:HA	20:Y:82:TYR:CE2	1.91	1.03
2:B:17:VAL:HG13	2:B:30:PHE:HB2	1.41	1.02
20:X:358:ALA:CB	20:X:382:ALA:CB	2.36	1.02
1:A:1114:ARG:CB	13:N:779:MET:HE3	1.89	1.02
2:B:15:LEU:N	2:B:31:ASN:O	1.91	1.02
13:N:180:PHE:CD1	13:N:299:TRP:HZ3	1.55	1.02
1:A:1116:THR:HG22	13:N:779:MET:HE1	1.05	1.01
2:B:42:ASP:HA	13:N:630:LYS:HG3	1.38	1.01
2:B:38:LYS:CB	13:N:562:LYS:HZ3	1.53	1.01
20:X:355:TYR:HD2	20:X:386:MET:CA	1.62	1.00
2:B:17:VAL:HA	2:B:30:PHE:HB3	1.44	1.00
20:X:343:VAL:O	20:X:378:LEU:HD21	1.63	0.99
1:A:1114:ARG:CB	13:N:779:MET:CE	2.40	0.99
20:X:400:ILE:HD13	20:X:413:LEU:HD13	1.41	0.99
13:N:435:VAL:CG1	13:N:515:PHE:CZ	2.26	0.99
13:N:120:UNK:O	13:N:124:PRO:HD2	1.61	0.99
20:Y:305:ILE:CG2	20:Y:340:GLU:OE1	2.10	0.99
20:X:347:CYS:CA	20:X:378:LEU:HD11	1.93	0.98
2:B:14:TRP:CH2	2:B:40:PRO:C	2.31	0.98
14:O:222:LEU:O	14:O:226:ASP:O	1.81	0.98
13:N:527:LEU:CD1	13:N:564:MET:SD	2.52	0.98
20:Y:373:VAL:HG11	20:Y:403:ALA:HB2	1.46	0.97
6:H:537:GLU:OE2	6:H:568:GLU:OE1	1.82	0.97
13:N:559:VAL:HG23	13:N:562:LYS:HD3	1.47	0.97
20:X:355:TYR:CD1	20:X:382:ALA:C	2.28	0.97
14:O:219:GLN:HE22	14:O:231:LEU:HD13	1.30	0.96
20:X:350:PHE:CZ	20:X:381:ALA:HB3	2.00	0.96
20:X:363:ALA:HB2	20:X:379:LYS:HZ2	1.30	0.96
13:N:527:LEU:CD1	13:N:564:MET:CG	2.43	0.96
1:A:1114:ARG:CG	13:N:779:MET:CG	2.43	0.96
2:B:16:TRP:CD1	2:B:46:LEU:HD21	2.01	0.95
13:N:343:GLU:O	13:N:347:ILE:N	1.97	0.95
20:X:363:ALA:HB2	20:X:379:LYS:NZ	1.80	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:359:LEU:HD12	20:X:383:LEU:HD11	1.49	0.95
20:Y:42:ARG:HA	20:Y:82:TYR:HE2	1.22	0.95
9:J:445:GLU:HG2	9:J:446:PRO:HD3	1.49	0.94
13:N:502:ILE:HG12	13:N:548:ARG:NH1	1.81	0.94
1:A:1114:ARG:CD	13:N:779:MET:CG	2.44	0.94
8:I:349:ILE:HD11	14:O:407:LEU:HD13	1.48	0.94
11:L:126:ASP:HB2	11:L:132:THR:CA	1.98	0.93
20:X:355:TYR:HD2	20:X:387:GLY:N	1.56	0.93
20:Y:491:LYS:O	20:Y:494:ASP:OD1	1.87	0.92
14:O:291:ASN:O	14:O:336:ASP:HB2	1.70	0.92
20:X:491:LYS:O	20:X:494:ASP:OD1	1.87	0.91
2:B:14:TRP:CE3	2:B:31:ASN:O	2.23	0.91
2:B:74:PRO:C	15:Q:125:LEU:HD11	1.91	0.91
13:N:527:LEU:HD13	13:N:564:MET:HG3	1.50	0.91
13:N:527:LEU:CD1	13:N:564:MET:HG3	1.99	0.91
13:N:180:PHE:HD1	13:N:299:TRP:HZ3	1.10	0.90
13:N:511:SER:HB2	13:N:789:GLU:CB	1.98	0.90
13:N:395:ASP:OD1	13:N:398:THR:N	2.05	0.90
20:X:350:PHE:CE2	20:X:381:ALA:HB3	2.06	0.90
20:X:355:TYR:CE2	20:X:387:GLY:N	2.39	0.90
20:X:358:ALA:CB	20:X:382:ALA:HB2	2.01	0.90
20:X:350:PHE:HD1	20:X:382:ALA:N	1.62	0.89
10:K:250:CYS:SG	10:K:274:THR:CG2	2.60	0.89
2:B:14:TRP:HH2	2:B:40:PRO:C	1.72	0.89
20:X:452:LEU:CD2	20:X:457:THR:O	2.20	0.89
20:X:355:TYR:HA	20:X:382:ALA:C	1.92	0.88
2:B:17:VAL:HA	2:B:30:PHE:CB	2.02	0.88
20:X:350:PHE:CZ	20:X:378:LEU:O	2.26	0.88
13:N:393:THR:O	13:N:395:ASP:HB3	1.73	0.88
20:Y:452:LEU:CD2	20:Y:457:THR:O	2.20	0.88
20:Y:196:LEU:O	20:Y:200:PRO:HA	1.74	0.88
20:X:350:PHE:CE1	20:X:381:ALA:CA	2.57	0.88
2:B:15:LEU:H	2:B:31:ASN:C	1.72	0.88
2:B:16:TRP:CD2	2:B:41:GLY:CA	2.56	0.87
10:K:214:LYS:O	10:K:216:SER:N	2.07	0.87
13:N:511:SER:O	13:N:512:LYS:HG3	1.74	0.87
2:B:16:TRP:HZ2	2:B:45:PRO:HA	0.72	0.87
1:A:1116:THR:HG23	13:N:779:MET:HE2	0.88	0.87
13:N:435:VAL:HG11	13:N:515:PHE:CE2	2.06	0.86
13:N:564:MET:HA	13:N:564:MET:HE2	1.54	0.86
1:A:1116:THR:HG22	13:N:779:MET:CE	1.77	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:452:LEU:HD22	20:X:461:ALA:N	1.90	0.86
13:N:538:GLU:HG2	13:N:561:LEU:HG	1.58	0.86
2:B:16:TRP:CD1	2:B:46:LEU:CD2	2.59	0.86
2:B:17:VAL:CG1	2:B:30:PHE:CB	2.50	0.86
2:B:16:TRP:O	2:B:17:VAL:CG1	2.24	0.86
1:A:1097:THR:HG23	14:O:340:LEU:HB3	1.57	0.85
8:I:145:LEU:HD13	8:I:267:LEU:HD22	1.57	0.85
13:N:60:UNK:O	13:N:63:UNK:CB	2.24	0.85
2:B:74:PRO:O	15:Q:125:LEU:HG	1.75	0.85
20:X:343:VAL:O	20:X:378:LEU:CD2	2.25	0.85
1:A:1114:ARG:HG3	13:N:779:MET:CG	2.07	0.84
6:F:130:ARG:HG2	20:Y:506:GLN:HE21	1.43	0.84
13:N:502:ILE:CD1	13:N:548:ARG:HH12	1.90	0.84
20:Y:452:LEU:HD22	20:Y:461:ALA:N	1.91	0.84
9:J:445:GLU:OE1	9:J:475:ILE:HG21	1.76	0.84
13:N:120:UNK:O	13:N:124:PRO:CD	2.24	0.84
13:N:609:LEU:HD21	13:N:662:VAL:HG12	1.58	0.84
11:L:126:ASP:HB2	11:L:132:THR:HA	1.60	0.84
20:X:359:LEU:HA	20:X:379:LYS:HG3	1.61	0.83
20:X:407:LEU:HD22	20:X:437:LEU:HD21	1.60	0.83
6:H:537:GLU:CD	6:H:568:GLU:OE1	2.16	0.83
2:B:14:TRP:HH2	2:B:41:GLY:N	1.36	0.83
20:X:350:PHE:CE1	20:X:381:ALA:C	2.52	0.83
2:B:16:TRP:CE2	2:B:41:GLY:CA	2.62	0.82
9:J:254:THR:HG23	9:J:271:HIS:CD2	2.13	0.82
13:N:289:PHE:O	13:N:291:LYS:N	2.11	0.82
9:J:451:LEU:HD12	9:J:467:TYR:CD2	2.13	0.82
2:B:16:TRP:CZ3	2:B:41:GLY:HA3	2.13	0.82
6:F:130:ARG:HG2	20:Y:506:GLN:NE2	1.93	0.82
20:Y:452:LEU:HD23	20:Y:457:THR:O	1.78	0.82
20:Y:503:LEU:O	20:Y:506:GLN:NE2	2.12	0.82
2:B:16:TRP:HB2	2:B:31:ASN:C	1.99	0.82
20:Y:407:LEU:HD22	20:Y:437:LEU:HD21	1.60	0.82
20:X:452:LEU:HD23	20:X:457:THR:O	1.78	0.82
13:N:202:GLU:O	13:N:204:ASP:N	2.12	0.82
2:B:16:TRP:CE3	2:B:41:GLY:CA	2.60	0.81
13:N:398:THR:HG21	15:Q:278:UNK:CB	2.10	0.81
1:A:1114:ARG:HE	13:N:779:MET:CB	1.85	0.81
2:B:46:LEU:O	13:N:632:MET:HE3	1.78	0.81
1:A:1235:LEU:CD1	1:A:1272:VAL:HG21	2.11	0.81
6:F:653:LEU:HA	6:F:656:MET:SD	2.21	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:17:ASP:HA	12:M:20:ARG:HG2	1.61	0.81
13:N:564:MET:HE3	13:N:596:LEU:CD2	2.10	0.81
1:A:1351:GLN:O	11:L:42:VAL:HG21	1.79	0.81
20:X:355:TYR:CD2	20:X:386:MET:C	2.41	0.81
13:N:180:PHE:CE1	13:N:299:TRP:CH2	2.63	0.81
20:X:359:LEU:HA	20:X:379:LYS:CG	2.11	0.81
20:X:347:CYS:N	20:X:378:LEU:HD11	1.95	0.80
20:Y:366:ILE:HD11	20:Y:379:LYS:HD2	1.63	0.80
9:J:445:GLU:HG2	9:J:446:PRO:CD	2.11	0.80
11:L:83:TYR:CD2	11:L:115:GLU:HA	2.16	0.80
20:X:355:TYR:CG	20:X:383:LEU:O	2.35	0.80
20:X:355:TYR:HB3	20:X:383:LEU:CA	2.11	0.80
13:N:564:MET:HE2	13:N:564:MET:CA	2.11	0.80
20:X:355:TYR:CD1	20:X:383:LEU:C	2.56	0.80
10:K:185:LEU:HD13	10:K:209:LEU:HD11	1.65	0.79
16:R:178:VAL:O	19:V:327:SER:O	1.99	0.79
13:N:699:TRP:HB3	13:N:705:LEU:HD23	1.63	0.79
20:X:350:PHE:HD1	20:X:382:ALA:CA	1.94	0.79
20:X:355:TYR:HD1	20:X:382:ALA:O	1.27	0.79
20:X:350:PHE:CZ	20:X:378:LEU:HA	2.18	0.79
8:I:224:SER:CB	8:I:229:SER:HA	2.13	0.78
10:K:62:SER:O	10:K:63:ARG:HG3	1.83	0.78
10:K:432:ILE:HD11	10:K:444:TRP:CD1	2.17	0.78
20:X:503:LEU:O	20:X:506:GLN:NE2	2.17	0.78
13:N:502:ILE:HG13	13:N:548:ARG:HH12	0.65	0.78
20:X:355:TYR:CD2	20:X:383:LEU:O	2.36	0.78
20:X:347:CYS:HA	20:X:378:LEU:CD1	2.13	0.78
2:B:46:LEU:O	13:N:632:MET:CE	2.31	0.78
15:Q:116:ASP:OD2	15:Q:121:LYS:NZ	2.11	0.78
2:B:48:TRP:HZ3	13:N:632:MET:HE3	1.47	0.78
11:L:126:ASP:N	11:L:132:THR:HG23	1.99	0.78
1:A:482:VAL:HG12	1:A:487:THR:O	1.83	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
1:A:1797:ILE:HG22	1:A:1852:ILE:HD11	1.66	0.77
13:N:368:THR:OG1	13:N:369:ASP:HA	1.84	0.77
20:X:358:ALA:CB	20:X:382:ALA:HB3	2.06	0.77
3:P:233:PHE:CZ	3:P:237:ILE:CD1	2.67	0.77
9:J:35:GLU:OE2	9:J:63:ARG:NE	2.18	0.77
13:N:395:ASP:HB2	13:N:397:ILE:H	1.49	0.77
20:X:406:ARG:HB2	20:X:409:CYS:SG	2.25	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:366:ILE:HD11	20:Y:379:LYS:CD	2.14	0.77
20:X:355:TYR:CG	20:X:383:LEU:C	2.58	0.77
2:B:15:LEU:O	2:B:17:VAL:CG2	2.30	0.77
20:X:40:HIS:HB3	20:Y:201:LEU:HD11	1.66	0.77
2:B:8:TRP:CD1	13:N:644:VAL:HG12	2.19	0.77
2:B:14:TRP:CZ3	2:B:41:GLY:N	2.38	0.77
2:B:16:TRP:CZ3	2:B:41:GLY:CA	2.68	0.77
10:K:254:THR:HG23	10:K:271:HIS:CD2	2.20	0.77
13:N:511:SER:OG	13:N:789:GLU:CB	2.33	0.77
14:O:581:ILE:HD11	14:O:619:LEU:HB3	1.67	0.77
13:N:393:THR:O	13:N:395:ASP:CB	2.33	0.76
13:N:564:MET:CE	13:N:596:LEU:HD23	2.14	0.76
3:P:358:LEU:O	3:P:362:PRO:HA	1.86	0.76
3:C:251:TYR:HB3	3:C:269:ILE:HD11	1.68	0.76
9:J:285:PHE:HB2	9:J:308:TYR:CE1	2.20	0.76
13:N:180:PHE:CD1	13:N:299:TRP:HH2	1.94	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
13:N:435:VAL:HG11	13:N:515:PHE:CD2	2.20	0.76
3:P:267:SER:OG	3:P:299:ASN:ND2	2.19	0.76
1:A:1114:ARG:NH2	13:N:775:ASN:O	2.18	0.76
6:F:89:GLU:OE1	6:F:130:ARG:NH2	2.18	0.76
13:N:443:UNK:CB	13:N:537:ARG:NH2	2.49	0.76
1:A:1637:LEU:HD13	1:A:1665:GLN:HE21	1.49	0.76
13:N:564:MET:HA	13:N:564:MET:CE	2.14	0.76
14:O:414:LEU:CD1	14:O:417:LEU:HB2	2.16	0.76
8:I:34:LEU:HD12	8:I:46:LEU:HD21	1.68	0.75
13:N:670:PHE:CE1	13:N:715:VAL:HB	2.21	0.75
6:F:533:VAL:O	6:F:568:GLU:OE1	2.04	0.75
11:L:126:ASP:HB2	11:L:132:THR:N	2.01	0.75
10:K:285:PHE:HB2	10:K:308:TYR:CE1	2.21	0.75
11:L:45:LEU:O	11:L:155:GLN:OE1	2.04	0.75
13:N:502:ILE:CG1	13:N:548:ARG:HH11	1.97	0.75
20:X:452:LEU:CD2	20:X:461:ALA:N	2.49	0.75
13:N:78:VAL:O	13:N:80:GLN:N	2.18	0.75
20:Y:294:PHE:CD1	20:Y:311:TYR:CD1	2.74	0.75
13:N:180:PHE:HE1	13:N:299:TRP:CZ3	2.02	0.75
11:L:33:LEU:HG	11:L:42:VAL:HG22	1.69	0.75
3:P:464:ASP:OD2	3:P:469:ALA:HB3	1.86	0.75
20:Y:406:ARG:HB2	20:Y:409:CYS:SG	2.26	0.75
20:Y:452:LEU:CD2	20:Y:461:ALA:N	2.49	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:520:ARG:NH2	20:X:101:THR:OG1	2.20	0.74
13:N:513:ASP:OD2	13:N:789:GLU:N	2.19	0.74
20:X:350:PHE:HE1	20:X:382:ALA:H	1.34	0.74
20:Y:196:LEU:O	20:Y:200:PRO:CA	2.35	0.74
13:N:509:TYR:O	13:N:511:SER:N	2.21	0.74
13:N:414:MET:SD	13:N:498:SER:N	2.60	0.74
14:O:32:PRO:O	14:O:35:ILE:HG22	1.87	0.74
6:F:152:PHE:HE1	6:F:162:PRO:HG2	1.53	0.74
9:J:219:VAL:HG12	9:J:221:PRO:HD3	1.68	0.74
13:N:564:MET:HE3	13:N:596:LEU:HD23	1.67	0.74
13:N:564:MET:CE	13:N:596:LEU:CD2	2.66	0.74
13:N:435:VAL:HG12	13:N:515:PHE:CD2	2.12	0.74
13:N:395:ASP:HB2	13:N:397:ILE:N	2.03	0.74
3:C:493:TYR:CZ	3:C:497:ILE:HD11	2.23	0.73
20:X:359:LEU:CA	20:X:379:LYS:HG3	2.18	0.73
6:H:655:GLU:OE2	6:H:684:LYS:NZ	2.22	0.73
20:Y:349:SER:HB2	20:Y:358:ALA:HB2	1.68	0.73
20:Y:452:LEU:HD21	20:Y:457:THR:O	1.87	0.73
2:B:18:ALA:HB2	2:B:48:TRP:HZ2	1.52	0.73
3:C:96:VAL:HG21	3:P:53:LYS:HD3	1.70	0.73
3:P:402:TRP:CH2	3:P:424:ARG:HG2	2.23	0.73
1:A:1279:ARG:NH1	1:A:1287:TYR:OH	2.21	0.73
13:N:443:UNK:CB	13:N:537:ARG:HH22	2.01	0.73
8:I:279:ILE:CD1	8:I:337:ILE:HA	2.19	0.73
14:O:539:ASN:HD22	14:O:542:GLU:CB	2.02	0.73
20:X:452:LEU:HD21	20:X:457:THR:O	1.87	0.73
20:X:362:GLY:HA3	20:X:379:LYS:HB2	1.69	0.73
1:A:1235:LEU:HD11	1:A:1272:VAL:HG21	1.70	0.73
1:A:207:LEU:HD12	1:A:208:PRO:HD3	1.70	0.72
1:A:1482:LEU:N	17:T:7:LEU:CB	2.52	0.72
3:P:233:PHE:CZ	3:P:237:ILE:HD12	2.24	0.72
9:J:167:PHE:O	9:J:170:LEU:HD23	1.89	0.72
15:Q:165:TYR:O	15:Q:169:THR:HG22	1.90	0.72
1:A:801:PRO:O	1:A:804:ASP:OD1	2.06	0.72
1:A:1082:VAL:HG22	1:A:1138:HIS:CD2	2.25	0.72
13:N:528:LEU:HD11	13:N:641:LEU:HD13	1.72	0.72
1:A:1191:LEU:HD11	16:R:62:HIS:CB	2.19	0.72
2:B:42:ASP:CA	13:N:630:LYS:HG2	2.18	0.72
8:I:279:ILE:HD11	8:I:337:ILE:HG23	1.72	0.72
8:I:56:TRP:CE3	8:I:98:PRO:HB3	2.25	0.71
13:N:425:ARG:CZ	13:N:507:SER:HB2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:36:GLN:HG2	15:Q:59:LEU:HD11	1.72	0.71
20:Y:462:LYS:HG2	20:Y:485:LEU:HD13	1.73	0.71
1:A:1191:LEU:HD11	16:R:62:HIS:HB2	1.73	0.71
11:L:44:GLN:HA	11:L:47:ASP:OD2	1.91	0.71
11:L:125:THR:HA	11:L:126:ASP:HB3	1.71	0.71
20:X:350:PHE:CE1	20:X:381:ALA:N	2.59	0.71
2:B:16:TRP:CE2	2:B:44:CYS:O	2.42	0.71
9:J:215:PRO:HG3	9:J:402:PRO:HG2	1.72	0.71
1:A:1274:LEU:HD11	1:A:1321:VAL:HG12	1.71	0.71
20:Y:452:LEU:HD22	20:Y:460:LYS:C	2.11	0.71
13:N:676:TRP:O	13:N:713:PHE:HB2	1.89	0.71
20:X:359:LEU:HB2	20:X:383:LEU:HD21	1.73	0.71
20:Y:373:VAL:HG11	20:Y:403:ALA:CB	2.20	0.71
1:A:1781:GLN:HB2	1:A:1783:THR:HG22	1.71	0.71
8:I:307:LEU:HD13	8:I:313:ALA:HB2	1.71	0.71
16:R:484:SER:HB3	16:R:485:VAL:HA	1.73	0.71
20:X:452:LEU:HD22	20:X:460:LYS:C	2.11	0.71
9:J:211:LYS:O	9:J:212:TYR:CD2	2.43	0.70
1:A:1114:ARG:HE	13:N:779:MET:HG3	0.54	0.70
2:B:17:VAL:HG12	2:B:30:PHE:CB	2.14	0.70
3:C:358:LEU:O	3:C:362:PRO:HA	1.92	0.70
14:O:539:ASN:HD22	14:O:542:GLU:HB2	1.56	0.70
3:P:233:PHE:CE1	3:P:237:ILE:HD11	2.26	0.70
9:J:441:VAL:HG21	9:J:444:TRP:HD1	1.55	0.70
2:B:16:TRP:CZ2	2:B:44:CYS:O	2.45	0.70
6:F:705:CYS:SG	6:F:706:LYS:N	2.65	0.70
1:A:1114:ARG:CB	13:N:779:MET:HE2	2.21	0.70
14:O:414:LEU:HD12	14:O:417:LEU:HB2	1.72	0.70
3:C:358:LEU:HD13	3:C:367:ALA:HB3	1.74	0.70
10:K:210:LYS:O	10:K:212:TYR:N	2.23	0.70
13:N:97:UNK:C	13:N:99:UNK:N	2.54	0.70
13:N:435:VAL:HA	13:N:438:ILE:HD12	1.74	0.70
2:B:17:VAL:CA	2:B:30:PHE:HB3	2.19	0.70
20:X:359:LEU:HG	20:X:379:LYS:HE2	1.74	0.70
11:L:78:CYS:SG	11:L:119:TRP:CE3	2.85	0.69
13:N:502:ILE:HG12	13:N:548:ARG:HH11	1.57	0.69
20:Y:294:PHE:CD1	20:Y:311:TYR:CE1	2.81	0.69
1:A:1186:THR:HG23	1:A:1215:ALA:HB1	1.73	0.69
2:B:39:VAL:CB	2:B:43:ASP:HB2	2.22	0.69
3:C:352:LEU:HD21	3:C:356:ARG:CZ	2.23	0.69
11:L:105:LEU:HD12	11:L:138:GLN:OE1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:180:PHE:CG	13:N:299:TRP:HH2	2.09	0.69
2:B:17:VAL:HG13	2:B:30:PHE:CB	2.17	0.69
1:A:1114:ARG:HB3	13:N:779:MET:CG	2.23	0.69
15:Q:61:LYS:NZ	15:Q:84:GLU:OE1	2.24	0.69
2:B:16:TRP:CE2	2:B:41:GLY:HA2	2.27	0.69
15:Q:78:ARG:HH21	15:Q:80:LYS:HE3	1.56	0.69
20:X:474:ASP:OD1	20:X:502:ALA:HA	1.92	0.69
13:N:341:ILE:O	13:N:344:LEU:HB3	1.92	0.69
20:X:462:LYS:HG2	20:X:485:LEU:HD13	1.74	0.69
1:A:1033:ARG:NH1	1:A:1531:GLY:O	2.25	0.69
1:A:1640:GLY:N	1:A:1645:GLU:O	2.26	0.69
3:C:388:TYR:HB2	3:C:405:LEU:HD13	1.75	0.69
14:O:490:LEU:HD13	14:O:511:ASP:HB2	1.73	0.69
20:X:434:TYR:HA	20:X:444:LEU:HD22	1.74	0.69
1:A:612:ILE:O	1:A:641:TRP:CZ3	2.46	0.69
20:Y:474:ASP:OD1	20:Y:502:ALA:HA	1.91	0.69
2:B:75:MET:N	15:Q:125:LEU:HD11	2.07	0.69
8:I:144:THR:HG21	8:I:159:GLU:HA	1.74	0.69
15:Q:47:ASP:OD2	15:Q:129:ARG:NE	2.25	0.69
15:Q:78:ARG:NH2	15:Q:80:LYS:HE3	2.08	0.69
11:L:94:ILE:HD12	11:L:113:LEU:HD11	1.75	0.68
13:N:596:LEU:HD13	13:N:601:TRP:CE2	2.28	0.68
3:P:252:GLN:O	3:P:255:ILE:HG22	1.93	0.68
1:A:1470:LEU:HA	1:A:1522:SER:OG	1.92	0.68
6:H:73:TYR:CD1	6:H:117:THR:HG22	2.29	0.68
3:P:358:LEU:CD1	3:P:368:TRP:CE2	2.76	0.68
1:A:1114:ARG:HB2	13:N:779:MET:HE2	1.76	0.68
1:A:1114:ARG:HB2	13:N:779:MET:CE	2.23	0.68
6:H:729:LEU:HD13	6:H:739:VAL:HG22	1.75	0.68
8:I:73:TRP:CZ2	8:I:80:LEU:HD22	2.28	0.68
20:X:400:ILE:HG21	20:X:413:LEU:HB2	1.73	0.68
13:N:511:SER:HB3	13:N:789:GLU:CB	2.20	0.68
1:A:1114:ARG:NH2	13:N:778:ARG:N	2.30	0.68
14:O:479:GLU:O	14:O:656:ALA:O	2.10	0.68
14:O:591:TYR:HA	14:O:594:SER:OG	1.93	0.68
6:F:729:LEU:HD13	6:F:739:VAL:HG22	1.74	0.67
9:J:254:THR:HG23	9:J:271:HIS:HD2	1.59	0.67
9:J:451:LEU:HD12	9:J:467:TYR:CE2	2.29	0.67
6:F:133:LYS:HA	6:F:136:GLU:OE1	1.94	0.67
10:K:174:HIS:HA	10:K:211:LYS:NZ	2.08	0.67
13:N:97:UNK:O	13:N:99:UNK:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:559:VAL:HA	13:N:562:LYS:HG2	1.76	0.67
20:X:359:LEU:HD12	20:X:383:LEU:CD1	2.23	0.67
13:N:202:GLU:HB2	13:N:282:GLU:OE2	1.95	0.67
20:X:201:LEU:CD1	20:Y:40:HIS:HB3	2.25	0.67
13:N:60:UNK:C	13:N:63:UNK:CB	2.72	0.67
3:P:404:GLY:O	3:P:408:THR:HG22	1.93	0.67
13:N:519:TYR:CE1	13:N:523:LEU:HD21	2.30	0.67
16:R:57:TRP:HE3	16:R:57:TRP:HA	1.59	0.67
2:B:48:TRP:CZ3	13:N:632:MET:HE3	2.30	0.67
9:J:476:PRO:HG2	3:P:182:LEU:HG	1.77	0.67
20:X:316:ALA:HB1	20:X:351:TYR:CE1	2.30	0.67
6:F:552:LEU:HG	6:F:576:CYS:SG	2.35	0.67
13:N:88:SER:HA	13:N:91:PHE:HB2	1.75	0.67
13:N:559:VAL:O	13:N:562:LYS:HG2	1.95	0.67
6:H:571:CYS:SG	6:H:606:LEU:HD12	2.35	0.67
20:Y:407:LEU:CD2	20:Y:437:LEU:HD21	2.25	0.67
2:B:14:TRP:HA	2:B:15:LEU:CG	2.25	0.66
13:N:571:ASN:OD1	13:N:592:TYR:CD1	2.48	0.66
3:P:368:TRP:HB3	3:P:391:ALA:HB2	1.77	0.66
20:X:215:LYS:O	20:X:219:VAL:HG23	1.95	0.66
20:Y:229:THR:HG21	20:Y:233:LEU:HD12	1.77	0.66
1:A:1287:TYR:CD1	1:A:1287:TYR:O	2.48	0.66
1:A:1380:ASN:HD22	1:A:1383:ILE:HD12	1.60	0.66
3:C:136:ASP:O	14:O:150:GLN:NE2	2.28	0.66
16:R:57:TRP:HA	16:R:57:TRP:CE3	2.30	0.66
6:F:571:CYS:SG	6:F:606:LEU:HD12	2.35	0.66
13:N:663:GLN:HE21	13:N:695:ARG:HG3	1.60	0.66
1:A:1481:ASN:HA	17:T:7:LEU:CB	2.25	0.66
2:B:75:MET:HA	15:Q:125:LEU:HD13	1.77	0.66
13:N:123:UNK:O	13:N:127:UNK:N	2.28	0.66
14:O:75:VAL:HG13	14:O:165:ASP:CB	2.25	0.66
20:X:355:TYR:CD1	20:X:384:ARG:N	2.62	0.66
8:I:186:GLU:OE1	8:I:197:ARG:NH1	2.29	0.66
6:F:131:LEU:HD11	6:F:158:ILE:HG23	1.78	0.66
6:H:552:LEU:HG	6:H:576:CYS:SG	2.35	0.66
6:F:73:TYR:CD1	6:F:117:THR:HG22	2.31	0.66
6:F:537:GLU:OE1	6:F:602:TYR:HB3	1.95	0.66
13:N:180:PHE:HD1	13:N:299:TRP:CZ3	1.82	0.66
3:P:402:TRP:CZ3	3:P:424:ARG:HG2	2.31	0.66
13:N:577:GLU:HG2	13:N:583:ALA:HB2	1.77	0.66
20:X:229:THR:HG21	20:X:233:LEU:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:434:TYR:HA	20:Y:444:LEU:HD22	1.76	0.66
13:N:435:VAL:CG1	13:N:515:PHE:HE2	1.96	0.66
20:X:445:THR:O	20:X:449:THR:HG23	1.96	0.66
6:H:481:CYS:HB3	6:H:512:LEU:HD13	1.78	0.65
2:B:16:TRP:C	2:B:17:VAL:HG22	2.16	0.65
16:R:153:VAL:O	16:R:157:SER:OG	2.13	0.65
20:Y:215:LYS:O	20:Y:219:VAL:HG23	1.95	0.65
1:A:126:ALA:HA	1:A:152:CYS:O	1.97	0.65
14:O:467:ALA:HB1	14:O:506:LEU:HD11	1.76	0.65
20:X:294:PHE:CD1	20:X:311:TYR:CD1	2.85	0.65
7:G:6:PRO:HB3	9:J:406:HIS:CD2	2.32	0.65
13:N:704:VAL:HG23	13:N:705:LEU:HD22	1.77	0.65
20:X:271:VAL:CG1	20:X:304:LEU:HD21	2.27	0.65
1:A:592:HIS:O	1:A:593:ASN:HB3	1.96	0.65
1:A:1076:ARG:HE	1:A:1543:HIS:CD2	2.12	0.65
13:N:699:TRP:CZ3	13:N:728:VAL:HG21	2.31	0.65
20:X:294:PHE:CE2	20:X:311:TYR:HB2	2.32	0.65
20:Y:445:THR:O	20:Y:449:THR:HG23	1.95	0.65
20:Y:271:VAL:CG1	20:Y:304:LEU:HD21	2.27	0.65
3:C:460:TYR:CE1	3:C:470:LEU:HD11	2.31	0.65
8:I:177:VAL:HG12	8:I:208:LEU:HD13	1.78	0.65
11:L:74:VAL:HG21	11:L:137:ILE:HD11	1.77	0.65
2:B:16:TRP:NE1	2:B:44:CYS:O	2.29	0.65
14:O:581:ILE:HG22	14:O:610:LEU:HD23	1.78	0.65
14:O:219:GLN:NE2	14:O:231:LEU:HD13	2.09	0.65
1:A:1405:LEU:HD13	1:A:1467:GLY:CA	2.27	0.65
8:I:297:THR:O	14:O:58:ARG:NH2	2.30	0.65
11:L:108:ILE:HB	11:L:125:THR:O	1.97	0.65
20:X:363:ALA:N	20:X:379:LYS:HD2	2.12	0.64
20:Y:226:VAL:HG22	20:Y:236:LEU:HD23	1.77	0.64
1:A:1113:PRO:HB2	13:N:778:ARG:HH21	1.63	0.64
1:A:1191:LEU:HD21	16:R:62:HIS:CG	2.32	0.64
6:F:537:GLU:CD	6:F:600:TYR:OH	2.35	0.64
13:N:796:GLN:O	13:N:800:GLN:HG3	1.97	0.64
13:N:519:TYR:OH	13:N:541:ASN:HB3	1.98	0.64
1:A:1770:LEU:HD23	1:A:1771:PHE:N	2.13	0.64
3:C:368:TRP:HB3	3:C:391:ALA:HB2	1.80	0.64
3:C:413:LYS:O	3:C:415:PRO:HD3	1.97	0.64
8:I:231:VAL:HG21	8:I:557:TYR:CZ	2.33	0.64
8:I:265:ILE:HD11	8:I:396:PHE:CE2	2.32	0.64
9:J:258:MET:HE1	9:J:271:HIS:CG	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:233:PHE:CZ	3:P:237:ILE:HD11	2.31	0.64
1:A:1175:PHE:CZ	1:A:1179:LEU:HD21	2.33	0.64
11:L:45:LEU:HD23	11:L:46:ARG:N	2.13	0.64
11:L:86:ASP:HB3	11:L:89:TYR:HB2	1.80	0.64
1:A:72:GLU:HG3	1:A:94:TYR:OH	1.97	0.64
2:B:76:CYS:O	2:B:77:ARG:HB2	1.98	0.64
3:C:327:ASP:O	3:C:333:THR:HG21	1.97	0.64
8:I:38:ALA:HB2	8:I:71:LEU:HD11	1.80	0.64
9:J:441:VAL:CG2	9:J:444:TRP:HD1	2.10	0.64
13:N:73:UNK:O	13:N:74:TRP:HB3	1.98	0.64
3:C:148:ASN:HB3	3:C:151:LEU:HG	1.80	0.64
8:I:88:LYS:O	8:I:106:VAL:HG22	1.98	0.64
11:L:73:THR:HG22	11:L:131:PRO:HB2	1.80	0.64
20:X:279:ASP:OD1	20:X:310:VAL:HG21	1.98	0.64
1:A:34:ALA:HB3	14:O:237:GLN:HE22	1.63	0.63
1:A:1084:ARG:NH2	1:A:1139:ASN:OD1	2.31	0.63
14:O:658:LEU:HD13	14:O:704:VAL:HG11	1.80	0.63
3:C:36:LEU:HD21	3:C:58:LEU:HB2	1.80	0.63
3:C:259:PHE:HB3	3:C:265:ILE:HD12	1.79	0.63
13:N:538:GLU:HG2	13:N:561:LEU:CG	2.28	0.63
1:A:1114:ARG:HB3	13:N:779:MET:HG3	1.79	0.63
6:H:537:GLU:OE1	6:H:568:GLU:OE1	2.15	0.63
16:R:484:SER:CB	16:R:485:VAL:HA	2.28	0.63
1:A:1114:ARG:CB	13:N:779:MET:CG	2.77	0.63
1:A:1531:GLY:HA3	1:A:1566:PHE:CE1	2.33	0.63
6:F:726:LEU:HD21	6:F:742:LEU:HD22	1.81	0.63
10:K:495:PHE:CZ	10:K:525:MET:HG2	2.33	0.63
13:N:611:VAL:HG11	13:N:637:TRP:CH2	2.33	0.63
20:X:226:VAL:HG22	20:X:236:LEU:HD23	1.78	0.63
1:A:620:THR:HG23	1:A:866:ILE:CD1	2.29	0.63
8:I:142:LEU:HD13	8:I:264:TYR:CD2	2.34	0.63
20:X:353:LYS:HA	20:X:385:ASN:HB3	1.79	0.63
20:Y:316:ALA:HB1	20:Y:351:TYR:CE1	2.34	0.63
6:H:726:LEU:HD21	6:H:742:LEU:HD22	1.81	0.63
10:K:384:SER:HB2	10:K:415:ASN:HD21	1.63	0.63
20:X:407:LEU:CD2	20:X:437:LEU:HD21	2.27	0.63
13:N:281:TYR:CZ	13:N:357:ALA:HA	2.34	0.63
6:F:130:ARG:CG	20:Y:506:GLN:HB2	2.29	0.62
11:L:78:CYS:SG	11:L:119:TRP:HE3	2.22	0.62
1:A:445:LEU:HD21	1:A:478:ASP:HA	1.80	0.62
13:N:274:GLU:OE2	13:N:278:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:MET:HE2	1:A:1564:LEU:CD1	2.29	0.62
1:A:1194:HIS:HB2	16:R:99:LEU:HD13	1.81	0.62
4:D:54:ILE:HD12	3:P:389:ARG:NH2	2.14	0.62
8:I:209:CYS:SG	8:I:584:HIS:CE1	2.92	0.62
13:N:181:LEU:HD22	13:N:299:TRP:CE2	2.33	0.62
13:N:386:LEU:O	13:N:388:HIS:N	2.33	0.62
1:A:436:LEU:HG	1:A:501:THR:HG23	1.82	0.62
1:A:1621:PRO:HG3	1:A:1653:ALA:HB3	1.82	0.62
3:P:286:PHE:HB3	3:P:303:PHE:CE2	2.35	0.62
20:Y:532:TYR:CE2	20:Y:548:GLY:HA3	2.35	0.62
1:A:1482:LEU:H	17:T:7:LEU:CB	2.13	0.62
2:B:20:ASP:CB	2:B:30:PHE:HE2	2.11	0.62
14:O:662:ARG:HD2	14:O:755:LEU:HD12	1.81	0.62
4:D:10:PRO:HG2	14:O:346:TRP:CZ2	2.34	0.62
9:J:281:ALA:HA	9:J:311:MET:CE	2.30	0.62
13:N:286:LEU:O	13:N:288:GLU:N	2.32	0.62
1:A:873:VAL:HG21	1:A:951:ILE:CG2	2.29	0.62
1:A:1220:MET:CG	1:A:1264:THR:HG21	2.30	0.62
2:B:14:TRP:HA	2:B:15:LEU:CB	2.28	0.62
6:H:537:GLU:CD	6:H:600:TYR:OH	2.38	0.62
13:N:86:ASN:C	13:N:89:PRO:HD2	2.20	0.62
13:N:418:GLU:OE2	13:N:495:UNK:O	2.18	0.62
20:X:430:ALA:CB	20:X:451:CYS:SG	2.88	0.62
3:P:460:TYR:CE1	3:P:470:LEU:HD11	2.34	0.62
3:C:233:PHE:CZ	3:C:237:ILE:HD12	2.35	0.62
3:P:327:ASP:O	3:P:333:THR:HG21	1.99	0.62
2:B:16:TRP:CZ3	2:B:41:GLY:C	2.39	0.61
20:X:373:VAL:HG11	20:X:403:ALA:HB2	1.81	0.61
1:A:1191:LEU:HD21	16:R:62:HIS:ND1	2.15	0.61
9:J:294:LEU:HD12	10:K:54:HIS:CD2	2.35	0.61
20:X:350:PHE:CZ	20:X:378:LEU:C	2.73	0.61
1:A:1672:ARG:O	1:A:1701:LEU:HD12	2.00	0.61
13:N:249:ARG:HB3	13:N:250:LEU:HD23	1.82	0.61
13:N:281:TYR:CE2	13:N:356:PRO:HB2	2.34	0.61
1:A:617:LEU:HD11	1:A:782:GLY:HA2	1.81	0.61
1:A:1624:VAL:HG22	1:A:1698:TYR:HD2	1.66	0.61
6:H:689:LEU:HD11	6:H:716:ASN:HD21	1.66	0.61
3:C:414:MET:CE	14:O:300:LEU:HD13	2.30	0.61
5:E:61:TYR:CE1	20:X:360:TYR:CE2	2.89	0.61
20:Y:294:PHE:CD1	20:Y:294:PHE:C	2.73	0.61
1:A:43:GLN:NE2	3:C:142:GLU:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:684:LYS:HG2	6:F:687:LYS:HB2	1.82	0.61
10:K:250:CYS:SG	10:K:274:THR:HG22	2.40	0.61
3:P:267:SER:CB	3:P:299:ASN:HD21	2.14	0.61
1:A:592:HIS:O	1:A:593:ASN:CB	2.46	0.61
20:X:100:TYR:HB2	20:X:142:LEU:CD2	2.30	0.61
13:N:426:ARG:NH2	13:N:793:GLN:HE22	1.97	0.61
20:X:347:CYS:SG	20:X:378:LEU:HD13	2.41	0.61
13:N:368:THR:CB	13:N:369:ASP:HA	2.31	0.61
1:A:869:ARG:NH2	1:A:946:THR:OG1	2.33	0.60
13:N:505:LEU:CD1	13:N:548:ARG:HD3	2.30	0.60
1:A:1113:PRO:HB2	13:N:778:ARG:NH2	2.15	0.60
2:B:17:VAL:CA	2:B:30:PHE:CB	2.77	0.60
6:H:730:LYS:HD3	6:H:740:TYR:HE1	1.65	0.60
13:N:281:TYR:CZ	13:N:284:SER:HB3	2.36	0.60
13:N:509:TYR:CD2	13:N:515:PHE:HE1	2.18	0.60
14:O:657:ILE:HD11	14:O:704:VAL:HG23	1.83	0.60
20:X:93:TYR:CE2	20:X:148:VAL:HG11	2.36	0.60
1:A:1312:ASN:O	1:A:1312:ASN:ND2	2.30	0.60
13:N:141:UNK:O	13:N:142:UNK:C	2.49	0.60
9:J:465:LEU:HA	9:J:488:ILE:CD1	2.32	0.60
6:H:130:ARG:HH12	10:K:473:VAL:HG22	1.66	0.60
8:I:289:LYS:O	8:I:293:GLU:N	2.32	0.60
10:K:292:VAL:HG21	12:M:57:TRP:CB	2.31	0.60
13:N:560:MET:HE3	13:N:560:MET:HA	1.81	0.60
20:X:94:ARG:CG	20:Y:334:ILE:O	2.49	0.60
1:A:617:LEU:HD11	1:A:782:GLY:CA	2.32	0.60
1:A:1797:ILE:HG22	1:A:1852:ILE:CD1	2.32	0.60
13:N:281:TYR:CE1	13:N:357:ALA:HA	2.37	0.60
14:O:417:LEU:HA	14:O:420:ILE:CG2	2.32	0.60
20:X:94:ARG:HG3	20:Y:334:ILE:O	2.00	0.60
1:A:1114:ARG:CD	13:N:779:MET:HA	2.25	0.60
6:F:146:PRO:HG3	6:F:167:THR:HA	1.83	0.60
8:I:309:LEU:HD23	14:O:64:LEU:HD11	1.82	0.60
20:X:203:LEU:HD21	20:X:239:TRP:CH2	2.36	0.60
1:A:873:VAL:HG21	1:A:951:ILE:HG21	1.84	0.60
9:J:193:LEU:O	9:J:197:GLU:HB2	2.02	0.60
1:A:956:ARG:NH1	1:A:1785:GLU:OE1	2.34	0.60
2:B:75:MET:CA	15:Q:125:LEU:CD1	2.58	0.60
6:H:115:CYS:SG	6:H:116:PHE:N	2.75	0.60
8:I:17:LYS:NZ	8:I:51:SER:O	2.34	0.60
9:J:35:GLU:OE2	9:J:63:ARG:NH2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:185:LEU:HD13	9:J:206:GLU:OE1	2.02	0.60
13:N:706:ARG:HB2	13:N:716:ILE:HD13	1.84	0.60
3:P:475:LYS:O	3:P:479:GLN:NE2	2.35	0.60
13:N:75:PHE:CD1	13:N:79:LEU:HD23	2.37	0.60
20:Y:339:ALA:O	20:Y:343:VAL:HG23	2.02	0.60
3:C:521:PHE:CD1	3:C:553:ILE:HG22	2.37	0.59
9:J:213:ASN:OD1	9:J:214:LYS:N	2.34	0.59
10:K:153:TYR:CE2	10:K:169:LEU:HD22	2.37	0.59
14:O:233:PRO:HA	14:O:263:ARG:HH21	1.66	0.59
20:Y:93:TYR:CE2	20:Y:148:VAL:HG11	2.37	0.59
3:C:120:TYR:CE2	3:C:124:LEU:HD11	2.37	0.59
8:I:218:SER:OG	8:I:584:HIS:ND1	2.35	0.59
20:Y:462:LYS:HG2	20:Y:485:LEU:CD1	2.33	0.59
14:O:119:PHE:CE1	14:O:136:LEU:HD11	2.37	0.59
14:O:351:GLY:O	14:O:352:GLN:HG3	2.02	0.59
20:X:271:VAL:HG13	20:X:304:LEU:HD21	1.84	0.59
1:A:860:TYR:CG	1:A:861:PRO:HD2	2.38	0.59
3:P:392:ILE:HD11	3:P:402:TRP:CH2	2.38	0.59
20:X:355:TYR:CA	20:X:382:ALA:C	2.63	0.59
2:B:17:VAL:HG13	2:B:31:ASN:N	2.13	0.59
6:F:115:CYS:SG	6:F:116:PHE:N	2.75	0.59
6:F:131:LEU:HD11	6:F:158:ILE:CG2	2.32	0.59
9:J:406:HIS:CE1	9:J:450:ASN:HD22	2.21	0.59
13:N:97:UNK:O	13:N:98:UNK:C	2.51	0.59
14:O:114:ASP:HA	14:O:117:ASP:OD1	2.02	0.59
1:A:629:LEU:HD11	1:A:634:ALA:HB2	1.82	0.59
13:N:77:GLU:O	13:N:78:VAL:HG23	2.02	0.59
1:A:811:PRO:HG3	1:A:1806:SER:O	2.03	0.59
1:A:1054:TYR:O	1:A:1056:GLU:N	2.31	0.59
10:K:271:HIS:O	10:K:274:THR:OG1	2.20	0.59
13:N:542:VAL:HG11	13:N:558:GLU:CD	2.23	0.59
3:P:120:TYR:CZ	3:P:124:LEU:HD11	2.38	0.59
1:A:1251:VAL:HG12	1:A:1294:TYR:HA	1.83	0.59
13:N:91:PHE:CD2	13:N:161:LEU:CD1	2.77	0.59
13:N:284:SER:OG	13:N:285:PHE:HB2	2.02	0.59
14:O:105:LEU:HD11	14:O:151:VAL:CG1	2.33	0.59
18:U:21:UNK:O	18:U:23:UNK:N	2.35	0.59
9:J:465:LEU:HA	9:J:488:ILE:HD12	1.85	0.59
11:L:98:VAL:HB	11:L:134:THR:HG21	1.84	0.59
13:N:285:PHE:O	13:N:289:PHE:HD1	1.86	0.59
