



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 10:11 PM UTC

PDB ID : 5G04 / pdb_00005g04
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 : 3.90 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:

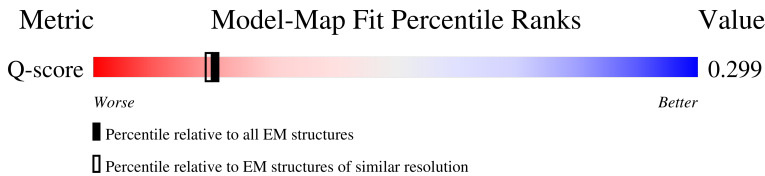
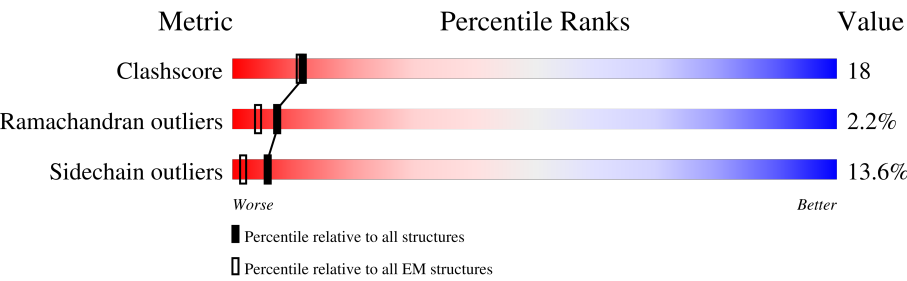
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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.



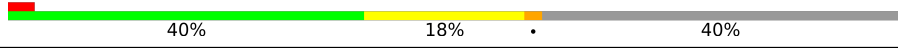
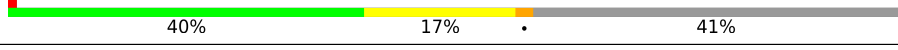
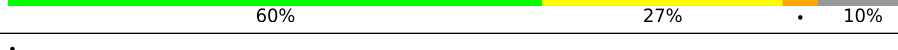
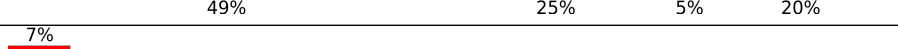
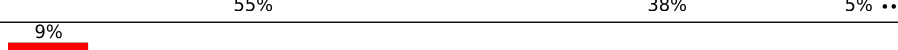
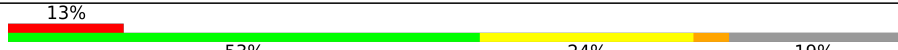
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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 $\leq 5\%$. 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	40%26%7%26% 98%
2	B	84	63%26%8% 98%
3	C	597	8%42%33%12%12% 98%
3	P	597	5%51%25%5%18% 98%

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Mol	Chain	Length	Quality of chain
4	D	121	
5	E	110	
6	F	824	
6	H	824	
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
1	A	1437	Total	C	N	O	S	0	0
			10925	7025	1849	1977	74		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	524	Total	C	N	O	S	0	0
			4306	2774	727	781	24		
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
4	D	55	Total	C	N	O	0	0
			436	277	73	86		

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

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

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

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

- 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		

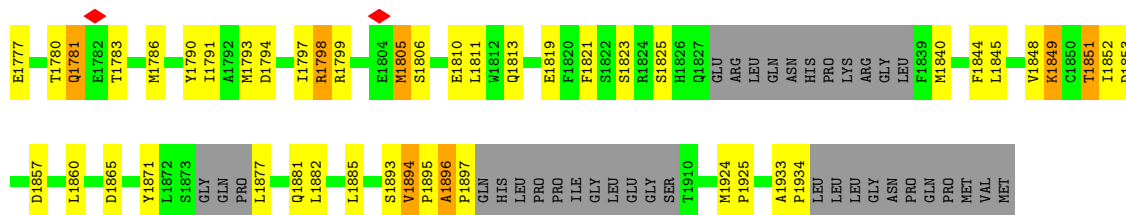
- Molecule 16 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 7.

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		

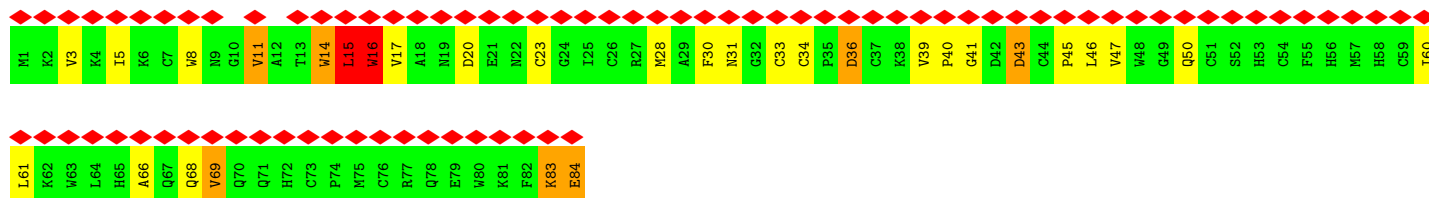
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

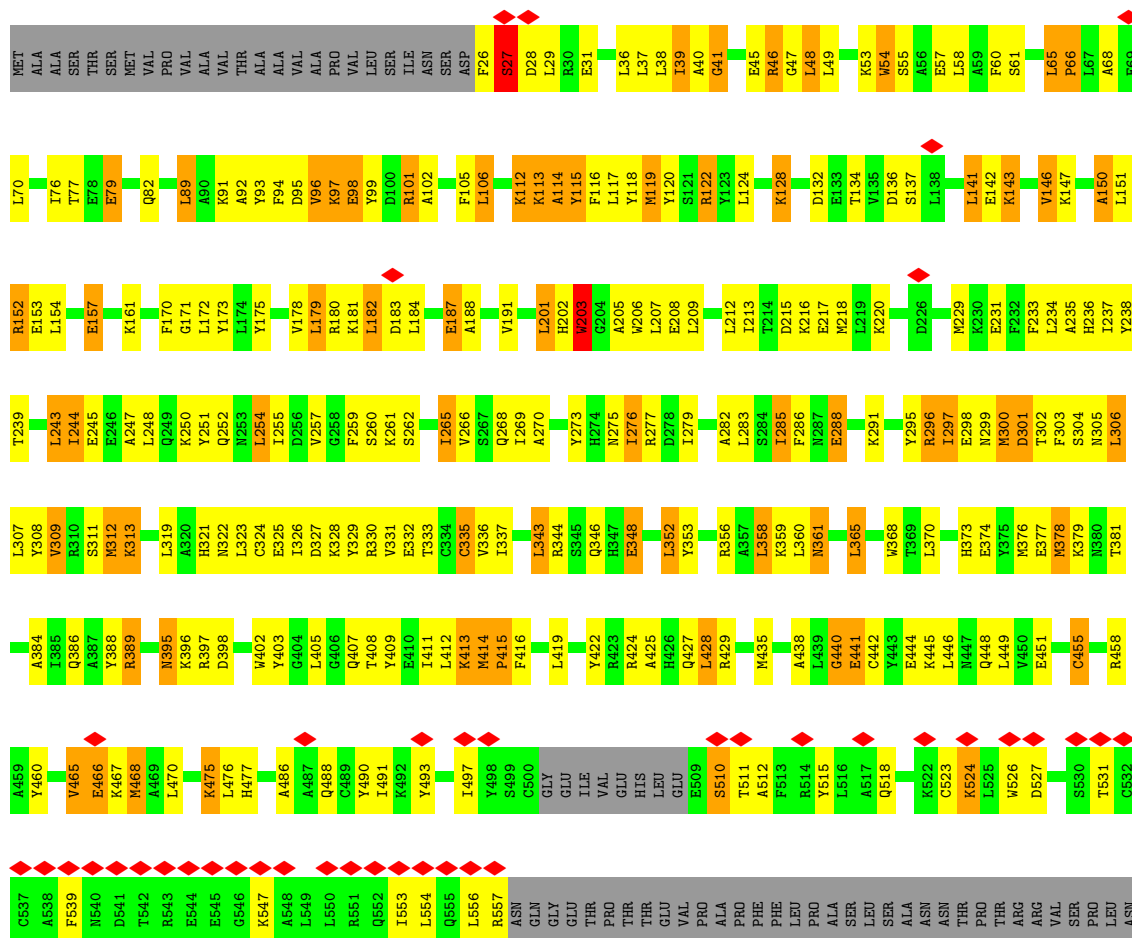
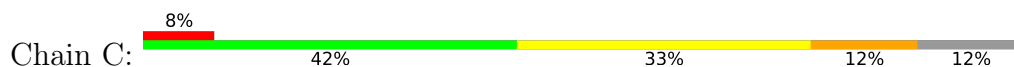




• Molecule 2: ANAPHASE-PROMOTING COMPLEX SUBUNIT 11

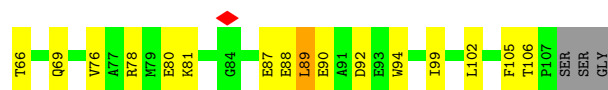


• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

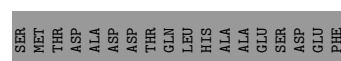
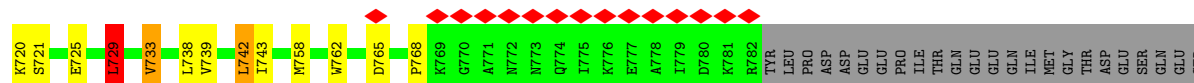
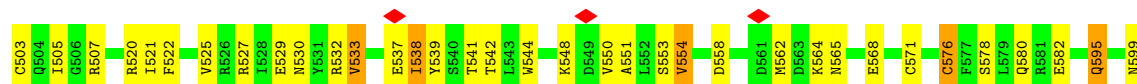
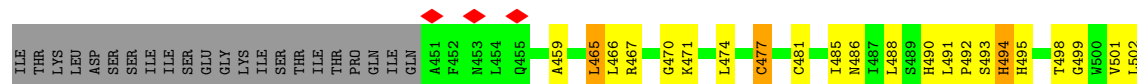
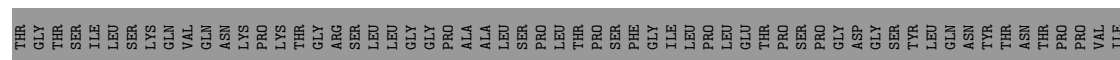
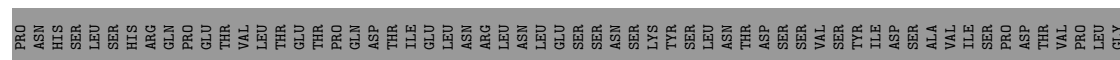
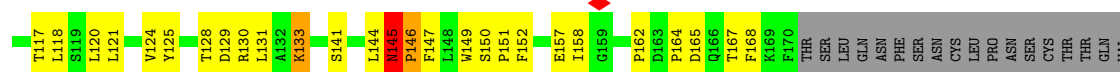
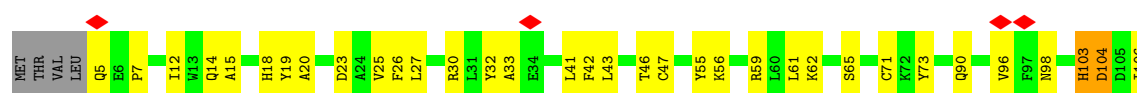


VAL
THR
PRO

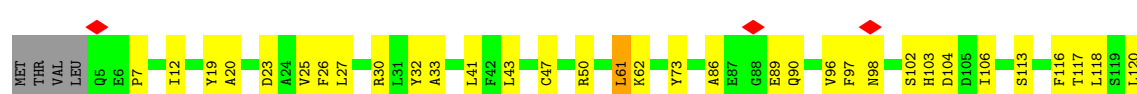
MET	ALA	ALA	SER	SER	SER	SER	SER	ALA	ALA	GLY	GLY	VAL	SER	GLY	SER	SER	SER	VAL	THR	GLY	GLY	GLY	PHE	SER	VAL	ASP	LEU	ALA	PRO	PRO	ARG	LYS	LYS	ALA	LEU	PHE	THR	TYR	PRO	PRO	LYS	GLY	ALA	GLY	GLU	MET	LEU	GLU	ASP	GLY	SER	GLU	R52	V58	F59	S60	Y61	Q62	V63
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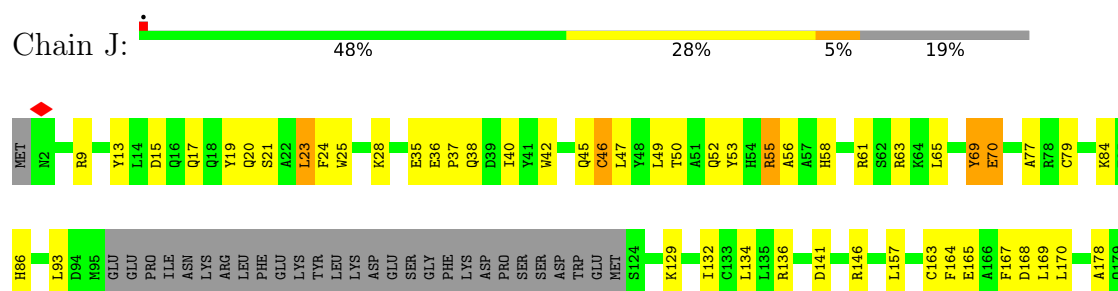


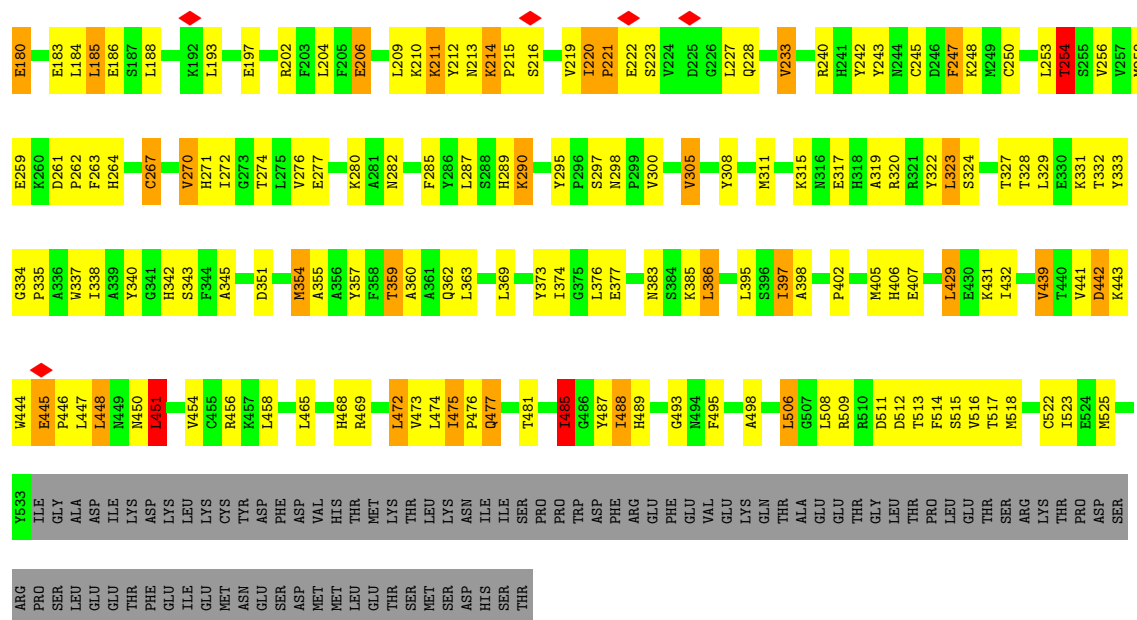
• Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG



