Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 10:53 am GMT

PDB ID	:	5G04
EMDB ID	:	EMD-3385
Title	:	Structure of the human APC-Cdc20-Hsl1 complex
Authors	:	Zhang, S.; Chang, L.; Alfieri, C.; Zhang, Z.; Yang, J.; Maslen, S.; Skehel, M.; Barford, D.
Deposited on	:	2016-03-16
Resolution	:	4.00 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:

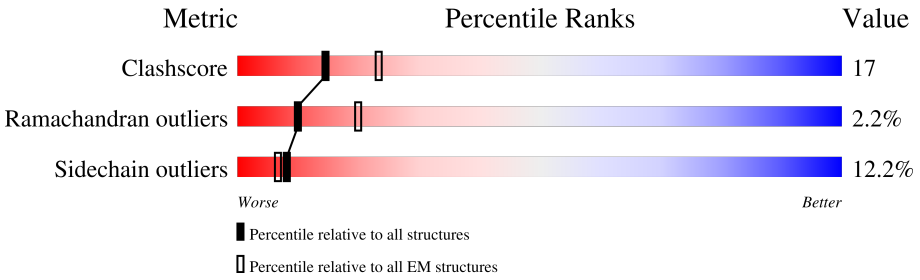
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.00 Å.

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



Metric	Whole archive (#Entries)	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	1944	41% 26% 6% 26%
2	B	84	98% 69% 23% 6%
3	C	597	8% 44% 34% 10% 12%
3	P	597	5% 53% 24% 5% 18%
4	D	121	26% 17% 55%
5	E	110	35% 15% 49%
6	F	824	41% 17% 40%
6	H	824	41% 16% 41%

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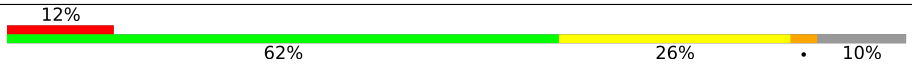
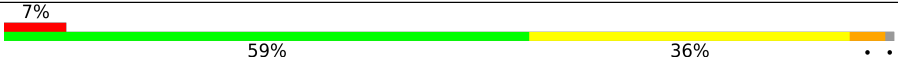
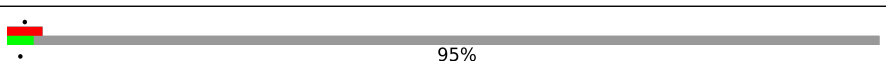
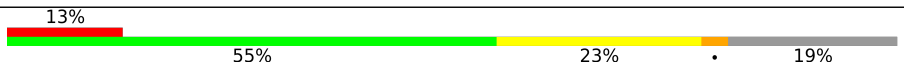
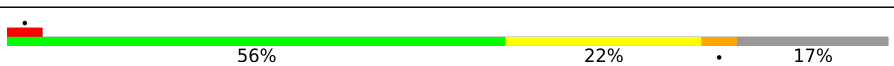
Mol	Chain	Length	Quality of chain
7	G	85	
7	W	85	
8	I	808	
9	J	620	
9	K	620	
10	L	184	
11	M	74	
12	N	822	
13	O	755	
14	R	499	
15	S	206	
16	X	599	
16	Y	599	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 65481 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
			Total	C	N	O	S		
1	A	1437	10925	7025	1849	1977	74	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	84	649	416	117	99	17	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	524	4306	2774	727	781	24	0	0
3	P	491	Total	C	N	O	S	0	0
			4039	2608	678	729	24		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	55	436	277	73	86	0	0

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

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

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

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

- 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
			213	133	40	39	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		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	504	Total	C	N	O	S	0	0
			4047	2601	684	737	25		
9	K	493	Total	C	N	O	S	0	0
			3988	2563	672	729	24		

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	ARG	deletion	UNP Q9UM13

- Molecule 11 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 13.

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

- Molecule 12 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	631	Total	C	N	O	S	0	0
			4837	3067	880	868	22		

- Molecule 13 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	685	Total	C	N	O	S	0	0
			5395	3440	940	987	28		

- Molecule 14 is a protein called CELL DIVISION CYCLE PROTEIN 20 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	370	Total	C	N	O	S	2	0
			2869	1801	524	532	12		

- Molecule 15 is a protein called PROBABLE SERINE/THREONINE-PROTEIN KINASE HSL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	S	10	Total	C	N	O	0	0
			72	42	14	16		

- Molecule 16 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	484	Total	C	N	O	S	0	0
			3767	2390	649	704	24		
16	Y	496	Total	C	N	O	S	0	0
			3859	2444	666	724	25		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

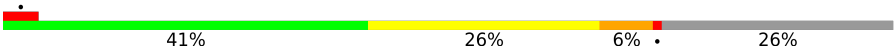
Mol	Chain	Residues	Atoms		AltConf
17	B	3	Total	Zn	0
			3	3	

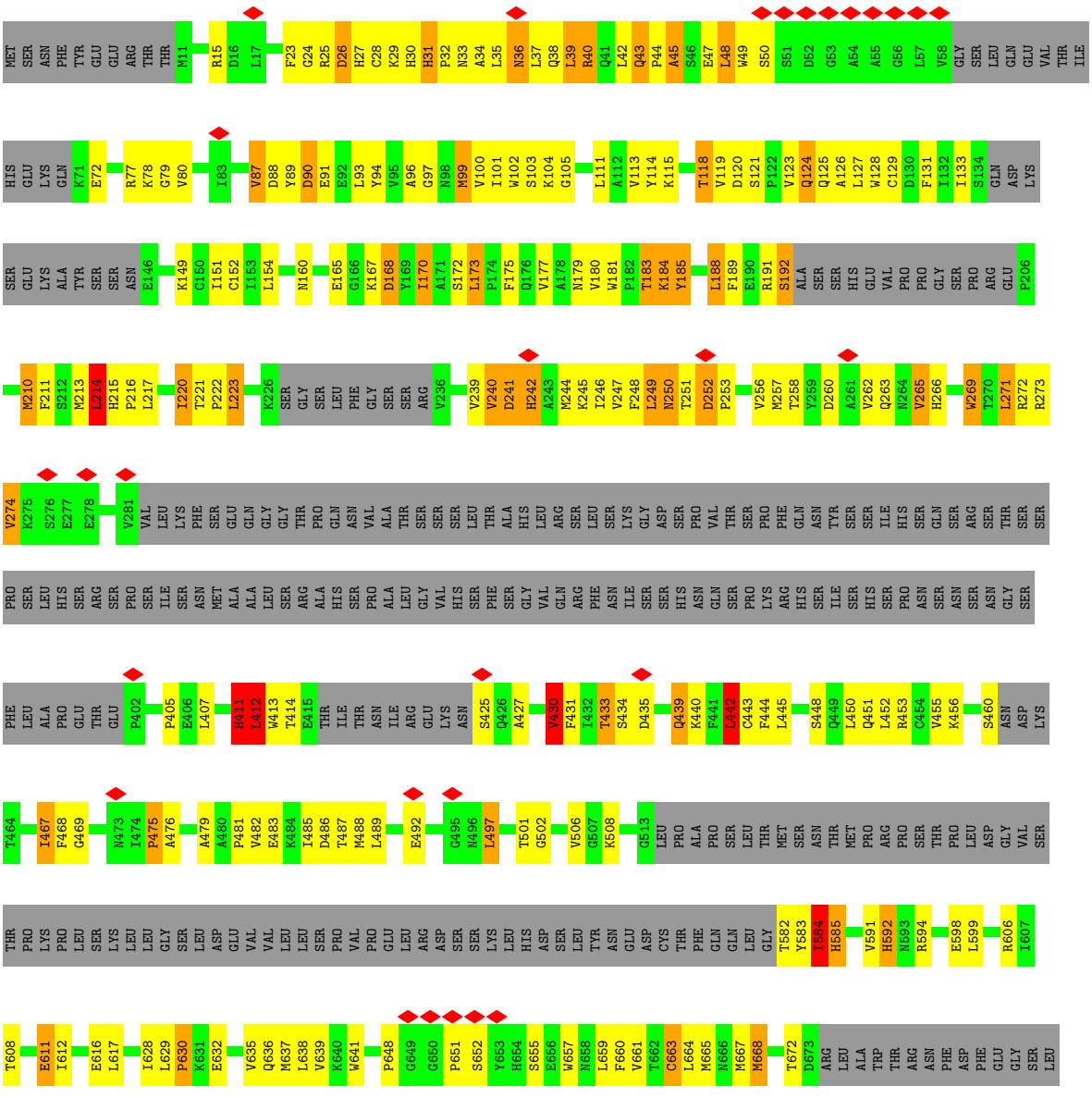
3 Residue-property plots (i)

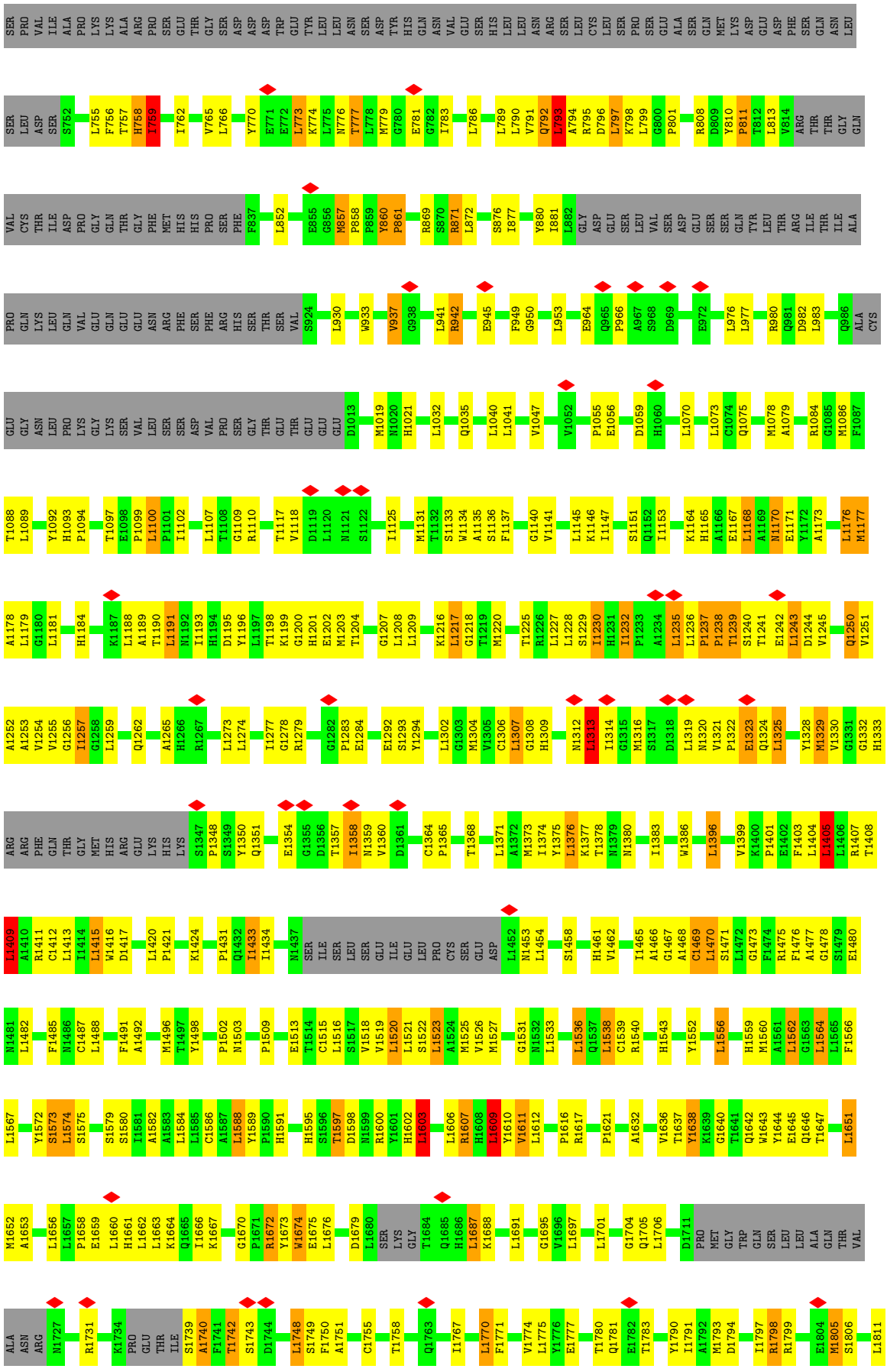
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

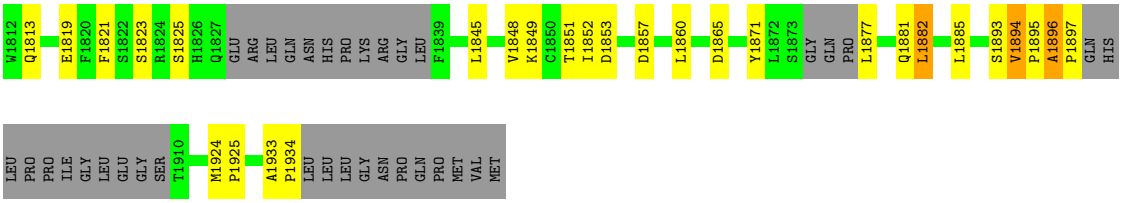
• Molecule 1: ANAPHASE-PROMOTING COMPLEX SUBUNIT 1

Chain A:



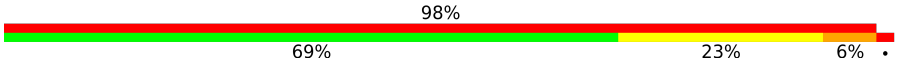


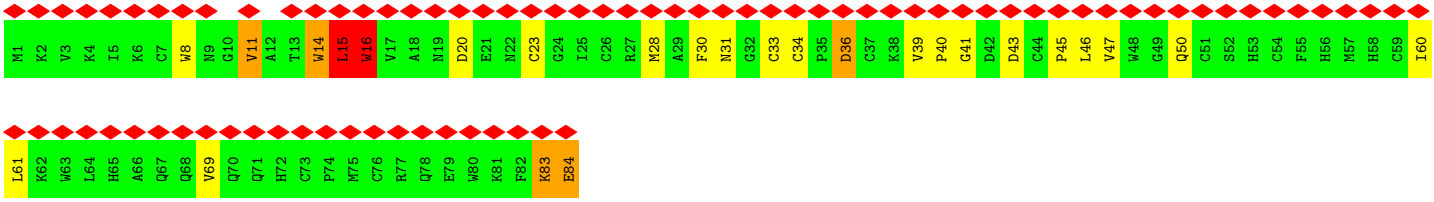




• Molecule 2: ANAPHASE-PROMOTING COMPLEX SUBUNIT 11

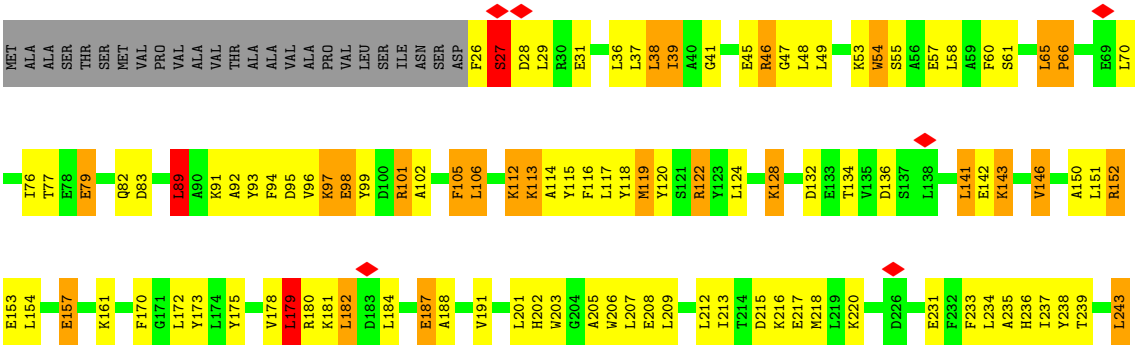
Chain B:

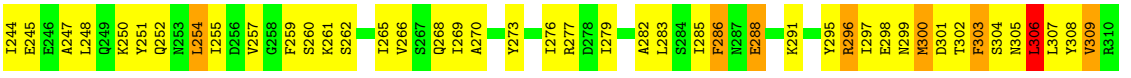


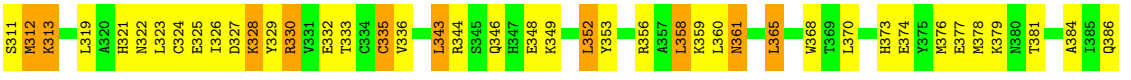


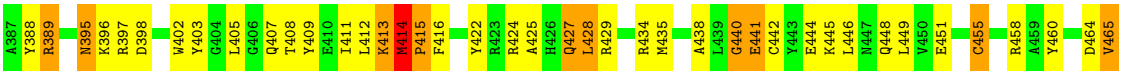
• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

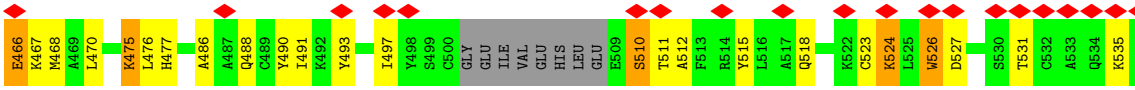
Chain C:

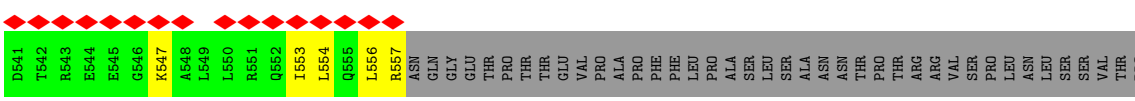






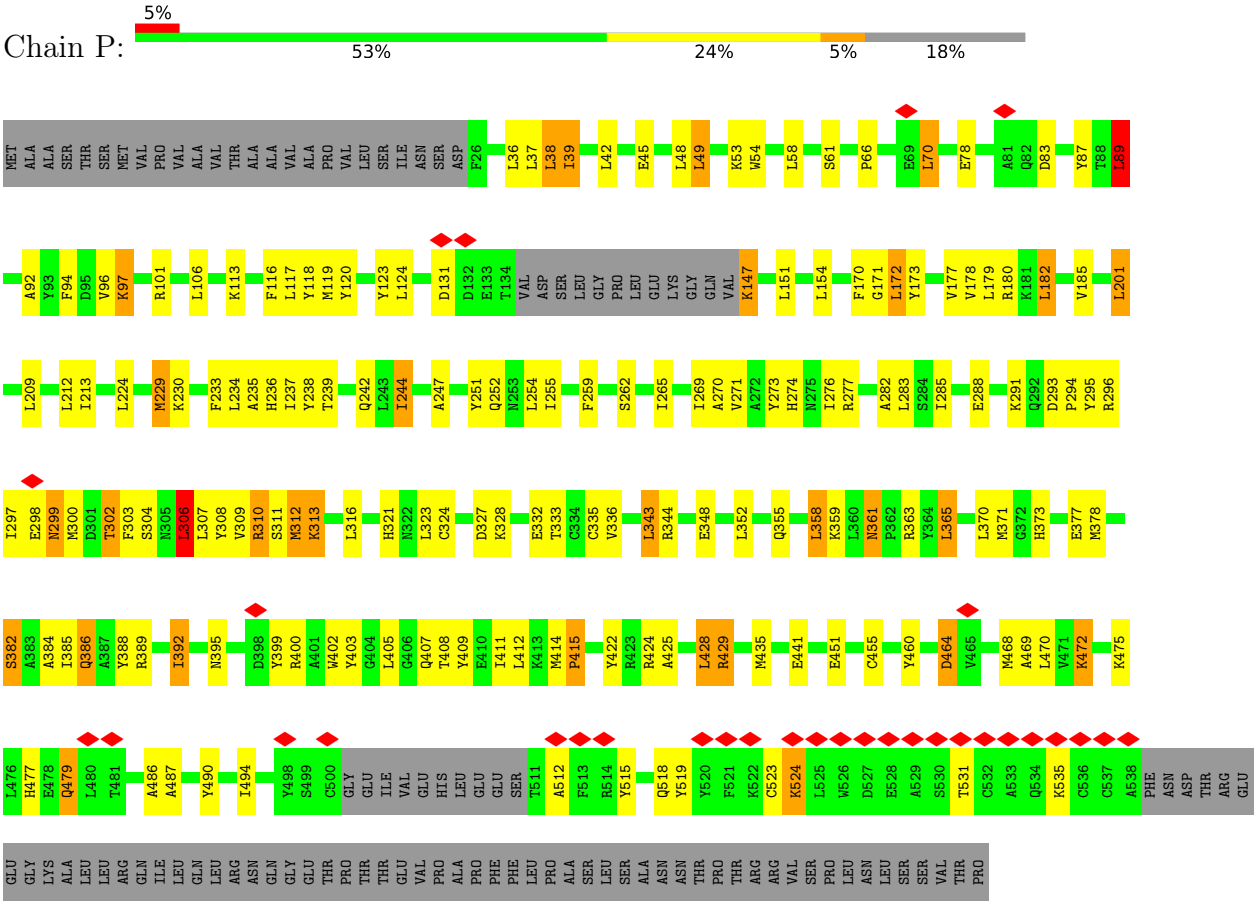






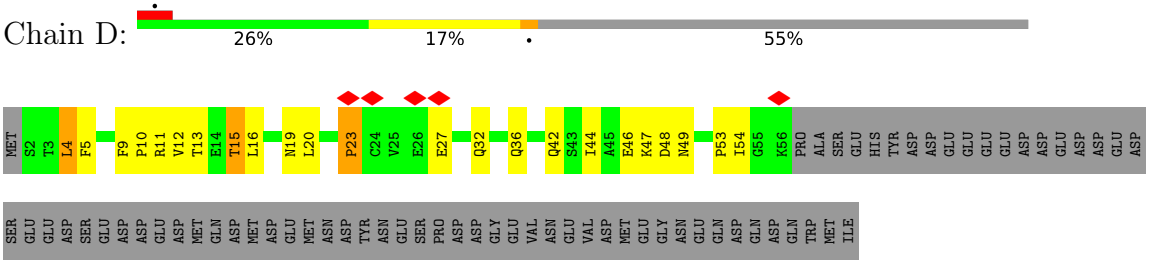
• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

Chain P:



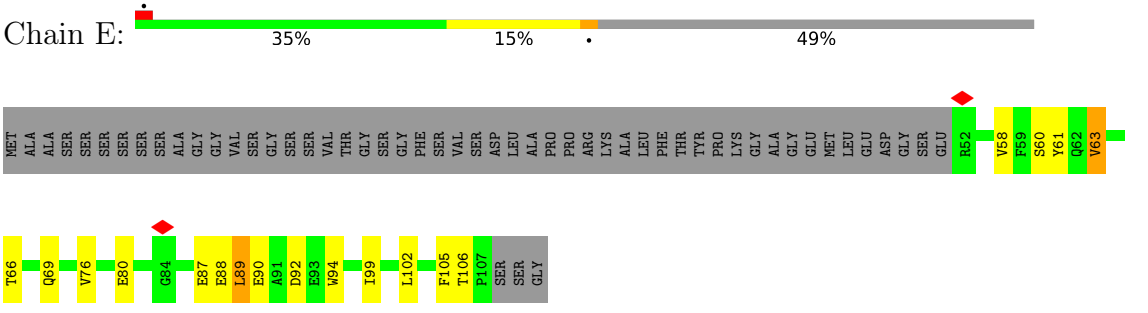
• Molecule 4: ANAPHASE-PROMOTING COMPLEX SUBUNIT 15

Chain D:



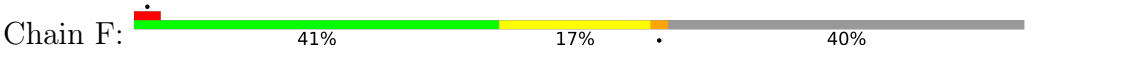
• Molecule 5: ANAPHASE-PROMOTING COMPLEX SUBUNIT 16

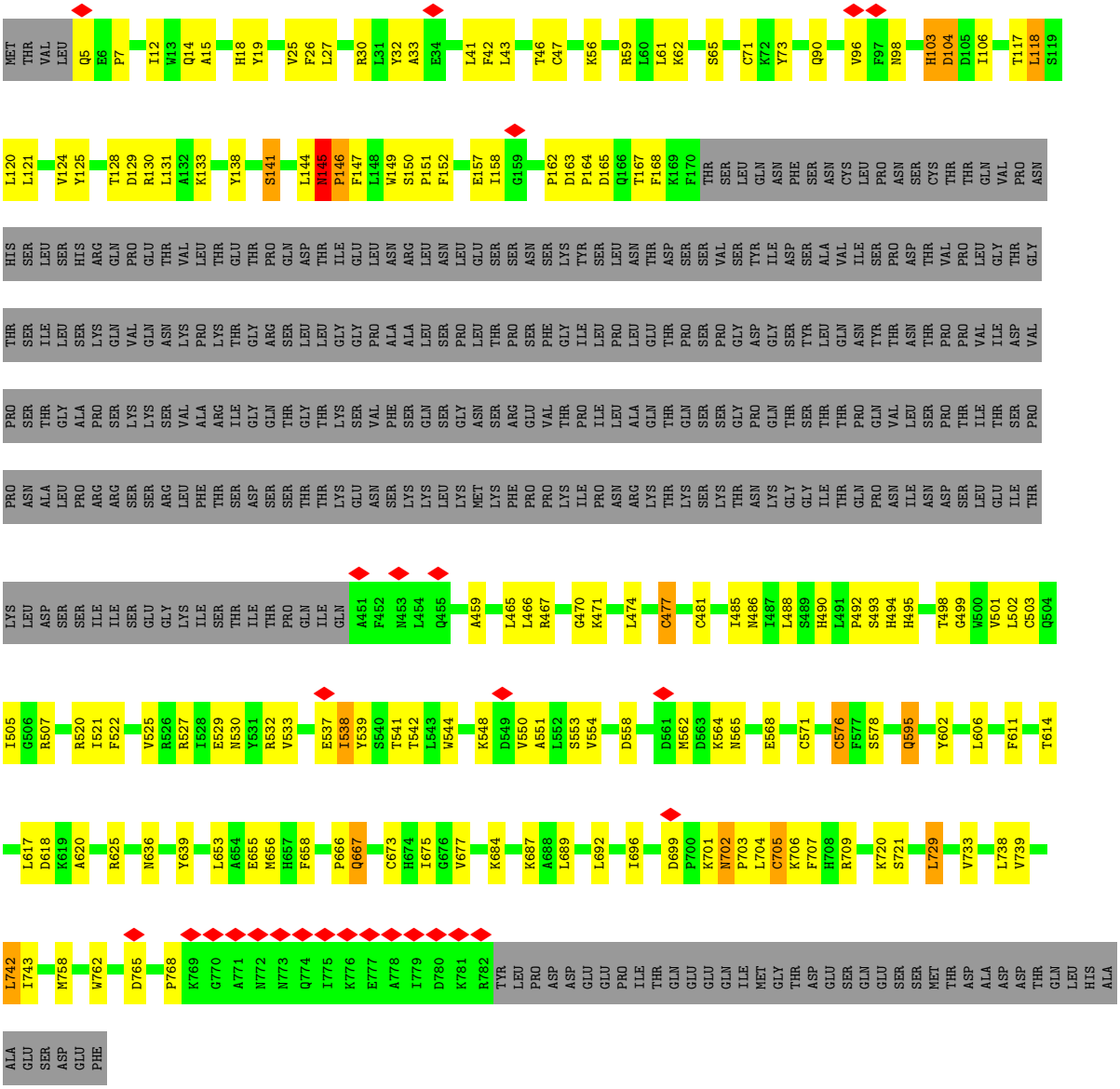
Chain E:



• Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

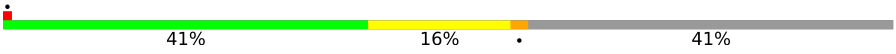
Chain F:

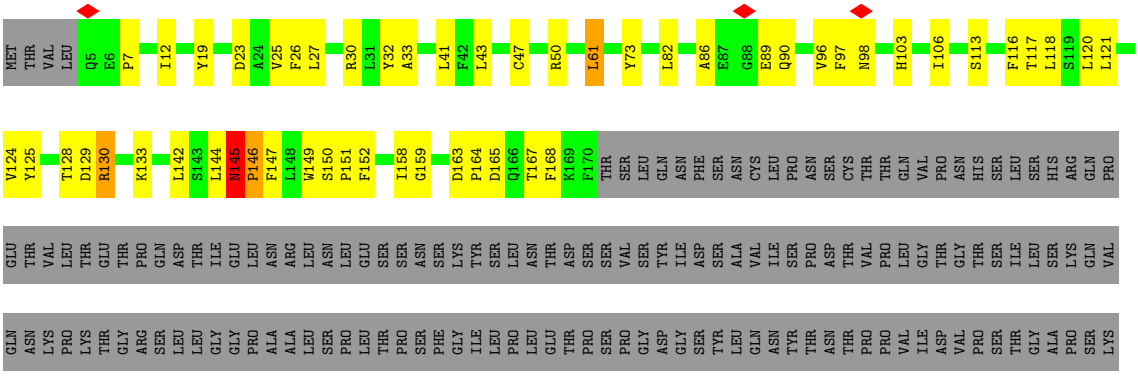


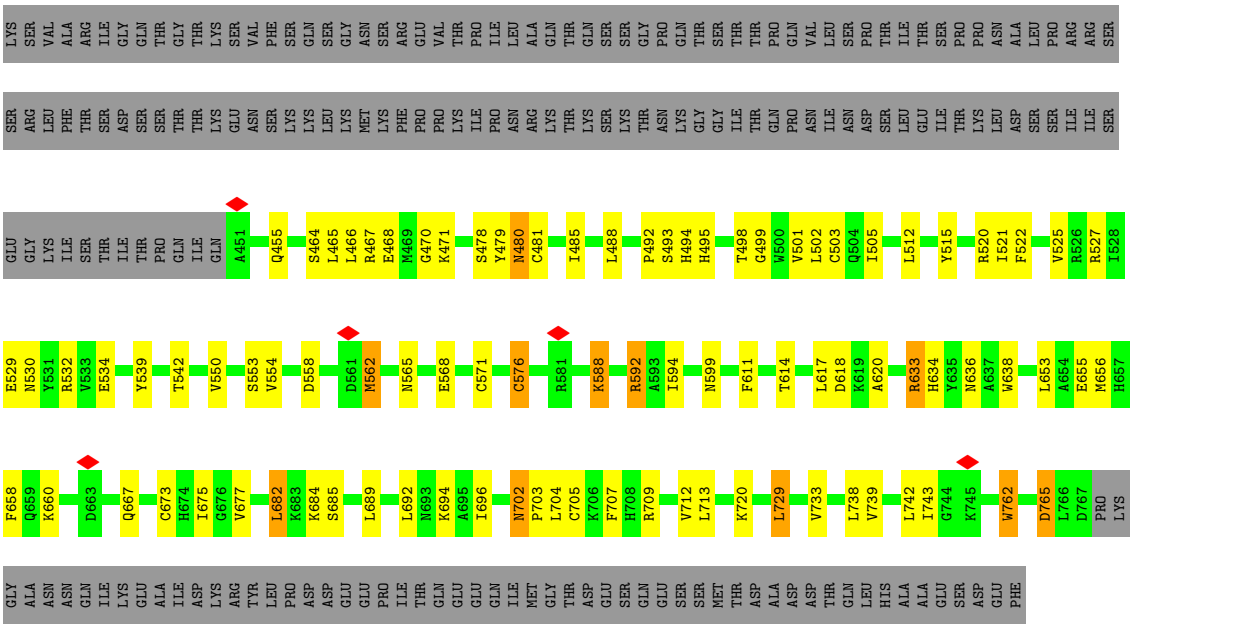


• Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG

Chain H:

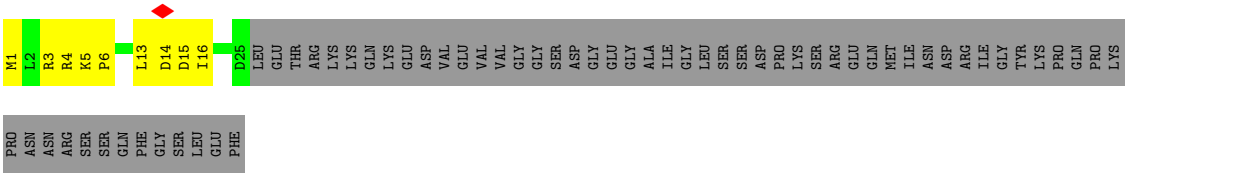






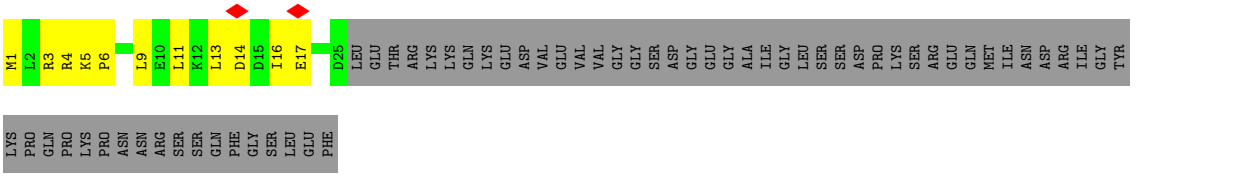
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

Chain G:



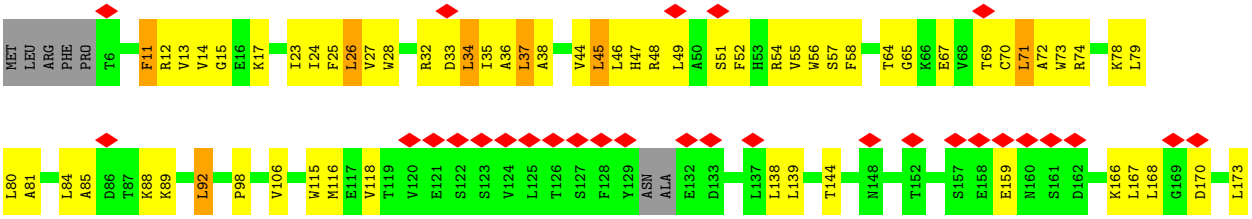
• Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

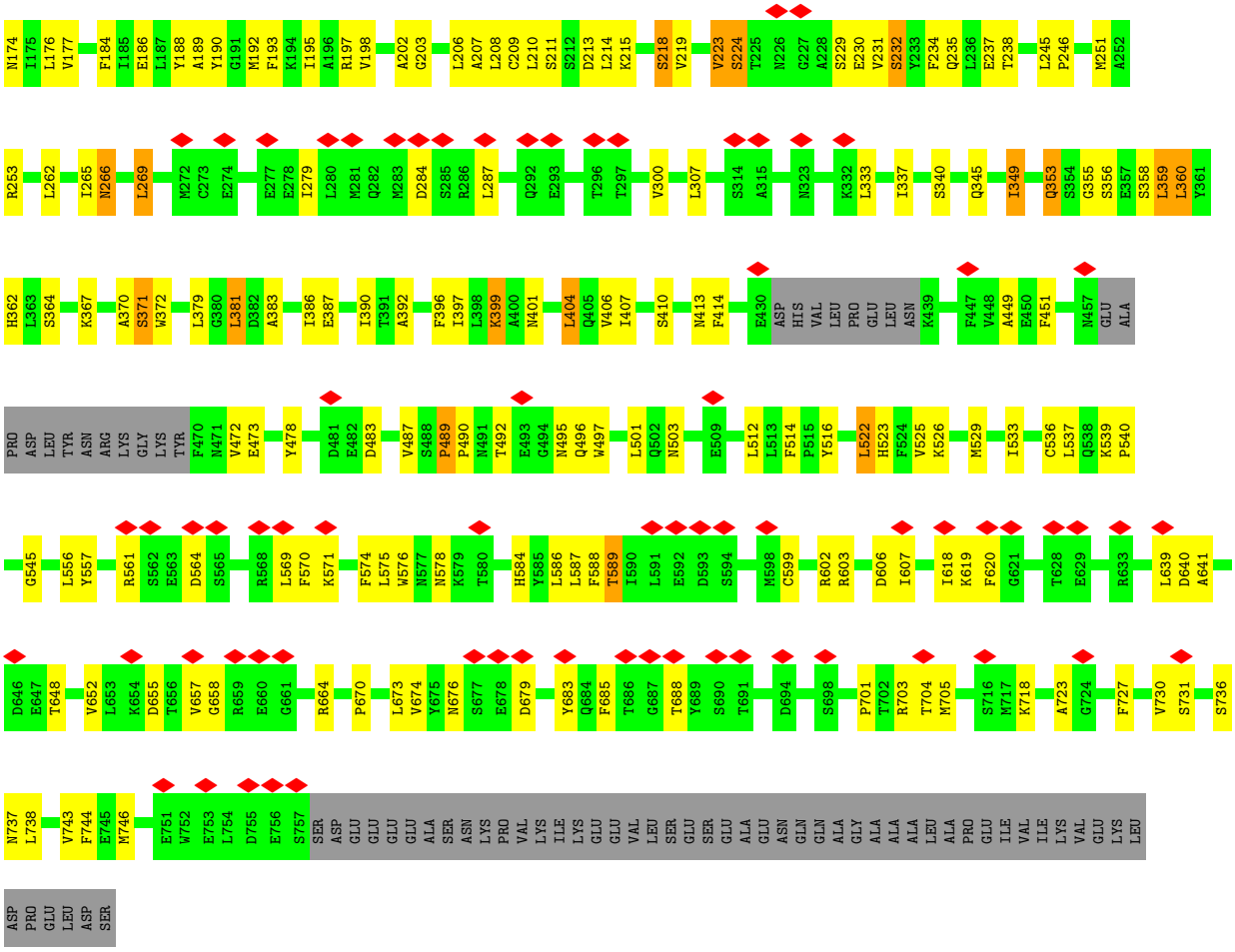
Chain W:



• Molecule 8: ANAPHASE-PROMOTING COMPLEX SUBUNIT 4

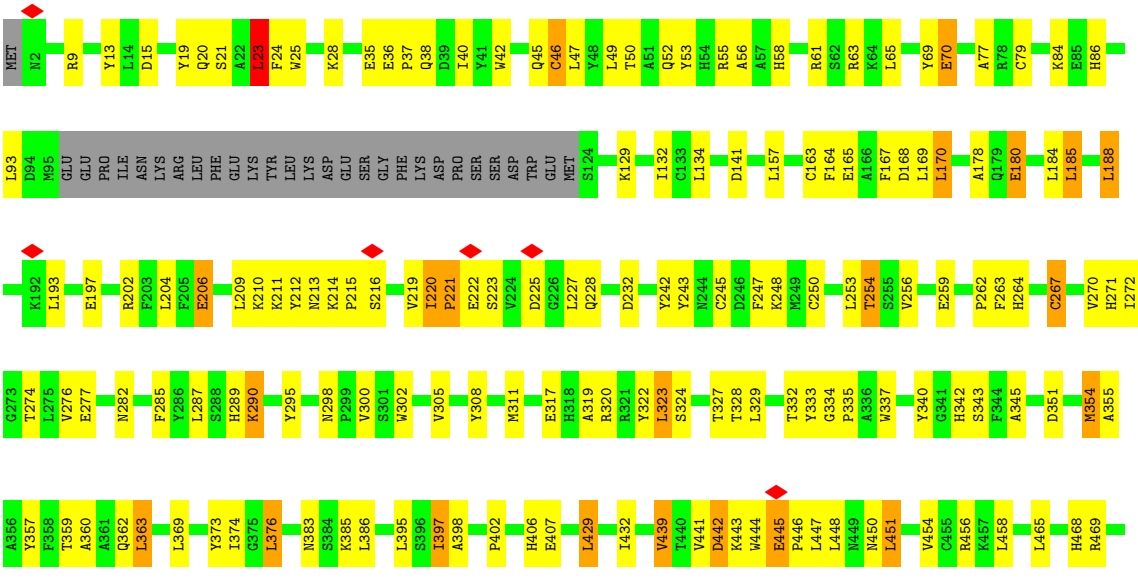
Chain I:

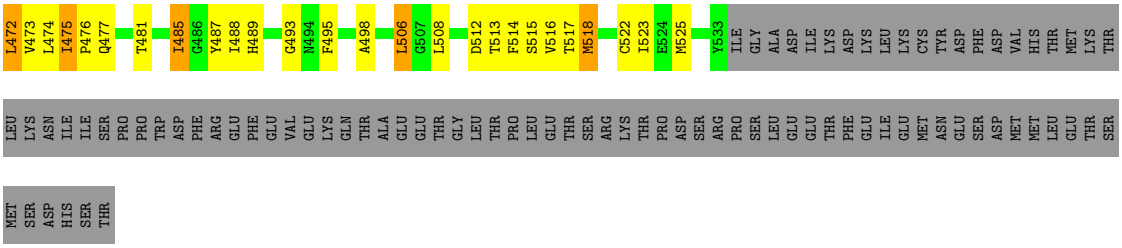




• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

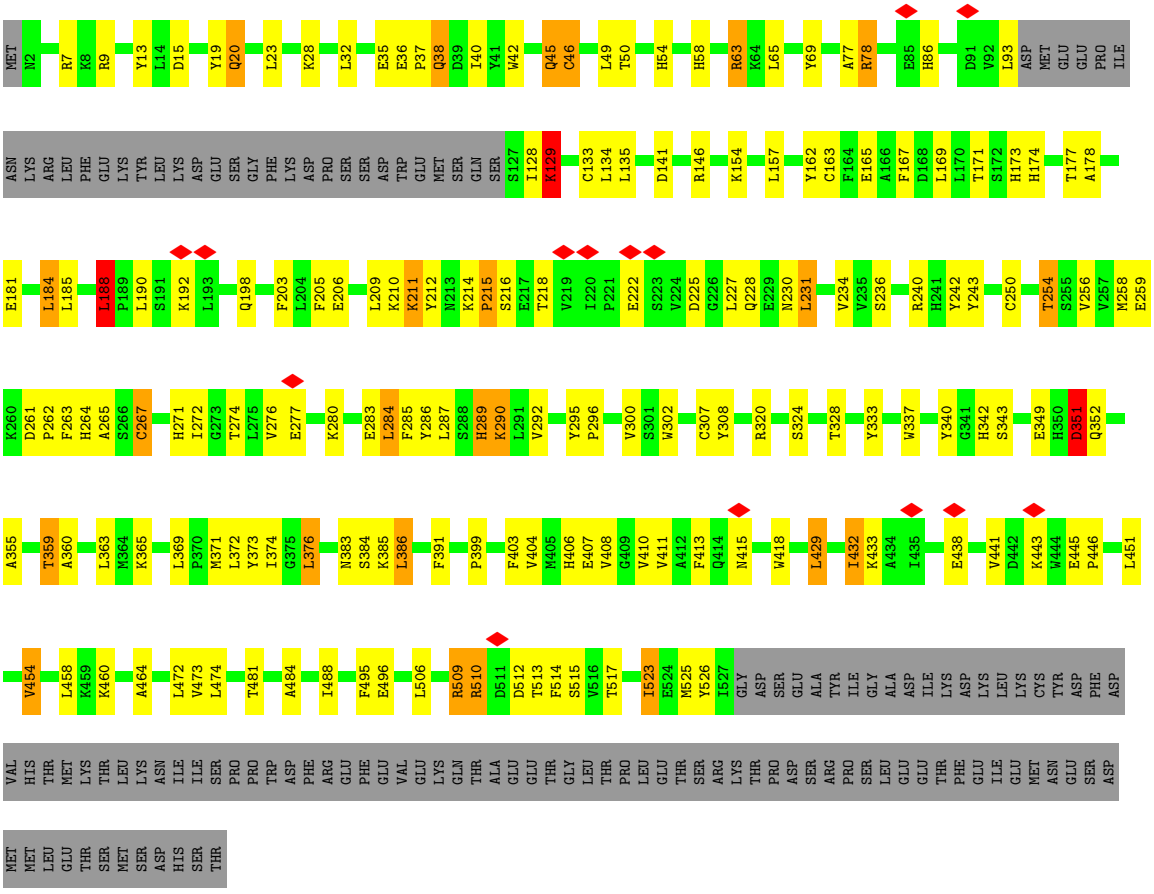
Chain J:





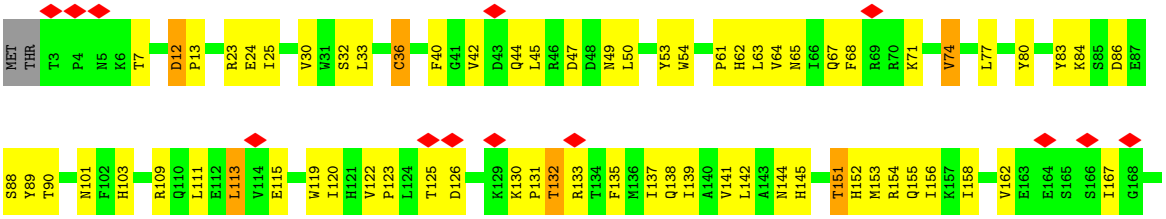
• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

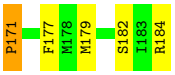
Chain K:



• Molecule 10: ANAPHASE-PROMOTING COMPLEX SUBUNIT 10

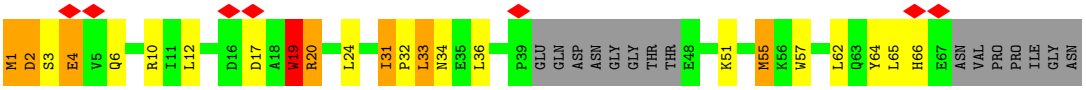
Chain L:





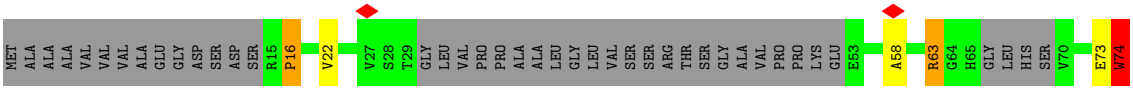
• Molecule 11: ANAPHASE-PROMOTING COMPLEX SUBUNIT 13

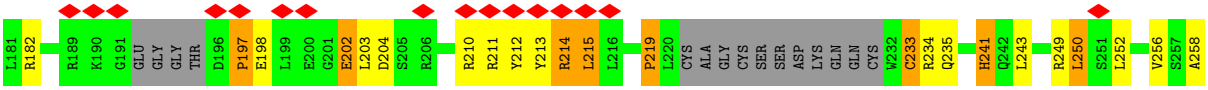
Chain M:

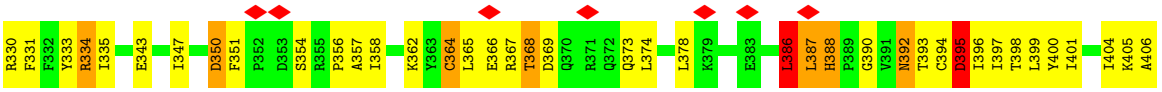


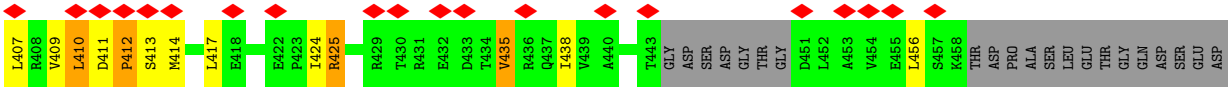
• Molecule 12: ANAPHASE-PROMOTING COMPLEX SUBUNIT 2

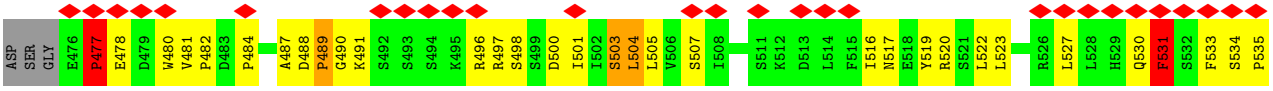
Chain N:

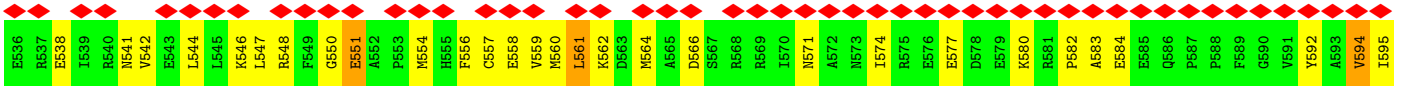


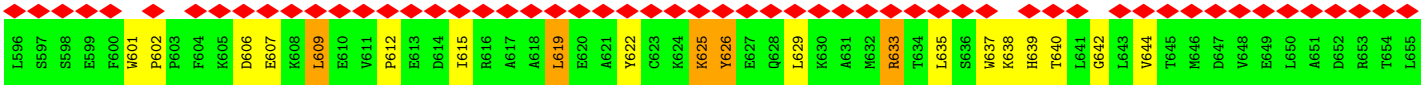


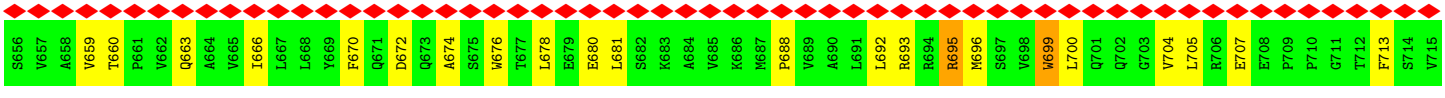


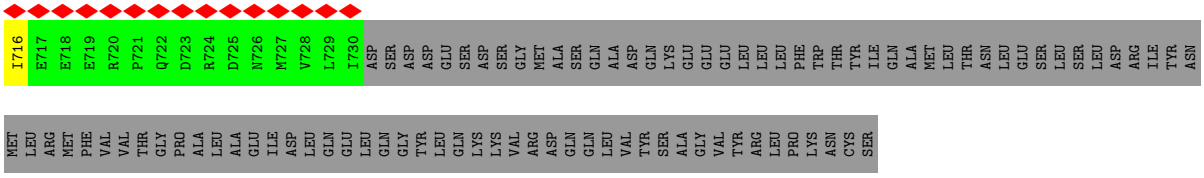






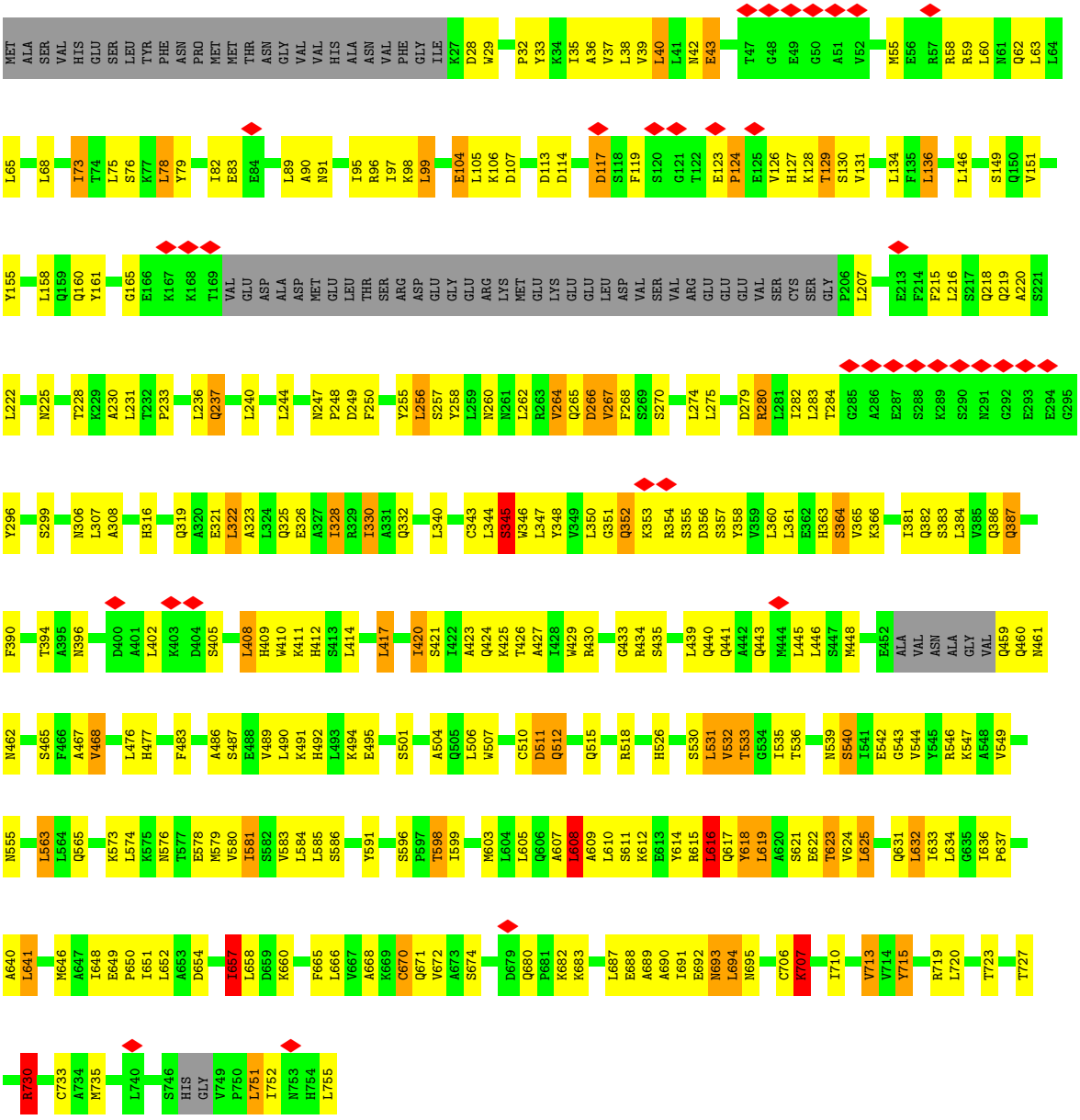






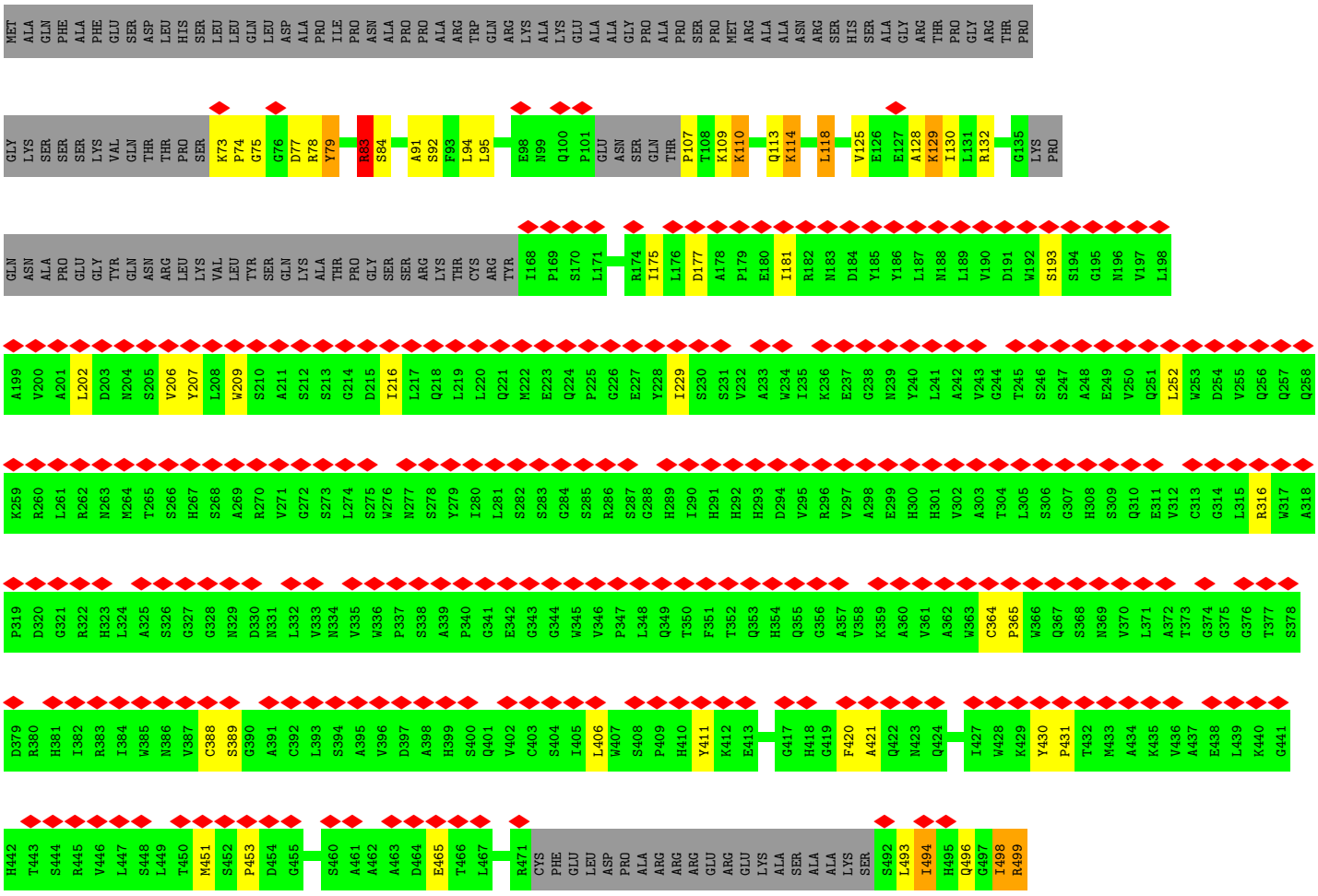
• Molecule 13: ANAPHASE-PROMOTING COMPLEX SUBUNIT 5

Chain O:



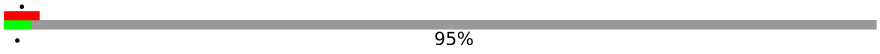
• Molecule 14: CELL DIVISION CYCLE PROTEIN 20 HOMOLOG

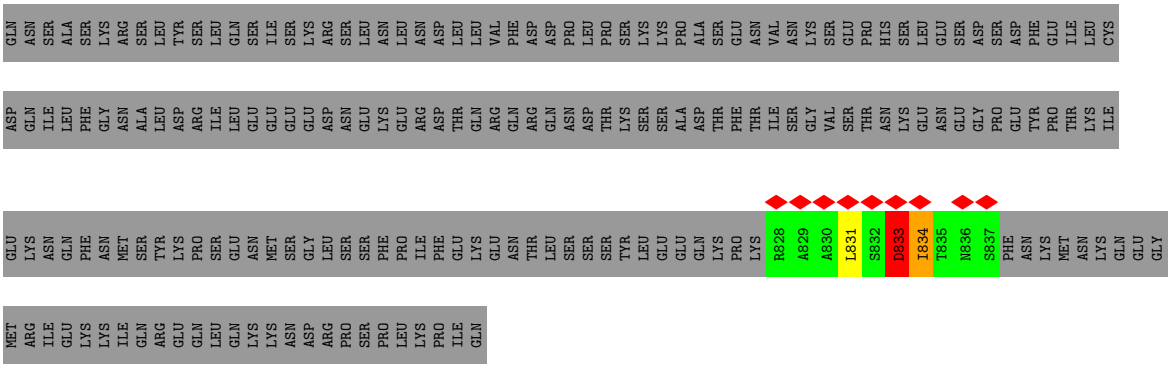
Chain R:



• Molecule 15: PROBABLE SERINE/THREONINE-PROTEIN KINASE HSL1

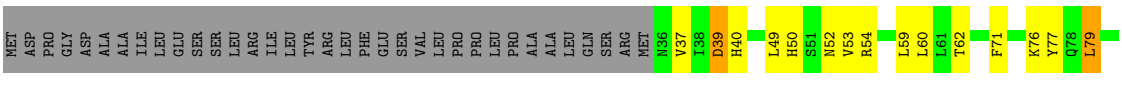
Chain S:

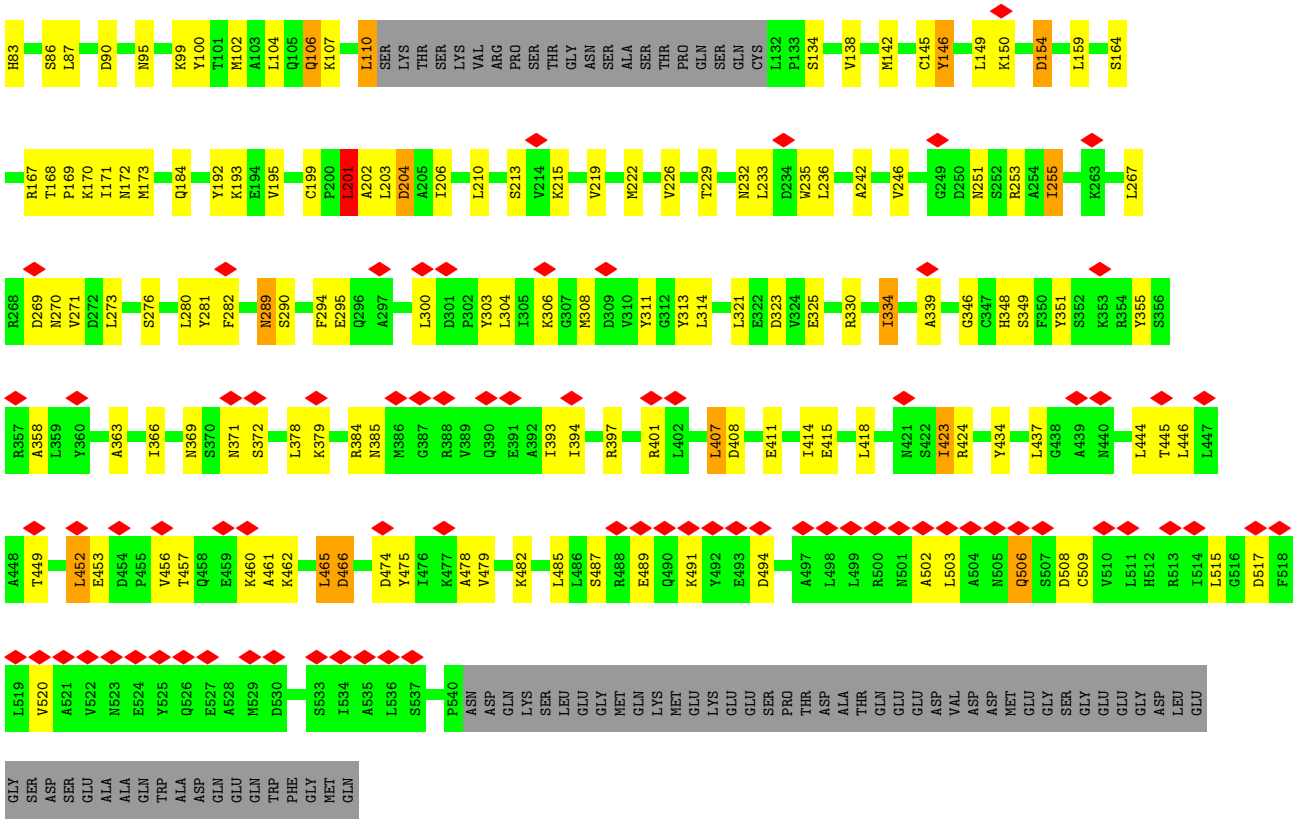




• Molecule 16: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

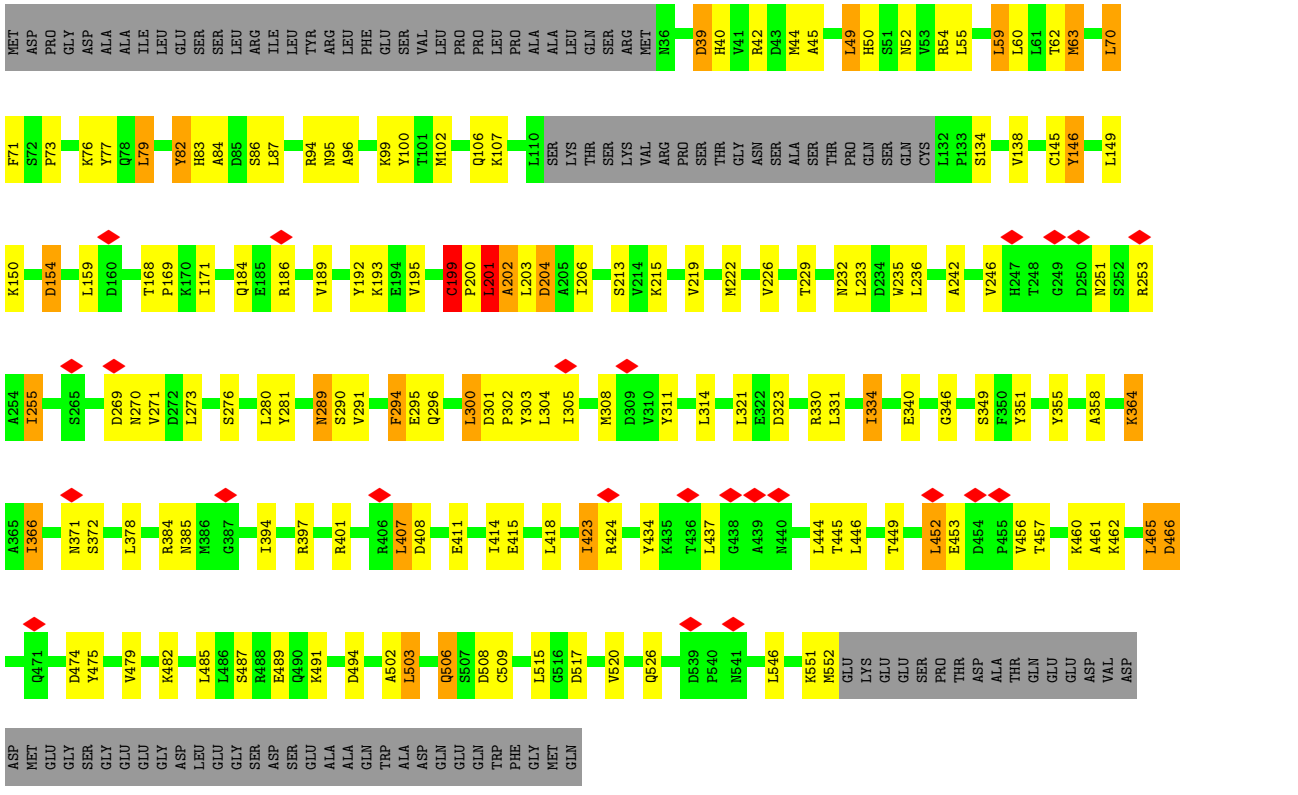
Chain X:





• Molecule 16: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	179660	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	27	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	0.392	Depositor
Minimum map value	-0.196	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	386.24, 386.24, 386.24	wwPDB
Map dimensions	284, 284, 284	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	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	0.58	0/11165	0.89	29/15204 (0.2%)
2	B	0.67	0/674	0.91	0/913
3	C	0.65	0/4404	0.94	8/5945 (0.1%)
3	P	0.63	0/4134	0.91	7/5583 (0.1%)
4	D	0.58	0/446	0.85	1/610 (0.2%)
5	E	0.57	0/459	0.78	0/619
6	F	0.58	0/4013	0.83	4/5428 (0.1%)
6	H	0.59	0/3942	0.82	3/5326 (0.1%)
7	G	0.59	0/214	0.92	1/284 (0.4%)
7	W	0.64	0/214	0.86	0/284
8	I	0.65	0/5827	0.93	12/7899 (0.2%)
9	J	0.69	1/4146 (0.0%)	0.94	6/5616 (0.1%)
9	K	0.70	1/4086 (0.0%)	0.93	5/5534 (0.1%)
10	L	0.67	0/1468	0.88	1/1993 (0.1%)
11	M	0.63	1/502 (0.2%)	0.95	0/680
12	N	0.54	0/4915	0.88	15/6645 (0.2%)
13	O	0.61	1/5493 (0.0%)	0.92	14/7421 (0.2%)
14	R	0.54	2/2940 (0.1%)	0.72	1/3996 (0.0%)
15	S	0.50	0/71	1.09	1/95 (1.1%)
16	X	0.55	0/3826	0.80	6/5177 (0.1%)
16	Y	0.55	0/3919	0.82	10/5301 (0.2%)
All	All	0.61	6/66858 (0.0%)	0.88	124/90553 (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	1
3	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1
6	H	0	1
8	I	0	3
9	J	0	1
10	L	0	1
11	M	0	1
12	N	0	4
16	Y	0	1
All	All	0	15

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	268	PHE	CG-CD2	7.98	1.50	1.38
9	J	302	TRP	CB-CG	-6.32	1.38	1.50
14	R	79	TYR	CB-CG	5.73	1.60	1.51
11	M	19	TRP	CB-CG	5.53	1.60	1.50
14	R	79	TYR	CE1-CZ	5.37	1.45	1.38
9	K	302	TRP	CB-CG	-5.22	1.40	1.50