13:N:609:LEU:HD22	13:N:639:HIS:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:354:ARG:CD	14:O:573:LYS:O	2.50	0.59
20:X:350:PHE:CZ	20:X:378:LEU:CA	2.84	0.59
20:Y:219:VAL:HG22	20:Y:240:ILE:HG22	1.85	0.59
14:O:216:LEU:HD22	14:O:256:LEU:HD12	1.85	0.59
3:P:228:TRP:O	3:P:231:GLU:N	2.36	0.59
20:X:350:PHE:CE1	20:X:381:ALA:HB3	2.37	0.59
20:Y:350:PHE:CZ	20:Y:378:LEU:HD12	2.38	0.59
6:F:152:PHE:CE1	6:F:162:PRO:HG2	2.37	0.58
6:F:696:ILE:HG12	6:F:705:CYS:SG	2.43	0.58
9:J:406:HIS:HE1	9:J:450:ASN:HD22	1.51	0.58
9:J:523:ILE:HD11	3:P:420:TYR:CB	2.33	0.58
13:N:670:PHE:CD1	13:N:715:VAL:HB	2.38	0.58
3:P:385:ILE:HD11	3:P:412:LEU:HD11	1.85	0.58
1:A:1747:LEU:HD23	1:A:1779:VAL:HG22	1.85	0.58
11:L:126:ASP:CB	11:L:132:THR:N	2.66	0.58
13:N:619:LEU:HG	13:N:637:TRP:CZ2	2.37	0.58
20:X:316:ALA:HB1	20:X:351:TYR:CZ	2.38	0.58
6:F:124:VAL:O	6:F:128:THR:OG1	2.14	0.58
6:F:128:THR:HG21	6:F:130:ARG:NH1	2.18	0.58
1:A:1079:ALA:HB1	1:A:1556:LEU:HA	1.85	0.58
1:A:1475:ARG:HG2	1:A:1476:PHE:CE1	2.38	0.58
2:B:41:GLY:O	2:B:45:PRO:HA	2.01	0.58
6:F:707:PHE:HB2	6:F:729:LEU:HD11	1.85	0.58
6:H:685:SER:O	6:H:689:LEU:HD12	2.04	0.58
13:N:409:VAL:O	13:N:410:ILE:HG13	2.03	0.58
14:O:731:ASN:HD21	18:U:5:UNK:H2	1.50	0.58
1:A:454:CYS:O	1:A:471:VAL:HA	2.03	0.58
1:A:1546:THR:OG1	1:A:1547:GLY:N	2.35	0.58
13:N:273:MET:CG	13:N:277:CYS:SG	2.91	0.58
13:N:273:MET:HG2	13:N:277:CYS:SG	2.43	0.58
13:N:393:THR:CG2	13:N:434:THR:HG22	2.34	0.58
13:N:513:ASP:CG	13:N:789:GLU:H	2.06	0.58
13:N:556:PHE:CZ	13:N:600:PHE:HA	2.38	0.58
20:X:350:PHE:CZ	20:X:381:ALA:CB	2.82	0.58
1:A:1477:ALA:HB1	1:A:1574:LEU:CD1	2.33	0.58
6:H:478:SER:HA	6:H:633:ARG:HH22	1.69	0.58
13:N:177:TYR:CD2	13:N:261:VAL:HG12	2.39	0.58
20:X:339:ALA:O	20:X:343:VAL:HG23	2.02	0.58
20:X:407:LEU:HD13	20:X:443:THR:HG21	1.84	0.58
1:A:79:ALA:HB1	1:A:89:TYR:CE1	2.39	0.58
3:C:493:TYR:CE2	3:C:497:ILE:HD11	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:455:UNK:CB	13:N:501:ILE:HD11	2.34	0.58
14:O:417:LEU:HA	14:O:420:ILE:HG22	1.85	0.58
20:Y:271:VAL:HG13	20:Y:304:LEU:HD21	1.83	0.58
20:Y:452:LEU:HD21	20:Y:460:LYS:HB2	1.85	0.58
3:C:93:TYR:OH	3:C:101:ARG:NH1	2.36	0.58
3:C:358:LEU:HD21	3:C:368:TRP:CE2	2.39	0.58
13:N:560:MET:HA	13:N:560:MET:CE	2.34	0.58
3:P:151:LEU:HD22	3:P:178:VAL:HG13	1.85	0.58
20:X:355:TYR:H	20:X:386:MET:HB2	1.68	0.58
20:X:462:LYS:HG2	20:X:485:LEU:CD1	2.33	0.58
20:Y:316:ALA:HB1	20:Y:351:TYR:CZ	2.38	0.58
1:A:32:PRO:CD	14:O:264:VAL:HG11	2.34	0.58
10:K:496:GLU:HB2	10:K:526:TYR:HE1	1.68	0.58
13:N:233:CYS:O	13:N:235:GLN:N	2.37	0.58
3:P:355:GLN:HA	3:P:358:LEU:HD23	1.84	0.58
2:B:16:TRP:CB	2:B:31:ASN:C	2.65	0.58
9:J:481:THR:O	9:J:485:ILE:HG12	2.04	0.58
11:L:77:LEU:HD12	11:L:78:CYS:N	2.17	0.58
1:A:79:ALA:HB1	1:A:89:TYR:CZ	2.39	0.57
1:A:1086:MET:CE	1:A:1564:LEU:HD13	2.33	0.57
3:C:53:LYS:HD2	3:P:93:TYR:CE1	2.39	0.57
6:H:102:SER:OG	6:H:104:ASP:OD1	2.16	0.57
8:I:168:LEU:HD22	8:I:192:MET:SD	2.44	0.57
11:L:144:ASN:ND2	11:L:151:THR:HG23	2.19	0.57
13:N:564:MET:HE3	13:N:596:LEU:HD22	1.86	0.57
14:O:635:GLY:O	14:O:637:PRO:HD3	2.03	0.57
3:P:392:ILE:CD1	3:P:402:TRP:CH2	2.86	0.57
2:B:15:LEU:HD22	13:N:634:THR:O	2.03	0.57
2:B:16:TRP:HD1	2:B:46:LEU:HD21	1.64	0.57
2:B:48:TRP:HZ3	13:N:632:MET:CE	1.89	0.57
3:C:120:TYR:CZ	3:C:124:LEU:HD11	2.39	0.57
6:F:104:ASP:OD1	6:F:104:ASP:N	2.37	0.57
6:F:168:PHE:CB	6:F:467:ARG:HD3	2.35	0.57
13:N:278:ARG:HB3	13:N:343:GLU:OE2	2.04	0.57
3:C:93:TYR:CE1	3:P:53:LYS:HD2	2.39	0.57
10:K:284:LEU:HD13	10:K:308:TYR:HB2	1.86	0.57
3:P:36:LEU:HD21	3:P:58:LEU:HB2	1.87	0.57
20:X:452:LEU:HD21	20:X:460:LYS:HB2	1.86	0.57
2:B:14:TRP:HA	2:B:15:LEU:HG	1.85	0.57
6:H:761:SER:O	6:H:765:ASP:HB2	2.05	0.57
13:N:395:ASP:OD2	13:N:397:ILE:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:LEU:HD22	1:A:779:MET:HG3	1.85	0.57
1:A:1230:ILE:HG13	16:R:94:LEU:HD22	1.85	0.57
1:A:1364:CYS:N	1:A:1365:PRO:HD2	2.19	0.57
3:C:259:PHE:HB3	3:C:265:ILE:CD1	2.34	0.57
20:X:437:LEU:HB2	20:X:444:LEU:HD21	1.85	0.57
1:A:1575:SER:O	1:A:1580:SER:OG	2.17	0.57
3:P:39:ILE:HD12	3:P:201:LEU:HB2	1.85	0.57
3:P:286:PHE:HB3	3:P:303:PHE:CD2	2.39	0.57
3:C:151:LEU:HD22	3:C:178:VAL:HG13	1.86	0.57
3:C:416:PHE:CE2	14:O:323:ALA:HB2	2.40	0.57
9:J:476:PRO:HB3	3:P:182:LEU:HB3	1.86	0.57
10:K:305:VAL:HG22	12:M:57:TRP:CZ3	2.40	0.57
13:N:505:LEU:HD13	13:N:548:ARG:HD3	1.87	0.57
14:O:529:ASP:O	14:O:532:VAL:HG12	2.04	0.57
20:X:100:TYR:HD1	20:X:138:VAL:HG13	1.70	0.57
1:A:174:PRO:O	1:A:295:UNK:C	2.53	0.57
1:A:1116:THR:HG21	13:N:779:MET:HE2	1.74	0.57
1:A:1293:SER:HB3	1:A:1600:ARG:O	2.04	0.57
2:B:38:LYS:CB	13:N:562:LYS:CE	2.79	0.57
8:I:56:TRP:HZ3	8:I:58:PHE:HB2	1.70	0.57
8:I:308:LEU:HD21	8:I:445:ILE:HG23	1.85	0.57
10:K:449:ASN:HD22	7:W:8:ARG:NH1	2.02	0.57
6:H:515:TYR:HE2	6:H:545:HIS:CD2	2.23	0.57
9:J:281:ALA:HA	9:J:311:MET:HE1	1.86	0.57
10:K:292:VAL:HG21	12:M:57:TRP:HB2	1.87	0.57
13:N:513:ASP:CG	13:N:789:GLU:CB	2.72	0.57
20:X:346:GLY:C	20:X:378:LEU:HD11	2.25	0.57
1:A:620:THR:HG23	1:A:866:ILE:HD13	1.87	0.57
1:A:763:PHE:CD1	1:A:793:LEU:HD22	2.39	0.57
1:A:1220:MET:HG2	1:A:1264:THR:HG21	1.87	0.57
1:A:1377:LYS:HG2	1:A:1416:TRP:CG	2.40	0.57
8:I:276:TRP:CH2	8:I:280:LEU:HD22	2.40	0.57
11:L:89:TYR:O	11:L:151:THR:HG22	2.04	0.57
13:N:531:PHE:O	13:N:533:PHE:HA	2.05	0.57
13:N:609:LEU:CD2	13:N:662:VAL:HG12	2.31	0.57
14:O:356:ASP:HA	14:O:357:SER:HB2	1.86	0.57
14:O:243:LEU:HD12	14:O:243:LEU:O	2.05	0.56
1:A:939:PHE:HZ	1:A:944:LEU:HD13	1.69	0.56
8:I:67:GLU:O	8:I:85:ALA:N	2.32	0.56
3:P:120:TYR:CE2	3:P:124:LEU:HD11	2.39	0.56
20:X:359:LEU:HA	20:X:379:LYS:HG2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD21	1:A:177:VAL:HG11	1.88	0.56
2:B:1:MET:CE	13:N:650:LEU:HD22	2.35	0.56
2:B:33:CYS:HB3	2:B:39:VAL:O	2.06	0.56
5:E:89:LEU:O	6:H:592:ARG:NH2	2.37	0.56
6:F:503:CYS:SG	6:F:535:GLY:HA3	2.45	0.56
9:J:37:PRO:HB3	9:J:69:TYR:OH	2.04	0.56
3:P:238:TYR:HB3	3:P:247:ALA:HB2	1.88	0.56
3:P:389:ARG:O	3:P:392:ILE:HG23	2.05	0.56
20:X:100:TYR:CD1	20:X:138:VAL:HG13	2.41	0.56
20:X:219:VAL:HG22	20:X:240:ILE:HG22	1.86	0.56
1:A:99:MET:HB3	1:A:118:THR:HG22	1.88	0.56
1:A:443:CYS:HB3	1:A:452:LEU:HD12	1.87	0.56
1:A:1037:VAL:HG21	1:A:1566:PHE:CE2	2.40	0.56
1:A:1162:LYS:HG3	1:A:1163:PRO:CD	2.35	0.56
1:A:1241:THR:OG1	1:A:1243:LEU:HD22	2.06	0.56
5:E:96:PHE:HB2	6:H:595:GLN:HE21	1.71	0.56
13:N:202:GLU:OE2	13:N:283:ARG:HB2	2.05	0.56
13:N:704:VAL:HA	13:N:719:GLU:CD	2.26	0.56
3:P:358:LEU:HD11	3:P:368:TRP:CZ2	2.40	0.56
1:A:47:GLU:OE1	1:A:48:UNK:N	2.39	0.56
1:A:1632:ALA:O	1:A:1653:ALA:HB2	2.06	0.56
8:I:24:ILE:O	8:I:569:LEU:HD22	2.06	0.56
13:N:520:ARG:HD2	13:N:556:PHE:CD1	2.40	0.56
6:H:168:PHE:CB	6:H:467:ARG:HD3	2.35	0.56
6:H:707:PHE:HB2	6:H:729:LEU:HD11	1.87	0.56
9:J:55:ARG:HH11	10:K:264:HIS:HA	1.69	0.56
13:N:91:PHE:HE2	13:N:161:LEU:HD13	1.52	0.56
13:N:281:TYR:CZ	13:N:357:ALA:N	2.73	0.56
13:N:395:ASP:OD1	13:N:398:THR:HG23	2.06	0.56
14:O:691:ILE:HD13	14:O:721:TYR:CE1	2.41	0.56
20:X:423:ILE:HG22	20:X:454:ASP:OD1	2.05	0.56
1:A:1099:PRO:O	1:A:1161:ASN:ND2	2.39	0.56
1:A:1674:TRP:N	1:A:1674:TRP:CD1	2.73	0.56
3:C:39:ILE:HD12	3:C:201:LEU:HB2	1.88	0.56
10:K:441:VAL:HG13	10:K:474:LEU:HD22	1.87	0.56
13:N:202:GLU:HB2	13:N:282:GLU:CD	2.26	0.56
14:O:620:ALA:O	14:O:624:VAL:HG23	2.05	0.56
20:X:343:VAL:CG1	20:X:378:LEU:HD22	2.35	0.56
1:A:213:MET:CE	1:A:216:PRO:HA	2.36	0.56
3:C:238:TYR:HB3	3:C:247:ALA:HB2	1.86	0.56
13:N:141:UNK:O	13:N:143:UNK:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:378:SER:HB2	14:O:408:LEU:HD11	1.87	0.56
1:A:1882:LEU:HD23	1:A:1883:SER:N	2.21	0.56
2:B:42:ASP:HA	13:N:630:LYS:HG2	1.78	0.56
6:H:20:ALA:O	6:H:23:ASP:OD1	2.24	0.56
8:I:32:ARG:HD3	13:N:388:HIS:CE1	2.41	0.56
9:J:441:VAL:O	9:J:442:ASP:HB3	2.06	0.56
1:A:1086:MET:CE	1:A:1564:LEU:CD1	2.84	0.56
8:I:115:TRP:CE3	8:I:176:LEU:HD22	2.41	0.56
10:K:254:THR:HG23	10:K:271:HIS:HD2	1.66	0.56
20:X:294:PHE:CD1	20:X:294:PHE:C	2.79	0.56
6:H:145:ASN:HB2	6:H:146:PRO:O	2.06	0.55
8:I:290:PHE:CE1	8:I:320:LEU:HD22	2.42	0.55
14:O:435:SER:HB3	14:O:654:ASP:HB2	1.88	0.55
20:X:365:ALA:HB3	20:X:375:ALA:HB1	1.88	0.55
2:B:16:TRP:HB2	2:B:32:GLY:N	2.21	0.55
14:O:123:GLU:N	14:O:124:PRO:HA	2.22	0.55
1:A:457:PHE:HB3	1:A:468:PHE:CD2	2.42	0.55
3:C:233:PHE:CZ	3:C:237:ILE:CD1	2.89	0.55
6:H:639:TYR:CE2	11:L:183:ILE:HG22	2.41	0.55
8:I:507:LEU:HD22	8:I:513:LEU:HD11	1.89	0.55
10:K:153:TYR:CZ	10:K:169:LEU:HD22	2.41	0.55
12:M:11:ILE:HG23	12:M:15:ILE:HD12	1.87	0.55
13:N:281:TYR:OH	13:N:357:ALA:HA	2.07	0.55
20:X:359:LEU:HB2	20:X:383:LEU:CD2	2.36	0.55
20:Y:100:TYR:HD1	20:Y:138:VAL:HG13	1.72	0.55
20:Y:219:VAL:HG22	20:Y:240:ILE:CG2	2.37	0.55
1:A:1799:ARG:HD3	1:A:1805:MET:HB3	1.88	0.55
10:K:19:TYR:CD1	10:K:49:LEU:HD13	2.41	0.55
20:Y:437:LEU:HB2	20:Y:444:LEU:HD21	1.87	0.55
2:B:47:VAL:HG21	2:B:60:ILE:HG21	1.88	0.55
3:C:60:PHE:HA	3:P:85:ASP:CG	2.27	0.55
6:H:128:THR:HG21	6:H:130:ARG:NH1	2.20	0.55
10:K:432:ILE:CD1	10:K:444:TRP:CG	2.89	0.55
16:R:154:SER:O	16:R:158:GLN:HG2	2.06	0.55
20:X:219:VAL:HG22	20:X:240:ILE:CG2	2.37	0.55
20:X:449:THR:HG21	20:X:465:LEU:CA	2.36	0.55
20:Y:294:PHE:CE2	20:Y:311:TYR:HB2	2.41	0.55
20:Y:449:THR:HG21	20:Y:465:LEU:CA	2.37	0.55
13:N:281:TYR:CE1	13:N:357:ALA:CA	2.90	0.55
6:H:503:CYS:SG	6:H:535:GLY:HA3	2.47	0.55
14:O:64:LEU:C	14:O:64:LEU:HD12	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:431:ASN:HA	3:P:462:VAL:HG21	1.89	0.55
1:A:87:VAL:HG12	1:A:88:ASP:N	2.22	0.55
1:A:1624:VAL:HG22	1:A:1698:TYR:CD2	2.41	0.55
6:F:145:ASN:HB2	6:F:146:PRO:C	2.26	0.55
8:I:15:GLY:O	8:I:743:VAL:N	2.37	0.55
8:I:45:LEU:HG	8:I:57:SER:HA	1.89	0.55
13:N:257:SER:O	13:N:261:VAL:HG13	2.06	0.55
8:I:341:TYR:CE1	8:I:475:VAL:HG21	2.42	0.55
9:J:190:LEU:HD13	9:J:202:ARG:HD3	1.88	0.55
11:L:144:ASN:CG	11:L:151:THR:HG23	2.27	0.55
13:N:650:LEU:HD12	13:N:651:ALA:N	2.22	0.55
20:X:494:ASP:OD1	20:X:494:ASP:N	2.40	0.55
6:F:149:TRP:CZ3	6:F:152:PHE:HD2	2.25	0.54
8:I:56:TRP:CD2	8:I:98:PRO:HB3	2.41	0.54
10:K:487:TYR:OH	7:W:15:ASP:O	2.23	0.54
13:N:190:LYS:O	13:N:196:UNK:N	2.41	0.54
13:N:281:TYR:CE1	13:N:357:ALA:HB2	2.42	0.54
13:N:347:ILE:HG21	13:N:358:ILE:HG23	1.89	0.54
20:X:350:PHE:HA	20:X:382:ALA:HA	1.88	0.54
8:I:262:LEU:HA	8:I:265:ILE:HG22	1.89	0.54
10:K:406:HIS:CE1	7:W:6:PRO:HB3	2.42	0.54
13:N:523:LEU:HD22	13:N:538:GLU:OE1	2.07	0.54
13:N:564:MET:HE2	13:N:564:MET:N	2.21	0.54
3:C:228:TRP:O	3:C:231:GLU:N	2.39	0.54
8:I:214:LEU:O	8:I:238:THR:OG1	2.26	0.54
9:J:19:TYR:CD1	9:J:49:LEU:HD13	2.43	0.54
10:K:46:CYS:O	10:K:50:THR:OG1	2.22	0.54
13:N:74:TRP:CH2	13:N:77:GLU:HB2	2.42	0.54
13:N:574:ILE:HD12	13:N:625:LYS:HG2	1.89	0.54
20:X:355:TYR:CB	20:X:386:MET:CB	2.72	0.54
1:A:1290:ASP:OD2	1:A:1600:ARG:HA	2.08	0.54
20:X:203:LEU:HD22	20:Y:55:LEU:HB3	1.89	0.54
1:A:95:VAL:HG13	1:A:100:VAL:HG22	1.88	0.54
1:A:860:TYR:CD2	1:A:861:PRO:HD2	2.43	0.54
1:A:1248:ASN:O	1:A:1251:VAL:HG22	2.07	0.54
6:H:621:LEU:O	6:H:625:ARG:HG3	2.08	0.54
9:J:322:TYR:HE1	12:M:36:LEU:HD11	1.72	0.54
14:O:114:ASP:O	14:O:117:ASP:OD1	2.26	0.54
20:X:350:PHE:CE1	20:X:381:ALA:CB	2.90	0.54
1:A:1540:ARG:CZ	13:N:486:UNK:O	2.56	0.54
3:C:368:TRP:CB	3:C:391:ALA:HB2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:344:LEU:HA	13:N:347:ILE:HB	1.90	0.54
6:H:146:PRO:HG3	6:H:167:THR:HA	1.89	0.54
13:N:345:PHE:CD1	13:N:385:ARG:CZ	2.91	0.54
13:N:386:LEU:HD12	13:N:387:LEU:N	2.22	0.54
14:O:648:ILE:CD1	14:O:663:ALA:HB1	2.37	0.54
20:Y:196:LEU:O	20:Y:200:PRO:HB3	2.07	0.54
20:Y:294:PHE:CE1	20:Y:311:TYR:CG	2.96	0.54
1:A:269:TRP:HB3	1:A:409:ILE:HG23	1.90	0.54
1:A:982:ASP:OD1	1:A:983:LEU:N	2.40	0.54
20:X:359:LEU:C	20:X:379:LYS:HG3	2.26	0.54
1:A:616:GLU:O	1:A:620:THR:OG1	2.20	0.54
1:A:1114:ARG:HD3	13:N:779:MET:HA	1.90	0.54
1:A:1786:MET:HA	1:A:1786:MET:CE	2.38	0.54
6:F:89:GLU:OE2	6:F:125:TYR:HE1	1.91	0.54
10:K:432:ILE:HD11	10:K:444:TRP:CG	2.43	0.54
13:N:191:GLY:O	13:N:196:UNK:N	2.40	0.54
13:N:782:VAL:HG22	13:N:788:ALA:O	2.08	0.54
1:A:1137:PHE:O	1:A:1141:VAL:HG23	2.07	0.54
1:A:1791:ILE:HB	14:O:598:THR:HG21	1.90	0.54
9:J:451:LEU:CD1	9:J:467:TYR:CE2	2.90	0.54
10:K:369:LEU:HD21	7:W:3:ARG:HG2	1.89	0.54
14:O:596:SER:OG	14:O:599:ILE:HD12	2.08	0.54
1:A:1241:THR:HG22	16:R:161:LEU:HD22	1.90	0.53
3:C:89:LEU:HD12	3:P:60:PHE:CG	2.43	0.53
3:C:276:ILE:O	3:C:276:ILE:HG22	2.08	0.53
3:C:304:SER:HB2	3:C:336:VAL:HG22	1.89	0.53
13:N:414:MET:SD	13:N:498:SER:CA	2.96	0.53
3:P:402:TRP:CZ2	3:P:424:ARG:HG2	2.43	0.53
20:Y:100:TYR:CD1	20:Y:138:VAL:HG13	2.42	0.53
1:A:129:CYS:SG	1:A:130:ASP:N	2.81	0.53
1:A:1677:LEU:HD12	1:A:1678:ILE:N	2.24	0.53
8:I:142:LEU:HD13	8:I:264:TYR:CE2	2.43	0.53
10:K:296:PRO:HB2	12:M:55:MET:HG3	1.89	0.53
14:O:348:TYR:CE2	14:O:361:LEU:HD11	2.43	0.53
1:A:857:ALA:CB	1:A:858:PRO:HD3	2.38	0.53
1:A:1304:MET:O	1:A:1307:LEU:HB2	2.09	0.53
1:A:1867:CYS:HB3	1:A:1881:GLN:CD	2.28	0.53
13:N:350:ASP:CB	13:N:351:PHE:HA	2.37	0.53
13:N:425:ARG:HG2	13:N:425:ARG:HH11	1.72	0.53
13:N:513:ASP:OD1	13:N:514:LEU:HD22	2.08	0.53
14:O:431:LEU:HD12	14:O:431:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:251:TYR:OH	3:P:268:GLN:HG3	2.09	0.53
20:X:40:HIS:HB3	20:Y:201:LEU:CD1	2.36	0.53
1:A:237:GLN:HG3	1:A:238:TYR:N	2.24	0.53
3:C:307:LEU:CD2	3:C:316:LEU:HD13	2.39	0.53
6:H:639:TYR:CD2	11:L:183:ILE:HG22	2.43	0.53
13:N:165:ALA:N	13:N:166:PRO:HA	2.23	0.53
14:O:439:LEU:HG	14:O:476:LEU:HD13	1.90	0.53
3:P:244:ILE:C	3:P:244:ILE:HD12	2.29	0.53
20:X:192:TYR:HA	20:X:195:VAL:HG22	1.89	0.53
1:A:612:ILE:O	1:A:641:TRP:CH2	2.62	0.53
1:A:1658:PRO:HG2	1:A:1663:LEU:HD13	1.90	0.53
8:I:24:ILE:HG22	8:I:38:ALA:O	2.09	0.53
8:I:26:LEU:HB3	8:I:37:LEU:HB3	1.91	0.53
9:J:37:PRO:HB3	9:J:69:TYR:CE2	2.42	0.53
10:K:248:LYS:N	10:K:438:GLU:OE2	2.41	0.53
20:X:423:ILE:HA	20:X:454:ASP:OD2	2.07	0.53
1:A:150:CYS:HB3	1:A:163:SER:HA	1.89	0.53
1:A:1064:GLU:HA	1:A:1125:ILE:HD11	1.89	0.53
1:A:1540:ARG:NH1	13:N:486:UNK:O	2.42	0.53
2:B:23:CYS:HA	2:B:30:PHE:CZ	2.43	0.53
3:C:550:LEU:O	3:C:553:ILE:HG12	2.08	0.53
13:N:394:CYS:O	13:N:395:ASP:CG	2.47	0.53
6:H:540:SER:OG	6:H:575:ASN:ND2	2.30	0.53
6:H:762:TRP:HA	6:H:765:ASP:HB3	1.89	0.53
8:I:65:GLY:H	8:I:84:LEU:HG	1.74	0.53
10:K:429:LEU:HA	10:K:432:ILE:HG22	1.90	0.53
13:N:289:PHE:HA	13:N:292:TRP:HB3	1.90	0.53
14:O:354:ARG:HD3	14:O:574:LEU:HA	1.89	0.53
14:O:710:ILE:O	14:O:711:ARG:C	2.47	0.53
3:P:441:GLU:HG3	3:P:472:LYS:HZ1	1.73	0.53
20:X:282:PHE:HD1	20:X:314:LEU:HD21	1.74	0.53
9:J:53:TYR:O	9:J:79:CYS:SG	2.67	0.53
3:P:420:TYR:OH	3:P:424:ARG:HD3	2.08	0.53
1:A:857:ALA:HB3	1:A:858:PRO:HD3	1.90	0.53
6:H:653:LEU:HD22	10:K:523:ILE:HG21	1.91	0.53
9:J:445:GLU:HA	9:J:474:LEU:HD23	1.89	0.53
10:K:185:LEU:HD21	10:K:205:PHE:CB	2.39	0.53
10:K:190:LEU:O	10:K:198:GLN:NE2	2.42	0.53
14:O:258:TYR:CE1	14:O:262:LEU:HD22	2.44	0.53
14:O:652:LEU:HD23	14:O:660:LYS:HG3	1.90	0.53
9:J:35:GLU:CD	9:J:63:ARG:HE	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:55:ARG:NH1	10:K:264:HIS:HA	2.25	0.53
12:M:4:GLU:HG2	3:P:50:HIS:CE1	2.43	0.53
13:N:527:LEU:HD11	13:N:561:LEU:HD22	1.90	0.53
1:A:213:MET:HE1	1:A:216:PRO:HA	1.90	0.52
1:A:1470:LEU:HD23	1:A:1470:LEU:C	2.28	0.52
3:C:199:LEU:HD23	3:C:199:LEU:O	2.10	0.52
3:C:422:TYR:OH	16:R:52:ARG:NH2	2.42	0.52
4:D:13:THR:HG22	14:O:255:TYR:HE2	1.73	0.52
8:I:74:ARG:HD2	8:I:174:ASN:HD22	1.74	0.52
9:J:37:PRO:HB3	9:J:69:TYR:CZ	2.45	0.52
10:K:176:LEU:HD12	10:K:181:GLU:HG2	1.91	0.52
13:N:88:SER:HA	13:N:91:PHE:CB	2.39	0.52
20:X:336:ASP:OD1	20:X:337:GLN:N	2.36	0.52
20:Y:309:ASP:HB2	20:Y:340:GLU:HG2	1.90	0.52
8:I:353:GLN:HA	8:I:353:GLN:HE21	1.73	0.52
10:K:250:CYS:SG	10:K:274:THR:HG21	2.46	0.52
13:N:563:ASP:OD2	13:N:597:SER:HB3	2.10	0.52
20:X:400:ILE:HD13	20:X:413:LEU:CD1	2.25	0.52
20:Y:551:LYS:HD3	20:Y:552:MET:N	2.24	0.52
1:A:1227:LEU:O	1:A:1230:ILE:HG22	2.09	0.52
6:F:704:LEU:HD21	16:R:488:LEU:HB3	1.90	0.52
13:N:273:MET:HG3	13:N:277:CYS:SG	2.50	0.52
13:N:364:CYS:O	13:N:367:ARG:O	2.26	0.52
3:P:233:PHE:CE1	3:P:237:ILE:CD1	2.90	0.52
1:A:77:ARG:HD3	1:A:128:TRP:CE3	2.45	0.52
1:A:504:VAL:HG11	1:A:635:VAL:HG13	1.90	0.52
1:A:1412:CYS:HB2	1:A:1471:SER:OG	2.10	0.52
9:J:277:GLU:OE1	9:J:278:LEU:HD23	2.09	0.52
3:P:407:GLN:HA	3:P:422:TYR:OH	2.10	0.52
1:A:956:ARG:CZ	1:A:1785:GLU:OE1	2.58	0.52
1:A:980:ARG:NH2	1:A:1674:TRP:O	2.43	0.52
9:J:383:ASN:HB3	9:J:386:LEU:HD13	1.91	0.52
13:N:102:UNK:HA	13:N:107:UNK:O	2.10	0.52
13:N:392:ASN:O	13:N:395:ASP:HA	2.10	0.52
20:Y:214:VAL:HG12	20:Y:217:ALA:HB3	1.91	0.52
9:J:355:ALA:O	9:J:359:THR:HG23	2.10	0.52
10:K:351:ASP:OD1	10:K:351:ASP:N	2.42	0.52
13:N:395:ASP:CG	13:N:398:THR:N	2.63	0.52
13:N:501:ILE:O	13:N:505:LEU:HG	2.09	0.52
13:N:527:LEU:HD11	13:N:564:MET:HG3	1.91	0.52
14:O:431:LEU:HD11	14:O:616:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:467:ALA:CB	14:O:506:LEU:HD11	2.39	0.52
3:C:409:TYR:HB2	3:C:418:CYS:HB3	1.92	0.52
3:C:478:GLU:CD	3:C:490:TYR:HH	2.13	0.52
9:J:276:VAL:HA	9:J:311:MET:SD	2.49	0.52
9:J:332:THR:HA	9:J:363:LEU:HD21	1.90	0.52
20:Y:192:TYR:HA	20:Y:195:VAL:HG22	1.89	0.52
1:A:1250:GLN:O	1:A:1254:VAL:HG23	2.10	0.52
1:A:1815:LYS:NZ	1:A:1893:SER:OG	2.29	0.52
2:B:46:LEU:C	13:N:632:MET:HE3	2.30	0.52
3:P:355:GLN:HA	3:P:358:LEU:CD2	2.40	0.52
20:Y:302:PRO:HG2	20:Y:303:TYR:CE2	2.45	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
6:H:743:ILE:CG2	6:H:759:ASN:HD21	2.21	0.52
9:J:211:LYS:O	9:J:212:TYR:CG	2.62	0.52
16:R:286:ARG:C	16:R:287:ASP:O	2.48	0.52
20:Y:350:PHE:HB2	20:Y:351:TYR:CD1	2.45	0.52
1:A:612:ILE:O	1:A:641:TRP:HZ3	1.92	0.52
6:F:755:LEU:HD13	9:J:393:GLN:HE22	1.74	0.52
13:N:321:LEU:HD22	13:N:324:TRP:CD2	2.45	0.52
13:N:435:VAL:HG11	13:N:515:PHE:CZ	2.33	0.52
13:N:509:TYR:CD2	13:N:515:PHE:CE1	2.98	0.52
3:P:304:SER:HB2	3:P:336:VAL:HG22	1.91	0.52
20:X:355:TYR:HB2	20:X:386:MET:HB2	1.80	0.52
3:C:370:LEU:HD22	16:R:47:ARG:CZ	2.40	0.51
6:F:146:PRO:CG	6:F:167:THR:HA	2.40	0.51
13:N:281:TYR:CE1	13:N:284:SER:HB3	2.45	0.51
13:N:540:ARG:O	13:N:544:LEU:HD22	2.09	0.51
3:P:199:LEU:O	3:P:199:LEU:HD23	2.09	0.51
3:P:276:ILE:HG22	3:P:277:ARG:N	2.25	0.51
3:P:388:TYR:O	3:P:392:ILE:HG22	2.10	0.51
20:X:350:PHE:HB2	20:X:351:TYR:CD1	2.44	0.51
1:A:174:PRO:HG2	1:A:175:PHE:CD1	2.45	0.51
1:A:1079:ALA:HB1	1:A:1556:LEU:CA	2.40	0.51
2:B:8:TRP:HD1	13:N:644:VAL:HG12	1.72	0.51
2:B:36:ASP:OD1	2:B:36:ASP:N	2.43	0.51
3:C:361:ASN:HB3	3:C:363:ARG:N	2.25	0.51
9:J:35:GLU:OE2	9:J:63:ARG:CZ	2.58	0.51
10:K:185:LEU:CD1	10:K:209:LEU:HD11	2.39	0.51
13:N:574:ILE:HD13	13:N:622:TYR:CE1	2.45	0.51
14:O:119:PHE:CZ	14:O:136:LEU:HD11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:251:TYR:HB3	3:P:269:ILE:HD11	1.91	0.51
16:R:155:ASN:O	16:R:158:GLN:HB2	2.10	0.51
20:Y:159:LEU:HD22	20:Y:171:ILE:HG23	1.91	0.51
20:Y:494:ASP:OD1	20:Y:494:ASP:N	2.40	0.51
3:C:251:TYR:CB	3:C:269:ILE:HD11	2.38	0.51
3:C:494:ILE:HA	3:C:497:ILE:HD12	1.91	0.51
6:H:537:GLU:OE2	6:H:600:TYR:CZ	2.62	0.51
16:R:44:HIS:CG	16:R:45:GLY:N	2.78	0.51
20:X:214:VAL:HG12	20:X:217:ALA:HB3	1.91	0.51
1:A:207:LEU:HD12	1:A:208:PRO:CD	2.40	0.51
1:A:1218:GLY:N	1:A:1259:LEU:O	2.44	0.51
1:A:1236:LEU:HD12	16:R:161:LEU:HD11	1.92	0.51
2:B:20:ASP:O	2:B:30:PHE:CD2	2.63	0.51
6:F:699:ASP:HB2	6:F:702:ASN:HD21	1.74	0.51
10:K:174:HIS:CE1	10:K:211:LYS:HD2	2.44	0.51
12:M:2:ASP:OD1	12:M:3:SER:N	2.42	0.51
1:A:42:LEU:HD23	3:C:142:GLU:HG2	1.93	0.51
1:A:1114:ARG:CB	13:N:779:MET:HG3	2.40	0.51
3:C:431:ASN:HA	3:C:462:VAL:HG21	1.91	0.51
6:F:537:GLU:CD	6:F:600:TYR:HH	2.14	0.51
8:I:344:ILE:O	8:I:348:VAL:HG23	2.11	0.51
13:N:156:MET:O	13:N:160:VAL:HG23	2.10	0.51
13:N:567:SER:HA	13:N:570:ILE:HG22	1.92	0.51
13:N:663:GLN:HB3	13:N:699:TRP:CZ2	2.45	0.51
3:P:122:ARG:HG2	3:P:154:LEU:HD11	1.92	0.51
3:P:358:LEU:CD1	3:P:368:TRP:CD2	2.94	0.51
16:R:196:SER:HB3	16:R:234:TRP:CE2	2.45	0.51
1:A:1265:ALA:HB2	1:A:1309:HIS:CD2	2.46	0.51
6:F:702:ASN:HB2	6:F:705:CYS:SG	2.51	0.51
6:H:689:LEU:HD11	6:H:716:ASN:ND2	2.25	0.51
9:J:495:PHE:CZ	9:J:525:MET:SD	3.04	0.51
10:K:443:LYS:O	10:K:446:PRO:HD2	2.11	0.51
11:L:89:TYR:CE2	11:L:152:HIS:CE1	2.98	0.51
14:O:348:TYR:CZ	14:O:361:LEU:HD11	2.45	0.51
20:Y:199:CYS:HB2	20:Y:200:PRO:C	2.31	0.51
20:Y:449:THR:HG22	20:Y:461:ALA:O	2.11	0.51
1:A:1274:LEU:HD21	1:A:1325:LEU:CD1	2.41	0.51
1:A:1651:LEU:HD12	1:A:1651:LEU:N	2.25	0.51
2:B:14:TRP:HE3	2:B:31:ASN:O	1.85	0.51
3:C:206:TRP:O	3:C:209:LEU:HB2	2.10	0.51
6:F:617:LEU:HD11	6:F:648:GLN:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:62:SER:O	10:K:63:ARG:CG	2.55	0.51
13:N:123:UNK:CB	13:N:250:LEU:HD11	2.41	0.51
13:N:386:LEU:C	13:N:388:HIS:HB3	2.31	0.51
13:N:662:VAL:CG2	13:N:695:ARG:HG2	2.41	0.51
14:O:78:LEU:HD12	14:O:78:LEU:O	2.11	0.51
14:O:354:ARG:HD2	14:O:573:LYS:O	2.11	0.51
20:X:359:LEU:CD1	20:X:383:LEU:HD11	2.33	0.51
1:A:852:LEU:HD11	1:A:1819:GLU:HB3	1.92	0.51
1:A:1230:ILE:HD11	16:R:94:LEU:HB3	1.92	0.51
3:C:516:LEU:HD22	3:C:520:TYR:CE2	2.45	0.51
8:I:115:TRP:CZ3	8:I:176:LEU:HD22	2.46	0.51
8:I:674:VAL:O	8:I:703:ARG:NH1	2.44	0.51
9:J:397:ILE:HG22	9:J:398:ALA:N	2.25	0.51
11:L:62:HIS:NE2	11:L:149:ARG:O	2.42	0.51
13:N:75:PHE:O	13:N:78:VAL:N	2.43	0.51
13:N:597:SER:HG	13:N:600:PHE:HB2	1.75	0.51
13:N:611:VAL:HG23	13:N:616:ARG:HG2	1.93	0.51
3:P:368:TRP:CB	3:P:391:ALA:HB2	2.41	0.51
15:Q:56:SER:OG	15:Q:57:ASP:N	2.44	0.51
6:F:75:LEU:HG	6:F:91:ILE:HD13	1.93	0.51
11:L:40:PHE:HA	11:L:44:GLN:OE1	2.10	0.51
13:N:670:PHE:CE2	13:N:705:LEU:HD11	2.46	0.51
20:X:267:LEU:CD1	20:Y:59:LEU:HD13	2.41	0.51
1:A:629:LEU:C	1:A:629:LEU:HD12	2.31	0.51
1:A:848:VAL:HG22	1:A:877:ILE:CD1	2.40	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
6:F:686:GLU:OE1	6:F:686:GLU:N	2.42	0.51
3:P:276:ILE:HG22	3:P:277:ARG:H	1.76	0.51
9:J:258:MET:HE2	9:J:271:HIS:CD2	2.45	0.50
9:J:393:GLN:O	9:J:396:SER:HB3	2.11	0.50
14:O:652:LEU:O	14:O:660:LYS:HD2	2.11	0.50
1:A:1086:MET:HE1	1:A:1564:LEU:HD13	1.93	0.50
3:C:296:ARG:HA	3:P:101:ARG:NH2	2.26	0.50
13:N:253:LEU:O	13:N:257:SER:OG	2.18	0.50
13:N:559:VAL:HG11	13:N:600:PHE:CZ	2.46	0.50
13:N:564:MET:HE1	13:N:596:LEU:HD23	1.92	0.50
20:Y:196:LEU:O	20:Y:200:PRO:CB	2.59	0.50
1:A:801:PRO:C	1:A:804:ASP:OD1	2.49	0.50
6:H:150:SER:O	6:H:154:SER:OG	2.29	0.50
6:H:730:LYS:HD3	6:H:740:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:63:LEU:HD22	11:L:138:GLN:HE21	1.76	0.50
13:N:511:SER:O	13:N:512:LYS:CG	2.55	0.50
13:N:513:ASP:OD2	13:N:788:ALA:HA	2.11	0.50
1:A:1191:LEU:HD23	1:A:1191:LEU:C	2.31	0.50
6:H:492:PRO:O	6:H:493:SER:CB	2.59	0.50
9:J:46:CYS:O	9:J:50:THR:OG1	2.22	0.50
9:J:397:ILE:O	9:J:398:ALA:C	2.50	0.50
13:N:425:ARG:NE	13:N:507:SER:HB2	2.25	0.50
14:O:513:LYS:HG2	14:O:542:GLU:OE1	2.12	0.50
20:X:509:CYS:SG	20:X:510:VAL:N	2.84	0.50
10:K:62:SER:C	10:K:63:ARG:CG	2.80	0.50
20:X:358:ALA:O	20:X:379:LYS:HA	2.11	0.50
1:A:174:PRO:HA	1:A:295:UNK:O	2.12	0.50
1:A:1262:GLN:HE21	1:A:1307:LEU:HD22	1.77	0.50
1:A:1469:CYS:O	1:A:1472:LEU:HB3	2.11	0.50
2:B:14:TRP:CZ3	2:B:31:ASN:O	2.65	0.50
3:C:167:LEU:HD23	3:C:172:LEU:HD13	1.94	0.50
13:N:74:TRP:CZ2	13:N:77:GLU:HB2	2.46	0.50
13:N:74:TRP:CG	13:N:75:PHE:N	2.79	0.50
14:O:40:LEU:HD22	14:O:82:ILE:HD12	1.94	0.50
14:O:490:LEU:HD13	14:O:511:ASP:CB	2.40	0.50
3:P:234:LEU:HD22	3:P:238:TYR:CE2	2.47	0.50
16:R:190:TYR:CE1	16:R:230:THR:HG23	2.47	0.50
1:A:1274:LEU:CD1	1:A:1321:VAL:HG12	2.39	0.50
1:A:1572:TYR:CE1	1:A:1616:PRO:HB3	2.46	0.50
2:B:15:LEU:HD21	13:N:635:LEU:HA	1.94	0.50
9:J:351:ASP:OD1	9:J:351:ASP:N	2.44	0.50
3:P:251:TYR:OH	3:P:268:GLN:CG	2.60	0.50
3:P:283:LEU:HD21	3:P:312:MET:HE3	1.93	0.50
3:P:332:GLU:N	3:P:332:GLU:OE1	2.45	0.50
16:R:57:TRP:CE3	16:R:57:TRP:CA	2.95	0.50
20:Y:384:ARG:HH22	20:Y:415:GLU:HB3	1.77	0.50
20:Y:509:CYS:SG	20:Y:510:VAL:N	2.85	0.50
1:A:1405:LEU:HD13	1:A:1467:GLY:HA2	1.94	0.50
6:F:492:PRO:O	6:F:493:SER:CB	2.60	0.50
8:I:52:PHE:CD1	8:I:743:VAL:HG21	2.46	0.50
9:J:55:ARG:NH1	10:K:261:ASP:OD2	2.44	0.50
13:N:501:ILE:H	13:N:501:ILE:HD12	1.77	0.50
14:O:621:SER:HB3	14:O:651:ILE:HG12	1.94	0.50
3:P:365:LEU:HB3	3:P:395:ASN:HD21	1.77	0.50
20:X:159:LEU:HD22	20:X:171:ILE:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:355:TYR:CE2	20:X:385:ASN:O	2.61	0.50
20:X:515:LEU:HD23	20:X:519:LEU:HG	1.94	0.50
1:A:1533:LEU:HD12	1:A:1534:LYS:N	2.26	0.50
3:C:251:TYR:OH	3:C:268:GLN:HG3	2.12	0.50
9:J:429:LEU:HA	9:J:432:ILE:HG22	1.94	0.50
13:N:418:GLU:OE2	13:N:495:UNK:C	2.60	0.50
13:N:644:VAL:HG21	13:N:664:ALA:CB	2.42	0.50
20:X:350:PHE:CD2	20:X:381:ALA:HB3	2.43	0.50
20:Y:376:LEU:HD21	20:Y:398:GLU:HG3	1.93	0.50
1:A:1427:ASP:O	1:A:1430:VAL:HG12	2.11	0.49
6:H:669:SER:HA	6:H:698:ILE:HD11	1.92	0.49
6:H:736:GLU:OE1	11:L:173:THR:O	2.29	0.49
8:I:46:LEU:HD22	8:I:56:TRP:HE1	1.77	0.49
10:K:292:VAL:HG21	12:M:57:TRP:HB3	1.93	0.49
13:N:202:GLU:O	13:N:202:GLU:OE1	2.30	0.49
13:N:286:LEU:HG	13:N:360:ASP:OD2	2.11	0.49
13:N:304:PHE:CD1	13:N:324:TRP:CH2	3.00	0.49
16:R:234:TRP:CZ3	16:R:255:VAL:HG21	2.47	0.49
20:X:355:TYR:CB	20:X:383:LEU:HA	2.22	0.49
1:A:260:ASP:OD1	1:A:262:VAL:HG22	2.12	0.49
1:A:881:ILE:O	1:A:882:LEU:HG	2.12	0.49
1:A:1086:MET:HE2	1:A:1564:LEU:HD12	1.94	0.49
6:H:128:THR:HG21	6:H:130:ARG:HH12	1.78	0.49
8:I:286:ARG:NH1	8:I:324:GLN:HB3	2.27	0.49
9:J:334:GLY:N	9:J:335:PRO:CD	2.75	0.49
10:K:324:SER:O	10:K:328:THR:HG23	2.12	0.49
13:N:87:ILE:O	13:N:90:GLU:HB2	2.12	0.49
13:N:681:LEU:HD23	13:N:692:LEU:HD11	1.93	0.49
14:O:631:GLN:HE22	14:O:643:LEU:HD13	1.77	0.49
14:O:632:LEU:C	14:O:632:LEU:HD12	2.33	0.49
3:P:303:PHE:CD1	3:P:303:PHE:C	2.84	0.49
16:R:47:ARG:O	16:R:48:PHE:CD1	2.64	0.49
1:A:641:TRP:CZ2	1:A:645:HIS:HB2	2.47	0.49