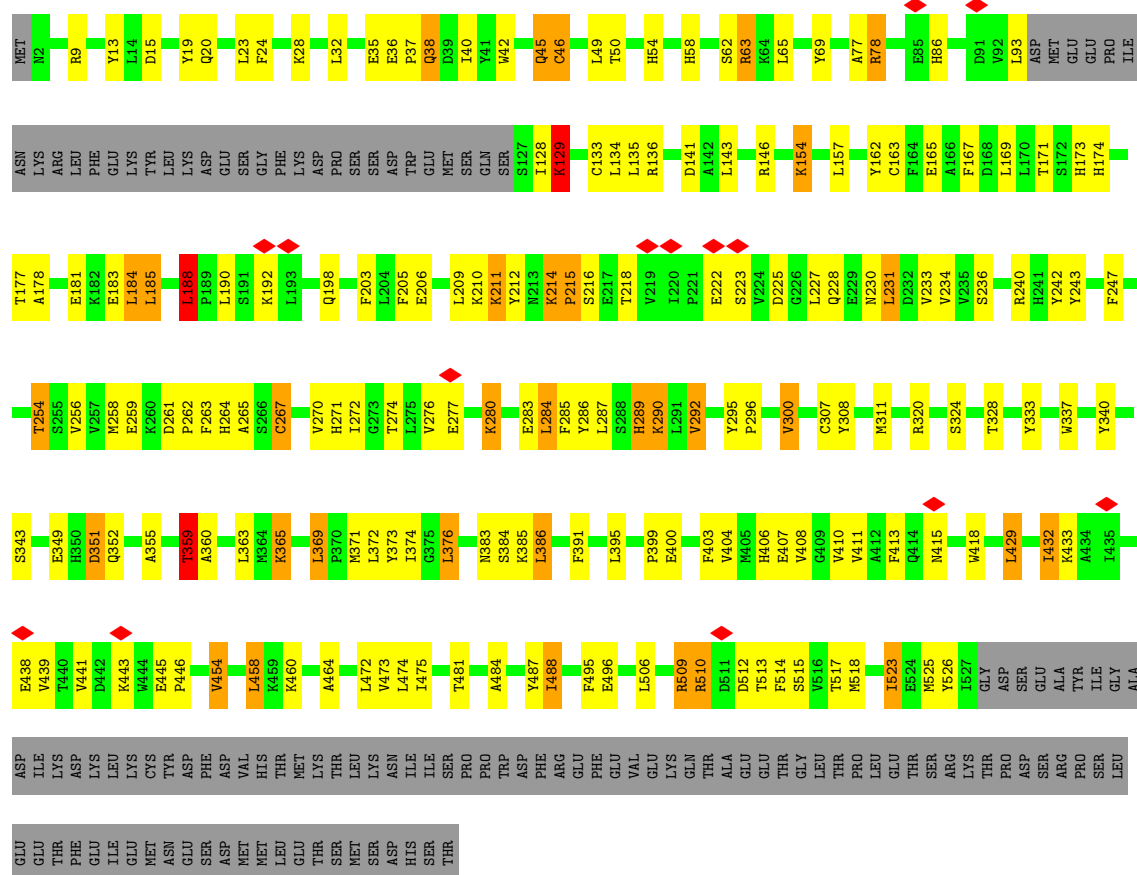
• Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG



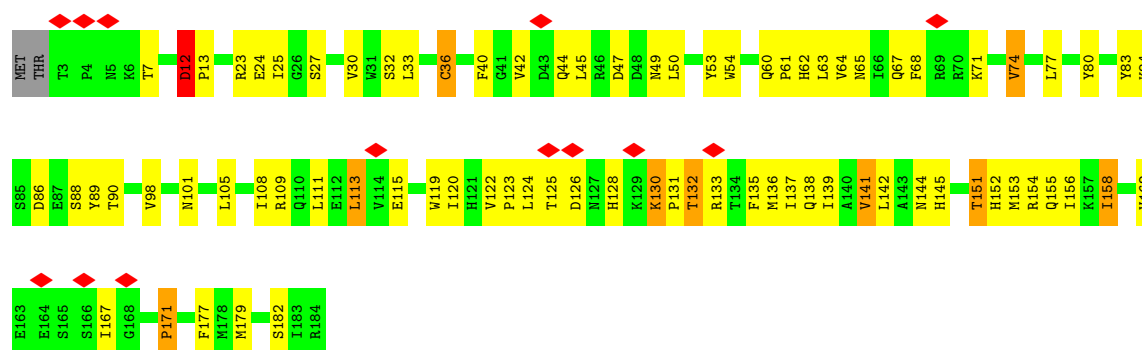




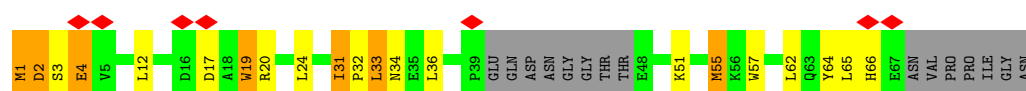
• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG



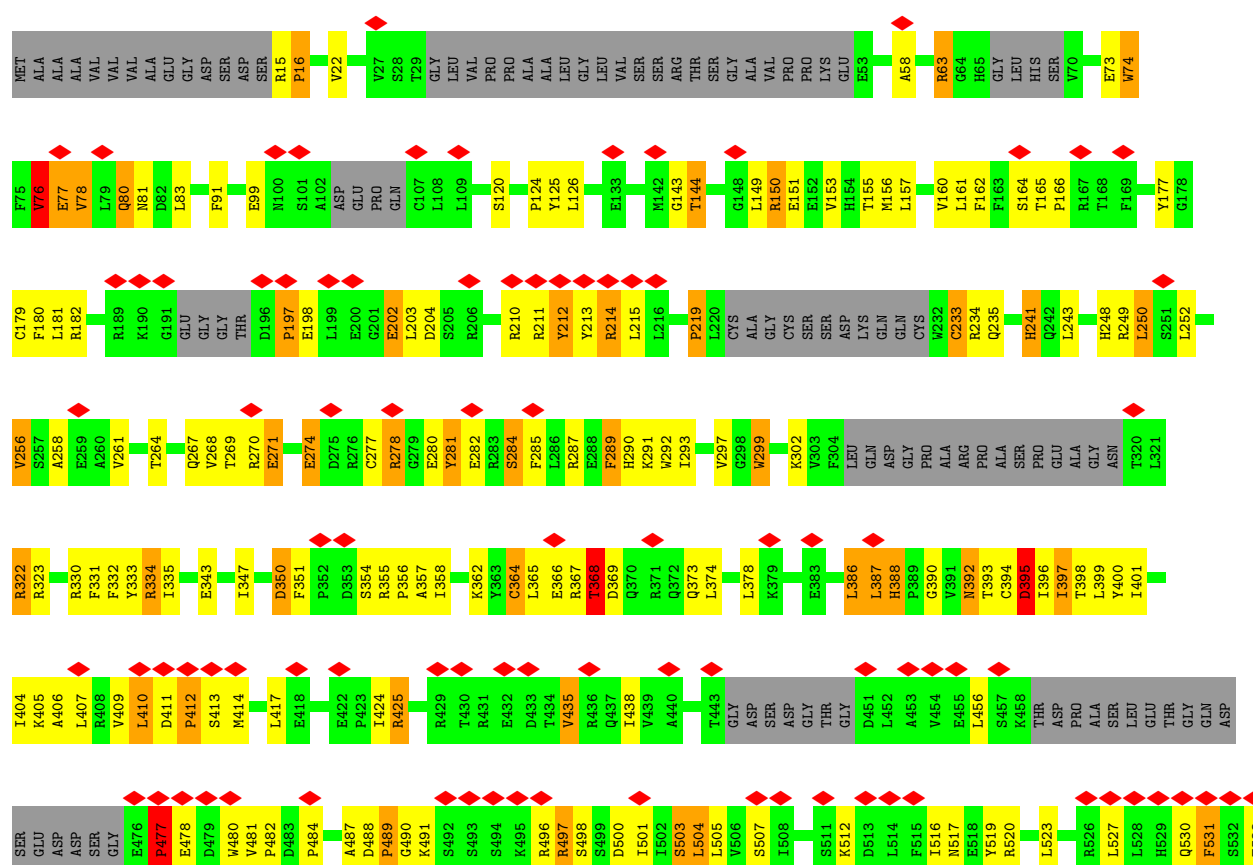
• Molecule 10: ANAPHASE-PROMOTING COMPLEX SUBUNIT 10

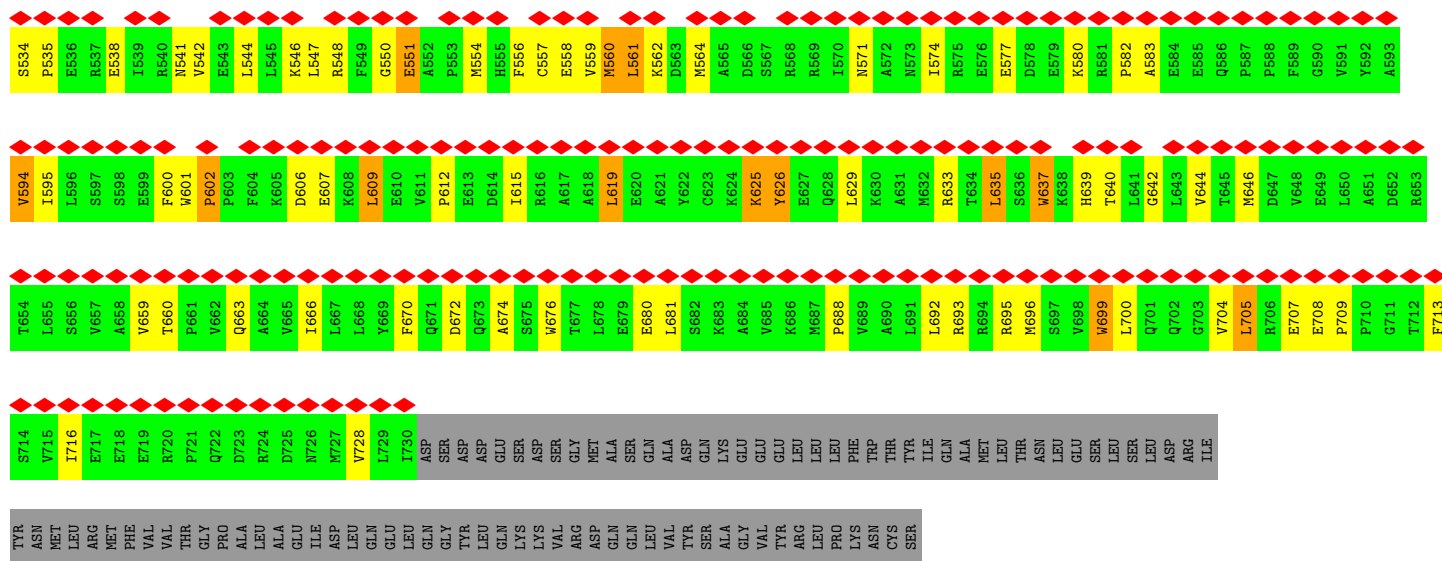


• Molecule 11: ANAPHASE-PROMOTING COMPLEX SUBUNIT 13

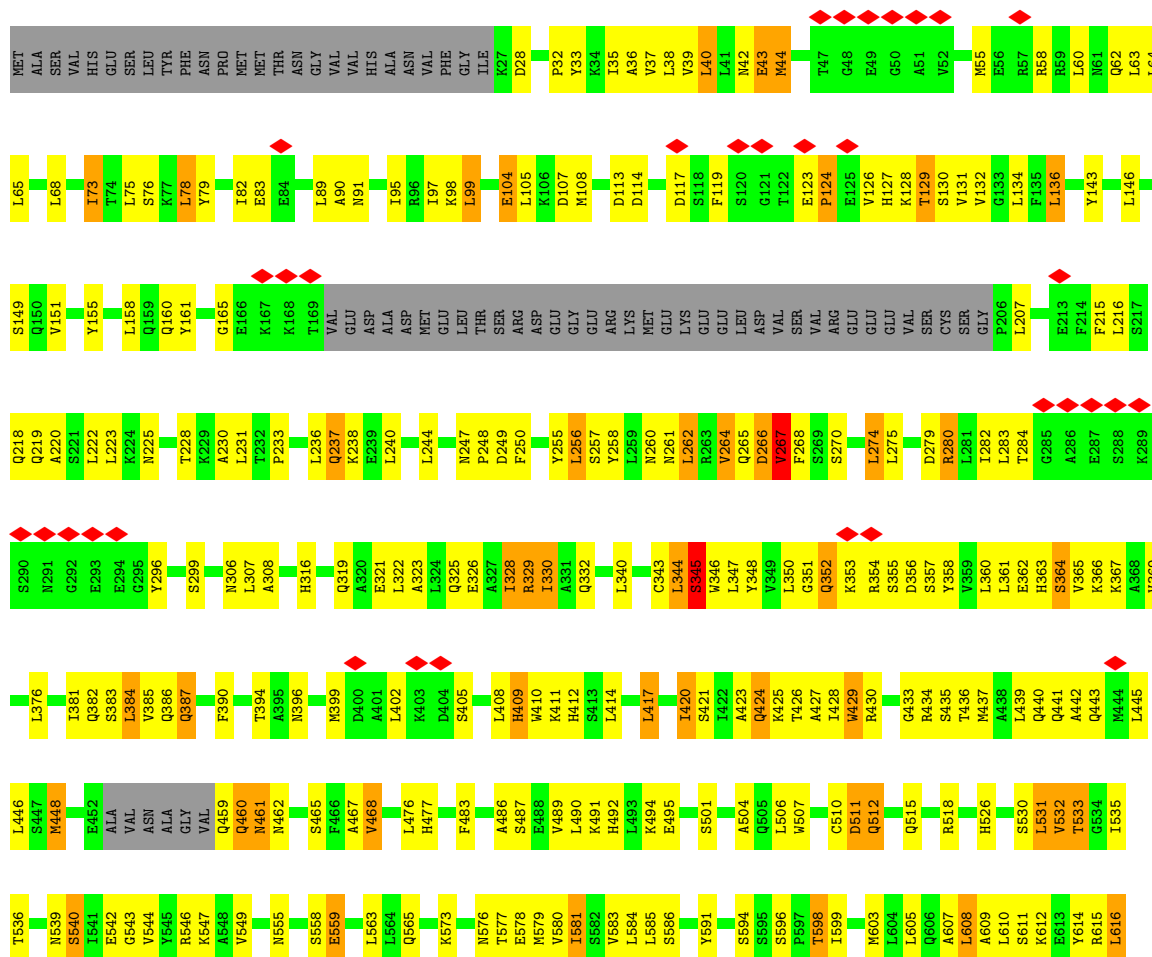


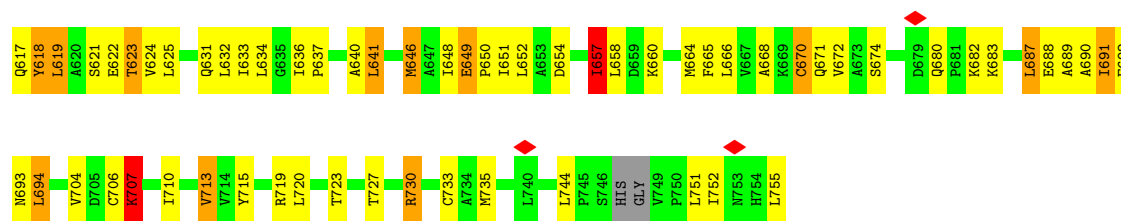
• Molecule 12: ANAPHASE-PROMOTING COMPLEX SUBUNIT 2



