Full wwPDB EM Validation Report

May 17, 2025 – 08:18 PM EDT

PDB ID	:	6XJA / pdb_00006xja
EMDB ID	:	EMD-22204
Title	:	Streptococcus Pneumoniae IgA1 Protease with IgA1 substrate
Authors	:	Eisenmesser, E.Z.; Zheng, H.
Deposited on	:	2020-06-23
Resolution	:	4.00 Å(reported)

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

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

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

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

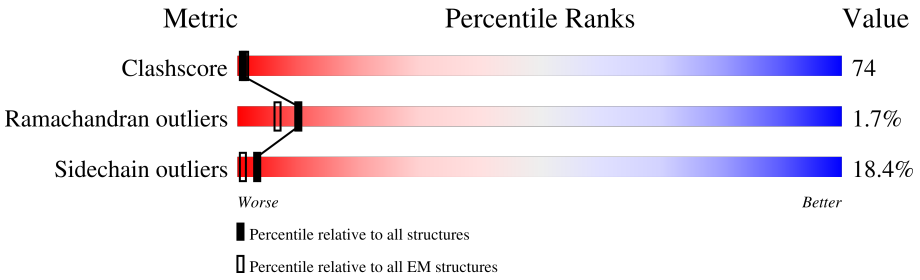
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	P	1299	12% 66% 29%
2	A	210	79% 20% 52% 24%
2	B	210	70% 17% 47% 31% 6%
3	L	219	10% 30% 47% 21%
4	H	232	10% 28% 45% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16441 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 Immunoglobulin A1 protease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	1286	Total	C	N	O	S	0	0
			10159	6402	1727	2012	18		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	1605	ALA	GLU	engineered mutation	UNP Q59947

- Molecule 2 is a protein called Immunoglobulin heavy constant alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	209	Total	C	N	O	S	0	0
			1598	1007	276	306	9		
2	B	210	Total	C	N	O	S	0	0
			1604	1010	277	307	10		

- Molecule 3 is a protein called Immunoglobulin alpha-1 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	219	Total	C	N	O	S	0	0
			1541	956	267	312	6		

- Molecule 4 is a protein called Immunoglobulin alpha-1 heavy chain.

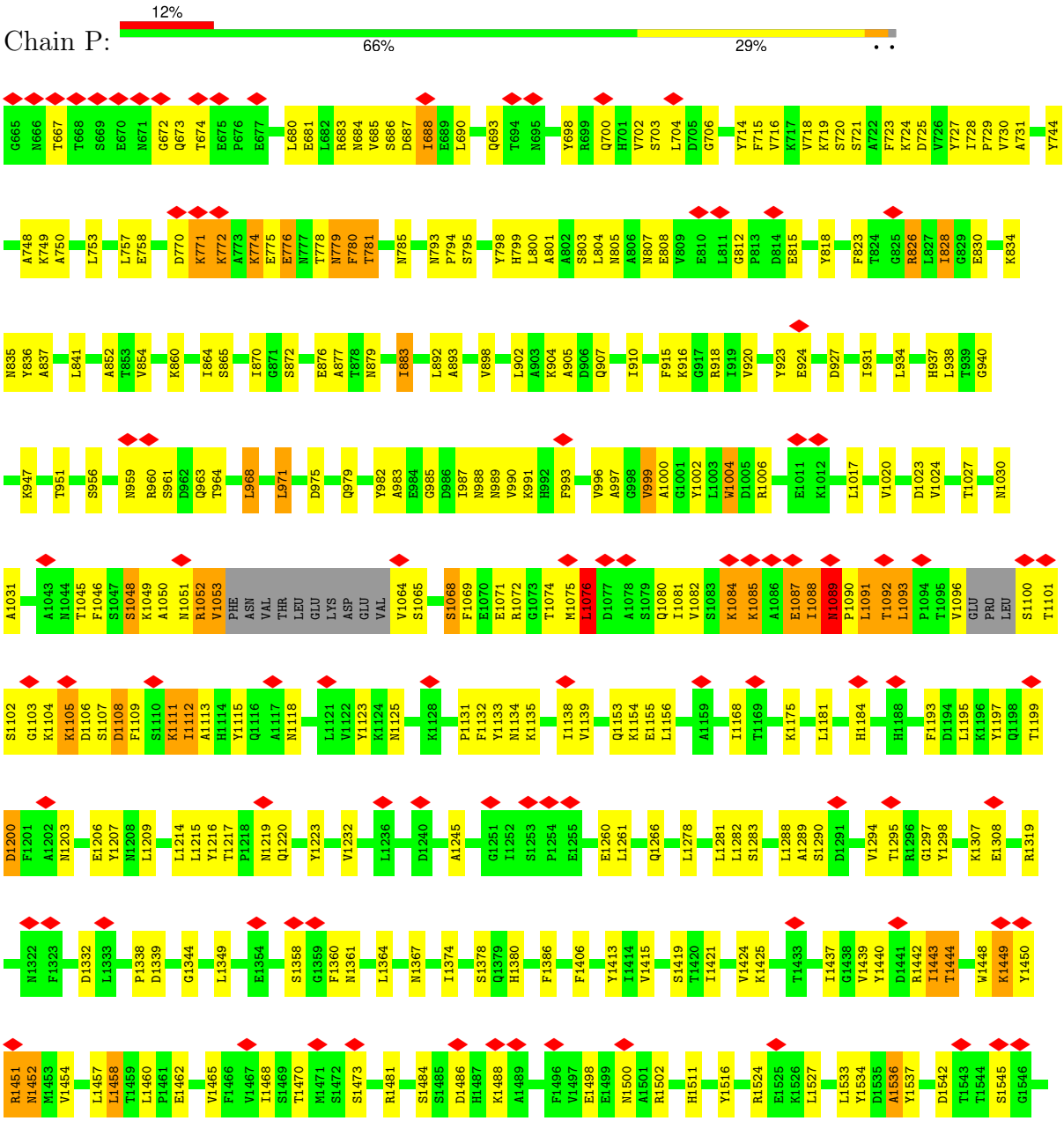
Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	232	Total	C	N	O	S	0	0
			1539	962	263	307	7		

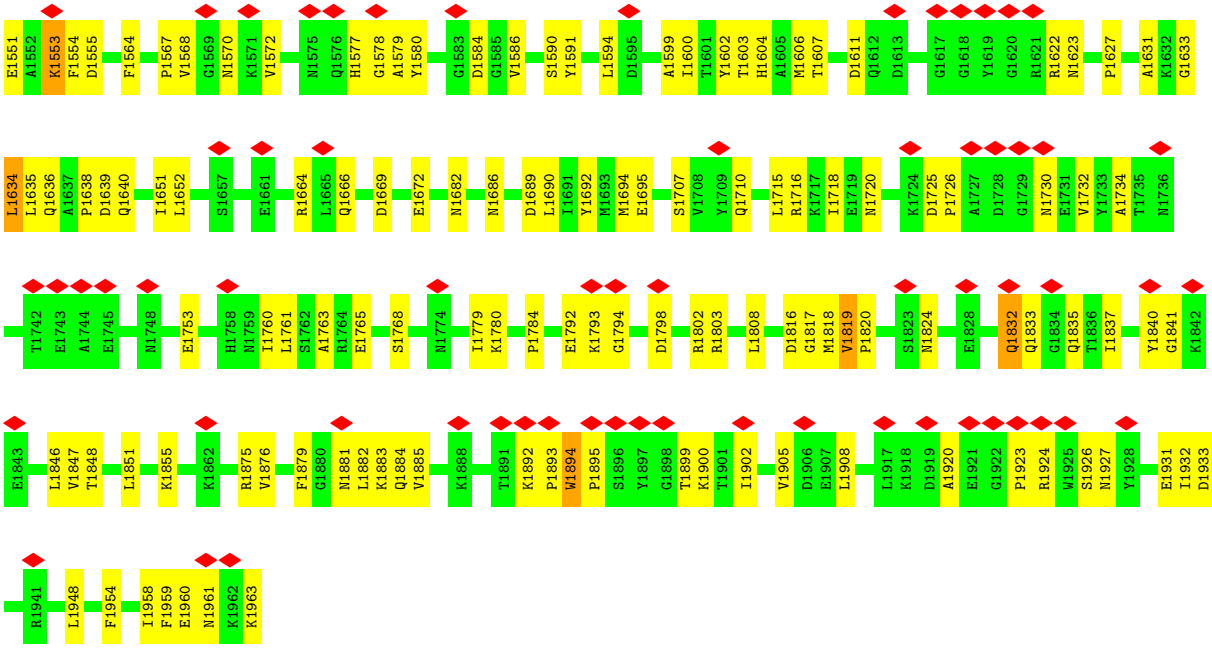
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Immunoglobulin A1 protease

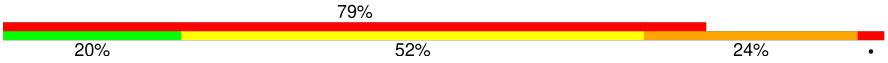
Chain P:

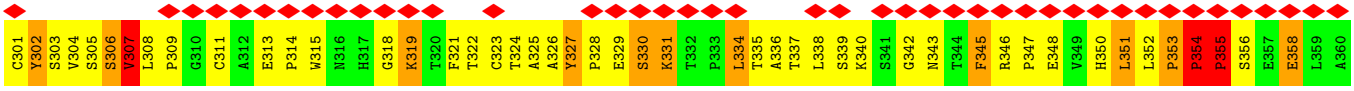


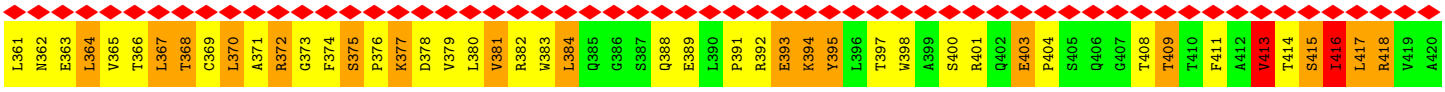


• Molecule 2: Immunoglobulin heavy constant alpha 1

Chain A:

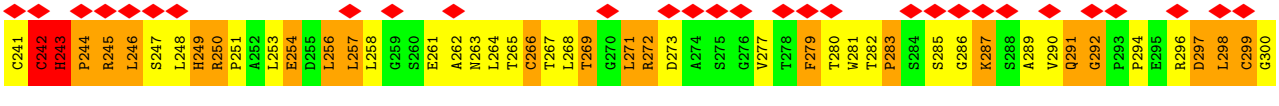


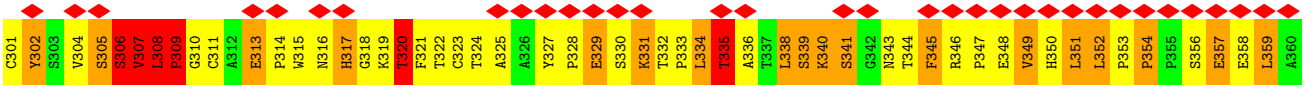


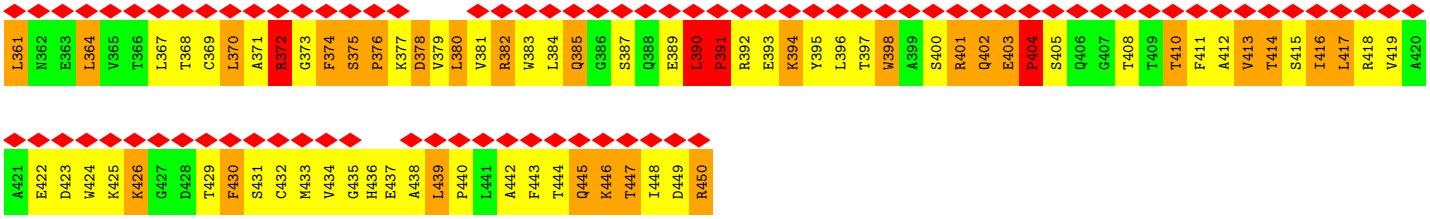


• Molecule 2: Immunoglobulin heavy constant alpha 1

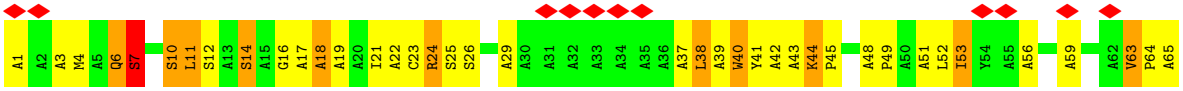
Chain B:

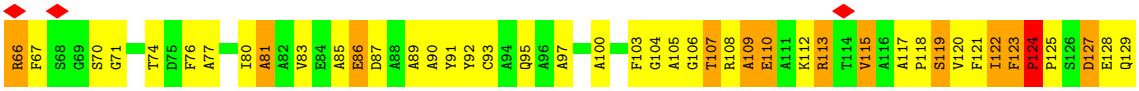


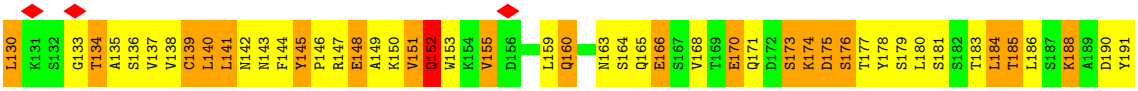


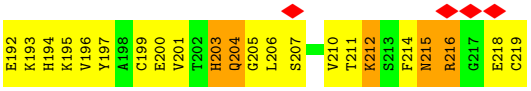


• Molecule 3: Immunoglobulin alpha-1 light chain

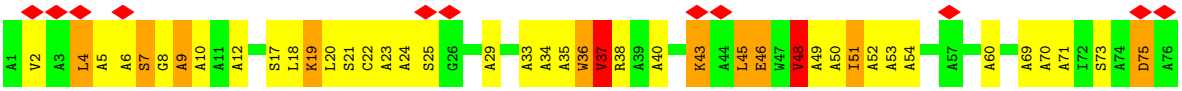


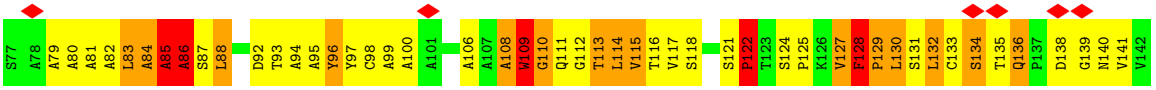


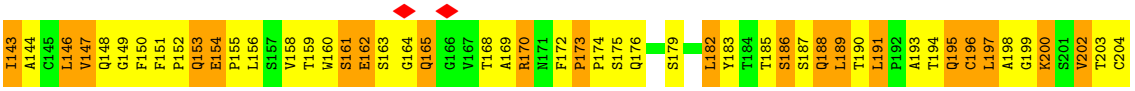


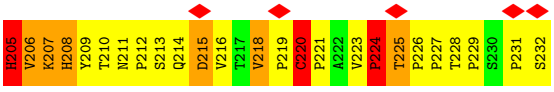


• Molecule 4: Immunoglobulin alpha-1 heavy chain









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100000	Depositor
Resolution determination method	FSC 3 SIGMA CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.751	Depositor
Minimum map value	-0.401	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	356.15997, 356.15997, 356.15997	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5899999, 1.5899999, 1.5899999	Depositor

5 Model quality

5.1 Standard geometry

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	P	0.55	0/10345	0.82	15/13970 (0.1%)
2	A	1.28	5/1639 (0.3%)	1.52	18/2238 (0.8%)
2	B	2.75	23/1645 (1.4%)	2.64	42/2246 (1.9%)
3	L	1.15	3/1570 (0.2%)	1.36	7/2140 (0.3%)
4	H	1.86	17/1574 (1.1%)	2.17	39/2177 (1.8%)
All	All	1.24	48/16773 (0.3%)	1.40	121/22771 (0.5%)

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	P	0	1
2	B	0	6
3	L	0	3
4	H	0	6
All	All	0	16

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	243	HIS	CA-CB	62.29	2.51	1.53
2	B	307	VAL	CA-CB	41.65	2.09	1.54
2	B	308	LEU	C-O	28.22	1.60	1.24
2	B	243	HIS	CB-CG	27.17	1.88	1.50
4	H	86	ALA	N-CA	27.00	1.77	1.46
2	B	307	VAL	CA-C	22.99	1.79	1.53
2	B	307	VAL	N-CA	22.85	1.80	1.45
4	H	109	TRP	C-O	22.19	1.51	1.23
2	A	251	PRO	N-CA	19.86	1.70	1.47
4	H	85	ALA	C-N	19.64	1.58	1.33
4	H	129	PRO	N-CA	18.95	1.70	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	309	PRO	N-CA	18.19	1.70	1.47
4	H	122	PRO	N-CA	18.10	1.70	1.47
2	B	404	PRO	N-CA	18.08	1.70	1.47
2	B	376	PRO	N-CA	18.07	1.70	1.47
2	B	391	PRO	N-CA	17.63	1.69	1.47
2	A	355	PRO	N-CA	17.06	1.69	1.47
2	B	306	SER	C-N	14.68	1.53	1.33
2	B	292	GLY	C-N	14.51	1.50	1.33
4	H	110	GLY	C-O	14.23	1.45	1.24
2	B	243	HIS	N-CA	13.40	1.65	1.46
4	H	128	PHE	C-N	11.98	1.46	1.33
4	H	86	ALA	CA-C	-11.67	1.38	1.52
3	L	124	PRO	N-CA	11.63	1.70	1.46
4	H	173	PRO	N-CA	11.46	1.70	1.46
4	H	109	TRP	C-N	10.87	1.45	1.34
4	H	109	TRP	CA-C	-10.87	1.39	1.52
4	H	172	PHE	C-N	10.66	1.46	1.33
2	B	243	HIS	CA-C	10.53	1.66	1.52
3	L	123	PHE	C-N	10.45	1.45	1.33
2	A	250	ARG	C-N	10.41	1.45	1.33
2	B	242	CYS	C-N	9.39	1.52	1.33
2	B	307	VAL	C-O	-8.81	1.12	1.23
4	H	86	ALA	C-O	-8.72	1.13	1.23
2	A	413	VAL	C-N	8.53	1.45	1.33
3	L	7	SER	C-N	8.52	1.50	1.34
4	H	85	ALA	CA-C	7.74	1.62	1.52
4	H	86	ALA	CA-CB	6.54	1.66	1.53
2	B	243	HIS	CE1-NE2	-6.42	1.26	1.32
2	B	307	VAL	C-N	6.02	1.46	1.33
4	H	37	VAL	C-O	-5.44	1.17	1.24
2	B	307	VAL	CB-CG1	5.24	1.69	1.52
4	H	121	SER	C-N	5.13	1.45	1.33
2	B	375	SER	C-N	5.13	1.45	1.33
2	B	390	LEU	C-N	5.12	1.45	1.33
2	B	403	GLU	C-N	5.09	1.45	1.33
2	A	354	PRO	C-N	5.09	1.45	1.33
2	B	308	LEU	C-N	5.07	1.45	1.33

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	242	CYS	O-C-N	-47.71	60.26	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	243	HIS	CA-CB-CG	39.10	152.90	113.80
4	H	109	TRP	CA-C-N	35.60	154.15	122.47
4	H	109	TRP	C-N-CA	35.60	154.15	122.47
2	B	306	SER	CA-C-N	29.89	167.21	123.27
2	B	306	SER	C-N-CA	29.89	167.21	123.27
2	B	307	VAL	CA-CB-CG1	23.59	150.50	110.40
2	B	307	VAL	CG1-CB-CG2	-19.24	68.48	110.80
4	H	85	ALA	CA-C-N	19.12	154.14	121.64
4	H	85	ALA	C-N-CA	19.12	154.14	121.64
3	L	123	PHE	CA-C-N	19.12	140.07	120.38
3	L	123	PHE	C-N-CA	19.12	140.07	120.38
2	B	243	HIS	CB-CA-C	19.07	147.73	110.17
4	H	172	PHE	CA-C-N	18.28	139.21	120.38
4	H	172	PHE	C-N-CA	18.28	139.21	120.38
2	B	307	VAL	CB-CA-C	17.86	136.34	111.34
2	B	307	VAL	CA-CB-CG2	17.67	140.44	110.40
2	A	250	ARG	CA-C-N	17.51	138.66	119.93
2	A	250	ARG	C-N-CA	17.51	138.66	119.93
2	A	354	PRO	CA-C-N	17.32	141.48	119.84
2	A	354	PRO	C-N-CA	17.32	141.48	119.84
2	B	292	GLY	CA-C-N	16.77	137.65	120.38
2	B	292	GLY	C-N-CA	16.77	137.65	120.38
2	B	375	SER	CA-C-N	16.33	140.25	119.84
2	B	375	SER	C-N-CA	16.33	140.25	119.84
2	B	390	LEU	CA-C-N	16.12	139.99	119.84
2	B	390	LEU	C-N-CA	16.12	139.99	119.84
2	B	308	LEU	CA-C-N	16.04	139.89	119.84
2	B	308	LEU	C-N-CA	16.04	139.89	119.84
2	B	403	GLU	CA-C-N	15.96	139.79	119.84
2	B	403	GLU	C-N-CA	15.96	139.79	119.84
4	H	121	SER	CA-C-N	15.80	139.59	119.84
4	H	121	SER	C-N-CA	15.80	139.59	119.84
4	H	128	PHE	CA-C-N	15.67	139.50	120.23
4	H	128	PHE	C-N-CA	15.67	139.50	120.23
4	H	86	ALA	N-CA-CB	15.55	136.86	110.57
2	B	307	VAL	CA-C-N	13.27	154.18	121.80
2	B	307	VAL	C-N-CA	13.27	154.18	121.80
2	B	309	PRO	O-C-N	-12.66	105.55	122.64
4	H	85	ALA	CA-C-O	-11.84	107.22	120.60
4	H	86	ALA	CA-C-O	-11.59	106.00	120.14
2	B	306	SER	CA-C-O	-11.35	108.21	120.24
2	A	354	PRO	N-CA-C	11.21	124.38	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	320	THR	O-C-N	11.20	135.86	122.75
2	A	355	PRO	CA-N-CD	-11.20	96.32	112.00
4	H	109	TRP	CA-C-O	-11.15	108.40	121.44
4	H	205	HIS	CA-C-N	10.99	137.54	123.14
4	H	205	HIS	C-N-CA	10.99	137.54	123.14
2	A	353	PRO	N-CA-C	-10.84	97.48	110.70
2	B	320	THR	CA-C-N	10.83	142.23	121.54
2	B	320	THR	C-N-CA	10.83	142.23	121.54
4	H	109	TRP	O-C-N	10.33	136.58	123.15
2	B	391	PRO	CA-N-CD	-10.08	97.89	112.00
4	H	173	PRO	CA-N-CD	-9.89	98.16	112.00
1	P	1819	VAL	N-CA-CB	9.88	116.72	110.50
2	B	307	VAL	CA-C-O	-9.50	110.61	121.44
2	B	376	PRO	CA-N-CD	-9.44	98.78	112.00
4	H	86	ALA	O-C-N	8.85	133.51	123.42
4	H	122	PRO	CA-N-CD	-8.78	99.70	112.00
4	H	110	GLY	CA-C-O	-8.75	111.70	121.77
2	B	404	PRO	CA-N-CD	-8.72	99.79	112.00
2	B	307	VAL	N-CA-CB	8.68	122.17	112.45
3	L	124	PRO	CA-N-CD	-8.65	99.89	112.00
2	B	244	PRO	CA-N-CD	-8.56	100.02	112.00
2	A	251	PRO	CA-N-CD	-8.55	100.03	112.00
2	A	307	VAL	CA-C-O	-8.51	110.97	120.84
2	B	309	PRO	CA-N-CD	-8.28	100.40	112.00
4	H	84	ALA	CA-C-N	8.19	134.20	121.99
4	H	84	ALA	C-N-CA	8.19	134.20	121.99
4	H	129	PRO	CA-N-CD	-8.10	100.66	112.00
3	L	109	ALA	O-C-N	8.05	132.03	122.46
2	B	307	VAL	N-CA-C	-7.69	99.43	108.82
4	H	109	TRP	CB-CA-C	-7.46	94.49	109.79
2	A	307	VAL	CA-C-N	-7.41	103.73	121.80
2	A	307	VAL	C-N-CA	-7.41	103.73	121.80
4	H	224	PRO	N-CA-CB	-7.38	95.50	103.25
2	A	250	ARG	CB-CA-C	7.32	117.37	111.00
1	P	1792	GLU	N-CA-C	-7.26	104.29	113.01
2	A	413	VAL	CA-C-O	-7.22	111.76	120.78
3	L	152	GLN	CB-CA-C	6.78	123.72	110.30
2	B	308	LEU	N-CA-CB	6.77	122.42	110.37
2	B	243	HIS	ND1-CG-CD2	-6.71	99.39	106.10
4	H	108	ALA	CA-C-N	-6.67	112.12	122.59
4	H	108	ALA	C-N-CA	-6.67	112.12	122.59
2	B	242	CYS	CA-C-N	-6.61	105.66	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	242	CYS	C-N-CA	-6.61	105.66	121.80
2	B	305	SER	CA-C-O	-6.46	114.51	121.36
1	P	1816	ASP	CB-CA-C	6.37	123.09	110.42
4	H	215	ASP	CA-C-N	-6.32	114.70	123.10
4	H	215	ASP	C-N-CA	-6.32	114.70	123.10
1	P	1088	ILE	CB-CA-C	6.27	116.63	111.05
1	P	1578	GLY	CA-C-O	-6.23	118.17	122.22
2	A	251	PRO	N-CA-C	-6.14	101.26	111.26
1	P	826	ARG	N-CA-C	-6.06	104.68	111.28
4	H	87	SER	CA-C-O	-6.01	114.69	122.14
1	P	780	PHE	CB-CA-C	-5.96	100.10	110.17
2	B	244	PRO	CA-C-O	-5.80	110.04	120.60
1	P	1536	ALA	CA-C-O	-5.68	114.53	120.55
1	P	1536	ALA	N-CA-C	5.66	117.44	111.28
4	H	106	ALA	N-CA-CB	5.57	120.04	111.46
1	P	1824	ASN	CA-CB-CG	5.51	118.11	112.60
4	H	36	TRP	CA-C-N	-5.49	116.01	122.93
4	H	36	TRP	C-N-CA	-5.49	116.01	122.93
2	B	243	HIS	CG-CD2-NE2	5.43	112.63	107.20
4	H	109	TRP	CA-CB-CG	-5.42	103.29	113.60
1	P	1794	GLY	N-CA-C	5.40	119.21	112.73
4	H	110	GLY	O-C-N	5.40	127.98	123.29
2	A	415	SER	CA-C-N	5.38	130.19	123.14
2	A	415	SER	C-N-CA	5.38	130.19	123.14
4	H	86	ALA	CA-C-N	-5.34	114.83	122.68
4	H	86	ALA	C-N-CA	-5.34	114.83	122.68
1	P	1568	VAL	CA-C-O	-5.21	118.10	122.63
3	L	151	VAL	CA-C-N	-5.21	114.07	122.82
3	L	151	VAL	C-N-CA	-5.21	114.07	122.82
2	A	416	ILE	CA-C-N	5.18	129.28	121.40
2	A	416	ILE	C-N-CA	5.18	129.28	121.40
1	P	1931	GLU	CB-CA-C	-5.13	110.25	117.23
2	B	335	THR	CB-CA-C	-5.12	105.08	111.43
4	H	85	ALA	N-CA-C	5.10	116.58	108.67
1	P	1818	MET	CA-C-N	-5.07	117.05	120.24
1	P	1818	MET	C-N-CA	-5.07	117.05	120.24

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	242	CYS	Mainchain

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Mol	Chain	Res	Type	Group
2	B	243	HIS	Peptide
2	B	306	SER	Peptide
2	B	307	VAL	Peptide
2	B	309	PRO	Mainchain
2	B	320	THR	Mainchain
4	H	109	TRP	Peptide
4	H	151	PHE	Peptide
4	H	205	HIS	Mainchain
4	H	85	ALA	Peptide
4	H	86	ALA	Mainchain
4	H	9	ALA	Mainchain
3	L	145	TYR	Peptide
3	L	151	VAL	Mainchain
3	L	7	SER	Peptide
1	P	1093	LEU	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	P	10159	0	9932	686	0
2	A	1598	0	1576	399	0
2	B	1604	0	1577	720	0
3	L	1541	0	1490	389	0
4	H	1539	0	1508	452	0
All	All	16441	0	16083	2398	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 74.