3:C:117:LEU:HD23	3:C:117:LEU:O	2.12	0.49
6:F:639:TYR:CD1	16:R:492:ILE:HG21	2.47	0.49
6:H:481:CYS:CB	6:H:512:LEU:HD13	2.42	0.49
8:I:414:PHE:HZ	8:I:472:VAL:HG13	1.76	0.49
13:N:165:ALA:O	13:N:169:PHE:HB3	2.12	0.49
13:N:659:VAL:HG23	13:N:728:VAL:HG23	1.94	0.49
20:X:359:LEU:HB2	20:X:383:LEU:CG	2.43	0.49
20:Y:294:PHE:HZ	20:Y:308:MET:SD	2.35	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
1:A:804:ASP:OD1	1:A:804:ASP:N	2.46	0.49
1:A:852:LEU:C	1:A:852:LEU:HD12	2.32	0.49
1:A:1637:LEU:CD1	1:A:1665:GLN:HE21	2.21	0.49
1:A:1888:PHE:CE2	1:A:1892:HIS:CD2	3.00	0.49
2:B:39:VAL:CB	2:B:43:ASP:CB	2.89	0.49
3:C:122:ARG:HG2	3:C:154:LEU:HD11	1.94	0.49
8:I:65:GLY:HA3	8:I:84:LEU:HB3	1.94	0.49
8:I:240:LEU:HD22	8:I:547:SER:CB	2.42	0.49
3:P:494:ILE:HD13	3:P:516:LEU:HD13	1.95	0.49
10:K:509:ARG:HG3	10:K:512:ASP:HB2	1.93	0.49
3:P:283:LEU:HD21	3:P:312:MET:CE	2.42	0.49
1:A:659:LEU:HD12	1:A:660:PHE:N	2.28	0.49
9:J:258:MET:CE	9:J:271:HIS:CG	2.96	0.49
10:K:297:SER:O	10:K:329:LEU:HD21	2.12	0.49
12:M:12:LEU:HD13	3:P:360:LEU:CD2	2.42	0.49
14:O:136:LEU:C	14:O:136:LEU:HD12	2.33	0.49
1:A:1469:CYS:HB2	1:A:1488:LEU:HD22	1.95	0.49
1:A:1511:ASN:HD22	1:A:1511:ASN:N	2.11	0.49
6:H:747:TYR:CZ	6:H:755:LEU:HD23	2.48	0.49
8:I:279:ILE:HD13	8:I:340:SER:HB2	1.95	0.49
14:O:264:VAL:O	14:O:265:GLN:HB2	2.13	0.49
20:X:363:ALA:HB2	20:X:379:LYS:CE	2.43	0.49
1:A:72:GLU:CG	1:A:94:TYR:OH	2.60	0.49
6:F:130:ARG:HG2	20:Y:506:GLN:HB2	1.93	0.49
8:I:46:LEU:HD22	8:I:56:TRP:NE1	2.28	0.49
9:J:77:ALA:CB	9:J:93:LEU:HD11	2.43	0.49
9:J:178:ALA:HB1	9:J:213:ASN:HD22	1.78	0.49
13:N:331:PHE:CZ	13:N:335:ILE:HD11	2.47	0.49
13:N:425:ARG:NH1	13:N:507:SER:HB2	2.28	0.49
13:N:519:TYR:HE1	13:N:523:LEU:HD21	1.76	0.49
20:X:350:PHE:O	20:X:385:ASN:OD1	2.31	0.49
20:Y:515:LEU:HD23	20:Y:519:LEU:HG	1.94	0.49
2:B:15:LEU:HD11	13:N:635:LEU:HD12	1.93	0.49
3:C:477:HIS:HD2	3:C:482:GLU:OE1	1.96	0.49
13:N:556:PHE:CE1	13:N:600:PHE:HA	2.48	0.49
13:N:669:TYR:CZ	13:N:684:ALA:HB1	2.48	0.49
14:O:539:ASN:HD22	14:O:542:GLU:HB3	1.74	0.49
15:Q:75:GLU:O	15:Q:76:ASP:HB2	2.13	0.49
1:A:268:VAL:HG12	1:A:412:LEU:HD21	1.94	0.49
1:A:1100:LEU:HB3	1:A:1101:PRO:CA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1134:TRP:CE2	1:A:1203:MET:HE2	2.48	0.49
1:A:1739:SER:N	1:A:1740:ALA:HB3	2.28	0.49
2:B:16:TRP:O	2:B:17:VAL:CB	2.60	0.49
8:I:679:ASP:OD1	8:I:703:ARG:NH2	2.46	0.49
9:J:354:MET:CE	9:J:354:MET:HA	2.43	0.49
10:K:230:ASN:OD1	10:K:231:LEU:N	2.46	0.49
13:N:281:TYR:CZ	13:N:357:ALA:CA	2.96	0.49
14:O:513:LYS:HE3	14:O:542:GLU:OE1	2.13	0.49
3:P:307:LEU:HD12	3:P:312:MET:HG3	1.95	0.49
20:X:52:ASN:HD22	20:Y:202:ALA:HB1	1.78	0.49
20:X:449:THR:HG22	20:X:461:ALA:O	2.11	0.49
1:A:154:LEU:HD13	1:A:159:ILE:HG13	1.95	0.48
1:A:175:PHE:CD2	1:A:191:ARG:HG3	2.48	0.48
1:A:813:LEU:O	1:A:814:ALA:HB2	2.12	0.48
1:A:1254:VAL:HG11	1:A:1298:ALA:HA	1.94	0.48
2:B:83:LYS:O	2:B:84:GLU:HB2	2.13	0.48
8:I:197:ARG:O	8:I:545:GLY:HA3	2.13	0.48
10:K:250:CYS:SG	10:K:274:THR:HG23	2.50	0.48
20:Y:442:GLN:HG2	20:Y:472:GLU:HB2	1.94	0.48
1:A:504:VAL:HG11	1:A:635:VAL:CG1	2.43	0.48
1:A:1089:LEU:HD11	1:A:1611:VAL:HG23	1.94	0.48
1:A:1793:MET:HA	1:A:1814:ILE:HD11	1.95	0.48
3:C:60:PHE:HA	3:P:85:ASP:OD2	2.13	0.48
8:I:73:TRP:CD2	8:I:80:LEU:HD13	2.47	0.48
9:J:268:LEU:N	9:J:269:PRO:HD2	2.28	0.48
11:L:125:THR:HA	11:L:126:ASP:O	2.12	0.48
14:O:341:GLN:HB3	14:O:376:LEU:HD23	1.95	0.48
20:X:376:LEU:HD21	20:X:398:GLU:HG3	1.95	0.48
1:A:1070:LEU:HD23	1:A:1120:LEU:HG	1.96	0.48
13:N:73:UNK:O	13:N:74:TRP:CB	2.59	0.48
13:N:527:LEU:HD11	13:N:564:MET:CG	2.39	0.48
13:N:669:TYR:CE1	13:N:684:ALA:HB1	2.48	0.48
14:O:657:ILE:HA	14:O:660:LYS:CB	2.43	0.48
16:R:149:SER:O	16:R:150:LEU:HG	2.12	0.48
1:A:170:ILE:HG21	3:C:427:GLN:HB2	1.94	0.48
1:A:1316:MET:O	1:A:1319:LEU:O	2.30	0.48
1:A:1470:LEU:HD12	1:A:1518:VAL:HG13	1.95	0.48
1:A:1656:LEU:H	1:A:1656:LEU:HD12	1.78	0.48
1:A:1800:LEU:HD11	1:A:1811:LEU:HD21	1.95	0.48
2:B:16:TRP:CZ2	2:B:45:PRO:CA	2.52	0.48
9:J:191:SER:O	9:J:193:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:445:GLU:CG	9:J:446:PRO:HD3	2.33	0.48
11:L:33:LEU:CG	11:L:42:VAL:HG22	2.40	0.48
13:N:296:VAL:O	13:N:299:TRP:HB3	2.14	0.48
13:N:655:LEU:HD11	13:N:726:ASN:HB2	1.94	0.48
20:X:266:LEU:HB3	20:Y:63:LEU:HD22	1.95	0.48
8:I:56:TRP:CE3	8:I:98:PRO:CB	2.96	0.48
9:J:324:SER:O	9:J:328:THR:HG23	2.13	0.48
13:N:542:VAL:HG11	13:N:558:GLU:CG	2.43	0.48
13:N:560:MET:SD	13:N:601:TRP:CD1	3.07	0.48
13:N:611:VAL:HG11	13:N:637:TRP:CZ2	2.47	0.48
3:P:234:LEU:CD2	3:P:238:TYR:CZ	2.96	0.48
3:P:303:PHE:C	3:P:303:PHE:HD1	2.16	0.48
20:X:343:VAL:HG12	20:X:378:LEU:HD22	1.95	0.48
20:X:466:ASN:O	20:X:470:THR:HG23	2.14	0.48
1:A:501:THR:HB	1:A:504:VAL:HG22	1.95	0.48
6:H:594:ILE:HD11	6:H:604:TYR:HA	1.96	0.48
8:I:72:ALA:O	8:I:80:LEU:HD12	2.14	0.48
8:I:73:TRP:CH2	8:I:80:LEU:HD22	2.48	0.48
8:I:209:CYS:HG	8:I:584:HIS:CE1	2.29	0.48
13:N:426:ARG:HH22	13:N:793:GLN:HE22	1.60	0.48
3:P:209:LEU:O	3:P:213:ILE:HG12	2.13	0.48
3:P:307:LEU:HD23	3:P:316:LEU:HD23	1.96	0.48
3:P:358:LEU:HD11	3:P:368:TRP:CE2	2.48	0.48
20:X:93:TYR:CZ	20:X:148:VAL:HG11	2.48	0.48
20:Y:294:PHE:CG	20:Y:311:TYR:CD1	3.01	0.48
1:A:90:ASP:HB3	1:A:591:VAL:HG21	1.96	0.48
1:A:250:ASN:OD1	1:A:432:ILE:HD12	2.13	0.48
5:E:102:LEU:HD13	6:H:594:ILE:HG22	1.95	0.48
6:H:145:ASN:CB	6:H:146:PRO:O	2.62	0.48
8:I:207:ALA:HB3	8:I:220:VAL:HB	1.95	0.48
13:N:281:TYR:HE2	13:N:356:PRO:HB2	1.77	0.48
13:N:791:ASP:OD1	13:N:794:GLU:HB2	2.14	0.48
3:P:117:LEU:HD23	3:P:117:LEU:O	2.12	0.48
20:Y:452:LEU:CD2	20:Y:460:LYS:HB2	2.43	0.48
1:A:1243:LEU:O	1:A:1243:LEU:HD23	2.12	0.48
1:A:1615:GLU:OE2	1:A:1617:ARG:HD3	2.12	0.48
1:A:1752:GLU:HB2	1:A:1753:TYR:HD1	1.78	0.48
2:B:23:CYS:HA	2:B:30:PHE:CE1	2.48	0.48
3:C:233:PHE:CE1	3:C:237:ILE:HD11	2.49	0.48
6:F:534:GLU:HA	6:F:568:GLU:OE1	2.14	0.48
6:H:75:LEU:HG	6:H:91:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:209:CYS:SG	8:I:577:ASN:HB2	2.54	0.48
9:J:258:MET:CE	9:J:271:HIS:CD2	2.96	0.48
14:O:513:LYS:CE	14:O:542:GLU:OE1	2.61	0.48
1:A:808:ARG:NH2	1:A:1894:VAL:O	2.46	0.48
1:A:1839:PHE:CD1	1:A:1840:MET:HG3	2.49	0.48
2:B:13:LEU:HD21	13:N:638:LYS:HD2	1.96	0.48
8:I:231:VAL:HG21	8:I:557:TYR:CE1	2.49	0.48
8:I:262:LEU:HD11	8:I:533:ILE:HG21	1.96	0.48
9:J:523:ILE:HD11	3:P:420:TYR:CG	2.49	0.48
12:M:10:ARG:HD3	12:M:14:LEU:HD12	1.95	0.48
13:N:269:THR:HG23	13:N:292:TRP:CZ3	2.49	0.48
3:P:234:LEU:CD2	3:P:238:TYR:CE2	2.97	0.48
15:Q:55:GLU:OE1	15:Q:61:LYS:HD3	2.14	0.48
20:X:425:GLU:O	20:X:429:MET:HE2	2.14	0.48
20:Y:407:LEU:HD13	20:Y:443:THR:HG21	1.96	0.48
20:Y:466:ASN:O	20:Y:470:THR:HG23	2.14	0.48
1:A:154:LEU:HD13	1:A:159:ILE:CG1	2.44	0.48
8:I:730:VAL:HG22	8:I:731:SER:N	2.29	0.48
9:J:320:ARG:HD3	9:J:344:PHE:CZ	2.48	0.48
10:K:417:GLU:HB2	10:K:420:THR:OG1	2.13	0.48
3:P:242:GLN:HE21	3:P:429:ARG:HA	1.79	0.48
3:P:274:HIS:O	3:P:276:ILE:O	2.32	0.48
20:X:294:PHE:HZ	20:X:308:MET:SD	2.37	0.48
20:X:350:PHE:HZ	20:X:378:LEU:CA	2.26	0.48
20:X:359:LEU:CB	20:X:383:LEU:HD21	2.43	0.48
20:X:452:LEU:CD2	20:X:460:LYS:HB2	2.44	0.48
1:A:184:LYS:O	1:A:185:TYR:HB2	2.13	0.47
9:J:441:VAL:O	9:J:442:ASP:CB	2.62	0.47
10:K:384:SER:HB3	10:K:415:ASN:OD1	2.13	0.47
13:N:164:ALA:HB3	13:N:165:ALA:HA	1.96	0.47
13:N:275:ASP:OD1	13:N:276:ARG:N	2.47	0.47
3:P:331:VAL:HG11	3:P:364:TYR:CD2	2.49	0.47
1:A:1078:MET:HB2	1:A:1552:TYR:CE1	2.49	0.47
3:C:238:TYR:CB	3:C:247:ALA:HB2	2.44	0.47
3:C:526:TRP:HE1	3:C:556:LEU:HD23	1.80	0.47
4:D:17:TRP:CD1	4:D:17:TRP:C	2.87	0.47
6:F:550:VAL:HG21	10:K:289:HIS:CB	2.45	0.47
6:H:86:ALA:HA	10:K:473:VAL:CG1	2.44	0.47
10:K:276:VAL:HA	10:K:311:MET:HE1	1.95	0.47
13:N:286:LEU:O	13:N:287:ARG:C	2.52	0.47
1:A:776:ASN:HD22	1:A:779:MET:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:LEU:HD12	3:C:141:LEU:O	2.13	0.47
4:D:8:LEU:HD23	14:O:420:ILE:HD11	1.97	0.47
5:E:87:GLU:OE1	5:E:87:GLU:N	2.47	0.47
6:H:481:CYS:SG	6:H:512:LEU:HB2	2.55	0.47
8:I:219:VAL:N	8:I:234:PHE:O	2.47	0.47
10:K:167:PHE:O	10:K:171:THR:HG22	2.13	0.47
11:L:33:LEU:HD13	11:L:54:TRP:CD2	2.49	0.47
13:N:556:PHE:CG	13:N:600:PHE:HD1	2.32	0.47
14:O:292:GLY:HA3	14:O:336:ASP:CB	2.43	0.47
16:R:56:ASN:N	16:R:56:ASN:OD1	2.45	0.47
20:Y:255:ILE:HD11	20:Y:281:TYR:OH	2.14	0.47
3:C:53:LYS:HD3	3:P:96:VAL:HG21	1.96	0.47
9:J:456:ARG:CG	9:J:488:ILE:HG22	2.44	0.47
14:O:405:SER:O	14:O:409:HIS:CD2	2.67	0.47
14:O:669:LYS:NZ	14:O:755:LEU:O	2.47	0.47
3:P:331:VAL:CG1	3:P:364:TYR:CD2	2.97	0.47
3:P:478:GLU:CD	3:P:490:TYR:OH	2.53	0.47
20:X:365:ALA:CB	20:X:375:ALA:HB1	2.44	0.47
20:Y:45:ALA:HB3	20:Y:82:TYR:CE2	2.50	0.47
20:Y:294:PHE:CE1	20:Y:311:TYR:CD1	3.03	0.47
20:Y:452:LEU:HD23	20:Y:461:ALA:HB2	1.96	0.47
20:Y:546:LEU:HD11	20:Y:550:GLN:HE21	1.79	0.47
1:A:1172:TYR:CZ	1:A:1176:LEU:HD23	2.48	0.47
1:A:1405:LEU:CD1	1:A:1467:GLY:HA2	2.44	0.47
1:A:1622:VAL:HA	1:A:1629:PRO:HA	1.95	0.47
2:B:18:ALA:HB2	2:B:48:TRP:CZ2	2.42	0.47
8:I:49:LEU:HD13	8:I:730:VAL:HG21	1.95	0.47
10:K:77:ALA:CB	10:K:93:LEU:HD11	2.45	0.47
11:L:21:THR:O	11:L:162:VAL:HG12	2.14	0.47
15:Q:58:ASN:HB2	15:Q:60:PHE:H	1.78	0.47
20:Y:425:GLU:O	20:Y:429:MET:HE2	2.13	0.47
1:A:21:VAL:HG23	1:A:25:ARG:NH2	2.29	0.47
1:A:273:ARG:O	1:A:274:VAL:HG23	2.14	0.47
1:A:1881:GLN:NE2	1:A:1885:LEU:HD12	2.29	0.47
6:F:96:VAL:HG12	6:F:97:PHE:CD1	2.50	0.47
8:I:116:MET:HE1	8:I:211:SER:O	2.15	0.47
13:N:78:VAL:O	13:N:80:GLN:C	2.50	0.47
13:N:363:TYR:OH	13:N:367:ARG:CZ	2.62	0.47
13:N:520:ARG:CG	13:N:557:CYS:SG	3.02	0.47
13:N:567:SER:OG	13:N:594:VAL:O	2.33	0.47
14:O:65:LEU:HB3	14:O:66:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:619:LEU:O	14:O:623:THR:HG22	2.15	0.47
20:X:442:GLN:HG2	20:X:472:GLU:HB2	1.95	0.47
20:Y:270:ASN:HB2	20:Y:273:LEU:CB	2.44	0.47
20:Y:496:ILE:HD13	20:Y:519:LEU:HD23	1.97	0.47
1:A:767:HIS:O	1:A:770:TYR:HB3	2.15	0.47
2:B:16:TRP:CD1	2:B:56:HIS:CD2	3.03	0.47
3:C:329:TYR:HB3	12:M:15:ILE:HD11	1.95	0.47
6:F:723:LEU:HG	6:F:746:VAL:HG11	1.97	0.47
8:I:231:VAL:HG11	8:I:556:LEU:HD12	1.95	0.47
12:M:5:VAL:HG13	12:M:5:VAL:O	2.14	0.47
12:M:31:ILE:HG22	12:M:33:LEU:HD22	1.95	0.47
13:N:97:UNK:O	13:N:99:UNK:CA	2.62	0.47
13:N:619:LEU:HG	13:N:637:TRP:CH2	2.50	0.47
16:R:48:PHE:O	16:R:49:ILE:HG13	2.14	0.47
20:Y:400:ILE:HG13	20:Y:401:ARG:N	2.30	0.47
20:Y:451:CYS:O	20:Y:455:PRO:HD2	2.15	0.47
3:C:96:VAL:N	3:C:97:LYS:HA	2.29	0.47
3:C:209:LEU:O	3:C:213:ILE:HG12	2.15	0.47
4:D:10:PRO:HG2	14:O:346:TRP:CE2	2.49	0.47
6:F:550:VAL:HG21	10:K:289:HIS:CG	2.49	0.47
6:H:621:LEU:HD13	6:H:625:ARG:HH22	1.79	0.47
8:I:279:ILE:HD11	8:I:337:ILE:HA	1.94	0.47
10:K:432:ILE:CD1	10:K:444:TRP:CD1	2.95	0.47
13:N:662:VAL:HB	13:N:687:MET:SD	2.54	0.47
14:O:39:VAL:HG11	14:O:97:ILE:HG13	1.96	0.47
3:P:308:TYR:CE1	3:P:343:LEU:HG	2.50	0.47
20:X:430:ALA:HB2	20:X:451:CYS:SG	2.55	0.47
1:A:772:GLU:HG3	1:A:867:CYS:HA	1.96	0.47
1:A:1313:LEU:HD13	1:A:1316:MET:CG	2.44	0.47
2:B:48:TRP:CZ3	13:N:632:MET:CE	2.81	0.47
3:C:93:TYR:CD1	3:P:53:LYS:HD2	2.50	0.47
6:F:118:LEU:CD2	6:F:140:LYS:HB3	2.44	0.47
9:J:167:PHE:O	9:J:171:THR:HG22	2.14	0.47
9:J:354:MET:HE1	9:J:374:ILE:HA	1.97	0.47
14:O:625:LEU:HD12	14:O:625:LEU:C	2.35	0.47
20:X:359:LEU:CG	20:X:379:LYS:HE2	2.43	0.47
1:A:184:LYS:N	1:A:251:THR:HG22	2.30	0.47
2:B:20:ASP:O	2:B:30:PHE:HD2	1.98	0.47
6:F:130:ARG:HD3	20:Y:506:GLN:HB2	1.97	0.47
8:I:289:LYS:HD2	8:I:324:GLN:HE22	1.79	0.47
9:J:180:GLU:O	9:J:184:LEU:N	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:350:HIS:ND1	10:K:377:GLU:OE1	2.48	0.47
13:N:75:PHE:O	13:N:76:VAL:C	2.53	0.47
13:N:120:UNK:O	13:N:124:PRO:HD3	2.13	0.47
14:O:624:VAL:HG11	14:O:647:ALA:HB2	1.96	0.47
16:R:99:LEU:O	16:R:100:LEU:HD23	2.15	0.47
20:X:37:VAL:N	20:Y:230:VAL:HG21	2.30	0.47
20:X:270:ASN:HB2	20:X:273:LEU:CB	2.45	0.47
20:X:376:LEU:HD11	20:X:398:GLU:OE2	2.15	0.47
20:Y:303:TYR:O	20:Y:304:LEU:HD23	2.14	0.47
1:A:42:LEU:HD23	3:C:142:GLU:CG	2.45	0.46
1:A:1621:PRO:HG2	1:A:1630:CYS:O	2.15	0.46
6:F:456:LYS:CB	6:F:460:GLU:OE2	2.62	0.46
8:I:206:LEU:HD22	8:I:570:PHE:CG	2.50	0.46
8:I:349:ILE:HD12	14:O:407:LEU:HA	1.96	0.46
9:J:230:ASN:OD1	9:J:231:LEU:N	2.48	0.46
10:K:268:LEU:N	10:K:269:PRO:HD2	2.31	0.46
13:N:611:VAL:HG12	13:N:639:HIS:CE1	2.50	0.46
14:O:599:ILE:O	14:O:602:PRO:HD2	2.14	0.46
3:P:392:ILE:HD12	3:P:402:TRP:CH2	2.50	0.46
20:X:452:LEU:HD23	20:X:461:ALA:HB2	1.96	0.46
1:A:249:LEU:HD12	1:A:250:ASN:N	2.31	0.46
1:A:951:ILE:HD13	1:A:1816:LEU:HD13	1.96	0.46
3:C:36:LEU:HD21	3:C:58:LEU:CB	2.44	0.46
3:C:389:ARG:NE	14:O:279:ASP:OD2	2.38	0.46
6:F:723:LEU:CD2	6:F:746:VAL:HG11	2.45	0.46
6:H:629:ARG:NE	10:K:508:LEU:HD21	2.30	0.46
8:I:289:LYS:O	8:I:293:GLU:CB	2.63	0.46
10:K:181:GLU:HB3	10:K:209:LEU:HD13	1.96	0.46
10:K:300:VAL:HG12	10:K:333:TYR:OH	2.15	0.46
13:N:148:GLY:HA3	13:N:152:GLU:OE2	2.15	0.46
13:N:414:MET:SD	13:N:497:UNK:C	3.03	0.46
14:O:159:GLN:O	14:O:163:GLN:HG2	2.15	0.46
3:P:128:LYS:HA	3:P:128:LYS:HE3	1.98	0.46
20:Y:376:LEU:HD11	20:Y:398:GLU:OE2	2.16	0.46
20:Y:458:GLN:O	20:Y:462:LYS:HG3	2.15	0.46
1:A:255:ILE:HA	1:A:269:TRP:O	2.16	0.46
2:B:11:VAL:HG13	13:N:642:GLY:HA2	1.96	0.46
6:F:594:ILE:HD11	6:F:604:TYR:HA	1.97	0.46
8:I:69:THR:HG23	8:I:85:ALA:HB2	1.98	0.46
9:J:247:PHE:HB3	9:J:278:LEU:HD21	1.98	0.46
10:K:185:LEU:HD13	10:K:209:LEU:CD1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:574:ILE:HA	13:N:625:LYS:HE2	1.96	0.46
3:P:47:GLY:O	3:P:49:LEU:HD12	2.15	0.46
3:P:441:GLU:HG3	3:P:472:LYS:CE	2.45	0.46
20:X:100:TYR:CB	20:X:142:LEU:HD21	2.42	0.46
20:X:255:ILE:HD11	20:X:281:TYR:OH	2.16	0.46
1:A:1049:VAL:HG23	1:A:1069:ARG:HG2	1.97	0.46
1:A:1242:GLU:HG3	1:A:1242:GLU:O	2.16	0.46
3:C:266:VAL:HG12	3:C:289:LEU:HD23	1.96	0.46
3:C:308:TYR:CE1	3:C:343:LEU:HG	2.50	0.46
3:C:352:LEU:HD23	3:C:352:LEU:C	2.35	0.46
3:C:420:TYR:CD2	14:O:275:LEU:HD23	2.51	0.46
10:K:277:GLU:OE1	10:K:277:GLU:HA	2.15	0.46
10:K:495:PHE:CE1	10:K:525:MET:HG2	2.50	0.46
14:O:527:LEU:HD12	14:O:527:LEU:O	2.15	0.46
16:R:421:LEU:CD2	16:R:442:VAL:HG11	2.46	0.46
1:A:170:ILE:HG22	1:A:171:ALA:O	2.15	0.46
1:A:1078:MET:N	1:A:1078:MET:SD	2.88	0.46
2:B:20:ASP:CB	2:B:30:PHE:CE2	2.94	0.46
6:H:492:PRO:O	6:H:493:SER:HB3	2.16	0.46
11:L:33:LEU:CD2	11:L:64:VAL:HG13	2.46	0.46
13:N:400:TYR:CZ	13:N:404:ILE:HD11	2.51	0.46
20:X:400:ILE:HG13	20:X:401:ARG:N	2.31	0.46
1:A:465:ALA:C	1:A:466:LEU:HD12	2.35	0.46
1:A:852:LEU:HD12	1:A:853:LYS:N	2.30	0.46
5:E:86:VAL:HG13	6:H:588:LYS:HD3	1.97	0.46
6:F:726:LEU:HD11	6:F:742:LEU:HD22	1.97	0.46
9:J:397:ILE:HG22	9:J:398:ALA:H	1.81	0.46
9:J:485:ILE:HD12	9:J:501:TYR:CE1	2.51	0.46
14:O:126:VAL:HG13	14:O:132:VAL:HG12	1.98	0.46
14:O:694:LEU:HD13	14:O:713:VAL:HG22	1.97	0.46
3:P:358:LEU:HD12	3:P:368:TRP:CE2	2.50	0.46
1:A:776:ASN:O	1:A:777:THR:HB	2.16	0.46
1:A:1181:LEU:HB3	1:A:1611:VAL:HG11	1.97	0.46
6:F:699:ASP:HB3	6:F:702:ASN:OD1	2.16	0.46
6:H:723:LEU:CD2	6:H:746:VAL:HG11	2.45	0.46
10:K:42:TRP:HA	10:K:42:TRP:CE3	2.51	0.46
11:L:98:VAL:CG1	11:L:108:ILE:HD13	2.45	0.46
13:N:520:ARG:HD2	13:N:556:PHE:HD1	1.81	0.46
20:Y:93:TYR:CZ	20:Y:148:VAL:HG11	2.50	0.46
1:A:1279:ARG:HG2	1:A:1280:PRO:HD2	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)
9:J:281:ALA:CA	9:J:311:MET:CE	2.93	0.46
9:J:351:ASP:CG	16:R:387:ILE:HG21	2.35	0.46
13:N:280:GLU:O	13:N:354:SER:HA	2.16	0.46
13:N:292:TRP:CZ3	13:N:296:VAL:HG21	2.51	0.46
20:Y:517:ASP:O	20:Y:520:VAL:HG22	2.16	0.46
1:A:1232:ILE:HD11	1:A:1235:LEU:HD22	1.98	0.46
1:A:1894:VAL:O	1:A:1894:VAL:HG23	2.16	0.46
2:B:1:MET:HE2	13:N:715:VAL:HG21	1.98	0.46
6:H:152:PHE:CD1	6:H:152:PHE:C	2.88	0.46
13:N:386:LEU:O	13:N:388:HIS:HB3	2.16	0.46
3:P:441:GLU:HG3	3:P:472:LYS:NZ	2.30	0.46
20:X:83:HIS:O	20:X:86:SER:OG	2.20	0.46
20:X:451:CYS:O	20:X:455:PRO:HD2	2.15	0.46
1:A:32:PRO:O	1:A:33:ASN:HB3	2.16	0.46
12:M:9:GLY:HA3	3:P:329:TYR:CB	2.46	0.46
13:N:659:VAL:HG22	13:N:663:GLN:HB2	1.98	0.46
3:P:358:LEU:O	3:P:362:PRO:CA	2.58	0.46
16:R:94:LEU:CD1	16:R:161:LEU:HD21	2.46	0.46
20:X:458:GLN:O	20:X:462:LYS:HG3	2.15	0.46
1:A:269:TRP:CZ3	1:A:411:HIS:HB2	2.50	0.45
3:C:478:GLU:CD	3:C:490:TYR:OH	2.54	0.45
3:C:480:LEU:O	3:C:482:GLU:N	2.49	0.45
6:F:492:PRO:O	6:F:493:SER:HB3	2.16	0.45
6:F:674:HIS:O	6:F:678:VAL:HG23	2.16	0.45
9:J:376:LEU:CD2	9:J:407:GLU:HG2	2.46	0.45
13:N:150:ARG:HE	13:N:150:ARG:N	2.13	0.45
14:O:657:ILE:CG1	14:O:704:VAL:HG23	2.45	0.45
20:Y:269:ASP:HB3	20:Y:300:LEU:HD21	1.98	0.45
2:B:1:MET:HE2	13:N:650:LEU:HD22	1.98	0.45
3:C:255:ILE:HG12	3:C:260:SER:HA	1.97	0.45
5:E:67:LEU:HD22	20:Y:342:TRP:HH2	1.81	0.45
6:F:537:GLU:OE1	6:F:600:TYR:CE2	2.70	0.45
6:F:553:SER:HA	6:F:576:CYS:SG	2.57	0.45
8:I:360:LEU:HD21	8:I:390:ILE:HG23	1.98	0.45
8:I:607:ILE:HD12	8:I:607:ILE:H	1.81	0.45
13:N:559:VAL:HA	13:N:562:LYS:CG	2.45	0.45
13:N:570:ILE:HA	13:N:573:ASN:ND2	2.32	0.45
13:N:666:ILE:HG12	13:N:681:LEU:HD21	1.97	0.45
3:P:119:MET:HG2	3:P:158:LEU:HD21	1.98	0.45
3:P:392:ILE:CD1	3:P:402:TRP:CZ2	2.99	0.45
20:X:363:ALA:CB	20:X:379:LYS:NZ	2.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:100:TYR:HB2	20:Y:142:LEU:HD13	1.99	0.45
1:A:1114:ARG:HB2	1:A:1116:THR:HG23	1.97	0.45
6:F:130:ARG:HH11	20:Y:506:GLN:HB3	1.80	0.45
6:F:145:ASN:N	6:F:145:ASN:OD1	2.48	0.45
6:F:462:LEU:HD23	6:H:8:VAL:HG21	1.98	0.45
6:H:761:SER:O	6:H:765:ASP:CB	2.64	0.45
9:J:294:LEU:HD12	10:K:54:HIS:NE2	2.31	0.45
13:N:559:VAL:CA	13:N:562:LYS:HG2	2.45	0.45
14:O:532:VAL:HA	14:O:535:ILE:HD12	1.98	0.45
3:P:68:ALA:O	3:P:69:GLU:CB	2.64	0.45
3:P:424:ARG:HG3	3:P:424:ARG:NH1	2.30	0.45
15:Q:75:GLU:O	15:Q:76:ASP:CB	2.64	0.45
20:X:267:LEU:HD11	20:Y:59:LEU:HD13	1.97	0.45
20:Y:506:GLN:HG3	20:Y:508:ASP:OD1	2.16	0.45
1:A:23:PHE:HB2	1:A:111:LEU:HD22	1.96	0.45
1:A:1057:LEU:HA	1:A:1061:GLU:OE1	2.16	0.45
1:A:1274:LEU:HG	1:A:1302:LEU:HD11	1.99	0.45
1:A:1531:GLY:HA2	1:A:1565:LEU:HB3	1.98	0.45
2:B:16:TRP:HD1	2:B:56:HIS:CD2	2.33	0.45
3:C:180:ARG:HG3	3:C:212:LEU:HD21	1.98	0.45
3:C:409:TYR:CB	3:C:418:CYS:HB3	2.45	0.45
11:L:98:VAL:HG11	11:L:108:ILE:HD13	1.98	0.45
13:N:552:ALA:HB3	13:N:553:PRO:HD3	1.98	0.45
14:O:33:TYR:CE1	14:O:37:VAL:HG21	2.51	0.45
14:O:669:LYS:HE3	14:O:751:LEU:HD13	1.99	0.45
14:O:706:CYS:HB3	14:O:709:ARG:HB3	1.97	0.45
20:X:168:THR:HB	20:X:169:PRO:HD2	1.98	0.45
20:X:506:GLN:HG3	20:X:508:ASP:OD1	2.17	0.45
20:X:517:ASP:O	20:X:520:VAL:HG22	2.16	0.45
1:A:1276:GLU:HB3	1:A:1294:TYR:HE1	1.82	0.45
1:A:1469:CYS:HB2	1:A:1488:LEU:CD2	2.47	0.45
6:F:653:LEU:O	6:F:656:MET:HG2	2.16	0.45
8:I:70:CYS:C	8:I:71:LEU:HD12	2.37	0.45
10:K:376:LEU:HG	10:K:407:GLU:OE1	2.16	0.45
13:N:519:TYR:CD2	13:N:554:MET:SD	3.09	0.45
20:Y:222:MET:O	20:Y:226:VAL:HG23	2.16	0.45
20:Y:519:LEU:HD13	20:Y:527:GLU:CB	2.46	0.45
1:A:93:LEU:HB2	1:A:128:TRP:CH2	2.52	0.45
1:A:658:ASN:O	1:A:662:THR:HG23	2.16	0.45
1:A:1364:CYS:N	1:A:1365:PRO:CD	2.78	0.45
6:H:592:ARG:HA	6:H:592:ARG:HD3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:726:LEU:HD11	6:H:742:LEU:HD22	1.98	0.45
9:J:247:PHE:CZ	9:J:277:GLU:HG3	2.51	0.45
9:J:478:ASN:OD1	9:J:479:ALA:N	2.48	0.45
11:L:111:LEU:HD11	11:L:122:VAL:HG22	1.99	0.45
13:N:180:PHE:CE2	13:N:240:PHE:HB3	2.52	0.45
13:N:522:LEU:HD13	13:N:523:LEU:HD23	1.99	0.45
14:O:105:LEU:HD11	14:O:151:VAL:HG12	1.99	0.45
3:P:238:TYR:CB	3:P:247:ALA:HB2	2.47	0.45
20:X:212:LEU:O	20:X:213:SER:CB	2.63	0.45
20:X:294:PHE:CE1	20:X:311:TYR:CG	3.05	0.45
20:Y:77:TYR:CE1	20:Y:107:LYS:HB2	2.51	0.45
20:Y:294:PHE:CZ	20:Y:311:TYR:CG	3.04	0.45
20:Y:503:LEU:HD12	20:Y:515:LEU:HD13	1.98	0.45
1:A:1205:SER:O	1:A:1209:LEU:HG	2.17	0.45
2:B:16:TRP:O	2:B:17:VAL:HG22	2.16	0.45
3:C:30:ARG:HG3	3:C:30:ARG:O	2.16	0.45
8:I:52:PHE:HD1	8:I:743:VAL:HG21	1.81	0.45
8:I:167:LEU:HD12	8:I:168:LEU:N	2.32	0.45
10:K:349:GLU:OE1	16:R:150:LEU:HD22	2.17	0.45
13:N:122:UNK:O	13:N:126:UNK:CB	2.65	0.45
13:N:512:LYS:HG2	13:N:549:PHE:CZ	2.52	0.45
14:O:75:VAL:HG13	14:O:165:ASP:CG	2.36	0.45
14:O:114:ASP:CA	14:O:117:ASP:OD1	2.64	0.45
14:O:516:PHE:HB2	14:O:535:ILE:HD11	1.99	0.45
3:P:266:VAL:HG12	3:P:289:LEU:HD23	1.98	0.45
3:P:344:ARG:HB3	3:P:344:ARG:CZ	2.46	0.45
16:R:146:SER:N	16:R:147:PRO:HD3	2.32	0.45
16:R:416:TYR:HA	16:R:417:SER:HA	1.75	0.45
20:X:261:LEU:HD22	20:X:267:LEU:HD23	1.97	0.45
1:A:845:TYR:CD1	1:A:951:ILE:HD11	2.51	0.45
3:C:48:LEU:N	3:C:48:LEU:HD23	2.31	0.45
6:F:65:SER:N	20:Y:296:GLN:HE22	2.14	0.45
6:F:149:TRP:CZ3	6:F:152:PHE:CD2	3.05	0.45
14:O:129:THR:O	14:O:130:SER:CB	2.64	0.45
20:X:355:TYR:CB	20:X:383:LEU:CA	2.88	0.45
1:A:629:LEU:HD22	1:A:633:ILE:HG22	1.97	0.45
1:A:1236:LEU:CB	16:R:153:VAL:HG21	2.47	0.45
2:B:1:MET:HE3	13:N:650:LEU:HD22	1.98	0.45
6:H:754:HIS:CE1	6:H:755:LEU:HD13	2.52	0.45
8:I:639:LEU:HB2	8:I:652:VAL:HG12	1.98	0.45
10:K:383:ASN:HB3	10:K:386:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:11:ILE:HG23	12:M:15:ILE:CD1	2.47	0.45
13:N:76:VAL:O	13:N:80:GLN:HB3	2.17	0.45
20:X:203:LEU:HA	20:X:206:ILE:HD12	1.99	0.45
20:Y:212:LEU:O	20:Y:213:SER:CB	2.63	0.45
1:A:256:VAL:O	1:A:268:VAL:HA	2.17	0.45
1:A:1114:ARG:CD	13:N:779:MET:HG3	2.26	0.45
3:C:403:TYR:CD1	3:C:403:TYR:C	2.90	0.45
6:H:723:LEU:HG	6:H:746:VAL:HG11	1.99	0.45
8:I:245:LEU:HB3	8:I:246:PRO:HD3	1.97	0.45
10:K:19:TYR:CE1	10:K:49:LEU:HD13	2.51	0.45
10:K:185:LEU:HD21	10:K:205:PHE:HB3	1.98	0.45
10:K:509:ARG:HG3	10:K:509:ARG:O	2.16	0.45
13:N:386:LEU:HD21	13:N:399:LEU:HD22	1.99	0.45
14:O:292:GLY:HA3	14:O:336:ASP:HB3	1.99	0.45
16:R:487:ASN:OD1	16:R:490:THR:HG23	2.17	0.45
20:X:271:VAL:CG1	20:X:304:LEU:CD2	2.95	0.45
20:X:491:LYS:C	20:X:494:ASP:OD1	2.54	0.45
20:Y:343:VAL:HG13	20:Y:378:LEU:HD22	1.99	0.45
1:A:254:SER:OG	1:A:271:LEU:HB2	2.18	0.44
1:A:759:ILE:N	1:A:760:PRO:HD2	2.33	0.44
1:A:944:LEU:HD12	1:A:944:LEU:O	2.17	0.44
1:A:1480:GLU:HA	1:A:1527:MET:HB3	1.98	0.44
8:I:209:CYS:SG	8:I:584:HIS:ND1	2.87	0.44
8:I:617:ALA:O	8:I:618:ILE:HD13	2.17	0.44
9:J:322:TYR:CE1	12:M:31:ILE:HD13	2.52	0.44
10:K:284:LEU:HD12	10:K:311:MET:CE	2.48	0.44
12:M:9:GLY:HA3	3:P:329:TYR:CG	2.52	0.44
13:N:676:TRP:CZ3	13:N:684:ALA:HB2	2.51	0.44
20:X:77:TYR:CE1	20:X:107:LYS:HB2	2.52	0.44
20:X:350:PHE:HZ	20:X:378:LEU:HA	1.73	0.44
1:A:1047:VAL:O	1:A:1109:GLY:HA2	2.17	0.44
1:A:1114:ARG:HB3	13:N:779:MET:SD	2.57	0.44
1:A:1477:ALA:HB1	1:A:1574:LEU:HD12	1.99	0.44
4:D:12:VAL:O	4:D:13:THR:OG1	2.29	0.44
6:F:50:ARG:HE	6:H:19:TYR:HE1	1.66	0.44
8:I:26:LEU:CB	8:I:37:LEU:HB3	2.46	0.44
9:J:322:TYR:CZ	12:M:31:ILE:HD13	2.52	0.44
9:J:413:PHE:CD1	9:J:454:VAL:HG12	2.53	0.44
14:O:706:CYS:O	14:O:708:GLU:N	2.50	0.44
3:P:180:ARG:HG3	3:P:212:LEU:HD21	1.99	0.44
16:R:106:LYS:HA	16:R:106:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:R:160:LEU:HD12	16:R:160:LEU:O	2.18	0.44
1:A:39:LEU:CD1	14:O:248:PRO:HB3	2.47	0.44
1:A:961:HIS:ND1	1:A:964:GLU:OE2	2.51	0.44
1:A:1080:LEU:HB2	1:A:1081:PRO:HD3	2.00	0.44
4:D:54:ILE:HG12	9:J:506:LEU:HD23	1.99	0.44
8:I:73:TRP:CG	8:I:80:LEU:HD13	2.52	0.44
9:J:295:TYR:OH	10:K:54:HIS:HB2	2.17	0.44
14:O:631:GLN:OE1	14:O:640:ALA:HA	2.17	0.44
20:X:100:TYR:CB	20:X:142:LEU:CD2	2.96	0.44
20:X:235:TRP:CZ2	20:Y:59:LEU:HD11	2.53	0.44
1:A:430:VAL:HG12	1:A:444:PHE:HA	1.98	0.44
1:A:793:LEU:HD23	1:A:793:LEU:C	2.38	0.44
1:A:1191:LEU:HD11	16:R:62:HIS:HB3	1.98	0.44
6:H:110:PHE:CD2	6:H:117:THR:HG21	2.52	0.44
8:I:32:ARG:CD	13:N:388:HIS:CE1	2.99	0.44
8:I:101:LEU:HD21	8:I:168:LEU:HD11	2.00	0.44
9:J:271:HIS:O	9:J:274:THR:HG22	2.16	0.44
9:J:497:ASN:N	9:J:497:ASN:OD1	2.49	0.44
10:K:373:TYR:CE1	7:W:4:ARG:HG2	2.52	0.44
13:N:564:MET:CA	13:N:564:MET:CE	2.86	0.44
20:X:281:TYR:HB3	20:X:290:SER:OG	2.18	0.44
20:Y:336:ASP:OD1	20:Y:337:GLN:N	2.41	0.44
20:Y:437:LEU:HD22	20:Y:444:LEU:CD2	2.47	0.44
1:A:286:UNK:O	1:A:290:GLY:N	2.42	0.44
1:A:625:ILE:O	1:A:629:LEU:HG	2.17	0.44
3:C:360:LEU:HD23	12:M:14:LEU:HD13	2.00	0.44
3:C:478:GLU:OE2	3:C:490:TYR:OH	2.35	0.44
6:F:42:PHE:HB2	6:F:71:CYS:SG	2.57	0.44
6:F:67:THR:HG21	20:Y:263:LYS:HD3	2.00	0.44
10:K:145:ASN:HB3	10:K:148:LEU:HB2	1.99	0.44
10:K:509:ARG:CG	10:K:512:ASP:HB2	2.48	0.44
13:N:528:LEU:CD1	13:N:641:LEU:HD13	2.45	0.44
13:N:655:LEU:HA	13:N:724:ARG:O	2.17	0.44
20:Y:45:ALA:HB2	20:Y:82:TYR:CD2	2.52	0.44
1:A:95:VAL:HG13	1:A:100:VAL:CG2	2.46	0.44
1:A:1236:LEU:HD12	16:R:161:LEU:CD1	2.47	0.44
1:A:1399:VAL:HG11	1:A:1404:LEU:HG	1.99	0.44
3:C:60:PHE:CG	3:P:89:LEU:HD12	2.53	0.44
10:K:288:SER:HB3	12:M:57:TRP:CZ3	2.53	0.44
3:P:248:LEU:HD21	3:P:273:TYR:CZ	2.53	0.44
3:P:251:TYR:CZ	3:P:268:GLN:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:222:MET:O	20:X:226:VAL:HG23	2.18	0.44
1:A:1675:GLU:CG	1:A:1676:LEU:N	2.81	0.44
8:I:116:MET:SD	8:I:210:LEU:HG	2.58	0.44
9:J:445:GLU:CA	9:J:474:LEU:HD23	2.48	0.44
13:N:276:ARG:O	13:N:277:CYS:C	2.55	0.44
13:N:520:ARG:HG3	13:N:557:CYS:SG	2.58	0.44
14:O:215:PHE:CD1	14:O:215:PHE:C	2.90	0.44
16:R:146:SER:N	16:R:147:PRO:CD	2.81	0.44
1:A:1818:LEU:HD21	1:A:1849:LYS:HB2	1.99	0.44
3:C:416:PHE:CD2	14:O:323:ALA:HB2	2.53	0.44
9:J:297:SER:O	9:J:329:LEU:HD11	2.17	0.44
13:N:61:UNK:O	13:N:64:UNK:CB	2.65	0.44
13:N:285:PHE:O	13:N:289:PHE:CD1	2.69	0.44
13:N:292:TRP:CH2	13:N:296:VAL:HG21	2.52	0.44
13:N:400:TYR:CE1	13:N:404:ILE:HD11	2.51	0.44
14:O:127:HIS:O	14:O:128:LYS:HB3	2.17	0.44
3:P:389:ARG:HA	3:P:392:ILE:CG2	2.48	0.44
20:Y:168:THR:HB	20:Y:169:PRO:HD2	1.99	0.44
1:A:939:PHE:CZ	1:A:944:LEU:HB2	2.52	0.44
3:C:407:GLN:HA	3:C:422:TYR:OH	2.18	0.44
6:H:747:TYR:CE2	6:H:755:LEU:HD23	2.53	0.44
8:I:34:LEU:CD1	8:I:46:LEU:HD21	2.44	0.44
8:I:266:ASN:HA	8:I:526:LYS:NZ	2.33	0.44
9:J:337:TRP:HB3	9:J:360:ALA:HB2	1.98	0.44
13:N:501:ILE:HD12	13:N:501:ILE:N	2.32	0.44