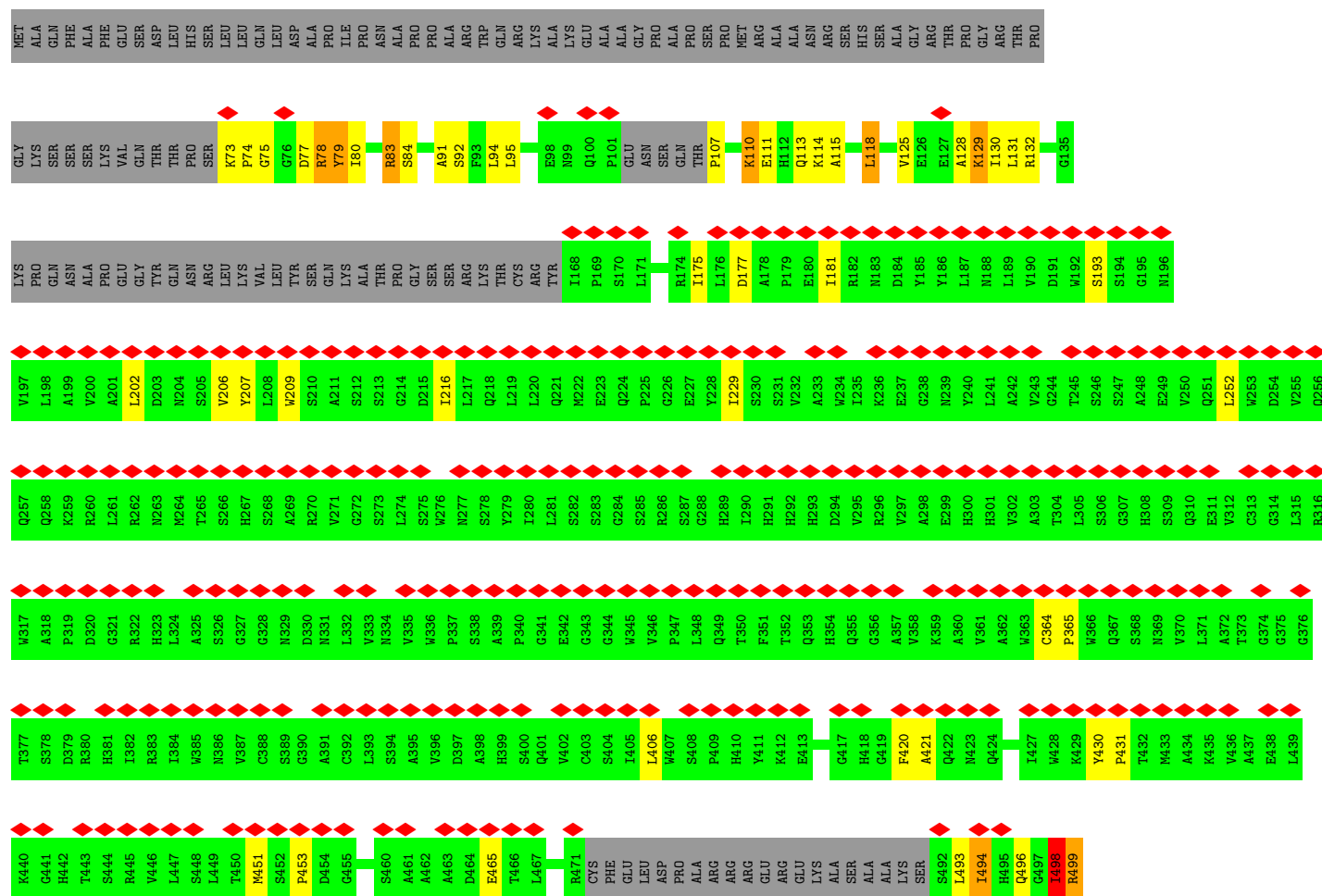


• Molecule 13: ANAPHASE-PROMOTING COMPLEX SUBUNIT 5

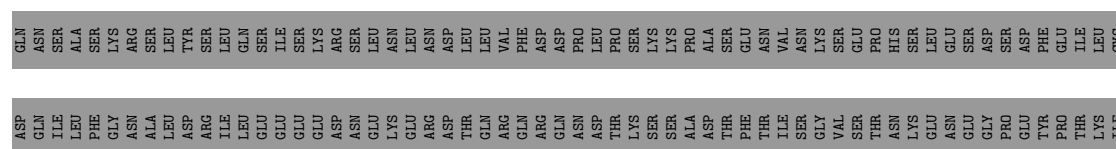


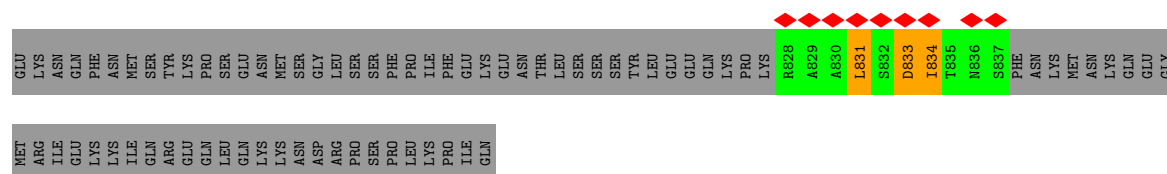


• Molecule 14: CELL DIVISION CYCLE PROTEIN 20 HOMOLOG

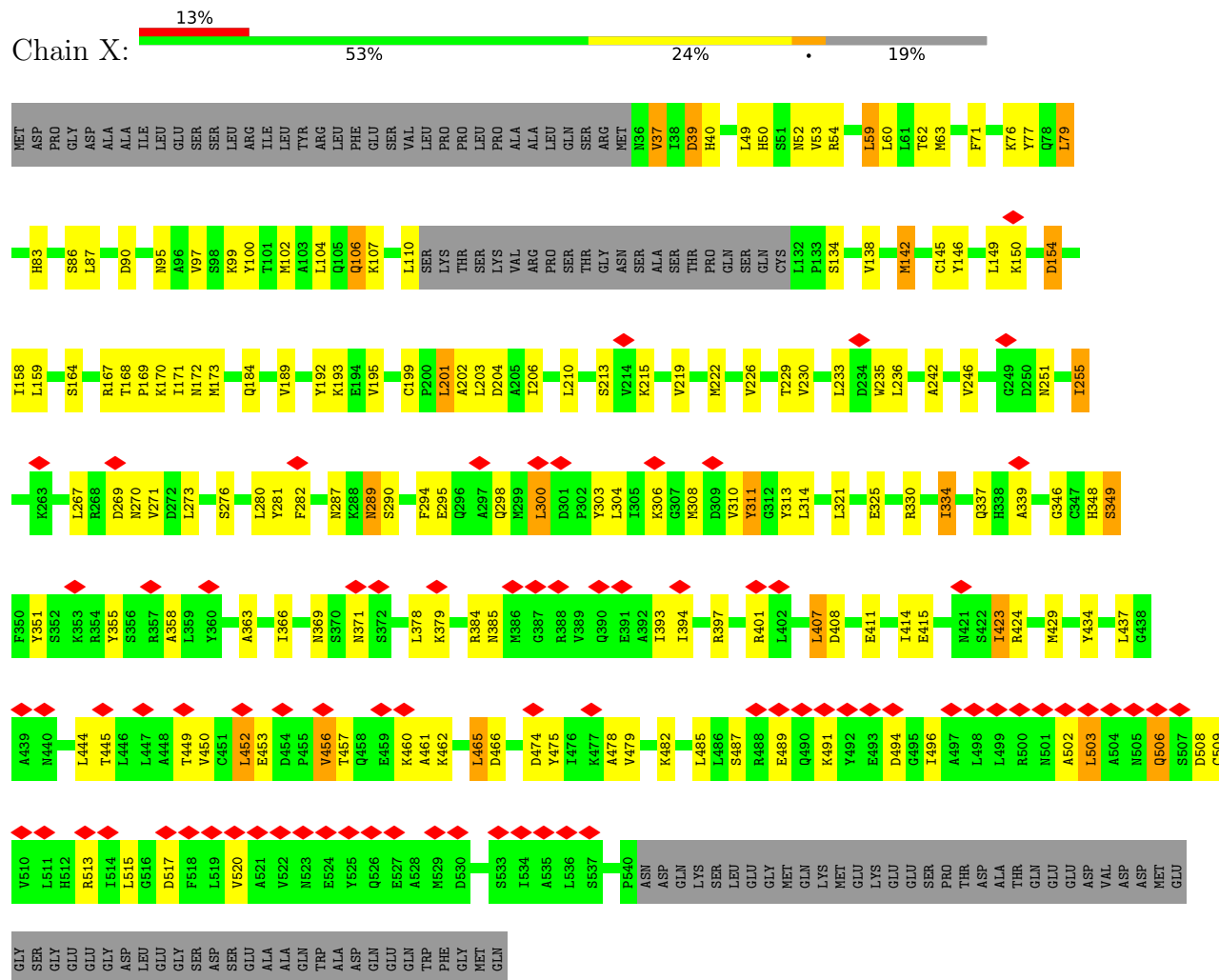


• Molecule 15: PROBABLE SERINE/THREONINE-PROTEIN KINASE HSL1

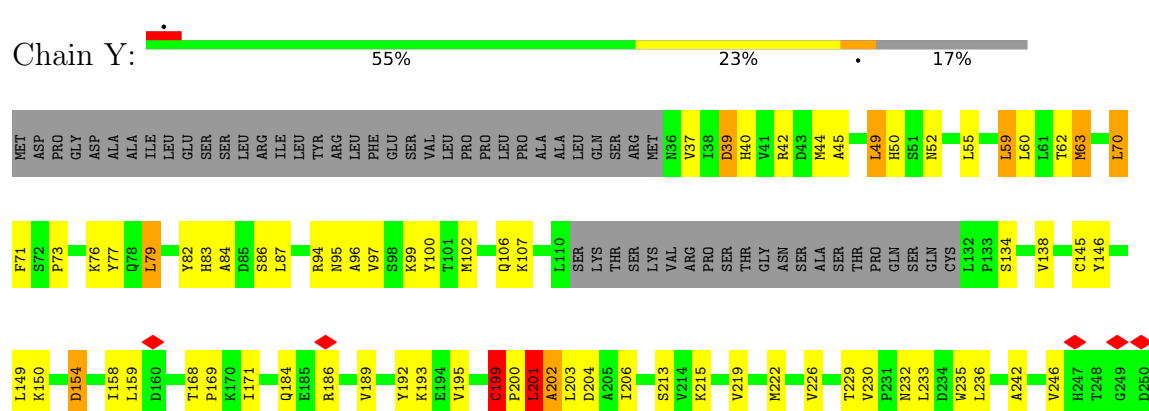


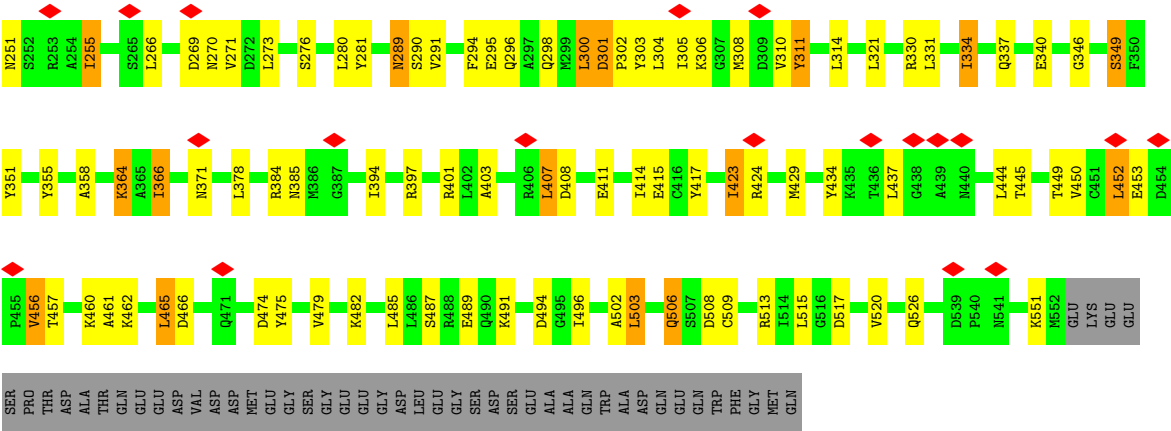


• Molecule 16: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7



• Molecule 16: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7





4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	386.24, 386.24, 386.24	wwPDB
Map dimensions	284, 284, 284	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.83	0/11165	1.31	60/15204 (0.4%)
2	B	0.91	0/674	1.21	1/913 (0.1%)
3	C	0.88	2/4404 (0.0%)	1.30	16/5945 (0.3%)
3	P	0.86	1/4134 (0.0%)	1.24	7/5583 (0.1%)
4	D	0.80	0/446	1.22	1/610 (0.2%)
5	E	0.81	0/459	1.30	1/619 (0.2%)
6	F	0.78	1/4013 (0.0%)	1.25	13/5428 (0.2%)
6	H	0.78	1/3942 (0.0%)	1.25	10/5326 (0.2%)
7	G	0.84	0/214	1.16	0/284
7	W	0.87	0/214	1.20	0/284
8	I	0.87	3/5827 (0.1%)	1.27	20/7899 (0.3%)
9	J	0.97	2/4146 (0.0%)	1.28	17/5616 (0.3%)
9	K	1.00	1/4086 (0.0%)	1.25	15/5534 (0.3%)
10	L	0.93	0/1468	1.26	7/1993 (0.4%)
11	M	0.79	0/502	1.25	0/680
12	N	0.77	2/4915 (0.0%)	1.32	33/6645 (0.5%)
13	O	0.84	2/5493 (0.0%)	1.31	22/7421 (0.3%)
14	R	0.75	2/2940 (0.1%)	0.96	2/3996 (0.1%)
15	S	0.83	0/71	1.22	0/95
16	X	0.77	1/3826 (0.0%)	1.24	6/5177 (0.1%)
16	Y	0.77	0/3919	1.25	10/5301 (0.2%)
All	All	0.84	18/66858 (0.0%)	1.27	241/90553 (0.3%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	261	ASP	N-CA	7.20	1.54	1.46
13	O	399	MET	C-O	-6.76	1.16	1.24
8	I	97	LYS	CA-C	-6.44	1.46	1.52
14	R	79	TYR	CA-C	6.29	1.61	1.52
3	P	41	GLY	C-O	-6.27	1.16	1.23
12	N	368	THR	CA-C	6.26	1.61	1.52
8	I	489	PRO	CA-C	5.85	1.57	1.52
12	N	709	PRO	CA-C	5.84	1.55	1.51
3	C	41	GLY	C-O	-5.72	1.17	1.23
13	O	268	PHE	CG-CD2	5.65	1.50	1.38
9	J	280	LYS	CA-C	-5.49	1.47	1.53
16	X	142	MET	CA-C	-5.49	1.45	1.52
9	K	280	LYS	CA-C	-5.45	1.47	1.53
6	H	20	ALA	CA-C	-5.42	1.46	1.53
3	C	115	TYR	C-O	-5.31	1.17	1.24
6	F	20	ALA	CA-C	-5.30	1.47	1.53
14	R	78	ARG	N-CA	5.27	1.52	1.45
8	I	187	LEU	CA-C	-5.12	1.46	1.52