All (2398) 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)
2:B:385:GLN:HG2	2:B:430:PHE:CB	1.20	1.67
1:P:836:TYR:CD1	1:P:1093:LEU:HD22	1.29	1.62
2:B:307:VAL:CA	2:B:307:VAL:HB	1.20	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:11:LEU:CD1	3:L:19:ALA:HB1	1.21	1.60
4:H:71:ALA:HB3	4:H:84:ALA:CB	1.16	1.60
2:B:402:GLN:HG2	2:B:411:PHE:CE2	1.14	1.59
2:A:281:TRP:CZ3	2:A:325:ALA:HB2	1.37	1.58
2:A:374:PHE:CB	2:A:411:PHE:HB2	1.13	1.58
2:A:299:CYS:SG	2:B:298:LEU:HD12	1.41	1.57
2:B:243:HIS:CB	2:B:243:HIS:CG	1.88	1.56
2:B:307:VAL:CG1	2:B:309:PRO:CG	1.78	1.56
1:P:1926:SER:HB2	2:B:243:HIS:CB	1.34	1.56
1:P:836:TYR:HD1	1:P:1093:LEU:CD2	1.13	1.55
3:L:123:PHE:CE1	4:H:132:LEU:HD13	1.40	1.55
3:L:18:ALA:HB2	3:L:83:VAL:CG2	1.10	1.55
2:B:307:VAL:CA	2:B:307:VAL:C	1.79	1.54
1:P:1883:LYS:C	1:P:1959:PHE:CB	1.78	1.54
2:A:374:PHE:HB3	2:A:411:PHE:CD2	1.39	1.53
1:P:719:LYS:CB	1:P:1101:THR:CG2	1.87	1.53
1:P:1885:VAL:HG13	1:P:1959:PHE:CE2	1.41	1.53
4:H:29:ALA:CB	4:H:54:ALA:HB2	1.33	1.52
2:B:272:ARG:NH1	2:B:301:CYS:H	1.04	1.52
3:L:86:GLU:HA	3:L:173:SER:CB	1.34	1.50
1:P:672:GLY:CA	1:P:674:THR:HG21	1.42	1.49
2:B:307:VAL:CG1	2:B:309:PRO:HG3	1.02	1.49
3:L:86:GLU:CA	3:L:173:SER:HB3	1.38	1.49
2:B:265:THR:CG2	2:B:292:GLY:HA3	1.33	1.49
2:B:385:GLN:CG	2:B:430:PHE:HB3	1.39	1.49
4:H:29:ALA:CB	4:H:54:ALA:CB	1.91	1.48
4:H:71:ALA:CB	4:H:84:ALA:CB	1.91	1.48
2:B:307:VAL:HG13	2:B:309:PRO:CB	1.42	1.48
3:L:123:PHE:CD1	4:H:132:LEU:HD13	1.45	1.48
4:H:29:ALA:HB3	4:H:54:ALA:CB	1.44	1.48
3:L:18:ALA:CB	3:L:83:VAL:CG2	1.91	1.47
4:H:86:ALA:N	4:H:86:ALA:CA	1.77	1.47
1:P:686:SER:HB3	1:P:1101:THR:C	1.35	1.47
1:P:1924:ARG:HB3	2:B:243:HIS:CB	1.45	1.46
3:L:146:PRO:HD2	3:L:203:HIS:NE2	1.24	1.45
1:P:704:LEU:CD1	1:P:772:LYS:O	1.64	1.45
2:B:307:VAL:CA	2:B:307:VAL:N	1.80	1.45
3:L:146:PRO:CD	3:L:203:HIS:CE1	2.00	1.45
4:H:71:ALA:CA	4:H:84:ALA:HB3	1.41	1.45
2:A:401:ARG:NH2	2:B:416:ILE:HB	1.26	1.45
3:L:124:PRO:N	3:L:124:PRO:CA	1.70	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1926:SER:HB3	2:B:242:CYS:SG	1.57	1.44
2:B:309:PRO:N	2:B:309:PRO:CA	1.70	1.44
2:B:256:LEU:CB	2:B:315:TRP:CZ3	1.81	1.44
2:B:391:PRO:N	2:B:391:PRO:CA	1.69	1.43
2:B:385:GLN:CB	2:B:430:PHE:HA	1.45	1.43
2:A:374:PHE:HB2	2:A:411:PHE:CB	1.47	1.43
1:P:719:LYS:HB2	1:P:1101:THR:CG2	0.95	1.42
2:B:402:GLN:CG	2:B:411:PHE:CE2	2.00	1.42
4:H:36:TRP:CG	4:H:83:LEU:HD22	1.55	1.41
2:A:355:PRO:CA	2:A:355:PRO:N	1.69	1.40
4:H:129:PRO:CB	4:H:218:VAL:HG12	1.48	1.40
2:A:281:TRP:CE3	2:A:325:ALA:HB2	1.56	1.40
4:H:36:TRP:CD1	4:H:83:LEU:HD22	1.55	1.40
2:B:404:PRO:N	2:B:404:PRO:CA	1.70	1.40
2:A:354:PRO:CA	2:B:352:LEU:HD13	1.50	1.39
4:H:71:ALA:C	4:H:84:ALA:HB3	1.48	1.39
2:A:251:PRO:N	2:A:251:PRO:CA	1.70	1.39
2:B:354:PRO:CD	2:B:450:ARG:NH1	1.86	1.39
4:H:129:PRO:N	4:H:129:PRO:CA	1.70	1.39
2:A:374:PHE:CB	2:A:411:PHE:CB	1.97	1.38
2:B:376:PRO:N	2:B:376:PRO:CA	1.70	1.38
2:B:320:THR:CA	2:B:339:SER:HA	1.53	1.38
1:P:1883:LYS:C	1:P:1959:PHE:HB3	1.38	1.37
4:H:173:PRO:N	4:H:173:PRO:CA	1.70	1.37
4:H:122:PRO:N	4:H:122:PRO:CA	1.70	1.37
2:B:264:LEU:N	2:B:309:PRO:HB3	1.35	1.37
2:B:345:PHE:CB	2:B:410:THR:HG21	1.52	1.37
1:P:687:ASP:CG	1:P:1101:THR:CG2	1.90	1.36
2:B:341:SER:OG	2:B:438:ALA:CB	1.71	1.36
3:L:40:TRP:HZ3	3:L:93:CYS:N	1.20	1.35
3:L:146:PRO:HD2	3:L:203:HIS:CD2	1.59	1.34
4:H:29:ALA:HB1	4:H:54:ALA:N	1.41	1.34
2:A:281:TRP:CZ3	2:A:325:ALA:CB	2.08	1.34
2:B:285:SER:CB	2:B:314:PRO:HB3	1.55	1.34
1:P:719:LYS:HB2	1:P:1101:THR:CB	1.55	1.34
2:B:320:THR:HB	2:B:339:SER:CB	1.56	1.33
2:B:272:ARG:HH12	2:B:301:CYS:N	0.88	1.33
2:B:376:PRO:HD3	2:B:436:HIS:ND1	1.41	1.33
3:L:145:TYR:C	3:L:203:HIS:HE1	1.33	1.33
1:P:1883:LYS:O	1:P:1959:PHE:CB	1.74	1.32
1:P:774:LYS:HB2	1:P:785:ASN:ND2	1.41	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:348:GLU:O	2:A:372:ARG:HG2	1.17	1.32
3:L:145:TYR:C	3:L:203:HIS:CE1	2.07	1.32
1:P:1580:TYR:HA	4:H:227:PRO:CD	1.58	1.32
4:H:6:ALA:CB	4:H:113:THR:HB	1.59	1.32
2:B:307:VAL:HG12	2:B:309:PRO:CG	1.42	1.31
1:P:1883:LYS:O	1:P:1959:PHE:CD2	1.82	1.31
1:P:1926:SER:HA	2:B:243:HIS:CA	1.60	1.31
1:P:687:ASP:CG	1:P:1101:THR:HG23	1.18	1.31
1:P:1884:GLN:N	1:P:1959:PHE:HB2	1.44	1.30
1:P:687:ASP:OD2	1:P:1101:THR:CG2	1.77	1.30
2:B:251:PRO:HB3	2:B:321:PHE:CD2	1.66	1.30
2:B:282:THR:OG1	2:B:283:PRO:HD3	1.20	1.30
3:L:40:TRP:CZ3	3:L:93:CYS:N	1.96	1.30
1:P:1924:ARG:CB	2:B:243:HIS:HB3	1.61	1.30
2:B:256:LEU:HB3	2:B:315:TRP:CH2	1.66	1.30
2:B:249:HIS:ND1	2:B:268:LEU:CD2	1.93	1.30
1:P:920:VAL:HG11	1:P:1374:ILE:CG2	1.60	1.29
3:L:103:PHE:CD2	4:H:37:VAL:HG23	1.68	1.29
2:A:354:PRO:CB	2:A:355:PRO:HD3	1.63	1.28
2:B:264:LEU:HB3	2:B:307:VAL:CA	1.64	1.28
2:B:350:HIS:CB	2:B:370:LEU:HB2	1.63	1.28
2:B:307:VAL:CA	2:B:307:VAL:CB	2.09	1.27
1:P:947:LYS:CD	1:P:1084:LYS:HB3	1.63	1.27
1:P:1580:TYR:CA	4:H:227:PRO:HD2	1.64	1.27
4:H:114:LEU:HB2	4:H:154:GLU:OE1	1.22	1.27
1:P:744:TYR:OH	1:P:772:LYS:HD3	1.32	1.26
1:P:1840:TYR:CA	4:H:138:ASP:HB2	1.66	1.26
1:P:719:LYS:CB	1:P:1101:THR:HG21	1.55	1.25
1:P:836:TYR:CE1	1:P:1093:LEU:HD13	1.70	1.25
1:P:721:SER:CA	1:P:1102:SER:HA	1.47	1.25
4:H:71:ALA:CB	4:H:84:ALA:HB1	1.60	1.25
2:A:299:CYS:SG	2:B:298:LEU:CD1	2.25	1.25
4:H:153:GLN:HG2	4:H:183:TYR:CD2	1.71	1.25
2:B:402:GLN:HG2	2:B:411:PHE:CD2	1.72	1.25
1:P:1926:SER:CB	2:B:243:HIS:CB	2.15	1.24
2:B:354:PRO:HD2	2:B:450:ARG:NH1	0.94	1.24
3:L:11:LEU:HD12	3:L:19:ALA:CB	1.65	1.24
2:B:268:LEU:CD1	2:B:325:ALA:HB3	1.68	1.24
3:L:40:TRP:CZ3	3:L:93:CYS:CB	2.21	1.24
2:B:307:VAL:CB	2:B:307:VAL:HA	1.65	1.24
4:H:71:ALA:CB	4:H:84:ALA:HB3	1.57	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:THR:CG2	2:B:292:GLY:CA	2.16	1.24
3:L:11:LEU:CD1	3:L:19:ALA:CB	2.14	1.24
1:P:1926:SER:CB	2:B:242:CYS:SG	2.17	1.24
1:P:1090:PRO:O	1:P:1092:THR:N	1.71	1.23
4:H:22:CYS:O	4:H:80:ALA:HB1	1.25	1.23
2:A:374:PHE:HB3	2:A:411:PHE:CG	1.72	1.23
3:L:146:PRO:CD	3:L:203:HIS:NE2	1.97	1.23
2:B:265:THR:HG21	2:B:292:GLY:CA	1.69	1.23
3:L:146:PRO:N	3:L:203:HIS:CE1	2.07	1.22
2:B:266:CYS:O	2:B:305:SER:OG	1.58	1.22
1:P:1091:LEU:C	1:P:1093:LEU:H	1.47	1.22
2:A:253:LEU:CD1	2:A:437:GLU:HB3	1.70	1.22
2:B:372:ARG:O	2:B:434:VAL:HB	1.34	1.22
4:H:19:LYS:HD3	4:H:83:LEU:O	1.12	1.22
2:A:401:ARG:HH22	2:B:416:ILE:CB	1.51	1.21
3:L:1:ALA:HB1	4:H:46:GLU:CG	1.68	1.21
1:P:684:ASN:CB	1:P:1104:LYS:O	1.89	1.20
3:L:124:PRO:HD3	4:H:133:CYS:CB	1.69	1.20
1:P:1883:LYS:O	1:P:1959:PHE:HB3	1.30	1.20
1:P:924:GLU:H	1:P:1361:ASN:CB	1.53	1.20
3:L:123:PHE:CE1	4:H:132:LEU:CD1	2.22	1.20
3:L:142:ASN:CA	3:L:179:SER:HB2	1.72	1.20
1:P:947:LYS:CD	1:P:1084:LYS:CB	2.18	1.19
2:B:253:LEU:HA	2:B:315:TRP:CH2	1.77	1.19
4:H:10:ALA:CB	4:H:152:PRO:HG2	1.71	1.19
1:P:1958:ILE:C	1:P:1959:PHE:N	2.01	1.19
2:A:279:PHE:CE2	2:A:291:GLN:HG2	1.76	1.19
4:H:4:LEU:HD22	4:H:98:CYS:O	1.37	1.19
2:B:256:LEU:HB3	2:B:315:TRP:CZ3	1.19	1.18
3:L:86:GLU:C	3:L:173:SER:HB3	1.68	1.18
2:B:264:LEU:CB	2:B:307:VAL:HA	1.73	1.18
2:B:372:ARG:O	2:B:434:VAL:CB	1.92	1.18
3:L:42:ALA:CB	3:L:91:TYR:CD1	2.27	1.17
4:H:129:PRO:HB3	4:H:218:VAL:CG1	1.74	1.17
1:P:727:TYR:HD2	1:P:1288:LEU:CD2	1.58	1.17
3:L:42:ALA:HB1	3:L:91:TYR:CE1	1.79	1.17
1:P:1882:LEU:HG	1:P:1960:GLU:HA	1.25	1.17
1:P:1883:LYS:O	1:P:1959:PHE:CG	1.98	1.17
3:L:108:ARG:O	3:L:110:GLU:CD	1.87	1.17
2:B:264:LEU:HB2	2:B:309:PRO:CA	1.74	1.16
2:B:354:PRO:CD	2:B:450:ARG:HH12	1.51	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:920:VAL:CG1	1:P:1374:ILE:HG23	1.76	1.16
4:H:6:ALA:HB1	4:H:113:THR:HB	1.19	1.16
1:P:719:LYS:CB	1:P:1101:THR:HB	1.75	1.16
1:P:1006:ARG:NH2	4:H:159:THR:HB	1.61	1.16
2:A:418:ARG:NH2	2:B:370:LEU:HD11	1.60	1.16
3:L:103:PHE:CD2	4:H:37:VAL:CG2	2.27	1.16
1:P:719:LYS:CG	1:P:1101:THR:HG21	1.75	1.15
1:P:1840:TYR:HA	4:H:138:ASP:CB	1.77	1.15
2:B:321:PHE:HB2	2:B:338:LEU:HB3	1.29	1.15
4:H:29:ALA:HB2	4:H:54:ALA:HB2	1.27	1.15
1:P:924:GLU:H	1:P:1361:ASN:HB3	1.08	1.15
2:B:320:THR:HB	2:B:339:SER:OG	1.46	1.15
1:P:704:LEU:HD13	1:P:772:LYS:O	1.38	1.15
2:B:353:PRO:HG3	2:B:450:ARG:H	1.04	1.14
2:B:385:GLN:NE2	2:B:430:PHE:HD1	1.43	1.14
1:P:836:TYR:HE1	1:P:1093:LEU:HD13	0.97	1.14
2:A:291:GLN:HA	2:A:306:SER:CA	1.78	1.14
2:A:348:GLU:CG	2:A:372:ARG:HD3	1.76	1.14
2:B:320:THR:HB	2:B:339:SER:CA	1.77	1.14
3:L:142:ASN:HA	3:L:179:SER:HB2	1.16	1.14
4:H:17:SER:CB	4:H:86:ALA:HA	1.76	1.13
2:B:256:LEU:HD13	2:B:315:TRP:CD2	1.71	1.13
1:P:1840:TYR:HA	4:H:138:ASP:HB2	1.14	1.13
2:A:354:PRO:HA	2:B:352:LEU:HD13	1.30	1.13
2:B:249:HIS:HB3	2:B:267:THR:O	1.46	1.13
1:P:686:SER:CB	1:P:1101:THR:C	2.21	1.13
1:P:721:SER:CA	1:P:1102:SER:CA	2.26	1.13
1:P:1091:LEU:O	1:P:1093:LEU:N	1.81	1.13
1:P:1885:VAL:CG1	1:P:1959:PHE:CE2	2.31	1.13
4:H:71:ALA:N	4:H:84:ALA:O	1.81	1.13
1:P:706:GLY:HA2	1:P:772:LYS:HE2	1.30	1.12
1:P:719:LYS:CB	1:P:1101:THR:CB	2.19	1.12
1:P:1883:LYS:C	1:P:1959:PHE:HB2	1.53	1.12
1:P:704:LEU:HD11	1:P:772:LYS:O	1.36	1.12
2:B:350:HIS:HB3	2:B:370:LEU:CB	1.78	1.12
4:H:131:SER:HB3	4:H:219:PRO:HG3	1.15	1.12
2:B:375:SER:HB3	2:B:436:HIS:CE1	1.83	1.12
3:L:11:LEU:HD11	3:L:19:ALA:HB1	1.27	1.12
2:B:307:VAL:HA	2:B:309:PRO:HD3	1.32	1.12
2:B:320:THR:HA	2:B:339:SER:HA	1.25	1.12
2:B:345:PHE:CD2	2:B:410:THR:OG1	2.02	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:LEU:HD12	2:B:369:CYS:HB3	1.23	1.12
3:L:142:ASN:CB	3:L:179:SER:HB2	1.80	1.12
4:H:71:ALA:H	4:H:84:ALA:C	1.56	1.12
3:L:124:PRO:HD3	4:H:133:CYS:HB2	1.16	1.12
4:H:125:PRO:HB3	4:H:150:PHE:HB2	1.31	1.12
4:H:131:SER:HB3	4:H:219:PRO:CG	1.78	1.12
1:P:721:SER:HA	1:P:1102:SER:HA	1.25	1.11
1:P:1090:PRO:C	1:P:1092:THR:N	2.08	1.11
2:A:280:THR:O	2:A:325:ALA:HA	1.50	1.11
4:H:71:ALA:O	4:H:84:ALA:CB	1.96	1.11
1:P:684:ASN:HB3	1:P:1104:LYS:C	1.76	1.11
2:B:264:LEU:HD12	2:B:308:LEU:C	1.74	1.11
4:H:153:GLN:HG2	4:H:183:TYR:CE2	1.85	1.11
2:A:417:LEU:CD2	2:B:401:ARG:NH2	2.15	1.10
3:L:108:ARG:NH1	3:L:147:ARG:CZ	2.14	1.10
1:P:1926:SER:CA	2:B:242:CYS:O	1.98	1.10
2:B:262:ALA:O	2:B:309:PRO:C	1.93	1.10
4:H:29:ALA:HB3	4:H:54:ALA:HB3	1.18	1.10
3:L:40:TRP:CZ3	3:L:93:CYS:HB3	1.83	1.10
4:H:97:TYR:HD1	4:H:112:GLY:HA3	1.15	1.10
1:P:672:GLY:HA2	1:P:674:THR:HG21	1.19	1.10
2:A:321:PHE:CE2	2:A:377:LYS:NZ	2.20	1.10
1:P:681:GLU:OE2	1:P:1134:ASN:CG	1.94	1.09
1:P:684:ASN:HB3	1:P:1104:LYS:O	0.94	1.09
2:A:374:PHE:CB	2:A:411:PHE:CD2	2.35	1.09
4:H:19:LYS:CD	4:H:83:LEU:O	1.99	1.09
2:B:256:LEU:CB	2:B:315:TRP:CH2	2.29	1.09
2:B:385:GLN:HB3	2:B:430:PHE:HA	1.13	1.09
2:B:256:LEU:CD1	2:B:315:TRP:CD2	2.31	1.09
2:B:349:VAL:HG13	2:B:432:CYS:HB2	1.27	1.09
1:P:728:ILE:HG22	1:P:1289:ALA:HB3	1.24	1.09
1:P:1883:LYS:O	1:P:1963:LYS:HD3	1.50	1.09
1:P:1924:ARG:HH12	2:B:243:HIS:CA	1.65	1.09
2:B:341:SER:OG	2:B:438:ALA:HB2	1.42	1.09
3:L:123:PHE:CD1	4:H:132:LEU:CD1	2.36	1.09
4:H:19:LYS:HZ3	4:H:83:LEU:C	1.59	1.09
2:A:354:PRO:CB	2:B:352:LEU:HD13	1.81	1.09
2:B:345:PHE:HB2	2:B:410:THR:HG21	1.18	1.09
4:H:40:ALA:HB2	4:H:94:ALA:CB	1.83	1.09
3:L:18:ALA:CB	3:L:83:VAL:HG22	1.69	1.08
1:P:1885:VAL:CG1	1:P:1959:PHE:HE2	1.65	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1924:ARG:HA	2:B:245:ARG:HB2	1.09	1.08
1:P:1927:ASN:N	2:B:242:CYS:HB2	1.66	1.08
2:A:290:VAL:O	2:A:307:VAL:N	1.86	1.08
4:H:12:ALA:HB3	4:H:117:VAL:HG22	1.29	1.08
4:H:71:ALA:O	4:H:84:ALA:N	1.86	1.08
2:B:272:ARG:NH1	2:B:301:CYS:N	1.72	1.08
2:B:375:SER:HB3	2:B:436:HIS:HE1	1.09	1.08
1:P:715:PHE:CD2	1:P:1295:THR:HG22	1.89	1.07
1:P:1439:VAL:HG12	1:P:1443:ILE:HD11	1.23	1.07
3:L:29:ALA:HB1	3:L:37:ALA:O	1.54	1.07
3:L:64:PRO:HB3	3:L:87:ASP:OD2	1.53	1.07
1:P:947:LYS:CG	1:P:1084:LYS:HB3	1.83	1.07
2:A:354:PRO:HB2	2:A:355:PRO:HD3	1.12	1.07
3:L:23:CYS:SG	3:L:76:PHE:HE1	1.76	1.07
1:P:780:PHE:HD1	1:P:799:HIS:O	1.35	1.07
1:P:1926:SER:HB2	2:B:243:HIS:HB2	1.37	1.07
2:A:244:PRO:HA	2:A:269:THR:O	1.53	1.07
2:A:417:LEU:HD21	2:B:401:ARG:NH2	1.68	1.07
2:B:385:GLN:HG2	2:B:430:PHE:CA	1.84	1.07
2:A:348:GLU:O	2:A:372:ARG:CG	2.02	1.07
4:H:71:ALA:O	4:H:84:ALA:HB3	1.54	1.07
3:L:18:ALA:HB2	3:L:83:VAL:HG22	1.21	1.06
1:P:686:SER:HB3	1:P:1101:THR:O	1.54	1.06
1:P:721:SER:N	1:P:1102:SER:HA	1.69	1.06
1:P:947:LYS:HD2	1:P:1084:LYS:CB	1.86	1.06
1:P:687:ASP:OD2	1:P:1101:THR:HG23	0.88	1.06
2:B:376:PRO:HD3	2:B:436:HIS:CE1	1.91	1.06
2:B:376:PRO:CB	2:B:437:GLU:HG3	1.84	1.06
2:B:376:PRO:HG2	2:B:437:GLU:H	1.18	1.06
3:L:144:PHE:HE2	3:L:149:ALA:CB	1.68	1.06
4:H:36:TRP:CG	4:H:83:LEU:CD2	2.37	1.06
2:B:264:LEU:HD13	2:B:307:VAL:C	1.80	1.06
3:L:40:TRP:CH2	3:L:93:CYS:SG	2.49	1.06
2:A:279:PHE:HE2	2:A:291:GLN:CG	1.69	1.05
2:A:299:CYS:SG	2:B:298:LEU:HB3	1.95	1.05
2:B:353:PRO:HG3	2:B:450:ARG:N	1.70	1.05
1:P:924:GLU:N	1:P:1361:ASN:CB	2.17	1.05
3:L:22:ALA:HB1	3:L:76:PHE:O	1.54	1.05
1:P:836:TYR:CD1	1:P:1093:LEU:CD2	2.05	1.05
1:P:924:GLU:N	1:P:1361:ASN:ND2	2.05	1.05
1:P:947:LYS:HD2	1:P:1084:LYS:CG	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:22:CYS:O	4:H:80:ALA:CB	2.05	1.05
3:L:18:ALA:N	3:L:83:VAL:HG21	1.71	1.05
4:H:10:ALA:HB1	4:H:152:PRO:CG	1.86	1.05
1:P:681:GLU:OE2	1:P:1134:ASN:CB	2.02	1.05
1:P:774:LYS:CB	1:P:785:ASN:ND2	2.19	1.05
4:H:17:SER:HB2	4:H:86:ALA:CA	1.87	1.05
3:L:18:ALA:CA	3:L:83:VAL:CG2	2.35	1.04
4:H:40:ALA:CA	4:H:94:ALA:HB1	1.86	1.04
2:B:251:PRO:HB3	2:B:321:PHE:HD2	0.91	1.04
2:B:327:TYR:CD1	2:B:328:PRO:HD2	1.92	1.04
3:L:6:GLN:OE1	3:L:106:GLY:N	1.87	1.04
2:A:348:GLU:HG2	2:A:372:ARG:CD	1.86	1.04
2:B:264:LEU:N	2:B:309:PRO:CB	2.20	1.04
2:B:272:ARG:HH12	2:B:300:GLY:C	1.65	1.04
3:L:1:ALA:HB1	4:H:46:GLU:HG2	1.39	1.04
4:H:29:ALA:HB1	4:H:54:ALA:CA	1.86	1.04
1:P:672:GLY:CA	1:P:674:THR:CG2	2.36	1.04
2:B:385:GLN:CB	2:B:430:PHE:CA	2.36	1.04
4:H:10:ALA:HA	4:H:116:THR:H	1.23	1.04
1:P:719:LYS:HB2	1:P:1101:THR:HG22	1.08	1.03
2:B:353:PRO:HB3	2:B:450:ARG:HD2	1.35	1.03
3:L:56:ALA:HB1	3:L:70:SER:HA	1.39	1.03
4:H:10:ALA:HB1	4:H:152:PRO:HG2	1.04	1.03
2:A:253:LEU:HD11	2:A:437:GLU:CB	1.87	1.03
4:H:12:ALA:HB3	4:H:117:VAL:CG2	1.88	1.03
1:P:724:LYS:HZ2	1:P:1219:ASN:HB2	1.17	1.03
2:B:345:PHE:HB2	2:B:410:THR:CG2	1.88	1.03
1:P:728:ILE:HG22	1:P:1289:ALA:CB	1.87	1.03
1:P:728:ILE:CG2	1:P:1289:ALA:HB3	1.87	1.03
1:P:920:VAL:HG11	1:P:1374:ILE:HG23	1.03	1.03
1:P:947:LYS:HD2	1:P:1084:LYS:HB3	1.37	1.03
2:B:385:GLN:HB3	2:B:430:PHE:CA	1.89	1.03
3:L:108:ARG:HH12	3:L:147:ARG:CZ	1.71	1.03
1:P:683:ARG:HH11	1:P:1138:ILE:HG13	1.19	1.03
1:P:923:TYR:C	1:P:1361:ASN:HD22	1.65	1.03
2:A:343:ASN:ND2	2:A:411:PHE:HE2	1.57	1.02
2:A:354:PRO:HA	2:B:352:LEU:CD1	1.89	1.02
3:L:40:TRP:CZ3	3:L:93:CYS:CA	2.41	1.02
1:P:780:PHE:CD1	1:P:799:HIS:O	2.12	1.02
2:A:401:ARG:NH2	2:B:416:ILE:CB	2.16	1.02
4:H:29:ALA:O	4:H:53:ALA:HB1	1.60	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:774:LYS:H	1:P:774:LYS:HD3	1.24	1.02
2:B:264:LEU:HB2	2:B:309:PRO:CB	1.90	1.02
3:L:40:TRP:CE3	3:L:93:CYS:HB3	1.94	1.02
4:H:29:ALA:CB	4:H:54:ALA:H	1.72	1.02
1:P:1924:ARG:NH1	2:B:243:HIS:CA	2.23	1.02
2:A:291:GLN:CB	2:A:306:SER:HB2	1.88	1.02
2:B:249:HIS:CE1	2:B:334:LEU:CD1	2.42	1.02
2:A:384:LEU:HD23	2:A:431:SER:O	1.56	1.02
2:B:376:PRO:HB2	2:B:437:GLU:HG3	1.39	1.02
2:A:257:LEU:HD21	2:A:315:TRP:HE1	1.20	1.01
2:B:307:VAL:HG13	2:B:309:PRO:HB3	1.38	1.01
2:B:376:PRO:CD	2:B:436:HIS:ND1	2.22	1.01
4:H:114:LEU:CB	4:H:154:GLU:OE1	2.05	1.01
1:P:727:TYR:CD2	1:P:1288:LEU:CD2	2.43	1.01
2:A:291:GLN:HA	2:A:306:SER:HA	1.04	1.01
2:A:417:LEU:CD1	2:B:404:PRO:HG3	1.89	1.01
2:B:351:LEU:CD1	2:B:369:CYS:HB3	1.91	1.01
2:B:361:LEU:HD23	2:B:361:LEU:H	1.26	1.01
4:H:21:SER:HA	4:H:81:ALA:O	1.60	1.01
1:P:729:PRO:HD3	1:P:1290:SER:HA	1.42	1.01
2:A:354:PRO:HB2	2:A:355:PRO:CD	1.89	1.01
1:P:686:SER:HB3	1:P:1101:THR:CA	1.90	1.01
1:P:1840:TYR:C	4:H:138:ASP:HB2	1.86	1.01
2:B:352:LEU:HG	2:B:353:PRO:HD2	1.38	1.01
3:L:140:LEU:HD23	3:L:181:SER:OG	1.61	1.01
1:P:724:LYS:NZ	1:P:1219:ASN:HB2	1.74	1.01
1:P:1105:LYS:O	1:P:1107:SER:N	1.93	1.01
1:P:1923:PRO:HD2	2:B:245:ARG:HD2	1.41	1.01
2:B:251:PRO:CB	2:B:321:PHE:CD2	2.44	1.01
4:H:127:VAL:HG11	4:H:206:VAL:HG11	1.42	1.01
2:B:285:SER:HB2	2:B:314:PRO:HB3	1.39	1.00
4:H:4:LEU:CD2	4:H:98:CYS:O	2.08	1.00
2:A:418:ARG:HH22	2:B:370:LEU:CD1	1.72	1.00
2:B:251:PRO:CB	2:B:321:PHE:HD2	1.72	1.00
2:B:307:VAL:CG1	2:B:309:PRO:CB	2.21	1.00
2:B:345:PHE:HB3	2:B:410:THR:HG21	1.44	1.00
3:L:144:PHE:HE2	3:L:149:ALA:HB2	1.24	1.00
1:P:1924:ARG:HA	2:B:245:ARG:CB	1.90	1.00
1:P:1926:SER:C	2:B:242:CYS:HB2	1.87	1.00
4:H:12:ALA:O	4:H:117:VAL:HG13	1.60	1.00
4:H:71:ALA:C	4:H:84:ALA:CB	2.33	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:114:LEU:HB2	4:H:154:GLU:CD	1.75	1.00
2:A:354:PRO:CA	2:B:352:LEU:CD1	2.40	1.00
2:B:256:LEU:HD13	2:B:315:TRP:CE2	1.97	1.00
2:B:345:PHE:CB	2:B:410:THR:CG2	2.40	1.00
3:L:108:ARG:O	3:L:110:GLU:OE1	1.80	1.00
3:L:146:PRO:HD2	3:L:203:HIS:CE1	1.83	1.00
1:P:1882:LEU:CG	1:P:1960:GLU:HA	1.91	0.99
4:H:6:ALA:HB1	4:H:113:THR:CB	1.92	0.99
3:L:18:ALA:CA	3:L:83:VAL:HG21	1.92	0.99
3:L:123:PHE:HE1	4:H:132:LEU:HD13	1.26	0.99
3:L:142:ASN:HA	3:L:179:SER:CB	1.93	0.99
1:P:685:VAL:H	1:P:1104:LYS:HD2	1.28	0.98
1:P:771:LYS:HD3	1:P:781:THR:HG21	1.44	0.98
1:P:1924:ARG:CZ	2:B:243:HIS:HB2	1.93	0.98
2:A:348:GLU:HG2	2:A:372:ARG:HD3	1.02	0.98
2:B:383:TRP:HD1	2:B:432:CYS:HA	1.24	0.98
4:H:71:ALA:CA	4:H:84:ALA:CB	2.31	0.98
1:P:1926:SER:HA	2:B:242:CYS:O	1.34	0.98
1:P:672:GLY:C	1:P:674:THR:HG21	1.70	0.98
2:B:249:HIS:CE1	2:B:334:LEU:HD13	1.98	0.98
1:P:719:LYS:HB3	1:P:1101:THR:HB	1.45	0.98
1:P:1933:ASP:CB	2:A:296:ARG:HD2	1.94	0.98
2:A:279:PHE:HE2	2:A:291:GLN:HG2	0.84	0.98
2:A:371:ALA:H	2:A:414:THR:CA	1.77	0.98
2:B:345:PHE:HD2	2:B:410:THR:OG1	1.36	0.98
3:L:108:ARG:O	3:L:110:GLU:OE2	1.80	0.98
4:H:34:ALA:O	4:H:51:ILE:HG22	1.63	0.98
1:P:924:GLU:N	1:P:1361:ASN:HD22	1.58	0.98
1:P:1926:SER:CA	2:B:243:HIS:CA	2.42	0.98
3:L:1:ALA:CB	4:H:46:GLU:HG2	1.93	0.98
2:B:385:GLN:NE2	2:B:430:PHE:CD1	2.22	0.98
1:P:687:ASP:HB3	1:P:1100:SER:HB3	1.44	0.98
1:P:1881:ASN:O	1:P:1963:LYS:HB2	1.62	0.98
3:L:18:ALA:CB	3:L:83:VAL:HG21	1.93	0.98
2:A:418:ARG:HH22	2:B:370:LEU:HD11	0.82	0.97
2:A:321:PHE:HE2	2:A:377:LYS:HZ1	1.12	0.97
2:B:372:ARG:C	2:B:434:VAL:HB	1.88	0.97
1:P:721:SER:HA	1:P:1102:SER:CA	1.88	0.97
1:P:727:TYR:CD2	1:P:1288:LEU:HD23	2.00	0.97
2:A:354:PRO:CG	2:A:355:PRO:HD3	1.94	0.97
3:L:86:GLU:HA	3:L:173:SER:HB2	1.42	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:97:TYR:CD1	4:H:112:GLY:HA3	1.98	0.97
2:B:320:THR:CB	2:B:339:SER:CB	2.43	0.97
4:H:19:LYS:NZ	4:H:83:LEU:C	2.23	0.97
2:A:381:VAL:HG13	2:A:416:ILE:N	1.79	0.97
2:A:381:VAL:HG13	2:A:416:ILE:H	1.27	0.97
4:H:29:ALA:O	4:H:53:ALA:CB	2.12	0.97
4:H:37:VAL:N	4:H:96:TYR:HB3	1.80	0.97
4:H:131:SER:CB	4:H:219:PRO:HG3	1.95	0.97
3:L:22:ALA:HB2	3:L:77:ALA:HA	1.46	0.96
1:P:683:ARG:NH1	1:P:1138:ILE:HG13	1.79	0.96
1:P:685:VAL:N	1:P:1104:LYS:HD2	1.79	0.96
1:P:947:LYS:HD3	1:P:1084:LYS:CB	1.93	0.96
3:L:42:ALA:HB1	3:L:91:TYR:CD1	1.96	0.96
2:B:282:THR:OG1	2:B:283:PRO:CD	2.13	0.96
2:B:307:VAL:CA	2:B:309:PRO:HD3	1.95	0.96
2:A:287:LYS:HD3	2:A:311:CYS:HB3	1.48	0.96
2:B:320:THR:CB	2:B:339:SER:HA	1.95	0.96
2:B:382:ARG:NH1	2:B:395:TYR:OH	1.98	0.96
3:L:40:TRP:HZ3	3:L:93:CYS:H	1.11	0.96
2:A:246:LEU:HD13	2:A:337:THR:H	1.27	0.95
3:L:11:LEU:HD11	3:L:19:ALA:CB	1.89	0.95
2:A:370:LEU:HA	2:A:414:THR:HA	1.48	0.95
2:B:423:ASP:CG	2:B:426:LYS:HZ1	1.74	0.95
2:B:307:VAL:HB	2:B:307:VAL:HA	0.95	0.95
2:B:327:TYR:CD1	2:B:328:PRO:CD	2.49	0.95
2:B:349:VAL:HG22	2:B:432:CYS:O	1.65	0.95
1:P:744:TYR:HH	1:P:772:LYS:HD3	1.21	0.95
3:L:1:ALA:HB1	4:H:46:GLU:HG3	1.43	0.95
4:H:17:SER:HB2	4:H:86:ALA:HA	0.95	0.95
2:A:417:LEU:HD22	2:B:404:PRO:CG	1.95	0.95
2:B:264:LEU:HD13	2:B:308:LEU:N	1.81	0.95
1:P:1440:TYR:CE2	1:P:1444:THR:HG21	2.00	0.95
2:B:307:VAL:CB	2:B:309:PRO:HG3	1.96	0.95
4:H:86:ALA:N	4:H:86:ALA:HA	1.80	0.95
1:P:836:TYR:HA	1:P:1093:LEU:CD2	1.97	0.95
1:P:1924:ARG:HD2	2:B:245:ARG:CB	1.95	0.94
2:B:307:VAL:HG13	2:B:309:PRO:CG	1.68	0.94
2:B:385:GLN:CG	2:B:430:PHE:HA	1.96	0.94
4:H:159:THR:O	4:H:205:HIS:N	1.98	0.94
1:P:836:TYR:CE1	1:P:1093:LEU:CD1	2.50	0.94
1:P:1091:LEU:C	1:P:1093:LEU:N	2.21	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:417:LEU:HD21	2:B:401:ARG:HH21	1.27	0.94
2:B:264:LEU:CB	2:B:309:PRO:HB3	1.96	0.94
2:B:354:PRO:HD2	2:B:450:ARG:HH11	1.24	0.94
3:L:146:PRO:HD3	3:L:203:HIS:CE1	2.01	0.94
4:H:40:ALA:HB2	4:H:94:ALA:HB2	1.47	0.94
1:P:924:GLU:CA	1:P:1361:ASN:ND2	2.29	0.94
4:H:36:TRP:CD1	4:H:83:LEU:CD2	2.48	0.94
2:B:320:THR:CB	2:B:339:SER:CA	2.45	0.94
3:L:119:SER:O	3:L:141:LEU:HA	1.67	0.94
1:P:920:VAL:CG1	1:P:1374:ILE:CG2	2.38	0.94
1:P:1884:GLN:CA	1:P:1959:PHE:HB2	1.98	0.94
2:B:272:ARG:CZ	2:B:301:CYS:H	1.79	0.94
4:H:114:LEU:HB3	4:H:154:GLU:C	1.89	0.94
2:A:245:ARG:N	2:A:269:THR:O	1.99	0.94
2:A:321:PHE:HE2	2:A:377:LYS:NZ	1.57	0.94
2:A:417:LEU:CD2	2:B:401:ARG:HH22	1.79	0.94
1:P:774:LYS:CB	1:P:785:ASN:HD21	1.79	0.94
2:A:273:ASP:HB2	2:A:329:GLU:OE1	1.68	0.94
3:L:42:ALA:HA	3:L:91:TYR:HD1	1.30	0.94
3:L:45:PRO:HG3	3:L:170:GLU:HB2	1.50	0.94
1:P:1439:VAL:HG12	1:P:1443:ILE:CD1	1.97	0.93
1:P:1439:VAL:CG1	1:P:1443:ILE:HD11	1.97	0.93
3:L:18:ALA:HB2	3:L:83:VAL:HG21	1.45	0.93
3:L:18:ALA:HB2	3:L:83:VAL:HG23	0.94	0.93
4:H:6:ALA:CB	4:H:113:THR:CB	2.45	0.93
4:H:129:PRO:CB	4:H:218:VAL:CG1	2.38	0.93
1:P:1627:PRO:HG2	4:H:225:THR:HG21	1.50	0.93
3:L:108:ARG:HH12	3:L:147:ARG:NH1	1.66	0.93
1:P:719:LYS:HB2	1:P:1101:THR:HG21	1.09	0.93
2:B:264:LEU:CD1	2:B:308:LEU:C	2.40	0.93
2:A:287:LYS:HE2	2:A:311:CYS:CB	1.98	0.93
4:H:156:LEU:HD12	4:H:208:HIS:HA	1.49	0.93
2:B:265:THR:HG23	2:B:292:GLY:N	1.83	0.93
4:H:153:GLN:CG	4:H:183:TYR:CE2	2.51	0.93
2:B:264:LEU:CA	2:B:309:PRO:HB3	1.98	0.93
1:P:924:GLU:N	1:P:1361:ASN:HB3	1.81	0.93
2:B:264:LEU:HB3	2:B:307:VAL:CB	1.99	0.93
3:L:10:SER:CA	3:L:110:GLU:OE1	2.16	0.93
1:P:771:LYS:HA	1:P:771:LYS:NZ	1.83	0.92
4:H:153:GLN:HG2	4:H:183:TYR:CG	2.03	0.92
2:A:343:ASN:HD22	2:A:411:PHE:HE2	1.11	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:374:PHE:HD1	2:A:436:HIS:HE1	1.01	0.92
2:B:251:PRO:HA	2:B:266:CYS:HB3	1.51	0.92
4:H:19:LYS:HZ3	4:H:83:LEU:CA	1.82	0.92
4:H:40:ALA:CB	4:H:94:ALA:HB1	1.99	0.92
1:P:836:TYR:HE1	1:P:1093:LEU:CD1	1.81	0.92
3:L:214:PHE:HB2	4:H:133:CYS:SG	2.10	0.92
2:A:403:GLU:OE2	2:B:416:ILE:HD12	1.70	0.92
3:L:124:PRO:CD	4:H:133:CYS:HB2	1.98	0.92
2:A:307:VAL:HB	2:A:309:PRO:HD3	1.50	0.92
3:L:103:PHE:CE2	4:H:37:VAL:CG2	2.52	0.92
2:B:264:LEU:HD22	2:B:307:VAL:N	1.85	0.92
2:A:291:GLN:CA	2:A:306:SER:HA	1.98	0.92
2:B:268:LEU:HD13	2:B:325:ALA:HB3	1.50	0.92
2:A:354:PRO:C	2:B:352:LEU:HD13	1.94	0.92
2:B:423:ASP:CG	2:B:426:LYS:NZ	2.29	0.91
1:P:1883:LYS:HB2	1:P:1963:LYS:HD2	1.49	0.91
2:A:281:TRP:HZ3	2:A:325:ALA:CB	1.65	0.91
2:B:272:ARG:NH1	2:B:300:GLY:HA2	1.85	0.91
3:L:6:GLN:CD	3:L:106:GLY:H	1.78	0.91
2:B:282:THR:HG1	2:B:283:PRO:HD3	1.33	0.91
2:B:400:SER:OG	2:B:413:VAL:HG12	1.68	0.91
2:B:249:HIS:CB	2:B:267:THR:O	2.18	0.91
2:B:262:ALA:O	2:B:309:PRO:HB2	1.70	0.91
2:B:285:SER:CB	2:B:314:PRO:CB	2.48	0.91
4:H:40:ALA:CB	4:H:94:ALA:CB	2.48	0.91
2:B:320:THR:CA	2:B:339:SER:CA	2.46	0.91
2:B:349:VAL:HA	2:B:370:LEU:O	1.70	0.91
2:B:249:HIS:ND1	2:B:268:LEU:HD21	1.82	0.91
3:L:86:GLU:O	3:L:173:SER:HB3	1.71	0.91
2:B:307:VAL:HG13	2:B:309:PRO:HB2	1.53	0.91
3:L:42:ALA:CB	3:L:91:TYR:CE1	2.52	0.91
3:L:113:ARG:HH21	3:L:113:ARG:HG3	1.36	0.91
3:L:123:PHE:CE2	3:L:140:LEU:CD1	2.53	0.91
1:P:1883:LYS:CA	1:P:1959:PHE:HB3	2.01	0.90
1:P:1627:PRO:CG	4:H:225:THR:HG21	2.01	0.90
4:H:220:CYS:H	4:H:221:PRO:HD3	1.36	0.90
2:B:253:LEU:HG	2:B:315:TRP:CE3	2.05	0.90
3:L:23:CYS:SG	3:L:76:PHE:CE1	2.65	0.90
1:P:683:ARG:NH1	1:P:1138:ILE:CG1	2.34	0.90
2:B:299:CYS:O	2:B:299:CYS:SG	2.29	0.90
3:L:42:ALA:CA	3:L:91:TYR:HD1	1.84	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:354:PRO:CB	2:A:355:PRO:CD	2.49	0.90
2:B:341:SER:OG	2:B:438:ALA:HB1	1.68	0.90
2:A:417:LEU:HD13	2:B:404:PRO:HG3	1.50	0.90
3:L:40:TRP:CZ3	3:L:93:CYS:SG	2.65	0.90
2:B:379:VAL:CG1	2:B:437:GLU:HG2	2.01	0.90
2:A:287:LYS:HZ2	2:A:319:LYS:NZ	1.70	0.90
1:P:836:TYR:HA	1:P:1093:LEU:HD23	1.54	0.89
2:A:253:LEU:HD11	2:A:437:GLU:HB3	0.91	0.89
2:A:371:ALA:H	2:A:414:THR:HA	1.35	0.89
3:L:40:TRP:CE3	3:L:93:CYS:CA	2.55	0.89
1:P:727:TYR:HD2	1:P:1288:LEU:HD21	1.38	0.89
1:P:771:LYS:HA	1:P:771:LYS:CE	2.02	0.89
2:B:249:HIS:CE1	2:B:334:LEU:HD11	2.07	0.89
1:P:680:LEU:HD11	1:P:1203:ASN:ND2	1.88	0.89
1:P:836:TYR:CG	1:P:1093:LEU:HD22	2.07	0.89
2:B:264:LEU:HB3	2:B:309:PRO:HD3	1.52	0.89
2:B:273:ASP:OD2	2:B:327:TYR:HE1	1.55	0.89
4:H:29:ALA:HB1	4:H:54:ALA:CB	1.90	0.89
2:A:343:ASN:ND2	2:A:411:PHE:CE2	2.41	0.89
3:L:42:ALA:HB2	3:L:91:TYR:CD1	2.06	0.89
3:L:103:PHE:HD2	4:H:37:VAL:HG23	1.37	0.89
2:A:371:ALA:HB3	2:A:414:THR:N	1.88	0.89
4:H:40:ALA:HB2	4:H:94:ALA:HB1	1.53	0.89
1:P:706:GLY:HA2	1:P:772:LYS:CE	2.02	0.89
2:B:320:THR:N	2:B:339:SER:HA	1.86	0.89
3:L:146:PRO:CD	3:L:203:HIS:CD2	2.48	0.89
2:A:417:LEU:HD22	2:B:404:PRO:HG2	1.52	0.89
2:A:417:LEU:HD23	2:B:401:ARG:NH2	1.87	0.89
3:L:6:GLN:CG	3:L:105:ALA:HB1	2.03	0.89
2:B:385:GLN:CG	2:B:430:PHE:CA	2.46	0.88
2:B:385:GLN:HB2	2:B:430:PHE:HA	1.54	0.88
3:L:150:LYS:NZ	3:L:152:GLN:HG3	1.88	0.88
1:P:721:SER:HA	1:P:1102:SER:CB	2.03	0.88
1:P:780:PHE:O	1:P:801:ALA:CB	2.21	0.88
2:B:318:GLY:O	2:B:340:LYS:HA	1.73	0.88
3:L:108:ARG:C	3:L:110:GLU:OE2	2.17	0.88
2:B:265:THR:HG23	2:B:292:GLY:CA	2.03	0.88
2:A:254:GLU:OE2	2:A:435:GLY:HA3	1.74	0.88
2:B:243:HIS:CB	2:B:243:HIS:CA	2.51	0.88
2:B:249:HIS:ND1	2:B:268:LEU:HD23	1.85	0.88
2:A:374:PHE:HB3	2:A:411:PHE:CB	1.85	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:144:PHE:HE1	3:L:179:SER:HA	1.38	0.88
2:B:341:SER:HG	2:B:438:ALA:CB	1.83	0.88
1:P:1604:HIS:NE2	4:H:227:PRO:HB3	1.89	0.88
2:A:287:LYS:CD	2:A:311:CYS:HB3	2.03	0.88
3:L:142:ASN:CB	3:L:179:SER:CB	2.51	0.88
4:H:156:LEU:CD1	4:H:208:HIS:HA	2.04	0.88
1:P:1885:VAL:HG13	1:P:1959:PHE:HE2	1.05	0.87
2:A:296:ARG:HB3	2:A:296:ARG:CZ	2.01	0.87
1:P:1924:ARG:HD2	2:B:245:ARG:HB2	1.56	0.87
2:A:361:LEU:HD13	2:A:364:LEU:HD12	1.56	0.87
2:A:415:SER:OG	2:A:434:VAL:HG22	1.74	0.87
3:L:45:PRO:CD	3:L:170:GLU:HG2	2.05	0.87
1:P:1924:ARG:HB3	2:B:243:HIS:CG	2.09	0.87
2:A:417:LEU:HD23	2:B:401:ARG:HH22	1.37	0.87
2:A:371:ALA:HB3	2:A:414:THR:H	1.39	0.87
3:L:118:PRO:HB2	3:L:141:LEU:HD12	1.57	0.87
2:B:287:LYS:HE3	2:B:308:LEU:HB3	1.56	0.87
2:B:372:ARG:O	2:B:434:VAL:CG2	2.23	0.87
4:H:204:CYS:SG	4:H:206:VAL:HG22	2.15	0.87
2:A:374:PHE:CD1	2:A:436:HIS:HE1	1.92	0.87
2:A:398:TRP:HB2	2:B:401:ARG:HD2	1.55	0.87
4:H:24:ALA:O	4:H:79:ALA:O	1.91	0.87
2:A:249:HIS:HE1	2:A:267:THR:HG22	1.38	0.87
1:P:1002:TYR:OH	4:H:163:SER:O	1.93	0.86
3:L:103:PHE:CE2	4:H:37:VAL:HB	2.09	0.86
3:L:123:PHE:HE1	4:H:132:LEU:CD1	1.81	0.86
4:H:19:LYS:HA	4:H:83:LEU:O	1.75	0.86
4:H:125:PRO:CB	4:H:150:PHE:HB2	2.05	0.86
4:H:153:GLN:CG	4:H:183:TYR:CD2	2.58	0.86
1:P:719:LYS:CD	1:P:1101:THR:HG21	2.04	0.86
1:P:780:PHE:O	1:P:801:ALA:HB3	1.74	0.86
1:P:1580:TYR:HA	4:H:227:PRO:HD2	0.88	0.86
2:A:398:TRP:HH2	2:B:414:THR:H	1.19	0.86
1:P:721:SER:HA	1:P:1102:SER:HB2	1.56	0.86
2:B:350:HIS:HB3	2:B:370:LEU:HB2	0.87	0.86
2:A:354:PRO:HB3	2:B:352:LEU:HB2	1.58	0.86
2:B:268:LEU:HD11	2:B:325:ALA:HB3	1.55	0.86
2:A:287:LYS:HE2	2:A:311:CYS:HB3	1.58	0.86
2:A:381:VAL:HG13	2:A:414:THR:O	1.75	0.86
2:B:291:GLN:HG3	2:B:305:SER:O	1.76	0.86
2:B:349:VAL:CG1	2:B:432:CYS:HB2	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:860:LYS:HD3	1:P:1091:LEU:HD21	1.57	0.86
1:P:1023:ASP:HB3	1:P:1048:SER:OG	1.75	0.86
3:L:113:ARG:HD2	3:L:176:SER:OG	1.75	0.86
1:P:923:TYR:CE1	1:P:1358:SER:O	2.28	0.85
2:B:264:LEU:H	2:B:309:PRO:HB3	1.40	0.85
4:H:69:ALA:O	4:H:86:ALA:N	2.09	0.85
1:P:681:GLU:CD	1:P:1134:ASN:HA	2.01	0.85
2:B:264:LEU:O	2:B:307:VAL:CA	2.24	0.85
3:L:66:ARG:HA	3:L:66:ARG:NE	1.91	0.85
1:P:1924:ARG:CA	2:B:245:ARG:HB2	2.02	0.85
2:B:249:HIS:ND1	2:B:268:LEU:HD22	1.88	0.85
2:A:374:PHE:HD1	2:A:436:HIS:CE1	1.93	0.85
1:P:947:LYS:HG2	1:P:1084:LYS:HB3	1.54	0.85
1:P:1096:VAL:HG13	1:P:1100:SER:OG	1.75	0.85
1:P:1883:LYS:O	1:P:1959:PHE:HD2	1.34	0.85
2:B:264:LEU:H	2:B:307:VAL:HG13	1.42	0.85
2:B:376:PRO:CD	2:B:436:HIS:CE1	2.60	0.85
4:H:131:SER:HA	4:H:219:PRO:HG2	1.57	0.85
2:B:345:PHE:CE1	2:B:408:THR:HB	2.10	0.85
3:L:41:TYR:O	3:L:92:TYR:N	2.09	0.85
3:L:144:PHE:CE2	3:L:149:ALA:HB2	2.10	0.85
3:L:147:ARG:HG3	3:L:178:TYR:CE2	2.11	0.85
4:H:208:HIS:CE1	4:H:214:GLN:OE1	2.28	0.85
2:B:245:ARG:NH2	2:B:331:LYS:HG2	1.91	0.85
2:B:265:THR:HG23	2:B:292:GLY:H	1.40	0.85
2:B:402:GLN:CG	2:B:411:PHE:HE2	1.63	0.85
3:L:86:GLU:CA	3:L:173:SER:CB	2.18	0.85
2:B:385:GLN:CG	2:B:430:PHE:CB	2.16	0.85
1:P:1933:ASP:OD2	2:A:296:ARG:CD	2.25	0.84
2:B:256:LEU:HB3	2:B:315:TRP:HZ3	1.03	0.84
2:B:307:VAL:HB	2:B:309:PRO:HD3	1.58	0.84
2:B:311:CYS:HB3	2:B:314:PRO:HG2	1.59	0.84
1:P:1579:ALA:O	4:H:227:PRO:HB2	1.76	0.84
4:H:37:VAL:H	4:H:96:TYR:HB3	1.42	0.84
2:A:381:VAL:HA	2:A:415:SER:HA	1.58	0.84
2:B:268:LEU:HD12	2:B:305:SER:HA	1.59	0.84
2:A:291:GLN:HA	2:A:306:SER:CB	2.08	0.84
2:A:342:GLY:O	2:A:375:SER:OG	1.93	0.84
2:A:350:HIS:O	2:A:368:THR:HG22	1.78	0.84
2:B:352:LEU:HG	2:B:353:PRO:CD	2.06	0.84
2:B:266:CYS:O	2:B:305:SER:CB	2.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:103:PHE:HE2	4:H:37:VAL:HB	1.43	0.84
2:A:371:ALA:H	2:A:414:THR:N	1.76	0.84
2:A:374:PHE:CG	2:A:411:PHE:HB2	2.11	0.84
2:B:249:HIS:HB3	2:B:268:LEU:HD23	1.60	0.84
2:B:423:ASP:OD1	2:B:426:LYS:NZ	2.11	0.84
4:H:29:ALA:HB1	4:H:54:ALA:H	1.05	0.84
3:L:18:ALA:CA	3:L:83:VAL:HG22	2.04	0.83
1:P:947:LYS:CD	1:P:1084:LYS:CG	2.53	0.83
2:B:264:LEU:O	2:B:307:VAL:N	2.10	0.83
3:L:104:GLY:HA2	4:H:45:LEU:HD12	1.60	0.83
1:P:1882:LEU:HA	1:P:1959:PHE:O	1.77	0.83
2:A:321:PHE:CD2	2:A:340:LYS:HB2	2.13	0.83
4:H:162:GLU:HG3	4:H:200:LYS:HE3	1.59	0.83
2:A:291:GLN:HB3	2:A:306:SER:HB2	1.61	0.83
2:B:307:VAL:CB	2:B:309:PRO:CG	2.53	0.83
1:P:683:ARG:HH11	1:P:1138:ILE:CG1	1.91	0.83
1:P:1926:SER:CB	2:B:243:HIS:CG	2.61	0.83
2:A:307:VAL:C	2:A:309:PRO:HD3	2.04	0.83
2:A:321:PHE:CD2	2:A:377:LYS:NZ	2.45	0.83
2:B:250:ARG:H	2:B:250:ARG:HD2	1.41	0.83
2:B:382:ARG:CZ	2:B:395:TYR:OH	2.27	0.83
3:L:42:ALA:CB	3:L:91:TYR:HD1	1.82	0.83
1:P:681:GLU:OE2	1:P:1134:ASN:HB3	1.76	0.83
2:B:285:SER:OG	2:B:314:PRO:HB3	1.77	0.83
2:B:264:LEU:HB3	2:B:307:VAL:HB	1.59	0.83
2:B:376:PRO:HB3	2:B:437:GLU:HG3	1.58	0.83
3:L:42:ALA:HB1	3:L:91:TYR:HE1	1.39	0.83
1:P:683:ARG:HG2	1:P:1135:LYS:HG3	1.59	0.83
4:H:208:HIS:NE2	4:H:214:GLN:OE1	2.12	0.83
1:P:1926:SER:CA	2:B:243:HIS:CB	2.56	0.83
3:L:195:LYS:O	3:L:195:LYS:HD3	1.79	0.83
4:H:40:ALA:HA	4:H:94:ALA:HB1	1.61	0.83
3:L:108:ARG:NH1	3:L:147:ARG:NH1	2.26	0.82
1:P:684:ASN:C	1:P:1104:LYS:HB3	2.04	0.82
3:L:144:PHE:CE1	3:L:179:SER:HA	2.13	0.82
2:A:417:LEU:CD2	2:B:404:PRO:CG	2.57	0.82
2:B:272:ARG:NH1	2:B:300:GLY:CA	2.43	0.82
3:L:123:PHE:HD1	4:H:132:LEU:HD13	1.36	0.82
4:H:131:SER:CB	4:H:219:PRO:CG	2.54	0.82
1:P:1440:TYR:CZ	1:P:1444:THR:HG21	2.15	0.82
2:B:320:THR:HA	2:B:339:SER:CA	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:THR:HA	2:B:338:LEU:O	1.77	0.82
2:B:385:GLN:HB3	2:B:431:SER:H	1.43	0.82
3:L:22:ALA:CB	3:L:76:PHE:O	2.27	0.82
2:A:343:ASN:HB3	2:A:375:SER:HA	1.59	0.82
2:B:251:PRO:HG2	2:B:338:LEU:HD12	1.61	0.82
2:A:299:CYS:CB	2:B:298:LEU:HD12	2.08	0.82
3:L:22:ALA:CB	3:L:77:ALA:HA	2.09	0.82
3:L:123:PHE:HE1	4:H:132:LEU:HD22	1.44	0.82
3:L:142:ASN:HB3	3:L:179:SER:HB2	1.61	0.82
1:P:1926:SER:HB2	2:B:243:HIS:CG	2.15	0.82
2:B:423:ASP:HA	2:B:426:LYS:HZ2	1.42	0.82
3:L:40:TRP:CE3	3:L:93:CYS:CB	2.59	0.82
3:L:10:SER:CB	3:L:110:GLU:OE1	2.28	0.81
3:L:123:PHE:HE1	4:H:132:LEU:CD2	1.93	0.81
4:H:220:CYS:H	4:H:221:PRO:CD	1.93	0.81
2:B:320:THR:CB	2:B:339:SER:OG	2.28	0.81
4:H:71:ALA:O	4:H:84:ALA:CA	2.28	0.81
4:H:52:ALA:HB2	4:H:60:ALA:HB2	1.63	0.81
1:P:1091:LEU:C	1:P:1092:THR:N	2.39	0.81
2:B:264:LEU:H	2:B:307:VAL:CG1	1.94	0.81
1:P:920:VAL:HG11	1:P:1374:ILE:HG21	1.62	0.81
1:P:947:LYS:HD3	1:P:1084:LYS:HB2	1.60	0.81
1:P:1885:VAL:HG13	1:P:1959:PHE:CD2	2.15	0.81
1:P:1924:ARG:CB	2:B:243:HIS:CG	2.64	0.81
2:B:385:GLN:CD	2:B:430:PHE:HB3	2.05	0.81
4:H:4:LEU:CB	4:H:22:CYS:SG	2.69	0.81
1:P:681:GLU:HB3	1:P:1134:ASN:HA	1.63	0.81
2:B:273:ASP:OD2	2:B:327:TYR:CE1	2.33	0.81
2:B:383:TRP:CD1	2:B:432:CYS:HA	2.14	0.80
4:H:19:LYS:HD3	4:H:83:LEU:C	2.06	0.80
2:A:271:LEU:HB2	2:A:302:TYR:O	1.81	0.80
3:L:10:SER:C	3:L:110:GLU:OE1	2.24	0.80
3:L:40:TRP:CZ3	3:L:92:TYR:C	2.58	0.80
4:H:43:LYS:HA	4:H:43:LYS:CE	2.10	0.80
2:B:379:VAL:HG23	2:B:381:VAL:CG2	2.12	0.80
4:H:19:LYS:NZ	4:H:84:ALA:N	2.29	0.80
2:A:355:PRO:HB2	2:A:358:GLU:HB3	1.62	0.80
2:A:374:PHE:CB	2:A:411:PHE:CG	2.44	0.80
2:A:374:PHE:CG	2:A:411:PHE:CB	2.64	0.80
1:P:1883:LYS:HB2	1:P:1963:LYS:CD	1.93	0.80
2:B:253:LEU:HG	2:B:315:TRP:CZ3	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:86:GLU:HA	3:L:173:SER:HB3	0.86	0.80
3:L:1:ALA:CB	4:H:46:GLU:CG	2.52	0.80
1:P:1924:ARG:CZ	2:B:243:HIS:CB	2.59	0.80
2:A:381:VAL:CG1	2:A:416:ILE:N	2.44	0.80
2:B:400:SER:OG	2:B:413:VAL:CG1	2.29	0.80
2:B:400:SER:OG	2:B:413:VAL:CB	2.29	0.80
3:L:113:ARG:CD	3:L:176:SER:OG	2.29	0.80
1:P:774:LYS:HB2	1:P:785:ASN:HD22	1.42	0.80
2:A:381:VAL:CG1	2:A:416:ILE:H	1.95	0.80
1:P:1046:PHE:CD1	1:P:1072:ARG:HG3	2.17	0.79
4:H:160:TRP:HE1	4:H:202:VAL:CG1	1.94	0.79
4:H:170:ARG:NH1	4:H:170:ARG:HA	1.97	0.79
2:A:291:GLN:CA	2:A:306:SER:HB2	2.12	0.79
1:P:836:TYR:HD1	1:P:1093:LEU:HD21	1.44	0.79
2:A:249:HIS:HE1	2:A:267:THR:CG2	1.96	0.79
2:A:371:ALA:CB	2:A:414:THR:H	1.95	0.79
2:B:264:LEU:HD22	2:B:307:VAL:CA	2.12	0.79
4:H:149:GLY:HA2	4:H:182:LEU:HD23	1.65	0.79
4:H:220:CYS:N	4:H:221:PRO:CD	2.45	0.79
1:P:1112:ILE:HG21	1:P:1139:VAL:HG11	1.63	0.79
3:L:123:PHE:CE1	4:H:132:LEU:HD22	2.18	0.79
2:B:398:TRP:CD1	2:B:398:TRP:H	1.99	0.79
2:A:244:PRO:CA	2:A:269:THR:O	2.30	0.79
2:B:345:PHE:HD2	2:B:410:THR:HG1	0.82	0.79
3:L:86:GLU:OE2	3:L:174:LYS:HA	1.83	0.79
4:H:95:ALA:HB2	4:H:114:LEU:HD12	1.62	0.79
1:P:1882:LEU:CD2	1:P:1960:GLU:HA	2.13	0.79
2:A:299:CYS:SG	2:B:298:LEU:CB	2.70	0.78
1:P:693:GLN:HB2	1:P:1294:VAL:HG23	1.65	0.78
3:L:147:ARG:HG3	3:L:178:TYR:CD2	2.18	0.78
1:P:685:VAL:H	1:P:1104:LYS:CD	1.96	0.78
1:P:724:LYS:HZ1	1:P:1219:ASN:C	1.91	0.78
1:P:1926:SER:HA	2:B:243:HIS:HA	1.65	0.78
2:A:271:LEU:HD13	2:A:303:SER:HA	1.63	0.78
2:B:268:LEU:CD1	2:B:325:ALA:CB	2.58	0.78
3:L:40:TRP:CE3	3:L:93:CYS:N	2.51	0.78
1:P:924:GLU:N	1:P:1361:ASN:CG	2.35	0.78
2:A:384:LEU:HD11	2:A:429:THR:HG23	1.62	0.78
4:H:4:LEU:HB3	4:H:22:CYS:SG	2.23	0.78
1:P:683:ARG:HH12	1:P:1138:ILE:HD11	1.47	0.78
1:P:1923:PRO:C	2:B:245:ARG:HG3	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:GLN:HB3	2:B:431:SER:N	1.97	0.78
3:L:144:PHE:CE2	3:L:149:ALA:CB	2.60	0.78
1:P:686:SER:HB2	1:P:1104:LYS:H	1.49	0.78
2:B:258:LEU:HD11	2:B:440:PRO:O	1.83	0.78
2:B:383:TRP:CZ2	2:B:413:VAL:HG22	2.19	0.78
3:L:146:PRO:HD3	3:L:203:HIS:ND1	1.99	0.78
1:P:1884:GLN:HA	1:P:1959:PHE:CG	2.19	0.78
2:B:265:THR:CB	2:B:292:GLY:HA3	2.13	0.78
2:A:287:LYS:CE	2:A:311:CYS:HB3	2.12	0.78
2:A:374:PHE:CB	2:A:411:PHE:HD2	1.84	0.78
2:B:448:ILE:HD12	2:B:448:ILE:O	1.84	0.78
3:L:40:TRP:CE3	3:L:40:TRP:HA	2.17	0.78
2:B:307:VAL:CB	2:B:309:PRO:HD3	2.14	0.78
1:P:1883:LYS:N	1:P:1959:PHE:HB3	1.98	0.78
1:P:1926:SER:N	2:B:243:HIS:CB	2.47	0.77
2:A:273:ASP:CB	2:A:329:GLU:OE1	2.32	0.77
2:A:436:HIS:O	2:A:440:PRO:HB3	1.84	0.77
4:H:19:LYS:NZ	4:H:82:ALA:C	2.42	0.77
4:H:159:THR:OG1	4:H:205:HIS:HB3	1.84	0.77
