Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 12:18 PM JST

PDB ID	:	5H53
EMDB ID	:	EMD-6664
Title	:	The structure of rabbit skeletal muscle actomyosin rigor complex at 5.2 angstrom.
Authors	:	Fujii, T.; Namba, K.
Deposited on	:	2016-11-04
Resolution	:	5.20 Å(reported)

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

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

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

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

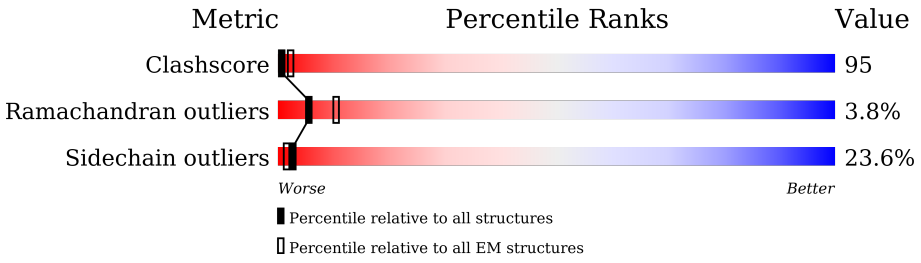
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 5.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	845	41% 19% 58% 20% ·
2	B	146	100% 18% 49% 25% 8%
3	C	153	90% 7% 49% 32% 12%
4	D	375	16% 29% 55% 15% ·
4	E	375	14% 35% 51% 13% ·

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15077 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 Skeletal muscle myosin heavy chain MyHC-EO/IIL.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	845	Total	C	N	O	S	0	0
			6795	4340	1155	1256	44		

- Molecule 2 is a protein called Myosin regulatory light chain 2, skeletal muscle isoform type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	146	Total	C	N	O	S	0	0
			1157	729	189	232	7		

- Molecule 3 is a protein called Myosin light chain 1/3, skeletal muscle isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	153	Total	C	N	O	S	0	0
			1203	751	199	246	7		

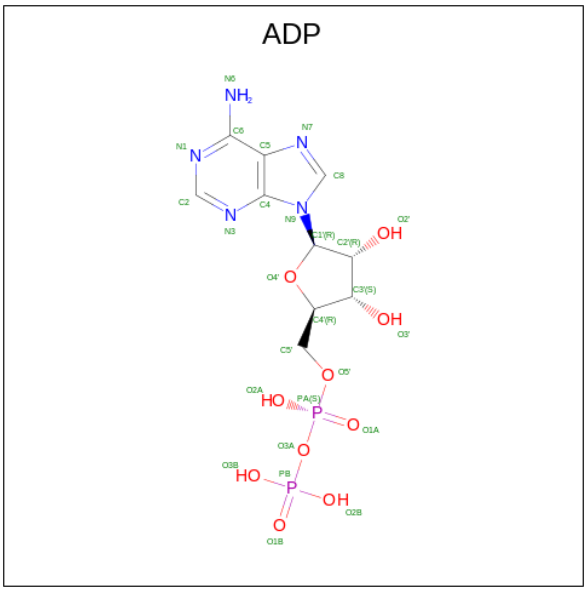
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	193	ASP	-	expression tag	UNP P02602

- Molecule 4 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
4	E	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