All (241) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	489	PRO	N-CA-C	11.79	125.08	110.70
3	P	96	VAL	N-CA-C	10.14	120.97	110.72
3	C	96	VAL	N-CA-C	9.56	120.38	110.72
3	C	440	GLY	N-CA-C	-9.38	90.94	113.18
8	I	488	SER	CA-C-N	9.07	129.72	120.38
8	I	488	SER	C-N-CA	9.07	129.72	120.38
9	J	511	ASP	N-CA-C	8.85	120.93	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	63	ARG	CA-C-N	8.53	137.05	121.70
12	N	63	ARG	C-N-CA	8.53	137.05	121.70
8	I	223	VAL	CB-CA-C	-8.12	98.51	110.62
12	N	477	PRO	N-CA-CB	8.10	111.76	103.25
4	D	23	PRO	N-CA-CB	8.09	111.74	103.25
1	A	457	PHE	N-CA-C	7.86	120.47	110.33
12	N	125	TYR	CA-C-N	7.77	135.68	121.70
12	N	125	TYR	C-N-CA	7.77	135.68	121.70
12	N	219	PRO	N-CA-CB	7.76	111.39	103.25
13	O	461	ASN	N-CA-C	7.61	119.65	111.36
1	A	1925	PRO	N-CA-CB	7.47	110.43	103.41
1	A	1675	GLU	N-CA-C	7.39	121.79	108.48
10	L	171	PRO	N-CA-CB	7.37	110.70	102.60
12	N	395	ASP	N-CA-C	7.34	126.44	110.80
8	I	657	VAL	N-CA-C	7.29	120.05	112.83
12	N	637	TRP	N-CA-C	7.27	119.11	111.03
16	Y	199	CYS	N-CA-C	7.25	125.82	109.81
9	J	331	LYS	N-CA-C	-7.24	100.51	110.35
1	A	133	ILE	N-CA-C	7.21	116.70	106.53
12	N	63	ARG	N-CA-C	7.15	126.03	110.80
12	N	602	PRO	N-CA-C	7.15	119.42	110.70
9	J	211	LYS	N-CA-C	-7.14	99.41	109.69
3	C	150	ALA	N-CA-C	-7.10	104.88	113.97
3	C	54	TRP	CB-CA-C	-7.06	99.75	110.90
12	N	15	ARG	CA-C-N	7.04	128.64	119.84
12	N	15	ARG	C-N-CA	7.04	128.64	119.84
1	A	1519	VAL	N-CA-C	6.91	117.41	110.23
8	I	722	VAL	N-CA-C	6.88	118.39	108.48
12	N	16	PRO	N-CA-CB	6.88	110.48	103.25
13	O	429	TRP	CA-C-N	6.87	129.79	120.38
13	O	429	TRP	C-N-CA	6.87	129.79	120.38
9	K	365	LYS	N-CA-C	6.85	119.59	111.71
12	N	489	PRO	N-CA-CB	6.82	110.41	103.25
12	N	212	TYR	N-CA-C	6.82	121.89	113.50
12	N	197	PRO	N-CA-CB	6.77	110.36	103.25
1	A	1934	PRO	N-CA-CB	6.76	110.43	103.00
1	A	240	VAL	CA-C-N	6.72	133.80	121.70
1	A	240	VAL	C-N-CA	6.72	133.80	121.70
6	H	701	LYS	N-CA-C	6.67	120.52	112.38
8	I	728	ARG	N-CA-C	-6.66	99.97	109.96
6	F	768	PRO	N-CA-CB	6.63	110.21	103.25
1	A	248	PHE	N-CA-C	6.62	120.40	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	HIS	CA-C-N	6.59	128.08	119.84
1	A	31	HIS	C-N-CA	6.59	128.08	119.84
5	E	78	ARG	N-CA-C	6.54	118.10	110.97
10	L	27	SER	N-CA-C	6.51	118.03	111.07
1	A	651	PRO	N-CA-CB	6.50	110.00	102.33
10	L	130	LYS	CA-C-N	-6.49	111.72	119.84
10	L	130	LYS	C-N-CA	-6.49	111.72	119.84
1	A	759	ILE	N-CA-C	6.49	122.90	108.88
9	J	451	LEU	N-CA-CB	6.45	120.27	110.28
8	I	628	THR	N-CA-C	6.42	117.94	111.07
1	A	1141	VAL	CB-CA-C	-6.42	103.47	112.14
1	A	113	VAL	CB-CA-C	6.38	118.55	111.08
12	N	484	PRO	N-CA-CB	6.38	109.62	102.60
12	N	708	GLU	CA-C-N	6.38	124.32	119.66
12	N	708	GLU	C-N-CA	6.38	124.32	119.66
9	K	359	THR	N-CA-CB	6.35	119.45	110.12
1	A	44	PRO	CA-C-N	6.32	133.08	121.70
1	A	44	PRO	C-N-CA	6.32	133.08	121.70
2	B	66	ALA	N-CA-C	6.32	117.96	111.14
8	I	659	ARG	N-CA-C	6.29	124.21	110.80
9	K	270	VAL	CB-CA-C	-6.27	103.56	112.22
12	N	144	THR	N-CA-C	6.24	124.10	110.80
12	N	482	PRO	N-CA-CB	6.23	109.94	102.72
3	C	114	ALA	N-CA-C	-6.22	100.08	109.60
3	P	358	LEU	CA-CB-CG	6.19	137.98	116.30
6	F	533	VAL	N-CA-C	-6.13	107.16	113.10
9	K	300	VAL	N-CA-CB	6.08	118.80	110.54
9	J	270	VAL	CB-CA-C	-6.07	103.84	112.22
3	C	203	TRP	N-CA-C	6.05	117.88	111.28
6	H	533	VAL	N-CA-C	-6.04	107.24	113.10
12	N	368	THR	CB-CA-C	6.04	122.44	110.42
6	F	651	PHE	N-CA-C	6.03	117.53	111.07
3	C	468	MET	N-CA-C	6.02	119.46	111.75
12	N	512	LYS	N-CA-C	-5.99	107.20	114.75
1	A	1167	GLU	N-CA-C	-5.95	100.86	110.32
9	J	247	PHE	N-CA-C	5.94	118.54	111.71
6	H	651	PHE	N-CA-C	5.93	117.42	111.07
1	A	810	TYR	CA-C-N	5.93	127.25	119.84
1	A	810	TYR	C-N-CA	5.93	127.25	119.84
1	A	613	ALA	N-CA-C	5.92	120.25	112.13
3	P	40	ALA	CA-C-N	5.91	126.67	119.99
3	P	40	ALA	C-N-CA	5.91	126.67	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	424	GLN	CA-C-N	5.88	128.44	120.38
13	O	424	GLN	C-N-CA	5.88	128.44	120.38
1	A	1589	TYR	CA-C-N	5.86	126.00	119.32
1	A	1589	TYR	C-N-CA	5.86	126.00	119.32
13	O	267	VAL	N-CA-C	-5.82	104.66	111.00
12	N	355	ARG	CA-C-N	-5.80	113.77	120.04
12	N	355	ARG	C-N-CA	-5.80	113.77	120.04
8	I	566	THR	N-CA-C	-5.80	100.24	109.23
3	C	40	ALA	CA-C-N	5.79	126.54	119.99
3	C	40	ALA	C-N-CA	5.79	126.54	119.99
12	N	125	TYR	N-CA-C	5.78	117.45	111.03
9	J	186	GLU	CA-C-N	5.77	128.02	120.28
9	J	186	GLU	C-N-CA	5.77	128.02	120.28
3	P	361	ASN	N-CA-C	5.77	122.56	109.81
1	A	1670	GLY	C-N-CD	-5.76	107.92	120.60
1	A	1653	ALA	CA-C-N	-5.73	112.67	119.84
1	A	1653	ALA	C-N-CA	-5.73	112.67	119.84
13	O	384	LEU	CA-C-N	5.72	128.30	120.46
13	O	384	LEU	C-N-CA	5.72	128.30	120.46
9	J	485	ILE	N-CA-CB	5.71	118.31	110.54
10	L	12	ASP	CA-C-N	5.70	125.82	119.32
10	L	12	ASP	C-N-CA	5.70	125.82	119.32
8	I	150	SER	N-CA-C	-5.69	106.10	113.16
9	J	233	VAL	N-CA-CB	5.69	117.85	110.57
1	A	1230	ILE	N-CA-C	5.68	118.19	111.09
12	N	497	ARG	N-CA-C	5.67	122.87	110.80
1	A	158	CYS	N-CA-C	5.66	116.87	108.60
3	C	276	ILE	CB-CA-C	-5.65	104.42	112.22
1	A	1321	VAL	N-CA-CB	5.64	114.05	110.50
13	O	261	ASN	N-CA-C	5.63	117.42	111.28
16	Y	403	ALA	CA-C-N	-5.62	114.18	120.14
16	Y	403	ALA	C-N-CA	-5.62	114.18	120.14
16	Y	301	ASP	CA-C-N	5.61	125.98	119.47
16	Y	301	ASP	C-N-CA	5.61	125.98	119.47
1	A	1849	LYS	CA-C-N	5.61	127.73	120.44
1	A	1849	LYS	C-N-CA	5.61	127.73	120.44
1	A	1518	VAL	N-CA-C	5.60	117.11	111.00
13	O	448	MET	N-CA-C	5.60	118.11	110.55
3	C	301	ASP	N-CA-CB	5.60	118.13	110.01
9	K	247	PHE	N-CA-C	5.59	118.14	111.71
1	A	221	THR	CA-C-N	-5.59	114.81	120.85
1	A	221	THR	C-N-CA	-5.59	114.81	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	N	256	VAL	N-CA-C	5.56	115.76	110.42
6	F	725	GLU	N-CA-C	5.56	117.42	111.36
12	N	322	ARG	N-CA-C	-5.55	106.36	113.02
13	O	442	ALA	N-CA-C	-5.55	104.45	111.11
9	J	69	TYR	N-CA-C	5.54	120.30	112.93
14	R	111	GLU	N-CA-C	5.54	118.25	111.82
9	J	254	THR	CB-CA-C	5.54	119.98	110.79
1	A	78	LYS	N-CA-C	-5.53	101.86	110.10
13	O	329	ARG	N-CA-C	5.52	116.98	111.07
8	I	721	TYR	N-CA-C	5.52	118.22	109.50
1	A	949	PHE	N-CA-C	5.52	118.00	111.33
1	A	1844	PHE	N-CA-C	-5.51	106.23	113.12
9	K	62	SER	N-CA-C	-5.50	102.74	110.50
9	K	369	LEU	CA-C-N	-5.50	112.94	119.05
9	K	369	LEU	C-N-CA	-5.50	112.94	119.05
6	H	491	LEU	CA-C-N	5.50	126.71	119.84
6	H	491	LEU	C-N-CA	5.50	126.71	119.84
6	H	725	GLU	N-CA-C	5.50	117.35	111.36
3	C	361	ASN	N-CA-C	5.48	121.92	109.81
3	P	203	TRP	N-CA-C	5.48	117.25	111.28
16	Y	37	VAL	CB-CA-C	-5.47	104.75	112.14
1	A	264	ASN	CA-C-N	5.46	131.53	121.70
1	A	264	ASN	C-N-CA	5.46	131.53	121.70
12	N	635	LEU	N-CA-C	5.46	119.14	109.96
1	A	240	VAL	CB-CA-C	5.46	120.24	111.29
3	C	68	ALA	N-CA-C	5.45	116.91	110.97
1	A	1420	LEU	CA-C-N	5.43	125.10	119.56
1	A	1420	LEU	C-N-CA	5.43	125.10	119.56
13	O	409	HIS	CB-CA-C	-5.43	102.36	110.88
3	C	275	ASN	CA-C-N	5.42	128.11	120.42
3	C	275	ASN	C-N-CA	5.42	128.11	120.42
12	N	284	SER	N-CA-C	5.41	118.32	110.42
16	X	158	ILE	CB-CA-C	-5.41	104.84	112.14
8	I	391	THR	N-CA-C	-5.40	105.30	111.07
1	A	1512	LEU	N-CA-C	5.39	117.23	111.36
9	J	136	ARG	N-CA-C	-5.39	104.65	111.11
13	O	559	GLU	N-CA-C	-5.39	105.41	111.28
6	F	729	LEU	CA-C-N	5.38	127.81	120.54
6	F	729	LEU	C-N-CA	5.38	127.81	120.54
13	O	428	ILE	N-CA-C	5.38	115.82	110.23
1	A	1628	THR	CA-C-N	-5.38	114.18	119.99
1	A	1628	THR	C-N-CA	-5.38	114.18	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	137	SER	N-CA-C	5.37	117.66	110.35
6	F	494	HIS	N-CA-C	-5.36	105.55	111.71
6	F	491	LEU	CA-C-N	5.35	126.52	119.84
6	F	491	LEU	C-N-CA	5.35	126.52	119.84
8	I	663	ASP	N-CA-C	5.33	119.89	113.17
8	I	209	CYS	CA-C-N	-5.33	115.65	123.00
8	I	209	CYS	C-N-CA	-5.33	115.65	123.00
6	F	23	ASP	CB-CA-C	-5.32	102.53	110.88
8	I	373	LYS	N-CA-C	5.31	116.88	111.14
1	A	1851	THR	CA-C-N	5.30	127.72	120.77
1	A	1851	THR	C-N-CA	5.30	127.72	120.77
9	K	136	ARG	N-CA-C	-5.30	104.75	111.11
3	P	365	LEU	N-CA-C	5.29	122.07	110.80
16	X	97	VAL	O-C-N	5.29	127.23	121.94
16	Y	97	VAL	O-C-N	5.29	127.23	121.94
13	O	385	VAL	N-CA-C	5.29	116.02	110.62
1	A	173	LEU	N-CA-C	5.28	117.60	110.31
1	A	1739	SER	CA-C-N	5.27	131.19	121.70
1	A	1739	SER	C-N-CA	5.27	131.19	121.70
16	Y	158	ILE	CB-CA-C	-5.26	105.03	112.14
6	F	133	LYS	CA-C-N	5.26	125.67	119.94
6	F	133	LYS	C-N-CA	5.26	125.67	119.94
9	K	223	SER	N-CA-C	-5.25	105.67	111.71
9	J	305	VAL	O-C-N	5.25	126.96	121.87
1	A	1235	LEU	CA-CB-CG	5.24	134.65	116.30
16	X	311	TYR	N-CA-C	5.24	117.73	111.71
8	I	191	GLY	N-CA-C	-5.22	108.41	115.36
13	O	437	MET	N-CA-C	5.22	116.97	111.28
10	L	124	LEU	N-CA-C	5.21	117.73	109.24
12	N	368	THR	CA-C-N	5.20	131.06	121.70
12	N	368	THR	C-N-CA	5.20	131.06	121.70
9	K	292	VAL	N-CA-CB	5.20	118.38	110.58
9	K	188	LEU	N-CA-CB	5.19	118.22	110.02
13	O	594	SER	N-CA-C	5.19	119.24	113.01
1	A	1206	ILE	N-CA-C	5.18	115.40	110.53
14	R	115	ALA	N-CA-C	-5.18	105.53	111.07
16	X	37	VAL	CB-CA-C	-5.18	105.15	112.14
13	O	362	GLU	CA-C-N	5.17	127.17	120.44
13	O	362	GLU	C-N-CA	5.17	127.17	120.44
1	A	1237	PRO	CA-C-N	-5.16	113.39	119.84
1	A	1237	PRO	C-N-CA	-5.16	113.39	119.84
1	A	1742	THR	N-CA-C	5.15	117.51	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	VAL	N-CA-C	5.15	120.05	109.34
1	A	1034	VAL	N-CA-C	5.15	117.53	111.09
1	A	57	LEU	N-CA-C	5.14	116.12	108.31
8	I	224	SER	N-CA-C	5.14	116.10	108.60
9	J	240	ARG	CA-C-O	-5.14	115.43	120.82
16	X	287	ASN	N-CA-C	5.14	116.56	111.07
6	H	733	VAL	CA-C-N	5.13	124.75	119.05
6	H	733	VAL	C-N-CA	5.13	124.75	119.05
9	K	214	LYS	CA-C-N	5.13	126.25	119.84
9	K	214	LYS	C-N-CA	5.13	126.25	119.84
16	X	349	SER	N-CA-C	5.12	116.94	111.36
9	J	297	SER	N-CA-C	5.11	116.93	111.36
9	K	270	VAL	CA-C-O	-5.10	115.44	120.85
9	J	359	THR	N-CA-CB	5.09	117.61	110.12
13	O	345	SER	CA-C-N	5.08	127.51	120.29
13	O	345	SER	C-N-CA	5.08	127.51	120.29
6	F	554	VAL	N-CA-CB	5.05	116.12	110.51
1	A	857	MET	CA-C-N	-5.05	115.18	120.38
1	A	857	MET	C-N-CA	-5.05	115.18	120.38
16	Y	311	TYR	N-CA-C	5.02	117.49	111.71
8	I	194	LYS	N-CA-C	5.02	116.82	107.99
6	H	164	PRO	CA-C-N	5.02	127.50	120.28
6	H	164	PRO	C-N-CA	5.02	127.50	120.28
16	Y	349	SER	N-CA-C	5.01	116.83	111.36

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

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Mol	Chain	Res	Type	Group
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	488	0
2	B	649	0	595	28	0
3	C	4306	0	4273	285	0
3	P	4039	0	3989	124	0
4	D	436	0	396	28	0
5	E	450	0	435	13	0
6	F	3923	0	3819	118	0
6	H	3853	0	3793	114	0
7	G	213	0	220	17	0
7	W	213	0	220	9	0
8	I	5709	0	5597	199	0
9	J	4047	0	3949	189	0
9	K	3988	0	3908	155	0
10	L	1435	0	1382	44	0
11	M	493	0	469	17	0
12	N	4837	0	4534	165	0
13	O	5395	0	5429	240	0
14	R	2869	0	2772	58	0
15	S	72	0	71	10	0
16	X	3767	0	3819	140	0
16	Y	3859	0	3908	155	0
17	B	3	0	0	0	0
All	All	65481	0	64247	2299	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 18.