1:P:774:LYS:HD3	1:P:774:LYS:N	1.97	0.77
1:P:960:ARG:NH2	4:H:203:THR:OG1	2.16	0.77
2:A:343:ASN:O	2:A:375:SER:HA	1.83	0.77
2:B:351:LEU:HD12	2:B:369:CYS:CB	2.11	0.77
1:P:1924:ARG:HH12	2:B:243:HIS:C	1.93	0.77
2:A:256:LEU:HD12	2:A:256:LEU:O	1.84	0.77
2:B:321:PHE:CD2	2:B:338:LEU:HD13	2.19	0.77
3:L:11:LEU:N	3:L:110:GLU:OE1	2.17	0.77
4:H:129:PRO:HB2	4:H:218:VAL:HG12	1.60	0.77
1:P:686:SER:CB	1:P:1101:THR:O	2.29	0.77
1:P:1633:GLY:HA3	1:P:1802:ARG:HD3	1.67	0.77
2:B:322:THR:HA	2:B:336:ALA:H	1.50	0.77
2:B:385:GLN:HE21	2:B:430:PHE:HD1	0.82	0.77
3:L:48:ALA:HA	4:H:97:TYR:CE2	2.20	0.77
2:B:285:SER:HB3	2:B:314:PRO:HB3	1.62	0.77
2:B:402:GLN:CD	2:B:411:PHE:CE2	2.61	0.77
3:L:11:LEU:HD12	3:L:19:ALA:HB1	0.77	0.77
2:B:249:HIS:HA	2:B:267:THR:O	1.85	0.77
1:P:686:SER:OG	1:P:1103:GLY:N	2.18	0.77
1:P:1932:ILE:CD1	2:A:293:PRO:HB3	2.15	0.77
2:A:257:LEU:CD2	2:A:315:TRP:HE1	1.96	0.77
3:L:86:GLU:O	3:L:173:SER:CB	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:146:PRO:CD	3:L:203:HIS:ND1	2.48	0.77
2:A:374:PHE:CD2	2:A:411:PHE:CB	2.68	0.77
1:P:719:LYS:HD3	1:P:1101:THR:HG21	1.67	0.76
2:B:375:SER:CB	2:B:436:HIS:CE1	2.68	0.76
1:P:681:GLU:HB3	1:P:1134:ASN:CA	2.15	0.76
1:P:1006:ARG:HH22	4:H:159:THR:HB	1.48	0.76
3:L:145:TYR:CA	3:L:203:HIS:HE1	1.97	0.76
3:L:150:LYS:HZ2	3:L:152:GLN:HG3	1.50	0.76
2:A:281:TRP:CE3	2:A:325:ALA:CB	2.50	0.76
2:A:354:PRO:HG2	2:A:355:PRO:HD3	1.65	0.76
2:B:376:PRO:CG	2:B:436:HIS:CE1	2.69	0.76
3:L:45:PRO:HG3	3:L:170:GLU:CB	2.14	0.76
3:L:41:TYR:N	3:L:92:TYR:O	2.17	0.76
4:H:169:ALA:HA	4:H:188:GLN:O	1.86	0.76
3:L:11:LEU:HG	3:L:11:LEU:O	1.86	0.76
4:H:114:LEU:O	4:H:155:PRO:HD3	1.85	0.76
1:P:724:LYS:NZ	1:P:1219:ASN:O	2.19	0.76
2:A:307:VAL:CB	2:A:309:PRO:HD3	2.15	0.76
4:H:36:TRP:CD2	4:H:83:LEU:HD22	2.19	0.76
1:P:720:SER:HA	1:P:1101:THR:O	1.86	0.76
3:L:3:ALA:HB2	3:L:25:SER:HA	1.66	0.76
4:H:129:PRO:HB3	4:H:218:VAL:HG12	0.79	0.76
1:P:686:SER:CB	1:P:1103:GLY:H	1.99	0.75
1:P:703:SER:OG	1:P:808:GLU:OE1	2.04	0.75
2:B:361:LEU:H	2:B:361:LEU:CD2	1.99	0.75
4:H:70:ALA:HA	4:H:85:ALA:HA	1.68	0.75
2:B:264:LEU:HB2	2:B:309:PRO:HA	1.64	0.75
3:L:95:GLN:OE1	3:L:95:GLN:N	2.18	0.75
1:P:672:GLY:HA2	1:P:674:THR:CG2	2.07	0.75
2:B:345:PHE:CG	2:B:410:THR:HG21	2.22	0.75
1:P:1281:LEU:HD21	1:P:1349:LEU:HD13	1.68	0.75
3:L:103:PHE:CD2	4:H:37:VAL:HG21	2.19	0.75
3:L:108:ARG:HH22	3:L:147:ARG:NE	1.84	0.75
3:L:113:ARG:HG3	3:L:113:ARG:NH2	1.97	0.75
2:A:281:TRP:HZ3	2:A:325:ALA:HB3	1.50	0.75
2:B:264:LEU:CB	2:B:309:PRO:CB	2.58	0.75
3:L:6:GLN:HG3	3:L:105:ALA:HB1	1.67	0.75
1:P:686:SER:CB	1:P:1103:GLY:N	2.49	0.75
1:P:1109:PHE:HE1	1:P:1138:ILE:HG21	1.51	0.75
2:A:374:PHE:HA	2:A:436:HIS:CE1	2.22	0.75
2:B:306:SER:OG	2:B:325:ALA:HB2	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:103:PHE:CE2	4:H:37:VAL:HG21	2.21	0.75
4:H:40:ALA:CA	4:H:94:ALA:CB	2.65	0.75
1:P:719:LYS:HB3	1:P:1101:THR:CB	2.07	0.75
1:P:727:TYR:O	1:P:1289:ALA:N	2.20	0.75
1:P:1883:LYS:O	1:P:1963:LYS:CD	2.33	0.75
2:A:371:ALA:N	2:A:414:THR:HA	2.02	0.75
3:L:123:PHE:CE2	3:L:140:LEU:HD11	2.20	0.75
1:P:836:TYR:CD1	1:P:1093:LEU:HD21	2.21	0.75
2:B:264:LEU:N	2:B:307:VAL:HG13	2.01	0.75
4:H:160:TRP:NE1	4:H:202:VAL:CG1	2.49	0.75
1:P:774:LYS:HB3	1:P:785:ASN:HD21	1.52	0.74
2:A:367:LEU:CD1	2:A:383:TRP:CH2	2.70	0.74
2:B:265:THR:HG21	2:B:292:GLY:HA3	0.75	0.74
3:L:66:ARG:HA	3:L:66:ARG:CZ	2.17	0.74
1:P:971:LEU:HD12	1:P:1002:TYR:HB3	1.69	0.74
2:B:253:LEU:HB2	2:B:321:PHE:HZ	1.51	0.74
2:B:329:GLU:OE2	2:B:329:GLU:HA	1.85	0.74
1:P:1105:LYS:C	1:P:1107:SER:N	2.37	0.74
2:B:350:HIS:CB	2:B:370:LEU:CB	2.52	0.74
2:B:379:VAL:HG23	2:B:381:VAL:HG23	1.67	0.74
3:L:166:GLU:HG3	3:L:180:LEU:HD11	1.67	0.74
1:P:672:GLY:HA3	1:P:674:THR:HG21	1.62	0.74
1:P:698:TYR:CE2	1:P:1294:VAL:O	2.40	0.74
2:A:374:PHE:HB3	2:A:411:PHE:HD2	0.99	0.74
2:B:256:LEU:HB2	2:B:315:TRP:CH2	2.21	0.74
1:P:1894:TRP:HE1	2:A:292:GLY:HA3	1.51	0.74
2:B:361:LEU:HD23	2:B:361:LEU:N	2.02	0.74
4:H:29:ALA:CB	4:H:54:ALA:CA	2.52	0.74
3:L:146:PRO:HG3	3:L:204:GLN:HB2	1.69	0.74
2:B:250:ARG:HB3	2:B:377:LYS:NZ	2.03	0.74
2:B:322:THR:HB	2:B:335:THR:HA	1.69	0.74
3:L:137:VAL:HG12	3:L:153:TRP:HH2	1.50	0.74
4:H:160:TRP:HE1	4:H:202:VAL:HG11	1.52	0.74
2:B:253:LEU:O	2:B:253:LEU:HD23	1.88	0.74
1:P:698:TYR:HE2	1:P:1294:VAL:CG2	2.00	0.74
1:P:720:SER:CA	1:P:1101:THR:O	2.36	0.74
2:A:287:LYS:HE2	2:A:311:CYS:HB2	1.68	0.74
4:H:4:LEU:N	4:H:4:LEU:HD12	2.02	0.74
1:P:924:GLU:OE2	1:P:1367:ASN:ND2	2.21	0.73
1:P:1580:TYR:CB	4:H:227:PRO:HD2	2.17	0.73
2:A:371:ALA:H	2:A:414:THR:H	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:TRP:HZ3	2:B:321:PHE:HA	1.53	0.73
3:L:123:PHE:HE1	4:H:132:LEU:CG	2.01	0.73
3:L:166:GLU:HG2	3:L:166:GLU:O	1.87	0.73
4:H:156:LEU:HD12	4:H:208:HIS:CA	2.18	0.73
1:P:684:ASN:ND2	1:P:1106:ASP:O	2.20	0.73
2:A:354:PRO:C	2:B:352:LEU:CD1	2.58	0.73
3:L:103:PHE:CE2	4:H:37:VAL:CB	2.70	0.73
1:P:729:PRO:HD3	1:P:1290:SER:CA	2.16	0.73
2:A:374:PHE:CD2	2:A:411:PHE:HB3	2.22	0.73
3:L:18:ALA:HB1	3:L:80:ILE:HG13	1.70	0.73
3:L:108:ARG:CZ	3:L:147:ARG:CZ	2.66	0.73
4:H:40:ALA:HA	4:H:95:ALA:H	1.52	0.73
4:H:127:VAL:HG11	4:H:206:VAL:CG1	2.17	0.73
2:B:379:VAL:HG13	2:B:437:GLU:HG2	1.67	0.73
3:L:45:PRO:HG3	3:L:170:GLU:HG2	1.68	0.73
4:H:38:ARG:N	4:H:48:VAL:HG23	2.02	0.73
4:H:40:ALA:HB3	4:H:45:LEU:HD22	1.70	0.73
2:A:287:LYS:NZ	2:A:319:LYS:NZ	2.36	0.73
3:L:45:PRO:CG	3:L:170:GLU:HG2	2.17	0.73
3:L:146:PRO:HD2	3:L:203:HIS:CG	2.23	0.73
1:P:1511:HIS:HB2	1:P:1651:ILE:HG12	1.69	0.73
3:L:180:LEU:HD23	3:L:180:LEU:C	2.13	0.73
3:L:40:TRP:CH2	3:L:93:CYS:HB3	2.24	0.73
4:H:7:SER:O	4:H:20:LEU:HD22	1.88	0.73
1:P:727:TYR:CD2	1:P:1288:LEU:HD21	2.16	0.73
2:B:354:PRO:HG3	2:B:367:LEU:HG	1.70	0.73
3:L:25:SER:O	3:L:74:THR:HB	1.89	0.73
3:L:53:ILE:HG22	3:L:59:ALA:HA	1.69	0.73
4:H:4:LEU:HB2	4:H:22:CYS:SG	2.29	0.73
4:H:9:ALA:CB	4:H:115:VAL:HG22	2.19	0.73
1:P:1004:TRP:CZ2	4:H:165:GLN:HA	2.24	0.73
1:P:1442:ARG:NH1	1:P:1470:THR:O	2.22	0.73
2:B:263:ASN:C	2:B:309:PRO:CB	2.61	0.72
2:B:308:LEU:N	2:B:309:PRO:CD	2.51	0.72
2:B:401:ARG:O	2:B:401:ARG:HD3	1.89	0.72
2:A:350:HIS:HB2	2:A:370:LEU:HD22	1.70	0.72
4:H:34:ALA:H	4:H:51:ILE:CG2	2.02	0.72
1:P:723:PHE:CD1	1:P:1132:PHE:CE1	2.77	0.72
2:B:345:PHE:CG	2:B:410:THR:CG2	2.71	0.72
4:H:191:LEU:HD23	4:H:191:LEU:H	1.53	0.72
1:P:686:SER:HB2	1:P:1103:GLY:N	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:323:CYS:HB2	2:A:336:ALA:HB3	1.71	0.72
3:L:40:TRP:CH2	3:L:93:CYS:CB	2.72	0.72
3:L:118:PRO:HB2	3:L:141:LEU:CD1	2.20	0.72
1:P:683:ARG:O	1:P:1104:LYS:HD3	1.90	0.72
2:A:343:ASN:HB2	2:A:375:SER:O	1.89	0.72
2:B:327:TYR:CD1	2:B:328:PRO:HD3	2.24	0.72
3:L:18:ALA:CB	3:L:83:VAL:HG23	1.89	0.72
3:L:115:VAL:HG21	3:L:205:GLY:HA2	1.68	0.72
4:H:43:LYS:HA	4:H:43:LYS:NZ	2.05	0.72
2:A:339:SER:O	2:A:377:LYS:HD2	1.89	0.72
2:A:398:TRP:CH2	2:B:414:THR:HB	2.25	0.72
1:P:680:LEU:CD1	1:P:1203:ASN:ND2	2.52	0.72
2:B:245:ARG:HH22	2:B:331:LYS:H	1.38	0.72
4:H:19:LYS:HZ3	4:H:83:LEU:N	1.87	0.72
4:H:40:ALA:HA	4:H:94:ALA:CA	2.19	0.72
1:P:1449:LYS:HD3	1:P:1584:ASP:HB3	1.72	0.72
2:A:257:LEU:HD21	2:A:315:TRP:NE1	2.02	0.72
2:B:250:ARG:H	2:B:250:ARG:CD	2.00	0.72
2:B:374:PHE:N	2:B:434:VAL:HG12	1.99	0.72
1:P:1933:ASP:HB3	2:A:296:ARG:HD2	1.72	0.71
2:A:354:PRO:HB3	2:B:352:LEU:CB	2.20	0.71
2:B:373:GLY:HA3	2:B:434:VAL:O	1.89	0.71
1:P:774:LYS:H	1:P:774:LYS:CD	2.02	0.71
2:B:402:GLN:NE2	2:B:411:PHE:CE2	2.59	0.71
2:A:382:ARG:O	2:A:433:MET:O	2.07	0.71
2:B:341:SER:HG	2:B:438:ALA:HB1	1.49	0.71
3:L:148:GLU:HA	3:L:148:GLU:OE2	1.90	0.71
1:P:1883:LYS:HG2	1:P:1963:LYS:HE3	1.69	0.71
2:B:327:TYR:CE1	2:B:328:PRO:HD2	2.25	0.71
2:B:374:PHE:CD2	2:B:381:VAL:HG21	2.25	0.71
2:B:271:LEU:HD12	2:B:327:TYR:HB2	1.72	0.71
1:P:774:LYS:HE2	1:P:774:LYS:O	1.90	0.71
3:L:45:PRO:HD3	3:L:170:GLU:HG2	1.70	0.71
2:A:358:GLU:OE2	2:B:446:LYS:HD3	1.90	0.71
4:H:40:ALA:HA	4:H:94:ALA:CB	2.20	0.71
1:P:700:GLN:HG2	1:P:807:ASN:HB3	1.73	0.71
2:A:371:ALA:N	2:A:414:THR:H	1.88	0.71
2:B:353:PRO:HG3	2:B:450:ARG:CA	2.21	0.71
3:L:124:PRO:HD3	4:H:133:CYS:CA	2.20	0.71
4:H:97:TYR:HA	4:H:112:GLY:HA2	1.73	0.71
4:H:127:VAL:CG1	4:H:206:VAL:HG11	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:99:ALA:HB2	4:H:110:GLY:CA	2.21	0.70
1:P:780:PHE:HE1	1:P:799:HIS:H	1.38	0.70
2:A:279:PHE:CE2	2:A:291:GLN:CG	2.56	0.70
2:A:367:LEU:HD13	2:A:383:TRP:CH2	2.26	0.70
2:B:264:LEU:CB	2:B:309:PRO:HD3	2.21	0.70
3:L:168:VAL:HG12	3:L:180:LEU:HD12	1.72	0.70
1:P:681:GLU:HB3	1:P:1134:ASN:N	2.06	0.70
2:A:301:CYS:SG	2:B:241:CYS:HB2	2.30	0.70
2:B:382:ARG:HB2	2:B:395:TYR:CE1	2.27	0.70
1:P:1959:PHE:HB3	1:P:1963:LYS:HD3	1.72	0.70
1:P:703:SER:OG	1:P:808:GLU:CD	2.35	0.70
2:A:256:LEU:HD12	2:A:256:LEU:C	2.16	0.70
2:A:299:CYS:SG	2:B:298:LEU:CG	2.80	0.70
1:P:1926:SER:C	2:B:242:CYS:O	2.34	0.70
2:B:327:TYR:CG	2:B:328:PRO:HD2	2.26	0.70
2:B:402:GLN:HG2	2:B:411:PHE:HE2	0.89	0.70
4:H:204:CYS:SG	4:H:206:VAL:CG2	2.79	0.70
1:P:1533:LEU:HD23	1:P:1586:VAL:HB	1.72	0.70
2:B:263:ASN:C	2:B:309:PRO:HB3	2.13	0.70
3:L:18:ALA:HA	3:L:83:VAL:HG22	1.73	0.70
4:H:160:TRP:NE1	4:H:202:VAL:HG11	2.07	0.70
1:P:1881:ASN:C	1:P:1963:LYS:HB2	2.16	0.70
3:L:11:LEU:CD2	3:L:107:THR:HG22	2.21	0.70
1:P:780:PHE:O	1:P:801:ALA:N	2.24	0.70
1:P:1924:ARG:HB3	2:B:243:HIS:HB3	0.73	0.70
2:A:374:PHE:CD2	2:A:411:PHE:CG	2.80	0.70
3:L:142:ASN:CA	3:L:179:SER:CB	2.58	0.70
4:H:153:GLN:HG2	4:H:183:TYR:CZ	2.26	0.70
4:H:156:LEU:HG	4:H:207:LYS:O	1.92	0.70
3:L:124:PRO:HB2	3:L:125:PRO:HD2	1.74	0.70
1:P:684:ASN:CB	1:P:1104:LYS:C	2.52	0.69
2:A:273:ASP:CG	2:A:329:GLU:OE1	2.35	0.69
4:H:4:LEU:HD11	4:H:109:TRP:C	2.17	0.69
4:H:10:ALA:HA	4:H:116:THR:N	2.04	0.69
2:A:251:PRO:N	2:A:251:PRO:C	2.50	0.69
2:A:278:THR:O	2:A:326:ALA:O	2.10	0.69
2:A:371:ALA:CB	2:A:414:THR:N	2.54	0.69
2:B:251:PRO:HB3	2:B:321:PHE:CE2	2.25	0.69
2:B:307:VAL:CA	2:B:307:VAL:H	2.03	0.69
4:H:136:GLN:H	4:H:136:GLN:CD	1.98	0.69
1:P:1958:ILE:O	1:P:1959:PHE:N	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:HIS:CA	2:B:267:THR:O	2.40	0.69
2:B:264:LEU:HB2	2:B:309:PRO:N	2.05	0.69
3:L:42:ALA:HA	3:L:91:TYR:CD1	2.22	0.69
1:P:680:LEU:HD11	1:P:1203:ASN:HD22	1.56	0.69
1:P:1580:TYR:HA	4:H:227:PRO:CG	2.21	0.69
1:P:1710:GLN:HG2	1:P:1920:ALA:HB1	1.72	0.69
1:P:1924:ARG:CD	2:B:245:ARG:CB	2.71	0.69
2:B:289:ALA:HA	2:B:308:LEU:HD23	1.74	0.69
1:P:1579:ALA:O	4:H:227:PRO:O	2.10	0.69
2:B:372:ARG:O	2:B:434:VAL:HG23	1.90	0.69
3:L:215:ASN:HB2	3:L:218:GLU:HG3	1.74	0.69
4:H:4:LEU:HD12	4:H:4:LEU:H	1.55	0.69
1:P:684:ASN:HA	1:P:1106:ASP:O	1.93	0.69
1:P:683:ARG:NE	1:P:1133:TYR:O	2.26	0.69
2:B:250:ARG:CB	2:B:378:ASP:OD2	2.40	0.69
2:B:382:ARG:NH1	2:B:395:TYR:HH	1.90	0.69
3:L:40:TRP:CE3	3:L:92:TYR:C	2.70	0.69
1:P:1926:SER:HB3	2:B:243:HIS:CG	2.28	0.69
2:A:246:LEU:HD11	2:A:336:ALA:HA	1.73	0.69
2:B:250:ARG:CD	2:B:267:THR:H	2.05	0.69
2:B:272:ARG:HG2	2:B:272:ARG:HH11	1.57	0.69
2:B:321:PHE:CG	2:B:338:LEU:HD13	2.26	0.69
2:B:382:ARG:HB2	2:B:395:TYR:HE1	1.56	0.69
3:L:146:PRO:CD	3:L:203:HIS:CG	2.76	0.69
1:P:681:GLU:CB	1:P:1134:ASN:HA	2.23	0.69
4:H:71:ALA:N	4:H:84:ALA:HB3	2.07	0.69
1:P:1579:ALA:O	4:H:227:PRO:CB	2.40	0.68
2:A:280:THR:O	2:A:325:ALA:CA	2.37	0.68
2:B:383:TRP:CH2	2:B:413:VAL:HG21	2.28	0.68
2:B:400:SER:OG	2:B:413:VAL:HB	1.93	0.68
2:B:262:ALA:O	2:B:309:PRO:CB	2.40	0.68
2:B:341:SER:OG	2:B:438:ALA:HB3	1.88	0.68
2:B:394:LYS:HG2	2:B:417:LEU:HD13	1.75	0.68
2:B:402:GLN:CG	2:B:411:PHE:CD2	2.53	0.68
4:H:12:ALA:HB2	4:H:18:LEU:HD22	1.74	0.68
2:B:254:GLU:HG3	2:B:380:LEU:HB2	1.74	0.68
2:A:318:GLY:HA3	2:A:340:LYS:HZ1	1.59	0.68
2:B:250:ARG:HD3	2:B:267:THR:H	1.56	0.68
2:B:265:THR:OG1	2:B:292:GLY:HA2	1.92	0.68
2:B:307:VAL:CB	2:B:309:PRO:CD	2.71	0.68
2:B:311:CYS:C	2:B:314:PRO:HD2	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:99:ALA:HB2	4:H:110:GLY:HA2	1.75	0.68
1:P:715:PHE:CD2	1:P:1295:THR:CG2	2.73	0.68
2:A:299:CYS:HG	2:B:298:LEU:HB3	1.56	0.68
2:B:264:LEU:HD12	2:B:309:PRO:N	2.09	0.68
3:L:6:GLN:HG2	3:L:105:ALA:HB1	1.74	0.68
4:H:160:TRP:CD1	4:H:202:VAL:CG1	2.76	0.68
2:A:318:GLY:HA3	2:A:340:LYS:NZ	2.09	0.68
2:B:249:HIS:CG	2:B:268:LEU:HD23	2.28	0.68
2:B:289:ALA:HA	2:B:307:VAL:O	1.93	0.68
2:B:258:LEU:CD1	2:B:440:PRO:O	2.40	0.68
2:B:291:GLN:CG	2:B:305:SER:O	2.41	0.68
3:L:108:ARG:CZ	3:L:147:ARG:NH2	2.57	0.68
1:P:836:TYR:CD1	1:P:1093:LEU:CD1	2.77	0.68
2:A:381:VAL:HG13	2:A:415:SER:HA	1.76	0.68
1:P:687:ASP:CG	1:P:1101:THR:HG22	2.10	0.67
2:B:318:GLY:O	2:B:340:LYS:CA	2.42	0.67
4:H:131:SER:CA	4:H:219:PRO:HG2	2.24	0.67
1:P:1591:TYR:OH	4:H:229:PRO:O	2.11	0.67
2:A:282:THR:OG1	2:A:283:PRO:HD3	1.94	0.67
2:A:417:LEU:HD11	2:B:404:PRO:HG3	1.76	0.67
2:B:347:PRO:HA	2:B:372:ARG:HB3	1.77	0.67
1:P:706:GLY:CA	1:P:772:LYS:HE2	2.18	0.67
2:A:401:ARG:HD2	2:B:414:THR:HG21	1.76	0.67
2:B:383:TRP:HH2	2:B:413:VAL:HG21	1.59	0.67
3:L:10:SER:HA	3:L:110:GLU:OE1	1.93	0.67
3:L:108:ARG:NH1	3:L:147:ARG:NH2	2.42	0.67
1:P:1926:SER:C	2:B:242:CYS:CB	2.66	0.67
2:A:300:GLY:HA3	2:B:242:CYS:N	2.08	0.67
2:A:388:GLN:OE1	2:A:388:GLN:HA	1.95	0.67
2:B:272:ARG:NH1	2:B:300:GLY:C	2.37	0.67
4:H:19:LYS:CD	4:H:83:LEU:C	2.64	0.67
3:L:44:LYS:HD3	3:L:89:ALA:HB2	1.77	0.67
3:L:45:PRO:HG3	3:L:170:GLU:CG	2.25	0.67
2:A:381:VAL:HG13	2:A:415:SER:CA	2.25	0.67
2:B:249:HIS:CG	2:B:268:LEU:CD2	2.78	0.67
2:B:372:ARG:O	2:B:434:VAL:N	2.28	0.67
4:H:23:ALA:HA	4:H:80:ALA:HB2	1.77	0.67
1:P:836:TYR:CD1	1:P:1093:LEU:HD13	2.28	0.67
3:L:45:PRO:CG	3:L:170:GLU:HB2	2.25	0.67
1:P:1933:ASP:OD2	2:A:296:ARG:HD3	1.95	0.67
2:A:339:SER:O	2:A:377:LYS:CD	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:HIS:H	2:B:249:HIS:CD2	2.12	0.67
2:B:354:PRO:CD	2:B:450:ARG:HH11	1.82	0.67
1:P:719:LYS:O	1:P:1101:THR:HA	1.95	0.67
2:A:268:LEU:HD11	2:A:334:LEU:O	1.95	0.67
2:B:266:CYS:SG	2:B:306:SER:O	2.53	0.67
2:B:285:SER:HB2	2:B:314:PRO:CB	2.20	0.67
2:B:313:GLU:HA	2:B:313:GLU:OE2	1.95	0.67
2:A:264:LEU:HD21	2:A:321:PHE:CZ	2.30	0.66
2:B:374:PHE:N	2:B:434:VAL:CG1	2.57	0.66
3:L:127:ASP:HA	3:L:130:LEU:HD22	1.77	0.66
4:H:19:LYS:CE	4:H:83:LEU:C	2.68	0.66
1:P:1840:TYR:CA	4:H:138:ASP:CB	2.51	0.66
2:A:417:LEU:HD13	2:B:404:PRO:CG	2.22	0.66
2:B:264:LEU:CB	2:B:309:PRO:CD	2.73	0.66
2:B:272:ARG:CZ	2:B:272:ARG:HB3	2.26	0.66
1:P:1933:ASP:CG	2:A:296:ARG:HD2	2.20	0.66
2:A:374:PHE:HD2	2:A:411:PHE:CG	2.14	0.66
2:B:249:HIS:CB	2:B:268:LEU:HD23	2.26	0.66
3:L:6:GLN:NE2	3:L:40:TRP:CH2	2.63	0.66
4:H:131:SER:CA	4:H:219:PRO:CG	2.74	0.66
4:H:168:THR:O	4:H:189:LEU:HA	1.93	0.66
2:B:253:LEU:HB2	2:B:321:PHE:CZ	2.31	0.66
3:L:115:VAL:CG2	3:L:205:GLY:HA2	2.25	0.66
1:P:947:LYS:CD	1:P:1084:LYS:HG2	2.25	0.66
4:H:40:ALA:HA	4:H:95:ALA:N	2.10	0.66
1:P:688:ILE:HG23	1:P:718:VAL:HG12	1.77	0.66
1:P:1730:ASN:HD22	1:P:1837:ILE:HG13	1.59	0.66
1:P:1924:ARG:CB	2:B:243:HIS:CB	2.41	0.66
2:A:246:LEU:CD1	2:A:337:THR:H	2.07	0.66
2:A:381:VAL:HG13	2:A:415:SER:C	2.21	0.66
2:A:381:VAL:HG22	2:A:413:VAL:O	1.94	0.66
1:P:961:SER:OG	4:H:162:GLU:HG2	1.96	0.66
2:A:287:LYS:HZ2	2:A:319:LYS:HZ1	1.43	0.66
2:B:250:ARG:HB3	2:B:377:LYS:HZ2	1.59	0.66
2:B:257:LEU:HG	2:B:440:PRO:HB3	1.76	0.66
2:B:376:PRO:HG3	2:B:436:HIS:CE1	2.30	0.66
1:P:1895:PRO:HG2	2:A:393:GLU:OE1	1.96	0.66
2:A:351:LEU:O	2:A:351:LEU:HD23	1.95	0.66
3:L:86:GLU:HA	3:L:173:SER:CA	2.21	0.66
1:P:1091:LEU:O	1:P:1093:LEU:CA	2.44	0.66
2:A:383:TRP:HE1	2:A:416:ILE:HA	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:VAL:O	2:B:307:VAL:CB	2.44	0.66
2:B:311:CYS:O	2:B:314:PRO:HD2	1.95	0.66
3:L:215:ASN:N	3:L:215:ASN:OD1	2.29	0.66
4:H:153:GLN:OE1	4:H:174:PRO:HG2	1.96	0.66
1:P:924:GLU:HA	1:P:1361:ASN:ND2	2.09	0.66
2:A:322:THR:HA	2:A:336:ALA:O	1.96	0.66
2:A:354:PRO:CB	2:B:352:LEU:CD1	2.69	0.66
2:B:321:PHE:CB	2:B:338:LEU:HB3	2.16	0.66
3:L:120:VAL:O	3:L:212:LYS:NZ	2.25	0.66
4:H:97:TYR:HA	4:H:112:GLY:CA	2.26	0.66
4:H:116:THR:OG1	4:H:152:PRO:HB3	1.95	0.66
1:P:683:ARG:HH12	1:P:1138:ILE:CD1	2.09	0.65
1:P:723:PHE:CE1	1:P:1132:PHE:CE1	2.84	0.65
1:P:1883:LYS:C	1:P:1963:LYS:HD3	2.17	0.65
2:B:402:GLN:CB	2:B:411:PHE:CE2	2.79	0.65
3:L:190:ASP:HA	3:L:193:LYS:HD2	1.78	0.65
4:H:160:TRP:CD1	4:H:202:VAL:HG12	2.31	0.65
1:P:750:ALA:HB3	1:P:753:LEU:HB2	1.77	0.65
1:P:1049:LYS:HE2	1:P:1071:GLU:OE2	1.97	0.65
2:B:265:THR:HG22	2:B:305:SER:HB3	1.77	0.65
1:P:877:ALA:HB2	1:P:902:LEU:HD13	1.77	0.65
1:P:1923:PRO:HD2	2:B:245:ARG:CD	2.21	0.65
3:L:40:TRP:HA	3:L:40:TRP:HE3	1.60	0.65
2:B:323:CYS:C	2:B:334:LEU:HB3	2.21	0.65
1:P:720:SER:C	1:P:1101:THR:O	2.39	0.65
2:A:291:GLN:CA	2:A:306:SER:CB	2.72	0.65
3:L:40:TRP:HZ3	3:L:92:TYR:C	1.99	0.65
4:H:19:LYS:HZ3	4:H:82:ALA:C	2.05	0.65
1:P:918:ARG:HD2	1:P:1378:SER:HB2	1.77	0.65
2:A:253:LEU:CD1	2:A:437:GLU:CB	2.61	0.65
2:B:265:THR:OG1	2:B:292:GLY:CA	2.45	0.65
2:B:390:LEU:H	2:B:390:LEU:HD12	1.61	0.65
3:L:150:LYS:HZ1	3:L:152:GLN:HG3	1.60	0.65
1:P:835:ASN:O	1:P:1093:LEU:HB2	1.96	0.65
2:A:370:LEU:CA	2:A:414:THR:HA	2.23	0.65
2:A:372:ARG:NH2	2:B:358:GLU:OE1	2.30	0.65
3:L:108:ARG:HB3	3:L:110:GLU:OE2	1.97	0.65
2:A:417:LEU:CD2	2:B:404:PRO:HD2	2.27	0.65
2:B:402:GLN:CB	2:B:411:PHE:CD2	2.80	0.65
4:H:140:ASN:HD22	4:H:190:THR:HG22	1.62	0.65
1:P:1481:ARG:HE	1:P:1536:ALA:HB3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:LEU:HB3	2:B:307:VAL:HA	0.77	0.65
2:B:264:LEU:HB2	2:B:309:PRO:HB3	1.59	0.65
4:H:19:LYS:HD2	4:H:83:LEU:N	2.11	0.65
3:L:29:ALA:CB	3:L:37:ALA:O	2.40	0.64
2:B:271:LEU:HG	2:B:304:VAL:HG22	1.78	0.64
4:H:22:CYS:C	4:H:80:ALA:HB1	2.16	0.64
4:H:33:ALA:HB1	4:H:51:ILE:O	1.98	0.64
2:B:394:LYS:HG2	2:B:417:LEU:CD1	2.27	0.64
2:B:423:ASP:O	2:B:426:LYS:HB2	1.96	0.64
3:L:123:PHE:CE1	4:H:132:LEU:CD2	2.76	0.64
1:P:1604:HIS:CD2	4:H:227:PRO:HB3	2.32	0.64
2:A:279:PHE:HA	2:A:326:ALA:O	1.96	0.64
3:L:145:TYR:O	3:L:203:HIS:CE1	2.48	0.64
4:H:48:VAL:HG21	4:H:96:TYR:CD1	2.32	0.64
4:H:17:SER:CA	4:H:86:ALA:HA	2.27	0.64
1:P:673:GLN:O	1:P:674:THR:CA	2.22	0.64
1:P:1932:ILE:HD12	2:A:293:PRO:HB3	1.78	0.64
4:H:9:ALA:HB1	4:H:115:VAL:HG22	1.78	0.64
1:P:687:ASP:HB3	1:P:1100:SER:CB	2.22	0.64
1:P:698:TYR:CZ	1:P:1294:VAL:O	2.50	0.64
1:P:703:SER:HG	1:P:808:GLU:CD	2.04	0.64
1:P:835:ASN:O	1:P:1093:LEU:CB	2.45	0.64
1:P:1883:LYS:HG2	1:P:1963:LYS:CE	2.26	0.64
1:P:1924:ARG:CA	2:B:243:HIS:HB3	2.27	0.64
3:L:6:GLN:OE1	3:L:106:GLY:CA	2.45	0.64
4:H:8:GLY:O	4:H:18:LEU:HD21	1.97	0.64
4:H:19:LYS:HZ1	4:H:84:ALA:N	1.93	0.64
4:H:40:ALA:N	4:H:94:ALA:HB1	2.12	0.64
4:H:12:ALA:CB	4:H:117:VAL:HG22	2.15	0.64
1:P:683:ARG:C	1:P:1106:ASP:O	2.41	0.64
1:P:719:LYS:C	1:P:1101:THR:HB	2.23	0.64
1:P:1577:HIS:HA	1:P:1590:SER:HB2	1.80	0.64
1:P:1716:ARG:NH2	1:P:1768:SER:OG	2.31	0.64
1:P:1881:ASN:O	1:P:1963:LYS:CB	2.42	0.64
1:P:1884:GLN:HA	1:P:1959:PHE:HB2	1.76	0.64
2:B:253:LEU:HA	2:B:315:TRP:CZ3	2.32	0.63
2:B:369:CYS:SG	2:B:415:SER:OG	2.55	0.63
3:L:175:ASP:N	3:L:175:ASP:OD1	2.31	0.63
1:P:729:PRO:CD	1:P:1290:SER:HA	2.25	0.63
1:P:1017:LEU:HD23	1:P:1020:VAL:HG11	1.79	0.63
2:A:445:GLN:OE1	2:A:445:GLN:HA	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:923:TYR:C	1:P:1361:ASN:ND2	2.44	0.63
2:B:251:PRO:CB	2:B:321:PHE:CE2	2.80	0.63
1:P:698:TYR:OH	1:P:1297:GLY:HA3	1.97	0.63
2:B:243:HIS:CG	2:B:243:HIS:HB2	2.23	0.63
4:H:29:ALA:O	4:H:53:ALA:CA	2.46	0.63
1:P:724:LYS:CE	1:P:1219:ASN:O	2.47	0.63
1:P:1111:LYS:HG3	1:P:1111:LYS:O	1.97	0.63
3:L:141:LEU:HD13	3:L:201:VAL:HG21	1.81	0.63
4:H:5:ALA:O	4:H:22:CYS:HA	1.98	0.63
4:H:127:VAL:HG12	4:H:147:VAL:HG13	1.81	0.63
1:P:685:VAL:N	1:P:1104:LYS:CD	2.57	0.63
1:P:1924:ARG:HB2	2:B:243:HIS:CG	2.33	0.63
2:A:291:GLN:NE2	2:A:291:GLN:O	2.32	0.63
4:H:146:LEU:HA	4:H:186:SER:OG	1.99	0.63
2:B:253:LEU:O	2:B:315:TRP:CZ3	2.52	0.63
2:B:317:HIS:O	2:B:340:LYS:HD3	1.99	0.63
2:B:390:LEU:HD12	2:B:390:LEU:N	2.13	0.63
2:B:402:GLN:N	2:B:411:PHE:HD2	1.97	0.63
3:L:144:PHE:CE1	3:L:178:TYR:O	2.52	0.63
2:A:415:SER:OG	2:A:434:VAL:CG2	2.47	0.62
2:A:436:HIS:O	2:A:440:PRO:CB	2.47	0.62
4:H:10:ALA:HB3	4:H:209:TYR:CZ	2.34	0.62
4:H:158:VAL:HA	4:H:206:VAL:HA	1.80	0.62
2:A:287:LYS:NZ	2:A:319:LYS:HZ1	1.97	0.62
3:L:137:VAL:HG12	3:L:153:TRP:CH2	2.34	0.62
1:P:703:SER:OG	1:P:808:GLU:OE2	2.16	0.62
1:P:860:LYS:HD3	1:P:1091:LEU:CD2	2.28	0.62
2:B:264:LEU:CB	2:B:307:VAL:CB	2.76	0.62
2:B:376:PRO:HB2	2:B:437:GLU:CG	2.22	0.62
3:L:63:VAL:HG21	3:L:66:ARG:HH21	1.64	0.62
1:P:1600:ILE:HG21	1:P:1639:ASP:HA	1.80	0.62
2:A:296:ARG:NH2	2:B:243:HIS:NE2	2.48	0.62
2:A:361:LEU:H	2:A:364:LEU:HB2	1.64	0.62
2:A:381:VAL:CA	2:A:415:SER:HA	2.30	0.62
3:L:24:ARG:HA	3:L:74:THR:O	1.99	0.62
3:L:122:ILE:HD13	3:L:139:CYS:HB2	1.80	0.62
4:H:71:ALA:HB3	4:H:84:ALA:HB1	0.63	0.62
4:H:114:LEU:HD21	4:H:153:GLN:HE21	1.64	0.62
4:H:199:GLY:H	4:H:221:PRO:HB3	1.64	0.62
1:P:1085:LYS:O	1:P:1085:LYS:NZ	2.26	0.62
2:A:313:GLU:OE1	2:A:314:PRO:HD3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:381:VAL:HG11	2:A:416:ILE:O	2.00	0.62
2:B:264:LEU:HB3	2:B:309:PRO:CD	2.28	0.62
2:B:379:VAL:HG12	2:B:437:GLU:HG2	1.81	0.62
2:B:402:GLN:N	2:B:411:PHE:CD2	2.67	0.62
4:H:69:ALA:HA	4:H:86:ALA:HB3	1.81	0.62
1:P:1841:GLY:N	4:H:138:ASP:HB2	2.14	0.62
2:A:249:HIS:CE1	2:A:267:THR:HG22	2.28	0.62
2:B:318:GLY:O	2:B:339:SER:C	2.43	0.62
1:P:1958:ILE:CA	1:P:1959:PHE:N	2.62	0.62
2:A:343:ASN:CB	2:A:375:SER:O	2.48	0.62
2:A:418:ARG:CZ	2:B:370:LEU:HD11	2.29	0.62
2:B:317:HIS:HB3	2:B:319:LYS:HE3	1.82	0.62
3:L:6:GLN:CD	3:L:106:GLY:N	2.49	0.62
3:L:86:GLU:OE2	3:L:174:LYS:CA	2.48	0.62
4:H:38:ARG:HH11	4:H:46:GLU:HB2	1.63	0.62
1:P:920:VAL:HG13	1:P:1374:ILE:HD13	1.82	0.62
3:L:40:TRP:CE3	3:L:93:CYS:HA	2.34	0.62
4:H:69:ALA:O	4:H:86:ALA:CA	2.47	0.62
2:B:268:LEU:HD11	2:B:325:ALA:CB	2.25	0.62
4:H:129:PRO:HB2	4:H:218:VAL:CB	2.30	0.62
4:H:176:GLN:NE2	4:H:176:GLN:HA	2.15	0.62
1:P:924:GLU:H	1:P:1361:ASN:HB2	1.55	0.61
2:A:433:MET:HG2	2:A:442:ALA:HB1	1.82	0.61
2:B:253:LEU:O	2:B:315:TRP:HZ3	1.83	0.61
4:H:19:LYS:NZ	4:H:82:ALA:O	2.31	0.61
4:H:100:ALA:HB3	4:H:108:ALA:H	1.65	0.61
4:H:127:VAL:HG21	4:H:206:VAL:HG21	1.81	0.61
4:H:139:GLY:O	4:H:193:ALA:N	2.33	0.61
2:B:375:SER:N	2:B:376:PRO:CD	2.63	0.61
2:B:375:SER:N	2:B:376:PRO:HD3	2.14	0.61
2:B:385:GLN:HB3	2:B:430:PHE:C	2.25	0.61
2:A:417:LEU:CD2	2:B:404:PRO:HG3	2.30	0.61
2:B:349:VAL:CG2	2:B:432:CYS:O	2.44	0.61
3:L:18:ALA:HA	3:L:83:VAL:CG2	2.28	0.61
4:H:37:VAL:O	4:H:96:TYR:HD1	1.83	0.61
1:P:1892:LYS:HB3	1:P:1893:PRO:HD2	1.80	0.61
2:A:252:ALA:HA	2:A:378:ASP:OD2	2.01	0.61
2:B:245:ARG:HH22	2:B:331:LYS:HG2	1.65	0.61
2:B:264:LEU:CB	2:B:307:VAL:CA	2.52	0.61
3:L:41:TYR:O	3:L:91:TYR:HA	2.00	0.61
1:P:1109:PHE:CE1	1:P:1123:TYR:HB3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1840:TYR:HA	4:H:138:ASP:CA	2.30	0.61
2:B:372:ARG:O	2:B:434:VAL:CA	2.49	0.61
4:H:158:VAL:HG13	4:H:206:VAL:HG22	1.81	0.61
1:P:771:LYS:CD	1:P:781:THR:HG21	2.24	0.61
1:P:1924:ARG:HH22	2:B:243:HIS:N	1.98	0.61
2:A:351:LEU:HA	2:A:368:THR:HG22	1.83	0.61
3:L:67:PHE:CG	3:L:81:ALA:HB3	2.36	0.61
3:L:115:VAL:HG23	3:L:115:VAL:O	2.01	0.61
3:L:135:ALA:N	3:L:186:LEU:O	2.34	0.61
4:H:153:GLN:CG	4:H:183:TYR:CZ	2.84	0.61
1:P:1924:ARG:NH1	2:B:243:HIS:CB	2.63	0.61
2:A:290:VAL:O	2:A:307:VAL:HG22	2.00	0.61
2:A:363:GLU:HG3	2:A:363:GLU:O	2.00	0.61
1:P:673:GLN:O	1:P:674:THR:N	2.32	0.61
3:L:146:PRO:N	3:L:203:HIS:NE2	2.36	0.61
3:L:199:CYS:O	3:L:211:THR:OG1	2.11	0.61
4:H:38:ARG:N	4:H:48:VAL:CG2	2.64	0.61
1:P:698:TYR:HE2	1:P:1294:VAL:HG22	1.65	0.61
2:B:398:TRP:H	2:B:398:TRP:HD1	1.48	0.61
1:P:771:LYS:HA	1:P:771:LYS:HZ1	1.66	0.60
1:P:1926:SER:O	2:B:242:CYS:O	2.19	0.60
2:A:291:GLN:HB2	2:A:305:SER:O	2.01	0.60
3:L:142:ASN:HB3	3:L:179:SER:CB	2.27	0.60
2:A:250:ARG:HG3	2:A:250:ARG:O	2.01	0.60
2:A:354:PRO:CB	2:B:352:LEU:HB2	2.30	0.60
4:H:19:LYS:HZ2	4:H:82:ALA:C	2.07	0.60
1:P:723:PHE:CD1	1:P:1132:PHE:HE1	2.17	0.60
1:P:918:ARG:NE	1:P:1378:SER:CB	2.65	0.60
1:P:1087:GLU:HB2	1:P:1089:ASN:HD21	1.65	0.60
2:A:265:THR:O	2:A:338:LEU:HD21	2.01	0.60
2:A:322:THR:O	2:A:322:THR:HG22	2.02	0.60
2:B:246:LEU:HD22	2:B:269:THR:O	2.00	0.60
3:L:110:GLU:CD	3:L:110:GLU:H	2.07	0.60
4:H:176:GLN:HA	4:H:176:GLN:HE21	1.66	0.60
1:P:1959:PHE:O	1:P:1963:LYS:NZ	2.35	0.60
2:A:381:VAL:O	2:A:381:VAL:HG12	2.02	0.60
2:B:243:HIS:CG	2:B:243:HIS:HB3	2.23	0.60
2:B:335:THR:O	2:B:335:THR:HG22	2.01	0.60
2:B:379:VAL:HG21	2:B:435:GLY:O	2.01	0.60
2:B:385:GLN:NE2	2:B:430:PHE:HB3	2.16	0.60
3:L:6:GLN:HG3	3:L:106:GLY:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:698:TYR:HE2	1:P:1294:VAL:HG23	1.67	0.60
1:P:1923:PRO:C	2:B:245:ARG:CG	2.75	0.60
2:A:277:VAL:HG11	2:A:304:VAL:HG11	1.83	0.60
2:B:272:ARG:HH11	2:B:272:ARG:CG	2.13	0.60
3:L:10:SER:HG	3:L:108:ARG:HH11	1.49	0.60
4:H:2:VAL:O	4:H:2:VAL:HG12	2.01	0.60
1:P:776:GLU:CD	1:P:776:GLU:H	2.04	0.60
1:P:1933:ASP:HB2	2:A:296:ARG:HD2	1.79	0.60
2:B:383:TRP:CH2	2:B:413:VAL:CG2	2.84	0.60
3:L:137:VAL:HG11	3:L:214:PHE:HE2	1.66	0.60
1:P:920:VAL:CG1	1:P:1374:ILE:HG21	2.23	0.60
1:P:1112:ILE:HG22	1:P:1115:TYR:HB2	1.82	0.60
1:P:1154:LYS:NZ	1:P:1155:GLU:O	2.35	0.60
2:A:368:THR:HG22	2:A:368:THR:O	2.02	0.60
2:A:244:PRO:C	2:A:269:THR:O	2.45	0.60
2:A:367:LEU:CD1	2:A:383:TRP:HH2	2.15	0.60
2:A:417:LEU:HD21	2:B:404:PRO:HD2	1.84	0.60
2:B:268:LEU:CD1	2:B:305:SER:HA	2.32	0.60
3:L:123:PHE:CD2	3:L:140:LEU:HD11	2.36	0.60
2:A:269:THR:HA	2:A:303:SER:HB2	1.83	0.59
1:P:780:PHE:HB3	1:P:801:ALA:HB2	1.82	0.59
1:P:1046:PHE:CD1	1:P:1072:ARG:CG	2.85	0.59
2:A:355:PRO:N	2:A:355:PRO:C	2.58	0.59
3:L:108:ARG:NH2	3:L:147:ARG:NE	2.50	0.59
3:L:118:PRO:CB	3:L:141:LEU:HD12	2.31	0.59
1:P:800:LEU:HD12	1:P:830:GLU:HG3	1.84	0.59
3:L:123:PHE:CD1	4:H:132:LEU:HA	2.38	0.59
4:H:40:ALA:CA	4:H:95:ALA:H	2.15	0.59
1:P:684:ASN:ND2	1:P:1106:ASP:C	2.27	0.59
2:A:307:VAL:C	2:A:309:PRO:CD	2.75	0.59
2:B:402:GLN:NE2	2:B:411:PHE:CZ	2.70	0.59
2:B:423:ASP:CA	2:B:426:LYS:HZ2	2.14	0.59
3:L:16:GLY:HA2	3:L:83:VAL:HB	1.82	0.59
3:L:146:PRO:CG	3:L:204:GLN:HB2	2.33	0.59
4:H:38:ARG:HB2	4:H:48:VAL:HG22	1.84	0.59
1:P:719:LYS:CB	1:P:1101:THR:HG22	1.89	0.59
2:A:256:LEU:HD13	2:A:262:ALA:HA	1.85	0.59
2:A:279:PHE:CE2	2:A:291:GLN:CD	2.80	0.59
4:H:168:THR:OG1	4:H:190:THR:HB	2.03	0.59
1:P:1926:SER:H	2:B:243:HIS:CG	2.20	0.59
2:A:370:LEU:O	2:A:370:LEU:HD23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:GLN:HA	2:B:305:SER:O	2.02	0.59
3:L:121:PHE:N	3:L:140:LEU:O	2.36	0.59
1:P:673:GLN:NE2	1:P:1113:ALA:HB1	2.18	0.59
1:P:1030:ASN:ND2	1:P:1068:SER:HB3	2.17	0.59
2:A:381:VAL:CG1	2:A:414:THR:O	2.48	0.59
2:B:273:ASP:CG	2:B:327:TYR:CE1	2.81	0.59
1:P:686:SER:CB	1:P:1101:THR:CA	2.74	0.59
2:A:296:ARG:HH21	2:B:243:HIS:CE1	2.20	0.59
2:A:350:HIS:O	2:A:368:THR:CG2	2.50	0.59
3:L:113:ARG:HH21	3:L:113:ARG:CG	2.13	0.59
1:P:1074:THR:HG22	1:P:1076:LEU:HD22	1.85	0.59
2:A:348:GLU:O	2:A:372:ARG:CD	2.51	0.59
3:L:122:ILE:HG13	3:L:214:PHE:CD2	2.38	0.59
3:L:64:PRO:CB	3:L:87:ASP:OD2	2.42	0.58
4:H:17:SER:HB2	4:H:86:ALA:CB	2.32	0.58
4:H:207:LYS:HE2	4:H:210:THR:HA	1.85	0.58
1:P:793:ASN:O	1:P:798:TYR:OH	2.20	0.58
2:A:354:PRO:CG	2:A:355:PRO:CD	2.78	0.58
2:B:264:LEU:HB2	2:B:309:PRO:CD	2.33	0.58
1:P:1023:ASP:HB3	1:P:1048:SER:HG	1.68	0.58
2:B:254:GLU:HB2	2:B:379:VAL:HA	1.85	0.58
2:B:290:VAL:HB	2:B:307:VAL:CB	2.33	0.58
1:P:1639:ASP:CG	4:H:231:PRO:HA	2.28	0.58
3:L:7:SER:HB2	3:L:22:ALA:O	2.03	0.58
2:A:371:ALA:HB3	2:A:413:VAL:C	2.28	0.58
2:B:311:CYS:HB3	2:B:314:PRO:CG	2.33	0.58
2:B:433:MET:N	2:B:433:MET:HE3	2.17	0.58
4:H:75:ASP:N	4:H:75:ASP:OD1	2.35	0.58
1:P:1926:SER:C	2:B:242:CYS:C	2.59	0.58
2:B:321:PHE:CD2	2:B:338:LEU:CD1	2.85	0.58
4:H:191:LEU:HD23	4:H:191:LEU:N	2.19	0.58
1:P:1603:THR:HB	1:P:1651:ILE:HD11	1.86	0.58
3:L:113:ARG:HD3	3:L:176:SER:HG	1.69	0.58
3:L:197:TYR:HB2	3:L:214:PHE:CE2	2.39	0.58
4:H:18:LEU:N	4:H:85:ALA:O	2.33	0.58
4:H:114:LEU:CB	4:H:154:GLU:CD	2.48	0.58
1:P:715:PHE:CE2	1:P:1295:THR:HG22	2.36	0.58
1:P:1876:VAL:HA	1:P:1879:PHE:CE2	2.39	0.58
2:A:321:PHE:HB3	2:A:338:LEU:HB2	1.84	0.58
2:B:307:VAL:CA	2:B:307:VAL:O	2.43	0.58
2:B:423:ASP:CG	2:B:426:LYS:HZ2	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:131:SER:HA	4:H:219:PRO:CG	2.30	0.58
4:H:153:GLN:HG2	4:H:183:TYR:CD1	2.38	0.58
4:H:160:TRP:NE1	4:H:202:VAL:HG12	2.19	0.58
2:A:354:PRO:HG2	2:A:355:PRO:CD	2.34	0.58
2:A:417:LEU:CD2	2:B:404:PRO:CD	2.81	0.58
3:L:40:TRP:O	3:L:52:LEU:HG	2.04	0.58
1:P:1902:ILE:HG21	1:P:1908:LEU:HB2	1.86	0.58
2:A:343:ASN:O	2:A:375:SER:HB2	2.04	0.58
2:A:383:TRP:CH2	2:A:432:CYS:HB3	2.39	0.58
1:P:687:ASP:N	1:P:1101:THR:HA	2.18	0.57
1:P:836:TYR:CD1	1:P:1093:LEU:CG	2.82	0.57
1:P:1926:SER:H	2:B:243:HIS:CD2	2.21	0.57
1:P:724:LYS:HE3	1:P:1219:ASN:O	2.03	0.57
1:P:1260:GLU:HB3	1:P:1364:LEU:HD11	1.86	0.57
1:P:1848:THR:HG23	1:P:1851:LEU:H	1.68	0.57
3:L:1:ALA:HB3	4:H:46:GLU:HG2	1.84	0.57
1:P:723:PHE:CE1	1:P:1132:PHE:CD1	2.91	0.57
1:P:731:ALA:HB2	1:P:749:LYS:HB2	1.86	0.57
1:P:757:LEU:HG	1:P:758:GLU:HG2	1.86	0.57
1:P:826:ARG:HD2	1:P:852:ALA:HB2	1.85	0.57
1:P:1715:LEU:HD13	1:P:1760:ILE:HD13	1.87	0.57
1:P:1933:ASP:CG	2:A:296:ARG:CD	2.76	0.57
2:A:374:PHE:HA	2:A:436:HIS:HE1	1.70	0.57
3:L:95:GLN:HE22	3:L:100:ALA:HB3	1.69	0.57
4:H:160:TRP:CD1	4:H:202:VAL:HG11	2.38	0.57
2:A:398:TRP:CZ3	2:B:414:THR:HB	2.39	0.57
2:B:254:GLU:CG	2:B:380:LEU:HB2	2.33	0.57
2:B:258:LEU:HD23	2:B:443:PHE:CZ	2.40	0.57
2:B:297:ASP:OD1	2:B:297:ASP:N	2.37	0.57
2:B:344:THR:HG22	2:B:346:ARG:HH12	1.70	0.57
2:B:385:GLN:HG2	2:B:430:PHE:HB3	0.58	0.57
2:B:400:SER:HB3	2:B:412:ALA:O	2.04	0.57
2:B:402:GLN:HE21	2:B:411:PHE:HE2	1.52	0.57
3:L:11:LEU:HD23	3:L:107:THR:HG22	1.86	0.57
1:P:1450:TYR:CE2	1:P:1570:ASN:ND2	2.73	0.57
1:P:1924:ARG:HD2	2:B:245:ARG:CA	2.34	0.57
2:B:250:ARG:HB3	2:B:378:ASP:OD2	2.04	0.57
1:P:947:LYS:HG2	1:P:1084:LYS:CB	2.30	0.57
2:B:376:PRO:CB	2:B:437:GLU:CG	2.72	0.57
2:B:383:TRP:CZ2	2:B:413:VAL:CG2	2.87	0.57
1:P:724:LYS:NZ	1:P:1219:ASN:CB	2.60	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1091:LEU:O	1:P:1093:LEU:C	2.48	0.57
2:B:279:PHE:CD1	2:B:279:PHE:N	2.73	0.57
3:L:45:PRO:CG	3:L:170:GLU:CB	2.83	0.57
2:A:321:PHE:HD2	2:A:340:LYS:HB2	1.68	0.57
2:A:394:LYS:HD3	2:A:394:LYS:C	2.29	0.57
2:B:400:SER:HG	2:B:413:VAL:HG12	1.69	0.57
2:B:415:SER:OG	2:B:415:SER:O	2.23	0.57
4:H:6:ALA:HB2	4:H:113:THR:HB	1.75	0.57
1:P:1473:SER:HB3	1:P:1533:LEU:HD11	1.87	0.57
2:A:375:SER:H	2:A:376:PRO:HD2	1.69	0.57
2:B:343:ASN:OD1	2:B:408:THR:CG2	2.53	0.57
3:L:117:ALA:HB1	3:L:206:LEU:HD11	1.86	0.57
4:H:139:GLY:O	4:H:193:ALA:HB2	2.05	0.57
4:H:159:THR:O	4:H:205:HIS:CA	2.52	0.57
1:P:960:ARG:NH2	4:H:161:SER:HB3	2.20	0.57
2:A:296:ARG:NH2	2:B:243:HIS:CE1	2.72	0.57
2:B:265:THR:OG1	2:B:307:VAL:HG22	2.05	0.57
2:B:390:LEU:HD13	2:B:395:TYR:HB2	1.86	0.57
3:L:144:PHE:CD1	3:L:178:TYR:O	2.57	0.57
3:L:195:LYS:HG3	3:L:196:VAL:HG23	1.87	0.57
1:P:1640:GLN:NE2	4:H:232:SER:O	2.37	0.56
1:P:1884:GLN:HA	1:P:1959:PHE:CB	2.34	0.56
2:A:354:PRO:HG3	2:B:350:HIS:NE2	2.19	0.56
2:B:264:LEU:HD13	2:B:308:LEU:C	2.29	0.56
3:L:11:LEU:O	3:L:109:ALA:HA	2.04	0.56
2:B:307:VAL:HG12	2:B:309:PRO:HG3	0.56	0.56
3:L:23:CYS:SG	3:L:40:TRP:CH2	2.98	0.56
1:P:947:LYS:HD2	1:P:1084:LYS:HG3	1.80	0.56
2:B:340:LYS:HE3	2:B:341:SER:HB2	1.86	0.56
2:B:343:ASN:O	2:B:375:SER:HB2	2.05	0.56
4:H:4:LEU:HD11	4:H:110:GLY:N	2.20	0.56
4:H:158:VAL:HG13	4:H:206:VAL:HG13	1.86	0.56
1:P:719:LYS:O	1:P:1101:THR:CA	2.53	0.56
1:P:1923:PRO:O	2:B:245:ARG:HG2	2.06	0.56
2:A:279:PHE:N	2:A:279:PHE:CD1	2.73	0.56
3:L:140:LEU:CD2	3:L:181:SER:OG	2.46	0.56
3:L:142:ASN:HB2	3:L:179:SER:CB	2.35	0.56
1:P:721:SER:OG	1:P:1104:LYS:C	2.48	0.56
1:P:1386:PHE:HE1	1:P:1454:VAL:HG11	1.71	0.56
2:B:307:VAL:CG1	2:B:309:PRO:HB3	2.14	0.56
1:P:728:ILE:HG23	1:P:1289:ALA:HB3	1.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1045:THR:O	1:P:1072:ARG:HG3	2.05	0.56
2:A:245:ARG:HB3	2:A:269:THR:OG1	2.06	0.56
2:A:287:LYS:HZ2	2:A:319:LYS:HZ2	1.48	0.56
3:L:124:PRO:CD	4:H:133:CYS:N	2.69	0.56
2:A:361:LEU:HB2	2:A:364:LEU:HG	1.86	0.56
1:P:681:GLU:CD	1:P:1134:ASN:CA	2.76	0.56
3:L:14:SER:H	3:L:17:ALA:HB3	1.71	0.56
3:L:184:LEU:HD13	3:L:186:LEU:HD11	1.88	0.56
1:P:828:ILE:HG23	1:P:854:VAL:HG23	1.88	0.56
1:P:836:TYR:HA	1:P:1093:LEU:HD22	1.72	0.56
1:P:927:ASP:O	1:P:963:GLN:NE2	2.39	0.56
2:B:439:LEU:HB3	2:B:442:ALA:HB2	1.87	0.56
3:L:86:GLU:OE1	3:L:86:GLU:N	2.39	0.56
4:H:29:ALA:O	4:H:53:ALA:HA	2.05	0.56
1:P:916:LYS:HG3	1:P:951:THR:HB	1.87	0.56
2:B:344:THR:HG22	2:B:346:ARG:NH1	2.21	0.56
2:B:345:PHE:CD2	2:B:410:THR:CG2	2.89	0.56
2:B:383:TRP:HZ2	2:B:413:VAL:HG22	1.71	0.56
2:A:264:LEU:HD21	2:A:321:PHE:HZ	1.70	0.55
2:A:371:ALA:CA	2:A:414:THR:H	2.17	0.55
1:P:1924:ARG:CD	2:B:245:ARG:HB3	2.35	0.55
3:L:124:PRO:CB	3:L:125:PRO:HD2	2.36	0.55
4:H:36:TRP:O	4:H:48:VAL:HB	2.06	0.55
4:H:131:SER:CB	4:H:219:PRO:HG2	2.36	0.55
1:P:683:ARG:HG2	1:P:1135:LYS:CG	2.31	0.55
1:P:1883:LYS:CG	1:P:1963:LYS:HE3	1.82	0.55
2:B:264:LEU:CD2	2:B:307:VAL:CA	2.84	0.55
3:L:65:ALA:HB1	3:L:80:ILE:O	2.06	0.55
2:A:343:ASN:O	2:A:375:SER:CA	2.54	0.55
2:B:263:ASN:CA	2:B:309:PRO:HB2	2.36	0.55
3:L:145:TYR:HE1	3:L:178:TYR:HD2	1.53	0.55
1:P:681:GLU:CB	1:P:1134:ASN:CA	2.82	0.55
1:P:1004:TRP:CH2	4:H:164:GLY:O	2.60	0.55
2:A:249:HIS:CE1	2:A:267:THR:CG2	2.86	0.55
2:A:391:PRO:HG2	2:A:394:LYS:HB3	1.87	0.55
2:B:251:PRO:CG	2:B:338:LEU:HD12	2.32	0.55
2:B:256:LEU:HD12	2:B:310:GLY:CA	2.37	0.55
2:B:263:ASN:C	2:B:309:PRO:HB2	2.31	0.55
2:B:327:TYR:CG	2:B:328:PRO:CD	2.88	0.55
2:B:374:PHE:HE1	2:B:411:PHE:O	1.90	0.55
3:L:191:TYR:CZ	3:L:216:ARG:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1927:ASN:N	2:B:242:CYS:CB	2.56	0.55
2:A:289:ALA:HA	2:A:307:VAL:O	2.07	0.55
3:L:39:ALA:O	3:L:93:CYS:HA	2.06	0.55
4:H:125:PRO:HA	4:H:150:PHE:HA	1.87	0.55
1:P:698:TYR:CE2	1:P:1294:VAL:HG23	2.42	0.55
1:P:1031:ALA:HB3	1:P:1069:PHE:CG	2.42	0.55
1:P:1882:LEU:CD2	1:P:1960:GLU:CA	2.77	0.55
1:P:1924:ARG:C	2:B:243:HIS:HB3	2.31	0.55
3:L:136:SER:CB	3:L:184:LEU:O	2.54	0.55
4:H:37:VAL:O	4:H:96:TYR:CD1	2.60	0.55
1:P:836:TYR:CA	1:P:1093:LEU:HD22	2.37	0.55
2:A:433:MET:CG	2:A:442:ALA:HB1	2.36	0.55
1:P:1960:GLU:O	1:P:1961:ASN:ND2	2.39	0.55
4:H:148:GLN:OE1	4:H:148:GLN:HA	2.07	0.55
1:P:683:ARG:CZ	1:P:1133:TYR:O	2.55	0.55
2:B:254:GLU:HB2	2:B:380:LEU:N	2.22	0.55
3:L:123:PHE:HD1	4:H:132:LEU:HA	1.72	0.55
4:H:37:VAL:C	4:H:96:TYR:HD1	2.15	0.55
4:H:129:PRO:HB2	4:H:218:VAL:CG1	2.25	0.55
1:P:968:LEU:HD23	1:P:982:TYR:O	2.07	0.54
1:P:1421:ILE:HB	1:P:1424:VAL:HG12	1.87	0.54
1:P:1695:GLU:HG2	1:P:1784:PRO:HB3	1.89	0.54
1:P:1882:LEU:CA	1:P:1959:PHE:O	2.52	0.54
2:A:287:LYS:NZ	2:A:319:LYS:HZ2	2.02	0.54
2:B:253:LEU:CA	2:B:315:TRP:CH2	2.71	0.54
2:B:264:LEU:HD12	2:B:308:LEU:O	2.07	0.54
2:B:264:LEU:O	2:B:307:VAL:CB	2.55	0.54
2:B:279:PHE:CD2	2:B:291:GLN:NE2	2.75	0.54
3:L:134:THR:O	3:L:134:THR:OG1	2.19	0.54
2:A:245:ARG:CB	2:A:269:THR:OG1	2.55	0.54
2:B:324:THR:O	2:B:324:THR:HG23	2.08	0.54
3:L:40:TRP:CD2	3:L:93:CYS:HB3	2.41	0.54
4:H:143:ILE:HG13	4:H:189:LEU:CD2	2.37	0.54
3:L:40:TRP:HH2	3:L:93:CYS:SG	2.26	0.54
1:P:1536:ALA:O	1:P:1537:TYR:HB2	2.07	0.54
1:P:1599:ALA:HB1	1:P:1651:ILE:HG21	1.90	0.54
3:L:195:LYS:HD3	3:L:195:LYS:C	2.33	0.54
4:H:159:THR:O	4:H:205:HIS:HB2	2.08	0.54
2:A:296:ARG:HB3	2:A:296:ARG:NH2	2.23	0.54
2:A:298:LEU:HA	2:B:243:HIS:CE1	2.43	0.54
2:B:353:PRO:HB3	2:B:450:ARG:CD	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:PRO:CG	2:B:436:HIS:ND1	2.70	0.54
3:L:29:ALA:HB1	3:L:37:ALA:HB3	1.89	0.54
2:B:249:HIS:CD2	2:B:249:HIS:N	2.76	0.54