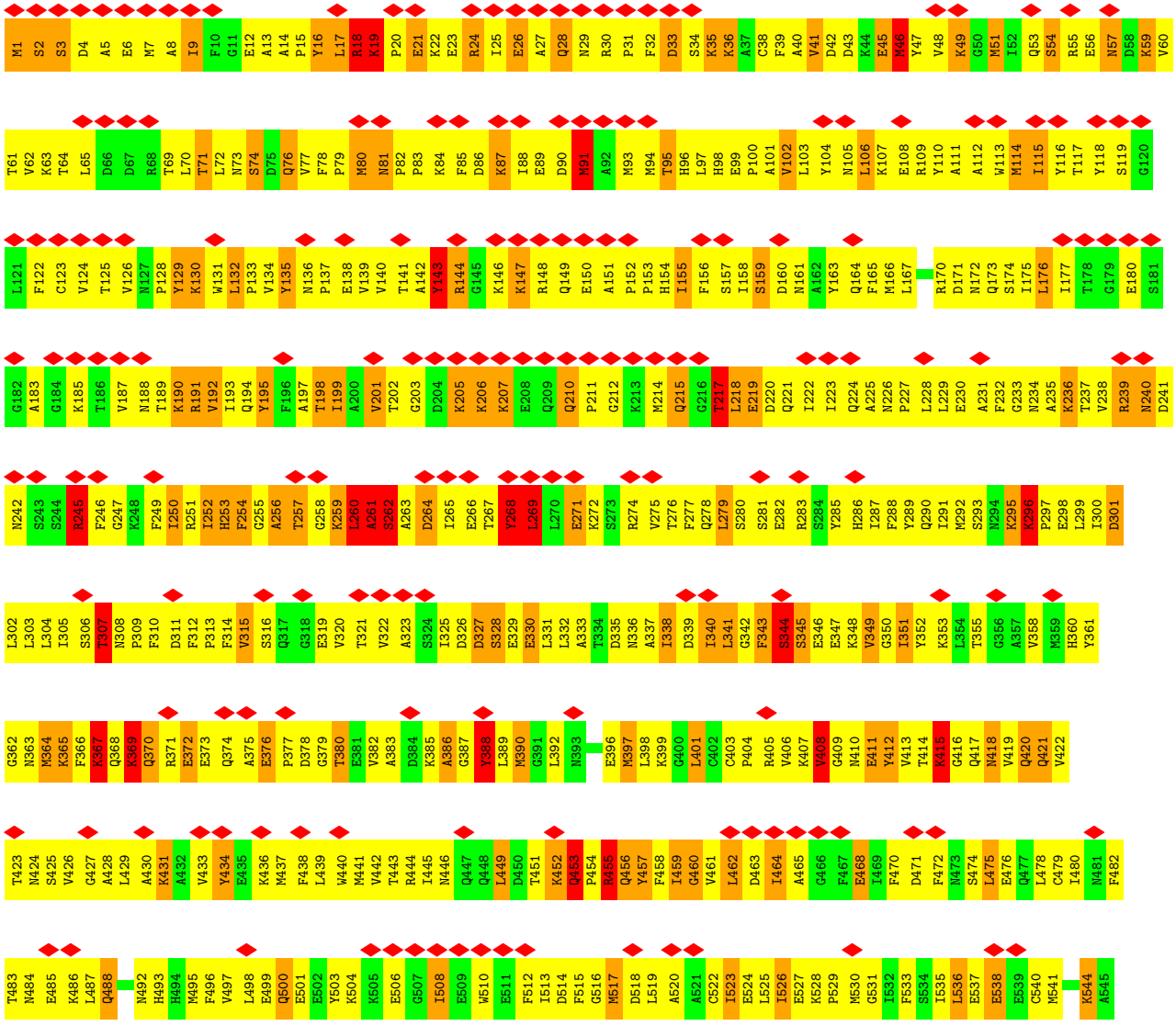
Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