All (2299) 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
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
14:R:177:ASP:CG	15:S:834:ILE:HD11	1.64	1.22
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
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
6:H:479:TYR:C	6:H:480:ASN:N	2.09	1.10
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
16:X:235:TRP:NE1	16:Y:63:MET:HE1	1.70	1.07
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
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
14:R:177:ASP:CG	15:S:834:ILE:CD1	2.33	1.02
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
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
16:X:235:TRP:HE1	16:Y:63:MET:HE1	1.20	0.99
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
9:J:354:MET:HE3	9:J:354:MET:HA	1.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:55:MET:SD	13:O:58:ARG:NH1	2.46	0.89
16:X:235:TRP:CD1	16:Y:63:MET:HE1	2.07	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
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
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
8:I:195:ILE:HD11	8:I:251:MET:HE3	1.60	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
3:C:234:LEU:HB3	3:C:250:LYS:HZ1	1.45	0.82
9:J:441:VAL:HG21	9:J:444:TRP:HD1	1.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:K:276:VAL:HA	9:K:311:MET:HE2	1.62	0.81
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
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
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
3:P:310:ARG:HB3	3:P:312:MET:HE2	1.62	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
10:L:105:LEU:HD11	10:L:136:MET:HE2	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
9:J:495:PHE:HD2	9:J:522:CYS:HG	1.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:625:ILE:HG21	1:A:637:MET:HE3	1.69	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
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:HA	9:J:354:MET:CE	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
12:N:560:MET:HE2	12:N:560:MET:HA	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:213:MET:HE2	1:A:216:PRO:HA	1.70	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
8:I:231:VAL:HG21	8:I:557:TYR:CZ	2.25	0.71
1:A:213:MET:HE3	1:A:220:ILE:HG22	1.72	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
3:C:413:LYS:C	3:C:415:PRO:HD2	2.16	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
1:A:1790:TYR:HE1	1:A:1840:MET:HE3	1.57	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
1:A:1610:TYR:CD1	1:A:1610:TYR:C	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:N:516:ILE:HG13	12:N:554:MET:HE3	1.72	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
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
16:X:235:TRP:CD1	16:Y:63:MET:HE3	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:234:LEU:HB3	3:C:250:LYS:NZ	2.06	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
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:1238:PRO:HA	1:A:1239:THR:C	2.21	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
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
9:K:174:HIS:HA	9:K:211:LYS:HZ3	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:J:354:MET:HE1	9:J:374:ILE:HA	1.79	0.65
1:A:1307:LEU:HD21	1:A:1579:SER:HA	1.79	0.64
1:A:1790:TYR:CE1	1:A:1840:MET:HE3	2.32	0.64
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
3:C:526:TRP:HE1	3:C:553:ILE:C	2.04	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:656:MET:HE2	9:K:523:ILE:HD13	1.79	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
7:G:23:ARG:HG2	9:J:525:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:M:2:ASP:CG	11:M:3:SER:H	2.06	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
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:J:35:GLU:CD	9:J:63:ARG:HE	2.06	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:93:TYR:HD1	3:C:98:GLU:CD	2.07	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
16:X:363:ALA:HB2	16:X:379:LYS:HZ2	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:H:145:ASN:HB2	6:H:146:PRO:C	2.25	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:F:656:MET:HE2	16:Y:526:GLN:H	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
1:A:1739:SER:HA	1:A:1740:ALA:CB	2.27	0.62
6:F:145:ASN:HB2	6:F:146:PRO:C	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1519:VAL:HG13	1:A:1520:LEU:N	2.15	0.61
3:C:416:PHE:H	13:O:326:GLU:CD	2.07	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
3:C:39:ILE:HG21	3:C:201:LEU:HG	1.80	0.61
3:C:93:TYR:CD1	3:C:98:GLU:CD	2.78	0.61
5:E:94:TRP:HZ3	6:F:564:LYS:HD2	1.65	0.61
8:I:11:PHE:CE1	8:I:746:MET:HE2	2.36	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
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: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
9:J:20:GLN:HB2	9:K:165:GLU:CD	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:I:364:SER:O	8:I:367:LYS:HB3	2.01	0.60
16:X:235:TRP:HD1	16:Y:63:MET:HE3	1.64	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
9:K:284:LEU:HD12	9:K:311:MET:HE3	1.84	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:I:27:VAL:C	8:I:35:ILE:HD12	2.28	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
1:A:1028:TRP:CD1	1:A:1033:ARG:HH11	2.21	0.58
6:F:130:ARG:CG	16:Y:506:GLN:HE21	2.16	0.58
8:I:618:ILE:HD12	8:I:705:MET:HE2	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
1:A:31:HIS:HB3	1:A:99:MET:HE2	1.86	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
12:N:333:TYR:HD1	12:N:364:CYS:HG	1.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1134:TRP:CE2	1:A:1203:MET:HE1	2.38	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
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
13:O:351:GLY:C	13:O:353:LYS:H	2.12	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:HD22	1:A:48:LEU:C	2.27	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
14:R:91:ALA:O	14:R:92:SER:C	2.46	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:560:MET:HE1	12:N:601:TRP:CD1	2.39	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:X:40:HIS:HB3	16:Y:201:LEU:HD13	1.87	0.56
16:X:203:LEU:HD23	16:X:203:LEU:C	2.30	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
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
1:A:1177:MET:HB2	1:A:1207:GLY:C	2.31	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
3:C:235:ALA:N	3:C:250:LYS:HZ2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
16:Y:294:PHE:CD1	16:Y:294:PHE:C	2.85	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:113:ASP:CG	3:P:344:ARG:HH22	2.12	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
3:P:348:GLU:HA	3:P:378:MET:HE1	1.87	0.55
1:A:663:CYS:O	1:A:667:MET:HE2	2.07	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:185:LEU:HD13	9:J:206:GLU:OE1	2.08	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
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:114:ASP:C	13:O:117:ASP:OD1	2.50	0.54
12:N:76:VAL:C	12:N:78:VAL:H	2.15	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
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
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
16:Y:298:GLN:HG3	16:Y:308:MET:HE1	1.90	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
3:P:332:GLU:O	3:P:333:THR:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:I:669:LEU:CD1	8:I:705:MET:HE1	2.38	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
3:C:206:TRP:CE3	3:C:233:PHE:CG	2.96	0.53
12:N:560:MET:HE3	12:N:600:PHE:HB2	1.90	0.53
13:O:236:LEU:HD23	13:O:260:ASN:HB2	1.90	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:332:GLU:O	3:C:333:THR:C	2.50	0.53
6:H:168:PHE:CB	6:H:467:ARG:HD3	2.38	0.53
10:L:63:LEU:HD22	10:L:138:GLN:NE2	2.24	0.53
11:M:19:TRP:CD1	11:M:19:TRP:C	2.87	0.53
16:X:76:LYS:CB	16:X:106:GLN:NE2	2.72	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
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
9:K:46:CYS:O	9:K:50:THR:OG1	2.23	0.52
1:A:1329:MET:HE2	1:A:1368:THR:HG22	1.90	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
16:X:63:MET:HE3	16:Y:266:LEU:HD13	1.92	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
8:I:248:VAL:HA	8:I:251:MET:HE2	1.92	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
16:X:298:GLN:HG3	16:X:308:MET:HE1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:303:PHE:HD1	3:C:303:PHE:C	2.18	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
8:I:44:VAL:C	8:I:45:LEU:HD12	2.35	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
3:C:98:GLU:CD	3:C:101:ARG:HB3	2.29	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
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
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
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
1:A:246:ILE:HD11	1:A:249:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASP:HB3	1:A:253:PRO:CD	2.34	0.52
3:C:114:ALA:C	3:C:116:PHE:N	2.68	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:33:ASN:HA	1:A:99:MET:HE1	1.93	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
8:I:116:MET:HE1	8:I:211:SER:O	2.11	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
16:X:294:PHE:C	16:X:294:PHE:CD1	2.88	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:136:LEU:C	13:O:136:LEU:HD12	2.36	0.51
13:O:146:LEU:HB2	13:O:151:VAL:CG2	2.40	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:354:MET:CE	9:J:374:ILE:HA	2.40	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
16:X:423:ILE:HG13	16:X:424:ARG:N	2.23	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
3:C:303:PHE:C	3:C:303:PHE:CD1	2.88	0.51
8:I:224:SER:HB3	8:I:229:SER:HA	1.90	0.51
8:I:372:TRP:CZ3	13:O:664:MET:HE1	2.46	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
1:A:1786:MET:HE2	1:A:1786:MET:HA	1.93	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
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:454:VAL:C	9:J:458:LEU:HD12	2.31	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
3:C:203:TRP:HA	3:C:229:MET:HE1	1.94	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:513:THR:O	9:K:517:THR:HG22	2.11	0.50
12:N:212:TYR:C	12:N:215:LEU:HB2	2.37	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
12:N:268:VAL:HA	12:N:271:GLU:CD	2.36	0.50
13:O:68:LEU:HD23	13:O:131:VAL:HG12	1.92	0.50
13:O:99:LEU:C	13:O:99:LEU:HD12	2.36	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
8:I:17:LYS:NZ	8:I:51:SER:O	2.44	0.50
1:A:33:ASN:HA	1:A:99:MET:CE	2.42	0.50
1:A:942:ARG:HD3	13:O:603:MET:HE1	1.94	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
9:J:397:ILE:O	9:J:398:ALA:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
3:C:285:ILE:HA	3:C:288:GLU:CD	2.37	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
8:I:195:ILE:HD11	8:I:251:MET:CE	2.37	0.49
9:J:245:CYS:SG	9:J:443:LYS:HD3	2.52	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
3:C:348:GLU:HA	3:C:378:MET:HE3	1.94	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
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:149:LEU:O	16:Y:150:LYS:HB2	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:I:399:LYS:HE3	8:I:478:TYR:HE1	1.77	0.49
9:K:509:ARG:HG3	9:K:509:ARG:O	2.11	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:91:GLU:CD	1:A:102:TRP:HE1	2.20	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
12:N:411:ASP:O	12:N:412:PRO:C	2.56	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
6:F:537:GLU:HG3	6:F:538:ILE:N	2.27	0.48
6:H:656:MET:HE3	6:H:660:LYS:HE2	1.95	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
4:D:45:ALA:HA	3:P:378:MET:HE2	1.95	0.48
5:E:60:SER:O	5:E:63:VAL:HG12	2.13	0.48
8:I:70:CYS:C	8:I:71:LEU:HD12	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:354:MET:HE2	9:J:374:ILE:HG23	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1405:LEU:C	1:A:1405:LEU:HD12	2.38	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:F:150:SER:N	6:F:151:PRO:HD2	2.29	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
8:I:669:LEU:HD11	8:I:705:MET:HE1	1.96	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
6:H:758:MET:HE1	16:X:429:MET:HG2	1.97	0.47
9:J:212:TYR:HB3	9:J:243:TYR:CD1	2.50	0.47
11:M:32:PRO:C	11:M:34:ASN:H	2.22	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
14:R:177:ASP:CG	15:S:834:ILE:HD12	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:I:202:ALA:C	8:I:223:VAL:HG22	2.39	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
12:N:554:MET:HE2	12:N:554:MET:HA	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
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
3:C:403:TYR:CD1	3:C:403:TYR:C	2.93	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
16:Y:294:PHE:C	16:Y:294:PHE:HD1	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:K:487:TYR:CE1	9:K:518:MET:HE3	2.50	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
3:C:493:TYR:CZ	3:C:497:ILE:HD11	2.50	0.46
7:G:3:ARG:HB2	9:J:443:LYS:HZ3	1.80	0.46
8:I:72:ALA:C	8:I:80:LEU:HD12	2.40	0.46
9:J:320:ARG:HB3	9:J:340:TYR:CE1	2.51	0.46
12:N:213:TYR:C	12:N:214:ARG:HA	2.40	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: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:1198:THR:C	1:A:1200:GLY:N	2.73	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:178:ALA:HA	9:K:181:GLU:CD	2.40	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
3:C:413:LYS:C	3:C:415:PRO:CD	2.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:598:GLU:HB2	1:A:604:MET:HE2	1.97	0.46
6:F:145:ASN:HB2	6:F:146:PRO:O	2.16	0.46
6:H:515:TYR:HB2	10:L:179:MET:HE3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
9:J:481:THR:O	9:J:485:ILE:HG12	2.16	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
2:B:5:ILE:HG12	12:N:646:MET:HE3	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:289:HIS:CD2	9:J:289:HIS:C	2.93	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:F:699:ASP:HB3	6:F:702:ASN:OD1	2.16	0.45
6:H:658:PHE:HB3	6:H:675:ILE:HG12	1.98	0.45
9:J:354:MET:HE1	9:J:377:GLU:HB2	1.97	0.45
12:N:542:VAL:HG11	12:N:558:GLU:CG	2.46	0.45
3:P:376:MET:HE1	3:P:408:THR:HA	1.98	0.45
16:Y:42:ARG:HG3	16:Y:82:TYR:HH	1.75	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
3:P:170:PHE:O	3:P:171:GLY:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:F:33:ALA:HB2	6:H:498:THR:HG21	1.99	0.45
6:F:55:TYR:CE2	6:H:562:MET:HE3	2.52	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
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
3:C:425:ALA:HB3	3:C:435:MET:HE2	1.98	0.45
3:C:435:MET:HA	3:C:435:MET:HE3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:11:PHE:CD1	8:I:746:MET:HE2	2.51	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
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
3:C:95:ASP:C	3:C:97:LYS:HG2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:I:578:ASN:C	8:I:578:ASN:OD1	2.59	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
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
6:F:537:GLU:CD	6:F:600:TYR:OH	2.60	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:231:VAL:HG12	8:I:232:SER:N	2.33	0.44
9:K:210:LYS:C	9:K:212:TYR:H	2.21	0.44
12:N:284:SER:HA	12:N:285:PHE:CG	2.53	0.44
12:N:531:PHE:C	12:N:533:PHE:HA	2.42	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:113:LYS:C	3:C:114:ALA:O	2.60	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
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
3:C:170:PHE:O	3:C:171:GLY:C	2.59	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:O	9:J:475:ILE:HG13	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
1:A:1391:ASP:CG	1:A:1431:PRO:HB3	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:397:ARG:C	3:C:428:LEU:HD21	2.43	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
12:N:180:PHE:CD1	12:N:180:PHE:C	2.97	0.43
12:N:560:MET:HA	12:N:560:MET:CE	2.44	0.43
16:X:52:ASN:CG	16:Y:204:ASP:HB2	2.44	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
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
9:K:487:TYR:HE1	9:K:518:MET:HE3	1.83	0.43
10:L:61:PRO:HB3	10:L:142:LEU:HA	2.00	0.43
12:N:560:MET:HE3	12:N:600:PHE:CB	2.48	0.43
12:N:693:ARG:HA	12:N:696:MET:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1329:MET:HE1	1:A:1371:LEU:HD12	2.01	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
8:I:526:LYS:HA	8:I:529:MET:HE2	2.00	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
16:Y:200:PRO:C	16:Y:202:ALA:H	2.21	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: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
13:O:646:MET:HA	13:O:646:MET:HE3	1.99	0.43
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:537:GLU:CD	6:H:600:TYR:OH	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
9:J:320:ARG:HG2	9:J:340:TYR:CE1	2.54	0.42
12:N:331:PHE:O	12:N:332:PHE:C	2.62	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
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
8:I:669:LEU:HD13	8:I:705:MET:HE1	2.01	0.42
9:J:214:LYS:HE2	9:J:216:SER:OG	2.20	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:44:MET:HE2	13:O:60:LEU:CD2	2.49	0.42
13:O:322:LEU:O	13:O:325:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:405:MET:HE1	9:J:431:LYS:HG3	2.01	0.42
12:N:212:TYR:C	12:N:215:LEU:H	2.27	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:667:MET:O	1:A:755:LEU:C	2.62	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:61:TYR:CD1	5:E:61:TYR:C	2.97	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:1611:VAL:CG1	1:A:1612:LEU:HD12	2.50	0.42
3:C:153:GLU:O	3:C:157:GLU:CD	2.63	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
9:K:24:PHE:CD1	9:K:24:PHE:C	2.97	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:110:LYS:HZ1	14:R:114:LYS:HG3	1.85	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
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
8:I:272:MET:HE3	8:I:479:LEU:HD21	2.02	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:347:ILE:HG21	12:N:358:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:X:204:ASP:HB2	16:Y:52:ASN:CG	2.45	0.42
16:Y:42:ARG:HA	16:Y:82:TYR:OH	2.17	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:102:SER:OG	6:H:104:ASP:OD1	2.30	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:HD1	16:Y:294:PHE:O	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:558:SER:O	13:O:559:GLU:C	2.63	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:O:344:LEU:O	13:O:345:SER:C	2.63	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:1373:MET:HE1	1:A:1582:ALA:HA	2.01	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: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
3:C:235:ALA:H	3:C:250:LYS:HZ2	1.67	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:143:TYR:CD1	13:O:143:TYR:C	2.99	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:591:VAL:O	1:A:592:HIS:C	2.63	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
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
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
8:I:251:MET:CE	8:I:379:LEU:HD13	2.51	0.41
9:J:475:ILE:HA	9:J:476:PRO:HD3	1.88	0.41
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
3:P:293:ASP:CG	3:P:296:ARG:HB2	2.46	0.41
16:Y:186:ARG:HA	16:Y:189:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1209:LEU:HD23	1:A:1209:LEU:HA	1.85	0.41
1:A:1216:LYS:O	1:A:1217:LEU:C	2.64	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:150:SER:OG	8:I:153:SER:O	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:44:MET:HE2	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
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:1253:ALA:O	1:A:1254:VAL:C	2.61	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:656:MET:HE3	9:K:526:TYR:CD2	2.56	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
1:A:780:GLY:C	1:A:782:GLY:H	2.30	0.40
3:C:306:LEU:HD12	3:C:306:LEU:C	2.46	0.40
3:C:397:ARG:O	3:C:428:LEU:HD21	2.21	0.40
6:F:580:GLN:C	6:F:582:GLU:H	2.29	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
13:O:539:ASN:ND2	13:O:542:GLU:HB2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:649:GLU:HB3	13:O:650:PRO:HD3	2.02	0.40
3:P:297:ILE:HD11	3:P:333:THR:HB	2.03	0.40
3:P:321:HIS:CD2	3:P:321:HIS:C	2.98	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:628:ILE:HG22	1:A:629:LEU:N	2.36	0.40
1:A:657:TRP:HA	1:A:660:PHE:HB3	2.02	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: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:237:GLU:CD	8:I:607:ILE:HD13	2.47	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
9:J:17:GLN:C	9:K:78:ARG:HH12	2.28	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
3:P:267:SER:OG	3:P:299:ASN:CG	2.64	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
16:Y:417:TYR:CD1	16:Y:429:MET:HE1	2.56	0.40
1:A:119:VAL:C	1:A:121:SER:H	2.29	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:1611:VAL:HG13	1:A:1612:LEU:N	2.36	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
13:O:351:GLY:C	13:O:353:LYS:N	2.79	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:183:THR:C	1:A:184:LYS:O	2.62	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
2:B:68:GLN:HA	2:B:69:VAL:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	2	20
2	B	83/84 (99%)	72 (87%)	7 (8%)	4 (5%)	2	18
3	C	520/597 (87%)	489 (94%)	23 (4%)	8 (2%)	8	37
3	P	485/597 (81%)	460 (95%)	20 (4%)	5 (1%)	12	45
4	D	53/121 (44%)	45 (85%)	7 (13%)	1 (2%)	6	33
5	E	54/110 (49%)	54 (100%)	0	0	100	100
6	F	494/824 (60%)	461 (93%)	25 (5%)	8 (2%)	7	36
6	H	477/824 (58%)	448 (94%)	22 (5%)	7 (2%)	8	37
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%)	18	53
9	J	500/620 (81%)	467 (93%)	29 (6%)	4 (1%)	16	50
9	K	489/620 (79%)	459 (94%)	24 (5%)	6 (1%)	10	41
10	L	180/184 (98%)	165 (92%)	11 (6%)	4 (2%)	5	31
11	M	55/74 (74%)	42 (76%)	10 (18%)	3 (6%)	1	17
12	N	601/822 (73%)	497 (83%)	58 (10%)	46 (8%)	1	12
13	O	677/755 (90%)	619 (91%)	46 (7%)	12 (2%)	6	34
14	R	361/499 (72%)	338 (94%)	20 (6%)	3 (1%)	16	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	S	8/206 (4%)	6 (75%)	0	2 (25%)	0	1
16	X	478/599 (80%)	463 (97%)	12 (2%)	3 (1%)	21	55
16	Y	492/599 (82%)	474 (96%)	14 (3%)	4 (1%)	16	50
All	All	8168/11057 (74%)	7474 (92%)	511 (6%)	183 (2%)	7	31