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	358	LEU	CA-CB-CG	9.86	137.98	115.30
13	O	730	ARG	NE-CZ-NH1	9.15	124.88	120.30
3	C	440	GLY	N-CA-C	-8.87	90.94	113.10
9	K	351	ASP	CB-CG-OD1	8.76	126.19	118.30
1	A	1235	LEU	CA-CB-CG	8.41	134.65	115.30
16	Y	70	LEU	CB-CG-CD1	7.62	123.96	111.00
3	P	89	LEU	CB-CG-CD2	7.55	123.84	111.00
3	C	179	LEU	CA-CB-CG	7.42	132.38	115.30
13	O	751	LEU	CA-CB-CG	7.31	132.12	115.30
13	O	117	ASP	CB-CG-OD1	-7.30	111.73	118.30
13	O	616	LEU	CA-CB-CG	7.10	131.62	115.30
12	N	477	PRO	N-CA-CB	7.05	111.76	103.30
4	D	23	PRO	N-CA-CB	7.03	111.74	103.30
12	N	63	ARG	C-N-CA	7.02	137.05	122.30
1	A	1415	LEU	CA-CB-CG	6.96	131.31	115.30
13	O	117	ASP	CB-CG-OD2	6.81	124.43	118.30
8	I	223	VAL	CB-CA-C	-6.78	98.51	111.40
12	N	219	PRO	N-CA-CB	6.74	111.39	103.30
13	O	632	LEU	CA-CB-CG	6.65	130.59	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	620	PHE	CG-CD1-CE1	6.53	127.98	120.80
9	J	188	LEU	CA-CB-CG	6.47	130.18	115.30
1	A	1168	LEU	CA-CB-CG	6.38	129.97	115.30
13	O	730	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	1748	LEU	CA-CB-CG	6.26	129.70	115.30
1	A	1409	LEU	CB-CG-CD2	6.26	121.64	111.00
12	N	215	LEU	CA-CB-CG	6.20	129.56	115.30
9	K	451	LEU	CB-CG-CD2	-6.19	100.48	111.00
10	L	171	PRO	N-CA-CB	6.17	110.70	103.30
13	O	625	LEU	CA-CB-CG	6.14	129.42	115.30
1	A	1556	LEU	CA-CB-CG	6.11	129.36	115.30
3	C	89	LEU	CA-CB-CG	6.11	129.35	115.30
16	Y	59	LEU	CA-CB-CG	6.11	129.34	115.30
16	X	110	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	1409	LEU	CA-CB-CG	5.99	129.08	115.30
12	N	16	PRO	N-CA-CB	5.98	110.48	103.30
12	N	386	LEU	CA-CB-CG	5.95	128.99	115.30
8	I	11	PHE	CB-CG-CD1	-5.95	116.64	120.80
1	A	1934	PRO	N-CA-CB	5.95	110.43	103.30
1	A	1925	PRO	N-CA-CB	5.94	110.43	103.30
12	N	489	PRO	N-CA-CB	5.93	110.41	103.30
1	A	1603	LEU	CA-CB-CG	5.90	128.86	115.30
16	Y	146	TYR	CB-CG-CD1	-5.89	117.46	121.00
6	F	689	LEU	CA-CB-CG	5.89	128.85	115.30
12	N	197	PRO	N-CA-CB	5.88	110.36	103.30
8	I	602	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	442	LEU	CA-CB-CG	5.84	128.73	115.30
13	O	608	LEU	CA-CB-CG	5.83	128.71	115.30
3	C	556	LEU	CA-CB-CG	5.83	128.70	115.30
6	H	682	LEU	CA-CB-CG	5.82	128.68	115.30
14	R	83	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	214	LEU	CA-CB-CG	5.79	128.61	115.30
9	J	23	LEU	CA-CB-CG	5.78	128.58	115.30
1	A	1770	LEU	CA-CB-CG	5.76	128.56	115.30
1	A	1670	GLY	C-N-CD	-5.76	107.92	120.60
6	F	768	PRO	N-CA-CB	5.76	110.21	103.30
8	I	589	THR	CA-CB-CG2	-5.76	104.34	112.40
16	X	446	LEU	CA-CB-CG	5.74	128.51	115.30
12	N	395	ASP	N-CA-C	5.72	126.44	111.00
1	A	412	LEU	CA-CB-CG	5.70	128.40	115.30
13	O	408	LEU	CA-CB-CG	5.69	128.38	115.30
13	O	574	LEU	CA-CB-CG	5.64	128.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	N	125	TYR	C-N-CA	5.59	135.68	121.70
1	A	271	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	651	PRO	N-CA-CB	5.58	110.00	103.30
16	Y	146	TYR	CB-CG-CD2	5.57	124.34	121.00
12	N	63	ARG	N-CA-C	5.57	126.03	111.00
16	X	418	LEU	CA-CB-CG	5.55	128.06	115.30
12	N	482	PRO	N-CA-CB	5.54	109.94	103.30
1	A	1313	LEU	CA-CB-CG	5.53	128.03	115.30
6	F	118	LEU	CA-CB-CG	5.53	128.02	115.30
16	X	201	LEU	CA-CB-CG	5.52	127.99	115.30
8	I	11	PHE	CB-CG-CD2	5.50	124.65	120.80
16	Y	199	CYS	N-CA-C	5.49	125.82	111.00
16	Y	446	LEU	CA-CB-CG	5.48	127.91	115.30
3	C	38	LEU	CA-CB-CG	5.45	127.83	115.30
8	I	307	LEU	CA-CB-CG	5.45	127.83	115.30
3	P	38	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	793	LEU	CA-CB-CG	5.43	127.79	115.30
13	O	563	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	1405	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	1609	LEU	CA-CB-CG	-5.39	102.91	115.30
3	P	358	LEU	CB-CA-C	5.37	120.39	110.20
16	Y	82	TYR	CB-CG-CD1	5.37	124.22	121.00
8	I	603	ARG	NE-CZ-NH1	5.35	122.97	120.30
3	C	54	TRP	CB-CA-C	-5.33	99.75	110.40
8	I	45	LEU	CB-CG-CD2	5.33	120.06	111.00
6	H	617	LEU	CA-CB-CG	5.30	127.50	115.30
8	I	606	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	773	LEU	CA-CB-CG	5.29	127.46	115.30
3	C	306	LEU	CA-CB-CG	5.28	127.43	115.30
1	A	1227	LEU	CA-CB-CG	5.27	127.42	115.30
12	N	484	PRO	N-CA-CB	5.27	109.62	103.30
3	P	172	LEU	CA-CB-CG	5.23	127.34	115.30
7	G	14	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	1882	LEU	CA-CB-CG	5.21	127.29	115.30
9	J	225	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	1059	ASP	CB-CG-OD2	5.20	122.98	118.30
16	Y	418	LEU	CA-CB-CG	5.20	127.25	115.30
15	S	833	ASP	CB-CG-OD2	5.19	122.97	118.30
16	Y	466	ASP	CB-CG-OD2	5.18	122.97	118.30
8	I	664	ARG	NE-CZ-NH1	5.18	122.89	120.30
12	N	522	LEU	CA-CB-CG	5.18	127.21	115.30
9	J	376	LEU	CA-CB-CG	5.17	127.18	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	X	466	ASP	CB-CG-OD2	5.16	122.94	118.30
16	X	146	TYR	CB-CG-CD1	-5.15	117.91	121.00
12	N	63	ARG	CA-C-N	5.14	126.49	116.20
3	P	229	MET	CG-SD-CE	5.14	108.42	100.20
1	A	797	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	1188	LEU	CA-CB-CG	5.12	127.07	115.30
9	K	188	LEU	CA-CB-CG	5.11	127.06	115.30
6	F	118	LEU	CB-CG-CD1	5.11	119.69	111.00
9	J	134	LEU	CA-CB-CG	5.10	127.04	115.30
1	A	1538	LEU	CA-CB-CG	5.10	127.03	115.30
16	Y	546	LEU	CA-CB-CG	5.10	127.03	115.30
9	K	451	LEU	CA-CB-CG	5.10	127.02	115.30
6	H	82	LEU	CA-CB-CG	5.06	126.94	115.30
13	O	322	LEU	CA-CB-CG	5.06	126.94	115.30
3	C	89	LEU	CB-CG-CD2	5.06	119.60	111.00
3	P	306	LEU	CA-CB-CG	5.05	126.92	115.30
13	O	268	PHE	CB-CG-CD2	5.03	124.32	120.80
1	A	1533	LEU	CA-CB-CG	5.03	126.87	115.30
8	I	683	TYR	CB-CG-CD2	5.03	124.02	121.00
9	J	232	ASP	CB-CG-OD1	5.03	122.82	118.30
9	K	7	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	GLN	Peptide
6	F	565	ASN	Peptide
6	H	565	ASN	Peptide
8	I	489	PRO	Peptide
8	I	658	GLY	Peptide
8	I	727	PHE	Peptide
9	J	220	ILE	Peptide
10	L	36	CYS	Peptide
11	M	62	LEU	Peptide
12	N	143	GLY	Peptide
12	N	367	ARG	Peptide
12	N	387	LEU	Peptide
12	N	394	CYS	Peptide
3	P	147	LYS	Peptide
16	Y	199	CYS	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	10925	0	10669	471	0
2	B	649	0	595	26	0
3	C	4306	0	4273	274	0
3	P	4039	0	3989	120	0
4	D	436	0	396	27	0
5	E	450	0	435	12	0
6	F	3923	0	3819	115	0
6	H	3853	0	3793	110	0
7	G	213	0	220	16	0
7	W	213	0	220	9	0
8	I	5709	0	5597	188	0
9	J	4047	0	3949	185	0
9	K	3988	0	3908	148	0
10	L	1435	0	1382	43	0
11	M	493	0	469	17	0
12	N	4837	0	4534	155	0
13	O	5395	0	5429	231	0
14	R	2869	0	2772	59	0
15	S	72	0	71	10	0
16	X	3767	0	3819	136	0
16	Y	3859	0	3908	150	0
17	B	3	0	0	0	0
All	All	65481	0	64247	2216	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 (2216) 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)
12:N:362:LYS:HG3	12:N:410:LEU:CD2	1.38	1.52
9:J:223:SER:CB	9:J:228:GLN:HE21	1.29	1.44
12:N:362:LYS:CG	12:N:410:LEU:HD23	1.60	1.31
12:N:362:LYS:CB	12:N:410:LEU:HD21	1.67	1.24
14:R:177:ASP:OD2	15:S:834:ILE:HD11	1.30	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1332:GLY:O	1:A:1358:ILE:HD12	1.34	1.23
12:N:362:LYS:CG	12:N:410:LEU:CD2	2.15	1.23
3:C:98:GLU:OE1	3:C:101:ARG:HB3	1.39	1.21
13:O:42:ASN:ND2	13:O:43:GLU:OE1	1.72	1.21
16:Y:42:ARG:HA	16:Y:82:TYR:CE2	1.75	1.20
14:R:177:ASP:CG	15:S:834:ILE:HD11	1.64	1.17
9:J:223:SER:CB	9:J:228:GLN:NE2	2.07	1.17
1:A:1229:SER:HA	1:A:1235:LEU:HG	1.17	1.16
9:J:383:ASN:HB3	9:J:386:LEU:HD13	1.24	1.16
9:K:250:CYS:SG	9:K:274:THR:HG21	1.85	1.14
1:A:39:LEU:HD13	13:O:248:PRO:HB3	1.30	1.11
9:J:223:SER:HB2	9:J:228:GLN:NE2	1.60	1.11
1:A:23:PHE:HB2	1:A:111:LEU:HD22	1.33	1.11
16:X:37:VAL:CG2	16:Y:232:ASN:HB2	1.81	1.09
3:C:101:ARG:HG2	3:C:101:ARG:HH11	1.02	1.08
1:A:1332:GLY:O	1:A:1358:ILE:CD1	2.01	1.07
9:K:129:LYS:O	9:K:133:CYS:SG	2.13	1.06
14:R:128:ALA:HB1	14:R:129:LYS:HA	1.37	1.06
6:H:479:TYR:C	6:H:480:ASN:N	2.09	1.05
8:I:56:TRP:CE3	8:I:98:PRO:HB3	1.92	1.04
14:R:177:ASP:OD2	15:S:834:ILE:CD1	2.06	1.03
16:X:37:VAL:HG21	16:Y:232:ASN:CB	1.89	1.03
12:N:362:LYS:HB2	12:N:410:LEU:HD21	1.39	1.02
3:C:251:TYR:HA	3:C:254:LEU:HD12	1.38	1.02
16:X:235:TRP:NE1	16:Y:63:MET:HE1	1.75	1.02
16:X:235:TRP:HE1	16:Y:63:MET:HE1	1.22	1.01
1:A:1237:PRO:HB2	1:A:1238:PRO:HD3	1.40	1.01
9:J:454:VAL:O	9:J:458:LEU:HD12	1.59	1.01
16:X:37:VAL:HG21	16:Y:232:ASN:HB2	1.05	1.01
12:N:414:MET:SD	12:N:498:SER:HA	2.02	0.99
1:A:1225:THR:O	1:A:1229:SER:N	1.96	0.99
12:N:425:ARG:HG2	12:N:425:ARG:HH11	1.26	0.98
8:I:209:CYS:SG	8:I:584:HIS:CE1	2.56	0.98
9:J:254:THR:HG23	9:J:271:HIS:HD2	1.27	0.97
14:R:177:ASP:CG	15:S:834:ILE:CD1	2.33	0.97
1:A:48:LEU:HD22	1:A:49:TRP:N	1.80	0.97
8:I:279:ILE:HD11	8:I:337:ILE:HA	1.44	0.96
9:K:263:PHE:HZ	9:K:290:LYS:HG2	1.30	0.96
12:N:538:GLU:HG2	12:N:561:LEU:HG	1.44	0.96
12:N:211:ARG:O	12:N:215:LEU:HG	1.66	0.96
3:C:98:GLU:OE2	3:C:101:ARG:HD3	1.66	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:233:PHE:CE2	3:P:237:ILE:HD11	1.99	0.96
9:J:223:SER:HB2	9:J:228:GLN:HE21	0.80	0.96
1:A:1433:ILE:H	1:A:1433:ILE:HD13	1.26	0.95
3:P:487:ALA:HB1	3:P:519:TYR:CD1	2.02	0.95
9:J:332:THR:HA	9:J:363:LEU:HD21	1.46	0.95
16:X:235:TRP:CD1	16:Y:63:MET:CE	2.50	0.94
6:F:130:ARG:HG3	16:Y:506:GLN:HB2	1.48	0.94
1:A:248:PHE:HB2	1:A:430:VAL:CG2	1.97	0.94
16:X:355:TYR:CZ	16:X:385:ASN:HB3	2.02	0.94
8:I:144:THR:HG21	8:I:159:GLU:HA	1.50	0.93
8:I:34:LEU:HD12	8:I:46:LEU:HD21	1.51	0.93
13:O:435:SER:HB3	13:O:654:ASP:HB2	1.50	0.93
3:C:283:LEU:HD13	3:C:306:LEU:CD1	1.97	0.93
16:Y:42:ARG:HG3	16:Y:82:TYR:OH	1.67	0.92
12:N:362:LYS:CB	12:N:410:LEU:CD2	2.44	0.92
3:C:296:ARG:CG	3:C:296:ARG:HH11	1.82	0.92
16:X:201:LEU:HD11	16:Y:40:HIS:HB3	1.52	0.92
3:C:441:GLU:HA	3:C:444:GLU:HB3	1.52	0.92
8:I:209:CYS:SG	8:I:584:HIS:ND1	2.43	0.92
3:C:54:TRP:HZ3	3:C:207:LEU:HD22	1.32	0.91
8:I:26:LEU:HB3	8:I:37:LEU:HB3	1.52	0.91
8:I:266:ASN:HA	8:I:526:LYS:HZ3	1.36	0.91
3:C:296:ARG:HH12	3:C:299:ASN:H	1.17	0.91
9:K:214:LYS:O	9:K:216:SER:N	2.04	0.91
3:C:296:ARG:HH11	3:C:296:ARG:HG3	1.34	0.91
3:C:414:MET:HG2	13:O:330:ILE:HG12	1.54	0.90
16:X:267:LEU:HD11	16:Y:59:LEU:HD11	1.49	0.90
1:A:1636:VAL:HB	1:A:1663:LEU:HD11	1.51	0.90
9:J:476:PRO:HG2	3:P:182:LEU:HG	1.54	0.90
9:K:174:HIS:CE1	9:K:211:LYS:HD3	2.06	0.90
13:O:55:MET:SD	13:O:58:ARG:CZ	2.60	0.90
1:A:1739:SER:HA	1:A:1740:ALA:HB3	1.54	0.90
9:K:472:LEU:HG	9:K:481:THR:HG21	1.52	0.90
16:X:235:TRP:NE1	16:Y:63:MET:CE	2.36	0.89
1:A:1145:LEU:HD22	1:A:1611:VAL:HG21	1.54	0.89
9:J:263:PHE:HZ	9:J:290:LYS:HG2	1.37	0.89
13:O:55:MET:SD	13:O:58:ARG:NH1	2.46	0.89
3:P:233:PHE:CZ	3:P:237:ILE:HD11	2.07	0.89
3:C:113:LYS:H	3:C:113:LYS:HE2	1.38	0.89
1:A:1255:VAL:HG11	1:A:1606:LEU:HD21	1.55	0.88
9:J:185:LEU:HD12	9:J:209:LEU:HD21	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PHE:HB3	1:A:257:MET:CB	2.03	0.88
8:I:514:PHE:HE2	13:O:440:GLN:HA	1.36	0.88
3:C:101:ARG:HG2	3:C:101:ARG:NH1	1.80	0.88
9:J:354:MET:HE1	9:J:374:ILE:HA	1.55	0.87
12:N:289:PHE:HA	12:N:292:TRP:HB3	1.56	0.87
3:C:46:ARG:HH21	3:C:48:LEU:HD11	1.39	0.87
3:C:234:LEU:HD23	3:C:250:LYS:HE3	1.56	0.87
4:D:9:PHE:HD2	13:O:346:TRP:CZ3	1.91	0.87
1:A:433:THR:HG22	1:A:481:PRO:HB3	1.55	0.87
9:J:295:TYR:OH	9:K:54:HIS:HB2	1.74	0.86
16:Y:42:ARG:HA	16:Y:82:TYR:HE2	1.34	0.86
1:A:1492:ALA:O	1:A:1496:MET:HG3	1.75	0.86
3:C:308:TYR:CD2	14:R:78:ARG:HD2	2.11	0.86
8:I:209:CYS:HG	8:I:584:HIS:CE1	1.92	0.86
1:A:1567:LEU:HD22	1:A:1574:LEU:HD23	1.58	0.86
1:A:1239:THR:HB	1:A:1240:SER:HA	1.56	0.86
1:A:1877:LEU:HD22	1:A:1881:GLN:HE22	1.39	0.86
1:A:1086:MET:SD	1:A:1564:LEU:HD13	2.16	0.86
1:A:1089:LEU:HD11	1:A:1611:VAL:HG23	1.57	0.85
1:A:252:ASP:HB3	1:A:253:PRO:HD3	1.57	0.85
8:I:186:GLU:OE2	8:I:197:ARG:NH1	2.10	0.85
9:J:254:THR:HG23	9:J:271:HIS:CD2	2.10	0.85
3:C:46:ARG:HH22	3:C:170:PHE:HB3	1.42	0.84
9:K:292:VAL:HG21	11:M:57:TRP:HB3	1.60	0.84
16:X:235:TRP:HE1	16:Y:63:MET:CE	1.89	0.84
16:X:267:LEU:HD11	16:Y:59:LEU:CD1	2.08	0.84
1:A:433:THR:CG2	1:A:481:PRO:HB3	2.09	0.83
3:C:449:LEU:HD22	3:C:476:LEU:CD2	2.09	0.83
16:Y:42:ARG:HA	16:Y:82:TYR:CZ	2.13	0.83
8:I:56:TRP:HZ3	8:I:58:PHE:HB2	1.42	0.83
1:A:1573:SER:OG	1:A:1656:LEU:HD22	1.77	0.83
1:A:1229:SER:CA	1:A:1235:LEU:HG	2.05	0.83
8:I:209:CYS:HG	8:I:584:HIS:HD1	1.27	0.82
9:J:441:VAL:HG21	9:J:444:TRP:HD1	1.42	0.82
9:K:383:ASN:HB3	9:K:386:LEU:HD13	1.60	0.82
12:N:531:PHE:O	12:N:533:PHE:HA	1.80	0.82
1:A:44:PRO:HA	1:A:45:ALA:HB2	1.62	0.82
13:O:231:LEU:HD23	13:O:236:LEU:HA	1.62	0.82
1:A:210:MET:HB3	1:A:223:LEU:HB2	1.63	0.81
3:C:61:SER:HB2	3:C:262:SER:HB2	1.62	0.81
3:C:283:LEU:HD13	3:C:306:LEU:HD11	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:406:HIS:CE1	9:J:450:ASN:HD22	1.98	0.81
13:O:578:GLU:HA	13:O:616:LEU:HD11	1.60	0.81
16:X:235:TRP:CD1	16:Y:63:MET:HE1	2.15	0.81
1:A:248:PHE:HB2	1:A:430:VAL:HG23	1.61	0.81
3:C:95:ASP:O	3:C:97:LYS:HG2	1.79	0.81
13:O:539:ASN:HD22	13:O:542:GLU:CB	1.93	0.81
1:A:185:TYR:HE1	1:A:273:ARG:HH11	1.28	0.80
9:J:167:PHE:O	9:J:170:LEU:HD23	1.80	0.80
8:I:356:SER:HB3	8:I:397:ILE:HG12	1.63	0.80
3:C:175:TYR:O	3:C:179:LEU:HD23	1.81	0.80
1:A:1373:MET:HA	1:A:1376:LEU:HD12	1.63	0.80
3:C:285:ILE:O	3:C:288:GLU:OE1	2.00	0.80
6:F:707:PHE:HB2	6:F:729:LEU:HD11	1.63	0.80
12:N:368:THR:OG1	12:N:369:ASP:HA	1.81	0.80
12:N:362:LYS:CA	12:N:410:LEU:HD21	2.11	0.79
1:A:1177:MET:HB2	1:A:1207:GLY:HA2	1.64	0.79
16:Y:84:ALA:HB1	16:Y:100:TYR:CE2	2.17	0.79
9:J:397:ILE:HG22	9:J:398:ALA:H	1.48	0.79
13:O:32:PRO:O	13:O:35:ILE:HG22	1.82	0.79
1:A:248:PHE:HB2	1:A:430:VAL:HG21	1.65	0.78
8:I:266:ASN:HA	8:I:526:LYS:NZ	1.97	0.78
13:O:539:ASN:HD22	13:O:542:GLU:HB3	1.45	0.78
8:I:73:TRP:CZ2	8:I:80:LEU:HD22	2.17	0.78
9:J:37:PRO:HB3	9:J:69:TYR:CE2	2.19	0.78
10:L:50:LEU:O	10:L:154:ARG:HD3	1.84	0.78
12:N:165:THR:H	12:N:166:PRO:HA	1.46	0.78
8:I:177:VAL:HG12	8:I:208:LEU:HD13	1.64	0.78
12:N:519:TYR:OH	12:N:541:ASN:HB3	1.83	0.78
1:A:1320:ASN:HB3	1:A:1323:GLU:HG2	1.65	0.78
1:A:1360:VAL:HB	1:A:1364:CYS:HB2	1.66	0.78
2:B:39:VAL:CB	2:B:43:ASP:HB2	2.14	0.78
11:M:2:ASP:HB2	3:P:123:TYR:CE2	2.18	0.78
11:M:2:ASP:HB2	3:P:123:TYR:HE2	1.49	0.78
13:O:581:ILE:HD11	13:O:619:LEU:HB3	1.66	0.78
1:A:1093:HIS:ND1	1:A:1151:SER:HB3	1.99	0.78
6:F:7:PRO:HG3	6:H:455:GLN:HG2	1.66	0.78
6:F:537:GLU:OE1	6:F:602:TYR:HB3	1.84	0.78
3:P:61:SER:HB2	3:P:262:SER:HB2	1.66	0.77
16:Y:45:ALA:HB3	16:Y:82:TYR:CE2	2.19	0.77
12:N:165:THR:N	12:N:166:PRO:HA	2.00	0.77
3:P:373:HIS:O	3:P:377:GLU:HG2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:438:ALA:HA	14:R:83:ARG:HH11	1.48	0.77
3:C:449:LEU:HD22	3:C:476:LEU:HD21	1.64	0.77
3:C:309:VAL:HG23	14:R:78:ARG:HG3	1.67	0.77
3:C:403:TYR:HD2	3:C:435:MET:SD	2.08	0.77
16:X:199:CYS:SG	16:Y:44:MET:HG2	2.25	0.77
3:C:206:TRP:HZ3	3:C:233:PHE:CD2	2.02	0.77
16:X:235:TRP:CD1	16:Y:63:MET:HE3	2.19	0.77
8:I:679:ASP:OD1	8:I:703:ARG:NH2	2.18	0.77
3:C:440:GLY:O	3:C:442:CYS:N	2.17	0.77
1:A:1332:GLY:O	1:A:1358:ILE:CG1	2.32	0.77
8:I:514:PHE:CE2	13:O:440:GLN:HA	2.20	0.77
3:C:54:TRP:HH2	3:C:207:LEU:HD13	1.50	0.76
3:C:370:LEU:HG	14:R:79:TYR:HE1	1.49	0.76
3:C:373:HIS:O	3:C:377:GLU:HG2	1.85	0.76
8:I:224:SER:CB	8:I:229:SER:HA	2.14	0.76
1:A:248:PHE:HB3	1:A:257:MET:HB2	1.65	0.76
3:C:54:TRP:CH2	3:C:207:LEU:HD13	2.21	0.76
9:J:55:ARG:HH11	9:K:264:HIS:HA	1.50	0.76
3:P:313:LYS:HE3	3:P:344:ARG:HD2	1.66	0.76
3:C:413:LYS:O	3:C:415:PRO:HD2	1.86	0.76
1:A:1791:ILE:HB	13:O:598:THR:HG21	1.67	0.76
9:J:441:VAL:HG21	9:J:444:TRP:CD1	2.19	0.76
3:C:46:ARG:NH2	3:C:170:PHE:HB3	2.01	0.75
12:N:213:TYR:N	12:N:215:LEU:H	1.82	0.75
6:H:653:LEU:HD22	9:K:523:ILE:HG21	1.66	0.75
3:P:487:ALA:HB1	3:P:519:TYR:HD1	1.50	0.75
1:A:1573:SER:HB2	1:A:1617:ARG:HH21	1.50	0.75
6:H:707:PHE:HB2	6:H:729:LEU:HD11	1.67	0.75
3:P:494:ILE:HG12	3:P:512:ALA:HB1	1.69	0.75
1:A:1409:LEU:HG	1:A:1470:LEU:HD23	1.69	0.75
9:K:177:THR:HG22	9:K:365:LYS:HB3	1.69	0.75
8:I:88:LYS:O	8:I:106:VAL:HG22	1.87	0.74
13:O:35:ILE:HG21	13:O:158:LEU:HD13	1.68	0.74
16:Y:271:VAL:HG12	16:Y:304:LEU:HD21	1.68	0.74
8:I:65:GLY:H	8:I:84:LEU:HG	1.51	0.74
16:X:452:LEU:HB3	16:X:461:ALA:HB2	1.70	0.74
1:A:39:LEU:HD13	13:O:248:PRO:CB	2.15	0.74
1:A:1433:ILE:HD13	1:A:1433:ILE:N	2.02	0.74
3:C:296:ARG:HH12	3:C:299:ASN:N	1.85	0.74
3:C:94:PHE:O	3:C:97:LYS:HB3	1.86	0.74
1:A:1877:LEU:HD22	1:A:1881:GLN:NE2	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:MET:O	3:C:122:ARG:HG2	1.88	0.74
3:C:114:ALA:O	3:C:116:PHE:N	2.20	0.74
9:K:45:GLN:HA	9:K:45:GLN:HE21	1.51	0.74
1:A:175:PHE:CD1	1:A:191:ARG:HG3	2.23	0.73
3:P:382:SER:HA	3:P:385:ILE:HD12	1.69	0.73
1:A:1293:SER:HB3	1:A:1600:ARG:O	1.88	0.73
3:C:115:TYR:OH	3:C:161:LYS:CD	2.36	0.73
10:L:126:ASP:HB2	10:L:132:THR:HG23	1.70	0.73
1:A:1229:SER:HA	1:A:1235:LEU:CG	2.09	0.73
3:C:99:TYR:HE2	3:C:128:LYS:HG3	1.52	0.73
8:I:26:LEU:CB	8:I:37:LEU:HB3	2.18	0.73
12:N:531:PHE:HB3	12:N:534:SER:HB2	1.71	0.73
16:X:62:THR:HG21	16:Y:270:ASN:HA	1.69	0.73
16:X:407:LEU:HD22	16:X:437:LEU:HD21	1.71	0.73
3:C:77:THR:OG1	3:C:79:GLU:OE1	2.06	0.73
9:J:354:MET:CE	9:J:354:MET:HA	2.19	0.73
1:A:431:PHE:O	1:A:431:PHE:CD1	2.42	0.73
16:Y:466:ASP:OD1	16:Y:482:LYS:HE3	1.88	0.73
4:D:9:PHE:HD2	13:O:346:TRP:HZ3	1.34	0.73
1:A:1470:LEU:HA	1:A:1522:SER:OG	1.89	0.73
16:Y:452:LEU:HB3	16:Y:461:ALA:HB2	1.70	0.73
6:F:502:LEU:HB3	6:F:525:VAL:HG22	1.69	0.72
8:I:48:ARG:HG3	8:I:55:VAL:HG22	1.71	0.72
14:R:177:ASP:OD1	15:S:834:ILE:HD11	1.88	0.72
13:O:652:LEU:HD23	13:O:660:LYS:HG3	1.70	0.72
1:A:793:LEU:HD22	1:A:794:ALA:HA	1.71	0.72
3:C:173:TYR:CD1	3:C:202:HIS:HE1	2.07	0.72
10:L:86:ASP:HB3	10:L:89:TYR:HB2	1.71	0.72
3:C:96:VAL:HG21	3:P:53:LYS:HD3	1.72	0.72
5:E:63:VAL:HG21	16:Y:364:LYS:HD2	1.70	0.72
8:I:674:VAL:O	8:I:703:ARG:NH1	2.22	0.72
9:J:465:LEU:HA	9:J:488:ILE:HD12	1.71	0.72
1:A:248:PHE:HB3	1:A:257:MET:HB3	1.70	0.72
1:A:1848:VAL:O	1:A:1852:ILE:HG12	1.90	0.72
6:H:502:LEU:HB3	6:H:525:VAL:HG22	1.72	0.72
8:I:46:LEU:HD22	8:I:56:TRP:HE1	1.55	0.72
3:P:271:VAL:HG22	3:P:302:THR:HG21	1.72	0.71
1:A:1791:ILE:HB	13:O:598:THR:CG2	2.21	0.71
6:H:703:PRO:HB3	6:H:733:VAL:HG21	1.71	0.71
6:H:765:ASP:OD1	16:X:397:ARG:HG2	1.90	0.71
9:K:63:ARG:HB2	9:K:65:LEU:CD1	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:231:VAL:HG21	8:I:557:TYR:CZ	2.25	0.71
1:A:87:VAL:HG12	1:A:88:ASP:N	2.05	0.71
3:C:296:ARG:HG3	3:C:296:ARG:NH1	2.06	0.71
3:C:407:GLN:O	3:C:411:ILE:HG12	1.91	0.71
9:J:254:THR:CG2	9:J:271:HIS:CD2	2.74	0.71
13:O:672:VAL:HG11	13:O:720:LEU:HD11	1.71	0.71
16:X:466:ASP:OD1	16:X:482:LYS:HE3	1.91	0.71
9:K:263:PHE:CZ	9:K:290:LYS:HG2	2.20	0.71
9:J:223:SER:OG	9:J:228:GLN:NE2	2.24	0.71
9:J:485:ILE:O	9:J:488:ILE:HG12	1.90	0.71
12:N:120:SER:O	12:N:124:PRO:HD3	1.91	0.71
3:P:276:ILE:HG22	3:P:277:ARG:N	2.06	0.71
6:F:130:ARG:HG3	16:Y:506:GLN:HE21	1.56	0.70
12:N:350:ASP:CB	12:N:351:PHE:HA	2.21	0.70
16:Y:77:TYR:HB2	16:Y:106:GLN:HG3	1.73	0.70
1:A:1405:LEU:HD13	1:A:1467:GLY:HA2	1.73	0.70
13:O:544:VAL:HA	13:O:547:LYS:HB3	1.73	0.70
14:R:114:LYS:HE2	14:R:118:LEU:HD12	1.73	0.70
6:F:738:LEU:HD12	14:R:494:ILE:HG12	1.72	0.70
6:H:685:SER:O	6:H:689:LEU:HD12	1.92	0.70
3:P:407:GLN:O	3:P:411:ILE:HG12	1.91	0.70
6:H:130:ARG:HH12	9:K:473:VAL:HG22	1.55	0.70
3:C:231:GLU:O	3:C:250:LYS:NZ	2.25	0.70
3:C:283:LEU:CD1	3:C:306:LEU:HD11	2.20	0.70
8:I:48:ARG:HG3	8:I:55:VAL:CG2	2.21	0.70
9:J:254:THR:CG2	9:J:271:HIS:HD2	2.01	0.70
3:C:53:LYS:HD3	3:P:96:VAL:HG21	1.73	0.70
6:H:689:LEU:HD11	6:H:712:VAL:HG12	1.72	0.70
1:A:1777:GLU:HA	1:A:1780:THR:HG22	1.74	0.70
9:J:305:VAL:HG11	11:M:31:ILE:HD11	1.74	0.70
1:A:1239:THR:CB	1:A:1240:SER:HA	2.22	0.70
1:A:641:TRP:HD1	1:A:663:CYS:HB2	1.56	0.70
3:C:99:TYR:CE2	3:C:128:LYS:HG3	2.27	0.70
3:C:259:PHE:HB3	3:C:265:ILE:HD12	1.74	0.70
8:I:56:TRP:CE3	8:I:98:PRO:CB	2.74	0.70
1:A:1177:MET:HB2	1:A:1207:GLY:CA	2.22	0.69
8:I:214:LEU:O	8:I:238:THR:OG1	2.10	0.69
8:I:269:LEU:HB2	8:I:526:LYS:HZ2	1.56	0.69
3:P:180:ARG:HG3	3:P:212:LEU:HD21	1.74	0.69
16:X:170:LYS:HA	16:Y:49:LEU:HD21	1.74	0.69
1:A:594:ARG:HB3	1:A:606:ARG:HE	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:TYR:HB2	1:A:1208:LEU:HD11	1.74	0.69
3:C:54:TRP:CZ3	3:C:207:LEU:HD22	2.22	0.69
12:N:663:GLN:HE21	12:N:695:ARG:HG3	1.57	0.69
16:X:170:LYS:HA	16:Y:49:LEU:CD2	2.22	0.69
1:A:272:ARG:O	1:A:407:LEU:HA	1.92	0.69
3:C:477:HIS:HB3	3:C:486:ALA:HB2	1.74	0.69
4:D:44:ILE:HA	4:D:47:LYS:HG2	1.74	0.69
8:I:116:MET:SD	8:I:210:LEU:HG	2.33	0.69
3:C:234:LEU:HB3	3:C:250:LYS:NZ	2.06	0.69
4:D:5:PHE:CE1	13:O:390:PHE:HZ	2.11	0.69
6:F:554:VAL:HG22	9:K:285:PHE:CD2	2.28	0.69
6:H:696:ILE:HG13	6:H:705:CYS:SG	2.33	0.69
1:A:1209:LEU:HD22	1:A:1228:LEU:HD23	1.75	0.69
7:G:6:PRO:HB3	9:J:406:HIS:CD2	2.27	0.69
1:A:125:GLN:HE21	1:A:179:ASN:HA	1.58	0.69
3:C:234:LEU:HB3	3:C:250:LYS:HZ1	1.57	0.69
8:I:24:ILE:O	8:I:569:LEU:HD22	1.92	0.69
16:X:201:LEU:HD11	16:Y:40:HIS:CB	2.22	0.69
8:I:353:GLN:HA	8:I:353:GLN:HE21	1.56	0.69
12:N:76:VAL:O	12:N:80:GLN:HB3	1.93	0.69
16:Y:503:LEU:O	16:Y:506:GLN:NE2	2.26	0.69
1:A:1237:PRO:HB2	1:A:1238:PRO:CD	2.20	0.68
1:A:1606:LEU:HD23	1:A:1609:LEU:HD13	1.75	0.68
8:I:279:ILE:CD1	8:I:337:ILE:HA	2.21	0.68
13:O:114:ASP:HA	13:O:117:ASP:OD1	1.94	0.68
13:O:426:THR:O	13:O:430:ARG:HB2	1.94	0.68
13:O:512:GLN:OE1	13:O:512:GLN:HA	1.93	0.68
9:K:184:LEU:O	9:K:188:LEU:HD23	1.93	0.68
1:A:629:LEU:HB2	1:A:630:PRO:HD2	1.76	0.68
8:I:251:MET:HE2	8:I:379:LEU:HD13	1.74	0.68
9:J:332:THR:CA	9:J:363:LEU:HD21	2.22	0.68
16:X:52:ASN:HD22	16:Y:202:ALA:HB1	1.57	0.68
1:A:185:TYR:O	1:A:214:LEU:HD23	1.94	0.68
3:C:46:ARG:NH2	3:C:170:PHE:CG	2.62	0.68
13:O:114:ASP:O	13:O:117:ASP:OD1	2.12	0.68
3:P:477:HIS:HB3	3:P:486:ALA:HB2	1.76	0.68
16:X:503:LEU:O	16:X:506:GLN:NE2	2.27	0.68
1:A:1145:LEU:CD2	1:A:1611:VAL:HG21	2.23	0.68
6:F:703:PRO:HB3	6:F:733:VAL:HG21	1.74	0.68
3:P:487:ALA:CB	3:P:519:TYR:HD1	2.07	0.68
9:K:372:LEU:HD22	9:K:404:VAL:HG22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:81:ALA:HB2	8:I:92:LEU:HB3	1.76	0.67
12:N:407:LEU:HB2	12:N:417:LEU:HD12	1.75	0.67
3:P:409:TYR:HA	3:P:412:LEU:HD12	1.75	0.67
1:A:24:GLY:O	1:A:28:CYS:N	2.24	0.67
1:A:1877:LEU:HD13	1:A:1885:LEU:CD1	2.25	0.67
16:X:235:TRP:HD1	16:Y:63:MET:HE3	1.57	0.67
1:A:1141:VAL:HA	1:A:1178:ALA:HB2	1.77	0.67
3:C:46:ARG:NH2	3:C:170:PHE:CB	2.57	0.67
6:F:502:LEU:CB	6:F:525:VAL:HG22	2.24	0.67
6:F:533:VAL:HG13	6:F:568:GLU:OE1	1.94	0.67
3:P:244:ILE:HG12	3:P:276:ILE:HG13	1.76	0.67
3:C:259:PHE:HB3	3:C:265:ILE:CD1	2.25	0.67
3:P:385:ILE:HD11	3:P:412:LEU:HD11	1.76	0.67
16:X:355:TYR:CE1	16:X:385:ASN:HB3	2.29	0.67
6:H:502:LEU:CB	6:H:525:VAL:HG22	2.25	0.67
9:J:263:PHE:HZ	9:J:290:LYS:CG	2.06	0.67
9:J:495:PHE:HD2	9:J:522:CYS:HG	1.41	0.67
9:K:210:LYS:O	9:K:212:TYR:N	2.23	0.67
13:O:648:ILE:HA	13:O:651:ILE:HD12	1.77	0.67
3:C:119:MET:HA	3:C:122:ARG:HD2	1.76	0.67
3:C:273:TYR:HB3	3:C:282:ALA:HB2	1.77	0.67
3:C:370:LEU:HG	14:R:79:TYR:CE1	2.29	0.67
4:D:9:PHE:CD2	13:O:346:TRP:HZ3	2.11	0.67
9:J:477:GLN:O	9:J:508:LEU:HD13	1.95	0.67
1:A:1181:LEU:HB3	1:A:1611:VAL:HG11	1.76	0.67
1:A:1239:THR:HB	1:A:1240:SER:CA	2.25	0.67
3:C:279:ILE:H	3:C:279:ILE:HD12	1.60	0.67
13:O:146:LEU:HB2	13:O:151:VAL:HG23	1.77	0.67
16:X:271:VAL:HG12	16:X:304:LEU:HD21	1.75	0.67
8:I:73:TRP:CG	8:I:80:LEU:HD13	2.30	0.67
9:J:19:TYR:CD1	9:J:49:LEU:HD13	2.29	0.67
11:M:2:ASP:OD2	3:P:177:VAL:HG13	1.95	0.67
6:H:656:MET:O	6:H:660:LYS:HG3	1.94	0.66
8:I:574:PHE:CE1	8:I:576:TRP:HB2	2.30	0.66
8:I:574:PHE:HE1	8:I:576:TRP:HB2	1.60	0.66
1:A:44:PRO:HA	1:A:45:ALA:CB	2.25	0.66
7:G:3:ARG:HA	9:J:373:TYR:OH	1.95	0.66
1:A:210:MET:HB3	1:A:223:LEU:CB	2.24	0.66
1:A:1229:SER:HB3	1:A:1236:LEU:HA	1.78	0.66
12:N:333:TYR:HD1	12:N:364:CYS:HG	1.43	0.66
3:C:413:LYS:C	3:C:415:PRO:HD2	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:3:ARG:NH1	9:J:243:TYR:HD1	1.93	0.66
8:I:26:LEU:HB3	8:I:37:LEU:CB	2.24	0.66
3:P:283:LEU:HD13	3:P:306:LEU:HD11	1.76	0.66
9:K:285:PHE:HB2	9:K:308:TYR:CE1	2.29	0.66
13:O:490:LEU:HD13	13:O:511:ASP:HB2	1.77	0.66
16:Y:304:LEU:O	16:Y:308:MET:HG2	1.95	0.66
8:I:13:VAL:HG22	8:I:744:PHE:CE2	2.30	0.66
3:P:242:GLN:HE22	3:P:429:ARG:HG3	1.60	0.66
3:C:416:PHE:HB3	13:O:326:GLU:HG2	1.77	0.66
12:N:362:LYS:HG3	12:N:410:LEU:HD23	0.68	0.66
13:O:328:ILE:O	13:O:332:GLN:HG3	1.96	0.66
13:O:609:ALA:HA	13:O:612:LYS:HE3	1.76	0.66
3:C:308:TYR:HD2	14:R:78:ARG:HD2	1.57	0.66
1:A:1674:TRP:N	1:A:1674:TRP:CD1	2.64	0.66
3:C:236:HIS:O	3:C:239:THR:HG22	1.95	0.66
3:C:386:GLN:HE22	13:O:282:ILE:HG12	1.60	0.66
13:O:477:HIS:HB3	13:O:486:ALA:HB2	1.77	0.66
13:O:641:LEU:HG	13:O:670:CYS:HB3	1.77	0.65
1:A:1610:TYR:CD1	1:A:1610:TYR:C	2.69	0.65
9:J:285:PHE:HB2	9:J:308:TYR:CE1	2.31	0.65
9:K:254:THR:HG23	9:K:271:HIS:CD2	2.32	0.65
12:N:538:GLU:CG	12:N:561:LEU:HG	2.25	0.65
12:N:666:ILE:HG12	12:N:681:LEU:HD21	1.77	0.65
3:P:236:HIS:O	3:P:239:THR:HG22	1.96	0.65
1:A:668:MET:HG2	1:A:759:ILE:HG12	1.79	0.65
1:A:1209:LEU:HD13	1:A:1253:ALA:HB2	1.76	0.65
3:C:208:GLU:OE1	3:C:208:GLU:HA	1.97	0.65
3:C:438:ALA:HA	14:R:83:ARG:NH1	2.11	0.65
13:O:343:CYS:O	13:O:347:LEU:HB2	1.97	0.65
8:I:269:LEU:HB2	8:I:526:LYS:NZ	2.11	0.65
9:J:55:ARG:NH1	9:K:264:HIS:HA	2.11	0.65
9:J:386:LEU:HD12	9:J:386:LEU:H	1.59	0.65
1:A:1255:VAL:HG21	1:A:1606:LEU:HD11	1.79	0.65
16:X:445:THR:O	16:X:449:THR:HG23	1.97	0.65
1:A:1193:ILE:HG23	1:A:1208:LEU:HD22	1.79	0.65
3:C:101:ARG:HH11	3:C:101:ARG:CG	1.92	0.65
16:Y:445:THR:O	16:Y:449:THR:HG23	1.96	0.65
1:A:799:LEU:O	1:A:801:PRO:HD2	1.97	0.65
8:I:73:TRP:CD1	8:I:80:LEU:HD13	2.31	0.65
9:J:263:PHE:CZ	9:J:290:LYS:HG2	2.27	0.65
1:A:1307:LEU:HD21	1:A:1579:SER:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:141:VAL:HG11	10:L:151:THR:HG21	1.78	0.64
14:R:209:TRP:HB2	15:S:831:LEU:HD13	1.77	0.64
1:A:1405:LEU:HD13	1:A:1467:GLY:CA	2.27	0.64
12:N:362:LYS:HA	12:N:410:LEU:HD21	1.79	0.64
1:A:185:TYR:CE1	1:A:273:ARG:HD3	2.33	0.64
16:Y:45:ALA:CB	16:Y:82:TYR:CE2	2.80	0.64
1:A:773:LEU:HD22	1:A:779:MET:HG3	1.79	0.64
6:F:550:VAL:HG21	9:K:289:HIS:CG	2.33	0.64
9:K:185:LEU:HA	9:K:188:LEU:HD21	1.79	0.64
13:O:420:ILE:O	13:O:424:GLN:N	2.26	0.64
6:H:89:GLU:HB2	6:H:124:VAL:HG11	1.80	0.64
6:H:478:SER:HA	6:H:633:ARG:HH22	1.61	0.64
8:I:15:GLY:O	8:I:743:VAL:N	2.27	0.64
8:I:206:LEU:HD22	8:I:570:PHE:CG	2.32	0.64
3:C:46:ARG:HH22	3:C:170:PHE:CB	2.11	0.64
3:C:475:LYS:HD2	3:C:490:TYR:OH	1.96	0.64
16:Y:349:SER:HB2	16:Y:358:ALA:HB2	1.80	0.64
8:I:72:ALA:O	8:I:80:LEU:HD12	1.97	0.64
9:K:19:TYR:CD1	9:K:49:LEU:HD13	2.33	0.64
9:K:300:VAL:HG12	9:K:333:TYR:OH	1.98	0.64
13:O:354:ARG:HD3	13:O:573:LYS:O	1.98	0.64
3:C:89:LEU:HD21	3:C:101:ARG:HH22	1.62	0.64
9:K:386:LEU:H	9:K:386:LEU:HD12	1.62	0.64
3:P:327:ASP:O	3:P:333:THR:HG21	1.98	0.64
3:C:93:TYR:CE2	3:C:101:ARG:NH2	2.65	0.64
3:C:389:ARG:HG2	13:O:279:ASP:HB3	1.80	0.64
3:P:273:TYR:HB3	3:P:282:ALA:HB2	1.80	0.64
2:B:14:TRP:HA	2:B:15:LEU:HG	1.80	0.63
8:I:67:GLU:O	8:I:85:ALA:N	2.25	0.63
13:O:220:ALA:HB2	13:O:256:LEU:HD21	1.80	0.63
1:A:15:ARG:HE	13:O:526:HIS:HB2	1.63	0.63
1:A:1413:LEU:HD22	1:A:1416:TRP:HZ3	1.63	0.63
3:C:115:TYR:OH	3:C:161:LYS:HD2	1.97	0.63
3:C:277:ARG:O	3:C:279:ILE:HD12	1.99	0.63
4:D:5:PHE:CZ	13:O:390:PHE:CZ	2.86	0.63
6:F:554:VAL:HG22	9:K:285:PHE:CE2	2.33	0.63
9:J:24:PHE:CE1	9:J:28:LYS:HE3	2.33	0.63
9:J:77:ALA:HB1	9:J:93:LEU:HD11	1.79	0.63
4:D:10:PRO:HD2	13:O:346:TRP:CE3	2.34	0.63
6:H:481:CYS:HB3	6:H:512:LEU:HD13	1.79	0.63
16:X:304:LEU:O	16:X:308:MET:HG2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:462:LYS:HG2	16:Y:485:LEU:HD13	1.80	0.63
1:A:78:LYS:HD3	1:A:592:HIS:HB2	1.80	0.63
3:C:409:TYR:HA	3:C:412:LEU:HD12	1.80	0.63
12:N:425:ARG:HG2	12:N:425:ARG:NH1	2.04	0.63
1:A:185:TYR:HE1	1:A:273:ARG:NH1	1.95	0.63
1:A:641:TRP:CD1	1:A:663:CYS:HB2	2.33	0.63
1:A:1638:TYR:N	1:A:1638:TYR:CD1	2.66	0.63
9:K:174:HIS:HA	9:K:211:LYS:HZ3	1.63	0.63
3:P:276:ILE:HG22	3:P:277:ARG:H	1.64	0.63
2:B:8:TRP:CD1	12:N:644:VAL:HG12	2.34	0.63
3:C:235:ALA:N	3:C:250:LYS:HZ2	1.97	0.63
9:J:429:LEU:HA	9:J:432:ILE:HG22	1.79	0.63
1:A:776:ASN:HD22	1:A:779:MET:HG2	1.64	0.63
1:A:1170:ASN:O	1:A:1173:ALA:HB3	1.99	0.63
1:A:1409:LEU:HD23	1:A:1471:SER:HA	1.81	0.63
9:J:219:VAL:HG12	9:J:221:PRO:HD3	1.80	0.62
16:X:462:LYS:HG2	16:X:485:LEU:HD13	1.81	0.62
1:A:585:HIS:HB3	1:A:598:GLU:O	1.99	0.62
3:C:327:ASP:O	3:C:333:THR:HG21	1.99	0.62
1:A:1218:GLY:N	1:A:1259:LEU:O	2.32	0.62
1:A:1595:HIS:NE2	1:A:1598:ASP:HB2	2.13	0.62
3:C:115:TYR:OH	3:C:161:LYS:HD3	1.98	0.62
7:G:4:ARG:HH21	9:J:345:ALA:HB1	1.63	0.62
13:O:275:LEU:HD11	13:O:307:LEU:HD13	1.82	0.62
8:I:231:VAL:HG21	8:I:557:TYR:CE1	2.34	0.62
16:X:104:LEU:HD11	16:X:142:MET:SD	2.39	0.62
1:A:950:GLY:H	1:A:1813:GLN:HG2	1.65	0.62
6:H:142:LEU:HD21	6:H:152:PHE:HB2	1.80	0.62
6:H:729:LEU:HD13	6:H:739:VAL:HG22	1.82	0.62
16:X:355:TYR:CE1	16:X:385:ASN:CB	2.82	0.62
16:Y:407:LEU:HD22	16:Y:437:LEU:HD21	1.81	0.62
2:B:14:TRP:HA	2:B:15:LEU:CG	2.30	0.62
3:C:265:ILE:O	3:C:269:ILE:HG12	1.99	0.62
9:J:167:PHE:HA	9:J:170:LEU:CD2	2.30	0.62
13:O:222:LEU:HB3	13:O:230:ALA:HB2	1.81	0.62
1:A:1536:LEU:HD23	1:A:1562:LEU:HD23	1.82	0.62
1:A:1877:LEU:HD13	1:A:1885:LEU:HD13	1.82	0.62
6:F:502:LEU:HA	6:F:505:ILE:HD12	1.82	0.62
9:K:250:CYS:SG	9:K:274:THR:CG2	2.76	0.62
1:A:1201:HIS:CE1	1:A:1203:MET:HB2	2.35	0.62
1:A:1323:GLU:HG3	1:A:1324:GLN:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1739:SER:HA	1:A:1740:ALA:CB	2.27	0.62
6:H:502:LEU:HA	6:H:505:ILE:HD12	1.82	0.62
8:I:607:ILE:HD12	8:I:607:ILE:H	1.65	0.62
12:N:404:ILE:HA	12:N:417:LEU:HD11	1.82	0.62
13:O:467:ALA:HB1	13:O:506:LEU:HD11	1.82	0.62
16:X:235:TRP:NE1	16:Y:63:MET:SD	2.73	0.62
3:C:58:LEU:HB3	3:C:259:PHE:HE2	1.65	0.61
6:H:673:CYS:O	6:H:677:VAL:HG23	2.00	0.61
8:I:28:TRP:NE1	8:I:723:ALA:O	2.30	0.61
9:K:472:LEU:HG	9:K:481:THR:CG2	2.27	0.61
12:N:258:ALA:HA	12:N:261:VAL:HG22	1.82	0.61
1:A:115:LYS:HD3	13:O:267:VAL:HG21	1.82	0.61
1:A:222:PRO:HD2	1:A:405:PRO:HA	1.82	0.61
1:A:1871:TYR:HB2	1:A:1877:LEU:HD21	1.81	0.61
6:F:541:THR:HG23	14:R:499:ARG:HG2	1.81	0.61
9:K:77:ALA:HB1	9:K:93:LEU:HD11	1.81	0.61
9:K:174:HIS:HA	9:K:211:LYS:NZ	2.14	0.61
3:P:39:ILE:HD13	3:P:201:LEU:HB2	1.81	0.61
3:P:304:SER:HB2	3:P:336:VAL:HG22	1.82	0.61
16:X:222:MET:O	16:X:226:VAL:HG23	2.00	0.61
9:K:280:LYS:HB3	9:K:283:GLU:HG2	1.82	0.61
9:K:372:LEU:HD11	9:K:407:GLU:HG3	1.80	0.61
13:O:657:ILE:HA	13:O:660:LYS:HB2	1.81	0.61
1:A:72:GLU:HG3	1:A:94:TYR:OH	2.00	0.61
1:A:1238:PRO:HA	1:A:1239:THR:C	2.21	0.61
1:A:1519:VAL:HG13	1:A:1520:LEU:N	2.15	0.61
3:C:486:ALA:HB3	3:C:515:TYR:OH	2.00	0.61
8:I:392:ALA:HB1	8:I:529:MET:HA	1.81	0.61
1:A:217:LEU:HD23	3:C:455:CYS:SG	2.41	0.61
1:A:594:ARG:HG2	1:A:608:THR:CG2	2.30	0.61
1:A:1378:THR:HG23	1:A:1380:ASN:H	1.65	0.61
3:P:58:LEU:HB3	3:P:259:PHE:HE2	1.66	0.61
1:A:445:LEU:HD22	1:A:479:ALA:H	1.65	0.61
3:C:262:SER:O	3:C:266:VAL:HG23	2.01	0.61
3:C:206:TRP:CZ3	3:C:233:PHE:CD2	2.88	0.61
9:J:397:ILE:HG22	9:J:398:ALA:N	2.16	0.61
9:K:429:LEU:HA	9:K:432:ILE:HG22	1.81	0.61
3:C:206:TRP:CZ3	3:C:233:PHE:CG	2.88	0.61
8:I:269:LEU:CB	8:I:526:LYS:HZ2	2.13	0.61
13:O:365:VAL:HG23	13:O:366:LYS:HD3	1.82	0.61
16:Y:222:MET:O	16:Y:226:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ILE:HG21	3:C:201:LEU:HG	1.80	0.61
5:E:94:TRP:HZ3	6:F:564:LYS:HD2	1.65	0.61
1:A:215:HIS:ND1	1:A:216:PRO:HD2	2.16	0.61
1:A:1877:LEU:CD2	1:A:1881:GLN:HE22	2.13	0.61
9:J:193:LEU:O	9:J:197:GLU:HB2	2.01	0.61
12:N:516:ILE:HG13	12:N:554:MET:HE2	1.83	0.61
13:O:348:TYR:CZ	13:O:361:LEU:HD11	2.36	0.61
16:X:349:SER:HB2	16:X:358:ALA:HB2	1.81	0.61
16:Y:305:ILE:HG23	16:Y:340:GLU:OE1	2.00	0.61
1:A:33:ASN:HA	1:A:99:MET:HE3	1.83	0.60
1:A:664:LEU:HA	1:A:667:MET:HB2	1.83	0.60
1:A:1262:GLN:HE22	1:A:1582:ALA:CB	2.14	0.60
1:A:1431:PRO:HG2	1:A:1434:ILE:HD12	1.83	0.60
3:C:277:ARG:NH1	14:R:77:ASP:OD2	2.30	0.60
6:F:729:LEU:HD13	6:F:739:VAL:HG22	1.82	0.60
13:O:274:LEU:HD11	13:O:306:ASN:HB3	1.81	0.60
1:A:188:LEU:HD12	1:A:211:PHE:O	2.01	0.60
3:C:39:ILE:HD13	3:C:201:LEU:HB3	1.83	0.60
7:G:3:ARG:NH1	9:J:243:TYR:CD1	2.68	0.60
13:O:619:LEU:O	13:O:623:THR:HG22	2.00	0.60
3:P:265:ILE:O	3:P:269:ILE:HG12	2.01	0.60
1:A:79:GLY:O	1:A:87:VAL:HG11	2.00	0.60
1:A:1145:LEU:HD22	1:A:1611:VAL:CG2	2.28	0.60
3:C:296:ARG:NH1	3:C:299:ASN:H	1.94	0.60
9:J:9:ARG:O	9:J:13:TYR:HD2	1.84	0.60
16:Y:251:ASN:O	16:Y:255:ILE:HG22	2.01	0.60
1:A:48:LEU:HD22	1:A:49:TRP:H	1.66	0.60
1:A:1516:LEU:O	1:A:1519:VAL:HG12	2.02	0.60
4:D:13:THR:HG22	13:O:255:TYR:HE2	1.67	0.60
16:X:100:TYR:CD1	16:X:138:VAL:HG13	2.37	0.60
3:C:352:LEU:O	3:C:356:ARG:HG3	2.01	0.60
9:K:77:ALA:CB	9:K:93:LEU:HD11	2.31	0.60
6:H:656:MET:HE2	9:K:523:ILE:HD13	1.83	0.60
8:I:364:SER:O	8:I:367:LYS:HB3	2.01	0.60
3:C:441:GLU:O	3:C:445:LYS:N	2.17	0.60
1:A:857:MET:CB	1:A:858:PRO:HD3	2.31	0.60
6:F:673:CYS:O	6:F:677:VAL:HG23	2.01	0.60
10:L:63:LEU:HD22	10:L:138:GLN:HE21	1.67	0.60
3:C:526:TRP:HE1	3:C:553:ILE:C	2.04	0.60
4:D:54:ILE:HD11	9:J:506:LEU:HB3	1.83	0.60
13:O:361:LEU:HD13	13:O:384:LEU:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:VAL:O	3:C:182:LEU:HD22	2.02	0.59
8:I:73:TRP:CE2	8:I:80:LEU:HD22	2.36	0.59
1:A:97:GLY:O	1:A:123:VAL:HG23	2.02	0.59
1:A:213:MET:HE1	1:A:216:PRO:HA	1.84	0.59
1:A:460:SER:HB3	1:A:467:ILE:HD11	1.83	0.59
6:H:481:CYS:CB	6:H:512:LEU:HD13	2.32	0.59
9:J:337:TRP:HB3	9:J:360:ALA:HB2	1.84	0.59
16:X:294:PHE:CE2	16:X:311:TYR:HB2	2.37	0.59
8:I:46:LEU:HD22	8:I:56:TRP:NE1	2.17	0.59
8:I:349:ILE:HG23	8:I:404:LEU:HD11	1.83	0.59
9:J:223:SER:HB3	9:J:228:GLN:HE21	1.54	0.59
9:K:441:VAL:HG13	9:K:474:LEU:HD22	1.84	0.59
12:N:531:PHE:CB	12:N:534:SER:HB2	2.32	0.59
12:N:704:VAL:HG23	12:N:705:LEU:HD22	1.85	0.59
13:O:727:THR:O	13:O:730:ARG:HB2	2.02	0.59
8:I:497:TRP:HE3	13:O:492:HIS:CD2	2.19	0.59
1:A:210:MET:HB2	1:A:239:VAL:HG21	1.83	0.59
1:A:1638:TYR:HD1	1:A:1638:TYR:H	1.49	0.59
3:C:101:ARG:NH1	3:C:101:ARG:CG	2.57	0.59
3:C:151:LEU:HD22	3:C:178:VAL:HG13	1.84	0.59
12:N:619:LEU:HG	12:N:637:TRP:CH2	2.38	0.59
16:X:159:LEU:HD22	16:X:171:ILE:HG23	1.83	0.59
16:Y:42:ARG:CG	16:Y:82:TYR:OH	2.46	0.59
1:A:93:LEU:HD22	1:A:128:TRP:CE2	2.38	0.59
3:C:510:SER:O	3:C:512:ALA:N	2.35	0.59
3:C:535:LYS:O	3:C:539:PHE:HD1	1.86	0.59
12:N:393:THR:O	12:N:395:ASP:HB3	2.02	0.59
12:N:435:VAL:HA	12:N:438:ILE:HD12	1.83	0.59
3:P:389:ARG:HA	3:P:392:ILE:HG23	1.84	0.59
16:X:52:ASN:ND2	16:Y:202:ALA:HB1	2.18	0.59
16:X:363:ALA:HB2	16:X:379:LYS:NZ	2.17	0.59
10:L:44:GLN:HA	10:L:47:ASP:OD2	2.03	0.59
10:L:113:LEU:HD13	10:L:120:ILE:HD13	1.85	0.59
11:M:2:ASP:CG	11:M:3:SER:H	2.06	0.59
16:Y:159:LEU:HD22	16:Y:171:ILE:HG23	1.84	0.59
16:Y:294:PHE:CE2	16:Y:311:TYR:HB2	2.36	0.59
2:B:14:TRP:HA	2:B:15:LEU:CB	2.32	0.59
16:Y:45:ALA:HB2	16:Y:82:TYR:CD2	2.37	0.59
16:X:270:ASN:HA	16:Y:62:THR:HG21	1.84	0.59
16:Y:100:TYR:HD1	16:Y:138:VAL:HG13	1.68	0.59
6:F:130:ARG:CG	16:Y:506:GLN:HE21	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:354:MET:HA	9:J:354:MET:HE3	1.85	0.58
16:Y:452:LEU:HD21	16:Y:460:LYS:HB2	1.85	0.58
1:A:1469:CYS:SG	1:A:1519:VAL:HA	2.43	0.58
10:L:88:SER:HA	10:L:145:HIS:O	2.03	0.58
1:A:877:ILE:HG23	1:A:881:ILE:HD12	1.84	0.58
8:I:588:PHE:CE1	8:I:599:CYS:HB2	2.39	0.58
3:C:397:ARG:HA	3:C:428:LEU:HD21	1.85	0.58
7:G:1:MET:HG2	9:J:335:PRO:HB3	1.86	0.58
9:K:185:LEU:HD13	9:K:209:LEU:HD11	1.86	0.58
16:X:251:ASN:O	16:X:255:ILE:HG22	2.02	0.58
16:Y:434:TYR:HA	16:Y:444:LEU:HD13	1.84	0.58
3:C:93:TYR:HD1	3:C:98:GLU:CD	2.07	0.58
6:H:522:PHE:HB3	6:H:539:TYR:CD1	2.38	0.58
8:I:24:ILE:HG22	8:I:38:ALA:O	2.04	0.58
13:O:262:LEU:HD13	13:O:270:SER:HB2	1.84	0.58
13:O:489:VAL:O	13:O:492:HIS:N	2.36	0.58
1:A:31:HIS:CD2	13:O:264:VAL:HG22	2.39	0.58
1:A:1176:LEU:HG	1:A:1208:LEU:HG	1.86	0.58
1:A:1470:LEU:HB2	1:A:1518:VAL:HG13	1.86	0.58
8:I:36:ALA:CB	8:I:80:LEU:HD21	2.33	0.58
9:J:35:GLU:CD	9:J:63:ARG:HE	2.06	0.58
10:L:45:LEU:O	10:L:155:GLN:OE1	2.21	0.58
12:N:350:ASP:HB2	12:N:351:PHE:HA	1.86	0.58
12:N:368:THR:CB	12:N:369:ASP:HA	2.34	0.58