13:N:509:TYR:HD2	13:N:515:PHE:CE1	2.35	0.44
13:N:562:LYS:HG3	13:N:563:ASP:OD1	2.18	0.44
13:N:681:LEU:HD22	13:N:713:PHE:CZ	2.52	0.44
14:O:657:ILE:HA	14:O:660:LYS:HB2	2.00	0.44
16:R:94:LEU:O	16:R:98:GLU:HG2	2.18	0.44
20:X:519:LEU:HD13	20:X:527:GLU:CB	2.47	0.44
20:Y:261:LEU:HD22	20:Y:267:LEU:HD23	1.99	0.44
20:Y:452:LEU:HB3	20:Y:461:ALA:HB2	2.00	0.44
1:A:39:LEU:HD12	14:O:248:PRO:HB3	1.99	0.43
1:A:1053:GLN:N	1:A:1053:GLN:OE1	2.51	0.43
1:A:1233:PRO:HA	1:A:1236:LEU:CD2	2.47	0.43
4:D:8:LEU:CD2	14:O:420:ILE:HD11	2.47	0.43
6:F:726:LEU:HD11	6:F:742:LEU:CD2	2.47	0.43
6:F:758:MET:O	6:F:762:TRP:CD1	2.70	0.43
6:H:545:HIS:HE1	11:L:182:SER:O	2.01	0.43
10:K:153:TYR:CE1	10:K:169:LEU:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:180:GLU:O	10:K:184:LEU:N	2.40	0.43
12:M:12:LEU:HD13	3:P:360:LEU:HD23	1.99	0.43
13:N:245:GLN:O	13:N:249:ARG:HG3	2.16	0.43
13:N:502:ILE:HA	13:N:505:LEU:HD12	2.00	0.43
14:O:416:GLU:O	14:O:420:ILE:HG22	2.18	0.43
14:O:643:LEU:C	14:O:643:LEU:HD23	2.38	0.43
16:R:94:LEU:HD11	16:R:161:LEU:HD21	2.00	0.43
16:R:492:ILE:HD13	16:R:492:ILE:HA	1.85	0.43
20:X:437:LEU:HD22	20:X:444:LEU:CD2	2.48	0.43
20:Y:491:LYS:C	20:Y:494:ASP:OD1	2.55	0.43
1:A:455:VAL:HB	1:A:471:VAL:HG12	2.00	0.43
1:A:1502:PRO:O	1:A:1503:ASN:CB	2.65	0.43
1:A:1640:GLY:HA2	1:A:1644:TYR:CE1	2.54	0.43
3:C:119:MET:HG2	3:C:158:LEU:HD21	2.00	0.43
3:C:483:SER:HA	3:C:515:TYR:OH	2.18	0.43
5:E:67:LEU:HD22	20:Y:342:TRP:CH2	2.53	0.43
5:E:105:PHE:HD1	10:K:510:ARG:HD3	1.83	0.43
8:I:13:VAL:HG22	8:I:744:PHE:CE2	2.52	0.43
9:J:185:LEU:HD11	9:J:205:PHE:HB2	1.99	0.43
11:L:113:LEU:HB3	11:L:116:PRO:HG3	2.00	0.43
13:N:414:MET:SD	13:N:498:SER:HA	2.58	0.43
14:O:114:ASP:C	14:O:117:ASP:OD1	2.56	0.43
14:O:143:TYR:C	14:O:143:TYR:CD1	2.91	0.43
14:O:699:ASN:O	14:O:702:ALA:HB3	2.17	0.43
20:X:201:LEU:O	20:X:203:LEU:N	2.52	0.43
20:X:294:PHE:CD1	20:X:311:TYR:CE1	3.06	0.43
20:Y:417:TYR:CD2	20:Y:429:MET:CE	3.01	0.43
20:Y:474:ASP:OD2	20:Y:505:ASN:ND2	2.50	0.43
1:A:93:LEU:HA	1:A:93:LEU:HD12	1.72	0.43
1:A:168:ASP:OD1	1:A:168:ASP:N	2.52	0.43
1:A:1060:HIS:O	1:A:1063:ILE:HG22	2.19	0.43
1:A:1239:THR:HG23	1:A:1241:THR:HG23	2.01	0.43
1:A:1274:LEU:HD23	1:A:1274:LEU:HA	1.87	0.43
1:A:1495:PHE:O	1:A:1499:LEU:HD13	2.19	0.43
3:C:413:LYS:O	3:C:415:PRO:CD	2.65	0.43
6:H:515:TYR:CE2	6:H:545:HIS:CD2	3.06	0.43
6:H:531:TYR:O	6:H:562:MET:HE3	2.19	0.43
6:H:553:SER:HA	6:H:576:CYS:SG	2.58	0.43
6:H:762:TRP:O	6:H:766:LEU:N	2.50	0.43
10:K:222:GLU:O	10:K:225:ASP:O	2.36	0.43
10:K:276:VAL:HA	10:K:311:MET:CE	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:13:PRO:HG3	11:L:78:CYS:SG	2.59	0.43
11:L:24:GLU:HG2	11:L:159:TYR:CE1	2.54	0.43
13:N:75:PHE:O	13:N:77:GLU:C	2.57	0.43
14:O:33:TYR:HA	14:O:161:TYR:OH	2.18	0.43
14:O:534:GLY:O	14:O:538:LEU:HD12	2.18	0.43
3:P:233:PHE:CE2	3:P:237:ILE:HD12	2.53	0.43
16:R:93:ALA:O	16:R:97:ASN:OD1	2.36	0.43
20:X:142:LEU:HD23	20:X:142:LEU:HA	1.85	0.43
20:X:503:LEU:HD12	20:X:515:LEU:HD13	1.99	0.43
20:Y:452:LEU:HG	20:Y:457:THR:OG1	2.18	0.43
1:A:1755:CYS:O	1:A:1768:LEU:HD21	2.18	0.43
3:C:153:GLU:O	3:C:157:GLU:HG2	2.17	0.43
6:F:128:THR:O	6:F:129:ASP:CB	2.66	0.43
6:H:531:TYR:O	6:H:562:MET:CE	2.66	0.43
6:H:726:LEU:HD11	6:H:742:LEU:CD2	2.48	0.43
9:J:42:TRP:CE3	9:J:42:TRP:HA	2.52	0.43
9:J:308:TYR:OH	12:M:27:GLU:O	2.24	0.43
10:K:185:LEU:HD21	10:K:205:PHE:HB2	2.00	0.43
3:P:36:LEU:HD21	3:P:58:LEU:CB	2.48	0.43
20:X:350:PHE:HZ	20:X:377:LEU:O	2.01	0.43
1:A:1191:LEU:HD12	16:R:59:VAL:HA	1.99	0.43
2:B:16:TRP:CZ3	2:B:42:ASP:N	2.83	0.43
6:F:563:ASP:OD1	6:F:564:LYS:O	2.37	0.43
9:J:19:TYR:CE1	9:J:49:LEU:HD13	2.53	0.43
13:N:102:UNK:HA	13:N:107:UNK:C	2.48	0.43
13:N:180:PHE:CG	13:N:299:TRP:CH2	2.86	0.43
13:N:304:PHE:CD1	13:N:324:TRP:HH2	2.37	0.43
14:O:652:LEU:HA	14:O:660:LYS:HG3	2.00	0.43
3:P:48:LEU:N	3:P:48:LEU:HD23	2.32	0.43
3:P:297:ILE:HG21	3:P:330:ARG:NH2	2.34	0.43
20:X:417:TYR:CD2	20:X:429:MET:CE	3.01	0.43
20:X:452:LEU:HG	20:X:457:THR:OG1	2.19	0.43
1:A:1191:LEU:HD21	16:R:62:HIS:CE1	2.53	0.43
1:A:1623:ASP:O	1:A:1624:VAL:HB	2.18	0.43
1:A:1699:VAL:HG23	1:A:1699:VAL:O	2.18	0.43
6:F:98:ASN:OD1	6:F:98:ASN:N	2.52	0.43
6:H:496:TYR:CE1	6:H:505:ILE:HD11	2.54	0.43
10:K:217:GLU:O	10:K:218:THR:OG1	2.20	0.43
10:K:497:ASN:OD1	10:K:497:ASN:N	2.51	0.43
13:N:655:LEU:HD12	13:N:724:ARG:O	2.18	0.43
14:O:64:LEU:HD12	14:O:65:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:294:PHE:CE2	20:X:311:TYR:CB	3.00	0.43
20:X:452:LEU:HB3	20:X:461:ALA:HB2	2.00	0.43
20:X:496:ILE:HD13	20:X:519:LEU:HD23	1.99	0.43
20:Y:549:MET:O	20:Y:552:MET:HG3	2.19	0.43
1:A:215:HIS:CD2	1:A:217:LEU:H	2.36	0.43
1:A:659:LEU:HD12	1:A:659:LEU:C	2.38	0.43
1:A:1333:HIS:HB2	1:A:1357:THR:HA	2.01	0.43
6:H:550:VAL:HG13	6:H:551:ALA:N	2.34	0.43
6:H:639:TYR:CZ	6:H:643:MET:SD	3.12	0.43
9:J:465:LEU:HG	9:J:488:ILE:HD11	2.01	0.43
10:K:208:LYS:O	10:K:211:LYS:HG2	2.19	0.43
10:K:227:LEU:O	10:K:230:ASN:N	2.52	0.43
10:K:355:ALA:O	10:K:359:THR:HG22	2.19	0.43
10:K:496:GLU:HB2	10:K:526:TYR:CE1	2.51	0.43
13:N:340:ARG:CB	13:N:361:LEU:HD13	2.49	0.43
13:N:409:VAL:O	13:N:410:ILE:CG1	2.66	0.43
13:N:612:PRO:HB3	13:N:665:VAL:HG23	2.00	0.43
13:N:774:TYR:CZ	13:N:778:ARG:HD3	2.54	0.43
20:X:309:ASP:OD1	20:X:343:VAL:HG11	2.19	0.43
20:X:474:ASP:OD2	20:X:505:ASN:ND2	2.50	0.43
1:A:105:GLY:O	1:A:111:LEU:HG	2.19	0.43
1:A:173:LEU:HA	1:A:174:PRO:HD2	1.89	0.43
1:A:591:VAL:O	1:A:591:VAL:HG23	2.18	0.43
1:A:593:ASN:OD1	1:A:609:ILE:O	2.37	0.43
8:I:73:TRP:CZ3	8:I:95:VAL:HG21	2.54	0.43
8:I:276:TRP:CE2	8:I:476:GLY:HA2	2.54	0.43
10:K:338:ILE:HG23	10:K:342:HIS:CE1	2.53	0.43
13:N:75:PHE:CG	13:N:79:LEU:HD23	2.53	0.43
13:N:354:SER:O	13:N:357:ALA:HB3	2.19	0.43
13:N:559:VAL:HA	13:N:562:LYS:CD	2.49	0.43
13:N:699:TRP:CB	13:N:705:LEU:HD23	2.42	0.43
14:O:359:VAL:HG13	14:O:360:LEU:HD12	1.99	0.43
7:W:14:ASP:OD1	7:W:14:ASP:N	2.52	0.43
20:X:99:LYS:HD3	20:X:102:MET:CE	2.49	0.43
20:Y:334:ILE:HG13	20:Y:335:SER:N	2.34	0.43
20:Y:552:MET:SD	20:Y:552:MET:C	2.97	0.43
1:A:1160:TYR:OH	14:O:337:HIS:ND1	2.44	0.43
2:B:16:TRP:NE1	2:B:46:LEU:CD2	2.80	0.43
3:C:510:SER:HB3	3:C:539:PHE:HB2	2.01	0.43
4:D:18:PHE:CE1	4:D:20:LEU:HD11	2.53	0.43
6:H:707:PHE:CD1	6:H:707:PHE:C	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:129:LYS:O	9:J:132:ILE:HG22	2.19	0.43
9:J:477:GLN:O	9:J:508:LEU:HD13	2.19	0.43
10:K:155:GLU:O	10:K:159:LEU:HD13	2.19	0.43
11:L:88:SER:HA	11:L:145:HIS:O	2.19	0.43
13:N:345:PHE:CD1	13:N:345:PHE:C	2.91	0.43
14:O:75:VAL:HG13	14:O:165:ASP:HB2	2.00	0.43
14:O:233:PRO:HA	14:O:263:ARG:NH2	2.34	0.43
15:Q:58:ASN:OD1	15:Q:58:ASN:N	2.47	0.43
16:R:48:PHE:O	16:R:49:ILE:CG1	2.67	0.43
1:A:1313:LEU:HD13	1:A:1316:MET:HB2	1.99	0.43
6:F:745:LYS:NZ	6:F:778:ALA:HB1	2.34	0.43
9:J:214:LYS:HD2	9:J:400:GLU:OE2	2.18	0.43
11:L:45:LEU:HD23	11:L:45:LEU:C	2.39	0.43
11:L:141:VAL:HG11	11:L:151:THR:HG21	2.00	0.43
13:N:559:VAL:HG11	13:N:600:PHE:CE1	2.54	0.43
14:O:312:CYS:SG	14:O:350:LEU:HD21	2.58	0.43
3:P:405:LEU:HD23	3:P:405:LEU:HA	1.95	0.43
20:X:242:ALA:O	20:X:246:VAL:HG23	2.19	0.43
1:A:32:PRO:HD2	14:O:264:VAL:HG11	2.01	0.42
6:F:639:TYR:CD1	6:F:639:TYR:C	2.93	0.42
9:J:177:THR:HG22	9:J:180:GLU:HG2	2.01	0.42
10:K:379:GLY:HA3	10:K:411:VAL:HG22	2.01	0.42
11:L:77:LEU:HD12	11:L:77:LEU:C	2.38	0.42
11:L:108:ILE:HD12	11:L:125:THR:O	2.19	0.42
14:O:631:GLN:HB2	14:O:640:ALA:HB2	2.00	0.42
20:Y:475:TYR:CE1	20:Y:477:LYS:HB2	2.54	0.42
1:A:13:ALA:HB3	1:A:648:PRO:HB3	2.01	0.42
1:A:174:PRO:HD2	1:A:220:ILE:HD12	2.02	0.42
1:A:1074:CYS:SG	1:A:1107:LEU:CB	3.07	0.42
1:A:1145:LEU:HD23	1:A:1145:LEU:HA	1.67	0.42
1:A:1531:GLY:HA3	1:A:1566:PHE:CZ	2.55	0.42
6:H:656:MET:O	6:H:660:LYS:HG3	2.18	0.42
9:J:476:PRO:HB2	3:P:148:ASN:HD21	1.85	0.42
13:N:76:VAL:O	13:N:78:VAL:N	2.53	0.42
14:O:530:SER:O	14:O:533:THR:HG22	2.19	0.42
20:Y:52:ASN:OD1	20:Y:52:ASN:N	2.52	0.42
20:Y:294:PHE:CE1	20:Y:311:TYR:CD2	3.07	0.42
1:A:612:ILE:HG22	1:A:642:TYR:CD2	2.54	0.42
2:B:13:LEU:HD22	13:N:598:SER:HA	2.01	0.42
2:B:68:GLN:HA	2:B:69:VAL:C	2.39	0.42
3:C:414:MET:HG2	14:O:330:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:60:SER:O	5:E:63:VAL:HG12	2.19	0.42
6:F:157:GLU:HA	6:F:477:CYS:SG	2.60	0.42
6:H:42:PHE:HB2	6:H:71:CYS:SG	2.59	0.42
8:I:48:ARG:HG3	8:I:55:VAL:CG2	2.49	0.42
10:K:487:TYR:CE2	10:K:491:LEU:HD11	2.54	0.42
11:L:113:LEU:HD13	11:L:120:ILE:CD1	2.50	0.42
13:N:181:LEU:HD22	13:N:299:TRP:NE1	2.34	0.42
13:N:342:GLU:OE2	13:N:342:GLU:HA	2.20	0.42
13:N:589:PHE:O	13:N:591:VAL:HG13	2.18	0.42
3:P:306:LEU:HD12	3:P:307:LEU:N	2.35	0.42
20:X:181:LYS:HE3	20:X:370:SER:HB2	2.00	0.42
20:X:347:CYS:N	20:X:378:LEU:HD21	2.34	0.42
1:A:79:ALA:CB	1:A:89:TYR:CE1	3.03	0.42
1:A:174:PRO:O	1:A:295:UNK:O	2.38	0.42
1:A:409:ILE:CG2	1:A:410:ASP:N	2.83	0.42
1:A:971:PRO:HG2	1:A:974:VAL:HG23	2.01	0.42
1:A:1481:ASN:OD1	1:A:1482:LEU:N	2.53	0.42
1:A:1624:VAL:HG22	1:A:1698:TYR:HB3	2.01	0.42
6:F:486:ASN:O	6:F:490:HIS:ND1	2.51	0.42
13:N:386:LEU:HD12	13:N:387:LEU:HG	2.01	0.42
13:N:782:VAL:HA	13:N:788:ALA:O	2.20	0.42
14:O:751:LEU:C	14:O:751:LEU:HD12	2.40	0.42
20:X:449:THR:HG21	20:X:465:LEU:HA	2.01	0.42
20:Y:83:HIS:O	20:Y:86:SER:OG	2.20	0.42
20:Y:229:THR:CG2	20:Y:233:LEU:HD12	2.46	0.42
1:A:1375:TYR:HB3	1:A:1378:THR:CG2	2.49	0.42
2:B:11:VAL:HB	13:N:594:VAL:CG1	2.50	0.42
6:F:118:LEU:HD21	6:F:140:LYS:HB3	2.01	0.42
6:F:540:SER:OG	6:F:575:ASN:ND2	2.33	0.42
8:I:224:SER:HB3	8:I:229:SER:HA	1.98	0.42
10:K:163:CYS:O	10:K:163:CYS:SG	2.77	0.42
10:K:406:HIS:ND1	7:W:6:PRO:HB3	2.35	0.42
10:K:465:LEU:HD23	10:K:465:LEU:HA	1.95	0.42
12:M:10:ARG:HD2	12:M:11:ILE:HD12	2.00	0.42
14:O:583:VAL:O	14:O:587:VAL:HG23	2.19	0.42
3:P:161:LEU:HD23	3:P:166:GLU:HB2	2.01	0.42
3:P:242:GLN:NE2	3:P:429:ARG:HA	2.33	0.42
20:X:294:PHE:CE1	20:X:311:TYR:CD1	3.08	0.42
20:X:355:TYR:HD1	20:X:382:ALA:CA	2.26	0.42
1:A:248:PHE:CB	1:A:430:VAL:HG22	2.49	0.42
1:A:1281:PRO:HB3	1:A:1352:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1552:TYR:CE2	1:A:1596:SER:HA	2.55	0.42
2:B:43:ASP:N	13:N:630:LYS:HE3	2.21	0.42
6:H:121:LEU:HG	6:H:125:TYR:CE1	2.54	0.42
6:H:128:THR:O	6:H:129:ASP:CB	2.67	0.42
8:I:719:ALA:HA	8:I:735:SER:HA	2.01	0.42
13:N:241:HIS:CE1	13:N:302:LYS:HE2	2.54	0.42
13:N:265:LEU:HD23	13:N:265:LEU:C	2.39	0.42
13:N:273:MET:HE3	13:N:332:PHE:CE1	2.55	0.42
13:N:395:ASP:OD1	13:N:398:THR:CB	2.68	0.42
20:X:269:ASP:HB3	20:X:300:LEU:HD21	2.02	0.42
20:X:359:LEU:HB2	20:X:383:LEU:HG	2.01	0.42
3:C:389:ARG:HD3	3:C:389:ARG:HA	1.77	0.42
6:H:98:ASN:OD1	6:H:98:ASN:N	2.53	0.42
6:H:486:ASN:O	6:H:490:HIS:HD2	2.01	0.42
6:H:674:HIS:O	6:H:678:VAL:HG23	2.20	0.42
8:I:717:MET:HG3	8:I:719:ALA:HB2	2.00	0.42
9:J:532:ALA:HB2	3:P:443:TYR:OH	2.20	0.42
13:N:434:THR:O	13:N:437:GLN:N	2.52	0.42
13:N:571:ASN:HA	13:N:574:ILE:HG22	2.01	0.42
13:N:700:LEU:HD13	13:N:707:GLU:HG3	2.01	0.42
14:O:378:SER:OG	14:O:409:HIS:CD2	2.72	0.42
3:P:170:PHE:O	3:P:173:TYR:HB3	2.19	0.42
20:Y:134:SER:N	20:Y:137:GLU:OE1	2.53	0.42
20:Y:169:PRO:HG3	20:Y:198:GLN:OE1	2.20	0.42
20:Y:271:VAL:CG1	20:Y:304:LEU:CD2	2.96	0.42
1:A:184:LYS:O	1:A:185:TYR:CB	2.67	0.42
1:A:246:ILE:O	1:A:246:ILE:HG23	2.19	0.42
1:A:1351:GLN:CG	11:L:36:CYS:HB3	2.50	0.42
1:A:1513:GLU:HB2	1:A:1554:PHE:CE2	2.55	0.42
1:A:1632:ALA:O	1:A:1653:ALA:CB	2.68	0.42
7:G:23:ARG:CG	9:J:525:MET:HE1	2.49	0.42
8:I:32:ARG:HB2	8:I:34:LEU:CD2	2.49	0.42
8:I:355:GLY:O	8:I:359:LEU:HB2	2.20	0.42
8:I:397:ILE:HD12	14:O:440:GLN:HG3	2.01	0.42
9:J:281:ALA:CA	9:J:311:MET:HE1	2.50	0.42
9:J:320:ARG:HD3	9:J:344:PHE:CE1	2.55	0.42
9:J:500:ASP:O	9:J:504:THR:HG23	2.20	0.42
13:N:88:SER:O	13:N:89:PRO:C	2.57	0.42
13:N:139:UNK:C	13:N:141:UNK:N	2.83	0.42
14:O:423:ALA:O	14:O:426:THR:HG23	2.19	0.42
14:O:657:ILE:CD1	14:O:704:VAL:HG23	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:294:PHE:CZ	20:X:311:TYR:CG	3.08	0.42
20:Y:242:ALA:O	20:Y:246:VAL:HG23	2.20	0.42
1:A:1236:LEU:HB3	16:R:153:VAL:HG21	2.02	0.42
1:A:1621:PRO:HA	1:A:1697:LEU:O	2.20	0.42
3:C:115:TYR:OH	3:C:161:LEU:CD1	2.68	0.42
3:C:477:HIS:CD2	3:C:482:GLU:OE1	2.73	0.42
8:I:90:ILE:HD12	8:I:106:VAL:HG11	2.01	0.42
11:L:89:TYR:CD2	11:L:152:HIS:CE1	3.08	0.42
13:N:393:THR:HG21	13:N:434:THR:HG22	2.01	0.42
14:O:127:HIS:O	14:O:128:LYS:CB	2.68	0.42
14:O:751:LEU:HD12	14:O:752:ILE:N	2.35	0.42
3:P:192:PHE:CB	3:P:209:LEU:HD13	2.50	0.42
3:P:308:TYR:CD1	3:P:343:LEU:HG	2.54	0.42
3:P:402:TRP:CE3	3:P:424:ARG:HG2	2.55	0.42
20:X:334:ILE:HG13	20:X:335:SER:N	2.35	0.42
20:X:414:ILE:HD11	20:X:451:CYS:SG	2.59	0.42
20:Y:373:VAL:HG12	20:Y:402:LEU:HB2	2.01	0.42
20:Y:430:ALA:HA	20:Y:433:VAL:HG12	2.01	0.42
1:A:174:PRO:CA	1:A:295:UNK:O	2.67	0.42
1:A:844:ILE:HD11	1:A:873:VAL:HG13	2.01	0.42
1:A:1276:GLU:CD	1:A:1294:TYR:OH	2.58	0.42
1:A:1487:CYS:SG	1:A:1488:LEU:N	2.92	0.42
3:C:358:LEU:O	3:C:362:PRO:CA	2.63	0.42
6:H:104:ASP:OD1	6:H:105:ASP:N	2.53	0.42
8:I:32:ARG:HB2	8:I:34:LEU:HD22	2.02	0.42
8:I:175:ILE:HG22	8:I:176:LEU:N	2.35	0.42
9:J:69:TYR:O	9:J:70:GLU:CB	2.68	0.42
9:J:245:CYS:HA	9:J:247:PHE:CE1	2.55	0.42
14:O:538:LEU:HD12	14:O:538:LEU:H	1.85	0.42
3:P:478:GLU:OE2	3:P:490:TYR:OH	2.38	0.42
15:Q:274:UNK:O	15:Q:275:UNK:CB	2.68	0.42
16:R:177:ARG:HD3	16:R:179:LEU:HD21	2.02	0.42
20:X:53:VAL:HG23	20:X:86:SER:HB3	2.02	0.42
20:Y:53:VAL:HG23	20:Y:86:SER:HB3	2.02	0.42
20:Y:291:VAL:CG2	20:Y:314:LEU:HD13	2.50	0.42
1:A:12:ILE:HD11	1:A:506:VAL:HG12	2.02	0.41
1:A:627:PHE:CD1	1:A:627:PHE:C	2.92	0.41
1:A:1532:ASN:O	1:A:1533:LEU:C	2.58	0.41
3:C:26:PHE:O	3:C:27:SER:CB	2.67	0.41
3:C:306:LEU:HD12	3:C:307:LEU:N	2.34	0.41
6:H:481:CYS:O	6:H:485:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:247:PHE:HB3	10:K:278:LEU:HD21	2.02	0.41
11:L:125:THR:CA	11:L:126:ASP:HB3	2.44	0.41
14:O:216:LEU:HD22	14:O:256:LEU:CD1	2.49	0.41
16:R:193:ILE:HD11	16:R:455:VAL:CG1	2.49	0.41
20:X:440:ASN:HA	20:X:471:GLN:HE22	1.85	0.41
1:A:1208:LEU:O	1:A:1212:VAL:HG23	2.20	0.41
1:A:1584:LEU:HD23	1:A:1584:LEU:HA	1.91	0.41
3:C:53:LYS:HD2	3:P:93:TYR:CD1	2.55	0.41
3:C:151:LEU:HB3	3:C:182:LEU:HD11	2.02	0.41
3:C:283:LEU:HD13	3:C:306:LEU:HD11	2.03	0.41
3:C:521:PHE:HD1	3:C:553:ILE:HG22	1.82	0.41
4:D:54:ILE:HD12	3:P:389:ARG:CZ	2.50	0.41
6:F:58:TYR:OH	6:F:87:GLU:OE2	2.35	0.41
8:I:231:VAL:CG1	8:I:556:LEU:HD12	2.50	0.41
8:I:685:PHE:HA	8:I:701:PRO:HD3	2.02	0.41
13:N:350:ASP:HB3	13:N:351:PHE:HA	2.02	0.41
13:N:556:PHE:CG	13:N:600:PHE:CD1	3.08	0.41
13:N:630:LYS:HB3	13:N:633:ARG:HD2	2.02	0.41
14:O:711:ARG:HA	14:O:740:LEU:HD12	2.03	0.41
16:R:493:ARG:HD3	16:R:493:ARG:C	2.40	0.41
20:Y:80:LEU:HD23	20:Y:80:LEU:HA	1.94	0.41
1:A:28:CYS:SG	1:A:101:ILE:HD12	2.60	0.41
1:A:88:ASP:O	1:A:594:ARG:NH2	2.53	0.41
1:A:94:TYR:O	1:A:100:VAL:HA	2.19	0.41
1:A:487:THR:OG1	1:A:499:LEU:HD11	2.20	0.41
1:A:1390:PRO:HG3	1:A:1396:LEU:HD23	2.02	0.41
1:A:1800:LEU:CD1	1:A:1811:LEU:HD21	2.49	0.41
4:D:40:TRP:CE2	4:D:44:ILE:HD11	2.55	0.41
11:L:22:VAL:HG12	11:L:161:PRO:HA	2.01	0.41
12:M:2:ASP:CG	12:M:3:SER:N	2.74	0.41
12:M:60:LEU:N	12:M:60:LEU:HD23	2.35	0.41
13:N:123:UNK:CB	13:N:124:PRO:HD3	2.50	0.41
13:N:359:GLU:O	13:N:362:LYS:HB3	2.20	0.41
3:P:96:VAL:N	3:P:97:LYS:HA	2.35	0.41
3:P:115:TYR:OH	3:P:161:LEU:CD1	2.68	0.41
20:X:134:SER:N	20:X:137:GLU:OE1	2.53	0.41
20:X:350:PHE:CE2	20:X:378:LEU:HD12	2.56	0.41
1:A:1512:LEU:HD23	1:A:1512:LEU:HA	1.90	0.41
3:C:409:TYR:HB2	3:C:418:CYS:CB	2.50	0.41
6:F:473:TYR:CD1	6:F:473:TYR:C	2.94	0.41
6:H:731:GLN:HE22	20:X:186:ARG:HG3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:69:TYR:O	9:J:70:GLU:HB3	2.21	0.41
10:K:203:PHE:HE1	10:K:218:THR:HB	1.85	0.41
13:N:668:LEU:O	13:N:671:GLN:HB3	2.21	0.41
14:O:68:LEU:HD23	14:O:131:VAL:HG12	2.02	0.41
14:O:462:ASN:O	14:O:463:THR:OG1	2.27	0.41
14:O:657:ILE:HG22	14:O:660:LYS:HE2	2.02	0.41
3:P:283:LEU:HD13	3:P:306:LEU:HD11	2.02	0.41
20:Y:437:LEU:HB2	20:Y:444:LEU:HD11	2.02	0.41
1:A:188:LEU:HD12	1:A:189:PHE:N	2.36	0.41
1:A:1839:PHE:CE1	1:A:1840:MET:HG3	2.55	0.41
1:A:1885:LEU:HD23	1:A:1885:LEU:O	2.20	0.41
3:C:85:ASP:OD2	3:P:33:LYS:NZ	2.52	0.41
8:I:44:VAL:C	8:I:45:LEU:HD12	2.40	0.41
8:I:359:LEU:O	8:I:363:LEU:HG	2.21	0.41
8:I:618:ILE:HG23	8:I:705:MET:HE2	2.01	0.41
10:K:71:ALA:HA	10:K:128:ILE:HD13	2.02	0.41
10:K:129:LYS:O	10:K:133:CYS:SG	2.66	0.41
10:K:195:ASN:OD1	10:K:195:ASN:N	2.54	0.41
13:N:393:THR:HG23	13:N:434:THR:HG22	2.02	0.41
13:N:560:MET:O	13:N:564:MET:HG2	2.21	0.41
14:O:89:LEU:HD12	14:O:89:LEU:HA	1.90	0.41
3:P:89:LEU:HD21	3:P:93:TYR:CE2	2.56	0.41
20:X:243:TYR:O	20:X:246:VAL:HB	2.21	0.41
20:X:316:ALA:HB1	20:X:351:TYR:CD1	2.56	0.41
20:X:350:PHE:HD1	20:X:382:ALA:HA	1.79	0.41
1:A:248:PHE:CD1	1:A:248:PHE:C	2.93	0.41
1:A:592:HIS:O	1:A:592:HIS:CD2	2.74	0.41
2:B:14:TRP:CZ3	2:B:41:GLY:CA	3.04	0.41
3:C:60:PHE:HA	3:P:85:ASP:OD1	2.21	0.41
3:C:94:PHE:O	3:C:97:LYS:HB2	2.21	0.41
6:F:130:ARG:CD	20:Y:506:GLN:HB2	2.51	0.41
9:J:61:ARG:NH1	9:J:92:VAL:HG22	2.35	0.41
10:K:174:HIS:CE1	10:K:211:LYS:CD	3.03	0.41
10:K:242:TYR:CD2	10:K:242:TYR:C	2.94	0.41
13:N:351:PHE:HB2	13:N:354:SER:OG	2.21	0.41
13:N:560:MET:CE	13:N:601:TRP:CD1	3.04	0.41
13:N:619:LEU:HD13	13:N:619:LEU:O	2.20	0.41
13:N:663:GLN:HE22	13:N:698:VAL:CG1	2.33	0.41
3:P:94:PHE:O	3:P:97:LYS:HB2	2.21	0.41
3:P:352:LEU:HD23	3:P:352:LEU:C	2.41	0.41
16:R:282:THR:HA	16:R:291:LEU:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:349:SER:CB	20:X:358:ALA:HB2	2.44	0.41
1:A:1332:GLY:O	1:A:1358:LEU:HB2	2.20	0.41
1:A:1571:ARG:NH1	1:A:1694:ASP:O	2.54	0.41
3:C:388:TYR:CB	3:C:405:LEU:HD13	2.48	0.41
3:C:478:GLU:OE2	3:C:490:TYR:CZ	2.74	0.41
6:F:89:GLU:CD	6:F:130:ARG:NH2	2.72	0.41
6:H:707:PHE:CZ	6:H:738:LEU:HD21	2.55	0.41
6:H:747:TYR:CD2	6:H:755:LEU:HB3	2.55	0.41
8:I:28:TRP:HZ3	8:I:33:ASP:O	2.03	0.41
8:I:264:TYR:O	8:I:268:SER:OG	2.22	0.41
9:J:306:GLY:HA3	9:J:323:LEU:HD13	2.02	0.41
10:K:167:PHE:CE1	10:K:171:THR:HG21	2.55	0.41
10:K:305:VAL:HG22	12:M:57:TRP:CE3	2.56	0.41
13:N:91:PHE:CE1	13:N:122:UNK:CB	3.04	0.41
13:N:602:PRO:N	13:N:603:PRO:HD2	2.34	0.41
14:O:394:THR:HA	14:O:615:ARG:NH1	2.35	0.41
3:P:248:LEU:HD21	3:P:273:TYR:CE1	2.56	0.41
16:R:484:SER:CB	16:R:485:VAL:CA	2.98	0.41
20:X:343:VAL:HG13	20:X:378:LEU:HD22	2.02	0.41
20:X:430:ALA:HA	20:X:433:VAL:HG12	2.01	0.41
20:Y:321:LEU:HD21	20:Y:351:TYR:CB	2.51	0.41
20:Y:377:LEU:HD12	20:Y:377:LEU:C	2.41	0.41
1:A:1110:ARG:HG2	1:A:1117:THR:HG22	2.02	0.41
1:A:1864:GLY:HA2	1:A:1867:CYS:SG	2.60	0.41
6:H:16:LEU:HD21	6:H:47:CYS:SG	2.61	0.41
13:N:639:HIS:CD2	13:N:661:PRO:HB2	2.56	0.41
20:X:63:LEU:HD22	20:Y:266:LEU:HB3	2.02	0.41
20:Y:203:LEU:HA	20:Y:206:ILE:HD12	2.01	0.41
20:Y:331:LEU:HD12	20:Y:344:VAL:HG11	2.03	0.41
1:A:257:MET:HE1	1:A:444:PHE:CZ	2.56	0.41
1:A:273:ARG:O	1:A:274:VAL:CB	2.69	0.41
1:A:466:LEU:HD12	1:A:466:LEU:N	2.36	0.41
1:A:613:ALA:O	1:A:614:THR:CB	2.69	0.41
1:A:1493:LYS:O	1:A:1497:THR:HG23	2.21	0.41
2:B:17:VAL:N	2:B:30:PHE:HB3	2.35	0.41
3:C:91:LYS:O	3:C:94:PHE:HB3	2.21	0.41
3:C:200:PRO:O	3:C:201:LEU:HB2	2.21	0.41
3:C:233:PHE:CE1	3:C:237:ILE:CD1	3.04	0.41
6:H:639:TYR:OH	6:H:643:MET:SD	2.64	0.41
8:I:17:LYS:CE	8:I:51:SER:O	2.69	0.41
8:I:65:GLY:O	8:I:84:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:238:THR:HG22	8:I:548:MET:SD	2.61	0.41
8:I:276:TRP:O	8:I:279:ILE:HG22	2.21	0.41
8:I:276:TRP:CZ2	8:I:476:GLY:HA3	2.56	0.41
9:J:167:PHE:HA	9:J:170:LEU:CD2	2.50	0.41
9:J:441:VAL:HG21	9:J:444:TRP:CD1	2.45	0.41
10:K:63:ARG:HB2	10:K:65:LEU:HD13	2.03	0.41
10:K:391:PHE:CE2	10:K:411:VAL:HG21	2.56	0.41
10:K:514:PHE:CZ	7:W:11:LEU:HD22	2.56	0.41
13:N:78:VAL:C	13:N:80:GLN:N	2.74	0.41
13:N:509:TYR:HD2	13:N:515:PHE:HE1	1.65	0.41
13:N:574:ILE:HG13	13:N:625:LYS:HE2	2.03	0.41
13:N:644:VAL:HG21	13:N:664:ALA:HB2	2.03	0.41
13:N:659:VAL:HG23	13:N:728:VAL:CG2	2.51	0.41
3:P:395:ASN:OD1	3:P:395:ASN:N	2.54	0.41
16:R:188:PHE:HA	16:R:443:LEU:HD22	2.02	0.41
20:X:50:HIS:HA	20:X:53:VAL:HG22	2.02	0.41
20:X:52:ASN:OD1	20:X:52:ASN:N	2.54	0.41
20:X:437:LEU:HB2	20:X:444:LEU:HD11	2.02	0.41
20:X:456:VAL:HG12	20:X:456:VAL:O	2.21	0.41
20:Y:349:SER:HA	20:Y:352:SER:OG	2.21	0.41
20:Y:366:ILE:HD11	20:Y:379:LYS:CE	2.51	0.41
1:A:155:GLN:HE22	1:A:160:ASN:ND2	2.19	0.41
1:A:257:MET:HA	1:A:267:SER:O	2.21	0.41
1:A:259:TYR:OH	1:A:424:ALA:O	2.17	0.41
1:A:1190:THR:HG23	1:A:1191:LEU:N	2.35	0.41
2:B:17:VAL:CA	2:B:30:PHE:HB2	2.48	0.41
2:B:69:VAL:HG12	2:B:70:GLN:N	2.36	0.41
3:C:66:PRO:HD2	3:C:68:ALA:O	2.21	0.41
4:D:17:TRP:O	4:D:18:PHE:HB3	2.20	0.41
5:E:67:LEU:HD13	20:Y:342:TRP:CZ3	2.56	0.41
6:F:8:VAL:HG21	6:H:462:LEU:HD23	2.03	0.41
6:F:90:GLN:OE1	20:Y:292:LEU:HG	2.20	0.41
6:H:621:LEU:HD13	6:H:625:ARG:NH2	2.36	0.41
10:K:248:LYS:HB2	10:K:438:GLU:OE2	2.20	0.41
10:K:384:SER:HB2	10:K:415:ASN:ND2	2.33	0.41
11:L:63:LEU:HD13	11:L:138:GLN:NE2	2.36	0.41
20:X:321:LEU:HD21	20:X:351:TYR:CB	2.51	0.41
20:X:349:SER:HA	20:X:352:SER:OG	2.21	0.41
20:X:362:GLY:C	20:X:379:LYS:HD2	2.41	0.41
20:X:397:ARG:O	20:X:400:ILE:HG12	2.21	0.41
20:X:408:ASP:O	20:X:411:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:496:ILE:CD1	20:Y:519:LEU:HD23	2.50	0.41
1:A:86:ASP:OD2	14:O:563:LEU:HD13	2.21	0.40
1:A:1369:LEU:HD23	1:A:1369:LEU:HA	1.84	0.40
3:C:161:LEU:HD23	3:C:166:GLU:HB2	2.03	0.40
6:H:73:TYR:HD1	6:H:117:THR:HG22	1.82	0.40
8:I:174:ASN:OD1	8:I:174:ASN:N	2.54	0.40
10:K:500:ASP:O	10:K:504:THR:HG23	2.21	0.40
11:L:44:GLN:HA	11:L:47:ASP:CG	2.41	0.40
13:N:259:GLU:O	13:N:263:THR:HG23	2.20	0.40
13:N:597:SER:OG	13:N:600:PHE:HB2	2.20	0.40
20:X:475:TYR:CE1	20:X:477:LYS:HB2	2.56	0.40
1:A:75:GLN:O	1:A:76:LEU:HD12	2.21	0.40
1:A:133:ILE:O	1:A:133:ILE:HD12	2.21	0.40
1:A:799:LEU:O	1:A:801:PRO:CD	2.69	0.40
1:A:1610:TYR:CD1	1:A:1610:TYR:C	2.94	0.40
3:C:68:ALA:O	3:C:69:GLU:CB	2.69	0.40
3:C:379:LYS:HG3	16:R:61:PHE:CE1	2.56	0.40
6:F:550:VAL:HG13	6:F:551:ALA:N	2.37	0.40
8:I:28:TRP:NE1	8:I:723:ALA:O	2.54	0.40
9:J:180:GLU:OE1	9:J:180:GLU:CA	2.69	0.40
9:J:432:ILE:HD11	9:J:444:TRP:NE1	2.36	0.40
11:L:25:ILE:HD11	11:L:74:VAL:HG12	2.02	0.40
11:L:86:ASP:HB2	11:L:90:THR:OG1	2.21	0.40
13:N:344:LEU:HD22	13:N:374:LEU:HD21	2.04	0.40
14:O:266:ASP:CB	14:O:269:SER:HB3	2.51	0.40
14:O:467:ALA:HB1	14:O:506:LEU:CD1	2.47	0.40
14:O:587:VAL:O	14:O:590:LEU:HB2	2.21	0.40
20:X:214:VAL:HG12	20:X:217:ALA:CB	2.51	0.40
20:X:350:PHE:CE2	20:X:378:LEU:HA	2.55	0.40
1:A:75:GLN:C	1:A:76:LEU:HD12	2.42	0.40
1:A:248:PHE:CG	1:A:249:LEU:N	2.88	0.40
1:A:435:ASP:HB2	1:A:501:THR:HG22	2.04	0.40
1:A:657:TRP:CD1	1:A:785:SER:OG	2.74	0.40
1:A:777:THR:O	14:O:594:SER:O	2.39	0.40
1:A:1405:LEU:HD12	1:A:1405:LEU:C	2.41	0.40
6:F:522:PHE:CB	6:F:539:TYR:CD1	3.04	0.40
6:H:146:PRO:CG	6:H:167:THR:HA	2.50	0.40
8:I:349:ILE:HG23	8:I:404:LEU:HD21	2.04	0.40
10:K:263:PHE:CD2	10:K:291:LEU:HD21	2.55	0.40
11:L:46:ARG:NH1	11:L:156:ILE:O	2.54	0.40
13:N:394:CYS:C	13:N:395:ASP:CG	2.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:409:VAL:C	13:N:410:ILE:HG13	2.42	0.40
14:O:614:TYR:CD1	14:O:614:TYR:N	2.90	0.40
16:R:131:SER:HB2	16:R:132:LEU:HA	2.03	0.40
1:A:961:HIS:HA	1:A:964:GLU:HG3	2.02	0.40
1:A:1265:ALA:HB2	1:A:1309:HIS:HD2	1.84	0.40
1:A:1352:ILE:HD12	11:L:32:SER:HB3	2.04	0.40
1:A:1770:LEU:HD21	1:A:1794:ASP:OD2	2.21	0.40
1:A:1775:LEU:HD23	1:A:1776:TYR:N	2.36	0.40
1:A:1867:CYS:CB	1:A:1881:GLN:CD	2.90	0.40
6:F:610:GLU:O	6:F:614:THR:OG1	2.37	0.40
6:H:656:MET:SD	10:K:523:ILE:HD13	2.61	0.40
9:J:185:LEU:CD1	9:J:206:GLU:OE1	2.68	0.40
10:K:413:PHE:CD1	10:K:454:VAL:HG23	2.56	0.40
13:N:368:THR:CG2	13:N:369:ASP:HA	2.52	0.40
13:N:370:GLN:HE21	13:N:373:GLN:HB3	1.86	0.40
13:N:533:PHE:C	13:N:535:PRO:HD3	2.41	0.40
13:N:556:PHE:CD1	13:N:600:PHE:HD1	2.39	0.40
13:N:611:VAL:HG11	13:N:637:TRP:CZ3	2.56	0.40
14:O:291:ASN:O	14:O:336:ASP:CB	2.56	0.40
14:O:712:ASP:OD2	14:O:751:LEU:HB3	2.21	0.40
3:P:368:TRP:CE2	3:P:390:HIS:HB3	2.56	0.40
16:R:220:VAL:HG13	16:R:258:ARG:CZ	2.51	0.40
20:X:482:LYS:O	20:X:486:LEU:HD13	2.22	0.40
1:A:32:PRO:CG	14:O:264:VAL:HG11	2.52	0.40
1:A:1229:SER:OG	1:A:1235:LEU:HD23	2.21	0.40
2:B:17:VAL:HG12	2:B:30:PHE:CD2	2.57	0.40
6:F:696:ILE:CG1	6:F:705:CYS:SG	3.09	0.40
8:I:272:MET:SD	8:I:348:VAL:HG22	2.61	0.40
9:J:207:ASN:OD1	9:J:208:LYS:N	2.54	0.40
10:K:19:TYR:CD1	10:K:49:LEU:CD1	3.04	0.40
11:L:54:TRP:CD1	11:L:55:GLN:N	2.90	0.40
15:Q:104:HIS:CE1	15:Q:142:PRO:HB3	2.57	0.40
20:Y:186:ARG:O	20:Y:189:VAL:HG12	2.20	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	1354/1441 (94%)	1217 (90%)	106 (8%)	31 (2%)	6 37
2	B	83/84 (99%)	69 (83%)	8 (10%)	6 (7%)	1 16
3	C	520/597 (87%)	495 (95%)	23 (4%)	2 (0%)	34 72
3	P	485/597 (81%)	459 (95%)	25 (5%)	1 (0%)	47 81
4	D	53/121 (44%)	46 (87%)	6 (11%)	1 (2%)	8 41
5	E	54/110 (49%)	54 (100%)	0	0	100 100
6	F	494/824 (60%)	477 (97%)	11 (2%)	6 (1%)	13 50
6	H	479/824 (58%)	462 (96%)	12 (2%)	5 (1%)	15 54
7	G	23/85 (27%)	23 (100%)	0	0	100 100
7	W	23/85 (27%)	23 (100%)	0	0	100 100
8	I	722/808 (89%)	690 (96%)	28 (4%)	4 (1%)	25 65
9	J	500/620 (81%)	467 (93%)	28 (6%)	5 (1%)	15 54
10	K	489/620 (79%)	458 (94%)	26 (5%)	5 (1%)	15 54
11	L	180/185 (97%)	169 (94%)	9 (5%)	2 (1%)	14 52
12	M	55/74 (74%)	46 (84%)	9 (16%)	0	100 100
13	N	572/703 (81%)	501 (88%)	33 (6%)	38 (7%)	1 18
14	O	677/755 (90%)	645 (95%)	24 (4%)	8 (1%)	13 50
15	Q	144/162 (89%)	139 (96%)	5 (4%)	0	100 100
16	R	374/386 (97%)	334 (89%)	35 (9%)	5 (1%)	12 48
17	T	2/21 (10%)	2 (100%)	0	0	100 100
19	V	11/13 (85%)	8 (73%)	1 (9%)	2 (18%)	0 2
20	X	480/599 (80%)	462 (96%)	15 (3%)	3 (1%)	25 65
20	Y	492/599 (82%)	471 (96%)	16 (3%)	5 (1%)	15 54
All	All	8266/10313 (80%)	7717 (93%)	420 (5%)	129 (2%)	13 45