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	941 (82%)	209 (18%)	2	11
2	B	65/75 (87%)	51 (78%)	14 (22%)	1	6
3	C	452/520 (87%)	357 (79%)	95 (21%)	1	7
3	P	421/520 (81%)	357 (85%)	64 (15%)	3	16
4	D	46/115 (40%)	37 (80%)	9 (20%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	47/89 (53%)	36 (77%)	11 (23%)	1	5
6	F	407/727 (56%)	366 (90%)	41 (10%)	7	27
6	H	408/727 (56%)	371 (91%)	37 (9%)	9	31
7	G	23/77 (30%)	20 (87%)	3 (13%)	4	19
7	W	23/77 (30%)	21 (91%)	2 (9%)	9	33
8	I	620/730 (85%)	573 (92%)	47 (8%)	12	37
9	J	424/548 (77%)	371 (88%)	53 (12%)	4	20
9	K	423/548 (77%)	370 (88%)	53 (12%)	4	20
10	L	155/169 (92%)	132 (85%)	23 (15%)	3	16
11	M	55/67 (82%)	45 (82%)	10 (18%)	2	11
12	N	460/724 (64%)	402 (87%)	58 (13%)	4	20
13	O	576/650 (89%)	465 (81%)	111 (19%)	1	9
14	R	304/411 (74%)	291 (96%)	13 (4%)	26	49
15	S	8/195 (4%)	7 (88%)	1 (12%)	4	20
16	X	406/513 (79%)	366 (90%)	40 (10%)	7	28
16	Y	416/513 (81%)	372 (89%)	44 (11%)	6	25
All	All	6889/9715 (71%)	5951 (86%)	938 (14%)	6	18

All (938) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
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	76	LEU
1	A	80	VAL
1	A	90	ASP

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Mol	Chain	Res	Type
1	A	103	SER
1	A	118	THR
1	A	124	GLN
1	A	129	CYS
1	A	132	ILE
1	A	133	ILE
1	A	149	LYS
1	A	151	ILE
1	A	153	ILE
1	A	167	LYS
1	A	168	ASP
1	A	170	ILE
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	244	MET
1	A	249	LEU
1	A	252	ASP
1	A	269	TRP
1	A	271	LEU
1	A	403	ILE
1	A	407	LEU
1	A	409	ILE
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

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Mol	Chain	Res	Type
1	A	453	ARG
1	A	456	LYS
1	A	467	ILE
1	A	482	VAL
1	A	483	GLU
1	A	490	VAL
1	A	497	LEU
1	A	584	ILE
1	A	595	VAL
1	A	609	ILE
1	A	611	GLU
1	A	616	GLU
1	A	617	LEU
1	A	628	ILE
1	A	636	GLN
1	A	637	MET
1	A	638	LEU
1	A	640	LYS
1	A	655	SER
1	A	659	LEU
1	A	663	CYS
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	793	LEU
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	1026	LEU

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Mol	Chain	Res	Type
1	A	1047	VAL
1	A	1075	GLN
1	A	1088	THR
1	A	1095	VAL
1	A	1100	LEU
1	A	1107	LEU
1	A	1118	VAL
1	A	1131	MET
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	1181	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	1227	LEU
1	A	1230	ILE
1	A	1232	ILE
1	A	1235	LEU
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	1314	ILE
1	A	1319	LEU
1	A	1323	GLU
1	A	1325	LEU
1	A	1329	MET

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Mol	Chain	Res	Type
1	A	1330	VAL
1	A	1352	ILE
1	A	1359	ASN
1	A	1373	MET
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	1417	ASP
1	A	1426	VAL
1	A	1433	ILE
1	A	1470	LEU
1	A	1482	LEU
1	A	1518	VAL
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	1556	LEU
1	A	1562	LEU
1	A	1564	LEU
1	A	1573	SER
1	A	1574	LEU
1	A	1588	LEU
1	A	1597	THR
1	A	1603	LEU
1	A	1607	ARG
1	A	1609	LEU
1	A	1611	VAL
1	A	1619	LEU
1	A	1620	VAL
1	A	1633	LEU
1	A	1638	TYR
1	A	1642	GLN
1	A	1646	GLN
1	A	1649	GLU
1	A	1651	LEU

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Mol	Chain	Res	Type
1	A	1652	MET
1	A	1660	LEU
1	A	1666	ILE
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	1744	ASP
1	A	1749	SER
1	A	1755	CYS
1	A	1756	LYS
1	A	1770	LEU
1	A	1781	GLN
1	A	1798	ARG
1	A	1805	MET
1	A	1810	GLU
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	3	VAL
2	B	11	VAL
2	B	14	TRP
2	B	15	LEU
2	B	16	TRP
2	B	17	VAL
2	B	28	MET
2	B	34	CYS
2	B	36	ASP
2	B	43	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

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Mol	Chain	Res	Type
3	C	37	LEU
3	C	38	LEU
3	C	39	ILE
3	C	46	ARG
3	C	48	LEU
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	89	LEU
3	C	91	LYS
3	C	97	LYS
3	C	98	GLU
3	C	101	ARG
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	147	LYS
3	C	152	ARG
3	C	157	GLU
3	C	172	LEU
3	C	179	LEU
3	C	182	LEU
3	C	183	ASP
3	C	187	GLU
3	C	201	LEU
3	C	203	TRP
3	C	216	LYS
3	C	243	LEU
3	C	244	ILE
3	C	254	LEU

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Mol	Chain	Res	Type
3	C	265	ILE
3	C	285	ILE
3	C	288	GLU
3	C	291	LYS
3	C	296	ARG
3	C	297	ILE
3	C	298	GLU
3	C	300	MET
3	C	302	THR
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	331	VAL
3	C	335	CYS
3	C	337	ILE
3	C	343	LEU
3	C	344	ARG
3	C	346	GLN
3	C	348	GLU
3	C	352	LEU
3	C	358	LEU
3	C	359	LYS
3	C	360	LEU
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	419	LEU
3	C	424	ARG
3	C	428	LEU
3	C	429	ARG
3	C	451	GLU
3	C	455	CYS
3	C	458	ARG
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	527	ASP
3	C	535	LYS
3	C	547	LYS
3	C	556	LEU
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	81	LYS
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	465	LEU
6	F	466	LEU

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Mol	Chain	Res	Type
6	F	474	LEU
6	F	477	CYS
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	599	ASN
6	F	614	THR
6	F	616	GLU
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	733	VAL
6	F	742	LEU
7	G	4	ARG
7	G	5	LYS
7	G	22	ILE
6	H	27	LEU
6	H	61	LEU
6	H	62	LYS
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	153	GLU
6	H	465	LEU

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Mol	Chain	Res	Type
6	H	466	LEU
6	H	474	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
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	655	GLU
6	H	667	GLN
6	H	677	VAL
6	H	694	LYS
6	H	702	ASN
6	H	720	LYS
6	H	729	LEU
6	H	733	VAL
6	H	742	LEU
6	H	758	MET
6	H	762	TRP
8	I	26	LEU
8	I	34	LEU
8	I	35	ILE
8	I	37	LEU
8	I	71	LEU
8	I	89	LYS
8	I	92	LEU
8	I	101	LEU
8	I	110	VAL
8	I	162	ASP
8	I	176	LEU
8	I	210	LEU
8	I	218	SER
8	I	224	SER
8	I	232	SER
8	I	266	ASN

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Mol	Chain	Res	Type
8	I	269	LEU
8	I	279	ILE
8	I	322	MET
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	372	TRP
8	I	381	LEU
8	I	387	GLU
8	I	397	ILE
8	I	399	LYS
8	I	401	ASN
8	I	404	LEU
8	I	473	GLU
8	I	492	THR
8	I	496	GLN
8	I	505	SER
8	I	512	LEU
8	I	522	LEU
8	I	523	HIS
8	I	537	LEU
8	I	564	ASP
8	I	571	LYS
8	I	609	GLN
8	I	652	VAL
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	55	ARG
9	J	61	ARG
9	J	134	LEU
9	J	141	ASP
9	J	146	ARG
9	J	157	LEU
9	J	163	CYS

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Mol	Chain	Res	Type
9	J	169	LEU
9	J	180	GLU
9	J	183	GLU
9	J	185	LEU
9	J	188	LEU
9	J	202	ARG
9	J	206	GLU
9	J	214	LYS
9	J	233	VAL
9	J	248	LYS
9	J	254	THR
9	J	258	MET
9	J	259	GLU
9	J	267	CYS
9	J	287	LEU
9	J	290	LYS
9	J	298	ASN
9	J	315	LYS
9	J	317	GLU
9	J	323	LEU
9	J	329	LEU
9	J	338	ILE
9	J	343	SER
9	J	351	ASP
9	J	354	MET
9	J	385	LYS
9	J	386	LEU
9	J	395	LEU
9	J	429	LEU
9	J	439	VAL
9	J	445	GLU
9	J	448	LEU
9	J	451	LEU
9	J	472	LEU
9	J	475	ILE
9	J	477	GLN
9	J	485	ILE
9	J	488	ILE
9	J	506	LEU
9	J	509	ARG
9	J	515	SER
9	J	523	ILE

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Mol	Chain	Res	Type
9	K	15	ASP
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	143	LEU
9	K	146	ARG
9	K	154	LYS
9	K	157	LEU
9	K	163	CYS
9	K	169	LEU
9	K	173	HIS
9	K	183	GLU
9	K	184	LEU
9	K	185	LEU
9	K	188	LEU
9	K	190	LEU
9	K	206	GLU
9	K	231	LEU
9	K	233	VAL
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	343	SER
9	K	351	ASP
9	K	359	THR
9	K	363	LEU
9	K	376	LEU
9	K	385	LYS
9	K	386	LEU
9	K	395	LEU
9	K	400	GLU
9	K	429	LEU
9	K	432	ILE

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Mol	Chain	Res	Type
9	K	438	GLU
9	K	439	VAL
9	K	454	VAL
9	K	458	LEU
9	K	475	ILE
9	K	488	ILE
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	60	GLN
10	L	65	ASN
10	L	67	GLN
10	L	74	VAL
10	L	77	LEU
10	L	84	LYS
10	L	98	VAL
10	L	101	ASN
10	L	108	ILE
10	L	113	LEU
10	L	128	HIS
10	L	132	THR
10	L	141	VAL
10	L	151	THR
10	L	158	ILE
10	L	162	VAL
10	L	182	SER
11	M	1	MET
11	M	12	LEU
11	M	17	ASP
11	M	19	TRP
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	76	VAL
12	N	77	GLU
12	N	80	GLN
12	N	83	LEU
12	N	150	ARG
12	N	162	PHE
12	N	181	LEU
12	N	202	GLU
12	N	214	ARG
12	N	233	CYS
12	N	241	HIS
12	N	243	LEU
12	N	248	HIS
12	N	250	LEU
12	N	256	VAL
12	N	269	THR
12	N	271	GLU
12	N	274	GLU
12	N	278	ARG
12	N	280	GLU
12	N	281	TYR
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	397	ILE
12	N	398	THR
12	N	425	ARG
12	N	435	VAL
12	N	503	SER
12	N	504	LEU

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Mol	Chain	Res	Type
12	N	505	LEU
12	N	517	ASN
12	N	544	LEU
12	N	547	LEU
12	N	557	CYS
12	N	560	MET
12	N	561	LEU
12	N	571	ASN
12	N	594	VAL
12	N	609	LEU
12	N	619	LEU
12	N	625	LYS
12	N	626	TYR
12	N	640	THR
12	N	670	PHE
12	N	699	TRP
12	N	705	LEU
12	N	728	VAL
13	O	28	ASP
13	O	38	LEU
13	O	40	LEU
13	O	43	GLU
13	O	44	MET
13	O	62	GLN
13	O	63	LEU
13	O	64	LEU
13	O	73	ILE
13	O	78	LEU
13	O	89	LEU
13	O	98	LYS
13	O	99	LEU
13	O	104	GLU
13	O	108	MET
13	O	129	THR
13	O	132	VAL
13	O	136	LEU
13	O	160	GLN
13	O	207	LEU
13	O	218	GLN
13	O	223	LEU
13	O	228	THR
13	O	237	GLN

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Mol	Chain	Res	Type
13	O	238	LYS
13	O	249	ASP
13	O	256	LEU
13	O	257	SER
13	O	262	LEU
13	O	264	VAL
13	O	265	GLN
13	O	266	ASP
13	O	267	VAL
13	O	274	LEU
13	O	280	ARG
13	O	283	LEU
13	O	299	SER
13	O	328	ILE
13	O	329	ARG
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	367	LYS
13	O	369	VAL
13	O	376	LEU
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	436	THR
13	O	460	GLN
13	O	465	SER
13	O	468	VAL
13	O	491	LYS
13	O	495	GLU
13	O	501	SER
13	O	510	CYS

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Mol	Chain	Res	Type
13	O	511	ASP
13	O	512	GLN
13	O	518	ARG
13	O	531	LEU
13	O	532	VAL
13	O	533	THR
13	O	535	ILE
13	O	563	LEU
13	O	577	THR
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	649	GLU
13	O	657	ILE
13	O	670	CYS
13	O	680	GLN
13	O	683	LYS
13	O	687	LEU
13	O	691	ILE
13	O	694	LEU
13	O	704	VAL
13	O	706	CYS
13	O	707	LYS
13	O	713	VAL
13	O	723	THR
13	O	730	ARG
13	O	735	MET
13	O	744	LEU

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Mol	Chain	Res	Type
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
3	P	78	GLU
3	P	89	LEU
3	P	98	GLU
3	P	119	MET
3	P	128	LYS
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	183	ASP
3	P	201	LEU
3	P	234	LEU
3	P	244	ILE
3	P	245	GLU
3	P	288	GLU
3	P	289	LEU
3	P	291	LYS
3	P	299	ASN
3	P	300	MET
3	P	302	THR
3	P	306	LEU
3	P	309	VAL
3	P	310	ARG
3	P	312	MET
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

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Mol	Chain	Res	Type
3	P	349	LYS
3	P	352	LEU
3	P	358	LEU
3	P	359	LYS
3	P	361	ASN
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
3	P	413	LYS
3	P	414	MET
3	P	419	LEU
3	P	428	LEU
3	P	429	ARG
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
3	P	535	LYS
14	R	73	LYS
14	R	80	ILE
14	R	83	ARG
14	R	110	LYS
14	R	118	LEU
14	R	125	VAL
14	R	129	LYS
14	R	131	LEU
14	R	132	ARG
14	R	252	LEU
14	R	496	GLN
14	R	498	ILE
14	R	499	ARG
15	S	831	LEU
7	W	5	LYS
7	W	22	ILE
16	X	39	ASP

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Mol	Chain	Res	Type
16	X	49	LEU
16	X	59	LEU
16	X	79	LEU
16	X	106	GLN
16	X	110	LEU
16	X	154	ASP
16	X	184	GLN
16	X	189	VAL
16	X	193	LYS
16	X	201	LEU
16	X	230	VAL
16	X	255	ILE
16	X	276	SER
16	X	289	ASN
16	X	295	GLU
16	X	300	LEU
16	X	303	TYR
16	X	306	LYS
16	X	310	VAL
16	X	334	ILE
16	X	337	GLN
16	X	366	ILE
16	X	371	ASN
16	X	401	ARG
16	X	407	LEU
16	X	414	ILE
16	X	423	ILE
16	X	450	VAL
16	X	452	LEU
16	X	453	GLU
16	X	456	VAL
16	X	457	THR
16	X	465	LEU
16	X	487	SER
16	X	496	ILE
16	X	503	LEU
16	X	506	GLN
16	X	513	ARG
16	X	515	LEU
16	Y	39	ASP
16	Y	49	LEU
16	Y	59	LEU

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Mol	Chain	Res	Type
16	Y	63	MET
16	Y	70	LEU
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	230	VAL
16	Y	255	ILE
16	Y	276	SER
16	Y	289	ASN
16	Y	295	GLU
16	Y	300	LEU
16	Y	303	TYR
16	Y	306	LYS
16	Y	310	VAL
16	Y	334	ILE
16	Y	337	GLN
16	Y	364	LYS
16	Y	366	ILE
16	Y	371	ASN
16	Y	401	ARG
16	Y	407	LEU
16	Y	414	ILE
16	Y	423	ILE
16	Y	450	VAL
16	Y	452	LEU
16	Y	453	GLU
16	Y	456	VAL
16	Y	457	THR
16	Y	465	LEU
16	Y	487	SER
16	Y	496	ILE
16	Y	503	LEU
16	Y	506	GLN
16	Y	513	ARG
16	Y	515	LEU
16	Y	551	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (190)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	33	ASN
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	623	GLN
1	A	658	ASN
1	A	776	ASN
1	A	1021	HIS
1	A	1165	HIS
1	A	1184	HIS
1	A	1201	HIS
1	A	1262	GLN
1	A	1266	HIS
1	A	1309	HIS
1	A	1327	GLN
1	A	1359	ASN
1	A	1380	ASN
1	A	1532	ASN
1	A	1543	HIS
1	A	1559	HIS
1	A	1604	GLN
1	A	1813	GLN
2	B	9	ASN
2	B	31	ASN
2	B	50	GLN
3	C	35	GLN
3	C	71	GLN
3	C	104	HIS
3	C	202	HIS
3	C	236	HIS
3	C	253	ASN
3	C	287	ASN
3	C	346	GLN
3	C	386	GLN
3	C	431	ASN
3	C	447	ASN