16:X:52:ASN:OD1	16:Y:204:ASP:HB2	2.03	0.58
16:X:271:VAL:CG1	16:X:304:LEU:HD21	2.33	0.58
1:A:1661:HIS:CE1	1:A:1662:LEU:HD23	2.38	0.58
3:C:134:THR:HG23	3:C:143:LYS:HG3	1.86	0.58
9:K:264:HIS:HD2	9:K:267:CYS:H	1.50	0.58
16:X:77:TYR:CE1	16:X:107:LYS:HB2	2.39	0.58
1:A:1409:LEU:HA	1:A:1471:SER:HB2	1.86	0.58
4:D:47:LYS:HD2	3:P:355:GLN:HE22	1.67	0.58
6:F:145:ASN:HB2	6:F:146:PRO:C	2.24	0.58
8:I:81:ALA:HA	8:I:92:LEU:HA	1.85	0.58
9:K:403:PHE:O	9:K:407:GLU:HG2	2.02	0.58
16:X:203:LEU:HD21	16:Y:55:LEU:HD23	1.86	0.58
16:X:452:LEU:HD21	16:X:460:LYS:HB2	1.85	0.58
1:A:852:LEU:HD11	1:A:1819:GLU:HB3	1.86	0.58
1:A:1465:ILE:HB	1:A:1491:PHE:HE2	1.69	0.58
1:A:1896:ALA:HB3	1:A:1897:PRO:HD3	1.86	0.58
3:C:46:ARG:CZ	3:C:170:PHE:CG	2.87	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:ARG:HB2	3:P:295:TYR:HB2	1.86	0.58
3:C:184:LEU:HB3	3:C:187:GLU:HG3	1.86	0.58
3:C:309:VAL:HG23	14:R:78:ARG:CG	2.32	0.58
4:D:9:PHE:HD2	13:O:346:TRP:CH2	2.21	0.58
9:J:77:ALA:CB	9:J:93:LEU:HD11	2.33	0.58
9:J:332:THR:HA	9:J:363:LEU:CD2	2.27	0.58
12:N:281:TYR:CZ	12:N:356:PRO:HB2	2.38	0.58
12:N:546:LYS:HA	12:N:550:GLY:CA	2.34	0.58
13:O:308:ALA:HA	13:O:323:ALA:HB3	1.86	0.58
3:P:252:GLN:O	3:P:255:ILE:HG22	2.04	0.58
16:X:282:PHE:HE1	16:X:313:TYR:HD2	1.52	0.58
1:A:125:GLN:NE2	1:A:179:ASN:HA	2.19	0.57
1:A:213:MET:CE	1:A:216:PRO:HA	2.34	0.57
3:C:526:TRP:HE1	3:C:553:ILE:CA	2.15	0.57
6:F:507:ARG:HH11	6:F:538:ILE:HD13	1.69	0.57
3:P:238:TYR:HB3	3:P:247:ALA:HB2	1.86	0.57
1:A:1089:LEU:HD12	1:A:1145:LEU:HB3	1.85	0.57
3:C:106:LEU:H	3:C:106:LEU:HD12	1.68	0.57
3:C:119:MET:HA	3:C:122:ARG:CD	2.34	0.57
3:C:381:THR:HG21	3:C:412:LEU:HD21	1.86	0.57
12:N:73:GLU:O	12:N:74:TRP:HB3	2.04	0.57
3:P:276:ILE:CG2	3:P:277:ARG:N	2.67	0.57
3:C:89:LEU:HD11	3:C:105:PHE:CD2	2.39	0.57
6:H:145:ASN:HB2	6:H:146:PRO:C	2.25	0.57
1:A:667:MET:O	1:A:755:LEU:O	2.23	0.57
1:A:1376:LEU:HD23	1:A:1377:LYS:HG3	1.85	0.57
1:A:1399:VAL:HG11	1:A:1404:LEU:HG	1.86	0.57
8:I:730:VAL:HG22	8:I:731:SER:N	2.19	0.57
9:J:445:GLU:HA	9:J:474:LEU:HD23	1.85	0.57
12:N:527:LEU:HD21	12:N:561:LEU:HD22	1.85	0.57
12:N:676:TRP:O	12:N:713:PHE:HB2	2.05	0.57
3:P:441:GLU:HG2	3:P:472:LYS:CE	2.34	0.57
1:A:44:PRO:HB2	3:C:181:LYS:HD3	1.84	0.57
1:A:1252:ALA:O	1:A:1256:GLY:N	2.36	0.57
3:C:93:TYR:CD1	3:C:98:GLU:CD	2.78	0.57
9:J:270:VAL:O	9:J:274:THR:HG22	2.05	0.57
3:C:120:TYR:CE2	3:C:124:LEU:HD11	2.39	0.57
6:F:684:LYS:HD3	6:F:687:LYS:HD2	1.86	0.57
9:K:373:TYR:CE1	7:W:4:ARG:HG2	2.39	0.57
10:L:153:MET:HG2	10:L:156:ILE:HD11	1.85	0.57
12:N:277:CYS:HA	12:N:285:PHE:CE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:231:LEU:HD23	13:O:236:LEU:CA	2.34	0.57
13:O:381:ILE:HG21	13:O:405:SER:HB2	1.85	0.57
13:O:578:GLU:HA	13:O:616:LEU:CD1	2.31	0.57
3:P:48:LEU:HD21	3:P:116:PHE:CZ	2.39	0.57
16:X:215:LYS:O	16:X:219:VAL:HG23	2.04	0.57
16:Y:215:LYS:O	16:Y:219:VAL:HG23	2.04	0.57
1:A:1433:ILE:H	1:A:1433:ILE:CD1	1.98	0.57
3:C:301:ASP:OD1	3:C:335:CYS:HB3	2.05	0.57
4:D:5:PHE:CZ	13:O:390:PHE:HZ	2.23	0.57
8:I:79:LEU:HD11	8:I:168:LEU:HD23	1.86	0.57
9:J:264:HIS:HD2	9:J:267:CYS:H	1.51	0.57
9:J:439:VAL:HG21	9:J:448:LEU:HD21	1.86	0.57
1:A:1032:LEU:HD12	1:A:1035:GLN:HB3	1.86	0.57
12:N:293:ILE:O	12:N:297:VAL:HG23	2.05	0.57
12:N:456:LEU:HA	12:N:548:ARG:HH21	1.69	0.57
13:O:386:GLN:HB2	13:O:424:GLN:HE22	1.70	0.57
3:C:238:TYR:HB3	3:C:247:ALA:HB2	1.87	0.57
8:I:17:LYS:CE	8:I:51:SER:O	2.53	0.57
8:I:32:ARG:HB2	8:I:34:LEU:CD2	2.35	0.57
12:N:164:SER:H	12:N:165:THR:HA	1.69	0.57
3:C:416:PHE:H	13:O:326:GLU:CD	2.07	0.56
16:X:40:HIS:HB3	16:Y:201:LEU:HD13	1.87	0.56
1:A:667:MET:O	1:A:756:PHE:N	2.37	0.56
1:A:1079:ALA:HB1	1:A:1556:LEU:HA	1.87	0.56
8:I:166:LYS:O	8:I:170:ASP:HB2	2.05	0.56
13:O:490:LEU:O	13:O:494:LYS:HB2	2.04	0.56
1:A:48:LEU:HD13	1:A:50:SER:CA	2.36	0.56
1:A:93:LEU:HB2	1:A:128:TRP:CH2	2.39	0.56
3:C:48:LEU:HD21	3:C:116:PHE:CZ	2.39	0.56
3:C:353:TYR:CZ	3:C:356:ARG:NH1	2.73	0.56
9:J:245:CYS:HA	9:J:247:PHE:CE1	2.39	0.56
13:O:530:SER:O	13:O:533:THR:HG23	2.04	0.56
3:P:276:ILE:CG2	3:P:277:ARG:H	2.17	0.56
16:Y:45:ALA:HB3	16:Y:82:TYR:HE2	1.71	0.56
16:Y:96:ALA:O	16:Y:100:TYR:HD2	1.88	0.56
1:A:248:PHE:CD1	1:A:430:VAL:O	2.58	0.56
6:H:689:LEU:HD21	6:H:713:LEU:HG	1.85	0.56
13:O:576:ASN:ND2	13:O:579:MET:HB2	2.20	0.56
4:D:9:PHE:CD2	13:O:346:TRP:CZ3	2.81	0.56
1:A:1236:LEU:HD21	1:A:1243:LEU:HD13	1.86	0.56
3:C:202:HIS:CE1	3:C:205:ALA:H	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:X:434:TYR:HA	16:X:444:LEU:HD13	1.86	0.56
1:A:257:MET:HG2	1:A:430:VAL:HG11	1.86	0.56
1:A:1251:VAL:O	1:A:1255:VAL:HG23	2.06	0.56
6:H:146:PRO:HG3	6:H:167:THR:HA	1.88	0.56
9:K:376:LEU:HG	9:K:407:GLU:OE1	2.06	0.56
9:K:418:TRP:HB3	9:K:458:LEU:HD12	1.87	0.56
13:O:605:LEU:HD23	13:O:608:LEU:HD12	1.87	0.56
3:P:296:ARG:HD2	3:P:298:GLU:HB3	1.87	0.56
3:C:47:GLY:HA3	3:C:94:PHE:HE2	1.70	0.56
6:F:59:ARG:HH22	6:H:562:MET:HB2	1.69	0.56
8:I:56:TRP:CZ3	8:I:58:PHE:HB2	2.31	0.56
13:O:104:GLU:N	13:O:107:ASP:OD2	2.39	0.56
1:A:79:GLY:O	1:A:87:VAL:CG1	2.53	0.56
4:D:10:PRO:HG3	13:O:345:SER:HB3	1.88	0.56
4:D:53:PRO:HB3	3:P:385:ILE:HD13	1.88	0.56
9:J:20:GLN:HB2	9:K:165:GLU:CD	2.26	0.56
9:J:495:PHE:CZ	9:J:525:MET:HG2	2.40	0.56
5:E:92:ASP:HB3	6:H:592:ARG:NH2	2.21	0.56
6:F:125:TYR:HD1	6:F:130:ARG:HE	1.50	0.56
16:X:77:TYR:N	16:X:106:GLN:HE21	2.04	0.56
1:A:1644:TYR:O	1:A:1645:GLU:HG2	2.06	0.55
3:C:376:MET:O	14:R:130:ILE:HG21	2.06	0.55
6:F:125:TYR:CD1	6:F:130:ARG:NE	2.69	0.55
9:K:272:ILE:HG23	9:K:307:CYS:SG	2.47	0.55
13:O:244:LEU:HD22	13:O:248:PRO:HA	1.88	0.55
1:A:118:THR:OG1	13:O:266:ASP:OD1	2.24	0.55
3:C:379:LYS:HE2	14:R:94:LEU:HB3	1.86	0.55
6:F:666:PRO:O	6:F:667:GLN:HG3	2.07	0.55
6:F:696:ILE:HG12	6:F:705:CYS:SG	2.46	0.55
3:C:170:PHE:O	3:C:173:TYR:N	2.40	0.55
13:O:123:GLU:N	13:O:124:PRO:HA	2.20	0.55
16:Y:269:ASP:HB3	16:Y:300:LEU:HD21	1.89	0.55
6:F:611:PHE:CB	6:F:620:ALA:HB2	2.36	0.55
6:H:128:THR:HG21	6:H:130:ARG:HH12	1.71	0.55
9:K:167:PHE:CE1	9:K:171:THR:HG21	2.42	0.55
12:N:519:TYR:O	12:N:523:LEU:HG	2.07	0.55
13:O:504:ALA:HA	13:O:507:TRP:NE1	2.21	0.55
16:Y:168:THR:HB	16:Y:169:PRO:HD2	1.88	0.55
1:A:39:LEU:HD12	1:A:40:ARG:HG2	1.87	0.55
1:A:762:ILE:O	1:A:765:VAL:HG12	2.06	0.55
2:B:8:TRP:HD1	12:N:644:VAL:HG12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:522:PHE:HB3	6:F:539:TYR:CD1	2.42	0.55
6:F:611:PHE:HB3	6:F:620:ALA:HB2	1.87	0.55
9:J:53:TYR:O	9:J:79:CYS:SG	2.65	0.55
9:J:178:ALA:HB1	9:J:213:ASN:HD22	1.71	0.55
10:L:50:LEU:HD21	10:L:119:TRP:HZ2	1.72	0.55
12:N:289:PHE:HA	12:N:292:TRP:CB	2.33	0.55
3:P:48:LEU:HD21	3:P:116:PHE:CE2	2.41	0.55
14:R:388[A]:CYS:HG	14:R:389:SER:N	2.04	0.55
1:A:48:LEU:HD13	1:A:50:SER:CB	2.37	0.55
1:A:189:PHE:HB2	1:A:211:PHE:HB2	1.88	0.55
1:A:1165:HIS:HD2	1:A:1167:GLU:HB2	1.71	0.55
1:A:1751:ALA:HA	1:A:1755:CYS:SG	2.47	0.55
3:C:217:GLU:HA	3:C:220:LYS:HD2	1.88	0.55
3:C:397:ARG:O	3:C:428:LEU:CD2	2.55	0.55
6:F:739:VAL:O	6:F:743:ILE:HG13	2.06	0.55
6:H:611:PHE:CB	6:H:620:ALA:HB2	2.37	0.55
9:J:25:TRP:NE1	9:K:162:TYR:O	2.31	0.55
12:N:289:PHE:O	12:N:291:LYS:N	2.38	0.55
13:O:536:THR:HA	13:O:543:GLY:HA3	1.87	0.55
13:O:688:GLU:O	13:O:691:ILE:HG22	2.06	0.55
14:R:177:ASP:OD1	15:S:834:ILE:CD1	2.50	0.55
16:Y:83:HIS:O	16:Y:86:SER:OG	2.19	0.55
1:A:1333:HIS:HB2	1:A:1357:THR:HA	1.89	0.55
1:A:1621:PRO:HA	1:A:1697:LEU:O	2.07	0.55
3:C:313:LYS:HG2	3:C:343:LEU:HD13	1.87	0.55
8:I:197:ARG:O	8:I:545:GLY:HA3	2.06	0.55
8:I:353:GLN:HA	8:I:353:GLN:NE2	2.22	0.55
6:H:611:PHE:HB3	6:H:620:ALA:HB2	1.89	0.55
8:I:28:TRP:CD1	8:I:723:ALA:HB1	2.42	0.55
9:J:37:PRO:HA	9:J:65:LEU:HD11	1.88	0.55
16:Y:70:LEU:HD12	16:Y:71:PHE:CE2	2.42	0.55
1:A:1502:PRO:O	1:A:1503:ASN:HB3	2.07	0.55
3:C:416:PHE:CD2	13:O:323:ALA:HB2	2.42	0.55
6:H:86:ALA:HB2	9:K:473:VAL:O	2.07	0.55
8:I:52:PHE:CD1	8:I:743:VAL:HG21	2.42	0.55
12:N:559:VAL:HA	12:N:562:LYS:HG2	1.89	0.55
16:Y:423:ILE:HG13	16:Y:424:ARG:N	2.22	0.55
1:A:77:ARG:HG2	1:A:78:LYS:O	2.07	0.55
1:A:1573:SER:HB2	1:A:1617:ARG:NH2	2.19	0.55
4:D:42:GLN:O	4:D:46:GLU:HG2	2.07	0.55
6:F:104:ASP:OD1	6:F:104:ASP:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:536:CYS:O	8:I:540:PRO:HD3	2.07	0.55
9:K:495:PHE:CZ	9:K:525:MET:HG2	2.41	0.55
13:O:356:ASP:HA	13:O:357:SER:HB2	1.88	0.55
1:A:1137:PHE:O	1:A:1141:VAL:HG23	2.07	0.54
3:C:93:TYR:CE1	3:C:98:GLU:OE2	2.60	0.54
3:C:554:LEU:HD13	9:K:386:LEU:HD11	1.88	0.54
8:I:115:TRP:CZ3	8:I:176:LEU:HD22	2.42	0.54
1:A:1094:PRO:HG2	1:A:1147:ILE:HG12	1.90	0.54
1:A:1251:VAL:HG12	1:A:1294:TYR:HA	1.88	0.54
3:C:173:TYR:CD1	3:C:202:HIS:CE1	2.93	0.54
6:H:653:LEU:HD22	9:K:523:ILE:CG2	2.36	0.54
9:J:185:LEU:HD13	9:J:206:GLU:OE1	2.08	0.54
12:N:542:VAL:HG11	12:N:558:GLU:HG2	1.89	0.54
13:O:119:PHE:CE1	13:O:136:LEU:HD11	2.42	0.54
16:X:168:THR:HB	16:X:169:PRO:HD2	1.89	0.54
16:Y:42:ARG:CA	16:Y:82:TYR:CE2	2.70	0.54
1:A:1332:GLY:O	1:A:1358:ILE:HG13	2.08	0.54
2:B:15:LEU:HD12	12:N:633:ARG:HG2	1.90	0.54
6:H:689:LEU:HD11	6:H:712:VAL:CG1	2.37	0.54
8:I:195:ILE:HD11	8:I:251:MET:HE3	1.88	0.54
9:J:319:ALA:O	9:J:323:LEU:HD22	2.08	0.54
9:J:322:TYR:HE1	11:M:36:LEU:HD11	1.72	0.54
9:K:355:ALA:O	9:K:359:THR:HG22	2.07	0.54
13:O:119:PHE:HE1	13:O:136:LEU:HD21	1.72	0.54
9:J:69:TYR:O	9:J:70:GLU:CB	2.56	0.54
12:N:425:ARG:HH11	12:N:425:ARG:CG	2.10	0.54
1:A:181:TRP:HB2	1:A:188:LEU:HB3	1.90	0.54
3:C:41:GLY:O	3:C:45:GLU:HG2	2.07	0.54
6:F:164:PRO:CG	6:F:471:LYS:HG3	2.38	0.54
6:H:553:SER:HA	6:H:576:CYS:SG	2.48	0.54
6:H:739:VAL:O	6:H:743:ILE:HG13	2.07	0.54
8:I:138:LEU:CD1	8:I:253:ARG:HA	2.37	0.54
8:I:195:ILE:HD11	8:I:251:MET:CE	2.37	0.54
13:O:76:SER:HB2	13:O:165:GLY:HA2	1.89	0.54
3:P:361:ASN:HD22	3:P:363:ARG:N	2.05	0.54
1:A:1019:MET:HB2	1:A:1021:HIS:CE1	2.42	0.54
1:A:1412:CYS:HB2	1:A:1471:SER:OG	2.08	0.54
1:A:1877:LEU:CD1	1:A:1885:LEU:CD1	2.85	0.54
3:C:244:ILE:HD13	3:C:276:ILE:HG12	1.89	0.54
3:C:493:TYR:CE2	3:C:497:ILE:HD11	2.43	0.54
6:F:146:PRO:HG3	6:F:167:THR:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:638:TRP:CZ3	6:H:660:LYS:HD2	2.43	0.54
16:Y:200:PRO:O	16:Y:202:ALA:N	2.28	0.54
3:C:46:ARG:HB3	3:C:116:PHE:CE2	2.43	0.54
9:K:391:PHE:CE2	9:K:411:VAL:HG21	2.42	0.54
3:P:238:TYR:CB	3:P:247:ALA:HB2	2.38	0.54
1:A:456:LYS:HB3	1:A:469:GLY:HA3	1.90	0.54
6:F:59:ARG:HH12	6:H:562:MET:HG3	1.73	0.54
1:A:1431:PRO:HG2	1:A:1434:ILE:CD1	2.38	0.54
1:A:1595:HIS:CE1	1:A:1598:ASP:HB2	2.43	0.54
1:A:34:ALA:O	13:O:237:GLN:NE2	2.41	0.53
1:A:250:ASN:HD22	1:A:251:THR:N	2.06	0.53
13:O:354:ARG:CD	13:O:573:LYS:O	2.57	0.53
3:P:117:LEU:HD23	3:P:117:LEU:O	2.07	0.53
3:P:270:ALA:HB2	3:P:285:ILE:HG22	1.90	0.53
16:X:269:ASP:HB3	16:X:300:LEU:HD21	1.91	0.53
1:A:1306:CYS:HB2	1:A:1374:ILE:HG12	1.88	0.53
1:A:1750:PHE:HD2	1:A:1775:LEU:HD12	1.73	0.53
8:I:218:SER:OG	8:I:584:HIS:ND1	2.41	0.53
9:J:253:LEU:O	9:J:256:VAL:HG22	2.08	0.53
12:N:165:THR:N	12:N:166:PRO:CA	2.71	0.53
16:X:192:TYR:HA	16:X:195:VAL:HG22	1.90	0.53
1:A:776:ASN:O	1:A:777:THR:HB	2.07	0.53
1:A:189:PHE:N	1:A:211:PHE:O	2.39	0.53
1:A:1794:ASP:HA	1:A:1797:ILE:HG12	1.91	0.53
3:C:79:GLU:OE1	3:C:79:GLU:N	2.39	0.53
3:C:238:TYR:CD1	3:C:243:LEU:HD12	2.44	0.53
6:H:762:TRP:HA	6:H:765:ASP:HB2	1.89	0.53
8:I:360:LEU:HD21	8:I:390:ILE:HG23	1.90	0.53
8:I:370:ALA:HB1	8:I:383:ALA:HA	1.91	0.53
9:K:258:MET:HG3	9:K:271:HIS:CD2	2.43	0.53
3:P:120:TYR:CZ	3:P:124:LEU:HD11	2.43	0.53
1:A:1243:LEU:O	1:A:1245:VAL:N	2.41	0.53
1:A:1329:MET:HE2	1:A:1368:THR:HG22	1.90	0.53
3:C:206:TRP:CE3	3:C:233:PHE:CG	2.96	0.53
13:O:236:LEU:HD23	13:O:260:ASN:HB2	1.90	0.53
13:O:351:GLY:C	13:O:353:LYS:H	2.12	0.53
16:X:76:LYS:HB3	16:X:106:GLN:HE22	1.73	0.53
1:A:248:PHE:CZ	1:A:250:ASN:HB2	2.43	0.53
1:A:412:LEU:O	1:A:468:PHE:HE2	1.91	0.53
1:A:966:PRO:HG3	1:A:980:ARG:HE	1.74	0.53
1:A:1543:HIS:CD2	1:A:1559:HIS:CE1	2.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:358:LEU:HD21	3:C:368:TRP:NE1	2.23	0.53
7:G:15:ASP:O	9:J:487:TYR:OH	2.23	0.53
13:O:33:TYR:CE2	13:O:73:ILE:HG13	2.44	0.53
8:I:207:ALA:HB1	8:I:575:LEU:HD12	1.90	0.53
9:J:227:LEU:HD12	9:K:32:LEU:HG	1.90	0.53
9:J:324:SER:O	9:J:328:THR:HG23	2.09	0.53
9:K:280:LYS:CB	9:K:283:GLU:HG2	2.38	0.53
3:P:170:PHE:O	3:P:173:TYR:N	2.41	0.53
1:A:31:HIS:CG	1:A:32:PRO:HD2	2.43	0.53
1:A:48:LEU:HD22	1:A:48:LEU:C	2.27	0.53
1:A:93:LEU:HD21	1:A:151:ILE:HG13	1.90	0.53
1:A:1672:ARG:HD2	1:A:1705:GLN:HB3	1.91	0.53
3:C:93:TYR:CD1	3:C:98:GLU:OE2	2.62	0.53
6:H:168:PHE:CB	6:H:467:ARG:HD3	2.38	0.53
8:I:27:VAL:C	8:I:35:ILE:HD12	2.28	0.53
10:L:63:LEU:HD22	10:L:138:GLN:NE2	2.24	0.53
16:X:76:LYS:CB	16:X:106:GLN:NE2	2.72	0.53
16:X:423:ILE:HG13	16:X:424:ARG:N	2.23	0.53
6:F:168:PHE:CB	6:F:467:ARG:HD3	2.39	0.53
6:H:128:THR:HG21	6:H:130:ARG:NH1	2.23	0.53
8:I:174:ASN:OD1	8:I:190:TYR:HA	2.08	0.53
9:J:406:HIS:HE1	9:J:450:ASN:HD22	1.55	0.53
9:J:442:ASP:OD1	9:J:475:ILE:HG22	2.09	0.53
12:N:78:VAL:O	12:N:81:ASN:N	2.42	0.53
12:N:503:SER:O	12:N:507:SER:HB3	2.09	0.53
12:N:612:PRO:HG2	12:N:615:ILE:HG12	1.91	0.53
13:O:83:GLU:HG3	13:O:90:ALA:CB	2.39	0.53
14:R:91:ALA:O	14:R:92:SER:C	2.46	0.53
1:A:1153:ILE:HD11	1:A:1184:HIS:HB3	1.91	0.53
2:B:11:VAL:HG13	12:N:642:GLY:HA2	1.90	0.53
3:C:152:ARG:HG3	3:C:153:GLU:N	2.23	0.53
4:D:48:ASP:OD2	3:P:386:GLN:HG2	2.09	0.53
8:I:639:LEU:HB2	8:I:652:VAL:HG12	1.91	0.53
10:L:126:ASP:OD2	10:L:130:LYS:O	2.27	0.53
16:X:203:LEU:CD2	16:Y:55:LEU:HD23	2.39	0.53
1:A:476:ALA:HB3	1:A:492:GLU:HA	1.91	0.52
1:A:641:TRP:CD1	1:A:663:CYS:CB	2.92	0.52
1:A:1078:MET:HB2	1:A:1552:TYR:CE1	2.44	0.52
3:C:141:LEU:HD22	3:C:368:TRP:HZ2	1.73	0.52
6:F:498:THR:HG21	6:H:33:ALA:HB2	1.90	0.52
8:I:207:ALA:CB	8:I:575:LEU:HD12	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:46:CYS:O	9:K:50:THR:OG1	2.23	0.52
3:C:416:PHE:CE2	13:O:323:ALA:HB2	2.43	0.52
7:G:4:ARG:HD2	9:J:373:TYR:CD1	2.44	0.52
1:A:506:VAL:HA	1:A:639:VAL:HG23	1.91	0.52
1:A:1165:HIS:CD2	1:A:1167:GLU:HB2	2.45	0.52
9:K:324:SER:O	9:K:328:THR:HG23	2.09	0.52
16:X:282:PHE:HE1	16:X:313:TYR:CD2	2.28	0.52
3:C:202:HIS:CE1	3:C:205:ALA:N	2.78	0.52
8:I:64:THR:HG22	8:I:84:LEU:HD11	1.90	0.52
8:I:65:GLY:HA3	8:I:84:LEU:HB3	1.91	0.52
9:K:429:LEU:O	9:K:433:LYS:HG3	2.10	0.52
12:N:202:GLU:O	12:N:204:ASP:N	2.42	0.52
13:O:608:LEU:HD22	13:O:612:LYS:HE2	1.91	0.52
14:R:175:ILE:O	15:S:833:ASP:O	2.28	0.52
3:C:304:SER:HB2	3:C:336:VAL:HG22	1.91	0.52
8:I:23:ILE:HD12	8:I:37:LEU:HD23	1.91	0.52
9:J:514:PHE:O	9:J:518:MET:HB2	2.10	0.52
12:N:249:ARG:HB3	12:N:250:LEU:HD23	1.91	0.52
13:O:355:SER:O	13:O:357:SER:HB2	2.10	0.52
16:Y:192:TYR:HA	16:Y:195:VAL:HG22	1.91	0.52
16:Y:308:MET:HG3	16:Y:331:LEU:HD21	1.91	0.52
1:A:1041:LEU:HD13	1:A:1084:ARG:HA	1.91	0.52
1:A:1658:PRO:HG2	1:A:1663:LEU:HD13	1.91	0.52
1:A:1767:ILE:HA	1:A:1798:ARG:NH2	2.25	0.52
2:B:47:VAL:HG21	2:B:60:ILE:HG21	1.90	0.52
7:G:4:ARG:HB2	9:J:373:TYR:HE1	1.73	0.52
8:I:269:LEU:HD11	8:I:522:LEU:HD13	1.91	0.52
9:J:28:LYS:HD3	9:K:230:ASN:HD21	1.75	0.52
1:A:791:VAL:O	1:A:793:LEU:N	2.42	0.52
6:F:553:SER:HA	6:F:576:CYS:SG	2.49	0.52
8:I:116:MET:HE1	8:I:211:SER:O	2.10	0.52
9:J:305:VAL:HG11	11:M:31:ILE:CD1	2.40	0.52
12:N:577:GLU:HB3	12:N:625:LYS:HE3	1.91	0.52
3:P:296:ARG:HH11	3:P:299:ASN:HD21	1.57	0.52
14:R:206:VAL:HG23	14:R:229:ILE:HD13	1.92	0.52
16:X:149:LEU:O	16:X:150:LYS:HB2	2.10	0.52
16:X:203:LEU:HD23	16:X:203:LEU:C	2.30	0.52
3:C:60:PHE:HB2	3:P:89:LEU:HD12	1.91	0.52
3:C:76:ILE:HD13	3:P:70:LEU:HD23	1.92	0.52
3:C:327:ASP:OD2	3:C:330:ARG:HD3	2.09	0.52
8:I:355:GLY:O	8:I:359:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1797:ILE:HG22	1:A:1852:ILE:HD11	1.91	0.52
3:C:365:LEU:HD11	3:C:395:ASN:HB2	1.92	0.52
6:F:130:ARG:HD2	6:F:133:LYS:HD3	1.90	0.52
7:G:3:ARG:HB2	9:J:443:LYS:NZ	2.25	0.52
8:I:381:LEU:HD12	8:I:386:ILE:HD11	1.91	0.52
14:R:110:LYS:HZ2	14:R:114:LYS:HB2	1.75	0.52
1:A:246:ILE:HD11	1:A:249:LEU:CD2	2.40	0.52
1:A:252:ASP:HB3	1:A:253:PRO:CD	2.34	0.52
6:F:544:TRP:CE3	14:R:499:ARG:HD3	2.45	0.52
1:A:246:ILE:HD11	1:A:249:LEU:HD22	1.91	0.51
1:A:1556:LEU:HD11	1:A:1607:ARG:HG2	1.92	0.51
1:A:1853:ASP:O	1:A:1857:ASP:HB2	2.10	0.51
4:D:4:LEU:HB3	13:O:468:VAL:HG12	1.92	0.51
9:J:355:ALA:O	9:J:359:THR:HG23	2.11	0.51
1:A:125:GLN:NE2	1:A:180:VAL:H	2.07	0.51
1:A:191:ARG:HG2	1:A:192:SER:H	1.75	0.51
1:A:439:GLN:OE1	1:A:456:LYS:HG2	2.11	0.51
1:A:668:MET:N	1:A:668:MET:SD	2.83	0.51
1:A:1799:ARG:HD3	1:A:1805:MET:HB2	1.92	0.51
9:K:154:LYS:HE2	9:K:184:LEU:HD22	1.92	0.51
16:Y:330:ARG:O	16:Y:334:ILE:HG23	2.10	0.51
16:Y:452:LEU:CD2	16:Y:460:LYS:HB2	2.41	0.51
1:A:811:PRO:HG3	1:A:1806:SER:O	2.11	0.51
1:A:1134:TRP:HD1	1:A:1597:THR:HA	1.75	0.51
1:A:1232:ILE:HG13	1:A:1235:LEU:HB3	1.91	0.51
6:F:150:SER:HB3	6:H:23:ASP:HB3	1.92	0.51
12:N:331:PHE:CE2	12:N:335:ILE:HD11	2.45	0.51
14:R:95:LEU:HG	14:R:130:ILE:HD11	1.93	0.51
1:A:36:ASN:HD22	1:A:36:ASN:H	1.58	0.51
3:C:93:TYR:CE2	3:C:101:ARG:CZ	2.94	0.51
3:C:414:MET:HG2	13:O:330:ILE:CG1	2.36	0.51
8:I:497:TRP:CE3	13:O:492:HIS:CD2	2.99	0.51
9:K:9:ARG:O	9:K:13:TYR:HD1	1.94	0.51
10:L:90:THR:HB	10:L:145:HIS:ND1	2.25	0.51
13:O:146:LEU:HB2	13:O:151:VAL:CG2	2.40	0.51
1:A:1177:MET:HB2	1:A:1207:GLY:C	2.31	0.51
8:I:218:SER:HA	8:I:235:GLN:HA	1.92	0.51
9:K:37:PRO:HB3	9:K:69:TYR:CE2	2.46	0.51
16:X:83:HIS:O	16:X:86:SER:OG	2.19	0.51
16:X:437:LEU:HB2	16:X:444:LEU:HD11	1.93	0.51
1:A:1509:PRO:O	1:A:1513:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:571:CYS:SG	6:F:606:LEU:HD12	2.51	0.51
8:I:279:ILE:HD11	8:I:337:ILE:CA	2.28	0.51
8:I:396:PHE:HA	8:I:525:VAL:HG11	1.93	0.51
13:O:114:ASP:CA	13:O:117:ASP:OD1	2.59	0.51
1:A:1078:MET:HB3	1:A:1135:ALA:HB2	1.92	0.51
6:H:527:ARG:HB3	16:Y:302:PRO:HG3	1.92	0.51
9:J:376:LEU:CD2	9:J:407:GLU:HG2	2.41	0.51
9:K:272:ILE:CG2	9:K:307:CYS:SG	2.98	0.51
3:P:310:ARG:HB3	3:P:312:MET:HE2	1.93	0.51
1:A:45:ALA:O	3:C:180:ARG:NH1	2.42	0.51
3:C:188:ALA:HA	3:C:191:VAL:HG22	1.92	0.51
8:I:224:SER:HB3	8:I:229:SER:HA	1.90	0.51
9:K:185:LEU:HD11	9:K:205:PHE:HB3	1.93	0.51
3:P:389:ARG:O	3:P:392:ILE:HG23	2.10	0.51
1:A:1092:TYR:O	1:A:1147:ILE:HA	2.10	0.51
1:A:1409:LEU:HD23	1:A:1471:SER:CA	2.41	0.51
1:A:1637:THR:O	1:A:1664:LYS:N	2.40	0.51
8:I:52:PHE:HD1	8:I:743:VAL:HG21	1.75	0.51
12:N:406:ALA:O	12:N:409:VAL:HB	2.11	0.51
16:Y:149:LEU:O	16:Y:150:LYS:HB2	2.10	0.51
16:Y:294:PHE:CD1	16:Y:294:PHE:C	2.85	0.51
1:A:89:TYR:HB3	13:O:536:THR:HG23	1.93	0.51
4:D:10:PRO:CG	13:O:345:SER:HB3	2.40	0.51
6:F:26:PHE:O	6:F:30:ARG:HG2	2.11	0.51
6:F:636:ASN:H	6:F:636:ASN:HD22	1.59	0.51
6:F:758:MET:HG2	6:F:762:TRP:CZ2	2.46	0.51
16:X:452:LEU:CD2	16:X:460:LYS:HB2	2.41	0.51
1:A:87:VAL:HG12	1:A:88:ASP:H	1.73	0.50
1:A:434:SER:HA	1:A:439:GLN:O	2.11	0.50
1:A:1396:LEU:HD11	1:A:1434:ILE:HD11	1.93	0.50
1:A:1617:ARG:HH11	1:A:1659:GLU:HA	1.77	0.50
8:I:358:SER:O	8:I:362:HIS:HD2	1.94	0.50
9:J:465:LEU:HA	9:J:488:ILE:CD1	2.40	0.50
12:N:362:LYS:HB2	12:N:410:LEU:CD2	2.22	0.50
12:N:409:VAL:O	12:N:410:LEU:HB2	2.11	0.50
13:O:427:ALA:O	13:O:430:ARG:HB3	2.10	0.50
13:O:580:VAL:HA	13:O:583:VAL:HG12	1.93	0.50
3:P:361:ASN:HD22	3:P:363:ARG:H	1.57	0.50
1:A:172:SER:OG	3:C:427:GLN:HG2	2.12	0.50
1:A:1278:GLY:HA3	1:A:1328:TYR:CE1	2.46	0.50
1:A:1672:ARG:HB2	1:A:1673:TYR:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1774:VAL:HG13	1:A:1790:TYR:HB3	1.93	0.50
2:B:11:VAL:HB	12:N:594:VAL:CG1	2.41	0.50
6:H:26:PHE:O	6:H:30:ARG:HG2	2.11	0.50
9:K:23:LEU:HA	9:K:46:CYS:SG	2.52	0.50
9:K:509:ARG:HG3	9:K:509:ARG:O	2.11	0.50
9:K:513:THR:O	9:K:517:THR:HG22	2.11	0.50
13:O:631:GLN:HB3	13:O:640:ALA:HB2	1.92	0.50
1:A:1573:SER:HG	1:A:1656:LEU:HD22	1.76	0.50
1:A:1704:GLY:H	1:A:1742:THR:HG21	1.76	0.50
3:C:323:LEU:HD12	3:C:336:VAL:HG11	1.92	0.50
3:C:402:TRP:HB3	3:C:425:ALA:HB2	1.92	0.50
6:H:73:TYR:CD1	6:H:117:THR:HG22	2.45	0.50
9:J:24:PHE:O	9:J:28:LYS:HG2	2.11	0.50
13:O:68:LEU:HD23	13:O:131:VAL:HG12	1.92	0.50
13:O:113:ASP:CG	3:P:344:ARG:HH22	2.12	0.50
16:Y:77:TYR:CE1	16:Y:107:LYS:HB2	2.46	0.50
16:Y:235:TRP:CE3	16:Y:236:LEU:HA	2.46	0.50
1:A:1209:LEU:HD22	1:A:1228:LEU:CD2	2.39	0.50
3:C:106:LEU:HD13	3:C:118:TYR:HB2	1.93	0.50
3:C:295:TYR:HD1	3:C:326:ILE:HG12	1.76	0.50
6:F:103:HIS:HA	6:F:106:ILE:HD12	1.93	0.50
10:L:119:TRP:HH2	10:L:155:GLN:HG2	1.76	0.50
12:N:212:TYR:HA	12:N:215:LEU:HB2	1.93	0.50
12:N:609:LEU:HD22	12:N:639:HIS:CD2	2.46	0.50
13:O:35:ILE:CG2	13:O:158:LEU:HD13	2.40	0.50
14:R:216:ILE:HG12	15:S:831:LEU:HB2	1.93	0.50
1:A:1097:THR:HG23	13:O:340:LEU:HB3	1.93	0.50
1:A:213:MET:HE3	1:A:220:ILE:HG22	1.93	0.50
1:A:1250:GLN:O	1:A:1254:VAL:HG23	2.12	0.50
3:C:449:LEU:HD22	3:C:476:LEU:HD22	1.88	0.50
13:O:657:ILE:HA	13:O:660:LYS:CB	2.41	0.50
16:X:203:LEU:HD22	16:Y:55:LEU:CD2	2.42	0.50
5:E:76:VAL:O	5:E:80:GLU:HB2	2.12	0.50
13:O:33:TYR:CE1	13:O:37:VAL:HG21	2.47	0.50
13:O:113:ASP:OD2	3:P:344:ARG:NH2	2.26	0.50
1:A:23:PHE:O	1:A:26:ASP:HB3	2.12	0.50
1:A:99:MET:HB3	1:A:118:THR:HG23	1.94	0.50
1:A:1032:LEU:HD12	1:A:1035:GLN:CB	2.41	0.50
1:A:1579:SER:O	1:A:1582:ALA:HB3	2.12	0.50
10:L:53:TYR:HE2	10:L:152:HIS:CE1	2.29	0.50
1:A:33:ASN:HA	1:A:99:MET:CE	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASN:HD22	1:A:251:THR:H	1.58	0.50
1:A:433:THR:HG21	1:A:481:PRO:HB3	1.90	0.50
1:A:487:THR:HG22	1:A:501:THR:HA	1.94	0.50
1:A:770:TYR:HB2	1:A:786:LEU:HD22	1.93	0.50
1:A:1519:VAL:CG1	1:A:1520:LEU:N	2.74	0.50
9:J:58:HIS:CD2	9:K:262:PRO:HD3	2.47	0.50
9:K:263:PHE:HZ	9:K:290:LYS:CG	2.14	0.50
10:L:40:PHE:HA	10:L:44:GLN:OE1	2.12	0.50
11:M:32:PRO:O	11:M:33:LEU:HB2	2.12	0.50
12:N:580:LYS:HB3	12:N:582:PRO:HD2	1.94	0.50
3:P:310:ARG:HB3	3:P:312:MET:CE	2.41	0.50
16:X:363:ALA:HB2	16:X:379:LYS:HZ3	1.75	0.50
16:Y:271:VAL:CG1	16:Y:304:LEU:HD21	2.40	0.50
1:A:1236:LEU:HD11	1:A:1243:LEU:HD22	1.93	0.49
6:F:656:MET:HG3	16:Y:526:GLN:HB2	1.94	0.49
8:I:116:MET:SD	8:I:210:LEU:HB3	2.52	0.49
9:J:245:CYS:SG	9:J:443:LYS:HD3	2.52	0.49
13:O:114:ASP:C	13:O:117:ASP:OD1	2.50	0.49
16:X:99:LYS:HD3	16:X:102:MET:CE	2.42	0.49
16:Y:437:LEU:HB2	16:Y:444:LEU:HD11	1.94	0.49
1:A:1196:TYR:HB2	1:A:1208:LEU:CD1	2.41	0.49
6:F:529:GLU:OE1	6:F:532:ARG:HB2	2.12	0.49
8:I:49:LEU:HD13	8:I:730:VAL:HG21	1.95	0.49
9:K:410:VAL:HG13	7:W:9:LEU:HD21	1.93	0.49
9:K:458:LEU:HB3	9:K:460:LYS:HG3	1.93	0.49
10:L:50:LEU:HD21	10:L:119:TRP:CZ2	2.47	0.49
10:L:83:TYR:CD1	10:L:115:GLU:HA	2.47	0.49
12:N:76:VAL:C	12:N:78:VAL:H	2.15	0.49
13:O:36:ALA:O	13:O:39:VAL:HG12	2.12	0.49
13:O:258:TYR:O	13:O:262:LEU:HB2	2.12	0.49
3:P:178:VAL:O	3:P:182:LEU:HD22	2.13	0.49
16:Y:186:ARG:O	16:Y:189:VAL:HG12	2.12	0.49
1:A:126:ALA:HA	1:A:152:CYS:O	2.12	0.49
3:C:308:TYR:CD1	3:C:343:LEU:HG	2.47	0.49
6:F:19:TYR:HE1	6:H:50:ARG:HE	1.59	0.49
3:P:36:LEU:HD21	3:P:58:LEU:HB2	1.93	0.49
16:Y:485:LEU:O	16:Y:489:GLU:HG2	2.12	0.49
1:A:442:LEU:O	1:A:455:VAL:HG12	2.13	0.49
1:A:1691:LEU:HA	1:A:1695:GLY:HA2	1.93	0.49
3:C:403:TYR:CD2	3:C:435:MET:SD	2.97	0.49
3:C:531:THR:O	3:C:535:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:537:GLU:HG3	6:F:538:ILE:N	2.27	0.49
8:I:399:LYS:HE3	8:I:478:TYR:HE1	1.77	0.49
13:O:580:VAL:O	13:O:583:VAL:HG12	2.12	0.49
3:P:531:THR:O	3:P:535:LYS:HG2	2.12	0.49
16:X:349:SER:CB	16:X:358:ALA:HB2	2.43	0.49
16:X:384:ARG:HH22	16:X:415:GLU:HB3	1.77	0.49
16:Y:349:SER:CB	16:Y:358:ALA:HB2	2.42	0.49
1:A:44:PRO:CA	1:A:45:ALA:CB	2.91	0.49
1:A:594:ARG:HG2	1:A:608:THR:HG23	1.94	0.49
1:A:1140:GLY:HA3	1:A:1171:GLU:O	2.13	0.49
1:A:1860:LEU:O	1:A:1865:ASP:HB2	2.12	0.49
2:B:23:CYS:HA	2:B:30:PHE:CZ	2.48	0.49
3:C:239:THR:HG21	3:C:268:GLN:HE21	1.76	0.49
12:N:546:LYS:HA	12:N:550:GLY:HA2	1.93	0.49
1:A:661:VAL:HG12	1:A:789:LEU:HD12	1.93	0.49
3:C:329:TYR:OH	11:M:20:ARG:HB2	2.13	0.49
8:I:48:ARG:HG2	12:N:390:GLY:HA2	1.95	0.49
8:I:224:SER:HB2	8:I:230:GLU:H	1.77	0.49
8:I:618:ILE:HD12	8:I:705:MET:HE1	1.94	0.49
13:O:91:ASN:O	13:O:95:ILE:HG12	2.13	0.49
13:O:433:GLY:HA2	13:O:618:TYR:HD2	1.77	0.49
16:X:203:LEU:HD13	16:Y:55:LEU:HB3	1.93	0.49
1:A:39:LEU:HD12	1:A:40:ARG:H	1.77	0.49
1:A:872:LEU:HD12	1:A:937:VAL:HG11	1.94	0.49
1:A:1047:VAL:O	1:A:1109:GLY:HA2	2.13	0.49
3:C:151:LEU:HD11	3:C:181:LYS:CB	2.42	0.49
3:C:370:LEU:CG	14:R:79:TYR:HE1	2.23	0.49
8:I:219:VAL:N	8:I:234:PHE:O	2.44	0.49
12:N:267:GLN:HG3	12:N:268:VAL:N	2.27	0.49
13:O:240:LEU:HD11	13:O:256:LEU:HB3	1.93	0.49
3:P:487:ALA:HB1	3:P:519:TYR:CE1	2.46	0.49
16:X:330:ARG:O	16:X:334:ILE:HG23	2.13	0.49
3:C:244:ILE:HD12	3:C:245:GLU:N	2.27	0.49
9:K:256:VAL:O	9:K:259:GLU:HG2	2.13	0.49
10:L:74:VAL:HG21	10:L:137:ILE:HD11	1.93	0.49
3:P:332:GLU:O	3:P:333:THR:C	2.51	0.49
14:R:493:LEU:O	14:R:494:ILE:HB	2.12	0.49
1:A:1611:VAL:CG1	1:A:1612:LEU:N	2.75	0.49
9:K:36:GLU:HG2	9:K:37:PRO:HD2	1.95	0.49
9:K:337:TRP:HB3	9:K:360:ALA:HB2	1.94	0.49
13:O:39:VAL:HG11	13:O:97:ILE:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:215:PHE:HD2	13:O:216:LEU:HD23	1.78	0.49
16:X:321:LEU:HD21	16:X:351:TYR:HB2	1.94	0.49
16:X:485:LEU:O	16:X:489:GLU:HG2	2.13	0.49
16:Y:226:VAL:HG22	16:Y:236:LEU:HD23	1.94	0.49
1:A:629:LEU:HB2	1:A:630:PRO:CD	2.42	0.49
1:A:1777:GLU:O	1:A:1781:GLN:HG2	2.13	0.49
3:C:119:MET:HA	3:C:122:ARG:HG2	1.95	0.49
3:C:234:LEU:HB3	3:C:250:LYS:CE	2.42	0.49
6:H:150:SER:N	6:H:151:PRO:HD2	2.28	0.49
8:I:56:TRP:CD2	8:I:98:PRO:HB3	2.43	0.49
9:J:45:GLN:O	9:J:49:LEU:HG	2.13	0.49
9:K:391:PHE:CZ	9:K:411:VAL:HG21	2.48	0.49
16:X:59:LEU:HD22	16:Y:270:ASN:ND2	2.27	0.49
1:A:1196:TYR:CB	1:A:1208:LEU:HD11	2.42	0.48
9:J:451:LEU:O	9:J:454:VAL:HG22	2.13	0.48
9:J:513:THR:O	9:J:517:THR:HG22	2.13	0.48
9:K:320:ARG:HB2	9:K:340:TYR:HE1	1.78	0.48
3:C:115:TYR:CZ	3:C:161:LYS:HD3	2.48	0.48
3:C:238:TYR:CB	3:C:247:ALA:HB2	2.43	0.48
3:C:270:ALA:HB2	3:C:285:ILE:HG22	1.94	0.48
8:I:673:LEU:HA	8:I:676:ASN:HB2	1.95	0.48
9:J:320:ARG:HB3	9:J:340:TYR:HE1	1.78	0.48
12:N:211:ARG:O	12:N:215:LEU:CG	2.50	0.48
14:R:110:LYS:NZ	14:R:114:LYS:HB2	2.28	0.48
14:R:420:PHE:HA	14:R:421:ALA:HA	1.65	0.48
16:X:146:TYR:CD1	16:X:154:ASP:HB2	2.48	0.48
16:X:204:ASP:HB2	16:Y:52:ASN:OD1	2.13	0.48
1:A:1377:LYS:HE2	1:A:1416:TRP:CE2	2.48	0.48
3:C:180:ARG:HG3	3:C:212:LEU:HD21	1.95	0.48
5:E:60:SER:O	5:E:63:VAL:HG12	2.13	0.48
8:I:571:LYS:HE2	8:I:571:LYS:HB3	1.65	0.48
9:K:277:GLU:HB3	9:K:443:LYS:NZ	2.28	0.48
13:O:672:VAL:HG13	13:O:687:LEU:HD11	1.96	0.48
1:A:90:ASP:HB3	1:A:591:VAL:HG21	1.94	0.48
1:A:1308:GLY:N	1:A:1373:MET:O	2.46	0.48
1:A:1401:PRO:HD3	10:L:135:PHE:CE2	2.48	0.48
1:A:1781:GLN:HB2	1:A:1783:THR:HG22	1.95	0.48
2:B:36:ASP:OD1	2:B:36:ASP:N	2.46	0.48
4:D:4:LEU:HD21	13:O:506:LEU:HB2	1.94	0.48
6:H:130:ARG:HD2	6:H:133:LYS:HD3	1.95	0.48
6:H:158:ILE:HG22	6:H:159:GLY:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLN:HG3	3:C:142:GLU:O	2.13	0.48
1:A:266:HIS:CE1	1:A:427:ALA:HB2	2.49	0.48
1:A:945:GLU:HG3	13:O:599:ILE:HG23	1.95	0.48
1:A:1313:LEU:HD13	1:A:1316:MET:HB2	1.95	0.48
1:A:1375:TYR:HB3	1:A:1378:THR:HG21	1.96	0.48
1:A:1672:ARG:HB2	1:A:1673:TYR:CE1	2.47	0.48
3:C:370:LEU:CG	14:R:79:TYR:CE1	2.96	0.48
9:K:242:TYR:O	7:W:3:ARG:NH2	2.45	0.48
13:O:405:SER:O	13:O:409:HIS:CD2	2.66	0.48
16:X:87:LEU:HD22	16:X:95:ASN:HD22	1.79	0.48
16:Y:491:LYS:O	16:Y:494:ASP:OD1	2.32	0.48
1:A:942:ARG:HG2	13:O:565:GLN:HG2	1.95	0.48
1:A:1454:LEU:O	1:A:1458:SER:HB2	2.14	0.48
1:A:1589:TYR:CE2	1:A:1591:HIS:HB2	2.48	0.48
1:A:1636:VAL:HG22	1:A:1651:LEU:HD11	1.95	0.48
3:C:332:GLU:O	3:C:333:THR:C	2.50	0.48
6:F:653:LEU:O	6:F:656:MET:HG2	2.14	0.48
6:H:529:GLU:OE1	6:H:532:ARG:HB2	2.12	0.48
9:J:36:GLU:HG2	9:J:37:PRO:HD2	1.96	0.48
11:M:19:TRP:CD1	11:M:19:TRP:C	2.87	0.48
12:N:179:CYS:HA	12:N:182:ARG:HB2	1.95	0.48
12:N:550:GLY:HA2	12:N:551:GLU:HB2	1.94	0.48
3:P:441:GLU:HG2	3:P:472:LYS:NZ	2.28	0.48
3:P:490:TYR:CD1	3:P:515:TYR:HB3	2.49	0.48
1:A:72:GLU:HB2	1:A:96:ALA:HA	1.95	0.48
1:A:982:ASP:OD1	1:A:983:LEU:N	2.46	0.48
1:A:1543:HIS:CD2	1:A:1559:HIS:HE1	2.31	0.48
3:C:296:ARG:HA	3:P:101:ARG:NH1	2.28	0.48
6:F:544:TRP:CD2	14:R:499:ARG:HD3	2.48	0.48
9:J:129:LYS:O	9:J:132:ILE:HG22	2.14	0.48
9:J:445:GLU:N	9:J:446:PRO:HD2	2.29	0.48
9:K:320:ARG:HB2	9:K:340:TYR:CE1	2.49	0.48
10:L:111:LEU:HD11	10:L:122:VAL:HG22	1.96	0.48
3:P:120:TYR:CE2	3:P:124:LEU:HD11	2.48	0.48
16:Y:146:TYR:CD1	16:Y:154:ASP:HB2	2.48	0.48
1:A:125:GLN:HG3	1:A:154:LEU:HD23	1.96	0.48
3:C:28:ASP:OD1	3:C:29:LEU:N	2.46	0.48
3:C:206:TRP:HE3	3:C:233:PHE:CD1	2.31	0.48
3:C:389:ARG:HG2	13:O:279:ASP:CB	2.44	0.48
7:G:4:ARG:HD3	9:J:376:LEU:HD12	1.95	0.48
8:I:17:LYS:HE3	8:I:51:SER:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:138:LEU:HD12	8:I:253:ARG:HA	1.96	0.48
12:N:395:ASP:HB2	12:N:397:ILE:H	1.79	0.48
3:P:87:TYR:CZ	3:P:113:LYS:HE2	2.48	0.48
16:X:100:TYR:HD1	16:X:138:VAL:HG13	1.78	0.48
16:Y:50:HIS:ND1	16:Y:86:SER:HA	2.28	0.48
16:Y:321:LEU:HD21	16:Y:351:TYR:HB2	1.95	0.48
1:A:105:GLY:O	1:A:111:LEU:HD23	2.14	0.48
1:A:1102:ILE:HG21	1:A:1171:GLU:OE1	2.13	0.48
1:A:1640:GLY:HA3	1:A:1645:GLU:O	2.13	0.48
1:A:1849:LYS:O	1:A:1852:ILE:HB	2.14	0.48
8:I:47:HIS:CE1	8:I:54:ARG:NH1	2.82	0.48
1:A:173:LEU:HD22	1:A:177:VAL:HG11	1.95	0.48
1:A:1475:ARG:HG2	1:A:1476:PHE:CE2	2.49	0.48
2:B:39:VAL:CB	2:B:43:ASP:CB	2.87	0.48
3:C:252:GLN:HA	3:C:255:ILE:HD12	1.96	0.48
6:F:152:PHE:CE1	6:F:162:PRO:HG2	2.48	0.48
8:I:74:ARG:HD2	8:I:174:ASN:HD22	1.78	0.48
9:J:242:TYR:HB2	9:J:250:CYS:SG	2.54	0.48
9:K:185:LEU:HA	9:K:188:LEU:CD2	2.43	0.48
9:K:227:LEU:O	9:K:230:ASN:N	2.46	0.48
16:X:40:HIS:HB3	16:Y:201:LEU:CD1	2.44	0.48
1:A:32:PRO:HD3	13:O:233:PRO:HB3	1.95	0.47
1:A:1253:ALA:O	1:A:1257:ILE:N	2.40	0.47
1:A:1502:PRO:O	1:A:1503:ASN:CB	2.62	0.47
1:A:1536:LEU:HD23	1:A:1562:LEU:CD2	2.44	0.47
7:G:3:ARG:HH22	9:J:243:TYR:HA	1.78	0.47
7:G:13:LEU:HA	7:G:16:ILE:HD12	1.96	0.47
8:I:17:LYS:NZ	8:I:51:SER:O	2.44	0.47
9:J:447:LEU:O	9:J:451:LEU:HD23	2.14	0.47
9:K:445:GLU:N	9:K:446:PRO:HD2	2.29	0.47
12:N:270:ARG:O	12:N:274:GLU:HB2	2.14	0.47
12:N:397:ILE:O	12:N:401:ILE:HG13	2.13	0.47
12:N:560:MET:CE	12:N:560:MET:HA	2.44	0.47
13:O:425:LYS:HB3	13:O:441:GLN:HG2	1.95	0.47
3:P:224:LEU:HB2	3:P:230:LYS:HD2	1.96	0.47
16:X:491:LYS:O	16:X:494:ASP:OD1	2.32	0.47
1:A:1771:PHE:O	1:A:1774:VAL:HB	2.13	0.47
2:B:83:LYS:O	2:B:84:GLU:HB2	2.14	0.47
3:C:412:LEU:O	3:C:414:MET:HG3	2.14	0.47
5:E:92:ASP:HB3	6:H:592:ARG:HH22	1.79	0.47
9:J:210:LYS:HE2	9:J:213:ASN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:477:HIS:CB	13:O:486:ALA:HB2	2.44	0.47
3:P:170:PHE:O	3:P:173:TYR:HB3	2.13	0.47
3:P:233:PHE:O	3:P:237:ILE:HG13	2.13	0.47
16:X:235:TRP:CE3	16:X:236:LEU:HA	2.48	0.47
1:A:1078:MET:HB2	1:A:1552:TYR:HE1	1.78	0.47
1:A:1871:TYR:HB2	1:A:1877:LEU:HD11	1.96	0.47
3:C:303:PHE:HD1	3:C:303:PHE:C	2.18	0.47
6:F:150:SER:N	6:F:151:PRO:HD2	2.29	0.47
8:I:44:VAL:C	8:I:45:LEU:HD12	2.35	0.47
8:I:45:LEU:HG	8:I:57:SER:HA	1.96	0.47
8:I:139:LEU:HD21	8:I:192:MET:CE	2.44	0.47
9:J:441:VAL:CG2	9:J:444:TRP:HD1	2.19	0.47
13:O:280:ARG:HA	13:O:280:ARG:HD2	1.67	0.47
13:O:411:LYS:HE2	13:O:412:HIS:CE1	2.48	0.47
13:O:467:ALA:HB1	13:O:506:LEU:CD1	2.43	0.47
3:P:94:PHE:O	3:P:97:LYS:HB2	2.14	0.47
16:X:226:VAL:HG22	16:X:236:LEU:HD23	1.95	0.47
6:F:692:LEU:HD13	6:F:709:ARG:HA	1.95	0.47
6:H:103:HIS:HA	6:H:106:ILE:HD12	1.96	0.47
9:J:212:TYR:HB3	9:J:243:TYR:CD1	2.50	0.47
13:O:146:LEU:CB	13:O:151:VAL:HG23	2.44	0.47
1:A:247:VAL:HG11	1:A:427:ALA:HB3	1.97	0.47
1:A:481:PRO:HA	1:A:488:MET:HA	1.97	0.47
1:A:1380:ASN:HD22	1:A:1383:ILE:HD12	1.79	0.47
2:B:16:TRP:CD1	2:B:46:LEU:HG	2.50	0.47
8:I:12:ARG:O	8:I:744:PHE:HA	2.14	0.47
9:K:167:PHE:O	9:K:171:THR:HG22	2.14	0.47
9:K:496:GLU:HB2	9:K:526:TYR:HE1	1.78	0.47
13:O:445:LEU:O	13:O:448:MET:HB2	2.14	0.47
3:P:402:TRP:HB3	3:P:425:ALA:HB2	1.96	0.47
1:A:15:ARG:HE	13:O:526:HIS:CB	2.26	0.47
1:A:582:THR:N	1:A:583:TYR:HA	2.29	0.47
1:A:770:TYR:CD1	1:A:783:ILE:HD11	2.49	0.47
3:C:526:TRP:NE1	3:C:553:ILE:HB	2.30	0.47
6:F:481:CYS:O	6:F:485:ILE:HG12	2.15	0.47
9:K:384:SER:HB3	9:K:415:ASN:OD1	2.15	0.47
12:N:387:LEU:HD21	12:N:424:ILE:HG12	1.96	0.47
13:O:421:SER:O	13:O:424:GLN:HB3	2.15	0.47
1:A:269:TRP:HA	1:A:411:HIS:HA	1.96	0.47
1:A:489:LEU:HD22	1:A:497:LEU:HD22	1.96	0.47
1:A:591:VAL:HG22	1:A:606:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:ALA:C	3:C:116:PHE:N	2.68	0.47
3:C:134:THR:OG1	3:C:146:VAL:HG21	2.15	0.47
3:C:303:PHE:CE1	3:C:307:LEU:HD12	2.49	0.47
6:F:554:VAL:HG22	9:K:285:PHE:HD2	1.77	0.47
7:G:4:ARG:HD2	9:J:373:TYR:HD1	1.80	0.47
8:I:166:LYS:O	8:I:170:ASP:N	2.45	0.47
9:J:21:SER:N	9:K:165:GLU:HG2	2.29	0.47
9:J:23:LEU:HA	9:J:46:CYS:SG	2.54	0.47
9:J:469:ARG:O	9:J:473:VAL:HG23	2.14	0.47
9:K:42:TRP:HA	9:K:42:TRP:CE3	2.49	0.47
9:K:45:GLN:O	9:K:49:LEU:HG	2.14	0.47
12:N:533:PHE:CZ	12:N:564:MET:HB3	2.50	0.47
13:O:515:GLN:HB3	13:O:531:LEU:HD11	1.96	0.47
14:R:181:ILE:HG22	14:R:465:GLU:HG2	1.96	0.47
16:X:203:LEU:CD2	16:Y:55:LEU:CD2	2.92	0.47
1:A:273:ARG:O	1:A:274:VAL:HB	2.14	0.47
4:D:27:GLU:HG3	13:O:134:LEU:HD21	1.97	0.47
6:F:73:TYR:CD1	6:F:117:THR:HG22	2.49	0.47
6:F:554:VAL:O	6:F:558:ASP:HB2	2.15	0.47
8:I:561:ARG:NH2	8:I:589:THR:O	2.47	0.47
9:J:55:ARG:NH1	9:K:265:ALA:H	2.12	0.47
9:K:93:LEU:HD12	9:K:93:LEU:N	2.30	0.47
13:O:707:LYS:HA	13:O:710:ILE:HG22	1.95	0.47
16:X:54:ARG:NH2	16:X:90:ASP:OD2	2.48	0.47
16:X:87:LEU:HD22	16:X:95:ASN:ND2	2.30	0.47
3:C:296:ARG:HH11	3:C:296:ARG:HG2	1.74	0.47
8:I:27:VAL:O	8:I:35:ILE:HD12	2.14	0.47
8:I:514:PHE:CD2	13:O:443:GLN:HG3	2.50	0.47
12:N:362:LYS:HA	12:N:410:LEU:CD2	2.44	0.47
13:O:40:LEU:HD22	13:O:82:ILE:HD12	1.96	0.47
13:O:247:ASN:HD21	13:O:250:PHE:HB2	1.79	0.47
13:O:539:ASN:HD22	13:O:542:GLU:HB2	1.79	0.47
3:P:384:ALA:O	3:P:388:TYR:CD2	2.68	0.47
16:X:76:LYS:HB2	16:X:106:GLN:NE2	2.29	0.47
1:A:240:VAL:H	1:A:241:ASP:CB	2.28	0.47
12:N:397:ILE:HA	12:N:400:TYR:HB3	1.97	0.47
13:O:641:LEU:HD11	13:O:671:GLN:HG2	1.97	0.47
3:P:251:TYR:HB3	3:P:269:ILE:HD11	1.95	0.47
3:P:308:TYR:CD1	3:P:343:LEU:HG	2.50	0.47
1:A:430:VAL:HA	1:A:443:CYS:O	2.15	0.46
3:C:233:PHE:O	3:C:237:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:493:TYR:CZ	3:C:497:ILE:HD11	2.50	0.46
9:J:320:ARG:HB3	9:J:340:TYR:CE1	2.51	0.46
12:N:550:GLY:HA2	12:N:551:GLU:CB	2.45	0.46
13:O:296:TYR:HE1	14:R:95:LEU:HB3	1.80	0.46
13:O:621:SER:HB3	13:O:651:ILE:HG12	1.97	0.46
13:O:665:PHE:CD1	13:O:713:VAL:HG23	2.50	0.46
16:X:294:PHE:C	16:X:294:PHE:CD1	2.88	0.46
16:Y:99:LYS:HD3	16:Y:102:MET:CE	2.45	0.46
1:A:263:GLN:HB2	1:A:265:VAL:HG11	1.96	0.46
1:A:1274:LEU:HG	1:A:1302:LEU:HD11	1.97	0.46
2:B:16:TRP:HB3	2:B:31:ASN:HA	1.97	0.46
4:D:10:PRO:HD2	13:O:346:TRP:CZ3	2.50	0.46
5:E:94:TRP:HE1	6:F:595:GLN:NE2	2.13	0.46
6:F:164:PRO:HG3	6:F:471:LYS:HG3	1.98	0.46
9:K:243:TYR:OH	7:W:1:MET:HG2	2.15	0.46
1:A:181:TRP:CZ2	1:A:246:ILE:O	2.69	0.46
1:A:183:THR:OG1	1:A:184:LYS:O	2.25	0.46
1:A:1145:LEU:HD13	1:A:1610:TYR:OH	2.15	0.46
1:A:1153:ILE:HG12	1:A:1184:HIS:CD2	2.50	0.46
5:E:102:LEU:HD13	6:H:594:ILE:HG22	1.98	0.46
6:F:149:TRP:HH2	6:F:470:GLY:HA2	1.80	0.46
6:H:121:LEU:HG	6:H:125:TYR:CE1	2.50	0.46
6:H:522:PHE:CB	6:H:539:TYR:CD1	2.98	0.46
9:J:445:GLU:OE1	9:J:475:ILE:HG21	2.14	0.46
12:N:149:LEU:HB3	12:N:150:ARG:H	1.46	0.46
12:N:213:TYR:H	12:N:214:ARG:N	2.12	0.46
13:O:546:ARG:HA	13:O:549:VAL:HG12	1.96	0.46
16:X:346:GLY:HA3	16:X:378:LEU:HD21	1.97	0.46
1:A:1351:GLN:HG3	10:L:36:CYS:SG	2.56	0.46
3:C:303:PHE:C	3:C:303:PHE:CD1	2.88	0.46
6:H:494:HIS:CD2	6:H:495:HIS:CD2	3.04	0.46
8:I:262:LEU:HA	8:I:265:ILE:HG22	1.98	0.46
9:K:37:PRO:HB3	9:K:69:TYR:CZ	2.50	0.46
12:N:74:TRP:CZ3	12:N:76:VAL:HG13	2.50	0.46
13:O:105:LEU:HD13	13:O:155:TYR:HB2	1.97	0.46
13:O:591:TYR:HE2	13:O:603:MET:HG3	1.79	0.46
7:W:13:LEU:HA	7:W:16:ILE:HD12	1.96	0.46
16:Y:60:LEU:HB3	16:Y:79:LEU:HD11	1.97	0.46
16:Y:281:TYR:CE1	16:Y:289:ASN:HB3	2.50	0.46
1:A:165:GLU:O	13:O:316:HIS:HB3	2.15	0.46
1:A:215:HIS:CG	1:A:216:PRO:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:145:ASN:HB2	6:F:146:PRO:O	2.16	0.46