2:B:400:SER:HG	2:B:413:VAL:CG1	2.20	0.54
1:P:795:SER:HA	1:P:826:ARG:HG3	1.88	0.54
1:P:1883:LYS:CB	1:P:1963:LYS:CD	2.60	0.54
2:B:307:VAL:C	2:B:309:PRO:HD3	2.33	0.54
2:B:389:GLU:OE2	2:B:395:TYR:CE2	2.61	0.54
3:L:41:TYR:HB2	3:L:92:TYR:O	2.07	0.54
4:H:19:LYS:CE	4:H:83:LEU:O	2.55	0.54
2:A:266:CYS:HB2	2:A:338:LEU:HD11	1.90	0.54
4:H:37:VAL:CG1	4:H:97:TYR:H	2.20	0.54
1:P:681:GLU:OE2	1:P:1134:ASN:CA	2.55	0.54
2:A:291:GLN:HB2	2:A:306:SER:HB2	1.86	0.54
4:H:109:TRP:HE3	4:H:110:GLY:HA3	1.73	0.54
4:H:130:LEU:HD12	4:H:144:ALA:O	2.07	0.54
4:H:131:SER:CA	4:H:219:PRO:HG3	2.37	0.54
1:P:1087:GLU:OE1	1:P:1087:GLU:N	2.41	0.54
1:P:1339:ASP:HB3	1:P:1344:GLY:HA2	1.89	0.54
1:P:1732:VAL:HG21	1:P:1846:LEU:HD21	1.90	0.54
1:P:1413:TYR:OH	1:P:1502:ARG:NH1	2.41	0.53
3:L:86:GLU:O	3:L:173:SER:OG	2.25	0.53
1:P:698:TYR:CE2	1:P:1294:VAL:CG2	2.88	0.53
1:P:1181:LEU:HD23	1:P:1209:LEU:HD21	1.89	0.53
2:B:250:ARG:CD	2:B:267:THR:N	2.66	0.53
4:H:153:GLN:OE1	4:H:174:PRO:CB	2.56	0.53
1:P:685:VAL:N	1:P:1104:LYS:HB3	2.23	0.53
2:A:343:ASN:O	2:A:375:SER:CB	2.56	0.53
2:B:290:VAL:O	2:B:307:VAL:CA	2.56	0.53
3:L:121:PHE:O	3:L:139:CYS:HA	2.07	0.53
4:H:43:LYS:CE	4:H:43:LYS:CA	2.85	0.53
4:H:143:ILE:HG13	4:H:189:LEU:HD23	1.90	0.53
4:H:153:GLN:CD	4:H:183:TYR:CZ	2.87	0.53
1:P:870:ILE:HD11	1:P:898:VAL:HG13	1.89	0.53
2:A:254:GLU:HB2	2:A:382:ARG:CZ	2.38	0.53
2:B:258:LEU:HB2	2:B:380:LEU:HB3	1.90	0.53
4:H:9:ALA:CB	4:H:115:VAL:CG2	2.87	0.53
4:H:96:TYR:O	4:H:112:GLY:HA2	2.09	0.53
1:P:698:TYR:CE1	1:P:1297:GLY:C	2.87	0.53
1:P:1640:GLN:CD	4:H:232:SER:O	2.52	0.53
1:P:1882:LEU:HD23	1:P:1960:GLU:CA	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:143:ASN:OD1	3:L:177:THR:OG1	2.25	0.53
4:H:156:LEU:HD12	4:H:208:HIS:O	2.08	0.53
1:P:1049:LYS:HE2	1:P:1071:GLU:CD	2.34	0.53
2:A:348:GLU:HG3	2:A:372:ARG:HD3	1.83	0.53
2:A:242:CYS:HB2	2:A:272:ARG:HE	1.74	0.53
2:B:374:PHE:CE1	2:B:411:PHE:O	2.61	0.53
3:L:128:GLU:OE2	4:H:129:PRO:HG2	2.09	0.53
4:H:12:ALA:HB3	4:H:117:VAL:HG21	1.84	0.53
4:H:22:CYS:O	4:H:80:ALA:CA	2.57	0.53
1:P:1933:ASP:OD2	2:A:296:ARG:HD2	2.03	0.53
2:A:395:TYR:HE1	2:A:417:LEU:HD11	1.74	0.53
2:B:249:HIS:HB3	2:B:268:LEU:CD2	2.36	0.53
2:B:262:ALA:O	2:B:309:PRO:CA	2.57	0.53
2:B:289:ALA:HA	2:B:307:VAL:C	2.34	0.53
3:L:121:PHE:O	3:L:140:LEU:N	2.39	0.53
1:P:744:TYR:HH	1:P:772:LYS:CD	2.07	0.52
1:P:920:VAL:CG1	1:P:1374:ILE:HD13	2.39	0.52
1:P:1109:PHE:CZ	1:P:1123:TYR:HB3	2.44	0.52
4:H:8:GLY:O	4:H:20:LEU:CD2	2.57	0.52
4:H:156:LEU:HD11	4:H:208:HIS:HA	1.91	0.52
2:A:374:PHE:CD1	2:A:436:HIS:CE1	2.81	0.52
3:L:21:ILE:CD1	3:L:91:TYR:HD2	2.20	0.52
3:L:128:GLU:N	3:L:128:GLU:OE1	2.42	0.52
4:H:6:ALA:HB3	4:H:113:THR:CB	2.37	0.52
4:H:36:TRP:NE1	4:H:83:LEU:HD22	2.16	0.52
2:A:384:LEU:C	2:A:384:LEU:HD12	2.35	0.52
2:B:272:ARG:NH1	2:B:272:ARG:HB3	2.22	0.52
2:B:402:GLN:NE2	2:B:411:PHE:HE2	2.00	0.52
2:A:254:GLU:H	2:A:254:GLU:CD	2.17	0.52
2:A:418:ARG:HH12	2:B:370:LEU:CD1	2.22	0.52
2:B:258:LEU:CB	2:B:380:LEU:HB3	2.39	0.52
2:B:439:LEU:HD23	2:B:440:PRO:HD2	1.92	0.52
4:H:8:GLY:O	4:H:20:LEU:HD21	2.08	0.52
1:P:683:ARG:NH1	1:P:1138:ILE:CD1	2.71	0.52
1:P:684:ASN:HA	1:P:1104:LYS:HG2	1.91	0.52
1:P:812:GLY:HA3	1:P:815:GLU:HB2	1.90	0.52
1:P:1627:PRO:HG3	4:H:225:THR:HG21	1.86	0.52
2:A:244:PRO:HA	2:A:270:GLY:HA3	1.92	0.52
2:A:246:LEU:CD1	2:A:336:ALA:HA	2.38	0.52
2:B:290:VAL:H	2:B:307:VAL:C	2.18	0.52
2:B:353:PRO:CG	2:B:450:ARG:H	1.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:113:ARG:HD3	3:L:176:SER:OG	2.06	0.52
3:L:146:PRO:HD3	3:L:203:HIS:CG	2.41	0.52
3:L:191:TYR:OH	3:L:216:ARG:HB2	2.10	0.52
1:P:1516:TYR:CZ	1:P:1524:ARG:HD3	2.44	0.52
1:P:1623:ASN:HD21	1:P:1846:LEU:HD12	1.74	0.52
1:P:1633:GLY:HA3	1:P:1802:ARG:CD	2.39	0.52
2:A:340:LYS:HD3	2:A:377:LYS:HZ3	1.73	0.52
2:A:414:THR:HB	2:A:416:ILE:HD11	1.91	0.52
1:P:1927:ASN:CA	2:B:242:CYS:HB2	2.37	0.52
2:A:348:GLU:C	2:A:372:ARG:HG2	2.18	0.52
2:B:381:VAL:HG13	2:B:434:VAL:HA	1.92	0.52
3:L:42:ALA:HA	3:L:91:TYR:HA	1.91	0.52
2:A:296:ARG:HH21	2:B:243:HIS:HE2	1.58	0.52
2:A:366:THR:HG22	2:A:418:ARG:HD3	1.91	0.52
2:A:381:VAL:HG22	2:A:414:THR:O	2.10	0.52
2:A:417:LEU:HD22	2:B:404:PRO:CD	2.37	0.52
2:B:318:GLY:O	2:B:339:SER:O	2.28	0.52
2:B:402:GLN:CD	2:B:411:PHE:HE2	2.12	0.52
3:L:141:LEU:HG	3:L:141:LEU:O	2.08	0.52
4:H:114:LEU:O	4:H:154:GLU:O	2.28	0.52
1:P:1924:ARG:HA	2:B:245:ARG:CG	2.40	0.52
2:A:398:TRP:HH2	2:B:414:THR:HB	1.73	0.52
2:A:417:LEU:HD21	2:B:404:PRO:CD	2.39	0.52
2:B:272:ARG:NH1	2:B:272:ARG:CG	2.73	0.52
3:L:6:GLN:CG	3:L:106:GLY:H	2.22	0.52
3:L:37:ALA:HB2	3:L:97:ALA:HB2	1.92	0.52
4:H:37:VAL:C	4:H:48:VAL:HG23	2.33	0.52
1:P:672:GLY:HA3	1:P:674:THR:CG2	2.30	0.51
1:P:1591:TYR:OH	4:H:231:PRO:HD3	2.10	0.51
2:A:373:GLY:O	2:A:436:HIS:NE2	2.43	0.51
3:L:19:ALA:O	3:L:80:ILE:HG12	2.11	0.51
4:H:125:PRO:CA	4:H:150:PHE:HB2	2.39	0.51
4:H:129:PRO:HB2	4:H:218:VAL:HA	1.93	0.51
1:P:1819:VAL:HG23	1:P:1820:PRO:HD3	1.92	0.51
2:A:327:TYR:CD1	2:A:327:TYR:N	2.77	0.51
3:L:10:SER:HB3	3:L:110:GLU:OE1	2.06	0.51
3:L:144:PHE:HE1	3:L:179:SER:CA	2.16	0.51
2:A:249:HIS:CG	2:A:265:THR:HG22	2.45	0.51
2:A:294:PRO:HB2	2:A:302:TYR:CZ	2.45	0.51
2:A:301:CYS:SG	2:B:241:CYS:CB	2.99	0.51
2:B:264:LEU:CD1	2:B:309:PRO:N	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:LEU:N	2:B:309:PRO:HD2	2.24	0.51
2:B:320:THR:CB	2:B:339:SER:HB3	2.35	0.51
2:B:385:GLN:HE21	2:B:430:PHE:CB	2.23	0.51
3:L:129:GLN:CD	4:H:128:PHE:CE1	2.89	0.51
2:A:384:LEU:HG	2:A:384:LEU:O	2.10	0.51
1:P:1524:ARG:HA	1:P:1527:LEU:HD13	1.91	0.51
1:P:1682:ASN:O	1:P:1686:ASN:ND2	2.44	0.51
2:A:374:PHE:HB2	2:A:411:PHE:HB2	0.51	0.51
3:L:136:SER:OG	3:L:185:THR:HA	2.11	0.51
2:A:339:SER:O	2:A:377:LYS:HD3	2.11	0.51
3:L:41:TYR:CE2	3:L:51:ALA:HB2	2.46	0.51
4:H:191:LEU:N	4:H:191:LEU:CD2	2.73	0.51
2:A:318:GLY:CA	2:A:340:LYS:HZ1	2.21	0.51
2:A:434:VAL:H	2:A:442:ALA:HA	1.75	0.51
2:B:285:SER:HB3	2:B:314:PRO:CB	2.31	0.51
2:B:344:THR:HG23	2:B:436:HIS:CG	2.45	0.51
1:P:876:GLU:HG2	1:P:904:LYS:HB3	1.92	0.51
3:L:133:GLY:O	3:L:188:LYS:N	2.44	0.51
4:H:2:VAL:HG13	4:H:109:TRP:O	2.10	0.51
4:H:170:ARG:HA	4:H:170:ARG:CZ	2.39	0.51
1:P:684:ASN:CA	1:P:1106:ASP:O	2.59	0.51
1:P:883:ILE:HB	1:P:910:ILE:HG12	1.93	0.51
1:P:985:GLY:C	1:P:1024:VAL:HG23	2.36	0.51
2:B:264:LEU:HD13	2:B:308:LEU:CA	2.39	0.51
4:H:40:ALA:HA	4:H:94:ALA:HA	1.90	0.51
3:L:123:PHE:CD2	3:L:140:LEU:CD1	2.94	0.51
1:P:716:VAL:HG23	1:P:730:VAL:HG12	1.93	0.50
2:A:318:GLY:C	2:A:340:LYS:NZ	2.69	0.50
2:B:289:ALA:CA	2:B:307:VAL:O	2.58	0.50
4:H:37:VAL:HG13	4:H:96:TYR:HA	1.93	0.50
4:H:140:ASN:HB3	4:H:190:THR:CG2	2.41	0.50
1:P:728:ILE:HG22	1:P:1289:ALA:HB1	1.84	0.50
2:A:321:PHE:CG	2:A:338:LEU:HB2	2.47	0.50
2:B:423:ASP:OD1	2:B:426:LYS:CE	2.59	0.50
4:H:17:SER:HB2	4:H:86:ALA:N	2.25	0.50
1:P:719:LYS:CA	1:P:1101:THR:HB	2.41	0.50
1:P:721:SER:N	1:P:1101:THR:O	2.44	0.50
1:P:960:ARG:HH22	4:H:205:HIS:CE1	2.29	0.50
2:B:394:LYS:CG	2:B:417:LEU:HD13	2.40	0.50
4:H:156:LEU:HD12	4:H:208:HIS:C	2.35	0.50
4:H:195:GLN:OE1	4:H:195:GLN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:719:LYS:CG	1:P:1101:THR:CG2	2.56	0.50
2:A:398:TRP:HH2	2:B:414:THR:N	1.99	0.50
3:L:129:GLN:HB2	4:H:128:PHE:CE2	2.46	0.50
1:P:672:GLY:C	1:P:674:THR:CG2	2.38	0.50
1:P:947:LYS:HD2	1:P:1084:LYS:HG2	1.82	0.50
2:A:242:CYS:SG	2:A:243:HIS:N	2.85	0.50
2:B:424:TRP:CZ3	2:B:425:LYS:HG3	2.46	0.50
3:L:6:GLN:CG	3:L:106:GLY:N	2.73	0.50
3:L:124:PRO:HD3	4:H:133:CYS:N	2.25	0.50
1:P:698:TYR:CE1	1:P:1298:TYR:N	2.79	0.50
1:P:960:ARG:HB3	1:P:963:GLN:OE1	2.12	0.50
1:P:1046:PHE:CE1	1:P:1072:ARG:HD2	2.47	0.50
2:A:266:CYS:CB	2:A:338:LEU:HD11	2.42	0.50
2:B:250:ARG:HD2	2:B:267:THR:N	2.27	0.50
2:B:353:PRO:HG3	2:B:450:ARG:HA	1.90	0.50
3:L:71:GLY:HA3	3:L:76:PHE:HB2	1.92	0.50
1:P:1448:TRP:HD1	1:P:1451:ARG:HA	1.77	0.50
2:B:265:THR:CB	2:B:292:GLY:CA	2.80	0.50
3:L:11:LEU:HD11	3:L:19:ALA:HB3	1.86	0.50
4:H:6:ALA:HB3	4:H:113:THR:HB	1.75	0.50
4:H:40:ALA:CB	4:H:94:ALA:HB2	2.27	0.50
4:H:140:ASN:HD22	4:H:190:THR:CG2	2.25	0.50
2:A:424:TRP:CE2	2:A:430:PHE:HB2	2.47	0.50
2:B:249:HIS:NE2	2:B:334:LEU:HD13	2.26	0.50
2:B:308:LEU:N	2:B:308:LEU:HD23	2.26	0.50
3:L:137:VAL:HG11	3:L:214:PHE:CE2	2.47	0.50
3:L:197:TYR:HB2	3:L:214:PHE:CZ	2.47	0.50
1:P:720:SER:C	1:P:1102:SER:HA	2.33	0.50
1:P:835:ASN:O	1:P:1093:LEU:HB3	2.12	0.49
2:B:391:PRO:HG2	2:B:417:LEU:HD11	1.95	0.49
2:B:400:SER:OG	2:B:413:VAL:CA	2.60	0.49
4:H:29:ALA:C	4:H:54:ALA:H	2.18	0.49
1:P:1168:ILE:HD11	1:P:1332:ASP:HB3	1.92	0.49
2:B:391:PRO:N	2:B:391:PRO:C	2.63	0.49
2:B:402:GLN:CA	2:B:411:PHE:CD2	2.96	0.49
3:L:137:VAL:CG1	3:L:153:TRP:HH2	2.21	0.49
2:A:384:LEU:HD21	2:A:431:SER:H	1.78	0.49
2:B:282:THR:CB	2:B:283:PRO:HD3	2.29	0.49
2:B:344:THR:CG2	2:B:346:ARG:HH12	2.25	0.49
2:B:353:PRO:CG	2:B:450:ARG:HA	2.41	0.49
3:L:171:GLN:HB2	3:L:178:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1500:ASN:HB3	1:P:1594:LEU:HD13	1.93	0.49
1:P:1707:SER:OG	1:P:1710:GLN:OE1	2.27	0.49
1:P:1926:SER:H	2:B:243:HIS:CB	2.22	0.49
2:A:374:PHE:CE1	2:A:379:VAL:HB	2.48	0.49
2:A:381:VAL:CG1	2:A:415:SER:HA	2.41	0.49
3:L:14:SER:H	3:L:17:ALA:CB	2.24	0.49
4:H:129:PRO:N	4:H:129:PRO:C	2.64	0.49
4:H:156:LEU:CG	4:H:207:LYS:O	2.59	0.49
1:P:683:ARG:O	1:P:1106:ASP:O	2.29	0.49
1:P:715:PHE:CG	1:P:1295:THR:HG22	2.41	0.49
1:P:1064:VAL:O	1:P:1064:VAL:HG23	2.12	0.49
2:B:308:LEU:N	2:B:309:PRO:HD3	2.26	0.49
4:H:29:ALA:CA	4:H:54:ALA:H	2.23	0.49
1:P:1089:ASN:N	1:P:1089:ASN:ND2	2.60	0.49
1:P:1452:ASN:HD22	1:P:1452:ASN:H	1.59	0.49
2:B:254:GLU:HG3	2:B:380:LEU:CB	2.40	0.49
2:B:254:GLU:HB2	2:B:379:VAL:CA	2.42	0.49
4:H:99:ALA:HB1	4:H:109:TRP:HA	1.94	0.49
4:H:173:PRO:N	4:H:173:PRO:C	2.62	0.49
1:P:686:SER:CB	1:P:1104:LYS:H	2.21	0.49
1:P:1109:PHE:CE1	1:P:1138:ILE:HG21	2.39	0.49
2:A:246:LEU:HD13	2:A:337:THR:N	2.11	0.49
2:B:308:LEU:H	2:B:309:PRO:HD2	1.78	0.49
2:B:380:LEU:HG	2:B:382:ARG:HE	1.77	0.49
3:L:160:GLN:HG3	3:L:163:ASN:HD21	1.77	0.49
1:P:1690:LEU:HG	1:P:1694:MET:HE2	1.95	0.49
2:B:376:PRO:HB3	2:B:437:GLU:CG	2.37	0.49
2:A:374:PHE:CG	2:A:411:PHE:CG	3.00	0.49
2:B:345:PHE:CG	2:B:410:THR:HG23	2.45	0.49
2:B:345:PHE:HE1	2:B:408:THR:HB	1.74	0.49
2:B:364:LEU:HD13	2:B:418:ARG:HD3	1.95	0.49
4:H:37:VAL:HG13	4:H:97:TYR:H	1.78	0.49
4:H:150:PHE:CD2	4:H:156:LEU:HD13	2.48	0.49
4:H:153:GLN:OE1	4:H:174:PRO:CG	2.59	0.49
1:P:1450:TYR:OH	1:P:1570:ASN:CG	2.56	0.49
2:B:254:GLU:HG3	2:B:380:LEU:CA	2.42	0.49
2:B:264:LEU:CB	2:B:309:PRO:N	2.75	0.49
2:B:340:LYS:HA	2:B:340:LYS:HD2	1.53	0.49
2:B:349:VAL:HG13	2:B:432:CYS:CB	2.20	0.49
3:L:6:GLN:NE2	3:L:40:TRP:HH2	2.07	0.49
1:P:1087:GLU:HB2	1:P:1089:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1108:ASP:HB3	1:P:1135:LYS:NZ	2.28	0.48
1:P:1406:PHE:HZ	1:P:1457:LEU:HD23	1.78	0.48
1:P:1570:ASN:O	1:P:1572:VAL:HG13	2.12	0.48
1:P:1631:ALA:O	1:P:1636:GLN:HB2	2.13	0.48
2:A:384:LEU:CD1	2:A:429:THR:HG23	2.37	0.48
4:H:160:TRP:CD2	4:H:189:LEU:HD22	2.48	0.48
1:P:987:ILE:HG13	1:P:1024:VAL:HG21	1.95	0.48
1:P:1207:TYR:N	1:P:1216:TYR:O	2.46	0.48
1:P:1732:VAL:HG22	1:P:1793:LYS:HB3	1.94	0.48
2:A:339:SER:O	2:A:339:SER:OG	2.20	0.48
2:B:320:THR:HB	2:B:339:SER:N	2.28	0.48
2:B:320:THR:HG22	2:B:339:SER:HB3	1.95	0.48
2:B:398:TRP:CD1	2:B:398:TRP:N	2.73	0.48
3:L:136:SER:HG	3:L:185:THR:HA	1.78	0.48
4:H:162:GLU:CG	4:H:200:LYS:HE3	2.39	0.48
1:P:681:GLU:CG	1:P:1134:ASN:HA	2.43	0.48
2:A:369:CYS:H	2:A:416:ILE:HG23	1.78	0.48
2:B:347:PRO:HB3	2:B:433:MET:HA	1.93	0.48
3:L:90:ALA:HA	3:L:107:THR:O	2.12	0.48
3:L:129:GLN:HE22	4:H:148:GLN:HB3	1.79	0.48
1:P:907:GLN:H	1:P:940:GLY:HA3	1.78	0.48
1:P:1091:LEU:O	1:P:1093:LEU:O	2.31	0.48
3:L:113:ARG:CD	3:L:176:SER:HG	2.21	0.48
4:H:150:PHE:CE2	4:H:153:GLN:HA	2.48	0.48
1:P:1206:GLU:HB3	1:P:1215:LEU:HD11	1.94	0.48
1:P:1607:THR:O	1:P:1611:ASP:HB2	2.13	0.48
2:B:320:THR:HA	2:B:338:LEU:C	2.38	0.48
2:B:350:HIS:C	2:B:350:HIS:CD2	2.90	0.48
2:B:379:VAL:HG23	2:B:381:VAL:HG22	1.91	0.48
4:H:71:ALA:H	4:H:84:ALA:CA	2.24	0.48
1:P:1484:SER:OG	1:P:1545:SER:O	2.31	0.48
2:A:374:PHE:HD2	2:A:411:PHE:CB	2.19	0.48
2:B:263:ASN:HA	2:B:309:PRO:HB2	1.95	0.48
3:L:122:ILE:CG1	3:L:214:PHE:HD2	2.26	0.48
1:P:780:PHE:HE1	1:P:799:HIS:N	2.10	0.48
1:P:1926:SER:CA	2:B:243:HIS:HA	2.32	0.48
3:L:37:ALA:HB1	3:L:95:GLN:HB2	1.94	0.48
3:L:164:SER:HA	3:L:184:LEU:HD23	1.94	0.48
4:H:19:LYS:CD	4:H:83:LEU:N	2.77	0.48
4:H:36:TRP:CE2	4:H:83:LEU:HD22	2.49	0.48
1:P:1440:TYR:CZ	1:P:1444:THR:CG2	2.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:271:LEU:HD12	2:A:271:LEU:N	2.29	0.48
2:A:375:SER:H	2:A:376:PRO:CD	2.26	0.48
2:B:402:GLN:HA	2:B:411:PHE:HA	1.94	0.48
4:H:140:ASN:HB3	4:H:190:THR:HG23	1.95	0.48
1:P:898:VAL:HB	1:P:931:ILE:HG13	1.96	0.48
1:P:1958:ILE:HA	1:P:1959:PHE:N	2.28	0.48
2:A:436:HIS:O	2:A:440:PRO:CD	2.62	0.48
2:B:320:THR:CG2	2:B:339:SER:HB3	2.43	0.48
2:B:331:LYS:HE2	2:B:331:LYS:N	2.29	0.48
2:B:404:PRO:N	2:B:404:PRO:C	2.65	0.48
3:L:119:SER:O	3:L:141:LEU:CA	2.51	0.48
1:P:771:LYS:CE	1:P:771:LYS:CA	2.86	0.48
1:P:1798:ASP:HB3	1:P:1802:ARG:HH12	1.78	0.48
2:A:371:ALA:HB3	2:A:413:VAL:CA	2.43	0.48
2:B:379:VAL:HG13	2:B:437:GLU:CG	2.40	0.48
3:L:85:ALA:C	3:L:173:SER:O	2.56	0.48
4:H:73:SER:OG	4:H:82:ALA:HB3	2.14	0.48
1:P:724:LYS:HZ2	1:P:1219:ASN:CB	2.08	0.47
1:P:803:SER:N	1:P:1093:LEU:HD21	2.29	0.47
2:B:280:THR:O	2:B:324:THR:CG2	2.62	0.47
3:L:45:PRO:CG	3:L:170:GLU:CG	2.87	0.47
3:L:108:ARG:NH2	3:L:147:ARG:CZ	2.76	0.47
3:L:128:GLU:HB2	4:H:128:PHE:HB3	1.94	0.47
1:P:865:SER:HA	1:P:893:ALA:O	2.13	0.47
2:A:265:THR:O	2:A:338:LEU:CD2	2.61	0.47
2:A:294:PRO:HB2	2:A:302:TYR:CE1	2.49	0.47
2:A:299:CYS:HB2	2:B:298:LEU:HD12	1.93	0.47
2:B:251:PRO:HB2	2:B:321:PHE:CD2	2.45	0.47
2:B:287:LYS:CE	2:B:308:LEU:HB3	2.36	0.47
2:B:331:LYS:HE2	2:B:331:LYS:CA	2.44	0.47
2:B:350:HIS:CA	2:B:370:LEU:HB2	2.37	0.47
3:L:123:PHE:HE2	3:L:140:LEU:CD1	2.19	0.47
4:H:12:ALA:CB	4:H:88:LEU:HD12	2.44	0.47
4:H:170:ARG:HG2	4:H:188:GLN:HE21	1.78	0.47
4:H:176:GLN:NE2	4:H:176:GLN:CA	2.73	0.47
1:P:1419:SER:O	1:P:1425:LYS:NZ	2.38	0.47
1:P:1600:ILE:HD11	1:P:1652:LEU:HD11	1.96	0.47
1:P:1924:ARG:CA	2:B:245:ARG:CB	2.79	0.47
2:A:279:PHE:CE2	2:A:291:GLN:OE1	2.67	0.47
2:A:366:THR:HG22	2:A:418:ARG:CD	2.45	0.47
2:B:373:GLY:CA	2:B:434:VAL:O	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1108:ASP:HB3	1:P:1135:LYS:HZ3	1.80	0.47
2:B:253:LEU:HG	2:B:315:TRP:CD2	2.49	0.47
2:B:258:LEU:N	2:B:258:LEU:HD12	2.30	0.47
3:L:23:CYS:HB3	3:L:40:TRP:CH2	2.49	0.47
4:H:97:TYR:HD1	4:H:112:GLY:CA	2.06	0.47
4:H:158:VAL:HG22	4:H:206:VAL:HG13	1.96	0.47
2:B:253:LEU:HA	2:B:315:TRP:HH2	1.64	0.47
2:B:272:ARG:HA	2:B:301:CYS:O	2.15	0.47
3:L:48:ALA:CB	4:H:97:TYR:CD2	2.98	0.47
4:H:36:TRP:CB	4:H:83:LEU:CD2	2.92	0.47
4:H:70:ALA:HA	4:H:85:ALA:CA	2.41	0.47
4:H:71:ALA:N	4:H:84:ALA:CB	2.72	0.47
4:H:86:ALA:CA	4:H:86:ALA:H	2.08	0.47
1:P:683:ARG:CD	1:P:1133:TYR:O	2.62	0.47
1:P:683:ARG:NH2	1:P:1133:TYR:H	2.13	0.47
1:P:836:TYR:CB	1:P:1093:LEU:HD22	2.45	0.47
1:P:1622:ARG:HE	1:P:1847:VAL:HG13	1.79	0.47
3:L:196:VAL:HG13	3:L:214:PHE:O	2.14	0.47
4:H:23:ALA:HA	4:H:80:ALA:CB	2.44	0.47
4:H:70:ALA:HA	4:H:84:ALA:O	2.14	0.47
4:H:153:GLN:HG2	4:H:183:TYR:CE1	2.50	0.47
1:P:690:LEU:HD11	1:P:714:TYR:HB3	1.97	0.47
1:P:1725:ASP:OD1	1:P:1725:ASP:N	2.48	0.47
2:A:430:PHE:HD1	2:A:430:PHE:O	1.97	0.47
2:B:347:PRO:CG	2:B:433:MET:HB2	2.45	0.47
3:L:190:ASP:HA	3:L:193:LYS:CD	2.44	0.47
1:P:1006:ARG:HH22	4:H:160:TRP:N	2.12	0.47
2:A:244:PRO:CB	2:A:334:LEU:HD12	2.45	0.47
2:A:367:LEU:HD13	2:A:383:TRP:HH2	1.71	0.47
2:B:254:GLU:HB2	2:B:379:VAL:C	2.40	0.47
2:B:397:THR:O	2:B:397:THR:HG22	2.15	0.47
3:L:145:TYR:CD2	3:L:146:PRO:HA	2.50	0.47
1:P:794:PRO:HB2	1:P:823:PHE:O	2.14	0.47
1:P:1156:LEU:HD12	1:P:1184:HIS:CE1	2.50	0.47
1:P:1442:ARG:NH2	1:P:1470:THR:O	2.48	0.47
2:A:281:TRP:HE3	2:A:325:ALA:HB2	1.57	0.47
2:B:250:ARG:HB3	2:B:377:LYS:HZ1	1.77	0.47
2:B:264:LEU:H	2:B:307:VAL:CG2	2.28	0.47
3:L:128:GLU:CB	4:H:128:PHE:HB3	2.45	0.47
1:P:1027:THR:HG22	1:P:1053:VAL:O	2.15	0.47
2:A:296:ARG:H	2:A:296:ARG:HG2	1.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:374:PHE:HD2	2:A:411:PHE:HB3	1.72	0.47
2:B:347:PRO:HG2	2:B:444:THR:OG1	2.16	0.47
2:B:401:ARG:CZ	2:B:403:GLU:HG3	2.45	0.47
3:L:122:ILE:HG13	3:L:214:PHE:HD2	1.77	0.47
3:L:123:PHE:CE2	3:L:140:LEU:HD13	2.48	0.47
4:H:160:TRP:HZ2	4:H:218:VAL:HG21	1.79	0.47
1:P:1718:ILE:HB	1:P:1761:LEU:HD22	1.97	0.46
2:A:433:MET:HG2	2:A:442:ALA:CB	2.44	0.46
3:L:25:SER:O	3:L:74:THR:CB	2.61	0.46
3:L:41:TYR:O	3:L:91:TYR:CA	2.63	0.46
4:H:153:GLN:HG3	4:H:183:TYR:CE2	2.43	0.46
1:P:681:GLU:HB3	1:P:1133:TYR:C	2.39	0.46
2:B:251:PRO:HB2	2:B:321:PHE:CE2	2.51	0.46
2:B:318:GLY:O	2:B:340:LYS:N	2.48	0.46
3:L:10:SER:HG	3:L:108:ARG:HD3	1.80	0.46
3:L:42:ALA:CA	3:L:91:TYR:CD1	2.71	0.46
3:L:122:ILE:O	4:H:132:LEU:HD12	2.14	0.46
3:L:141:LEU:HD11	3:L:144:PHE:CD2	2.50	0.46
4:H:191:LEU:HD11	4:H:196:CYS:SG	2.55	0.46
1:P:680:LEU:CD1	1:P:1203:ASN:HD21	2.28	0.46
1:P:723:PHE:CE1	1:P:1132:PHE:HE1	2.30	0.46
1:P:924:GLU:HB2	1:P:1361:ASN:HB2	1.12	0.46
1:P:1030:ASN:HD21	1:P:1068:SER:HB3	1.80	0.46
1:P:1195:LEU:HD22	1:P:1207:TYR:HB3	1.98	0.46
1:P:1765:GLU:HB3	1:P:1780:LYS:HG3	1.97	0.46
2:A:321:PHE:HD2	2:A:377:LYS:NZ	2.11	0.46
2:B:261:GLU:O	2:B:261:GLU:HG3	2.15	0.46
2:B:431:SER:HA	2:B:447:THR:CG2	2.45	0.46
2:B:439:LEU:CB	2:B:442:ALA:HB2	2.46	0.46
3:L:142:ASN:HD22	4:H:170:ARG:HG3	1.80	0.46
4:H:17:SER:HB2	4:H:86:ALA:HB2	1.97	0.46
4:H:160:TRP:CB	4:H:189:LEU:HD13	2.46	0.46
1:P:1052:ARG:HA	1:P:1052:ARG:HD2	1.64	0.46
2:B:249:HIS:HE1	2:B:334:LEU:CD1	2.20	0.46
2:B:344:THR:HG23	2:B:436:HIS:CD2	2.51	0.46
2:B:373:GLY:C	2:B:434:VAL:O	2.58	0.46
3:L:184:LEU:HD23	3:L:184:LEU:HA	1.76	0.46
1:P:1884:GLN:CA	1:P:1959:PHE:CG	2.97	0.46
3:L:11:LEU:CD2	3:L:107:THR:CG2	2.92	0.46
4:H:154:GLU:HA	4:H:155:PRO:HA	1.75	0.46
1:P:1639:ASP:OD2	4:H:231:PRO:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1879:PHE:CD1	1:P:1905:VAL:HG11	2.50	0.46
2:A:313:GLU:N	2:A:314:PRO:CD	2.77	0.46
2:A:318:GLY:CA	2:A:340:LYS:NZ	2.76	0.46
2:B:435:GLY:HA2	2:B:442:ALA:O	2.15	0.46
4:H:125:PRO:HB3	4:H:150:PHE:CB	2.23	0.46
1:P:673:GLN:HE22	1:P:1113:ALA:HB1	1.80	0.46
1:P:702:VAL:HG21	1:P:805:ASN:HB3	1.98	0.46
1:P:923:TYR:CZ	1:P:1358:SER:O	2.69	0.46
1:P:1413:TYR:CZ	1:P:1498:GLU:HG3	2.51	0.46
2:B:334:LEU:HD22	2:B:334:LEU:HA	1.73	0.46
3:L:110:GLU:CD	3:L:110:GLU:N	2.73	0.46
1:P:804:LEU:HD23	1:P:804:LEU:H	1.81	0.46
1:P:892:LEU:HD13	1:P:915:PHE:HZ	1.80	0.46
1:P:920:VAL:HG13	1:P:1374:ILE:CD1	2.46	0.46
3:L:137:VAL:CG1	3:L:153:TRP:CH2	2.96	0.46
1:P:963:GLN:OE1	1:P:963:GLN:N	2.49	0.46
1:P:1197:TYR:CZ	1:P:1200:ASP:HB3	2.49	0.46
1:P:1879:PHE:HD1	1:P:1905:VAL:HG11	1.81	0.46
2:B:424:TRP:HE1	2:B:450:ARG:HG2	1.81	0.46
3:L:22:ALA:CA	3:L:76:PHE:O	2.63	0.46
3:L:129:GLN:OE1	4:H:128:PHE:CE1	2.69	0.46
4:H:36:TRP:CD2	4:H:83:LEU:CD2	2.89	0.46
4:H:141:VAL:O	4:H:190:THR:HA	2.16	0.46
1:P:1084:LYS:HD2	1:P:1084:LYS:O	2.15	0.46
2:B:246:LEU:HB3	2:B:247:SER:H	1.52	0.46
2:B:256:LEU:HD21	2:B:257:LEU:HD23	1.98	0.46
4:H:70:ALA:C	4:H:84:ALA:O	2.53	0.46
4:H:188:GLN:O	4:H:188:GLN:HG3	2.15	0.46
1:P:776:GLU:OE2	1:P:776:GLU:N	2.40	0.45
1:P:1634:LEU:HD12	1:P:1635:LEU:HG	1.98	0.45
3:L:214:PHE:CD1	3:L:214:PHE:C	2.95	0.45
4:H:35:ALA:HA	4:H:50:ALA:HA	1.98	0.45
1:P:1131:PRO:HD2	1:P:1217:THR:HG23	1.97	0.45
1:P:1307:LYS:NZ	1:P:1308:GLU:OE2	2.48	0.45
2:A:401:ARG:CD	2:B:414:THR:HG21	2.45	0.45
2:B:253:LEU:CA	2:B:315:TRP:CZ3	2.99	0.45
2:B:351:LEU:HD13	2:B:369:CYS:HB3	1.91	0.45
2:B:374:PHE:HD1	2:B:374:PHE:H	1.63	0.45
3:L:21:ILE:CD1	3:L:91:TYR:CD2	2.99	0.45
4:H:159:THR:OG1	4:H:205:HIS:CB	2.60	0.45
1:P:698:TYR:CZ	1:P:1298:TYR:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:961:SER:HB2	4:H:200:LYS:HE2	1.97	0.45
1:P:1924:ARG:NH2	2:B:243:HIS:HB2	2.30	0.45
2:A:249:HIS:CD2	2:A:265:THR:CG2	2.99	0.45
2:B:287:LYS:NZ	2:B:308:LEU:HB2	2.32	0.45
2:B:289:ALA:CB	2:B:307:VAL:O	2.64	0.45
2:B:313:GLU:HB3	2:B:314:PRO:HD3	1.97	0.45
3:L:110:GLU:OE2	3:L:110:GLU:N	2.49	0.45
1:P:997:ALA:HB3	1:P:1000:ALA:O	2.16	0.45
1:P:1338:PRO:HA	1:P:1380:HIS:HD1	1.81	0.45
1:P:1599:ALA:HA	1:P:1602:TYR:HB3	1.99	0.45
1:P:1924:ARG:CD	2:B:245:ARG:HB2	2.37	0.45
2:B:343:ASN:OD1	2:B:408:THR:HG23	2.15	0.45
2:B:354:PRO:HD2	2:B:450:ARG:HH12	0.63	0.45
3:L:115:VAL:CG2	3:L:205:GLY:CA	2.93	0.45
4:H:4:LEU:HD11	4:H:109:TRP:O	2.16	0.45
4:H:12:ALA:O	4:H:117:VAL:CG1	2.50	0.45
4:H:29:ALA:C	4:H:53:ALA:HB1	2.38	0.45
3:L:199:CYS:C	3:L:211:THR:HG1	2.15	0.45
4:H:34:ALA:H	4:H:51:ILE:HG22	1.79	0.45
1:P:834:LYS:HG2	1:P:1092:THR:HB	1.97	0.45
1:P:1533:LEU:HD21	1:P:1606:MET:HE2	1.97	0.45
2:A:257:LEU:CD2	2:A:315:TRP:NE1	2.70	0.45
2:A:417:LEU:CD1	2:B:404:PRO:CG	2.78	0.45
2:B:358:GLU:HG2	2:B:358:GLU:O	2.16	0.45
2:B:400:SER:HB3	2:B:412:ALA:C	2.41	0.45
1:P:1288:LEU:HD22	1:P:1295:THR:HB	1.99	0.45
2:A:426:LYS:HD3	2:A:426:LYS:HA	1.58	0.45
4:H:71:ALA:N	4:H:84:ALA:C	2.42	0.45
2:A:321:PHE:CB	2:A:338:LEU:HB2	2.47	0.45
2:B:320:THR:N	2:B:339:SER:CA	2.69	0.45
4:H:153:GLN:OE1	4:H:174:PRO:HB2	2.16	0.45
1:P:1087:GLU:N	1:P:1087:GLU:CD	2.75	0.45
2:B:285:SER:HB3	2:B:314:PRO:CG	2.46	0.45
4:H:36:TRP:CE2	4:H:83:LEU:HB2	2.52	0.45
1:P:728:ILE:CG2	1:P:1289:ALA:CB	2.67	0.45
1:P:1448:TRP:HA	1:P:1448:TRP:CE3	2.52	0.45
2:A:371:ALA:N	2:A:414:THR:N	2.50	0.45
2:B:350:HIS:CD2	2:B:350:HIS:O	2.71	0.45
3:L:6:GLN:HB2	3:L:106:GLY:O	2.17	0.45
3:L:49:PRO:HD3	4:H:97:TYR:CE2	2.52	0.45
3:L:130:LEU:HD12	3:L:130:LEU:HA	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1808:LEU:HD12	1:P:1808:LEU:HA	1.83	0.44
2:B:271:LEU:CD1	2:B:327:TYR:HB2	2.46	0.44
2:B:307:VAL:C	2:B:307:VAL:N	2.74	0.44
4:H:207:LYS:CE	4:H:210:THR:HA	2.45	0.44
1:P:684:ASN:HA	1:P:1104:LYS:CG	2.47	0.44
1:P:776:GLU:CD	1:P:776:GLU:N	2.73	0.44
1:P:1923:PRO:O	2:B:245:ARG:CG	2.64	0.44
1:P:1924:ARG:NE	2:B:243:HIS:HB2	2.29	0.44
2:B:417:LEU:HD13	2:B:417:LEU:HA	1.76	0.44
3:L:3:ALA:CB	3:L:25:SER:HA	2.43	0.44
3:L:43:ALA:HB2	3:L:49:PRO:CB	2.47	0.44
4:H:6:ALA:HB1	4:H:113:THR:CG2	2.46	0.44
4:H:159:THR:O	4:H:205:HIS:CB	2.65	0.44
2:A:251:PRO:HG3	2:A:264:LEU:HD12	1.98	0.44
2:A:282:THR:N	2:A:283:PRO:CD	2.80	0.44
2:A:318:GLY:C	2:A:340:LYS:HZ1	2.24	0.44
2:A:348:GLU:OE1	2:B:357:GLU:OE1	2.35	0.44
2:B:262:ALA:HB1	2:B:310:GLY:CA	2.47	0.44
2:B:389:GLU:OE2	2:B:395:TYR:CD2	2.71	0.44
2:B:258:LEU:HD23	2:B:443:PHE:HZ	1.83	0.44
2:B:271:LEU:HG	2:B:304:VAL:CG2	2.48	0.44
2:B:320:THR:CG2	2:B:339:SER:CB	2.94	0.44
1:P:904:LYS:HG3	1:P:937:HIS:HB3	1.99	0.44
1:P:1232:VAL:HG13	1:P:1278:LEU:HD21	1.99	0.44
2:B:368:THR:O	2:B:368:THR:OG1	2.32	0.44
2:B:374:PHE:O	2:B:374:PHE:CD1	2.70	0.44
1:P:905:ALA:HB3	1:P:938:LEU:HD23	2.00	0.44
1:P:1926:SER:CB	2:B:243:HIS:CA	2.95	0.44
2:A:395:TYR:CE1	2:A:417:LEU:HD11	2.53	0.44
2:B:287:LYS:O	2:B:308:LEU:HD22	2.18	0.44
2:B:313:GLU:N	2:B:314:PRO:CD	2.81	0.44
2:B:415:SER:OG	2:B:432:CYS:SG	2.74	0.44
1:P:818:TYR:HE2	1:P:841:LEU:HD22	1.83	0.44
1:P:1817:GLY:O	1:P:1820:PRO:HD2	2.17	0.44
2:A:371:ALA:HB1	2:A:413:VAL:HG13	2.00	0.44
2:A:395:TYR:HE1	2:A:417:LEU:CD1	2.31	0.44
2:B:264:LEU:C	2:B:307:VAL:CB	2.91	0.44
2:B:391:PRO:HB2	2:B:394:LYS:HB2	2.00	0.44
3:L:142:ASN:OD1	3:L:142:ASN:N	2.51	0.44
1:P:1415:VAL:HG13	1:P:1468:ILE:HA	2.00	0.44
1:P:1443:ILE:H	1:P:1443:ILE:HG13	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:21:ILE:HD13	3:L:91:TYR:HD2	1.81	0.44
3:L:155:VAL:HG22	3:L:194:HIS:CB	2.48	0.44
3:L:199:CYS:O	3:L:212:LYS:N	2.43	0.44
1:P:1900:LYS:HD2	1:P:1900:LYS:HA	1.85	0.44
2:A:255:ASP:OD2	2:A:392:ARG:CZ	2.66	0.44
2:B:294:PRO:CB	2:B:302:TYR:HD2	2.30	0.44
3:L:153:TRP:HZ2	3:L:197:TYR:HD2	1.66	0.44
4:H:36:TRP:NE1	4:H:83:LEU:HB2	2.32	0.44
1:P:715:PHE:CD1	1:P:1294:VAL:HG22	2.53	0.43
2:A:296:ARG:CZ	2:A:296:ARG:CB	2.85	0.43
2:A:374:PHE:O	2:A:411:PHE:HD2	2.01	0.43
2:A:383:TRP:CE3	2:A:432:CYS:HA	2.53	0.43
2:B:250:ARG:CD	2:B:250:ARG:N	2.73	0.43
2:B:251:PRO:CB	2:B:338:LEU:HD12	2.48	0.43
2:B:264:LEU:HG	2:B:315:TRP:HZ2	1.82	0.43
2:B:343:ASN:O	2:B:375:SER:CB	2.66	0.43
2:B:345:PHE:CD2	2:B:410:THR:CB	2.96	0.43
3:L:65:ALA:HB2	3:L:80:ILE:HB	1.98	0.43
1:P:687:ASP:H	1:P:1101:THR:HA	1.83	0.43
1:P:937:HIS:NE2	1:P:971:LEU:HD23	2.33	0.43
1:P:1669:ASP:HB3	1:P:1672:GLU:HB2	1.99	0.43
1:P:1841:GLY:N	4:H:138:ASP:OD2	2.51	0.43
1:P:1883:LYS:CG	1:P:1963:LYS:CE	2.64	0.43
2:B:371:ALA:HB3	2:B:412:ALA:HB1	2.00	0.43
1:P:956:SER:O	1:P:989:ASN:HA	2.18	0.43
1:P:1072:ARG:HD3	1:P:1072:ARG:HA	1.78	0.43
1:P:1883:LYS:CA	1:P:1959:PHE:CB	2.72	0.43
2:A:367:LEU:HD23	2:A:367:LEU:HA	1.80	0.43
2:A:394:LYS:HD3	2:A:395:TYR:N	2.33	0.43
2:B:257:LEU:CG	2:B:440:PRO:HB3	2.47	0.43
1:P:864:ILE:HD12	1:P:872:SER:HA	2.00	0.43
2:A:248:LEU:HG	2:A:250:ARG:HB3	2.00	0.43
2:A:348:GLU:H	2:A:372:ARG:CG	2.31	0.43
2:A:354:PRO:HA	2:B:352:LEU:HD11	1.90	0.43
2:B:390:LEU:HD22	2:B:417:LEU:HD21	2.00	0.43
4:H:129:PRO:HB2	4:H:218:VAL:CA	2.49	0.43
4:H:153:GLN:OE1	4:H:183:TYR:CE1	2.71	0.43
4:H:197:LEU:O	4:H:200:LYS:HB2	2.19	0.43
1:P:729:PRO:HD3	1:P:1289:ALA:O	2.18	0.43
2:A:340:LYS:HA	2:A:377:LYS:CE	2.49	0.43
2:A:367:LEU:HD13	2:A:383:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:725:ASP:OD1	1:P:725:ASP:N	2.51	0.43
1:P:990:VAL:HG12	1:P:991:LYS:HG3	1.99	0.43
1:P:999:VAL:HG21	1:P:1020:VAL:HG22	2.00	0.43
2:B:256:LEU:HD11	2:B:315:TRP:CD2	2.42	0.43
2:B:318:GLY:HA3	2:B:340:LYS:HD2	2.00	0.43
3:L:6:GLN:OE1	3:L:106:GLY:HA2	2.19	0.43
3:L:38:LEU:HD13	3:L:38:LEU:HA	1.73	0.43
4:H:191:LEU:H	4:H:191:LEU:CD2	2.26	0.43
1:P:804:LEU:HD23	1:P:804:LEU:N	2.34	0.43
1:P:836:TYR:CA	1:P:1093:LEU:CD2	2.83	0.43
1:P:959:ASN:HA	1:P:993:PHE:HD2	1.83	0.43
2:B:256:LEU:CD1	2:B:315:TRP:CG	2.98	0.43
2:B:401:ARG:HD3	2:B:401:ARG:C	2.42	0.43
3:L:118:PRO:CB	3:L:141:LEU:CD1	2.95	0.43
1:P:1779:ILE:HD13	1:P:1803:ARG:HA	2.01	0.43
1:P:1832:GLN:HE21	1:P:1832:GLN:HB3	1.65	0.43
2:A:254:GLU:CG	2:A:435:GLY:HA3	2.49	0.43
2:B:264:LEU:CD1	2:B:308:LEU:CA	2.97	0.43
3:L:48:ALA:HA	4:H:97:TYR:CD2	2.53	0.43
3:L:123:PHE:HA	3:L:124:PRO:HD2	1.80	0.43
4:H:211:ASN:HB3	4:H:212:PRO:HD2	2.00	0.43
1:P:800:LEU:HD13	1:P:804:LEU:HD21	2.01	0.43
1:P:1564:PHE:C	1:P:1567:PRO:HD2	2.44	0.43
1:P:1580:TYR:CB	4:H:227:PRO:CD	2.93	0.43
2:A:345:PHE:HE2	2:A:409:THR:HG23	1.84	0.43
2:A:371:ALA:HB3	2:A:413:VAL:H	1.84	0.43
2:B:364:LEU:HD11	2:B:418:ARG:HH11	1.84	0.43
1:P:681:GLU:CD	1:P:1134:ASN:CB	2.89	0.43
1:P:698:TYR:CE2	1:P:1294:VAL:HG22	2.49	0.43
1:P:985:GLY:O	1:P:1024:VAL:HG23	2.19	0.43
1:P:1050:ALA:HB3	1:P:1052:ARG:NH1	2.33	0.43
1:P:1155:GLU:HG2	1:P:1156:LEU:O	2.18	0.43
1:P:1627:PRO:HG3	4:H:225:THR:CG2	2.48	0.43
1:P:1692:TYR:HB2	1:P:1875:ARG:HG2	2.01	0.43
1:P:1726:PRO:HB2	4:H:135:THR:HB	2.00	0.43
2:A:348:GLU:O	2:A:372:ARG:HD3	2.19	0.43
2:B:353:PRO:CB	2:B:450:ARG:HD2	2.25	0.43
3:L:144:PHE:O	3:L:144:PHE:CG	2.72	0.43
1:P:721:SER:OG	1:P:1104:LYS:O	2.37	0.42
1:P:1046:PHE:HA	1:P:1072:ARG:CG	2.49	0.42
2:A:331:LYS:HD3	2:A:331:LYS:HA	1.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:443:PHE:CD1	2:A:443:PHE:C	2.96	0.42
1:P:918:ARG:CD	1:P:1378:SER:HB2	2.46	0.42
1:P:1023:ASP:CB	1:P:1048:SER:OG	2.56	0.42
1:P:1046:PHE:HD1	1:P:1072:ARG:HB3	1.84	0.42
1:P:1720:ASN:HB2	1:P:1734:ALA:HB1	2.00	0.42
1:P:1881:ASN:O	1:P:1961:ASN:O	2.38	0.42
2:B:356:SER:HB3	2:B:359:LEU:HD12	2.01	0.42
4:H:37:VAL:H	4:H:96:TYR:CB	2.24	0.42
1:P:1084:LYS:C	1:P:1084:LYS:CD	2.92	0.42
1:P:1109:PHE:CD1	1:P:1123:TYR:HB3	2.53	0.42
2:A:242:CYS:HA	2:A:272:ARG:HB2	2.00	0.42
2:B:264:LEU:CG	2:B:307:VAL:CA	2.97	0.42
2:B:294:PRO:HB3	2:B:302:TYR:HD2	1.85	0.42
3:L:124:PRO:CD	4:H:133:CYS:CA	2.95	0.42
3:L:129:GLN:HB2	4:H:128:PHE:CZ	2.55	0.42
1:P:1883:LYS:C	1:P:1963:LYS:CD	2.78	0.42
2:A:264:LEU:O	2:A:308:LEU:N	2.43	0.42
3:L:123:PHE:CE2	3:L:140:LEU:HD12	2.50	0.42
3:L:155:VAL:HG22	3:L:194:HIS:HB2	2.01	0.42
3:L:168:VAL:O	3:L:168:VAL:HG23	2.18	0.42
4:H:156:LEU:CD1	4:H:207:LYS:O	2.67	0.42
1:P:715:PHE:CG	1:P:1295:THR:CG2	3.02	0.42
1:P:947:LYS:HD3	1:P:1084:LYS:HG2	1.98	0.42
1:P:1046:PHE:HA	1:P:1072:ARG:HG3	2.00	0.42
1:P:1209:LEU:HD12	1:P:1214:LEU:HB2	2.01	0.42
3:L:124:PRO:CD	4:H:133:CYS:H	2.33	0.42
4:H:83:LEU:HD12	4:H:84:ALA:N	2.34	0.42
1:P:684:ASN:ND2	1:P:1105:LYS:N	2.59	0.42
1:P:719:LYS:O	1:P:1101:THR:O	2.37	0.42
1:P:918:ARG:CD	1:P:1378:SER:CB	2.97	0.42
4:H:37:VAL:C	4:H:48:VAL:CG2	2.92	0.42
1:P:1440:TYR:CD2	1:P:1444:THR:HG21	2.51	0.42
1:P:1443:ILE:HA	1:P:1448:TRP:CD1	2.55	0.42
2:A:249:HIS:CD2	2:A:265:THR:HG21	2.54	0.42
2:A:264:LEU:HD21	2:A:321:PHE:CE1	2.54	0.42
2:B:332:THR:N	2:B:333:PRO:CD	2.83	0.42
2:B:380:LEU:C	2:B:380:LEU:HD12	2.44	0.42
3:L:145:TYR:HE1	3:L:178:TYR:CD2	2.34	0.42
4:H:124:SER:HA	4:H:125:PRO:HD3	1.94	0.42
4:H:132:LEU:HD13	4:H:132:LEU:HA	1.85	0.42
1:P:1125:ASN:ND2	1:P:1153:GLN:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1855:LYS:HA	1:P:1855:LYS:HD3	1.79	0.42
2:A:277:VAL:HG13	2:A:328:PRO:HD3	2.02	0.42
2:A:327:TYR:HB2	2:A:328:PRO:HD2	2.01	0.42
2:A:401:ARG:NH2	2:B:416:ILE:CG2	2.81	0.42
2:B:250:ARG:O	2:B:266:CYS:HA	2.20	0.42
3:L:145:TYR:CA	3:L:203:HIS:CE1	2.86	0.42
4:H:149:GLY:CA	4:H:182:LEU:HD23	2.41	0.42
1:P:681:GLU:CD	1:P:1134:ASN:CG	2.80	0.42
1:P:883:ILE:H	1:P:883:ILE:HG12	1.66	0.42
1:P:1458:LEU:HD12	1:P:1458:LEU:HA	1.71	0.42
1:P:1948:LEU:HD12	1:P:1954:PHE:HE1	1.85	0.42
2:A:374:PHE:C	2:A:411:PHE:HD2	2.26	0.42
2:B:256:LEU:HA	2:B:262:ALA:HB1	2.01	0.42
2:B:349:VAL:HG23	2:B:446:LYS:CE	2.50	0.42
2:B:367:LEU:HD23	2:B:367:LEU:HA	1.89	0.42
2:B:381:VAL:CG1	2:B:434:VAL:HA	2.48	0.42
3:L:122:ILE:HD12	3:L:123:PHE:H	1.85	0.42
4:H:150:PHE:HE2	4:H:153:GLN:HA	1.84	0.42
1:P:1175:LYS:HD2	1:P:1175:LYS:HA	1.81	0.42
1:P:728:ILE:HD12	1:P:748:ALA:HB1	2.02	0.41
1:P:1112:ILE:HD12	1:P:1112:ILE:HA	1.72	0.41
1:P:1488:LYS:HA	1:P:1542:ASP:OD1	2.20	0.41
2:A:364:LEU:HD23	2:A:364:LEU:HA	1.80	0.41
2:B:394:LYS:HE3	2:B:418:ARG:HB2	2.02	0.41
3:L:10:SER:OG	3:L:108:ARG:NH1	2.39	0.41
4:H:170:ARG:HG2	4:H:170:ARG:H	1.63	0.41
2:B:268:LEU:HD12	2:B:325:ALA:HB3	1.86	0.41
3:L:200:GLU:O	3:L:200:GLU:HG2	2.20	0.41
4:H:19:LYS:HZ1	4:H:84:ALA:HB2	1.85	0.41
1:P:688:ILE:HG23	1:P:718:VAL:CG1	2.46	0.41
1:P:698:TYR:CD1	1:P:1298:TYR:HA	2.56	0.41
1:P:1220:GLN:NE2	1:P:1283:SER:O	2.53	0.41
1:P:1450:TYR:OH	1:P:1570:ASN:OD1	2.38	0.41
1:P:1689:ASP:OD1	1:P:1875:ARG:HG3	2.20	0.41
2:B:394:LYS:HB3	2:B:417:LEU:CD1	2.50	0.41
3:L:14:SER:N	3:L:17:ALA:HB3	2.35	0.41
3:L:180:LEU:C	3:L:180:LEU:CD2	2.86	0.41
4:H:203:THR:HB	4:H:215:ASP:OD1	2.20	0.41
4:H:223:VAL:HG23	4:H:223:VAL:O	2.20	0.41
1:P:771:LYS:HD3	1:P:781:THR:CG2	2.32	0.41
1:P:1553:LYS:O	1:P:1554:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:137:VAL:CG1	3:L:214:PHE:HE2	2.32	0.41
1:P:719:LYS:HB3	1:P:719:LYS:HE3	1.93	0.41
2:B:258:LEU:HD22	2:B:380:LEU:HB3	2.02	0.41
3:L:145:TYR:CZ	3:L:147:ARG:HB2	2.56	0.41
3:L:159:LEU:HD12	3:L:159:LEU:HA	1.88	0.41
1:P:719:LYS:HG3	1:P:1101:THR:HG21	1.88	0.41
1:P:800:LEU:HD13	1:P:804:LEU:CD2	2.50	0.41
1:P:934:LEU:HB3	1:P:968:LEU:O	2.21	0.41
2:A:307:VAL:HB	2:A:309:PRO:CD	2.35	0.41
2:A:446:LYS:HD3	2:A:446:LYS:HA	1.39	0.41
2:B:290:VAL:H	2:B:307:VAL:CA	2.33	0.41
2:B:354:PRO:HB3	2:B:367:LEU:HD21	2.02	0.41
3:L:6:GLN:CD	3:L:106:GLY:CA	2.93	0.41
3:L:142:ASN:HA	3:L:179:SER:CA	2.47	0.41
4:H:86:ALA:N	4:H:86:ALA:C	2.64	0.41
1:P:684:ASN:O	1:P:1104:LYS:O	2.39	0.41
1:P:988:ASN:HA	1:P:1027:THR:OG1	2.20	0.41
1:P:1932:ILE:HD12	2:A:293:PRO:CB	2.49	0.41
2:B:250:ARG:CA	2:B:378:ASP:OD2	2.69	0.41
2:B:350:HIS:N	2:B:370:LEU:HB2	2.35	0.41
4:H:12:ALA:HB1	4:H:88:LEU:HD12	2.02	0.41
4:H:127:VAL:HG11	4:H:206:VAL:CB	2.51	0.41
1:P:667:THR:HG23	1:P:667:THR:O	2.20	0.41
1:P:698:TYR:OH	1:P:1294:VAL:O	2.34	0.41
1:P:771:LYS:HA	1:P:771:LYS:HZ2	1.79	0.41
1:P:1006:ARG:HH22	4:H:160:TRP:H	1.69	0.41
2:A:430:PHE:O	2:A:430:PHE:CD1	2.74	0.41
2:A:433:MET:HA	2:A:442:ALA:HB1	2.02	0.41
2:A:441:LEU:HD12	2:A:441:LEU:HA	1.83	0.41
2:B:245:ARG:HH21	2:B:331:LYS:HG2	1.80	0.41
2:B:374:PHE:CE1	2:B:434:VAL:HG21	2.55	0.41
2:B:394:LYS:CE	2:B:418:ARG:HB2	2.50	0.41
2:B:401:ARG:NH2	2:B:403:GLU:HG3	2.36	0.41
1:P:684:ASN:CG	1:P:1104:LYS:C	2.89	0.41
1:P:780:PHE:O	1:P:801:ALA:CA	2.69	0.41
1:P:780:PHE:O	1:P:801:ALA:HB2	2.16	0.41
1:P:780:PHE:CE1	1:P:799:HIS:HB2	2.56	0.41
1:P:834:LYS:HB3	1:P:1092:THR:HB	2.03	0.41
1:P:1223:TYR:OH	1:P:1282:LEU:HB3	2.20	0.41
1:P:1245:ALA:HB1	1:P:1308:GLU:HG2	2.03	0.41
2:A:254:GLU:CD	2:A:435:GLY:HA3	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:256:LEU:C	2:A:256:LEU:CD1	2.85	0.41
2:A:296:ARG:NH2	2:A:296:ARG:CB	2.84	0.41
2:A:327:TYR:CE2	2:A:330:SER:HB2	2.55	0.41
2:A:395:TYR:CE1	2:A:417:LEU:CD1	3.04	0.41
2:B:272:ARG:NH2	2:B:301:CYS:H	2.15	0.41
2:B:349:VAL:HG11	2:B:432:CYS:H	1.86	0.41
2:B:429:THR:HG22	2:B:449:ASP:HB3	2.03	0.41
4:H:17:SER:HA	4:H:86:ALA:N	2.35	0.41
4:H:48:VAL:HB	4:H:49:ALA:H	1.71	0.41
4:H:125:PRO:HA	4:H:150:PHE:HB2	2.02	0.41
4:H:147:VAL:HG12	4:H:150:PHE:HB3	2.02	0.41
2:A:255:ASP:OD2	2:A:392:ARG:NH1	2.54	0.41
3:L:129:GLN:HB2	4:H:128:PHE:CD2	2.56	0.41
1:P:1027:THR:HG22	1:P:1053:VAL:C	2.46	0.40
1:P:1193:PHE:HD1	1:P:1193:PHE:HA	1.81	0.40
2:A:398:TRP:CH2	2:B:414:THR:N	2.76	0.40
2:A:417:LEU:HD23	2:A:417:LEU:HA	1.81	0.40
2:B:345:PHE:CZ	2:B:408:THR:HB	2.52	0.40
2:B:350:HIS:HB3	2:B:370:LEU:CG	2.44	0.40
2:B:385:GLN:HE21	2:B:430:PHE:HB3	1.80	0.40
3:L:104:GLY:CA	4:H:45:LEU:HB2	2.50	0.40
3:L:122:ILE:HD12	3:L:123:PHE:N	2.36	0.40
4:H:19:LYS:HD3	4:H:19:LYS:HA	1.65	0.40
4:H:131:SER:HB3	4:H:219:PRO:CB	2.45	0.40
1:P:1266:GLN:HG2	1:P:1319:ARG:HB2	2.03	0.40
1:P:1457:LEU:HD12	1:P:1457:LEU:HA	1.90	0.40
1:P:1835:GLN:O	1:P:1846:LEU:HB3	2.21	0.40
2:A:290:VAL:O	2:A:306:SER:OG	2.39	0.40
2:A:379:VAL:HG11	2:A:400:SER:HB2	2.03	0.40
2:B:258:LEU:CD2	2:B:443:PHE:CZ	3.04	0.40
3:L:66:ARG:CZ	3:L:66:ARG:CA	2.93	0.40
4:H:202:VAL:HB	4:H:218:VAL:HG22	2.03	0.40
1:P:779:ASN:CB	1:P:785:ASN:C	2.94	0.40
1:P:947:LYS:HG2	1:P:1084:LYS:H	1.86	0.40
1:P:1002:TYR:OH	4:H:163:SER:HB2	2.20	0.40
1:P:1923:PRO:CD	2:B:245:ARG:HD2	2.31	0.40
2:B:431:SER:HB3	2:B:445:GLN:HA	2.04	0.40
3:L:67:PHE:HB2	3:L:80:ILE:O	2.20	0.40
4:H:109:TRP:HE3	4:H:110:GLY:CA	2.34	0.40
4:H:160:TRP:HB3	4:H:189:LEU:HD13	2.03	0.40
4:H:198:ALA:HB1	4:H:223:VAL:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:837:ALA:HB2	1:P:1091:LEU:HD11	2.02	0.40
1:P:918:ARG:NE	1:P:1378:SER:HB3	2.34	0.40
2:B:285:SER:HB3	2:B:314:PRO:HG3	2.02	0.40
2:B:374:PHE:CE2	2:B:381:VAL:HG21	2.57	0.40
3:L:22:ALA:HB1	3:L:77:ALA:HA	2.00	0.40
3:L:43:ALA:HB2	3:L:49:PRO:HB3	2.03	0.40
3:L:67:PHE:CD1	3:L:81:ALA:HB3	2.56	0.40
3:L:122:ILE:HG22	4:H:134:SER:OG	2.20	0.40
1:P:1118:ASN:OD1	1:P:1118:ASN:N	2.53	0.40
1:P:1261:LEU:HG	1:P:1360:PHE:HE1	1.85	0.40
1:P:1638:PRO:HG3	1:P:1666:GLN:HG3	2.04	0.40
1:P:1716:ARG:HG2	1:P:1763:ALA:HB2	2.03	0.40
2:B:250:ARG:HD2	2:B:267:THR:H	1.84	0.40
2:B:374:PHE:HB3	2:B:435:GLY:N	2.37	0.40
3:L:1:ALA:HB1	4:H:46:GLU:CB	2.43	0.40
4:H:29:ALA:HB3	4:H:54:ALA:HB2	1.22	0.40
4:H:88:LEU:HD22	4:H:88:LEU:HA	1.92	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	P	1272/1299 (98%)	1197 (94%)	69 (5%)	6 (0%)	25 61
2	A	207/210 (99%)	178 (86%)	19 (9%)	10 (5%)	2 20
2	B	208/210 (99%)	178 (86%)	20 (10%)	10 (5%)	2 20
3	L	217/219 (99%)	205 (94%)	8 (4%)	4 (2%)	7 36
4	H	230/232 (99%)	209 (91%)	14 (6%)	7 (3%)	3 27
All	All	2134/2170 (98%)	1967 (92%)	130 (6%)	37 (2%)	10 37