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Mol	Chain	Res	Type
3	C	518	GLN
4	D	36	GLN
4	D	37	HIS
4	D	38	GLN
4	D	49	ASN
5	E	69	GLN
5	E	75	GLN
6	F	100	GLN
6	F	495	HIS
6	F	545	HIS
6	F	547	GLN
6	F	580	GLN
6	F	583	HIS
6	F	595	GLN
6	F	626	ASN
6	F	634	HIS
6	F	636	ASN
6	F	648	GLN
6	F	659	GLN
6	H	14	GLN
6	H	70	GLN
6	H	480	ASN
6	H	494	HIS
6	H	495	HIS
6	H	517	GLN
6	H	545	HIS
6	H	547	GLN
6	H	580	GLN
6	H	634	HIS
6	H	648	GLN
6	H	659	GLN
6	H	680	HIS
6	H	708	HIS
8	I	18	GLN
8	I	323	ASN
8	I	345	GLN
8	I	353	GLN
8	I	362	HIS
8	I	374	GLN
8	I	471	ASN
8	I	523	HIS
8	I	604	HIS

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Mol	Chain	Res	Type
8	I	613	ASN
8	I	684	GLN
9	J	17	GLN
9	J	38	GLN
9	J	45	GLN
9	J	52	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	362	GLN
9	J	382	ASN
9	J	406	HIS
9	J	449	ASN
9	J	453	HIS
9	K	16	GLN
9	K	17	GLN
9	K	20	GLN
9	K	38	GLN
9	K	86	HIS
9	K	198	GLN
9	K	271	HIS
9	K	316	ASN
9	K	352	GLN
9	K	382	ASN
9	K	449	ASN
9	K	453	HIS
10	L	49	ASN
10	L	103	HIS
10	L	128	HIS
10	L	138	GLN
10	L	152	HIS
12	N	86	ASN
12	N	388	HIS
12	N	639	HIS
12	N	663	GLN
12	N	702	GLN
12	N	726	ASN

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Mol	Chain	Res	Type
13	O	62	GLN
13	O	69	GLN
13	O	91	ASN
13	O	211	GLN
13	O	218	GLN
13	O	237	GLN
13	O	242	ASN
13	O	247	ASN
13	O	319	GLN
13	O	332	GLN
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	552	GLN
13	O	555	ASN
13	O	556	GLN
13	O	695	ASN
13	O	728	GLN
3	P	71	GLN
3	P	236	HIS
3	P	242	GLN
3	P	287	ASN
3	P	305	ASN
3	P	321	HIS
3	P	346	GLN
3	P	427	GLN
3	P	447	ASN
14	R	99	ASN
14	R	196	ASN
14	R	263	ASN
14	R	323	HIS
14	R	355	GLN
14	R	369	ASN
14	R	423	ASN
14	R	496	GLN
16	X	36	ASN
16	X	50	HIS

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Mol	Chain	Res	Type
16	X	67	ASN
16	X	89	HIS
16	X	95	ASN
16	X	105	GLN
16	X	106	GLN
16	X	184	GLN
16	X	287	ASN
16	X	298	GLN
16	X	337	GLN
16	X	367	GLN
16	X	371	ASN
16	X	506	GLN
16	Y	67	ASN
16	Y	184	GLN
16	Y	270	ASN
16	Y	287	ASN
16	Y	296	GLN
16	Y	298	GLN
16	Y	337	GLN
16	Y	367	GLN
16	Y	371	ASN
16	Y	506	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
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

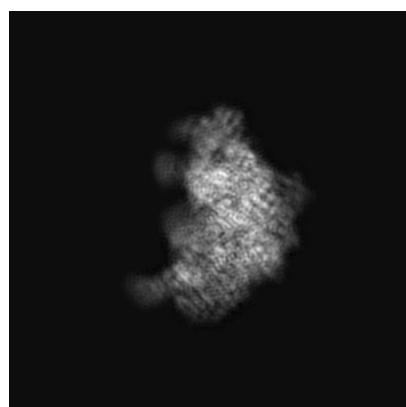
6 Map visualisation [i](#)

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.

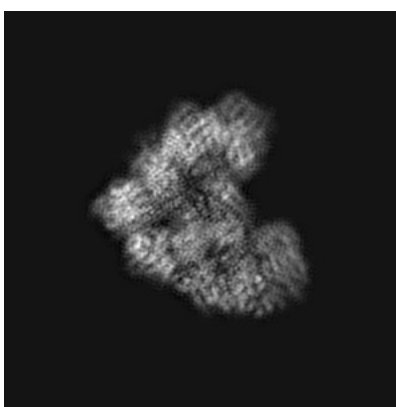
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

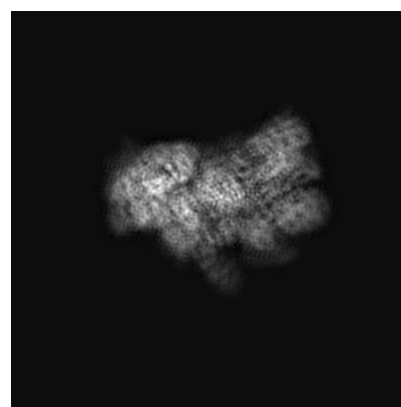
6.1.1 Primary map



X



Y

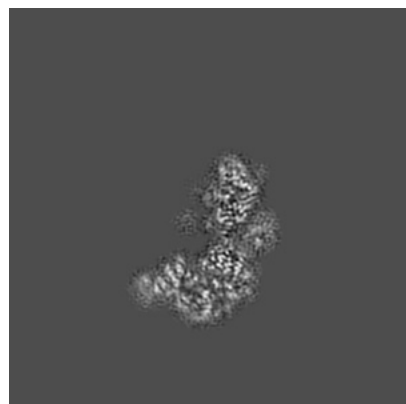


Z

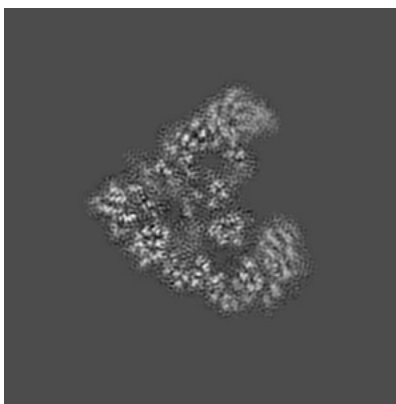
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

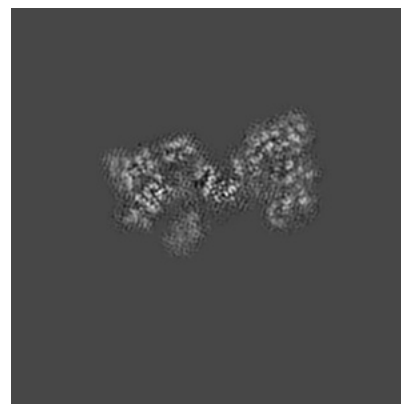
6.2.1 Primary map



X Index: 142



Y Index: 142

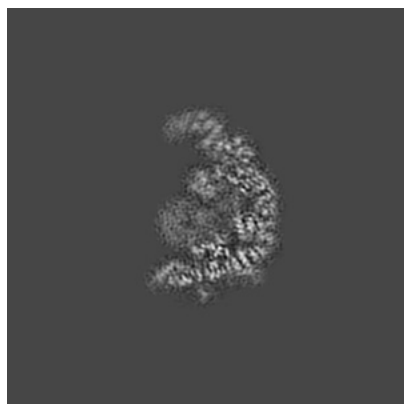


Z Index: 142

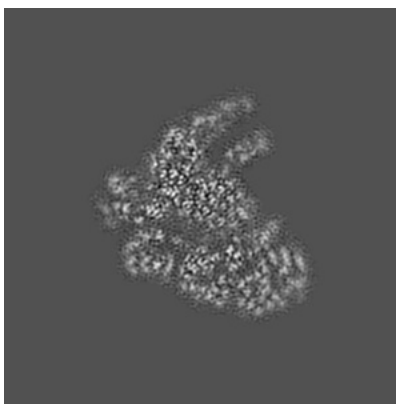
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

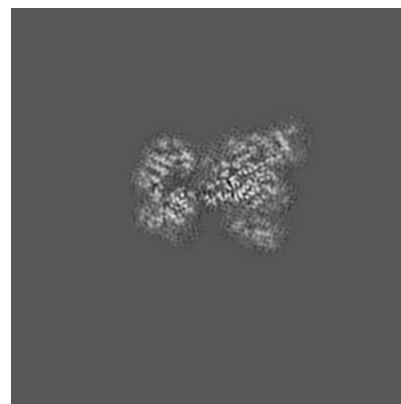
6.3.1 Primary map



X Index: 121



Y Index: 156

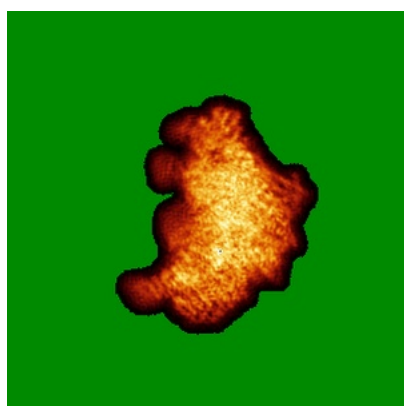


Z Index: 113

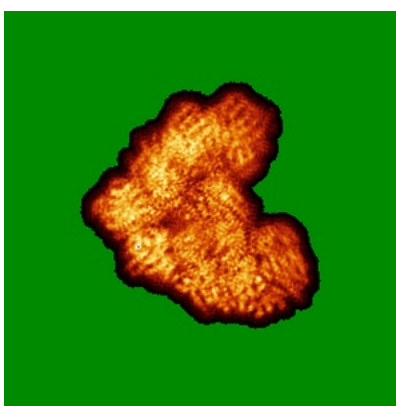
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

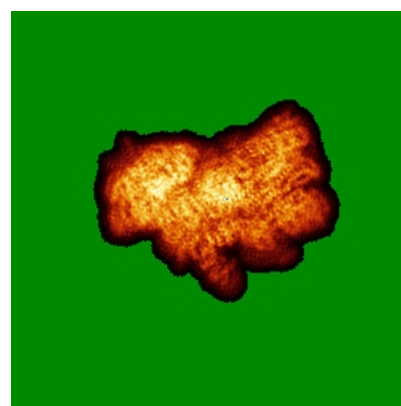
6.4.1 Primary map



X



Y

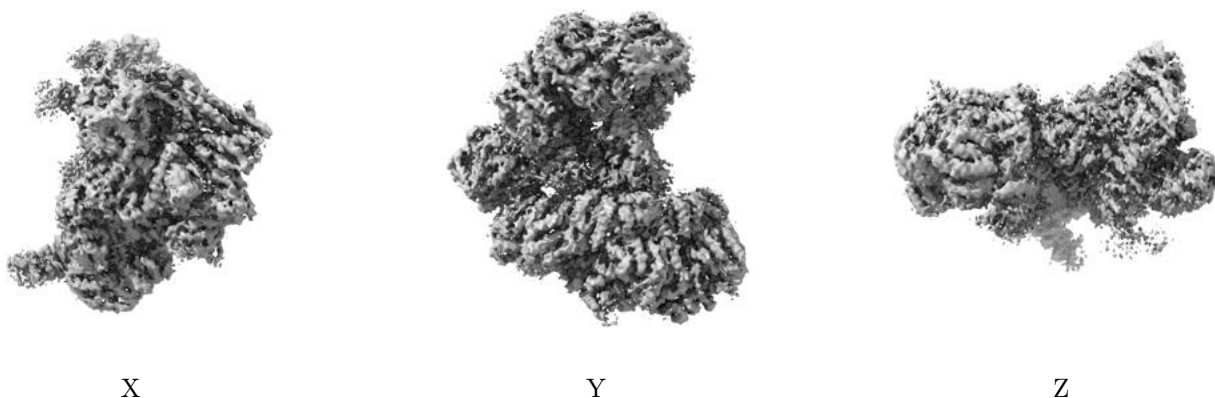


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

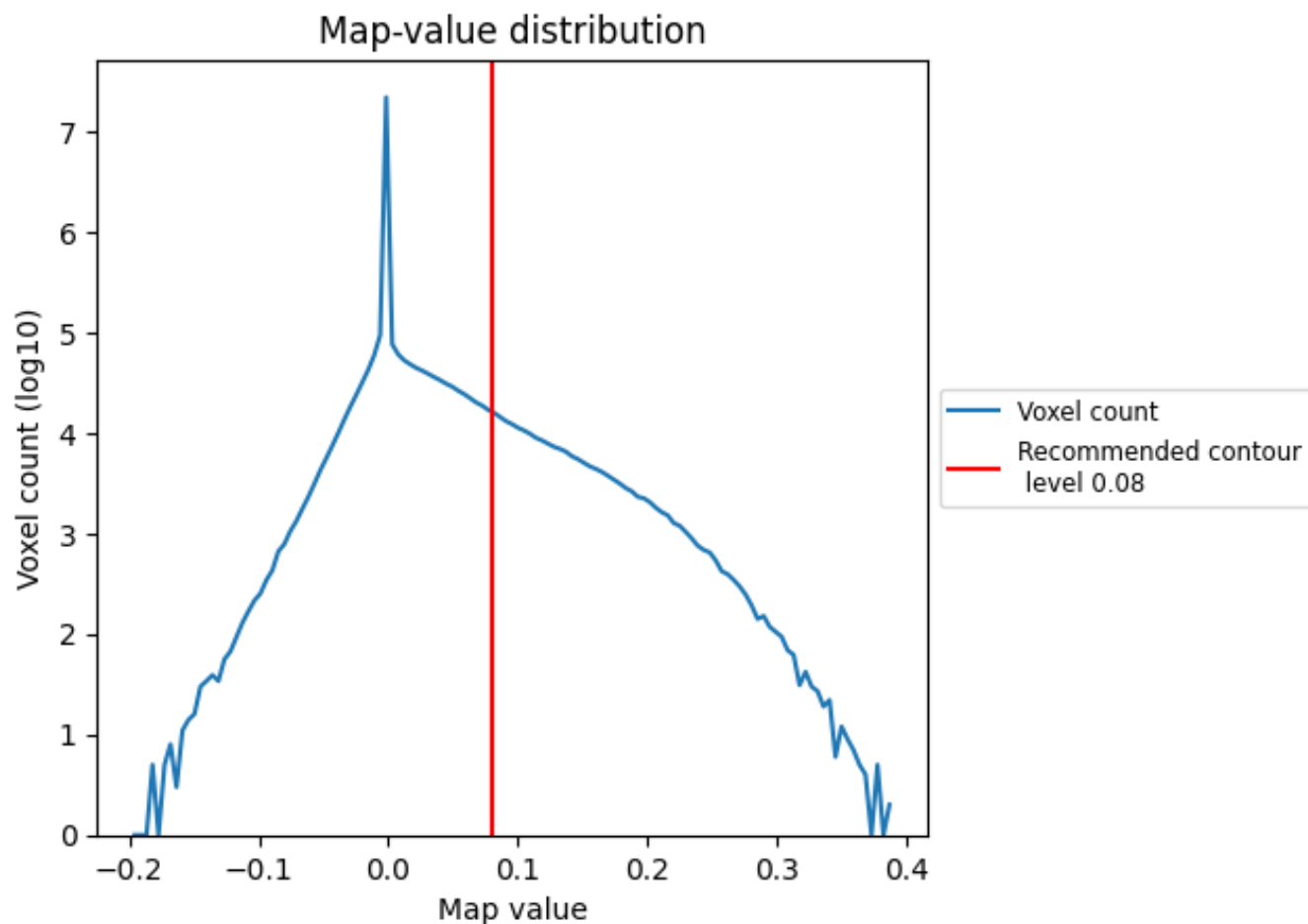
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