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	VAL
1	A	630	PRO
1	A	857	ALA
1	A	860	TYR
1	A	1125	ILE
2	B	15	LEU
2	B	17	VAL
6	F	147	PHE
6	F	493	SER
6	H	493	SER
8	I	489	PRO
8	I	503	ASN
9	J	221	PRO
10	K	211	LYS
10	K	215	PRO
13	N	74	TRP
13	N	75	PHE
13	N	78	VAL
13	N	79	LEU
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	530	GLN
13	N	606	ASP
13	N	674	ALA
13	N	716	ILE
16	R	153	VAL
16	R	223	CYS
19	V	328	VAL
20	X	213	SER
20	Y	201	LEU
20	Y	213	SER
1	A	1099	PRO
1	A	1307	LEU

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Mol	Chain	Res	Type
1	A	1314	ILE
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	278	ARG
13	N	350	ASP
13	N	353	ASP
13	N	512	LYS
13	N	595	ILE
13	N	672	ASP
16	R	384	ASN
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	531	PHE
13	N	550	GLY
13	N	629	LEU
14	O	126	VAL
14	O	555	ASN
14	O	707	LYS
3	P	415	PRO
16	R	154	SER
19	V	327	SER
20	X	202	ALA
1	A	653	TYR
1	A	781	GLU
1	A	1055	PRO
1	A	1283	PRO