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	779	ASN
1	P	1089	ASN
2	A	354	PRO
2	B	244	PRO
2	B	302	TYR
1	P	772	LYS
1	P	1108	ASP
2	A	270	GLY
2	B	372	ARG
4	H	224	PRO
1	P	983	ALA
2	A	355	PRO
2	A	362	ASN
2	B	283	PRO
4	H	48	VAL
4	H	122	PRO
1	P	1076	LEU
2	B	286	GLY
2	B	341	SER
3	L	18	ALA
3	L	115	VAL
4	H	225	THR
2	A	283	PRO
2	A	347	PRO
2	A	375	SER
2	A	404	PRO
2	B	354	PRO
2	B	391	PRO
2	B	404	PRO
4	H	111	GLN
3	L	81	ALA
4	H	220	CYS
4	H	226	PRO
2	A	353	PRO
2	A	381	VAL
2	B	243	HIS
3	L	124	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	P	1096/1118 (98%)	1032 (94%)	64 (6%)	17 40
2	A	179/180 (99%)	109 (61%)	70 (39%)	0 0
2	B	180/180 (100%)	107 (59%)	73 (41%)	0 0
3	L	145/145 (100%)	92 (63%)	53 (37%)	0 1
4	H	142/142 (100%)	82 (58%)	60 (42%)	0 0
All	All	1742/1765 (99%)	1422 (82%)	320 (18%)	3 9