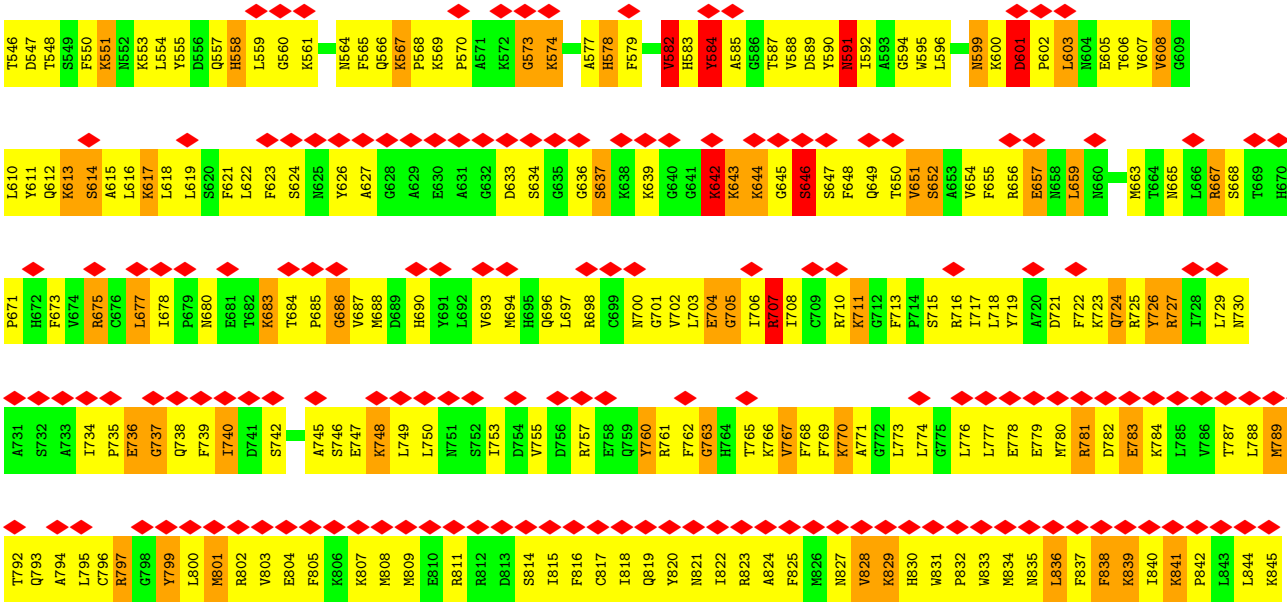
3 Residue-property plots (i)

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: Skeletal muscle myosin heavy chain MyHC-EO/IIL

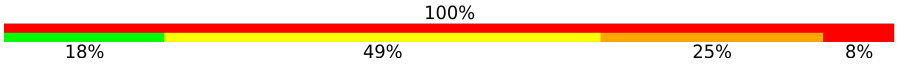
Chain A:

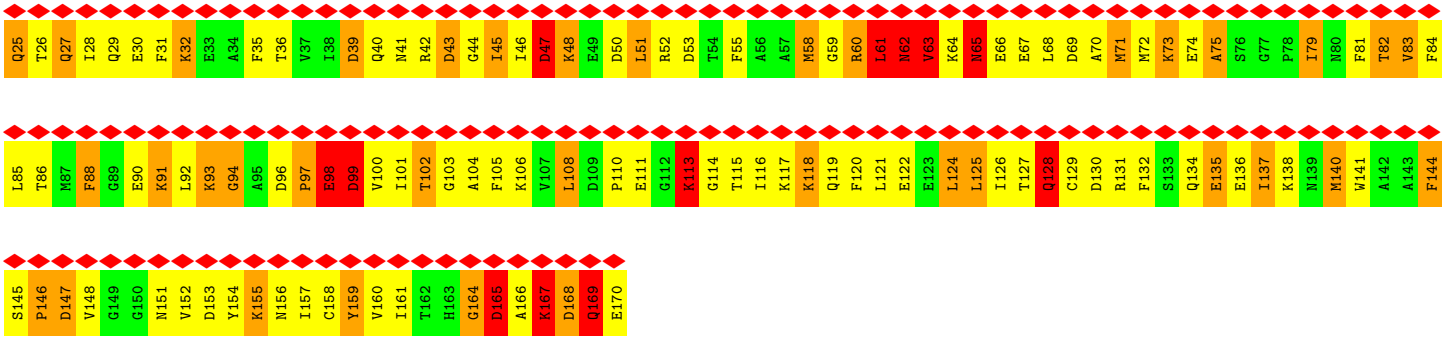




• Molecule 2: Myosin regulatory light chain 2, skeletal muscle isoform type 1

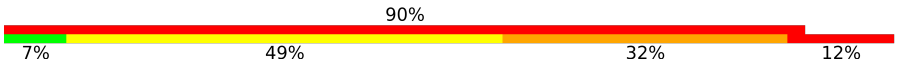
Chain B:

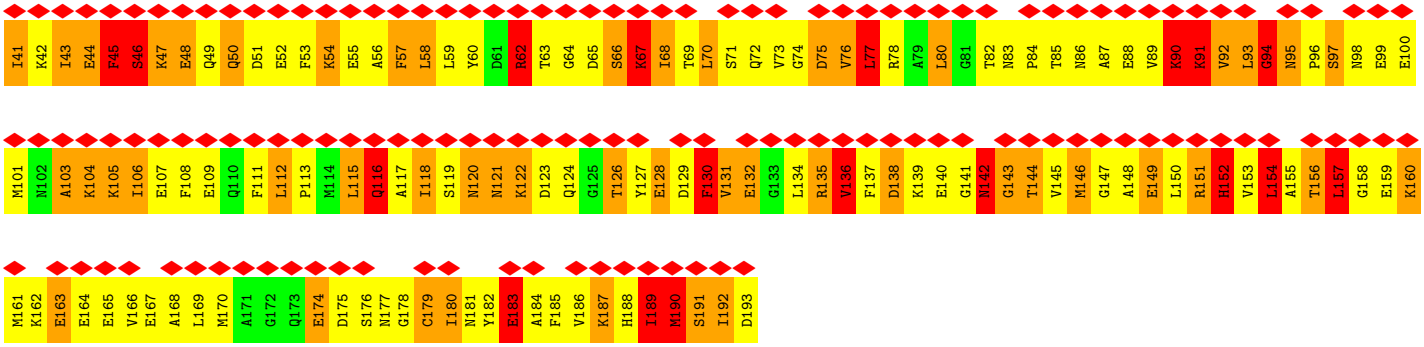




• Molecule 3: Myosin light chain 1/3, skeletal muscle isoform

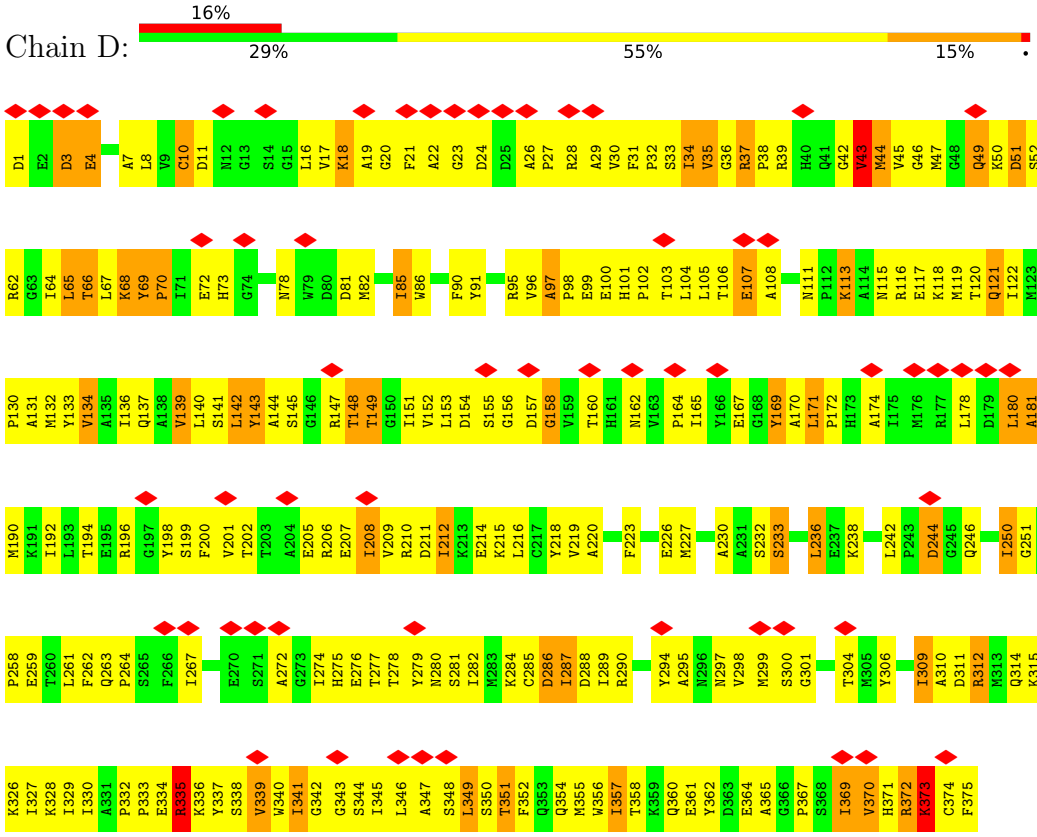
Chain C:





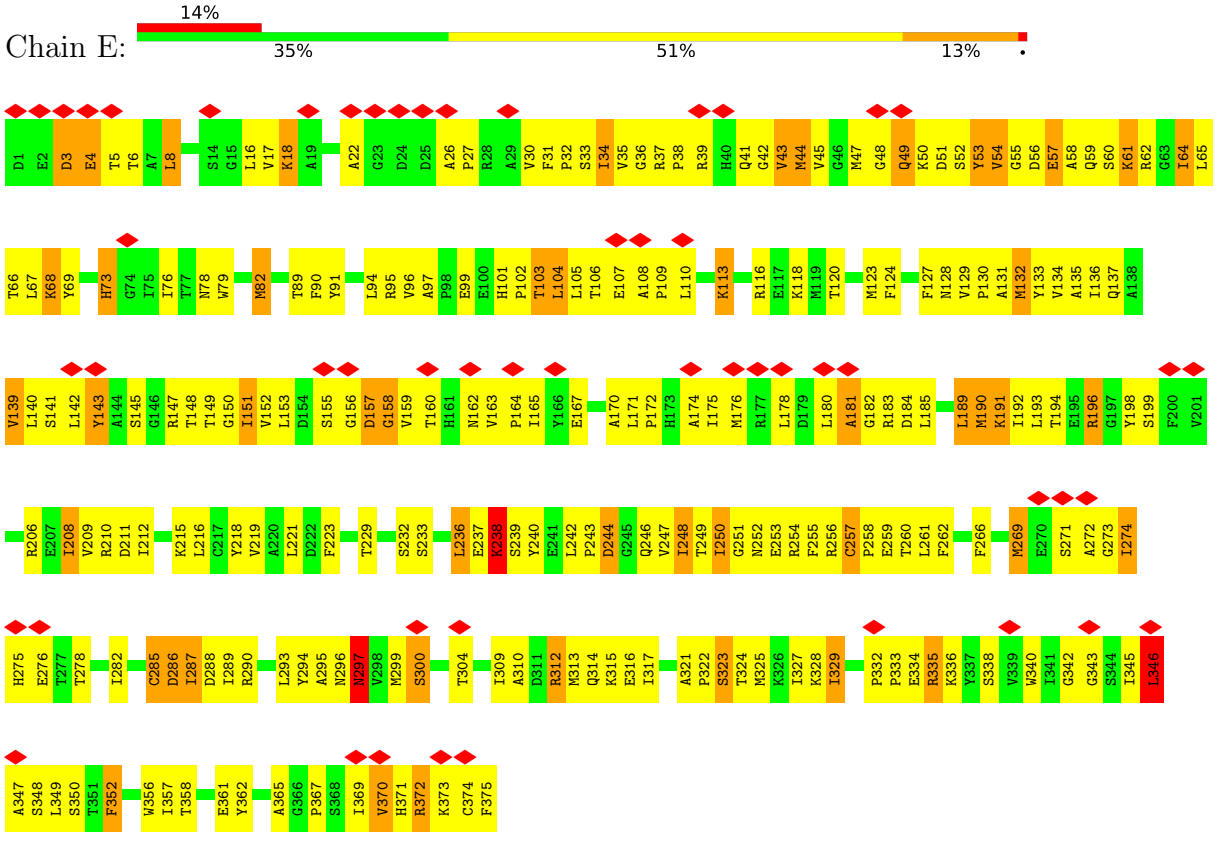
• Molecule 4: Actin, alpha skeletal muscle

Chain D:



• Molecule 4: Actin, alpha skeletal muscle

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=166.7°, rise=27.6 Å, axial sym=C1	Depositor
Number of segments used	31535	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	9.438	Depositor
Minimum map value	-6.853	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.746	Depositor
Recommended contour level	1.52	Depositor
Map size (Å)	337.5, 337.5, 337.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.03	3/6941 (0.0%)	1.45	52/9343 (0.6%)
2	B	0.96	1/1175 (0.1%)	1.78	8/1578 (0.5%)
3	C	1.02	1/1218 (0.1%)	1.33	4/1632 (0.2%)
4	D	1.02	5/2984 (0.2%)	1.15	4/4040 (0.1%)
4	E	0.97	0/2984	1.14	6/4040 (0.1%)
All	All	1.01	10/15302 (0.1%)	1.36	74/20633 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	31
2	B	0	18
3	C	0	22
4	D	0	2
4	E	0	2
All	All	0	75

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	538	GLU	CD-OE2	11.79	1.38	1.25
1	A	538	GLU	CG-CD	-10.73	1.35	1.51
4	D	212	ILE	C-N	8.81	1.54	1.34
1	A	538	GLU	CB-CG	7.55	1.66	1.52
3	C	183	GLU	CB-CG	6.51	1.64	1.52
4	D	351	THR	CB-CG2	6.17	1.72	1.52
4	D	70	PRO	C-N	-5.80	1.20	1.34
4	D	339	VAL	C-N	5.72	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	214	GLU	C-N	5.70	1.47	1.34
2	B	99	ASP	CB-CG	5.07	1.62	1.51