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Mol	Chain	Res	Type
1	A	1422	ASN
1	A	1503	ASN
2	B	18	ALA
4	D	23	PRO
6	F	145	ASN
6	H	145	ASN
13	N	76	VAL
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
1	A	1624	VAL
1	A	1822	SER
3	C	228	TRP
6	H	96	VAL
9	J	398	ALA
13	N	282	GLU
16	R	227	ASN
9	J	397	ILE
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

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Mol	Chain	Res	Type
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	1150/1206 (95%)	988 (86%)	162 (14%)	3 19
2	B	65/75 (87%)	54 (83%)	11 (17%)	2 13
3	C	452/520 (87%)	399 (88%)	53 (12%)	5 23
3	P	422/520 (81%)	373 (88%)	49 (12%)	5 24
4	D	46/115 (40%)	41 (89%)	5 (11%)	6 26
5	E	47/89 (53%)	37 (79%)	10 (21%)	1 7
6	F	407/729 (56%)	367 (90%)	40 (10%)	8 29
6	H	408/729 (56%)	372 (91%)	36 (9%)	10 34
7	G	22/77 (29%)	20 (91%)	2 (9%)	9 32
7	W	23/77 (30%)	22 (96%)	1 (4%)	29 55
8	I	620/730 (85%)	572 (92%)	48 (8%)	13 39
9	J	424/546 (78%)	368 (87%)	56 (13%)	4 20
10	K	423/549 (77%)	380 (90%)	43 (10%)	7 28
11	L	155/170 (91%)	140 (90%)	15 (10%)	8 29
12	M	55/67 (82%)	44 (80%)	11 (20%)	1 8
13	N	516/526 (98%)	459 (89%)	57 (11%)	6 25
14	O	578/651 (89%)	491 (85%)	87 (15%)	3 17
15	Q	122/127 (96%)	122 (100%)	0	100 100
16	R	326/334 (98%)	295 (90%)	31 (10%)	8 30
17	T	1/2 (50%)	1 (100%)	0	100 100
19	V	10/10 (100%)	7 (70%)	3 (30%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	X	407/513 (79%)	378 (93%)	29 (7%)	14 41
20	Y	418/513 (82%)	382 (91%)	36 (9%)	10 35
All	All	7097/8875 (80%)	6312 (89%)	785 (11%)	9 25