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	688	ILE
1	P	770	ASP
1	P	771	LYS
1	P	774	LYS
1	P	775	GLU
1	P	776	GLU
1	P	778	THR
1	P	781	THR
1	P	828	ILE
1	P	879	ASN
1	P	883	ILE
1	P	964	THR
1	P	968	LEU
1	P	971	LEU
1	P	975	ASP
1	P	979	GLN
1	P	996	VAL
1	P	999	VAL
1	P	1004	TRP
1	P	1048	SER
1	P	1051	ASN
1	P	1052	ARG
1	P	1053	VAL

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Mol	Chain	Res	Type
1	P	1065	SER
1	P	1068	SER
1	P	1075	MET
1	P	1076	LEU
1	P	1080	GLN
1	P	1081	ILE
1	P	1082	VAL
1	P	1084	LYS
1	P	1085	LYS
1	P	1087	GLU
1	P	1088	ILE
1	P	1089	ASN
1	P	1091	LEU
1	P	1092	THR
1	P	1105	LYS
1	P	1111	LYS
1	P	1112	ILE
1	P	1199	THR
1	P	1200	ASP
1	P	1437	ILE
1	P	1443	ILE
1	P	1444	THR
1	P	1449	LYS
1	P	1451	ARG
1	P	1452	ASN
1	P	1458	LEU
1	P	1460	LEU
1	P	1462	GLU
1	P	1465	VAL
1	P	1486	ASP
1	P	1534	TYR
1	P	1551	GLU
1	P	1553	LYS
1	P	1555	ASP
1	P	1634	LEU
1	P	1664	ARG
1	P	1753	GLU
1	P	1832	GLN
1	P	1833	GLN
1	P	1894	TRP
1	P	1899	THR
2	A	250	ARG