8:I:36:ALA:HB2	8:I:80:LEU:HD21	1.97	0.46
9:J:211:LYS:O	9:J:212:TYR:CD2	2.67	0.46
9:K:35:GLU:HB3	9:K:40:ILE:HD11	1.98	0.46
13:O:361:LEU:HD12	13:O:387:GLN:NE2	2.30	0.46
3:P:296:ARG:NH1	3:P:299:ASN:HD21	2.13	0.46
14:R:430:TYR:HA	14:R:431:PRO:HA	1.77	0.46
1:A:1177:MET:HB2	1:A:1207:GLY:O	2.15	0.46
1:A:1469:CYS:HB2	1:A:1488:LEU:CD2	2.45	0.46
3:C:384:ALA:O	3:C:388:TYR:CD2	2.68	0.46
6:F:131:LEU:HD11	6:F:158:ILE:HG12	1.98	0.46
6:F:541:THR:HG23	14:R:499:ARG:CG	2.46	0.46
8:I:685:PHE:HA	8:I:701:PRO:HD3	1.98	0.46
9:J:55:ARG:HD2	9:K:261:ASP:OD1	2.15	0.46
9:J:93:LEU:HD12	9:J:93:LEU:N	2.31	0.46
9:J:165:GLU:HG3	9:K:20:GLN:HB2	1.98	0.46
9:K:181:GLU:HB3	9:K:209:LEU:HD13	1.98	0.46
13:O:146:LEU:HD12	13:O:151:VAL:HG22	1.98	0.46
13:O:321:GLU:HG3	13:O:350:LEU:HD22	1.98	0.46
1:A:1659:GLU:O	1:A:1662:LEU:HG	2.15	0.46
3:C:48:LEU:HD21	3:C:116:PHE:HZ	1.81	0.46
3:C:328:LYS:HB3	3:C:329:TYR:CE2	2.50	0.46
4:D:5:PHE:CE1	13:O:390:PHE:CZ	2.98	0.46
8:I:74:ARG:HD2	8:I:174:ASN:ND2	2.31	0.46
13:O:727:THR:HG22	13:O:730:ARG:HD2	1.97	0.46
3:P:274:HIS:ND1	3:P:306:LEU:HB3	2.30	0.46
3:P:405:LEU:HD23	3:P:405:LEU:HA	1.78	0.46
3:C:321:HIS:HA	11:M:24:LEU:CD1	2.45	0.46
3:C:441:GLU:HB2	3:C:445:LYS:HE3	1.97	0.46
6:F:59:ARG:NH1	6:H:562:MET:HG3	2.30	0.46
9:J:454:VAL:C	9:J:458:LEU:HD12	2.31	0.46
13:O:361:LEU:HD13	13:O:384:LEU:CA	2.46	0.46
16:X:267:LEU:CD1	16:Y:59:LEU:CD1	2.89	0.46
16:Y:466:ASP:OD1	16:Y:482:LYS:CE	2.62	0.46
1:A:1894:VAL:HA	1:A:1895:PRO:HD3	1.69	0.46
3:C:112:LYS:H	3:C:112:LYS:HD2	1.81	0.46
3:C:300:MET:HG3	3:C:319:LEU:HD11	1.98	0.46
3:C:465:VAL:HG23	3:C:466:GLU:H	1.81	0.46
6:H:145:ASN:HB2	6:H:146:PRO:O	2.16	0.46
8:I:213:ASP:OD1	8:I:215:LYS:N	2.29	0.46
9:J:35:GLU:HB3	9:J:40:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:481:THR:O	9:J:485:ILE:HG12	2.16	0.46
12:N:212:TYR:C	12:N:215:LEU:HB2	2.37	0.46
13:O:136:LEU:C	13:O:136:LEU:HD12	2.36	0.46
16:X:203:LEU:HD22	16:Y:55:LEU:HB3	1.96	0.46
16:Y:233:LEU:HD22	16:Y:235:TRP:CZ2	2.51	0.46
16:Y:301:ASP:HA	16:Y:302:PRO:HD2	1.76	0.46
1:A:1321:VAL:HG23	1:A:1322:PRO:HD3	1.97	0.46
3:C:46:ARG:CZ	3:C:170:PHE:CD2	2.99	0.46
3:C:209:LEU:O	3:C:213:ILE:HG12	2.16	0.46
3:C:234:LEU:CD2	3:C:250:LYS:HE3	2.37	0.46
3:C:422:TYR:CE2	3:C:438:ALA:HB1	2.51	0.46
6:F:762:TRP:CE2	9:J:362:GLN:HB2	2.51	0.46
6:H:488:LEU:HD22	6:H:501:VAL:HG13	1.98	0.46
6:H:499:GLY:O	6:H:503:CYS:HB2	2.16	0.46
6:H:502:LEU:HB2	6:H:525:VAL:HG22	1.98	0.46
9:J:9:ARG:O	9:J:13:TYR:CD2	2.67	0.46
9:J:46:CYS:O	9:J:50:THR:OG1	2.22	0.46
9:J:262:PRO:HD3	9:K:58:HIS:CD2	2.51	0.46
9:J:272:ILE:O	9:J:276:VAL:HG23	2.16	0.46
9:J:493:GLY:HA2	9:J:495:PHE:CE1	2.51	0.46
9:K:386:LEU:H	9:K:386:LEU:CD1	2.29	0.46
12:N:268:VAL:HA	12:N:271:GLU:CD	2.36	0.46
13:O:99:LEU:C	13:O:99:LEU:HD12	2.36	0.46
3:P:251:TYR:HA	3:P:254:LEU:HD12	1.98	0.46
1:A:168:ASP:OD1	1:A:168:ASP:N	2.49	0.45
6:F:459:ALA:HB2	6:H:7:PRO:HG2	1.97	0.45
8:I:67:GLU:HB2	8:I:85:ALA:HB3	1.98	0.45
8:I:203:GLY:HA3	8:I:223:VAL:HG22	1.98	0.45
8:I:237:GLU:CG	8:I:607:ILE:HD13	2.47	0.45
13:O:585:LEU:HD21	13:O:623:THR:HB	1.98	0.45
13:O:715:TYR:HE1	13:O:719:ARG:HE	1.64	0.45
3:P:45:GLU:O	3:P:87:TYR:OH	2.33	0.45
16:Y:168:THR:OG1	16:Y:171:ILE:CD1	2.64	0.45
1:A:1201:HIS:HE1	1:A:1203:MET:HB2	1.81	0.45
6:H:12:ILE:CG2	6:H:43:LEU:HD21	2.46	0.45
6:H:149:TRP:HH2	6:H:470:GLY:HA2	1.81	0.45
8:I:115:TRP:CE3	8:I:176:LEU:HD22	2.50	0.45
12:N:659:VAL:HG22	12:N:660:THR:H	1.82	0.45
16:X:281:TYR:CE1	16:X:289:ASN:HB3	2.51	0.45
3:C:206:TRP:O	3:C:209:LEU:HB2	2.16	0.45
3:C:255:ILE:O	3:C:260:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:699:ASP:HB3	6:F:702:ASN:OD1	2.16	0.45
7:G:3:ARG:HB2	9:J:443:LYS:HZ1	1.81	0.45
6:H:656:MET:HE3	6:H:660:LYS:HE2	1.99	0.45
6:H:658:PHE:HB3	6:H:675:ILE:HG12	1.98	0.45
9:J:397:ILE:O	9:J:398:ALA:C	2.55	0.45
12:N:542:VAL:HG11	12:N:558:GLU:CG	2.46	0.45
16:Y:346:GLY:HA3	16:Y:378:LEU:HD21	1.98	0.45
16:Y:517:ASP:O	16:Y:520:VAL:HG22	2.16	0.45
1:A:173:LEU:HD22	1:A:177:VAL:CG1	2.46	0.45
1:A:256:VAL:HG23	1:A:271:LEU:HD22	1.98	0.45
1:A:584:ILE:O	1:A:598:GLU:O	2.33	0.45
1:A:1177:MET:CB	1:A:1207:GLY:HA2	2.42	0.45
1:A:1819:GLU:O	1:A:1823:SER:HB3	2.16	0.45
2:B:20:ASP:O	2:B:30:PHE:CD2	2.69	0.45
3:C:389:ARG:HD3	3:C:389:ARG:HA	1.52	0.45
3:C:416:PHE:CB	13:O:326:GLU:HG2	2.45	0.45
3:C:441:GLU:OE2	14:R:83:ARG:NH1	2.50	0.45
9:J:47:LEU:HD21	9:J:55:ARG:HH21	1.80	0.45
9:J:58:HIS:CG	9:K:262:PRO:HD3	2.51	0.45
9:J:290:LYS:HA	9:J:290:LYS:HE3	1.98	0.45
10:L:62:HIS:H	10:L:62:HIS:CD2	2.35	0.45
16:Y:394:ILE:HA	16:Y:397:ARG:HD3	1.97	0.45
1:A:451:GLN:HA	1:A:475:PRO:O	2.16	0.45
1:A:810:TYR:HA	1:A:811:PRO:HD2	1.68	0.45
1:A:1304:MET:O	1:A:1307:LEU:HB2	2.17	0.45
1:A:1354:GLU:HA	10:L:30:VAL:HG12	1.99	0.45
6:F:12:ILE:CG2	6:F:43:LEU:HD21	2.47	0.45
9:J:468:HIS:HB3	9:J:485:ILE:HG23	1.99	0.45
13:O:423:ALA:HA	13:O:426:THR:HG22	1.98	0.45
13:O:608:LEU:HD23	13:O:624:VAL:HG22	1.97	0.45
16:X:54:ARG:CZ	16:X:90:ASP:OD2	2.64	0.45
16:X:168:THR:OG1	16:X:171:ILE:CD1	2.65	0.45
1:A:1274:LEU:O	1:A:1277:ILE:HG22	2.16	0.45
3:C:96:VAL:N	3:C:97:LYS:HA	2.31	0.45
3:C:285:ILE:HA	3:C:288:GLU:CD	2.37	0.45
6:F:33:ALA:HB2	6:H:498:THR:HG21	1.99	0.45
9:K:272:ILE:O	9:K:276:VAL:HG23	2.16	0.45
12:N:241:HIS:NE2	12:N:302:LYS:HE2	2.31	0.45
13:O:127:HIS:O	13:O:128:LYS:HB3	2.17	0.45
14:R:128:ALA:HB1	14:R:129:LYS:CA	2.27	0.45
16:X:517:ASP:O	16:X:520:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:294:PHE:CD1	16:Y:294:PHE:O	2.69	0.45
1:A:1485:PHE:CD1	1:A:1523:LEU:HD21	2.52	0.45
1:A:1572:TYR:CE2	1:A:1616:PRO:HB3	2.52	0.45
1:A:1638:TYR:N	1:A:1638:TYR:HD1	2.10	0.45
3:C:122:ARG:HG3	3:C:154:LEU:HD11	1.98	0.45
6:F:59:ARG:NH2	6:H:562:MET:HB2	2.32	0.45
9:K:236:SER:O	9:K:240:ARG:HG3	2.16	0.45
9:K:464:ALA:HB1	9:K:488:ILE:HD12	1.99	0.45
13:O:402:LEU:HD23	13:O:402:LEU:HA	1.89	0.45
10:L:125:THR:HA	10:L:126:ASP:HB3	1.98	0.45
12:N:233:CYS:O	12:N:235:GLN:N	2.49	0.45
3:P:201:LEU:HA	3:P:229:MET:SD	2.57	0.45
16:Y:506:GLN:HG3	16:Y:508:ASP:OD1	2.17	0.45
1:A:1640:GLY:N	1:A:1645:GLU:O	2.50	0.45
2:B:33:CYS:HB3	2:B:39:VAL:O	2.17	0.45
3:C:277:ARG:O	3:C:279:ILE:CD1	2.65	0.45
6:H:656:MET:HE3	9:K:526:TYR:CD2	2.51	0.45
8:I:116:MET:SD	8:I:210:LEU:CG	3.05	0.45
8:I:262:LEU:HD21	8:I:533:ILE:HD13	1.99	0.45
8:I:269:LEU:HD22	8:I:526:LYS:HD2	1.99	0.45
9:J:476:PRO:HB3	3:P:182:LEU:HB3	1.98	0.45
9:K:38:GLN:HE21	9:K:38:GLN:HB2	1.68	0.45
3:P:61:SER:HB2	3:P:262:SER:CB	2.43	0.45
3:P:151:LEU:HD23	3:P:151:LEU:HA	1.85	0.45
3:P:209:LEU:O	3:P:213:ILE:HG12	2.17	0.45
3:P:405:LEU:HA	3:P:408:THR:HG22	1.97	0.45
16:X:60:LEU:HB3	16:X:79:LEU:HD11	1.98	0.45
1:A:1189:ALA:O	1:A:1191:LEU:N	2.50	0.45
1:A:1262:GLN:HE22	1:A:1582:ALA:HB1	1.82	0.45
1:A:1480:GLU:HA	1:A:1527:MET:HA	1.98	0.45
6:H:554:VAL:O	6:H:558:ASP:HB2	2.17	0.45
8:I:167:LEU:HD12	8:I:168:LEU:N	2.32	0.45
13:O:262:LEU:HD13	13:O:270:SER:CB	2.47	0.45
13:O:581:ILE:HG22	13:O:610:LEU:HD23	1.99	0.45
16:X:168:THR:OG1	16:X:171:ILE:HD12	2.17	0.45
16:X:173:MET:SD	16:Y:49:LEU:HB3	2.57	0.45
1:A:1417:ASP:HA	1:A:1643:TRP:CZ2	2.51	0.44
2:B:15:LEU:HD12	12:N:626:TYR:HE2	1.82	0.44
3:C:48:LEU:HD21	3:C:116:PHE:CE2	2.52	0.44
3:C:405:LEU:HA	3:C:408:THR:HG22	1.99	0.44
5:E:63:VAL:HA	5:E:66:THR:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:639:TYR:CZ	14:R:498:ILE:HG13	2.52	0.44
9:J:52:GLN:HG2	9:K:295:TYR:HE2	1.82	0.44
9:J:69:TYR:O	9:J:70:GLU:HB3	2.16	0.44
9:K:78:ARG:HG3	9:K:135:LEU:HD22	1.98	0.44
9:K:284:LEU:HD13	9:K:308:TYR:HB2	2.00	0.44
12:N:659:VAL:HG22	12:N:660:THR:N	2.32	0.44
16:Y:270:ASN:HB2	16:Y:273:LEU:HB3	1.99	0.44
1:A:260:ASP:OD1	1:A:262:VAL:HG22	2.17	0.44
1:A:872:LEU:HA	1:A:933:TRP:HH2	1.82	0.44
1:A:1637:THR:HA	1:A:1647:THR:O	2.17	0.44
6:H:130:ARG:HH12	9:K:473:VAL:CG2	2.26	0.44
8:I:371:SER:HB3	13:O:652:LEU:HB3	1.99	0.44
9:J:512:ASP:O	9:J:516:VAL:HG23	2.17	0.44
9:K:222:GLU:O	9:K:225:ASP:O	2.35	0.44
9:K:413:PHE:HD1	9:K:454:VAL:HG23	1.82	0.44
12:N:197:PRO:HA	12:N:198:GLU:HA	1.77	0.44
12:N:350:ASP:HB3	12:N:351:PHE:HA	1.96	0.44
13:O:219:GLN:O	13:O:222:LEU:HB2	2.17	0.44
13:O:350:LEU:HD23	13:O:350:LEU:HA	1.76	0.44
1:A:1642:GLN:HG3	1:A:1643:TRP:CE2	2.52	0.44
1:A:1675:GLU:HG3	1:A:1676:LEU:N	2.31	0.44
3:C:170:PHE:O	3:C:173:TYR:HB3	2.16	0.44
6:F:522:PHE:CB	6:F:539:TYR:CD1	2.99	0.44
6:F:539:TYR:O	6:F:542:THR:HB	2.17	0.44
8:I:38:ALA:HB2	8:I:71:LEU:HD11	1.99	0.44
8:I:287:LEU:HD22	8:I:300:VAL:HG11	2.00	0.44
9:J:337:TRP:CZ3	9:J:340:TYR:HD2	2.36	0.44
9:K:192:LYS:HG2	9:K:198:GLN:HE21	1.82	0.44
12:N:330:ARG:HB2	12:N:334:ARG:NH2	2.32	0.44
1:A:38:GLN:HG3	3:C:396:LYS:H	1.82	0.44
1:A:131:PHE:CE1	1:A:216:PRO:HD3	2.52	0.44
3:C:112:LYS:HB2	3:C:113:LYS:NZ	2.32	0.44
3:C:286:PHE:HB3	3:C:303:PHE:CE2	2.53	0.44
6:F:18:HIS:O	6:H:73:TYR:OH	2.18	0.44
6:F:488:LEU:HD22	6:F:501:VAL:HG13	2.00	0.44
8:I:186:GLU:OE2	8:I:197:ARG:CZ	2.62	0.44
9:J:206:GLU:HA	9:J:209:LEU:HG	1.98	0.44
12:N:281:TYR:HB3	12:N:282:GLU:H	1.55	0.44
12:N:574:ILE:HD12	12:N:625:LYS:HG2	1.99	0.44
13:O:668:ALA:CB	13:O:694:LEU:HD23	2.47	0.44
3:P:54:TRP:CH2	3:P:58:LEU:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:323:LEU:HD12	3:P:336:VAL:HG11	2.00	0.44
3:P:475:LYS:O	3:P:479:GLN:NE2	2.50	0.44
1:A:191:ARG:HG2	1:A:192:SER:N	2.32	0.44
1:A:880:TYR:HB2	1:A:930:LEU:HD22	1.98	0.44
3:C:235:ALA:H	3:C:250:LYS:HZ2	1.62	0.44
8:I:399:LYS:HG2	8:I:525:VAL:HG21	1.98	0.44
9:J:342:HIS:CD2	9:J:357:TYR:OH	2.70	0.44
9:J:506:LEU:HD21	9:J:516:VAL:HA	1.98	0.44
9:K:406:HIS:CE1	7:W:6:PRO:HB3	2.53	0.44
12:N:400:TYR:CZ	12:N:404:ILE:HD11	2.53	0.44
14:R:406:LEU:HD13	14:R:451[B]:MET:HB2	1.99	0.44
16:X:134:SER:O	16:X:138:VAL:HG23	2.17	0.44
16:Y:384:ARG:HH22	16:Y:415:GLU:HB3	1.82	0.44
1:A:91:GLU:CD	1:A:102:TRP:HE1	2.20	0.44
1:A:632:GLU:O	1:A:635:VAL:HB	2.17	0.44
1:A:1478:GLY:O	1:A:1617:ARG:NH2	2.50	0.44
1:A:1589:TYR:HE2	1:A:1591:HIS:HB2	1.82	0.44
1:A:1674:TRP:HD1	1:A:1674:TRP:H	1.65	0.44
2:B:23:CYS:HA	2:B:30:PHE:CE1	2.53	0.44
6:F:15:ALA:HA	6:H:116:PHE:CE1	2.52	0.44
6:H:121:LEU:O	6:H:125:TYR:CD1	2.70	0.44
9:J:37:PRO:HB3	9:J:69:TYR:CZ	2.52	0.44
9:K:290:LYS:HA	9:K:290:LYS:HE3	1.99	0.44
9:K:369:LEU:O	9:K:373:TYR:CD2	2.71	0.44
12:N:180:PHE:CD1	12:N:299:TRP:HZ3	2.35	0.44
12:N:411:ASP:O	12:N:412:PRO:C	2.56	0.44
3:P:399:TYR:HB3	3:P:428:LEU:HD22	1.99	0.44
16:X:201:LEU:CD1	16:Y:40:HIS:HB3	2.36	0.44
16:X:229:THR:HG21	16:X:233:LEU:HD12	1.99	0.44
16:X:394:ILE:HA	16:X:397:ARG:HD3	2.00	0.44
1:A:100:VAL:HG23	1:A:123:VAL:HG21	1.98	0.44
1:A:1070:LEU:HA	1:A:1073:LEU:HD12	1.99	0.44
1:A:1821:PHE:CD1	1:A:1845:LEU:HD13	2.53	0.44
3:C:39:ILE:CG2	3:C:201:LEU:HG	2.47	0.44
3:C:311:SER:O	3:C:311:SER:OG	2.34	0.44
3:C:488:GLN:O	3:C:491:ILE:HG13	2.17	0.44
6:F:499:GLY:O	6:F:503:CYS:HB2	2.18	0.44
8:I:69:THR:HG23	8:I:85:ALA:HB2	1.99	0.44
8:I:189:ALA:N	8:I:193:PHE:O	2.50	0.44
8:I:396:PHE:CE1	8:I:522:LEU:HD22	2.53	0.44
8:I:586:LEU:HD12	8:I:587:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:465:LEU:CA	9:J:488:ILE:HD12	2.44	0.44
12:N:264:THR:HA	12:N:267:GLN:HG2	2.00	0.44
13:O:78:LEU:HD12	13:O:78:LEU:O	2.17	0.44
13:O:129:THR:O	13:O:130:SER:CB	2.65	0.44
14:R:74:PRO:HA	14:R:75:GLY:HA2	1.79	0.44
16:Y:134:SER:O	16:Y:138:VAL:HG23	2.18	0.44
16:Y:474:ASP:OD1	16:Y:502:ALA:HA	2.18	0.44
1:A:435:ASP:HB2	1:A:501:THR:HG22	2.00	0.44
1:A:1265:ALA:HB2	1:A:1309:HIS:CD2	2.53	0.44
1:A:1477:ALA:HB1	1:A:1574:LEU:HD12	2.00	0.44
6:F:25:VAL:HG22	6:F:47:CYS:HB3	2.00	0.44
6:F:502:LEU:HB2	6:F:525:VAL:HG22	1.99	0.44
9:K:40:ILE:CD1	9:K:65:LEU:HD21	2.48	0.44
10:L:33:LEU:HD12	10:L:42:VAL:HG22	2.00	0.44
12:N:477:PRO:HA	12:N:478:GLU:HA	1.72	0.44
12:N:676:TRP:HE3	12:N:680:GLU:HB3	1.83	0.44
3:P:185:VAL:HG13	3:P:212:LEU:HD22	2.00	0.44
14:R:107:PRO:HA	14:R:110:LYS:HB3	2.00	0.44
16:X:506:GLN:HG3	16:X:508:ASP:OD1	2.17	0.44
16:Y:70:LEU:O	16:Y:70:LEU:HD13	2.17	0.44
16:Y:168:THR:OG1	16:Y:171:ILE:HD12	2.18	0.44
1:A:93:LEU:HD11	1:A:151:ILE:CD1	2.48	0.44
1:A:269:TRP:CD2	1:A:411:HIS:HB3	2.53	0.44
1:A:1466:ALA:HB2	1:A:1515:CYS:HB2	2.00	0.44
6:F:56:LYS:HE3	6:H:532:ARG:HA	1.98	0.44
8:I:70:CYS:C	8:I:71:LEU:HD12	2.38	0.44
8:I:231:VAL:HG12	8:I:232:SER:N	2.33	0.44
12:N:284:SER:HA	12:N:285:PHE:CG	2.53	0.44
13:O:402:LEU:HD13	13:O:425:LYS:HG3	2.00	0.44
7:W:14:ASP:O	7:W:17:GLU:HB2	2.18	0.44
16:Y:229:THR:HG21	16:Y:233:LEU:HD12	2.00	0.44
1:A:941:LEU:HD12	1:A:977:LEU:O	2.18	0.43
2:B:16:TRP:NE1	2:B:46:LEU:HG	2.32	0.43
3:C:370:LEU:HD23	3:C:370:LEU:HA	1.91	0.43
6:F:639:TYR:CD2	14:R:498:ILE:HG21	2.53	0.43
9:J:164:PHE:CZ	9:J:168:ASP:HB2	2.53	0.43
12:N:519:TYR:CE1	12:N:523:LEU:HD21	2.53	0.43
12:N:577:GLU:HG2	12:N:583:ALA:HB2	1.99	0.43
16:X:204:ASP:OD1	16:Y:55:LEU:HB2	2.18	0.43
16:X:233:LEU:HD22	16:X:235:TRP:CZ2	2.53	0.43
16:X:474:ASP:OD1	16:X:502:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:HD3	3:C:142:GLU:HG3	2.00	0.43
1:A:104:LYS:HE2	1:A:114:TYR:CD1	2.53	0.43
1:A:1473:GLY:HA2	1:A:1526:VAL:CG1	2.48	0.43
2:B:20:ASP:CB	2:B:30:PHE:HE2	2.30	0.43
3:C:60:PHE:CB	3:P:89:LEU:HD12	2.47	0.43
6:F:61:LEU:HD23	6:F:61:LEU:HA	1.94	0.43
6:F:765:ASP:OD2	9:J:359:THR:HG22	2.19	0.43
8:I:449:ALA:HB2	13:O:65:LEU:HD21	1.99	0.43
9:J:475:ILE:HG13	9:J:475:ILE:O	2.17	0.43
16:Y:39:ASP:OD1	16:Y:39:ASP:N	2.51	0.43
1:A:160:ASN:OD1	1:A:170:ILE:HG23	2.18	0.43
1:A:1198:THR:O	1:A:1200:GLY:N	2.51	0.43
3:C:36:LEU:HD21	3:C:58:LEU:HB2	1.98	0.43
6:F:658:PHE:HB3	6:F:675:ILE:HG12	1.99	0.43
6:H:707:PHE:CE2	6:H:738:LEU:HG	2.53	0.43
8:I:74:ARG:HH21	8:I:78:LYS:HB2	1.83	0.43
8:I:202:ALA:O	8:I:223:VAL:CG2	2.66	0.43
8:I:413:ASN:HB3	8:I:451:PHE:CE1	2.53	0.43
9:J:211:LYS:O	9:J:212:TYR:CG	2.71	0.43
9:J:369:LEU:O	9:J:373:TYR:CD2	2.72	0.43
9:K:45:GLN:HA	9:K:45:GLN:NE2	2.27	0.43
12:N:392:ASN:O	12:N:395:ASP:HA	2.18	0.43
13:O:596:SER:OG	13:O:599:ILE:HD12	2.18	0.43
16:X:50:HIS:HA	16:X:53:VAL:HG22	2.00	0.43
16:X:355:TYR:CE1	16:X:385:ASN:HB2	2.51	0.43
16:Y:355:TYR:CZ	16:Y:385:ASN:HB3	2.53	0.43
1:A:269:TRP:CE3	1:A:411:HIS:HB3	2.52	0.43
3:C:234:LEU:HB3	3:C:250:LYS:HE3	2.00	0.43
3:C:353:TYR:HA	3:C:356:ARG:HD2	2.00	0.43
6:H:121:LEU:CD1	6:H:125:TYR:HE1	2.32	0.43
6:H:689:LEU:CD2	6:H:713:LEU:HG	2.48	0.43
8:I:501:LEU:HD23	8:I:516:TYR:HE2	1.83	0.43
9:K:371:MET:HA	9:K:374:ILE:HD12	1.99	0.43
12:N:157:LEU:O	12:N:161:LEU:HG	2.17	0.43
1:A:776:ASN:HA	1:A:869:ARG:NE	2.33	0.43
1:A:1230:ILE:HD13	1:A:1236:LEU:HD13	2.00	0.43
1:A:1230:ILE:HA	1:A:1236:LEU:HB3	2.01	0.43
3:C:321:HIS:HA	11:M:24:LEU:HD13	1.99	0.43
6:F:46:THR:HG23	6:H:19:TYR:OH	2.18	0.43
6:H:164:PRO:HB2	6:H:467:ARG:HG3	2.01	0.43
8:I:184:PHE:HB2	8:I:198:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:520:ARG:HD3	12:N:556:PHE:HB3	2.00	0.43
3:C:414:MET:HA	13:O:326:GLU:OE1	2.19	0.43
3:C:416:PHE:HA	3:C:446:LEU:HD11	2.01	0.43
6:F:550:VAL:HG21	9:K:289:HIS:HB3	2.01	0.43
6:F:554:VAL:HG21	9:K:286:TYR:HD1	1.83	0.43
6:H:539:TYR:O	6:H:542:THR:HB	2.18	0.43
8:I:32:ARG:HG2	12:N:388:HIS:CE1	2.54	0.43
9:J:247:PHE:CD2	9:J:277:GLU:HB3	2.53	0.43
9:J:305:VAL:CG1	11:M:31:ILE:HD11	2.46	0.43
9:J:506:LEU:HD12	9:J:506:LEU:HA	1.79	0.43
9:K:349:GLU:HB3	9:K:352:GLN:HE21	1.84	0.43
10:L:61:PRO:HB3	10:L:142:LEU:HA	2.00	0.43
12:N:693:ARG:HA	12:N:696:MET:HB3	2.00	0.43
12:N:699:TRP:HA	12:N:699:TRP:CE3	2.53	0.43
16:X:39:ASP:OD1	16:X:39:ASP:N	2.51	0.43
16:Y:475:TYR:O	16:Y:479:VAL:HG23	2.19	0.43
1:A:1405:LEU:C	1:A:1405:LEU:HD12	2.38	0.43
3:C:150:ALA:O	3:C:154:LEU:HD13	2.18	0.43
6:F:554:VAL:HG21	9:K:286:TYR:CD1	2.53	0.43
3:P:389:ARG:HA	3:P:392:ILE:CG2	2.49	0.43
16:X:408:ASP:O	16:X:411:GLU:HG2	2.19	0.43
1:A:114:TYR:O	1:A:115:LYS:HG3	2.18	0.43
1:A:248:PHE:CB	1:A:430:VAL:HG21	2.44	0.43
1:A:412:LEU:HD12	1:A:468:PHE:CZ	2.54	0.43
1:A:876:SER:HB2	1:A:930:LEU:HD11	2.00	0.43
5:E:105:PHE:HA	9:K:510:ARG:HG2	2.00	0.43
6:H:121:LEU:HD11	6:H:125:TYR:HE1	1.83	0.43
8:I:11:PHE:HD1	8:I:746:MET:HA	1.84	0.43
13:O:319:GLN:O	13:O:322:LEU:HB2	2.19	0.43
16:X:270:ASN:HB2	16:X:273:LEU:HB3	2.01	0.43
1:A:183:THR:HG22	1:A:249:LEU:HG	2.00	0.43
1:A:755:LEU:HA	1:A:756:PHE:HA	1.74	0.43
1:A:1660:LEU:HD21	1:A:1687:LEU:HB3	2.01	0.43
3:C:446:LEU:HD23	3:C:448:GLN:OE1	2.19	0.43
6:F:157:GLU:HG2	6:F:477:CYS:SG	2.57	0.43
8:I:619:LYS:HE3	8:I:704:THR:HG23	2.01	0.43
9:J:354:MET:HA	9:J:354:MET:HE2	1.98	0.43
9:K:296:PRO:HB2	11:M:55:MET:HG3	2.00	0.43
12:N:268:VAL:HA	12:N:271:GLU:CG	2.48	0.43
12:N:523:LEU:O	12:N:527:LEU:HG	2.19	0.43
13:O:610:LEU:HD12	13:O:614:TYR:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:523:CYS:O	3:P:524:LYS:HG3	2.18	0.43
16:Y:45:ALA:CB	16:Y:82:TYR:CD2	3.00	0.43
16:Y:71:PHE:O	16:Y:76:LYS:HE3	2.19	0.43
1:A:949:PHE:N	1:A:1813:GLN:HE21	2.16	0.43
1:A:1364:CYS:N	1:A:1365:PRO:HD2	2.34	0.43
3:C:102:ALA:O	3:C:106:LEU:HD12	2.18	0.43
3:C:248:LEU:HD21	3:C:276:ILE:HD11	2.01	0.43
3:C:296:ARG:CG	3:C:296:ARG:NH1	2.53	0.43
6:F:65:SER:N	16:Y:296:GLN:HE22	2.17	0.43
6:F:120:LEU:O	6:F:124:VAL:HG23	2.19	0.43
6:H:702:ASN:HA	6:H:703:PRO:HD3	1.92	0.43
8:I:497:TRP:HB3	13:O:460:GLN:NE2	2.34	0.43
8:I:556:LEU:HD11	8:I:586:LEU:HD21	1.99	0.43
9:J:180:GLU:CA	9:J:180:GLU:OE1	2.67	0.43
9:J:456:ARG:CG	9:J:488:ILE:HG22	2.49	0.43
9:K:231:LEU:HA	9:K:234:VAL:HG22	2.00	0.43
9:K:406:HIS:ND1	7:W:6:PRO:HB3	2.32	0.43
10:L:80:TYR:HD2	10:L:154:ARG:HB2	1.84	0.43
11:M:32:PRO:C	11:M:34:ASN:H	2.22	0.43
12:N:151:GLU:O	12:N:155:THR:HG23	2.19	0.43
16:Y:508:ASP:HB3	16:Y:509:CYS:H	1.65	0.43
1:A:1110:ARG:HG2	1:A:1117:THR:HG22	2.01	0.42
1:A:1774:VAL:CG1	1:A:1790:TYR:HB3	2.49	0.42
2:B:41:GLY:O	2:B:45:PRO:HA	2.19	0.42
6:F:164:PRO:HG2	6:F:471:LYS:HG3	2.01	0.42
8:I:202:ALA:C	8:I:223:VAL:HG22	2.39	0.42
9:J:320:ARG:HG2	9:J:340:TYR:CE1	2.54	0.42
13:O:539:ASN:ND2	13:O:542:GLU:CB	2.71	0.42
3:P:460:TYR:CE1	3:P:470:LEU:HD11	2.53	0.42
16:Y:73:PRO:O	16:Y:106:GLN:OE1	2.37	0.42
16:Y:203:LEU:HA	16:Y:206:ILE:HD12	2.01	0.42
1:A:591:VAL:O	1:A:591:VAL:HG23	2.19	0.42
1:A:1377:LYS:HG2	1:A:1416:TRP:CG	2.54	0.42
3:C:112:LYS:H	3:C:112:LYS:CD	2.32	0.42
3:C:523:CYS:O	3:C:524:LYS:HG3	2.19	0.42
8:I:640:ASP:OD1	8:I:641:ALA:N	2.52	0.42
9:J:472:LEU:O	9:J:476:PRO:HA	2.19	0.42
10:L:24:GLU:HA	10:L:158:ILE:O	2.19	0.42
13:O:584:LEU:HD13	13:O:607:ALA:HB2	2.01	0.42
16:X:304:LEU:HD23	16:X:304:LEU:HA	1.87	0.42
16:Y:294:PHE:C	16:Y:294:PHE:HD1	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ARG:HH21	13:O:526:HIS:HB3	1.84	0.42
1:A:31:HIS:CD2	13:O:264:VAL:CG2	3.01	0.42
1:A:1262:GLN:NE2	1:A:1582:ALA:CB	2.81	0.42
3:C:61:SER:CB	3:C:262:SER:HB2	2.42	0.42
3:C:215:ASP:HB3	3:C:218:MET:HG3	2.01	0.42
8:I:25:PHE:CD1	8:I:71:LEU:HD13	2.54	0.42
9:J:214:LYS:HE2	9:J:216:SER:OG	2.20	0.42
9:K:178:ALA:HA	9:K:181:GLU:CD	2.40	0.42
9:K:203:PHE:HE1	9:K:218:THR:HB	1.84	0.42
12:N:333:TYR:HD1	12:N:364:CYS:SG	2.41	0.42
13:O:322:LEU:O	13:O:325:GLN:HB2	2.19	0.42
13:O:382:GLN:HG3	13:O:417:LEU:HD13	2.02	0.42
13:O:394:THR:HG22	13:O:615:ARG:HH12	1.84	0.42
3:P:96:VAL:N	3:P:97:LYS:HA	2.34	0.42
3:P:414:MET:HA	3:P:415:PRO:HD3	1.86	0.42
16:X:246:VAL:HG13	16:X:280:LEU:HD21	2.01	0.42
1:A:584:ILE:HG13	1:A:599:LEU:HD23	2.02	0.42
3:C:279:ILE:HD11	14:R:77:ASP:OD1	2.19	0.42
6:H:12:ILE:HG21	6:H:43:LEU:CD2	2.50	0.42
8:I:345:GLN:HB2	8:I:407:ILE:HG21	2.00	0.42
8:I:514:PHE:HE2	13:O:440:GLN:CA	2.20	0.42
9:J:342:HIS:HD2	9:J:357:TYR:OH	2.01	0.42
9:J:495:PHE:HD2	9:J:522:CYS:SG	2.39	0.42
13:O:361:LEU:HD13	13:O:384:LEU:HA	2.01	0.42
13:O:672:VAL:HG21	13:O:720:LEU:HD21	2.01	0.42
13:O:730:ARG:O	13:O:733:CYS:HB2	2.20	0.42
3:P:293:ASP:HA	3:P:294:PRO:HD3	1.96	0.42
16:X:242:ALA:O	16:X:246:VAL:HG23	2.20	0.42
16:X:281:TYR:HB3	16:X:290:SER:OG	2.19	0.42
16:Y:84:ALA:HB1	16:Y:100:TYR:CZ	2.54	0.42
1:A:1632:ALA:H	1:A:1653:ALA:HB3	1.84	0.42
3:C:58:LEU:O	3:C:61:SER:HB3	2.20	0.42
3:C:365:LEU:HD23	3:C:365:LEU:HA	1.84	0.42
3:C:403:TYR:CD1	3:C:403:TYR:C	2.93	0.42
3:C:526:TRP:NE1	3:C:553:ILE:O	2.49	0.42
6:H:32:TYR:CE1	6:H:41:LEU:HB2	2.54	0.42
6:H:481:CYS:O	6:H:485:ILE:HG12	2.20	0.42
9:J:220:ILE:HG22	9:J:222:GLU:H	1.85	0.42
9:J:443:LYS:O	9:J:446:PRO:HD2	2.19	0.42
12:N:73:GLU:O	12:N:74:TRP:CB	2.67	0.42
12:N:150:ARG:HA	12:N:153:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:581:ILE:HD13	13:O:611:SER:HB3	2.02	0.42
16:X:203:LEU:HA	16:X:206:ILE:HD12	2.01	0.42
16:Y:42:ARG:HG3	16:Y:82:TYR:HH	1.79	0.42
16:Y:145:CYS:O	16:Y:149:LEU:HG	2.20	0.42
16:Y:281:TYR:HB3	16:Y:290:SER:OG	2.19	0.42
1:A:247:VAL:HG12	1:A:257:MET:O	2.20	0.42
1:A:1329:MET:CE	1:A:1371:LEU:HD12	2.50	0.42
1:A:1403:PHE:O	1:A:1407:ARG:HB2	2.19	0.42
1:A:1790:TYR:O	1:A:1793:MET:HB2	2.19	0.42
3:C:46:ARG:NH2	3:C:48:LEU:HD11	2.21	0.42
3:C:244:ILE:HD12	3:C:245:GLU:H	1.85	0.42
6:F:762:TRP:NE1	9:J:362:GLN:HB2	2.34	0.42
6:H:532:ARG:HG3	6:H:534:GLU:H	1.84	0.42
8:I:269:LEU:HD23	8:I:523:HIS:CE1	2.55	0.42
9:J:300:VAL:HG22	9:J:333:TYR:OH	2.19	0.42
9:J:445:GLU:CA	9:J:474:LEU:HD23	2.48	0.42
10:L:33:LEU:HD13	10:L:54:TRP:CD2	2.55	0.42
12:N:520:ARG:HD2	12:N:556:PHE:CD1	2.55	0.42
1:A:612:ILE:O	1:A:641:TRP:CH2	2.73	0.42
1:A:980:ARG:NH2	1:A:1674:TRP:O	2.52	0.42
1:A:1329:MET:HE1	1:A:1371:LEU:HD12	2.02	0.42
1:A:1611:VAL:CG1	1:A:1612:LEU:HD12	2.50	0.42
6:F:704:LEU:HD13	14:R:494:ILE:H	1.84	0.42
6:H:465:LEU:HD22	6:H:495:HIS:CE1	2.55	0.42
9:J:167:PHE:HA	9:J:170:LEU:HD21	2.01	0.42
9:J:323:LEU:O	9:J:327:THR:HG22	2.20	0.42
12:N:523:LEU:HD22	12:N:538:GLU:OE1	2.20	0.42
13:O:439:LEU:HG	13:O:476:LEU:HD13	2.02	0.42
13:O:657:ILE:HG13	13:O:658:LEU:N	2.35	0.42
14:R:202:LEU:HD12	14:R:207:TYR:CD2	2.55	0.42
16:Y:465:LEU:HD23	16:Y:485:LEU:HD11	2.02	0.42
1:A:871:ARG:HG3	1:A:872:LEU:N	2.34	0.42
1:A:1586:CYS:HB3	1:A:1606:LEU:HD22	2.01	0.42
2:B:20:ASP:O	2:B:30:PHE:HD2	2.03	0.42
9:J:180:GLU:O	9:J:184:LEU:N	2.37	0.42
9:K:404:VAL:O	9:K:408:VAL:HG23	2.20	0.42
10:L:12:ASP:HA	10:L:13:PRO:HD2	1.84	0.42
16:X:475:TYR:O	16:X:479:VAL:HG23	2.19	0.42
16:Y:291:VAL:HG22	16:Y:314:LEU:HB3	2.01	0.42
1:A:93:LEU:HD11	1:A:151:ILE:HD11	2.02	0.42
1:A:1350:TYR:O	10:L:42:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1531:GLY:HA3	1:A:1566:PHE:CE2	2.55	0.42
2:B:11:VAL:HB	12:N:594:VAL:HG12	2.00	0.42
3:C:115:TYR:CZ	3:C:161:LYS:CD	3.03	0.42
3:C:395:ASN:HB3	3:C:398:ASP:H	1.85	0.42
3:C:413:LYS:C	3:C:415:PRO:CD	2.86	0.42
8:I:72:ALA:C	8:I:80:LEU:HD12	2.40	0.42
9:J:84:LYS:HD3	9:J:86:HIS:NE2	2.34	0.42
9:K:509:ARG:HG3	9:K:512:ASP:HB2	2.02	0.42
12:N:213:TYR:C	12:N:214:ARG:HA	2.40	0.42
12:N:347:ILE:HG21	12:N:358:ILE:HG23	2.02	0.42
12:N:681:LEU:HD23	12:N:692:LEU:HD21	2.01	0.42
13:O:360:LEU:O	13:O:364:SER:HB2	2.19	0.42
16:Y:42:ARG:HA	16:Y:82:TYR:OH	2.17	0.42
1:A:425:SER:N	1:A:448:SER:HG	2.17	0.42
1:A:1198:THR:C	1:A:1200:GLY:N	2.73	0.42
3:C:153:GLU:O	3:C:157:GLU:OE1	2.38	0.42
3:C:306:LEU:HD12	3:C:307:LEU:N	2.35	0.42
6:H:550:VAL:O	6:H:554:VAL:HG23	2.20	0.42
8:I:188:TYR:HA	8:I:193:PHE:O	2.20	0.42
9:K:514:PHE:CZ	7:W:11:LEU:HD22	2.55	0.42
12:N:22:VAL:CB	12:N:58:ALA:HA	2.50	0.42
12:N:156:MET:O	12:N:160:VAL:HG23	2.20	0.42
12:N:210:ARG:HB3	12:N:214:ARG:CZ	2.50	0.42
12:N:700:LEU:HD13	12:N:707:GLU:HG3	2.01	0.42
3:P:58:LEU:O	3:P:61:SER:HB3	2.20	0.42
14:R:110:LYS:O	14:R:113:GLN:HB2	2.19	0.42
16:X:87:LEU:HD11	16:X:99:LYS:HG3	2.01	0.42
16:X:393:ILE:HG22	16:X:397:ARG:HH11	1.85	0.42
16:Y:294:PHE:O	16:Y:294:PHE:HD1	2.03	0.42
3:C:297:ILE:O	3:C:297:ILE:HG12	2.18	0.41
6:H:120:LEU:O	6:H:124:VAL:HG23	2.20	0.41
6:H:704:LEU:HA	10:L:177:PHE:CZ	2.55	0.41
8:I:349:ILE:HD13	13:O:410:TRP:CD1	2.55	0.41
8:I:497:TRP:CD1	13:O:446:LEU:O	2.73	0.41
10:L:109:ARG:NH2	10:L:123:PRO:HD2	2.35	0.41
12:N:281:TYR:HE1	12:N:357:ALA:HA	1.83	0.41
12:N:331:PHE:CZ	12:N:335:ILE:HD11	2.55	0.41
13:O:690:ALA:O	13:O:693:ASN:HB2	2.20	0.41
16:X:508:ASP:HB3	16:X:509:CYS:H	1.65	0.41
1:A:23:PHE:HE2	1:A:113:VAL:HB	1.84	0.41
1:A:101:ILE:HG23	1:A:113:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1560:MET:O	1:A:1564:LEU:HD22	2.20	0.41
1:A:1584:LEU:HD22	1:A:1588:LEU:CD2	2.50	0.41
1:A:1672:ARG:O	1:A:1701:LEU:HA	2.20	0.41
3:C:119:MET:HA	3:C:122:ARG:CG	2.50	0.41
3:C:526:TRP:HE1	3:C:553:ILE:HA	1.85	0.41
6:F:705:CYS:SG	6:F:706:LYS:N	2.92	0.41
8:I:34:LEU:HA	8:I:47:HIS:O	2.20	0.41
8:I:206:LEU:HD22	8:I:570:PHE:CD2	2.55	0.41
9:J:450:ASN:O	9:J:454:VAL:HG13	2.20	0.41
9:J:489:HIS:HB3	9:J:498:ALA:HB2	2.02	0.41
9:K:369:LEU:O	9:K:373:TYR:HD2	2.03	0.41
9:K:495:PHE:CE2	9:K:525:MET:HG2	2.56	0.41
13:O:225:ASN:O	13:O:461:ASN:O	2.38	0.41
13:O:247:ASN:HA	13:O:248:PRO:HD3	1.82	0.41
3:P:92:ALA:O	3:P:96:VAL:HG23	2.20	0.41
16:X:71:PHE:O	16:X:76:LYS:HE3	2.20	0.41
16:X:145:CYS:O	16:X:149:LEU:HG	2.20	0.41
16:X:206:ILE:O	16:X:210:LEU:HG	2.20	0.41
16:X:270:ASN:HB2	16:X:273:LEU:CB	2.50	0.41
1:A:594:ARG:HG2	1:A:608:THR:HG22	2.02	0.41
1:A:1093:HIS:CD2	1:A:1093:HIS:N	2.88	0.41
1:A:1521:LEU:O	1:A:1525:MET:HB2	2.21	0.41
3:C:305:ASN:OD1	14:R:78:ARG:HD3	2.19	0.41
6:F:550:VAL:CG2	9:K:289:HIS:CG	3.03	0.41
6:H:25:VAL:HG22	6:H:47:CYS:HB3	2.02	0.41
6:H:692:LEU:HD13	6:H:709:ARG:HA	2.02	0.41
8:I:25:PHE:CE1	8:I:27:VAL:HG23	2.55	0.41
9:J:386:LEU:H	9:J:386:LEU:CD1	2.30	0.41
3:P:106:LEU:CB	3:P:118:TYR:HB2	2.50	0.41
3:P:355:GLN:HG3	3:P:371:MET:HE1	2.01	0.41
3:P:464:ASP:OD2	3:P:469:ALA:HB3	2.20	0.41
16:X:167:ARG:HB3	16:X:172:ASN:OD1	2.20	0.41
16:X:339:ALA:HB2	16:X:369:ASN:HB2	2.01	0.41
16:Y:242:ALA:O	16:Y:246:VAL:HG23	2.19	0.41
1:A:248:PHE:CE1	1:A:430:VAL:O	2.73	0.41
6:F:5:GLN:HA	6:H:455:GLN:HG3	2.02	0.41
6:F:32:TYR:CE1	6:F:41:LEU:HB2	2.55	0.41
6:F:128:THR:O	6:F:129:ASP:HB3	2.20	0.41
6:H:12:ILE:HG21	6:H:43:LEU:HD21	2.01	0.41
9:J:334:GLY:N	9:J:335:PRO:CD	2.84	0.41
12:N:177:TYR:O	12:N:180:PHE:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:79:TYR:HA	13:O:82:ILE:HG22	2.03	0.41
3:P:311:SER:HA	3:P:343:LEU:HD11	2.03	0.41
16:X:465:LEU:HD23	16:X:485:LEU:HD11	2.02	0.41
16:Y:270:ASN:HB2	16:Y:273:LEU:CB	2.50	0.41
1:A:119:VAL:O	1:A:121:SER:N	2.50	0.41
1:A:485:ILE:HG12	1:A:611:GLU:HA	2.03	0.41
3:C:377:GLU:HA	14:R:130:ILE:HG22	2.02	0.41
6:F:15:ALA:HA	6:H:116:PHE:CZ	2.56	0.41
6:F:486:ASN:O	6:F:490:HIS:ND1	2.52	0.41
6:H:61:LEU:HD12	6:H:61:LEU:HA	1.85	0.41
8:I:414:PHE:HZ	8:I:472:VAL:HG13	1.85	0.41
8:I:655:ASP:OD1	8:I:657:VAL:HG22	2.20	0.41
9:K:337:TRP:CZ3	9:K:340:TYR:HD2	2.39	0.41
10:L:53:TYR:CE2	10:L:152:HIS:CE1	3.08	0.41
10:L:68:PHE:HE1	10:L:137:ILE:HD12	1.84	0.41
12:N:343:GLU:O	12:N:347:ILE:N	2.52	0.41
12:N:386:LEU:HD23	12:N:399:LEU:HD13	2.00	0.41
13:O:483:PHE:O	13:O:487:SER:N	2.46	0.41
13:O:668:ALA:HB3	13:O:694:LEU:HD23	2.02	0.41
14:R:364:CYS:HA	14:R:365:PRO:HD3	1.89	0.41
16:Y:408:ASP:O	16:Y:411:GLU:HG2	2.20	0.41
1:A:1408:THR:HG21	1:A:1468:ALA:HB2	2.02	0.41
1:A:1519:VAL:CG1	1:A:1520:LEU:H	2.34	0.41
3:C:26:PHE:O	3:C:27:SER:OG	2.31	0.41
3:C:92:ALA:O	3:C:96:VAL:HG23	2.21	0.41
6:F:639:TYR:CE2	14:R:498:ILE:HG13	2.56	0.41
8:I:231:VAL:HG11	8:I:556:LEU:HD12	2.02	0.41
8:I:578:ASN:C	8:I:578:ASN:OD1	2.59	0.41
9:J:42:TRP:CE3	9:J:42:TRP:HA	2.55	0.41
13:O:35:ILE:HG21	13:O:158:LEU:CD1	2.44	0.41
13:O:215:PHE:CD2	13:O:216:LEU:HD23	2.55	0.41
13:O:532:VAL:HG21	13:O:547:LYS:HA	2.02	0.41
13:O:657:ILE:HG22	13:O:660:LYS:HE2	2.01	0.41
14:R:177:ASP:CG	15:S:834:ILE:HD12	2.31	0.41
16:X:154:ASP:OD1	16:X:154:ASP:N	2.53	0.41
1:A:88:ASP:O	1:A:594:ARG:NH2	2.54	0.41
1:A:240:VAL:HG13	1:A:241:ASP:CB	2.50	0.41
1:A:1434:ILE:CG2	1:A:1461:HIS:HB2	2.51	0.41
6:F:146:PRO:CG	6:F:167:THR:HA	2.50	0.41
6:H:164:PRO:HG3	6:H:471:LYS:HG3	2.03	0.41
9:J:475:ILE:HA	9:J:476:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:607:GLU:HG2	12:N:688:PRO:HG2	2.03	0.41
12:N:663:GLN:HB3	12:N:699:TRP:CZ2	2.55	0.41
13:O:608:LEU:CD2	13:O:612:LYS:HE2	2.50	0.41
3:P:242:GLN:NE2	3:P:429:ARG:HG3	2.31	0.41
16:Y:186:ARG:HA	16:Y:189:VAL:HG12	2.01	0.41
1:A:27:HIS:CE1	1:A:31:HIS:CD2	3.09	0.41
1:A:1453:ASN:ND2	10:L:133:ARG:HD2	2.36	0.41
1:A:1575:SER:O	1:A:1580:SER:OG	2.36	0.41
1:A:1743:SER:HA	1:A:1748:LEU:HD22	2.03	0.41
3:C:46:ARG:HB3	3:C:116:PHE:HE2	1.84	0.41
6:F:12:ILE:HG21	6:F:43:LEU:CD2	2.50	0.41
6:F:465:LEU:HD22	6:F:495:HIS:CE1	2.56	0.41
6:F:550:VAL:O	6:F:554:VAL:HG23	2.21	0.41
6:H:682:LEU:HD13	6:H:684:LYS:HE3	2.02	0.41
9:J:19:TYR:CE1	9:J:49:LEU:HD13	2.55	0.41
9:J:215:PRO:HG2	9:J:402:PRO:HG2	2.02	0.41
3:P:307:LEU:HD12	3:P:307:LEU:HA	1.84	0.41
1:A:87:VAL:CG1	1:A:88:ASP:N	2.73	0.41
1:A:245:LYS:O	1:A:258:THR:HA	2.21	0.41
1:A:628:ILE:HG22	1:A:629:LEU:N	2.36	0.41
1:A:1209:LEU:HD23	1:A:1209:LEU:HA	1.85	0.41
1:A:1236:LEU:H	1:A:1236:LEU:HD23	1.85	0.41
1:A:1237:PRO:CB	1:A:1238:PRO:CD	2.95	0.41
1:A:1325:LEU:HD23	1:A:1371:LEU:HG	2.03	0.41
1:A:1602:HIS:O	1:A:1603:LEU:HB3	2.20	0.41
1:A:1673:TYR:CZ	1:A:1701:LEU:HD13	2.56	0.41
1:A:1739:SER:CA	1:A:1740:ALA:CB	2.98	0.41
2:B:15:LEU:HD21	12:N:635:LEU:HA	2.02	0.41
3:C:261:LYS:HD2	3:C:261:LYS:HA	1.89	0.41
4:D:15:THR:HB	4:D:19:ASN:HD22	1.86	0.41
4:D:53:PRO:HD3	3:P:382:SER:OG	2.21	0.41
5:E:63:VAL:HG11	16:Y:364:LYS:NZ	2.36	0.41
6:F:18:HIS:NE2	6:H:113:SER:HB2	2.35	0.41
7:G:1:MET:CG	9:J:335:PRO:HB3	2.51	0.41
6:H:146:PRO:CG	6:H:167:THR:HA	2.50	0.41
8:I:118:VAL:HG12	8:I:173:LEU:O	2.21	0.41
8:I:349:ILE:HD13	13:O:410:TRP:HD1	1.86	0.41
8:I:397:ILE:HD12	13:O:440:GLN:HG3	2.03	0.41
8:I:618:ILE:HD12	8:I:705:MET:CE	2.51	0.41
8:I:737:ASN:OD1	8:I:738:LEU:N	2.54	0.41
9:J:276:VAL:HA	9:J:311:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:289:HIS:CD2	9:J:289:HIS:C	2.93	0.41
9:J:485:ILE:HG22	9:J:488:ILE:HD11	2.02	0.41
9:K:42:TRP:HA	9:K:42:TRP:HE3	1.84	0.41
9:K:351:ASP:OD1	9:K:351:ASP:N	2.46	0.41
9:K:418:TRP:HB3	9:K:458:LEU:CD1	2.50	0.41
10:L:68:PHE:CE1	10:L:137:ILE:HD12	2.56	0.41
10:L:88:SER:O	10:L:144:ASN:HB3	2.21	0.41
12:N:527:LEU:HD22	12:N:564:MET:CG	2.51	0.41
12:N:601:TRP:HA	12:N:602:PRO:HD2	1.97	0.41
13:O:40:LEU:HD11	13:O:60:LEU:HD21	2.03	0.41
13:O:75:LEU:HB2	13:O:161:TYR:CE2	2.56	0.41
13:O:119:PHE:CZ	13:O:136:LEU:HD11	2.55	0.41
3:P:235:ALA:HB1	3:P:251:TYR:CE2	2.55	0.41
3:P:402:TRP:CE2	3:P:424:ARG:HG2	2.56	0.41
16:X:199:CYS:SG	16:Y:44:MET:CG	3.04	0.41
16:Y:84:ALA:HB1	16:Y:100:TYR:CD2	2.55	0.41
16:Y:154:ASP:N	16:Y:154:ASP:OD1	2.53	0.41
1:A:23:PHE:O	1:A:26:ASP:N	2.50	0.41
1:A:794:ALA:HB1	1:A:797:LEU:HB3	2.02	0.41
1:A:860:TYR:HA	1:A:861:PRO:HD3	1.98	0.41
1:A:1409:LEU:HD23	1:A:1471:SER:CB	2.51	0.41
3:C:93:TYR:CZ	3:C:101:ARG:NE	2.90	0.41
3:C:235:ALA:HB1	3:C:251:TYR:CE2	2.56	0.41
6:F:550:VAL:HG21	9:K:289:HIS:CB	2.50	0.41
6:F:636:ASN:HD22	6:F:636:ASN:N	2.18	0.41
6:F:707:PHE:CE1	6:F:742:LEU:HD13	2.56	0.41
6:H:515:TYR:HD1	10:L:179:MET:HE2	1.86	0.41
9:K:484:ALA:O	9:K:488:ILE:HG12	2.20	0.41
10:L:64:VAL:HB	10:L:139:ILE:HB	2.03	0.41
12:N:456:LEU:HA	12:N:548:ARG:NH2	2.36	0.41
13:O:467:ALA:CB	13:O:506:LEU:HD11	2.49	0.41
3:P:306:LEU:HD12	3:P:307:LEU:N	2.36	0.41
1:A:89:TYR:HB3	13:O:536:THR:CG2	2.51	0.40
3:C:397:ARG:O	3:C:428:LEU:HD21	2.21	0.40
6:H:128:THR:O	6:H:129:ASP:HB3	2.21	0.40
6:H:634:HIS:CE1	6:H:636:ASN:HB2	2.56	0.40
8:I:231:VAL:HG21	8:I:557:TYR:CE2	2.55	0.40
9:K:214:LYS:HA	9:K:215:PRO:HD2	1.84	0.40
12:N:281:TYR:CE2	12:N:356:PRO:HB2	2.56	0.40
13:O:119:PHE:CE1	13:O:136:LEU:HD21	2.53	0.40
13:O:275:LEU:HD12	13:O:275:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:539:ASN:ND2	13:O:542:GLU:HB2	2.35	0.40
13:O:649:GLU:HB3	13:O:650:PRO:HD3	2.02	0.40
3:P:170:PHE:O	3:P:171:GLY:C	2.59	0.40
3:P:297:ILE:HD11	3:P:333:THR:HB	2.03	0.40
3:P:370:LEU:HD23	3:P:370:LEU:HA	1.89	0.40
3:P:403:TYR:CD1	3:P:422:TYR:HE1	2.39	0.40
16:X:325:GLU:HG3	16:X:348:HIS:CD2	2.56	0.40
16:X:475:TYR:HB3	16:X:478:ALA:HB3	2.03	0.40
16:Y:366:ILE:H	16:Y:366:ILE:HG13	1.72	0.40
1:A:213:MET:HE3	1:A:220:ILE:CG2	2.51	0.40
1:A:657:TRP:HA	1:A:660:PHE:HB3	2.02	0.40
1:A:1611:VAL:HG13	1:A:1612:LEU:N	2.36	0.40
3:C:46:ARG:NH2	3:C:170:PHE:CD1	2.89	0.40
3:C:322:ASN:N	9:J:282:ASN:ND2	2.69	0.40
4:D:54:ILE:CD1	9:J:506:LEU:HB3	2.48	0.40
5:E:89:LEU:HD22	6:H:588:LYS:HB3	2.03	0.40
6:F:138:TYR:O	6:F:141:SER:OG	2.33	0.40
6:F:548:LYS:HB3	6:F:551:ALA:HB3	2.03	0.40
8:I:28:TRP:HZ3	8:I:33:ASP:O	2.04	0.40
8:I:406:VAL:O	8:I:410:SER:HB2	2.21	0.40
9:J:204:LEU:HD22	9:K:28:LYS:NZ	2.36	0.40
9:J:489:HIS:CB	9:J:498:ALA:HB2	2.51	0.40
9:K:40:ILE:HD13	9:K:65:LEU:HD21	2.03	0.40
10:L:40:PHE:O	10:L:54:TRP:HA	2.21	0.40
12:N:501:ILE:O	12:N:504:LEU:HB2	2.22	0.40
13:O:666:LEU:O	13:O:666:LEU:HG	2.20	0.40
1:A:23:PHE:CE2	1:A:113:VAL:HB	2.57	0.40
1:A:1040:LEU:HG	1:A:1543:HIS:CE1	2.57	0.40
3:C:117:LEU:HD23	3:C:117:LEU:O	2.21	0.40
3:C:397:ARG:CA	3:C:428:LEU:HD21	2.50	0.40
3:C:460:TYR:CE1	3:C:470:LEU:HD11	2.57	0.40
6:F:42:PHE:HB2	6:F:71:CYS:SG	2.61	0.40
12:N:386:LEU:HD13	12:N:396:ILE:HG23	2.02	0.40
13:O:435:SER:HB2	13:O:618:TYR:HE2	1.86	0.40
13:O:536:THR:O	13:O:540:SER:HA	2.21	0.40
13:O:637:PRO:HB2	13:O:674:SER:HB3	2.03	0.40
13:O:689:ALA:O	13:O:692:GLU:HB2	2.22	0.40
3:P:49:LEU:H	3:P:49:LEU:HD12	1.86	0.40
14:R:83:ARG:HE	14:R:83:ARG:HA	1.86	0.40
14:R:193:SER:O	14:R:453:PRO:HG3	2.20	0.40
16:X:164:SER:HA	16:X:167:ARG:NE	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:87:LEU:HD11	16:Y:99:LYS:HG3	2.04	0.40
1:A:188:LEU:HD23	1:A:249:LEU:HD21	2.03	0.40
1:A:244:MET:SD	1:A:244:MET:N	2.94	0.40
1:A:433:THR:HG22	1:A:481:PRO:CB	2.39	0.40
1:A:1462:VAL:O	1:A:1465:ILE:HG13	2.21	0.40
1:A:1473:GLY:HA2	1:A:1526:VAL:HG13	2.03	0.40
1:A:1673:TYR:CE2	1:A:1701:LEU:HD13	2.56	0.40
3:C:26:PHE:CD2	3:C:257:VAL:HG21	2.56	0.40
3:C:65:LEU:HD13	3:C:66:PRO:HD2	2.03	0.40
6:H:464:SER:O	6:H:468:GLU:HG2	2.21	0.40
6:H:592:ARG:HA	6:H:592:ARG:HD3	1.77	0.40
8:I:14:VAL:N	8:I:743:VAL:O	2.55	0.40
9:J:441:VAL:O	9:J:442:ASP:CB	2.69	0.40
12:N:386:LEU:HD21	12:N:399:LEU:HD22	2.03	0.40
14:R:209:TRP:HD1	14:R:216:ILE:HG13	1.87	0.40
16:X:203:LEU:HD22	16:Y:55:LEU:CB	2.52	0.40
16:Y:246:VAL:HG13	16:Y:280:LEU:HD21	2.03	0.40
1:A:1420:LEU:HA	1:A:1421:PRO:HD3	1.91	0.40
1:A:1640:GLY:CA	1:A:1645:GLU:O	2.70	0.40
3:C:151:LEU:CD1	3:C:181:LYS:CB	2.99	0.40
3:C:312:MET:H	3:C:312:MET:HG2	1.67	0.40
4:D:48:ASP:OD1	4:D:48:ASP:N	2.54	0.40
6:H:128:THR:HG21	9:K:473:VAL:HG22	2.03	0.40
6:H:692:LEU:HB3	6:H:709:ARG:HG3	2.04	0.40
8:I:32:ARG:HG2	12:N:388:HIS:HE1	1.85	0.40
8:I:245:LEU:HB3	8:I:246:PRO:HD3	2.03	0.40
8:I:279:ILE:HD12	8:I:279:ILE:HA	1.83	0.40
8:I:495:ASN:HA	13:O:459:GLN:HA	2.03	0.40
8:I:648:THR:HG22	8:I:670:PRO:HA	2.02	0.40
9:J:56:ALA:HB3	9:J:79:CYS:SG	2.61	0.40
9:J:376:LEU:HD23	9:J:407:GLU:HG2	2.03	0.40
11:M:1:MET:SD	11:M:4:GLU:HB2	2.62	0.40
12:N:210:ARG:O	12:N:214:ARG:N	2.55	0.40
12:N:401:ILE:HG22	12:N:405:LYS:HE3	2.04	0.40
13:O:381:ILE:CG2	13:O:405:SER:HB2	2.50	0.40
16:X:232:ASN:O	16:Y:63:MET:HE1	2.22	0.40
16:X:311:TYR:HA	16:X:314:LEU:HD12	2.04	0.40
16:Y:100:TYR:CD1	16:Y:138:VAL:HG13	2.51	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	1393/1944 (72%)	1186 (85%)	149 (11%)	58 (4%)	3 25
2	B	83/84 (99%)	72 (87%)	7 (8%)	4 (5%)	2 23
3	C	520/597 (87%)	489 (94%)	23 (4%)	8 (2%)	10 45
3	P	485/597 (81%)	460 (95%)	20 (4%)	5 (1%)	15 53
4	D	53/121 (44%)	45 (85%)	7 (13%)	1 (2%)	8 40
5	E	54/110 (49%)	54 (100%)	0	0	100 100
6	F	494/824 (60%)	461 (93%)	25 (5%)	8 (2%)	9 44
6	H	477/824 (58%)	448 (94%)	22 (5%)	7 (2%)	10 45
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%)	683 (95%)	34 (5%)	5 (1%)	22 61
9	J	500/620 (81%)	467 (93%)	29 (6%)	4 (1%)	19 58
9	K	489/620 (79%)	459 (94%)	24 (5%)	6 (1%)	13 49
10	L	180/184 (98%)	165 (92%)	11 (6%)	4 (2%)	6 37
11	M	55/74 (74%)	42 (76%)	10 (18%)	3 (6%)	2 21
12	N	601/822 (73%)	497 (83%)	58 (10%)	46 (8%)	1 14
13	O	677/755 (90%)	619 (91%)	46 (7%)	12 (2%)	8 41
14	R	361/499 (72%)	338 (94%)	20 (6%)	3 (1%)	19 58
15	S	8/206 (4%)	6 (75%)	0	2 (25%)	0 1
16	X	478/599 (80%)	463 (97%)	12 (2%)	3 (1%)	25 63
16	Y	492/599 (82%)	474 (96%)	14 (3%)	4 (1%)	19 58
All	All	8168/11057 (74%)	7474 (92%)	511 (6%)	183 (2%)	10 37