All (785) 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
1	A	1706	LEU
1	A	1731	ARG
1	A	1744	ASP
1	A	1748	LEU
1	A	1756	LYS
1	A	1770	LEU
1	A	1775	LEU
1	A	1798	ARG
1	A	1805	MET
1	A	1806	SER
1	A	1821	PHE
1	A	1825	SER
1	A	1851	THR
1	A	1858	GLN
1	A	1869	HIS
1	A	1871	TYR

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Mol	Chain	Res	Type
1	A	1878	LEU
1	A	1882	LEU
2	B	11	VAL
2	B	14	TRP
2	B	15	LEU
2	B	16	TRP
2	B	17	VAL
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
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

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Mol	Chain	Res	Type
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	26	GLU
4	D	30	LEU
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	232	ASP
10	K	254	THR
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
13	N	787	LEU
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
16	R	44	HIS
16	R	57	TRP
16	R	89	LEU
16	R	94	LEU
16	R	99	LEU
16	R	106	LYS
16	R	127	LEU
16	R	128	PHE
16	R	132	LEU
16	R	148	TYR
16	R	150	LEU
16	R	157	SER
16	R	160	LEU
16	R	162	ARG
16	R	203	VAL
16	R	221	HIS
16	R	251	GLU
16	R	256	MET
16	R	297	MET
16	R	304	THR
16	R	310	GLN

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Mol	Chain	Res	Type
16	R	387	ILE
16	R	390	SER
16	R	407	THR
16	R	410	LEU
16	R	422	THR
16	R	463	LEU
16	R	468	LEU
16	R	470	ASP
16	R	488	LEU
16	R	492	ILE
19	V	321	PHE
19	V	326	LYS
19	V	327	SER
7	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
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

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS

Continued on next page...