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	99	ASP	CB-CG-OD1	-40.40	81.94	118.30
2	B	99	ASP	CB-CG-OD2	-25.09	95.72	118.30
1	A	180	GLU	CG-CD-OE1	-23.88	70.54	118.30
1	A	747	GLU	CG-CD-OE1	-23.65	71.00	118.30
1	A	747	GLU	CG-CD-OE2	-23.28	71.74	118.30
1	A	180	GLU	CG-CD-OE2	-23.07	72.15	118.30
1	A	538	GLU	CG-CD-OE1	-16.37	85.56	118.30
1	A	747	GLU	OE1-CD-OE2	16.18	142.72	123.30
1	A	180	GLU	OE1-CD-OE2	16.14	142.67	123.30
1	A	538	GLU	OE1-CD-OE2	15.52	141.93	123.30
1	A	261	ALA	CB-CA-C	-14.74	87.98	110.10
1	A	261	ALA	N-CA-CB	13.44	128.92	110.10
1	A	388	TYR	CB-CG-CD2	11.45	127.87	121.00
1	A	582	VAL	CA-CB-CG1	-11.23	94.05	110.90
1	A	129	TYR	CA-CB-CG	-8.35	97.53	113.40
1	A	16	TYR	CA-CB-CG	-8.22	97.78	113.40
1	A	260	LEU	C-N-CA	-8.12	101.40	121.70
1	A	218	LEU	C-N-CA	8.08	141.90	121.70
1	A	81	ASN	CA-CB-CG	-7.86	96.11	113.40
1	A	143	TYR	CA-CB-CG	-7.85	98.48	113.40
1	A	726	TYR	CA-CB-CG	-7.62	98.93	113.40
4	E	190	MET	CG-SD-CE	-7.56	88.10	100.20
4	D	351	THR	OG1-CB-CG2	7.55	127.37	110.00
1	A	195	TYR	CA-CB-CG	-7.49	99.16	113.40
1	A	434	TYR	CA-CB-CG	-7.43	99.27	113.40
1	A	135	TYR	CA-CB-CG	-7.41	99.33	113.40
1	A	455	ARG	CA-CB-CG	7.30	129.47	113.40
3	C	183	GLU	OE1-CD-OE2	7.27	132.03	123.30
1	A	114	MET	CG-SD-CE	-7.03	88.95	100.20
1	A	388	TYR	CB-CG-CD1	-6.96	116.82	121.00
1	A	254	PHE	CB-CA-C	-6.94	96.52	110.40
2	B	79	ILE	C-N-CA	6.86	138.86	121.70
2	B	167	LYS	C-N-CA	6.48	137.89	121.70
1	A	386	ALA	CB-CA-C	-6.43	100.45	110.10
1	A	268	TYR	CB-CG-CD1	6.42	124.86	121.00
1	A	16	TYR	CB-CG-CD2	6.19	124.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	838	PHE	CA-CB-CG	-6.16	99.11	113.90
2	B	98	GLU	C-N-CA	6.09	136.94	121.70
1	A	578	HIS	CA-CB-CG	-6.05	103.32	113.60
1	A	262	SER	N-CA-CB	6.04	119.57	110.50
1	A	155	ILE	CB-CA-C	-6.01	99.57	111.60
1	A	455	ARG	CD-NE-CZ	-5.99	115.21	123.60
4	D	351	THR	N-CA-CB	5.94	121.58	110.30
4	E	352	PHE	CA-CB-CG	-5.93	99.66	113.90
1	A	91	MET	CG-SD-CE	-5.93	90.71	100.20
2	B	146	PRO	C-N-CA	-5.90	106.94	121.70
1	A	591	ASN	C-N-CA	5.88	136.40	121.70
1	A	558	HIS	CA-CB-CG	-5.74	103.84	113.60
2	B	114	GLY	C-N-CA	5.69	135.92	121.70
4	D	335	ARG	O-C-N	-5.67	113.62	122.70
1	A	538	GLU	CB-CG-CD	-5.67	98.89	114.20
1	A	16	TYR	CB-CG-CD1	-5.64	117.62	121.00
3	C	130	PHE	CB-CG-CD1	5.63	124.74	120.80
1	A	218	LEU	CB-CA-C	-5.58	99.60	110.20
1	A	218	LEU	N-CA-C	-5.49	96.17	111.00
1	A	388	TYR	CA-CB-CG	5.47	123.79	113.40
4	E	346	LEU	CB-CA-C	5.42	120.50	110.20
4	E	91	TYR	CA-CB-CG	-5.34	103.26	113.40
4	D	169	TYR	CB-CG-CD2	-5.29	117.82	121.00
2	B	61	LEU	CA-CB-CG	5.29	127.46	115.30
3	C	183	GLU	CB-CG-CD	-5.29	99.92	114.20
1	A	268	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	A	18	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	252	ILE	C-N-CA	-5.17	108.78	121.70
1	A	799	TYR	CA-CB-CG	-5.14	103.64	113.40
1	A	268	TYR	O-C-N	5.13	130.91	122.70
3	C	152	HIS	CB-CA-C	-5.13	100.14	110.40
1	A	657	GLU	CB-CG-CD	-5.12	100.38	114.20
1	A	633	ASP	CA-CB-CG	-5.08	102.23	113.40
4	E	127	PHE	CA-CB-CG	-5.05	101.79	113.90
1	A	80	MET	CG-SD-CE	-5.03	92.15	100.20
1	A	760	TYR	CA-CB-CG	-5.02	103.86	113.40
1	A	245	ARG	C-N-CA	-5.00	109.19	121.70
4	E	53	TYR	CA-CB-CG	-5.00	103.89	113.40

There are no chirality outliers.

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	TYR	Peptide
1	A	18	ARG	Peptide
1	A	203	GLY	Peptide
1	A	217	THR	Peptide
1	A	239	ARG	Peptide
1	A	256	ALA	Peptide
1	A	261	ALA	Mainchain
1	A	268	TYR	Peptide
1	A	296	LYS	Peptide
1	A	343	PHE	Peptide
1	A	349	VAL	Peptide
1	A	367	LYS	Peptide
1	A	371	ARG	Peptide
1	A	379	GLY	Peptide
1	A	415	LYS	Peptide
1	A	421	GLN	Peptide
1	A	455	ARG	Sidechain
1	A	460	GLY	Peptide
1	A	538	GLU	Sidechain
1	A	573	GLY	Peptide
1	A	584	TYR	Peptide
1	A	594	GLY	Peptide
1	A	599	ASN	Peptide
1	A	667	ARG	Sidechain
1	A	686	GLY	Peptide
1	A	704	GLU	Peptide
1	A	707	ARG	Sidechain
1	A	736	GLU	Peptide
1	A	737	GLY	Peptide
1	A	763	GLY	Peptide
1	A	771	ALA	Peptide
2	B	102	THR	Peptide
2	B	113	LYS	Peptide
2	B	125	LEU	Peptide
2	B	128	GLN	Peptide
2	B	144	PHE	Peptide
2	B	147	ASP	Peptide
2	B	164	GLY	Peptide
2	B	169	GLN	Peptide
2	B	43	ASP	Peptide
2	B	47	ASP	Peptide
2	B	61	LEU	Peptide
2	B	63	VAL	Peptide