All (183) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ALA
1	A	241	ASP
1	A	274	VAL
1	A	411	HIS
1	A	413	TRP
1	A	414	THR
1	A	430	VAL
1	A	475	PRO
1	A	672	THR
1	A	857	MET
1	A	1099	PRO
1	A	1190	THR
1	A	1237	PRO
1	A	1358	ILE
1	A	1924	MET
2	B	15	LEU
3	C	361	ASN
3	C	441	GLU
3	C	511	THR
4	D	23	PRO
6	F	103	HIS
6	F	165	ASP
8	I	483	ASP
8	I	487	VAL
8	I	489	PRO
9	J	221	PRO
9	K	211	LYS
9	K	215	PRO
10	L	71	LYS
10	L	171	PRO
11	M	2	ASP
12	N	16	PRO
12	N	63	ARG
12	N	74	TRP
12	N	91	PHE
12	N	126	LEU
12	N	144	THR
12	N	203	LEU
12	N	219	PRO
12	N	368	THR
12	N	395	ASP
12	N	412	PRO
12	N	477	PRO

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Mol	Chain	Res	Type
12	N	481	VAL
12	N	488	ASP
12	N	489	PRO
12	N	496	ARG
12	N	497	ARG
12	N	530	GLN
12	N	674	ALA
12	N	716	ILE
13	O	555	ASN
3	P	361	ASN
3	P	365	LEU
3	P	464	ASP
14	R	494	ILE
15	S	834	ILE
16	Y	201	LEU
1	A	120	ASP
1	A	265	VAL
1	A	584	ILE
1	A	592	HIS
1	A	630	PRO
1	A	758	HIS
1	A	1125	ILE
1	A	1199	LYS
1	A	1238	PRO
1	A	1242	GLU
1	A	1244	ASP
1	A	1314	ILE
3	C	27	SER
6	F	147	PHE
6	H	147	PHE
8	I	503	ASN
9	J	70	GLU
9	J	397	ILE
9	K	86	HIS
9	K	129	LYS
9	K	228	GLN
10	L	167	ILE
11	M	4	GLU
12	N	76	VAL
12	N	78	VAL
12	N	99	GLU
12	N	234	ARG