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Mol	Chain	Res	Type
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	776	ASN
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	1795	GLN
1	A	1813	GLN
1	A	1892	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
11	L	152	HIS
13	N	266	HIS
13	N	370	GLN
13	N	571	ASN
13	N	639	HIS
13	N	663	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
14	O	731	ASN
3	P	50	HIS
3	P	71	GLN
3	P	236	HIS
3	P	249	GLN
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
16	R	60	ASN
16	R	438	HIS
16	R	444	HIS

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Mol	Chain	Res	Type
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 monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	20
13	N	10
16	R	5
15	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	173:GLN	C	272:UNK	N	71.87
1	A	986:ALA	C	1013:ASP	N	34.04
1	N	730:ILE	C	747:LYS	N	25.53
1	N	458:UNK	C	476:UNK	N	22.96
1	R	132:LEU	C	146:SER	N	22.90
1	A	814:ALA	C	839:SER	N	21.92
1	R	470:ASP	C	483:VAL	N	21.45
1	A	1333:HIS	C	1347:SER	N	21.12
1	A	58:UNK	C	71:LYS	N	19.22
1	A	1711:ASP	C	1727:ALA	N	18.14
1	R	67:ASN	C	88:GLY	N	17.14
1	A	192:SER	C	206:PRO	N	16.61
1	A	295:UNK	C	402:PRO	N	15.84
1	A	1897:PRO	C	1910:UNK	N	15.76
1	R	108:GLN	C	125:LYS	N	14.90
1	A	513:ALA	C	582:THR	N	14.59
1	R	163:SER	C	169:ARG	N	13.98
1	A	670:TYR	C	757:THR	N	13.68
1	A	414:ALA	C	424:ALA	N	13.23
1	N	304:PHE	C	320:THR	N	13.22
1	N	29:UNK	C	53:UNK	N	13.14
1	A	882:LEU	C	924:SER	N	12.37
1	A	1827:GLN	C	1839:PHE	N	10.98
1	A	1873:SER	C	1877:PRO	N	10.50
1	A	134:SER	C	146:GLU	N	9.68
1	N	443:UNK	C	451:UNK	N	9.67
1	A	1437:ASN	C	1452:LEU	N	9.33

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1734:LYS	C	1739:SER	N	7.00
1	A	226:LYS	C	236:ALA	N	5.32
1	N	65:UNK	C	70:UNK	N	5.16
1	A	1680:LEU	C	1684:THR	N	4.88
1	N	102:UNK	C	107:UNK	N	4.68
1	A	460:SER	C	464:THR	N	4.61
1	N	510:GLY	C	511:SER	N	4.14
1	N	220:UNK	C	232:TRP	N	3.98
1	N	191:GLY	C	196:UNK	N	3.40

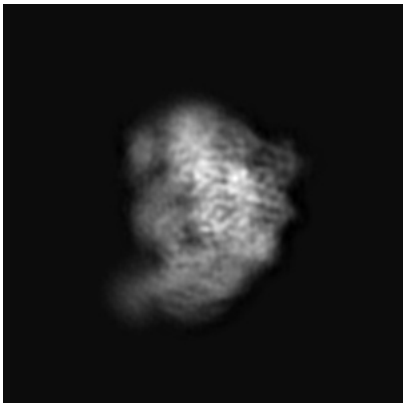
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2925. These allow visual inspection of the internal detail of the map and identification of artifacts.

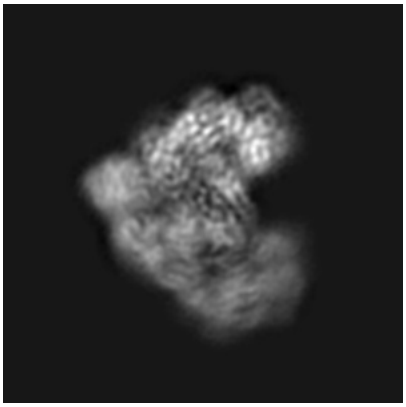
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

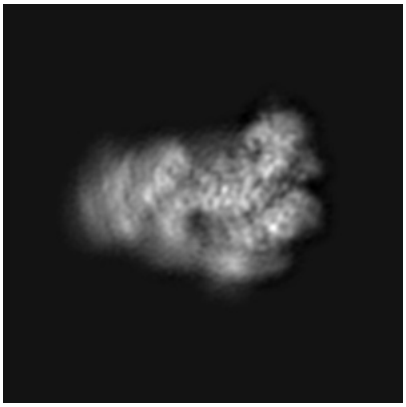
6.1.1 Primary map



X



Y

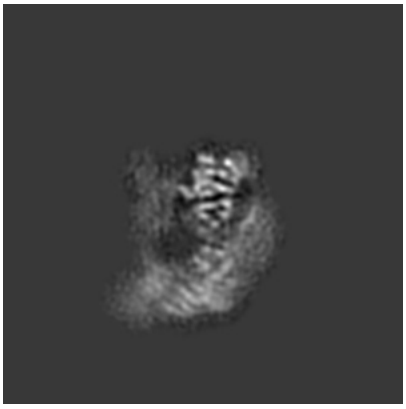


Z

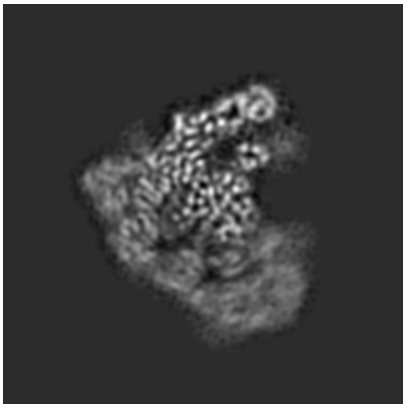
The images above show the map projected in three orthogonal directions.

6.2 Central slices

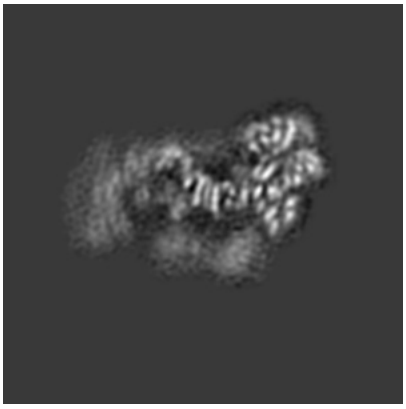
6.2.1 Primary map



X Index: 100



Y Index: 100



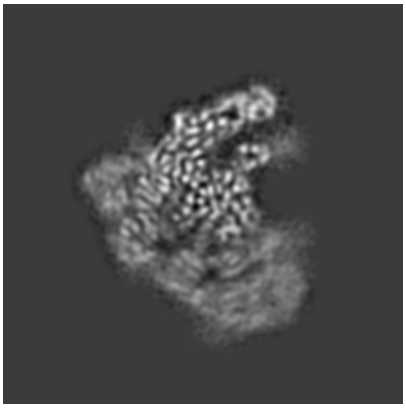
Z Index: 100

The images above show central slices of the map in three orthogonal directions.

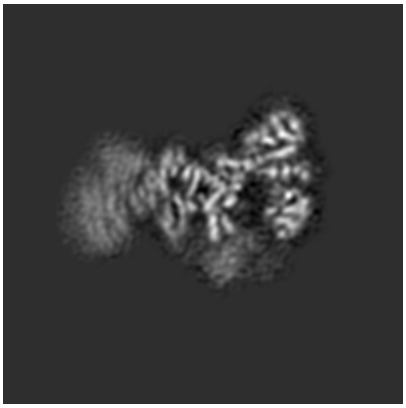
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 136



Y Index: 101



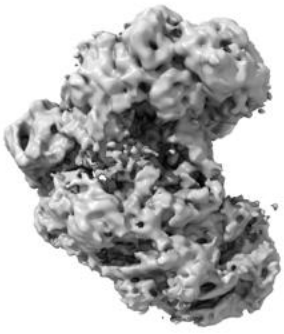
Z Index: 112

The images above show the largest variance slices of the map in three orthogonal directions.

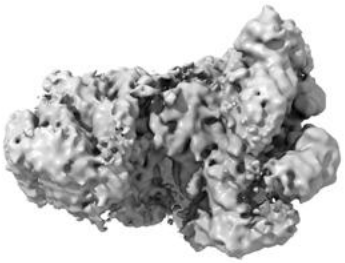
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

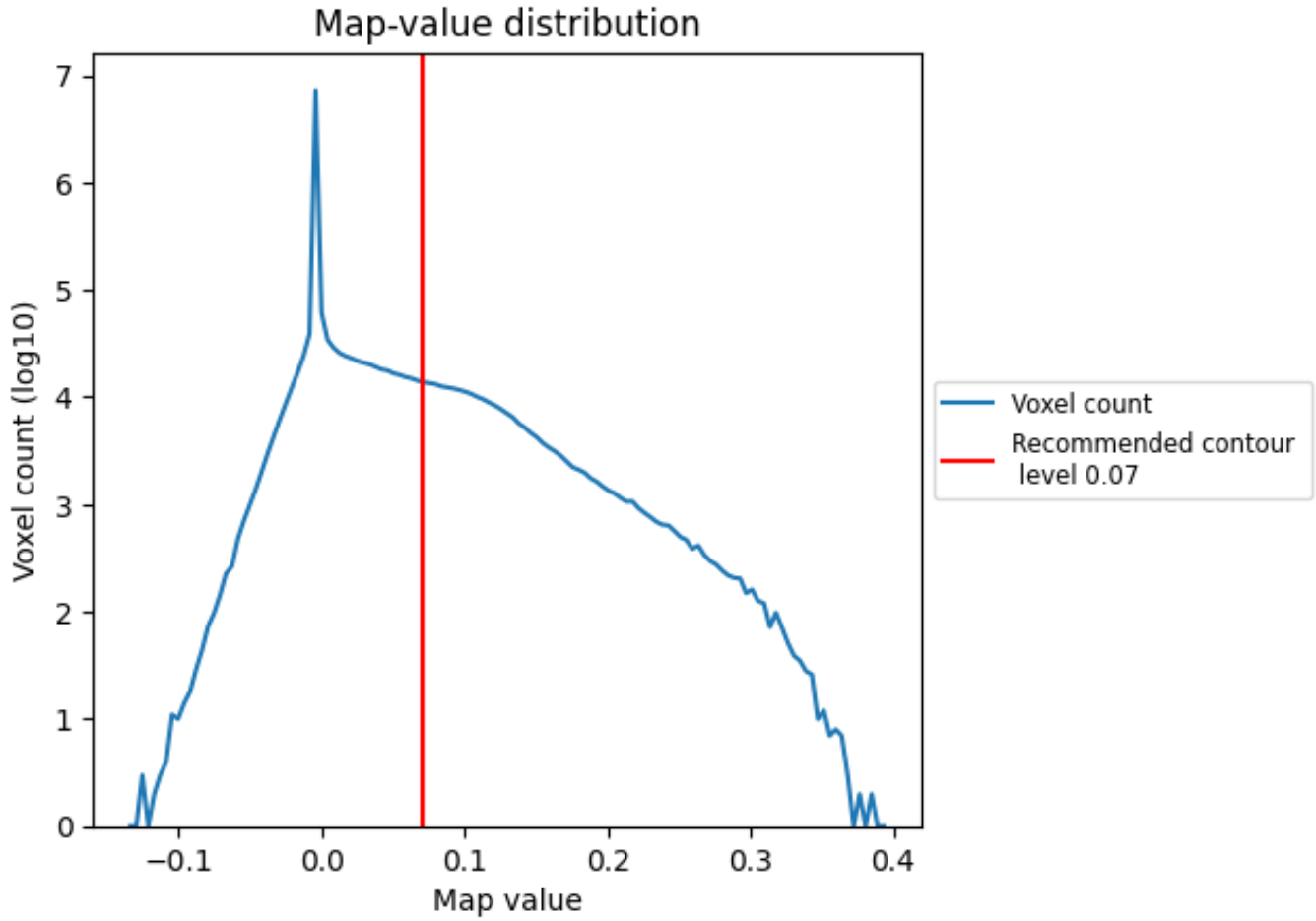
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

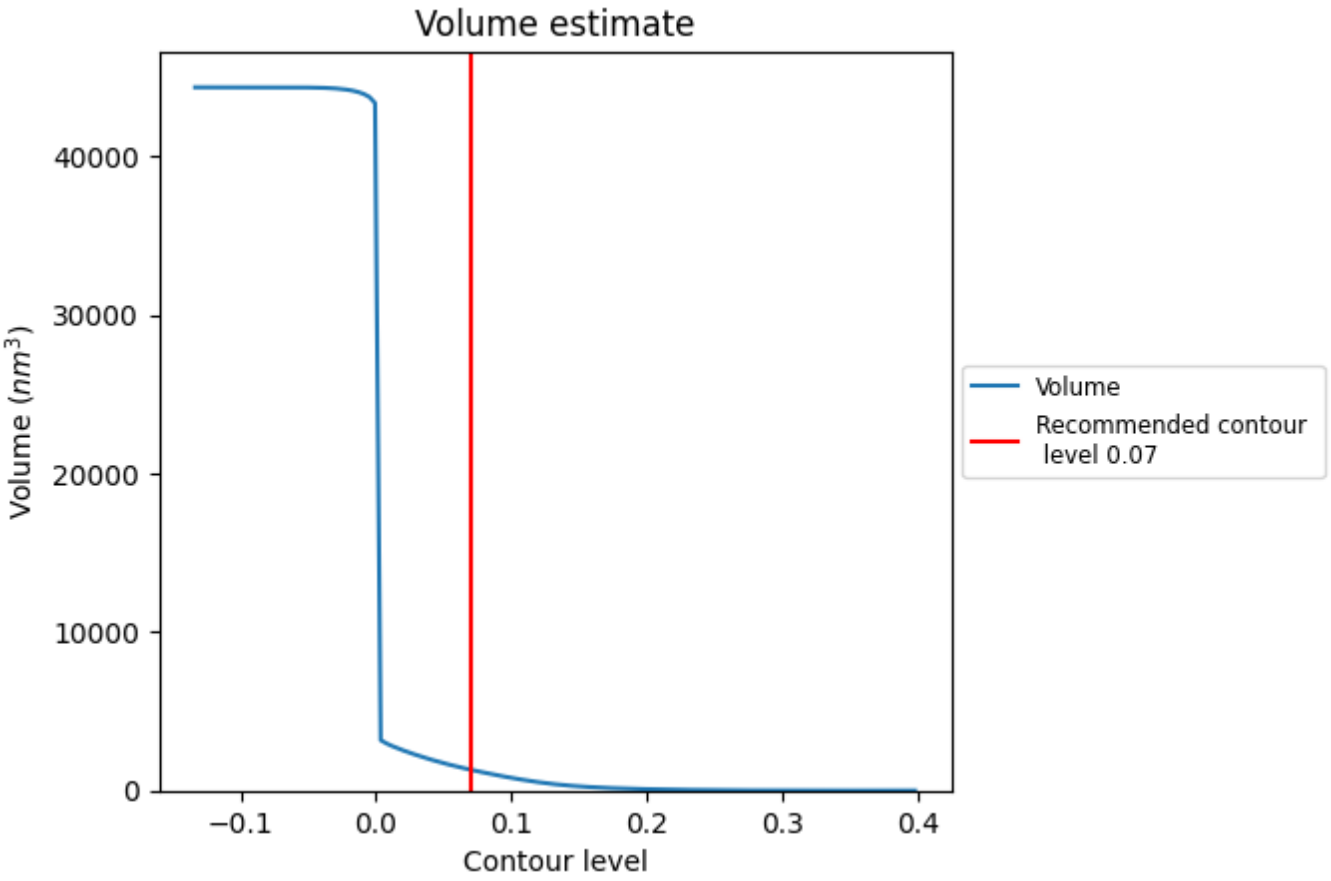
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

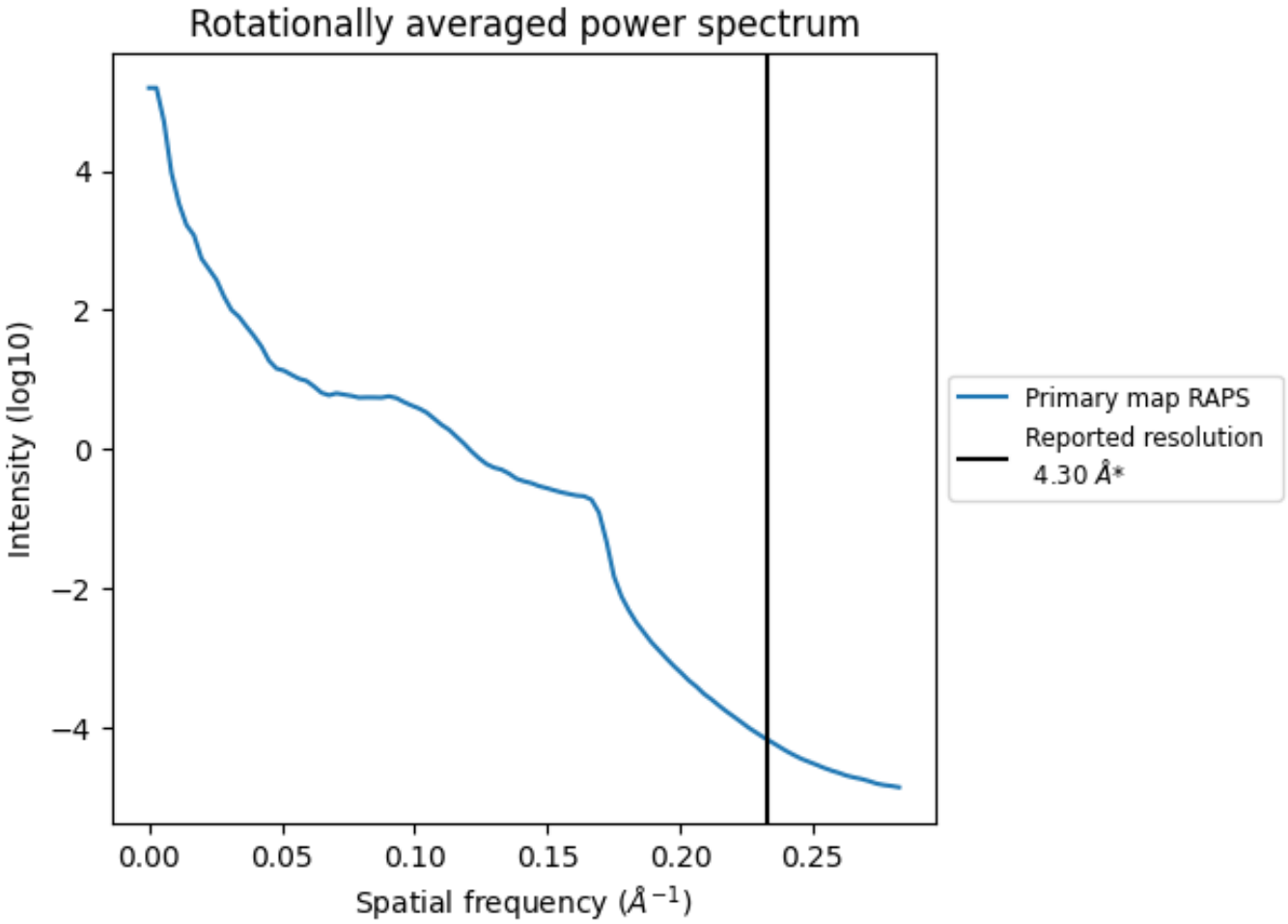
7.2 Volume estimate



The volume at the recommended contour level is 1309 nm^3; this corresponds to an approximate mass of 1182 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

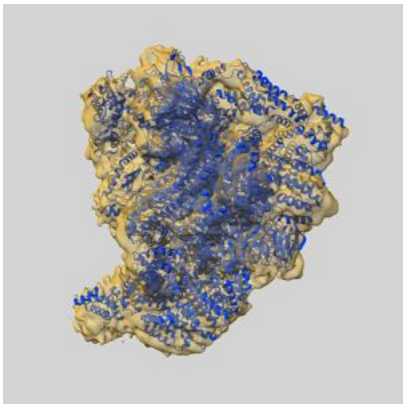
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

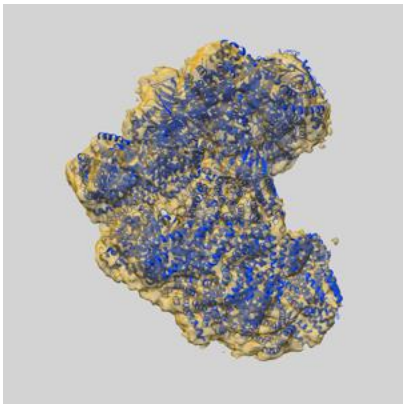
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2925 and PDB model 5A31. Per-residue inclusion information can be found in section 3 on page 9.

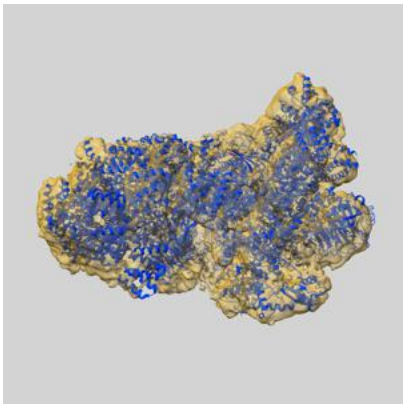
9.1 Map-model overlay



X



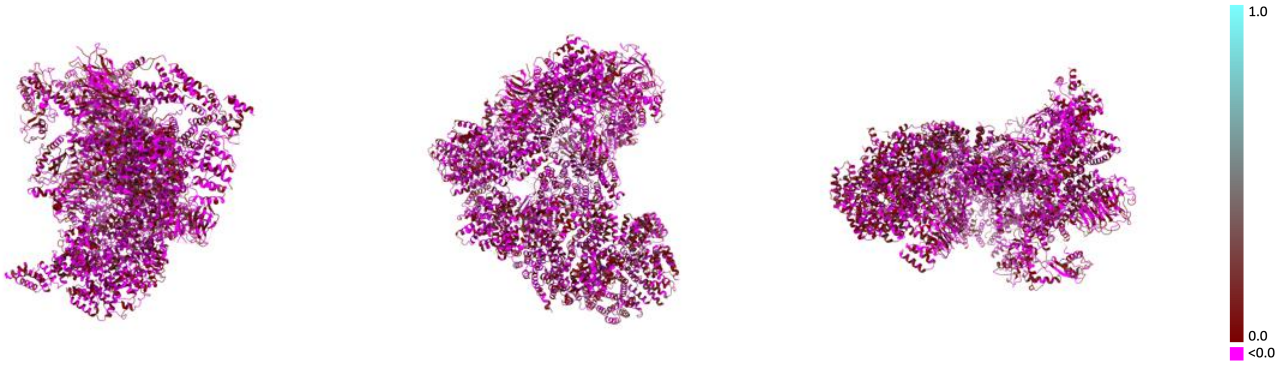
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

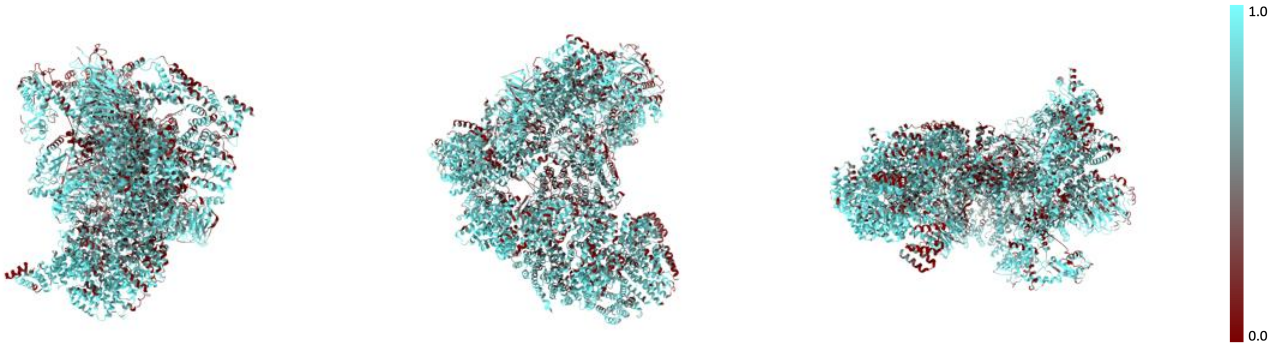
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

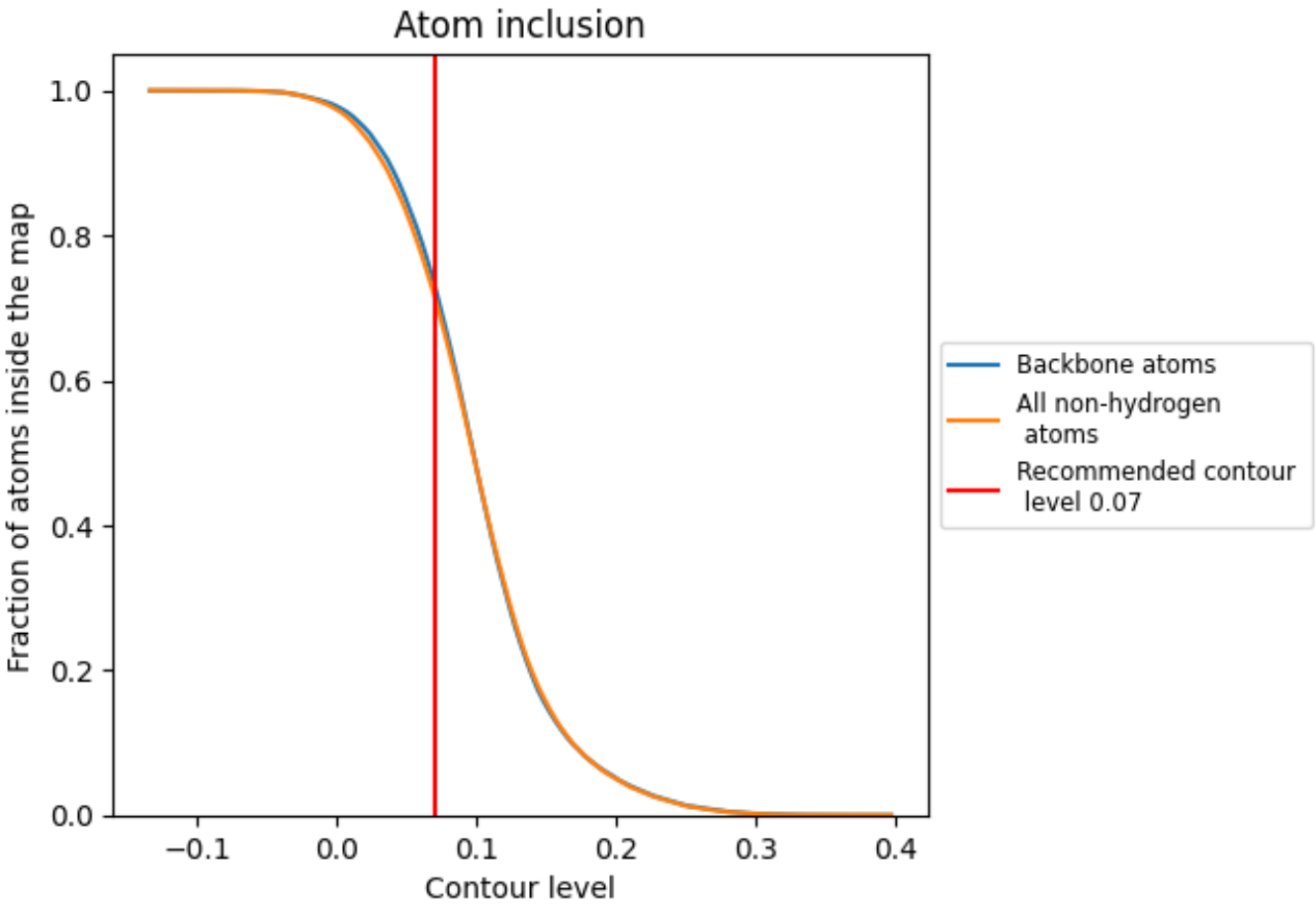
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7182	0.0070
A	0.6672	-0.0150
B	0.8150	0.0470
C	0.6676	-0.0110
D	0.6019	0.0420
E	0.6104	0.0040
F	0.7774	-0.0020
G	0.5665	-0.0150
H	0.7160	0.0300
I	0.7467	0.0370
J	0.7996	-0.0120
K	0.7544	0.0240
L	0.6690	0.0160
M	0.4555	-0.0260
N	0.6779	-0.0050
O	0.7117	0.0230
P	0.8138	-0.0260
Q	0.8292	0.0480
R	0.6395	-0.0080
T	0.5321	-0.0430
U	0.6500	-0.0220
V	0.5052	0.0200
W	0.7707	0.0460
X	0.6952	0.0350
Y	0.7888	0.0250