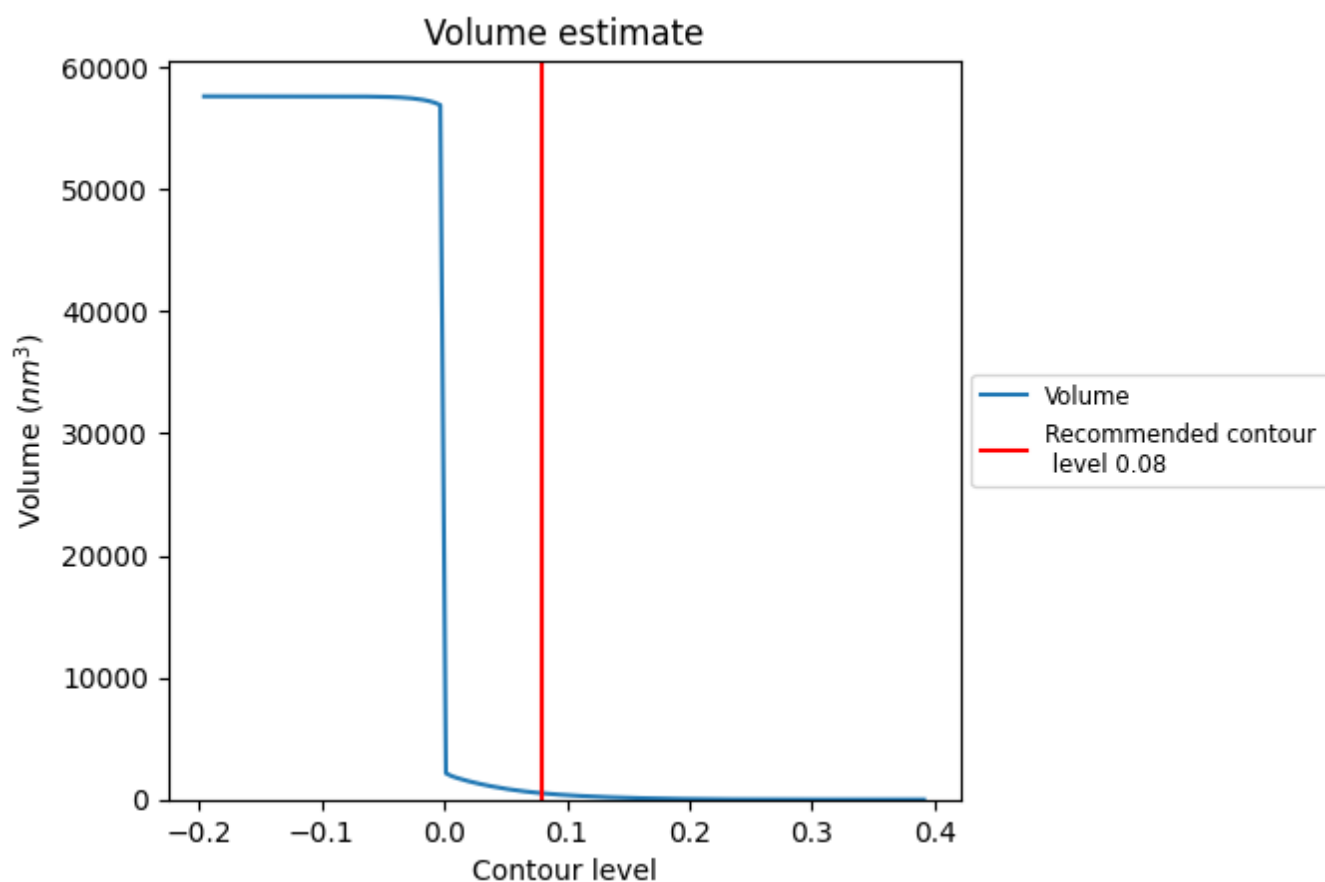
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

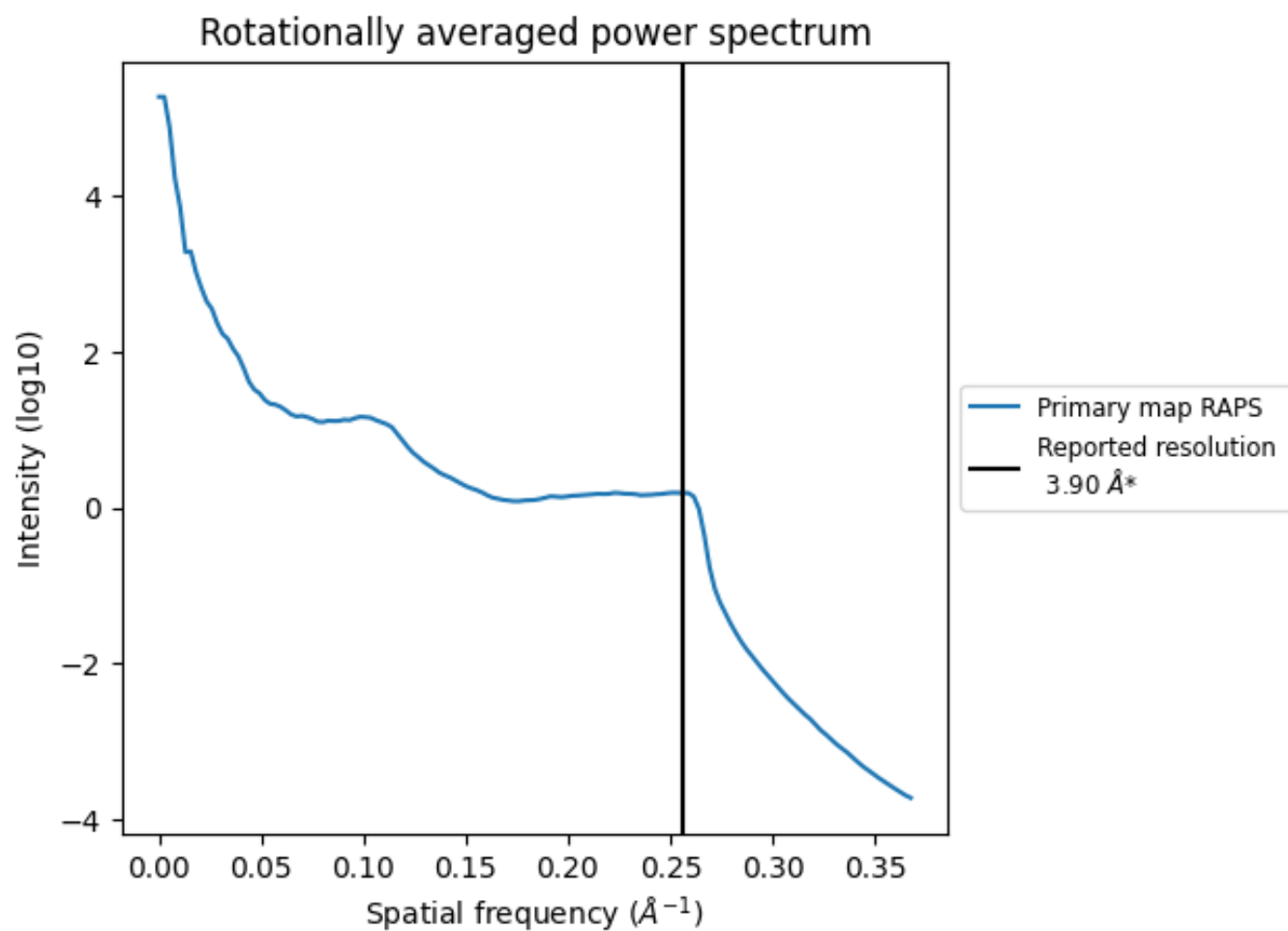
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 516 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

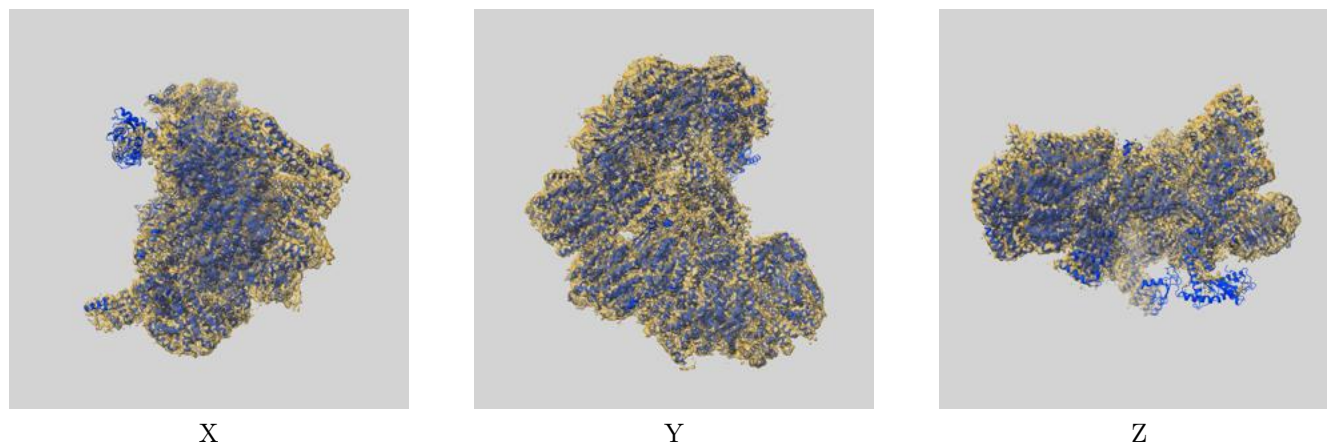
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

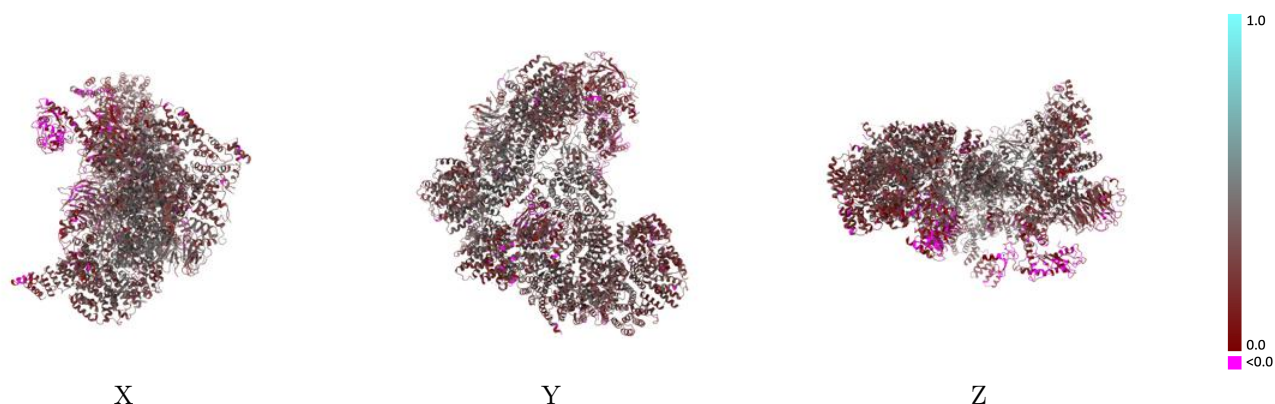
This section contains information regarding the fit between EMDB map EMD-3385 and PDB model 5G04. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



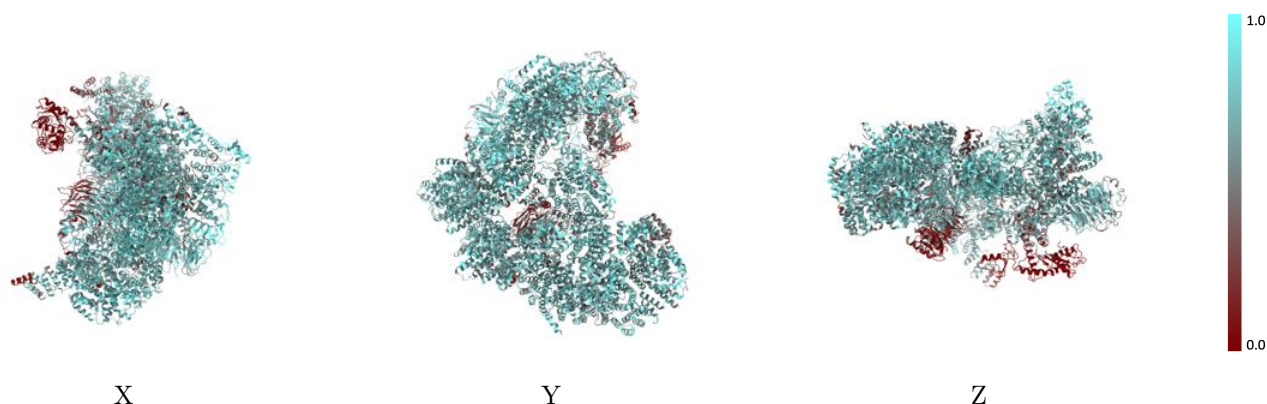
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



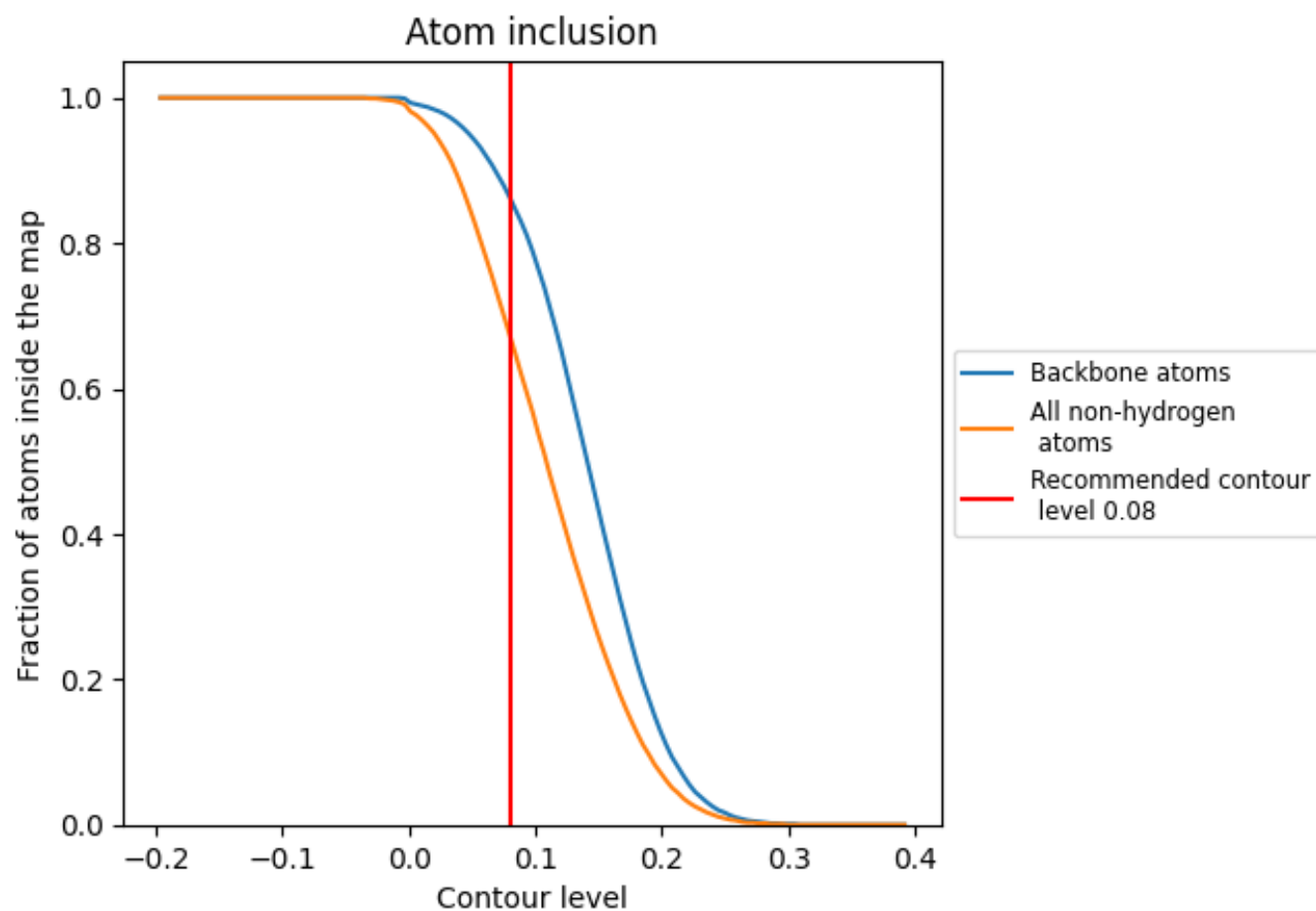
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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	 0.6720	 0.2990
A	 0.7500	 0.3600
B	 0.0130	 -0.0100
C	 0.7180	 0.3580
D	 0.6990	 0.3480
E	 0.7050	 0.3400
F	 0.7380	 0.3320
G	 0.7510	 0.3370
H	 0.7570	 0.3410
I	 0.6690	 0.2710
J	 0.7630	 0.3370
K	 0.7340	 0.3110
L	 0.7030	 0.3400
M	 0.6290	 0.3370
N	 0.4350	 0.1830
O	 0.7420	 0.3550
P	 0.7140	 0.3010
R	 0.2670	 0.1400
S	 0.0860	 0.0850
W	 0.6340	 0.3120
X	 0.6320	 0.2210
Y	 0.6880	 0.2530