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Mol	Chain	Res	Type
12	N	290	HIS
12	N	350	ASP
12	N	500	ASP
12	N	531	PHE
12	N	595	ILE
12	N	606	ASP
13	O	462	ASN
13	O	657	ILE
14	R	498	ILE
16	X	202	ALA
16	X	213	SER
16	Y	213	SER
1	A	30	HIS
1	A	757	THR
1	A	777	THR
1	A	790	LEU
1	A	1100	LEU
1	A	1217	LEU
1	A	1284	GLU
1	A	1307	LEU
1	A	1740	ALA
1	A	1758	THR
2	B	16	TRP
3	C	510	SER
6	F	493	SER
6	H	493	SER
8	I	490	PRO
12	N	77	GLU
12	N	278	ARG
12	N	289	PHE
12	N	410	LEU
12	N	413	SER
12	N	480	TRP
12	N	487	ALA
12	N	491	LYS
12	N	672	ASP
13	O	126	VAL
13	O	149	SER
13	O	284	THR
13	O	345	SER
13	O	352	GLN
13	O	682	LYS

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Mol	Chain	Res	Type
13	O	707	LYS
16	X	456	VAL
16	Y	202	ALA
16	Y	456	VAL
1	A	87	VAL
1	A	486	ASP
1	A	585	HIS
1	A	652	SER
1	A	793	LEU
1	A	811	PRO
1	A	1055	PRO
1	A	1164	LYS
2	B	69	VAL
3	C	414	MET
6	F	145	ASN
6	H	145	ASN
10	L	131	PRO
12	N	354	SER
12	N	490	GLY
12	N	535	PRO
12	N	629	LEU
13	O	540	SER
14	R	84	SER
15	S	833	ASP
1	A	242	HIS
1	A	860	TYR
1	A	1056	GLU
1	A	1896	ALA
1	A	1933	ALA
6	F	96	VAL
6	H	97	PHE
9	J	442	ASP
11	M	66	HIS
12	N	252	LEU
12	N	287	ARG
3	P	66	PRO
1	A	184	LYS
1	A	648	PRO
1	A	759	ILE
1	A	792	GLN
2	B	40	PRO
3	C	66	PRO

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Mol	Chain	Res	Type
6	H	96	VAL
12	N	551	GLU
3	P	415	PRO
1	A	861	PRO
1	A	1348	PRO
3	C	415	PRO
6	F	492	PRO
6	H	492	PRO
1	A	502	GLY
1	A	1283	PRO
9	K	399	PRO
6	F	146	PRO
6	H	146	PRO
13	O	124	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1150/1720 (67%)	970 (84%)	180 (16%)	2 16
2	B	65/75 (87%)	54 (83%)	11 (17%)	2 14
3	C	452/520 (87%)	357 (79%)	95 (21%)	1 6
3	P	421/520 (81%)	363 (86%)	58 (14%)	3 20
4	D	46/115 (40%)	37 (80%)	9 (20%)	1 8
5	E	47/89 (53%)	37 (79%)	10 (21%)	1 6
6	F	407/727 (56%)	369 (91%)	38 (9%)	9 32
6	H	408/727 (56%)	374 (92%)	34 (8%)	11 38
7	G	23/77 (30%)	22 (96%)	1 (4%)	29 56
7	W	23/77 (30%)	22 (96%)	1 (4%)	29 56
8	I	620/730 (85%)	584 (94%)	36 (6%)	20 48
9	J	424/548 (77%)	382 (90%)	42 (10%)	8 29
9	K	423/548 (77%)	379 (90%)	44 (10%)	7 28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	L	155/169 (92%)	136 (88%)	19 (12%)	4 23
11	M	55/67 (82%)	42 (76%)	13 (24%)	1 4
12	N	460/724 (64%)	398 (86%)	62 (14%)	4 21
13	O	576/650 (89%)	478 (83%)	98 (17%)	2 13
14	R	304/411 (74%)	290 (95%)	14 (5%)	27 54
15	S	8/195 (4%)	8 (100%)	0	100 100
16	X	406/513 (79%)	373 (92%)	33 (8%)	11 39
16	Y	416/513 (81%)	375 (90%)	41 (10%)	8 29
All	All	6889/9715 (71%)	6050 (88%)	839 (12%)	8 23

All (839) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	26	ASP
1	A	29	LYS
1	A	31	HIS
1	A	35	LEU
1	A	36	ASN
1	A	37	LEU
1	A	39	LEU
1	A	40	ARG
1	A	42	LEU
1	A	43	GLN
1	A	47	GLU
1	A	48	LEU
1	A	80	VAL
1	A	90	ASP
1	A	99	MET
1	A	103	SER
1	A	118	THR
1	A	124	GLN
1	A	127	LEU
1	A	129	CYS
1	A	133	ILE
1	A	149	LYS
1	A	167	LYS
1	A	168	ASP
1	A	170	ILE

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Mol	Chain	Res	Type
1	A	173	LEU
1	A	183	THR
1	A	185	TYR
1	A	188	LEU
1	A	192	SER
1	A	210	MET
1	A	214	LEU
1	A	220	ILE
1	A	221	THR
1	A	223	LEU
1	A	240	VAL
1	A	242	HIS
1	A	249	LEU
1	A	250	ASN
1	A	252	ASP
1	A	269	TRP
1	A	411	HIS
1	A	412	LEU
1	A	430	VAL
1	A	433	THR
1	A	439	GLN
1	A	440	LYS
1	A	442	LEU
1	A	444	PHE
1	A	450	LEU
1	A	452	LEU
1	A	453	ARG
1	A	467	ILE
1	A	482	VAL
1	A	483	GLU
1	A	497	LEU
1	A	508	LYS
1	A	584	ILE
1	A	611	GLU
1	A	616	GLU
1	A	617	LEU
1	A	636	GLN
1	A	637	MET
1	A	638	LEU
1	A	655	SER
1	A	659	LEU
1	A	663	CYS

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Mol	Chain	Res	Type
1	A	665	MET
1	A	668	MET
1	A	758	HIS
1	A	759	ILE
1	A	766	LEU
1	A	774	LYS
1	A	781	GLU
1	A	792	GLN
1	A	795	ARG
1	A	796	ASP
1	A	798	LYS
1	A	808	ARG
1	A	813	LEU
1	A	871	ARG
1	A	937	VAL
1	A	942	ARG
1	A	953	LEU
1	A	964	GLU
1	A	976	LEU
1	A	1075	GLN
1	A	1088	THR
1	A	1100	LEU
1	A	1107	LEU
1	A	1118	VAL
1	A	1131	MET
1	A	1133	SER
1	A	1136	SER
1	A	1146	LYS
1	A	1168	LEU
1	A	1170	ASN
1	A	1176	LEU
1	A	1177	MET
1	A	1179	LEU
1	A	1191	LEU
1	A	1195	ASP
1	A	1202	GLU
1	A	1204	THR
1	A	1216	LYS
1	A	1217	LEU
1	A	1220	MET
1	A	1230	ILE
1	A	1232	ILE

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Mol	Chain	Res	Type
1	A	1239	THR
1	A	1241	THR
1	A	1243	LEU
1	A	1250	GLN
1	A	1257	ILE
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	1325	LEU
1	A	1329	MET
1	A	1330	VAL
1	A	1359	ASN
1	A	1376	LEU
1	A	1386	TRP
1	A	1396	LEU
1	A	1405	LEU
1	A	1409	LEU
1	A	1411	ARG
1	A	1415	LEU
1	A	1424	LYS
1	A	1433	ILE
1	A	1469	CYS
1	A	1470	LEU
1	A	1482	LEU
1	A	1487	CYS
1	A	1498	TYR
1	A	1520	LEU
1	A	1523	LEU
1	A	1536	LEU
1	A	1538	LEU
1	A	1539	CYS
1	A	1540	ARG
1	A	1562	LEU
1	A	1564	LEU
1	A	1573	SER
1	A	1574	LEU
1	A	1588	LEU
1	A	1597	THR

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Mol	Chain	Res	Type
1	A	1603	LEU
1	A	1607	ARG
1	A	1609	LEU
1	A	1611	VAL
1	A	1638	TYR
1	A	1646	GLN
1	A	1651	LEU
1	A	1652	MET
1	A	1666	ILE
1	A	1667	LYS
1	A	1672	ARG
1	A	1674	TRP
1	A	1679	ASP
1	A	1687	LEU
1	A	1688	LYS
1	A	1706	LEU
1	A	1731	ARG
1	A	1742	THR
1	A	1749	SER
1	A	1770	LEU
1	A	1798	ARG
1	A	1805	MET
1	A	1811	LEU
1	A	1825	SER
1	A	1851	THR
1	A	1882	LEU
1	A	1893	SER
1	A	1894	VAL
2	B	11	VAL
2	B	14	TRP
2	B	15	LEU
2	B	16	TRP
2	B	28	MET
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	27	SER
3	C	31	GLU
3	C	37	LEU

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Mol	Chain	Res	Type
3	C	38	LEU
3	C	39	ILE
3	C	46	ARG
3	C	49	LEU
3	C	55	SER
3	C	57	GLU
3	C	65	LEU
3	C	70	LEU
3	C	79	GLU
3	C	82	GLN
3	C	83	ASP
3	C	89	LEU
3	C	91	LYS
3	C	97	LYS
3	C	98	GLU
3	C	101	ARG
3	C	105	PHE
3	C	106	LEU
3	C	112	LYS
3	C	113	LYS
3	C	119	MET
3	C	122	ARG
3	C	128	LYS
3	C	132	ASP
3	C	136	ASP
3	C	141	LEU
3	C	143	LYS
3	C	146	VAL
3	C	152	ARG
3	C	157	GLU
3	C	172	LEU
3	C	179	LEU
3	C	182	LEU
3	C	187	GLU
3	C	203	TRP
3	C	216	LYS
3	C	243	LEU
3	C	254	LEU
3	C	286	PHE
3	C	288	GLU
3	C	291	LYS
3	C	296	ARG

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Mol	Chain	Res	Type
3	C	298	GLU
3	C	300	MET
3	C	302	THR
3	C	303	PHE
3	C	306	LEU
3	C	309	VAL
3	C	312	MET
3	C	313	LYS
3	C	324	CYS
3	C	325	GLU
3	C	328	LYS
3	C	330	ARG
3	C	335	CYS
3	C	343	LEU
3	C	344	ARG
3	C	346	GLN
3	C	348	GLU
3	C	349	LYS
3	C	352	LEU
3	C	358	LEU
3	C	359	LYS
3	C	360	LEU
3	C	361	ASN
3	C	365	LEU
3	C	374	GLU
3	C	378	MET
3	C	389	ARG
3	C	395	ASN
3	C	413	LYS
3	C	414	MET
3	C	424	ARG
3	C	427	GLN
3	C	428	LEU
3	C	429	ARG
3	C	434	ARG
3	C	451	GLU
3	C	455	CYS
3	C	458	ARG
3	C	464	ASP
3	C	465	VAL
3	C	466	GLU
3	C	467	LYS

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Mol	Chain	Res	Type
3	C	468	MET
3	C	475	LYS
3	C	518	GLN
3	C	524	LYS
3	C	526	TRP
3	C	527	ASP
3	C	547	LYS
3	C	557	ARG
4	D	4	LEU
4	D	11	ARG
4	D	12	VAL
4	D	15	THR
4	D	16	LEU
4	D	20	LEU
4	D	32	GLN
4	D	36	GLN
4	D	49	ASN
5	E	58	VAL
5	E	61	TYR
5	E	63	VAL
5	E	69	GLN
5	E	87	GLU
5	E	88	GLU
5	E	89	LEU
5	E	90	GLU
5	E	99	ILE
5	E	106	THR
6	F	14	GLN
6	F	27	LEU
6	F	62	LYS
6	F	90	GLN
6	F	98	ASN
6	F	104	ASP
6	F	118	LEU
6	F	121	LEU
6	F	141	SER
6	F	144	LEU
6	F	145	ASN
6	F	163	ASP
6	F	466	LEU
6	F	474	LEU
6	F	477	CYS

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Mol	Chain	Res	Type
6	F	494	HIS
6	F	520	ARG
6	F	521	ILE
6	F	527	ARG
6	F	530	ASN
6	F	538	ILE
6	F	562	MET
6	F	576	CYS
6	F	578	SER
6	F	595	GLN
6	F	614	THR
6	F	617	LEU
6	F	618	ASP
6	F	625	ARG
6	F	655	GLU
6	F	667	GLN
6	F	701	LYS
6	F	702	ASN
6	F	705	CYS
6	F	720	LYS
6	F	721	SER
6	F	729	LEU
6	F	742	LEU
7	G	5	LYS
6	H	27	LEU
6	H	61	LEU
6	H	90	GLN
6	H	98	ASN
6	H	118	LEU
6	H	130	ARG
6	H	144	LEU
6	H	145	ASN
6	H	163	ASP
6	H	165	ASP
6	H	466	LEU
6	H	480	ASN
6	H	520	ARG
6	H	521	ILE
6	H	530	ASN
6	H	562	MET
6	H	568	GLU
6	H	571	CYS

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Mol	Chain	Res	Type
6	H	576	CYS
6	H	588	LYS
6	H	592	ARG
6	H	599	ASN
6	H	614	THR
6	H	618	ASP
6	H	633	ARG
6	H	655	GLU
6	H	667	GLN
6	H	694	LYS
6	H	702	ASN
6	H	720	LYS
6	H	729	LEU
6	H	742	LEU
6	H	762	TRP
6	H	765	ASP
8	I	26	LEU
8	I	34	LEU
8	I	37	LEU
8	I	71	LEU
8	I	89	LYS
8	I	92	LEU
8	I	218	SER
8	I	224	SER
8	I	232	SER
8	I	266	ASN
8	I	269	LEU
8	I	284	ASP
8	I	333	LEU
8	I	340	SER
8	I	349	ILE
8	I	353	GLN
8	I	359	LEU
8	I	360	LEU
8	I	371	SER
8	I	372	TRP
8	I	381	LEU
8	I	387	GLU
8	I	399	LYS
8	I	401	ASN
8	I	404	LEU
8	I	473	GLU