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Mol	Chain	Res	Type
2	A	256	LEU
2	A	257	LEU
2	A	258	LEU
2	A	260	SER
2	A	263	ASN
2	A	264	LEU
2	A	265	THR
2	A	267	THR
2	A	268	LEU
2	A	269	THR
2	A	272	ARG
2	A	275	SER
2	A	278	THR
2	A	279	PHE
2	A	280	THR
2	A	284	SER
2	A	285	SER
2	A	295	GLU
2	A	296	ARG
2	A	298	LEU
2	A	299	CYS
2	A	302	TYR
2	A	306	SER
2	A	307	VAL
2	A	319	LYS
2	A	324	THR
2	A	327	TYR
2	A	330	SER
2	A	331	LYS
2	A	334	LEU
2	A	335	THR
2	A	345	PHE
2	A	346	ARG
2	A	351	LEU
2	A	352	LEU
2	A	356	SER
2	A	358	GLU
2	A	364	LEU
2	A	365	VAL
2	A	367	LEU
2	A	368	THR
2	A	370	LEU

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Mol	Chain	Res	Type
2	A	372	ARG
2	A	377	LYS
2	A	380	LEU
2	A	384	LEU
2	A	389	GLU
2	A	393	GLU
2	A	394	LYS
2	A	395	TYR
2	A	397	THR
2	A	403	GLU
2	A	408	THR
2	A	409	THR
2	A	413	VAL
2	A	416	ILE
2	A	417	LEU
2	A	418	ARG
2	A	422	GLU
2	A	426	LYS
2	A	430	PHE
2	A	433	MET
2	A	441	LEU
2	A	443	PHE
2	A	446	LYS
2	A	447	THR
2	A	448	ILE
2	A	449	ASP
2	A	450	ARG
2	B	245	ARG
2	B	246	LEU
2	B	248	LEU
2	B	249	HIS
2	B	250	ARG
2	B	254	GLU
2	B	256	LEU
2	B	257	LEU
2	B	266	CYS
2	B	269	THR
2	B	271	LEU
2	B	272	ARG
2	B	277	VAL
2	B	279	PHE
2	B	287	LYS