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Mol	Chain	Res	Type
8	I	492	THR
8	I	496	GLN
8	I	512	LEU
8	I	522	LEU
8	I	537	LEU
8	I	539	LYS
8	I	564	ASP
8	I	688	THR
8	I	718	LYS
8	I	736	SER
9	J	15	ASP
9	J	23	LEU
9	J	38	GLN
9	J	46	CYS
9	J	61	ARG
9	J	141	ASP
9	J	157	LEU
9	J	163	CYS
9	J	169	LEU
9	J	170	LEU
9	J	180	GLU
9	J	185	LEU
9	J	188	LEU
9	J	202	ARG
9	J	206	GLU
9	J	248	LYS
9	J	254	THR
9	J	259	GLU
9	J	267	CYS
9	J	287	LEU
9	J	290	LYS
9	J	298	ASN
9	J	317	GLU
9	J	323	LEU
9	J	329	LEU
9	J	343	SER
9	J	351	ASP
9	J	354	MET
9	J	363	LEU
9	J	385	LYS
9	J	395	LEU
9	J	429	LEU

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Mol	Chain	Res	Type
9	J	439	VAL
9	J	445	GLU
9	J	451	LEU
9	J	472	LEU
9	J	475	ILE
9	J	485	ILE
9	J	506	LEU
9	J	515	SER
9	J	518	MET
9	J	523	ILE
9	K	15	ASP
9	K	20	GLN
9	K	38	GLN
9	K	45	GLN
9	K	46	CYS
9	K	63	ARG
9	K	78	ARG
9	K	128	ILE
9	K	129	LYS
9	K	134	LEU
9	K	141	ASP
9	K	146	ARG
9	K	157	LEU
9	K	163	CYS
9	K	169	LEU
9	K	173	HIS
9	K	184	LEU
9	K	188	LEU
9	K	190	LEU
9	K	206	GLU
9	K	231	LEU
9	K	254	THR
9	K	267	CYS
9	K	284	LEU
9	K	287	LEU
9	K	289	HIS
9	K	290	LYS
9	K	342	HIS
9	K	343	SER
9	K	351	ASP
9	K	359	THR
9	K	363	LEU

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Mol	Chain	Res	Type
9	K	376	LEU
9	K	385	LYS
9	K	386	LEU
9	K	429	LEU
9	K	432	ILE
9	K	438	GLU
9	K	454	VAL
9	K	506	LEU
9	K	509	ARG
9	K	510	ARG
9	K	515	SER
9	K	523	ILE
10	L	7	THR
10	L	12	ASP
10	L	23	ARG
10	L	25	ILE
10	L	32	SER
10	L	49	ASN
10	L	65	ASN
10	L	67	GLN
10	L	74	VAL
10	L	77	LEU
10	L	84	LYS
10	L	101	ASN
10	L	103	HIS
10	L	113	LEU
10	L	132	THR
10	L	151	THR
10	L	162	VAL
10	L	182	SER
10	L	184	ARG
11	M	1	MET
11	M	6	GLN
11	M	10	ARG
11	M	12	LEU
11	M	17	ASP
11	M	19	TRP
11	M	20	ARG
11	M	31	ILE
11	M	33	LEU
11	M	51	LYS
11	M	55	MET

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Mol	Chain	Res	Type
11	M	64	TYR
11	M	65	LEU
12	N	74	TRP
12	N	75	PHE
12	N	76	VAL
12	N	77	GLU
12	N	80	GLN
12	N	150	ARG
12	N	162	PHE
12	N	180	PHE
12	N	202	GLU
12	N	214	ARG
12	N	233	CYS
12	N	241	HIS
12	N	243	LEU
12	N	250	LEU
12	N	256	VAL
12	N	271	GLU
12	N	274	GLU
12	N	280	GLU
12	N	281	TYR
12	N	285	PHE
12	N	299	TRP
12	N	322	ARG
12	N	323	ARG
12	N	334	ARG
12	N	364	CYS
12	N	365	LEU
12	N	366	GLU
12	N	373	GLN
12	N	374	LEU
12	N	378	LEU
12	N	386	LEU
12	N	388	HIS
12	N	392	ASN
12	N	398	THR
12	N	425	ARG
12	N	435	VAL
12	N	503	SER
12	N	504	LEU
12	N	505	LEU
12	N	517	ASN

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Mol	Chain	Res	Type
12	N	531	PHE
12	N	544	LEU
12	N	547	LEU
12	N	557	CYS
12	N	561	LEU
12	N	566	ASP
12	N	571	ASN
12	N	584	GLU
12	N	592	TYR
12	N	594	VAL
12	N	609	LEU
12	N	619	LEU
12	N	622	TYR
12	N	625	LYS
12	N	626	TYR
12	N	633	ARG
12	N	638	LYS
12	N	640	THR
12	N	670	PHE
12	N	678	LEU
12	N	695	ARG
12	N	699	TRP
13	O	28	ASP
13	O	29	TRP
13	O	38	LEU
13	O	40	LEU
13	O	43	GLU
13	O	59	ARG
13	O	62	GLN
13	O	63	LEU
13	O	73	ILE
13	O	78	LEU
13	O	89	LEU
13	O	96	ARG
13	O	98	LYS
13	O	99	LEU
13	O	104	GLU
13	O	106	LYS
13	O	129	THR
13	O	136	LEU
13	O	160	GLN
13	O	207	LEU

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Mol	Chain	Res	Type
13	O	218	GLN
13	O	228	THR
13	O	237	GLN
13	O	249	ASP
13	O	256	LEU
13	O	257	SER
13	O	264	VAL
13	O	265	GLN
13	O	266	ASP
13	O	267	VAL
13	O	280	ARG
13	O	283	LEU
13	O	299	SER
13	O	328	ILE
13	O	330	ILE
13	O	344	LEU
13	O	345	SER
13	O	352	GLN
13	O	358	TYR
13	O	363	HIS
13	O	364	SER
13	O	383	SER
13	O	387	GLN
13	O	396	ASN
13	O	408	LEU
13	O	414	LEU
13	O	417	LEU
13	O	420	ILE
13	O	429	TRP
13	O	434	ARG
13	O	465	SER
13	O	468	VAL
13	O	491	LYS
13	O	495	GLU
13	O	501	SER
13	O	510	CYS
13	O	511	ASP
13	O	512	GLN
13	O	518	ARG
13	O	531	LEU
13	O	532	VAL
13	O	533	THR

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Mol	Chain	Res	Type
13	O	535	ILE
13	O	563	LEU
13	O	581	ILE
13	O	586	SER
13	O	598	THR
13	O	608	LEU
13	O	616	LEU
13	O	617	GLN
13	O	618	TYR
13	O	619	LEU
13	O	622	GLU
13	O	623	THR
13	O	625	LEU
13	O	632	LEU
13	O	633	ILE
13	O	634	LEU
13	O	636	ILE
13	O	641	LEU
13	O	646	MET
13	O	657	ILE
13	O	670	CYS
13	O	680	GLN
13	O	683	LYS
13	O	693	ASN
13	O	694	LEU
13	O	695	ASN
13	O	706	CYS
13	O	707	LYS
13	O	713	VAL
13	O	715	TYR
13	O	723	THR
13	O	730	ARG
13	O	735	MET
13	O	751	LEU
13	O	752	ILE
13	O	755	LEU
3	P	37	LEU
3	P	38	LEU
3	P	39	ILE
3	P	42	LEU
3	P	49	LEU
3	P	70	LEU

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Mol	Chain	Res	Type
3	P	78	GLU
3	P	83	ASP
3	P	89	LEU
3	P	97	LYS
3	P	119	MET
3	P	131	ASP
3	P	147	LYS
3	P	154	LEU
3	P	172	LEU
3	P	179	LEU
3	P	182	LEU
3	P	201	LEU
3	P	234	LEU
3	P	244	ILE
3	P	288	GLU
3	P	291	LYS
3	P	299	ASN
3	P	300	MET
3	P	302	THR
3	P	303	PHE
3	P	306	LEU
3	P	309	VAL
3	P	310	ARG
3	P	312	MET
3	P	313	LYS
3	P	316	LEU
3	P	321	HIS
3	P	324	CYS
3	P	328	LYS
3	P	335	CYS
3	P	343	LEU
3	P	348	GLU
3	P	352	LEU
3	P	358	LEU
3	P	359	LYS
3	P	365	LEU
3	P	378	MET
3	P	382	SER
3	P	386	GLN
3	P	392	ILE
3	P	395	ASN
3	P	400	ARG

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Mol	Chain	Res	Type
3	P	428	LEU
3	P	429	ARG
3	P	435	MET
3	P	451	GLU
3	P	455	CYS
3	P	468	MET
3	P	472	LYS
3	P	479	GLN
3	P	518	GLN
3	P	524	LYS
14	R	73	LYS
14	R	83	ARG
14	R	109	LYS
14	R	110	LYS
14	R	114	LYS
14	R	118	LEU
14	R	125	VAL
14	R	129	LYS
14	R	132	ARG
14	R	252	LEU
14	R	316	ARG
14	R	411	TYR
14	R	496	GLN
14	R	499	ARG
7	W	5	LYS
16	X	39	ASP
16	X	49	LEU
16	X	79	LEU
16	X	106	GLN
16	X	110	LEU
16	X	154	ASP
16	X	184	GLN
16	X	193	LYS
16	X	201	LEU
16	X	204	ASP
16	X	253	ARG
16	X	255	ILE
16	X	276	SER
16	X	289	ASN
16	X	295	GLU
16	X	303	TYR
16	X	306	LYS

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Mol	Chain	Res	Type
16	X	323	ASP
16	X	334	ILE
16	X	366	ILE
16	X	371	ASN
16	X	372	SER
16	X	401	ARG
16	X	407	LEU
16	X	414	ILE
16	X	423	ILE
16	X	452	LEU
16	X	453	GLU
16	X	457	THR
16	X	465	LEU
16	X	487	SER
16	X	506	GLN
16	X	515	LEU
16	Y	39	ASP
16	Y	49	LEU
16	Y	54	ARG
16	Y	63	MET
16	Y	79	LEU
16	Y	94	ARG
16	Y	95	ASN
16	Y	154	ASP
16	Y	184	GLN
16	Y	193	LYS
16	Y	199	CYS
16	Y	201	LEU
16	Y	204	ASP
16	Y	253	ARG
16	Y	255	ILE
16	Y	276	SER
16	Y	289	ASN
16	Y	294	PHE
16	Y	295	GLU
16	Y	300	LEU
16	Y	303	TYR
16	Y	323	ASP
16	Y	334	ILE
16	Y	364	LYS
16	Y	366	ILE
16	Y	371	ASN

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Mol	Chain	Res	Type
16	Y	372	SER
16	Y	401	ARG
16	Y	407	LEU
16	Y	414	ILE
16	Y	423	ILE
16	Y	452	LEU
16	Y	453	GLU
16	Y	457	THR
16	Y	465	LEU
16	Y	487	SER
16	Y	503	LEU
16	Y	506	GLN
16	Y	515	LEU
16	Y	551	LYS
16	Y	552	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	36	ASN
1	A	38	GLN
1	A	124	GLN
1	A	125	GLN
1	A	162	HIS
1	A	250	ASN
1	A	263	GLN
1	A	593	ASN
1	A	658	ASN
1	A	666	ASN
1	A	776	ASN
1	A	936	ASN
1	A	1021	HIS
1	A	1161	ASN
1	A	1165	HIS
1	A	1184	HIS
1	A	1201	HIS
1	A	1262	GLN
1	A	1266	HIS
1	A	1327	GLN
1	A	1380	ASN
1	A	1543	HIS

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Mol	Chain	Res	Type
1	A	1559	HIS
1	A	1604	GLN
1	A	1813	GLN
2	B	9	ASN
2	B	50	GLN
3	C	202	HIS
3	C	236	HIS
3	C	249	GLN
3	C	287	ASN
3	C	373	HIS
3	C	386	GLN
4	D	36	GLN
4	D	37	HIS
4	D	38	GLN
4	D	49	ASN
5	E	75	GLN
6	F	100	GLN
6	F	495	HIS
6	F	583	HIS
6	F	595	GLN
6	F	634	HIS
6	F	636	ASN
6	F	754	HIS
6	H	14	GLN
6	H	480	ASN
6	H	494	HIS
6	H	495	HIS
6	H	545	HIS
6	H	634	HIS
6	H	648	GLN
6	H	680	HIS
6	H	708	HIS
8	I	18	GLN
8	I	266	ASN
8	I	323	ASN
8	I	345	GLN
8	I	351	HIS
8	I	353	GLN
8	I	362	HIS
8	I	471	ASN
8	I	523	HIS
9	J	17	GLN

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Mol	Chain	Res	Type
9	J	38	GLN
9	J	45	GLN
9	J	58	HIS
9	J	173	HIS
9	J	228	GLN
9	J	271	HIS
9	J	289	HIS
9	J	316	ASN
9	J	342	HIS
9	J	352	GLN
9	J	382	ASN
9	J	406	HIS
9	K	17	GLN
9	K	20	GLN
9	K	38	GLN
9	K	45	GLN
9	K	198	GLN
9	K	271	HIS
9	K	316	ASN
9	K	352	GLN
9	K	382	ASN
10	L	49	ASN
10	L	103	HIS
10	L	128	HIS
10	L	138	GLN
10	L	152	HIS
12	N	370	GLN
12	N	388	HIS
12	N	571	ASN
12	N	639	HIS
12	N	663	GLN
12	N	702	GLN
12	N	726	ASN
13	O	62	GLN
13	O	69	GLN
13	O	91	ASN
13	O	211	GLN
13	O	219	GLN
13	O	237	GLN
13	O	242	ASN
13	O	247	ASN
13	O	319	GLN

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Mol	Chain	Res	Type
13	O	387	GLN
13	O	412	HIS
13	O	424	GLN
13	O	443	GLN
13	O	460	GLN
13	O	462	ASN
13	O	492	HIS
13	O	539	ASN
13	O	556	GLN
13	O	565	GLN
13	O	576	ASN
13	O	717	GLN
13	O	753	ASN
3	P	236	HIS
3	P	242	GLN
3	P	249	GLN
3	P	287	ASN
3	P	305	ASN
3	P	321	HIS
14	R	87	GLN
14	R	99	ASN
16	X	50	HIS
16	X	89	HIS
16	X	95	ASN
16	X	106	GLN
16	X	298	GLN
16	X	337	GLN
16	X	371	ASN
16	X	395	HIS
16	X	506	GLN
16	Y	270	ASN
16	Y	296	GLN
16	Y	298	GLN
16	Y	337	GLN
16	Y	371	ASN
16	Y	395	HIS
16	Y	505	ASN
16	Y	506	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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
12	N	6
14	R	2
16	X	1
1	A	1
6	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	510:GLY	C	511:SER	N	3.32
1	N	213:TYR	C	214:ARG	N	3.24
1	X	386:MET	C	387:GLY	N	3.24

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	92:TRP	C	93:ASN	N	3.21
1	R	388[A]:CYS	C	389:SER	N	3.09
1	N	166:PRO	C	167:ARG	N	2.97
1	N	549:PHE	C	550:GLY	N	2.95
1	R	388[B]:CYS	C	389:SER	N	2.94
1	A	1228:LEU	C	1229:SER	N	2.89
1	N	563:ASP	C	564:MET	N	2.82
1	H	479:TYR	C	480:ASN	N	2.09

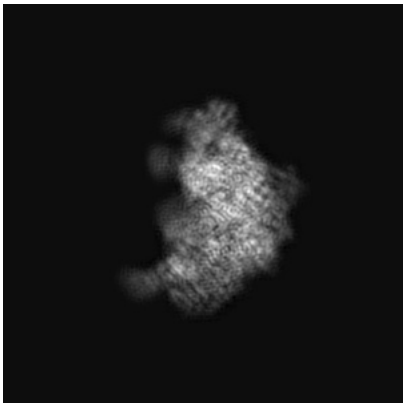
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3385. These allow visual inspection of the internal detail of the map and identification of artifacts.

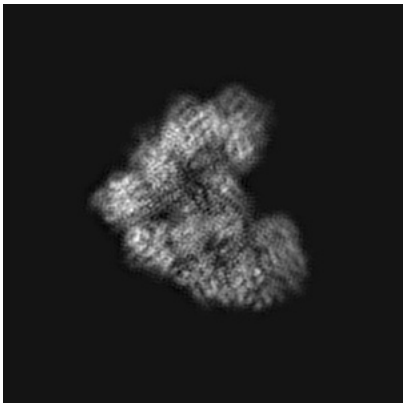
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

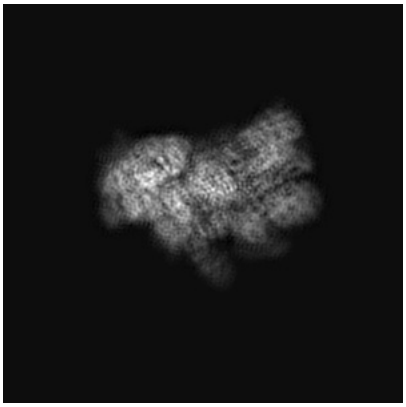
6.1.1 Primary map



X



Y

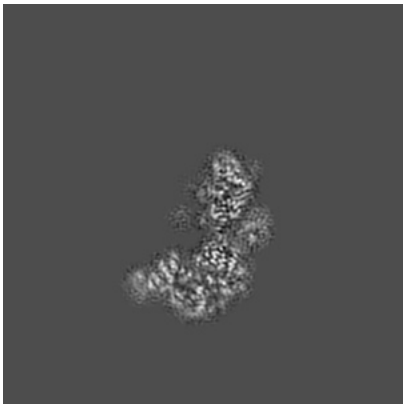


Z

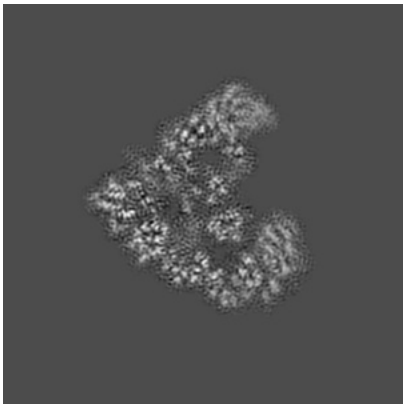
The images above show the map projected in three orthogonal directions.

6.2 Central slices

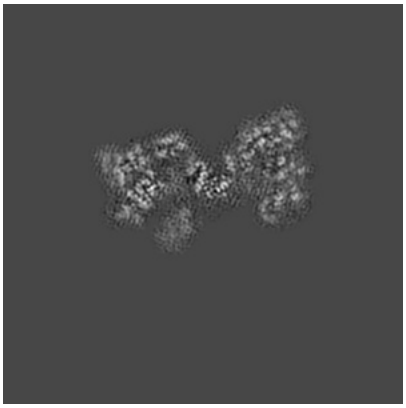
6.2.1 Primary map



X Index: 142



Y Index: 142



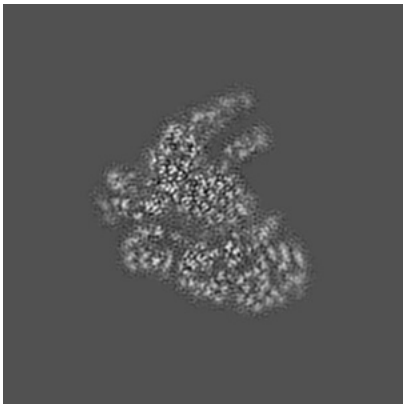
Z Index: 142

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

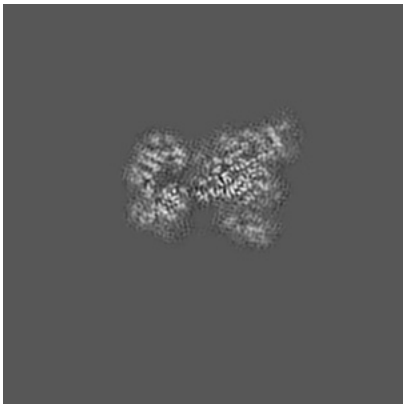
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 121



Y Index: 156

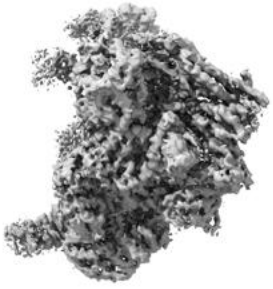


Z Index: 113

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 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

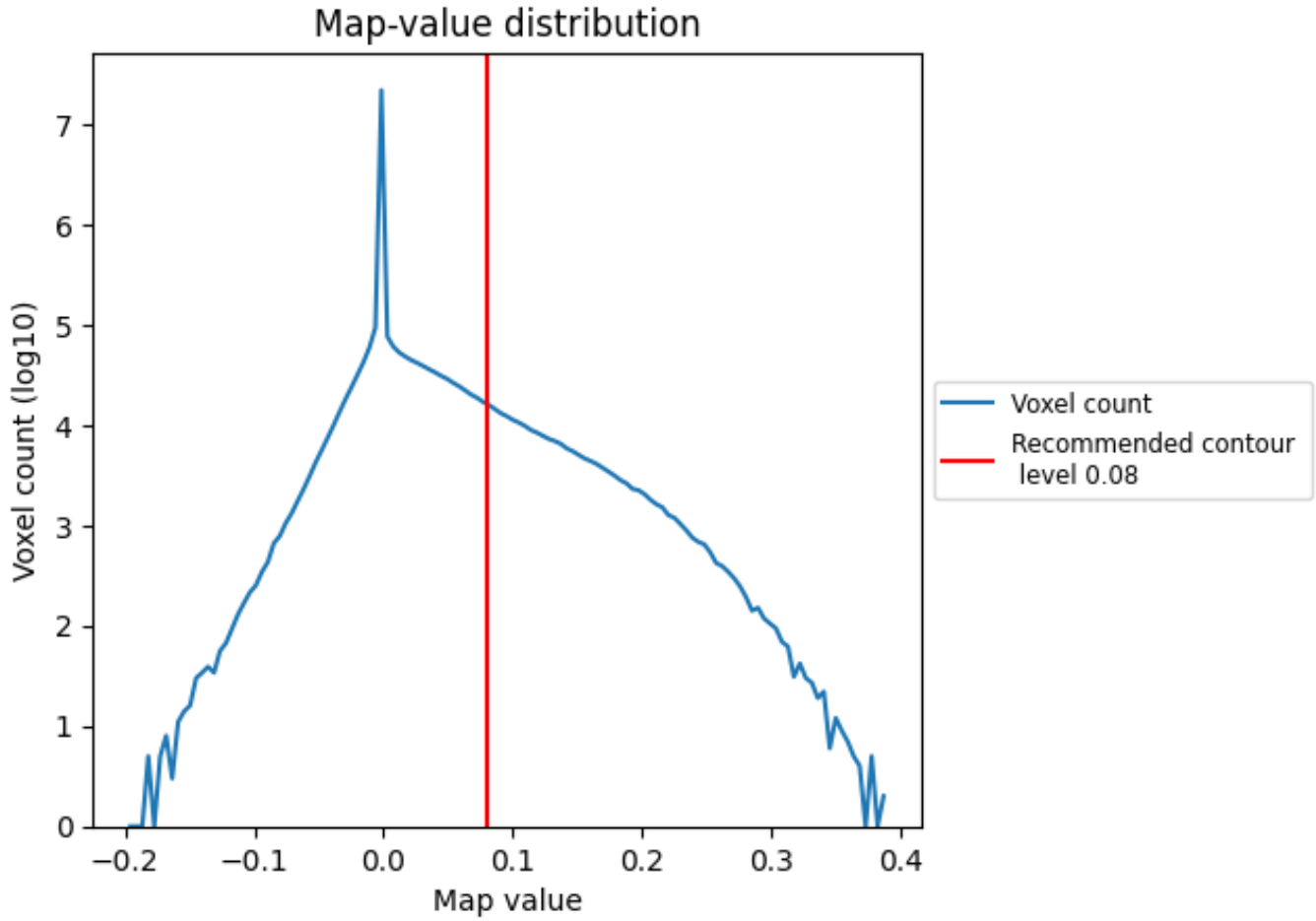
6.5 Mask visualisation (i)

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

7 Map analysis

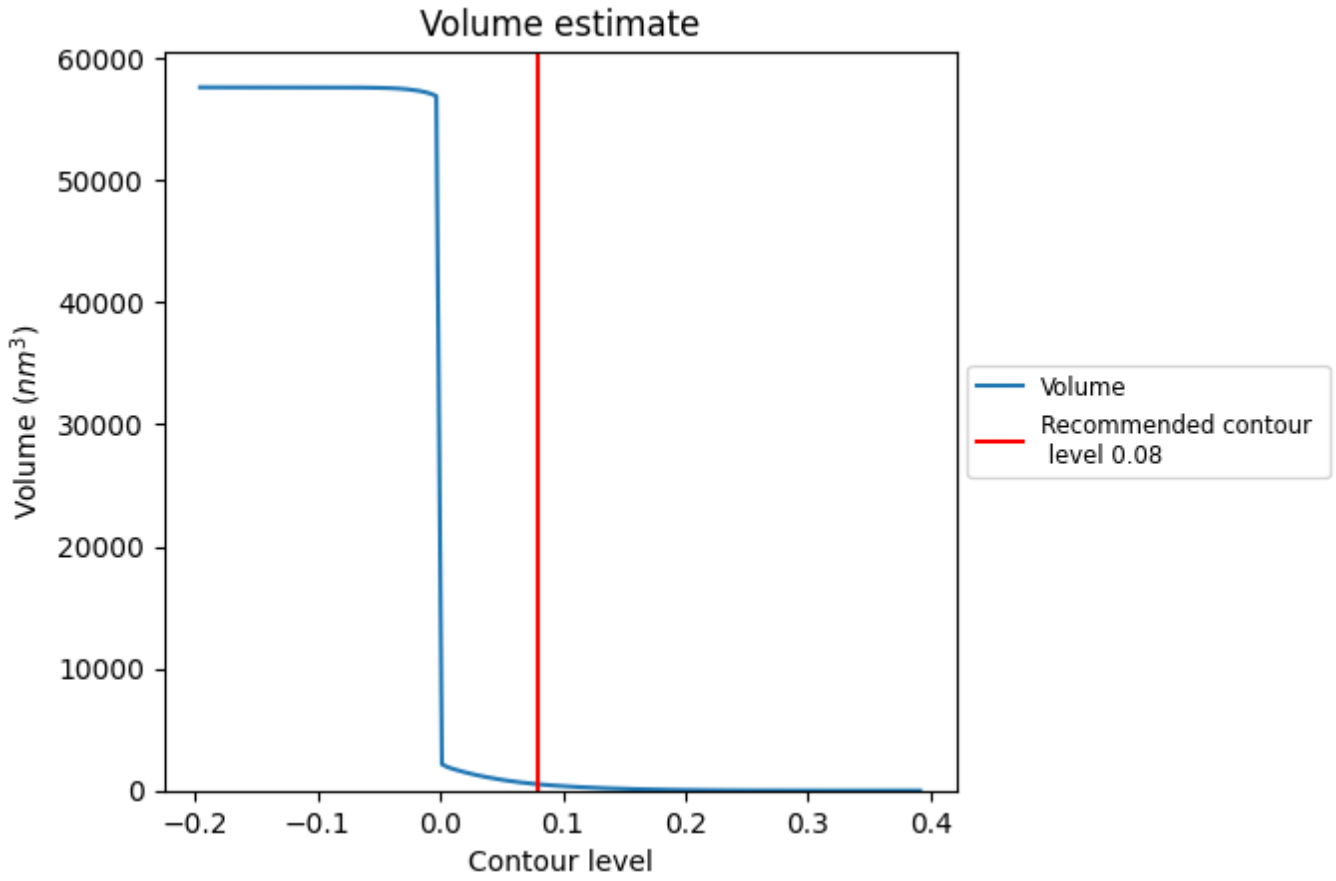
This section contains the results of statistical analysis of the map.

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.

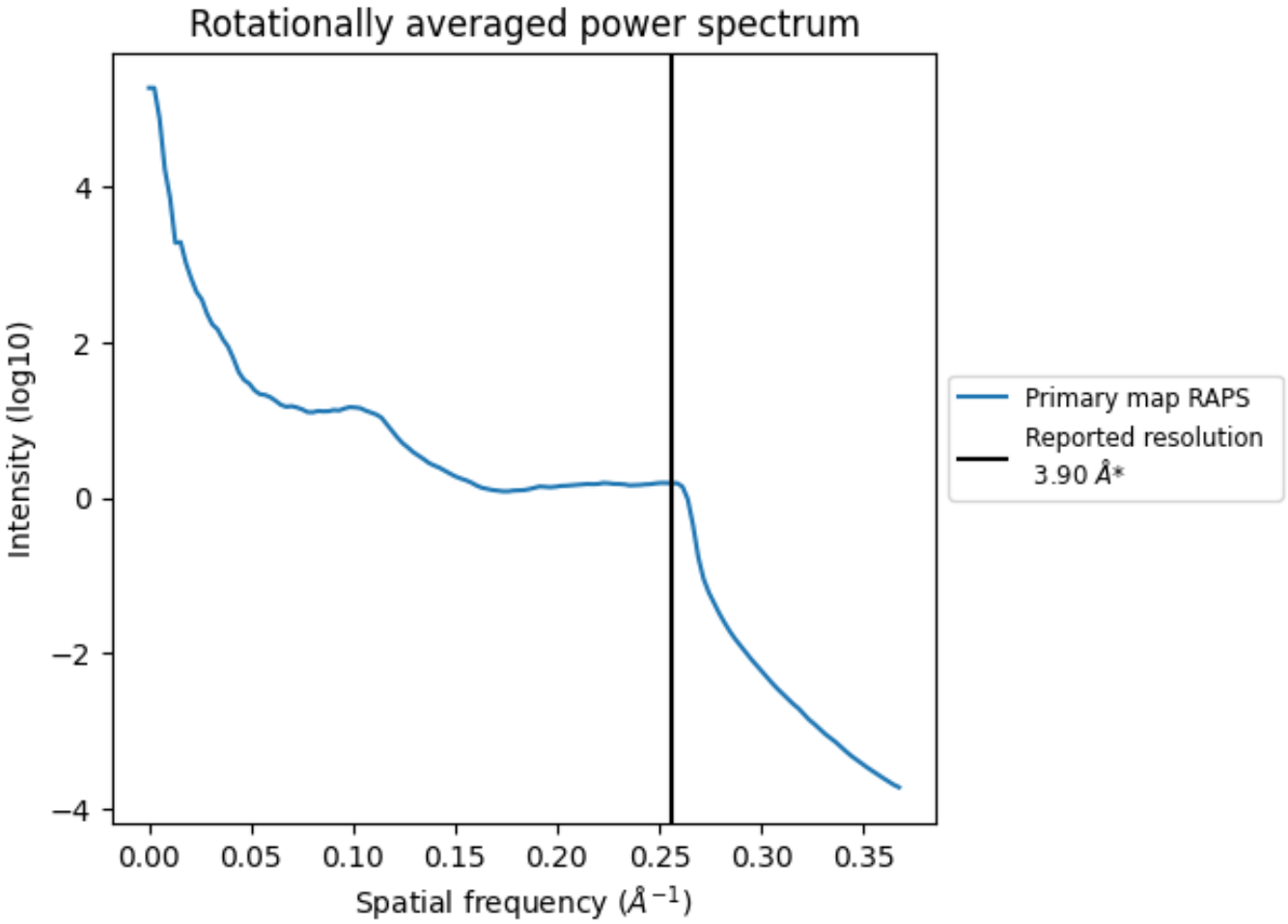
7.2 Volume estimate



The volume at the recommended contour level is 516 nm^3; this corresponds to an approximate mass of 466 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 0.256 Å^{-1}

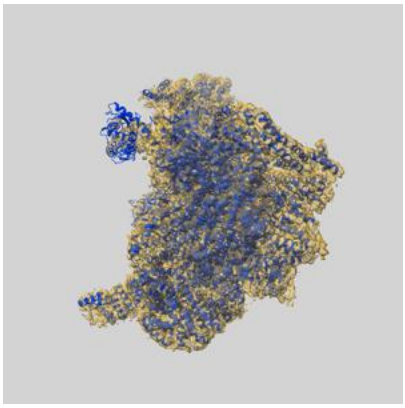
8 Fourier-Shell correlation

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

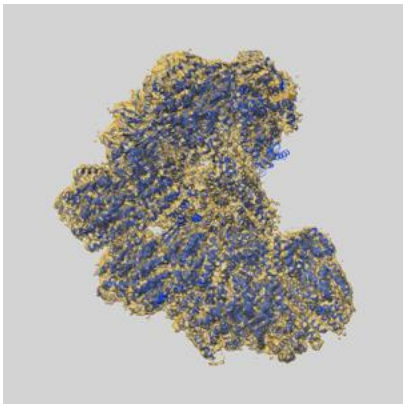
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3385 and PDB model 5G04. Per-residue inclusion information can be found in section 3 on page 7.

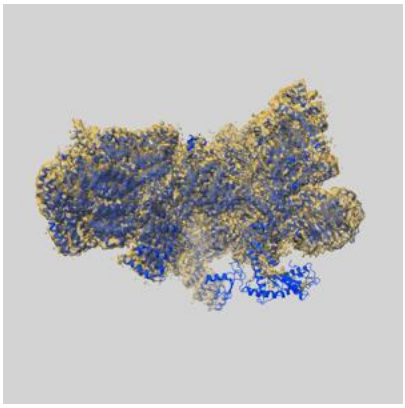
9.1 Map-model overlay



X



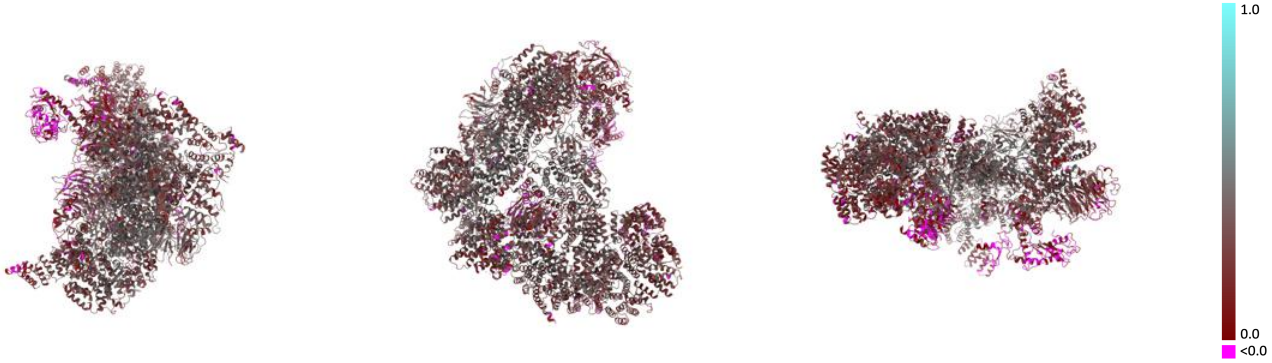
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

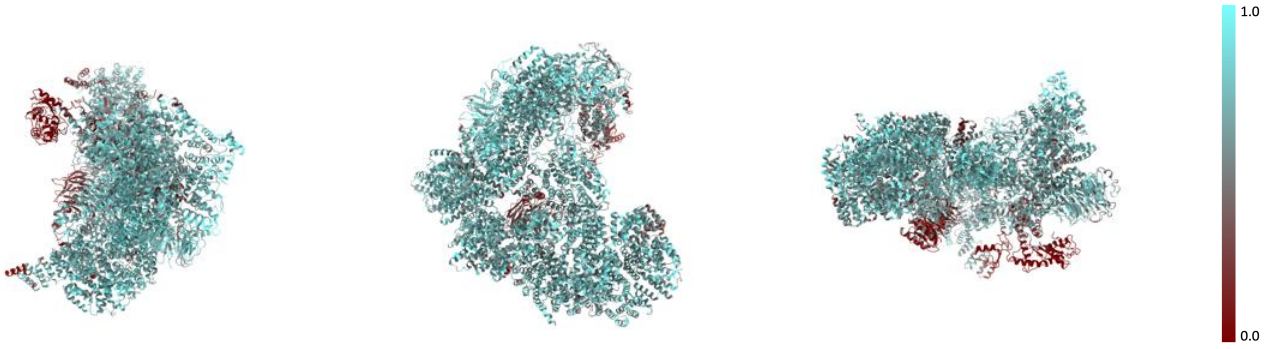
9.2 Q-score mapped to coordinate model (i)



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.

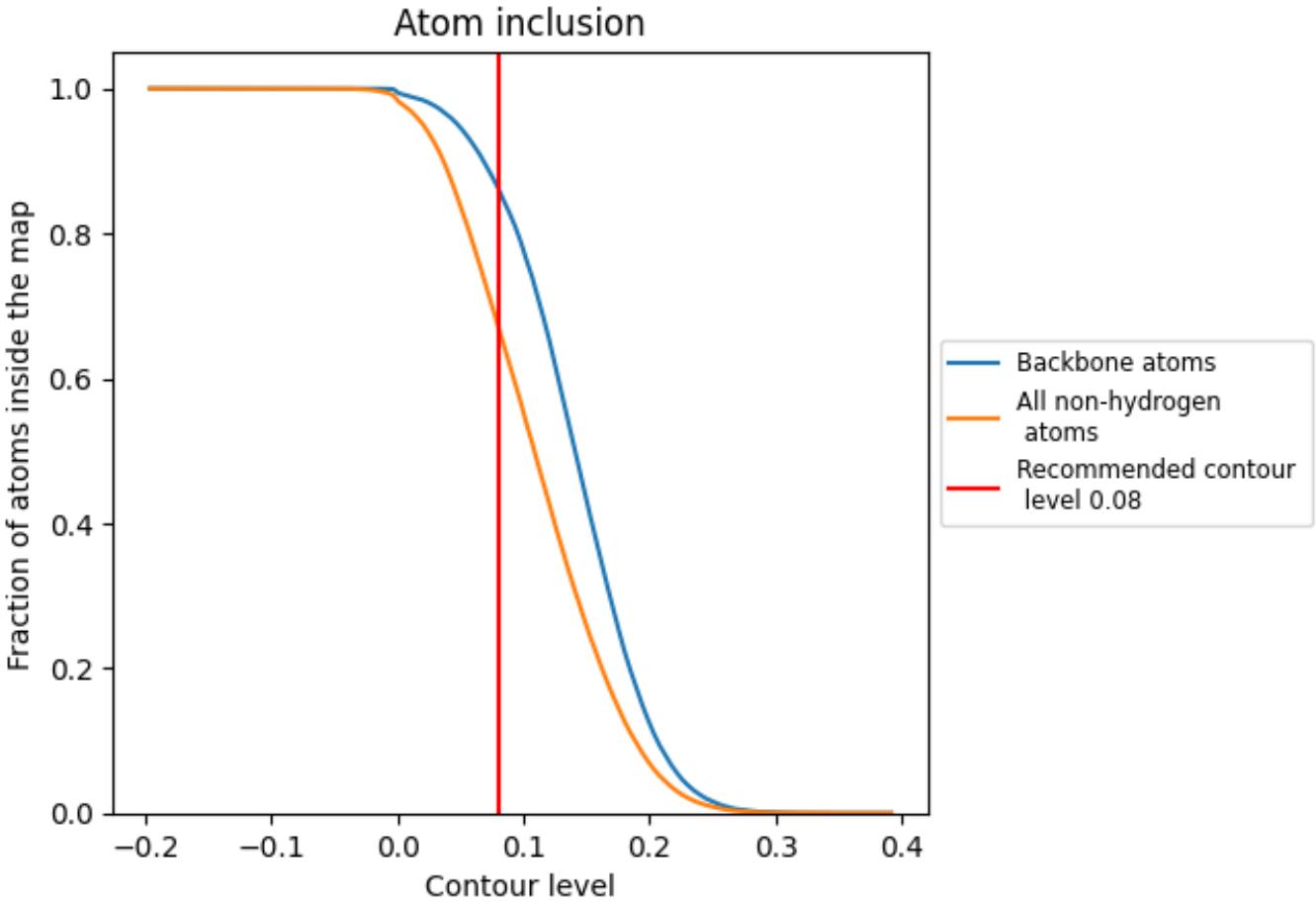
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 67% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6718	0.2990
A	0.7500	0.3600
B	0.0126	-0.0160
C	0.7182	0.3580
D	0.6991	0.3480
E	0.7050	0.3400
F	0.7375	0.3320
G	0.7512	0.3370
H	0.7567	0.3410
I	0.6692	0.2710
J	0.7630	0.3370
K	0.7337	0.3110
L	0.7026	0.3400
M	0.6294	0.3370
N	0.4352	0.1830
O	0.7416	0.3550
P	0.7135	0.3010
R	0.2669	0.1400
S	0.0857	0.0850
W	0.6341	0.3120
X	0.6322	0.2210
Y	0.6881	0.2530