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Mol	Chain	Res	Type
2	B	291	GLN
2	B	296	ARG
2	B	297	ASP
2	B	298	LEU
2	B	299	CYS
2	B	308	LEU
2	B	313	GLU
2	B	316	ASN
2	B	317	HIS
2	B	329	GLU
2	B	330	SER
2	B	331	LYS
2	B	334	LEU
2	B	335	THR
2	B	338	LEU
2	B	339	SER
2	B	340	LYS
2	B	345	PHE
2	B	348	GLU
2	B	349	VAL
2	B	351	LEU
2	B	352	LEU
2	B	357	GLU
2	B	359	LEU
2	B	361	LEU
2	B	364	LEU
2	B	370	LEU
2	B	372	ARG
2	B	374	PHE
2	B	378	ASP
2	B	380	LEU
2	B	382	ARG
2	B	384	LEU
2	B	385	GLN
2	B	387	SER
2	B	390	LEU
2	B	392	ARG
2	B	393	GLU
2	B	394	LYS
2	B	396	LEU
2	B	398	TRP
2	B	401	ARG

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Mol	Chain	Res	Type
2	B	402	GLN
2	B	405	SER
2	B	410	THR
2	B	413	VAL
2	B	414	THR
2	B	416	ILE
2	B	417	LEU
2	B	419	VAL
2	B	422	GLU
2	B	426	LYS
2	B	430	PHE
2	B	439	LEU
2	B	445	GLN
2	B	446	LYS
2	B	447	THR
2	B	450	ARG
3	L	4	MET
3	L	6	GLN
3	L	7	SER
3	L	10	SER
3	L	11	LEU
3	L	12	SER
3	L	14	SER
3	L	24	ARG
3	L	26	SER
3	L	38	LEU
3	L	40	TRP
3	L	44	LYS
3	L	53	ILE
3	L	63	VAL
3	L	66	ARG
3	L	86	GLU
3	L	107	THR
3	L	110	GLU
3	L	112	LYS
3	L	113	ARG
3	L	119	SER
3	L	122	ILE
3	L	127	ASP
3	L	130	LEU
3	L	134	THR
3	L	138	VAL

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Mol	Chain	Res	Type
3	L	139	CYS
3	L	140	LEU
3	L	141	LEU
3	L	148	GLU
3	L	152	GLN
3	L	155	VAL
3	L	160	GLN
3	L	165	GLN
3	L	166	GLU
3	L	170	GLU
3	L	173	SER
3	L	174	LYS
3	L	175	ASP
3	L	176	SER
3	L	183	THR
3	L	184	LEU
3	L	185	THR
3	L	188	LYS
3	L	192	GLU
3	L	203	HIS
3	L	204	GLN
3	L	207	SER
3	L	210	VAL
3	L	212	LYS
3	L	215	ASN
3	L	216	ARG
3	L	219	CYS
4	H	4	LEU
4	H	7	SER
4	H	19	LYS
4	H	25	SER
4	H	37	VAL
4	H	43	LYS
4	H	45	LEU
4	H	46	GLU
4	H	48	VAL
4	H	51	ILE
4	H	75	ASP
4	H	83	LEU
4	H	88	LEU
4	H	92	ASP
4	H	93	THR

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Mol	Chain	Res	Type
4	H	96	TYR
4	H	113	THR
4	H	114	LEU
4	H	115	VAL
4	H	118	SER
4	H	127	VAL
4	H	128	PHE
4	H	130	LEU
4	H	132	LEU
4	H	134	SER
4	H	136	GLN
4	H	143	ILE
4	H	146	LEU
4	H	147	VAL
4	H	153	GLN
4	H	154	GLU
4	H	161	SER
4	H	162	GLU
4	H	165	GLN
4	H	170	ARG
4	H	175	SER
4	H	179	SER
4	H	182	LEU
4	H	185	THR
4	H	186	SER
4	H	187	SER
4	H	188	GLN
4	H	189	LEU
4	H	191	LEU
4	H	194	THR
4	H	195	GLN
4	H	196	CYS
4	H	197	LEU
4	H	200	LYS
4	H	202	VAL
4	H	205	HIS
4	H	206	VAL
4	H	207	LYS
4	H	208	HIS
4	H	213	SER
4	H	216	VAL
4	H	218	VAL

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Mol	Chain	Res	Type
4	H	220	CYS
4	H	224	PRO
4	H	228	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	666	ASN
1	P	684	ASN
1	P	785	ASN
1	P	835	ASN
1	P	840	ASN
1	P	848	ASN
1	P	879	ASN
1	P	989	ASN
1	P	1089	ASN
1	P	1203	ASN
1	P	1220	GLN
1	P	1237	GLN
1	P	1361	ASN
1	P	1362	ASN
1	P	1403	ASN
1	P	1428	GLN
1	P	1452	ASN
1	P	1487	HIS
1	P	1640	GLN
1	P	1666	GLN
1	P	1759	ASN
1	P	1825	GLN
1	P	1832	GLN
1	P	1937	HIS
1	P	1961	ASN
2	A	243	HIS
2	A	249	HIS
2	A	263	ASN
2	A	402	GLN
2	A	436	HIS
2	B	350	HIS
3	L	27	GLN
3	L	129	GLN
3	L	152	GLN
3	L	203	HIS

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Mol	Chain	Res	Type
4	H	140	ASN
4	H	176	GLN
4	H	188	GLN
4	H	205	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	P	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	1106:ASP	C	1107:SER	N	3.16
1	P	673:GLN	C	674:THR	N	2.88
1	P	1091:LEU	C	1092:THR	N	2.39

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	1958:ILE	C	1959:PHE	N	2.01

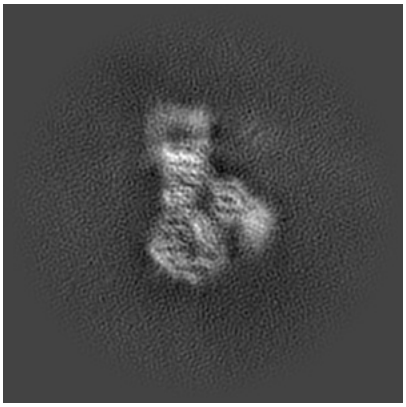
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22204. These allow visual inspection of the internal detail of the map and identification of artifacts.

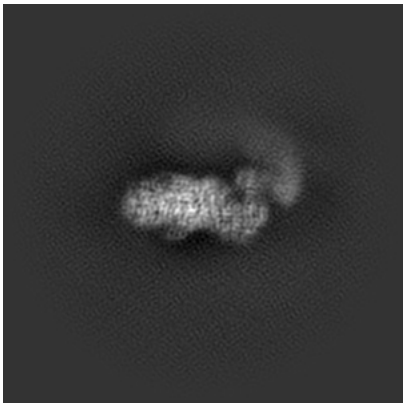
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

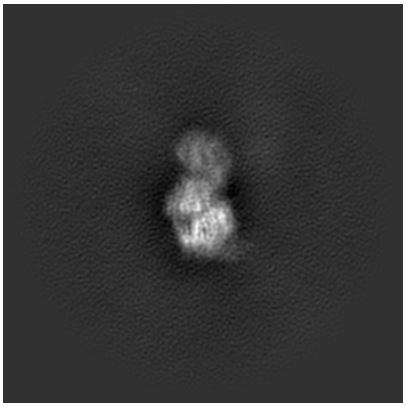
6.1.1 Primary map



X



Y

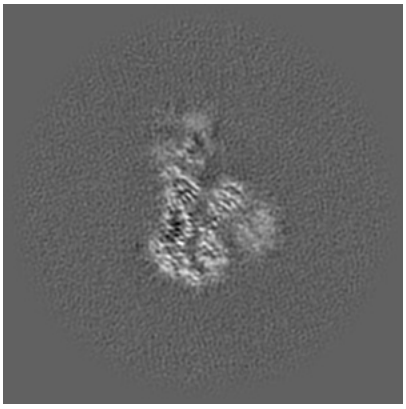


Z

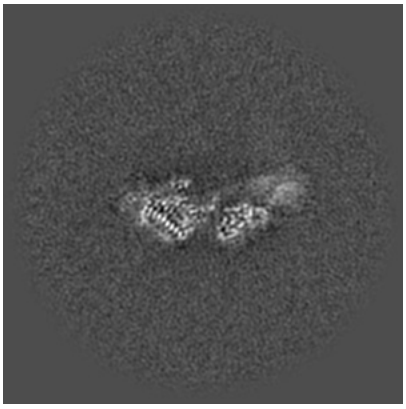
The images above show the map projected in three orthogonal directions.

6.2 Central slices

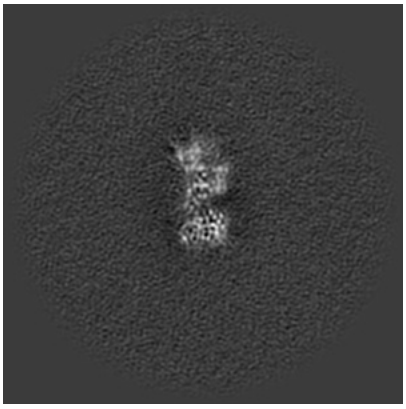
6.2.1 Primary map



X Index: 112



Y Index: 112

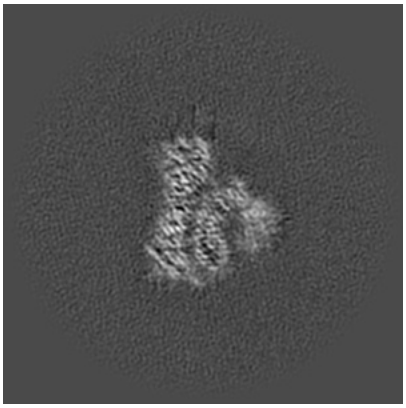


Z Index: 112

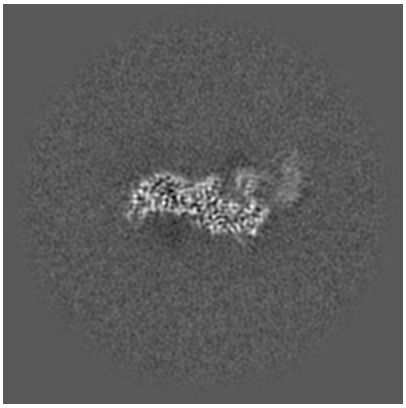
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

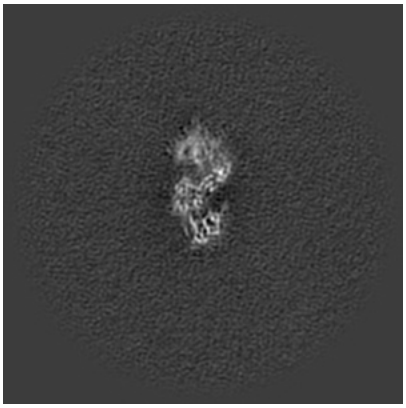
6.3.1 Primary map



X Index: 108



Y Index: 99

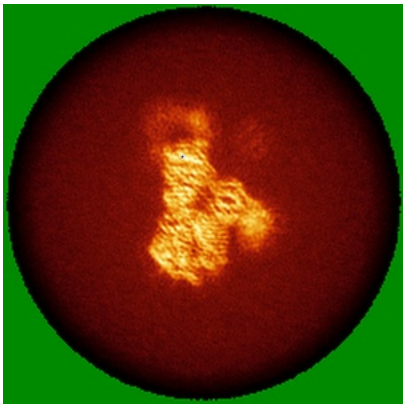


Z Index: 105

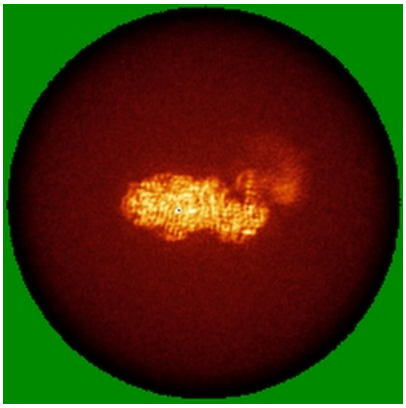
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

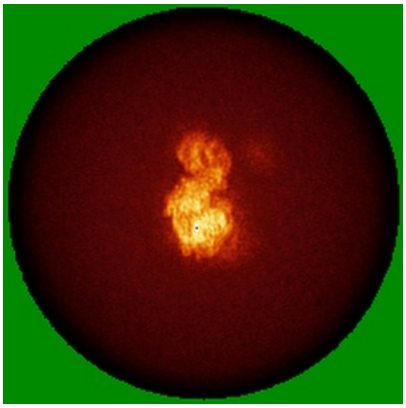
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

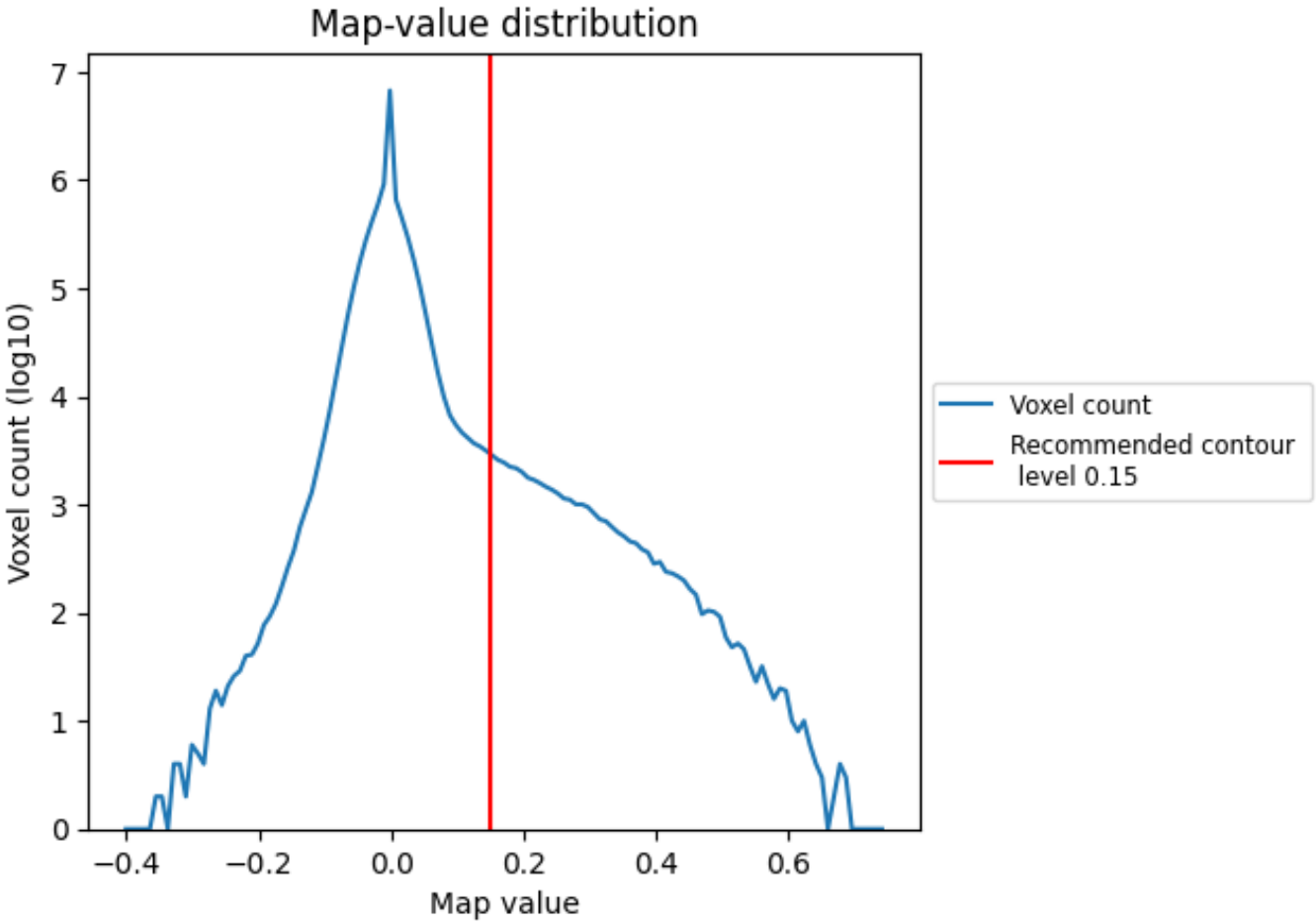
6.6 Mask visualisation (i)

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

7 Map analysis

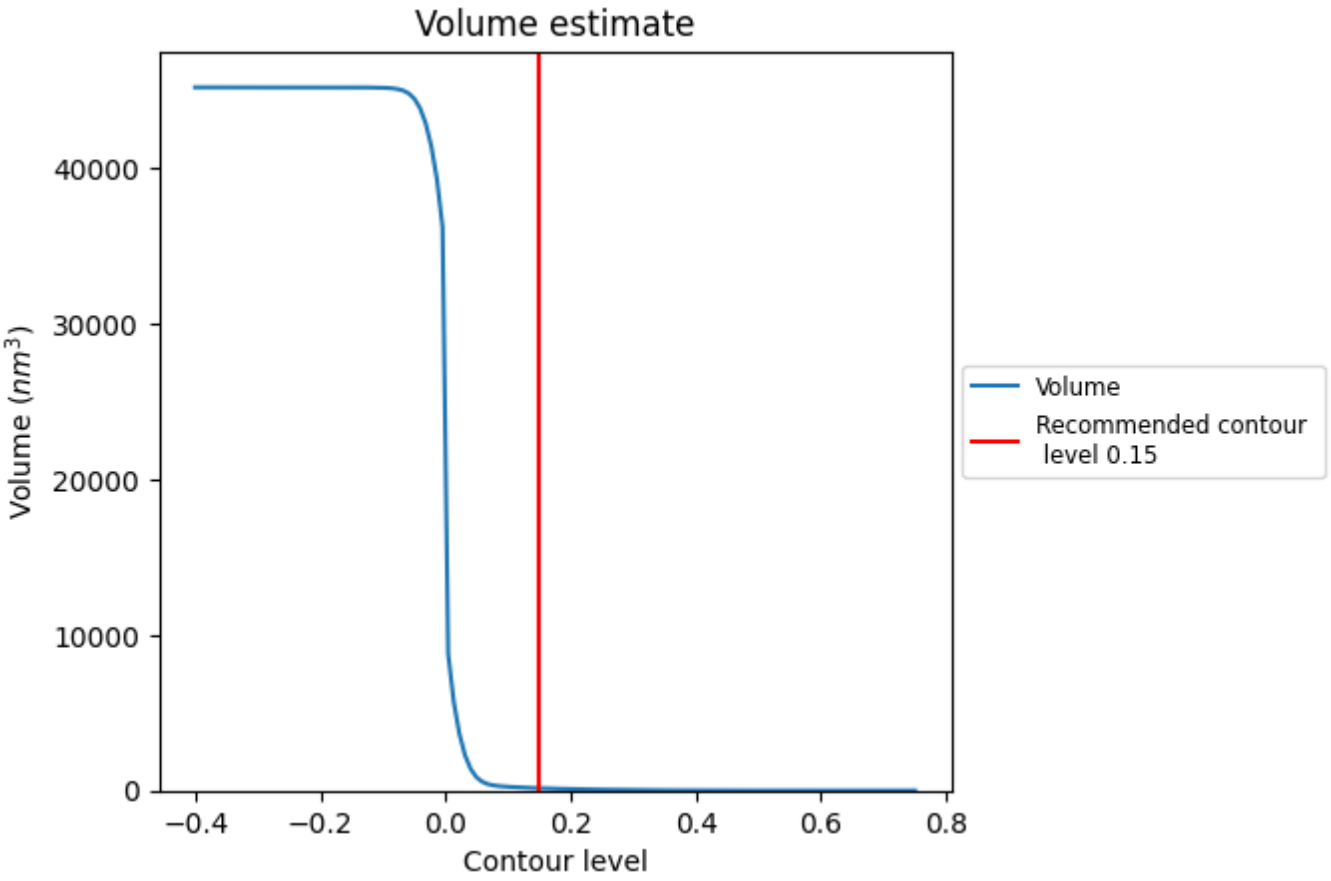
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

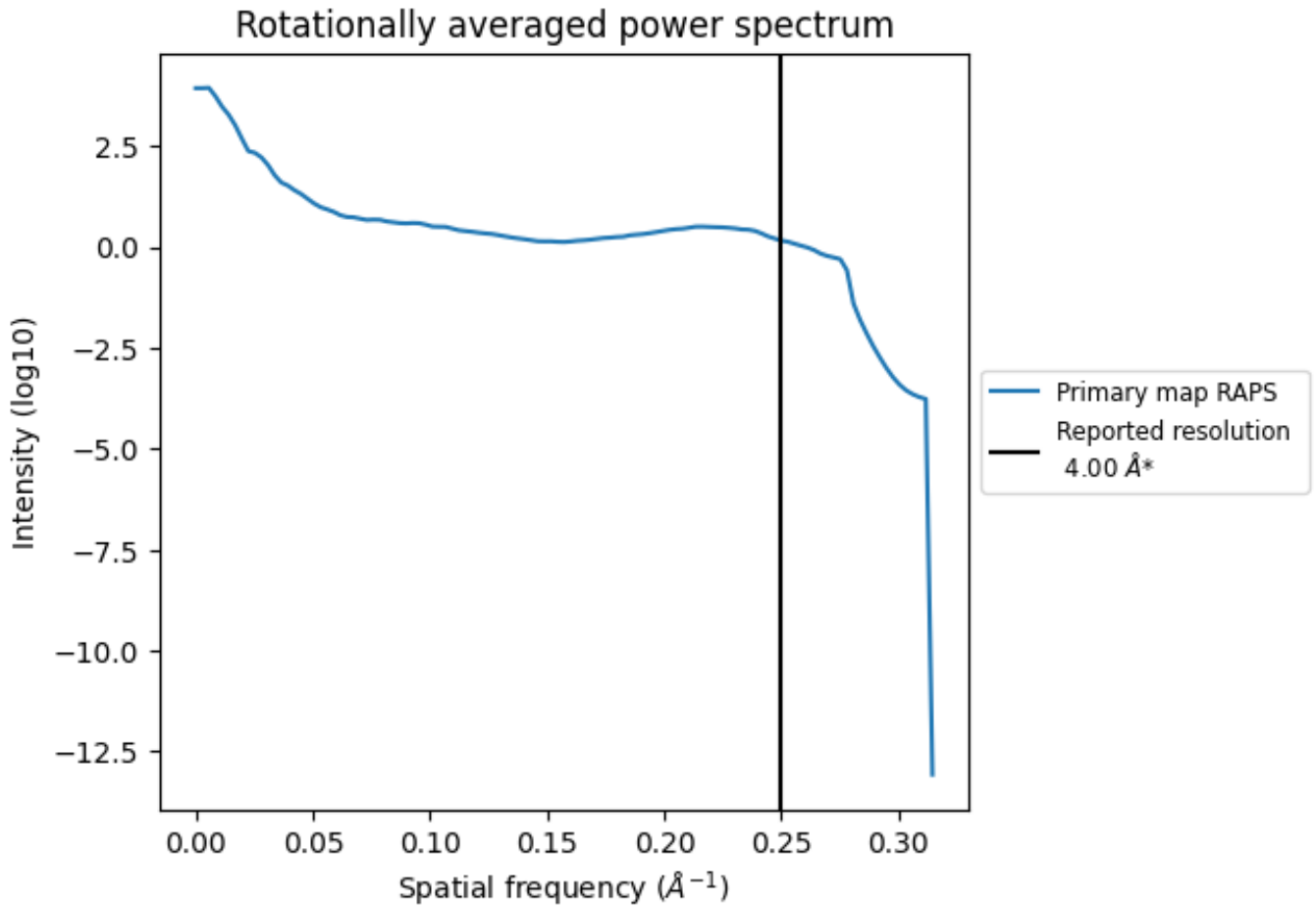
7.2 Volume estimate



The volume at the recommended contour level is 152 nm^3; this corresponds to an approximate mass of 137 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.250 $Å^{-1}$

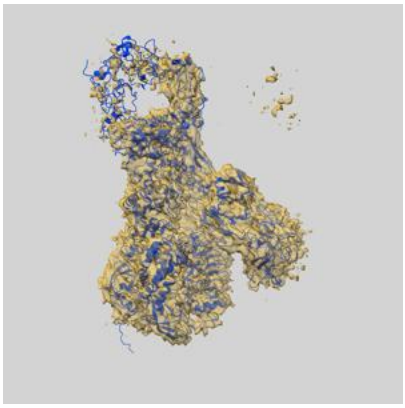
8 Fourier-Shell correlation

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

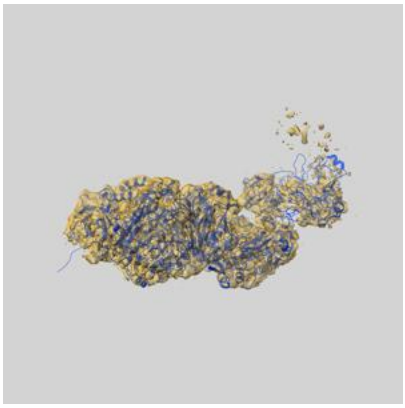
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22204 and PDB model 6XJA. Per-residue inclusion information can be found in section 3 on page 4.

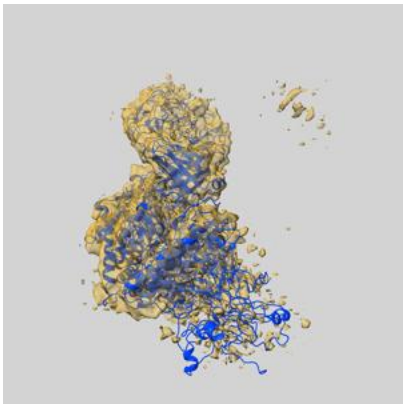
9.1 Map-model overlay



X



Y



Z

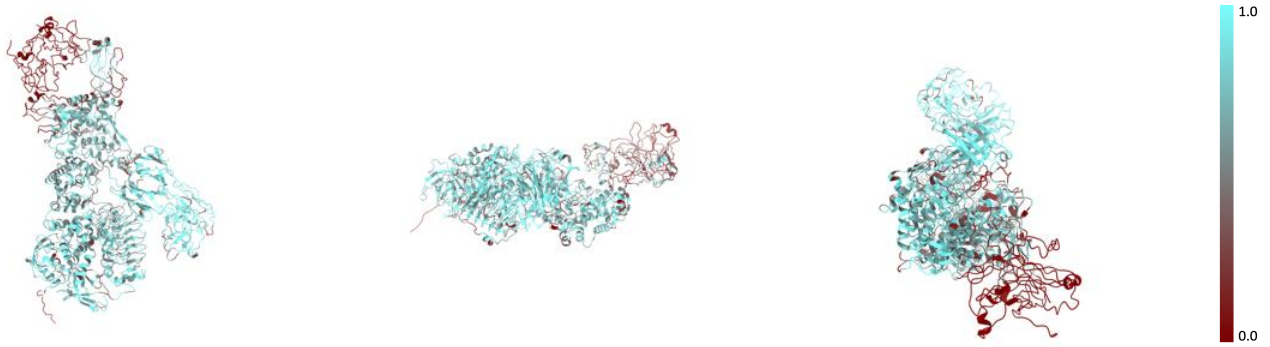
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

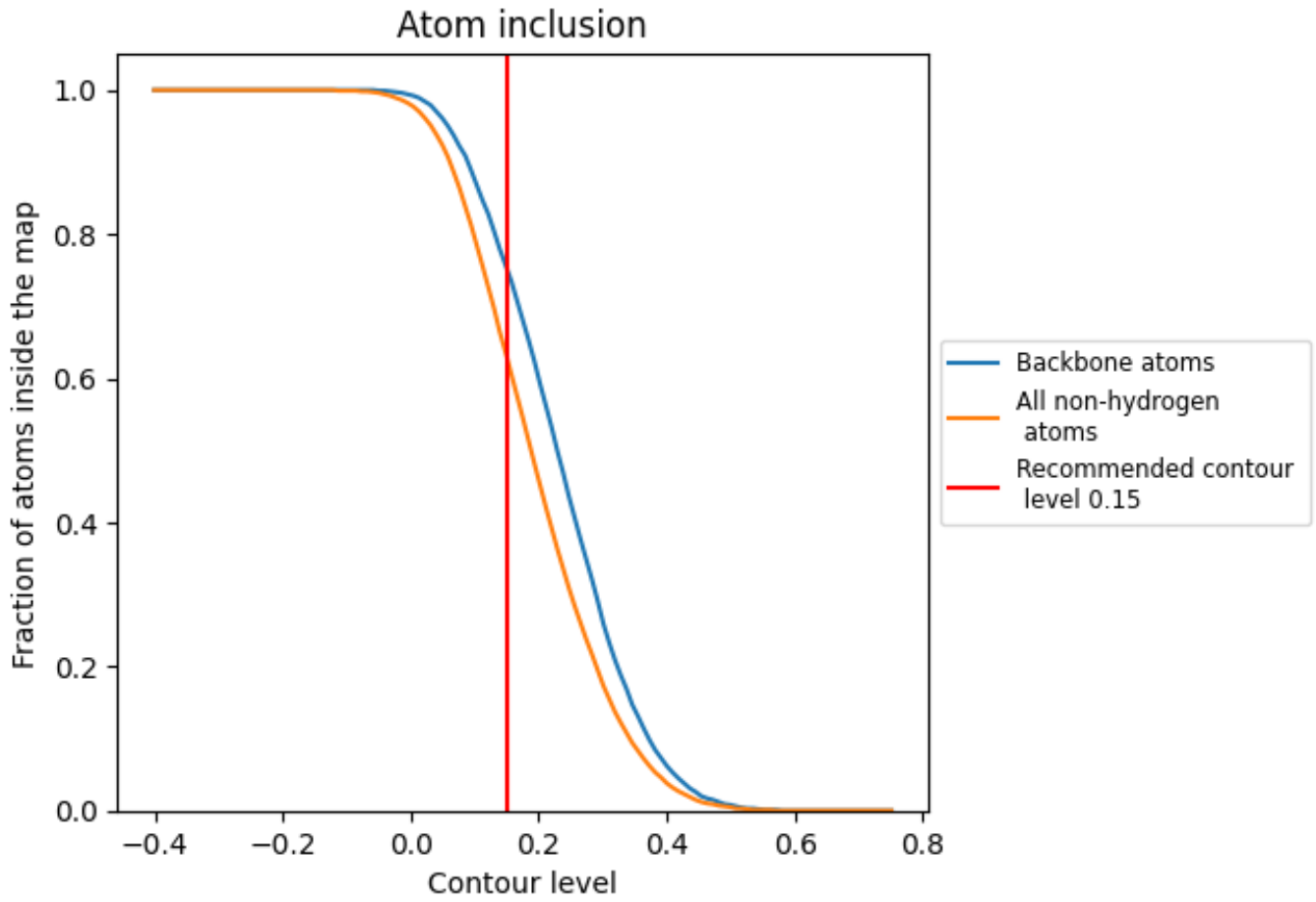
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 63% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6300	0.2430
A	0.2020	0.2520
B	0.2880	0.1810
H	0.8040	0.2800
L	0.8040	0.2640
P	0.6980	0.2430