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Mol	Chain	Res	Type	Group
2	B	65	ASN	Peptide
2	B	88	PHE	Peptide
2	B	94	GLY	Peptide
2	B	97	PRO	Peptide
2	B	99	ASP	Peptide,Sidechain
3	C	103	ALA	Peptide
3	C	116	GLN	Peptide
3	C	118	ILE	Peptide
3	C	121	ASN	Peptide
3	C	142	ASN	Peptide
3	C	143	GLY	Peptide
3	C	146	MET	Peptide
3	C	154	LEU	Peptide
3	C	168	ALA	Peptide
3	C	175	ASP	Peptide
3	C	189	ILE	Peptide
3	C	190	MET	Peptide
3	C	191	SER	Peptide
3	C	44	GLU	Peptide
3	C	45	PHE	Peptide
3	C	62	ARG	Peptide,Sidechain
3	C	66	SER	Peptide
3	C	77	LEU	Peptide
3	C	91	LYS	Peptide
3	C	93	LEU	Peptide
3	C	94	GLY	Peptide
4	D	201	VAL	Peptide
4	D	341	ILE	Peptide
4	E	297	ASN	Peptide
4	E	64	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6795	0	6785	1589	0
2	B	1157	0	1127	222	0
3	C	1203	0	1176	410	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2934	0	2894	381	0
4	E	2934	0	2895	382	0
5	D	27	0	12	7	0
5	E	27	0	12	4	0
All	All	15077	0	14901	2860	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 95.

All (2860) 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:79:ILE:HG13	2:B:83:VAL:HG13	1.20	1.19
4:E:361:GLU:HB3	4:E:369:ILE:HD13	1.25	1.19
1:A:390:MET:HB3	1:A:392:LEU:HD23	1.19	1.18
1:A:800:LEU:HG	3:C:162:LYS:HE2	1.19	1.17
4:D:142:LEU:HD21	4:D:165:ILE:HD13	1.17	1.17
1:A:833:TRP:HA	1:A:836:LEU:HD12	1.20	1.16
1:A:17:LEU:HB3	1:A:152:PRO:HG2	1.17	1.15
1:A:193:ILE:HG21	1:A:219:GLU:HB3	1.15	1.15
2:B:116:ILE:HG21	2:B:121:LEU:HD12	1.31	1.13
3:C:191:SER:HA	3:C:192:ILE:HG22	1.17	1.12
1:A:729:LEU:HD21	1:A:781:ARG:HB3	1.30	1.12
2:B:108:LEU:HD22	2:B:116:ILE:HD13	1.20	1.12
1:A:390:MET:HG2	1:A:618:LEU:HD22	1.12	1.12
1:A:115:ILE:HG22	1:A:126:VAL:HG23	1.13	1.11
4:D:154:ASP:HA	4:D:300:SER:HB3	1.30	1.11
1:A:207:LYS:HD2	1:A:454:PRO:HD2	1.13	1.10
1:A:32:PHE:HB3	1:A:83:PRO:HG3	1.34	1.10
1:A:360:HIS:HB3	1:A:382:VAL:HG13	1.29	1.09
3:C:68:ILE:HD12	3:C:95:ASN:HB2	1.32	1.09
4:D:212:ILE:HG23	4:D:216:LEU:HD12	1.35	1.09
4:E:76:ILE:HG21	4:E:82:MET:HG2	1.21	1.09
4:D:185:LEU:HD11	4:D:261:LEU:HD21	1.18	1.08
4:D:251:GLY:HA2	4:D:254:ARG:HG3	1.32	1.08
1:A:611:TYR:HB3	1:A:622:LEU:HD13	1.09	1.08
3:C:42:LYS:HA	3:C:43:ILE:HB	1.30	1.08
1:A:530:MET:HE1	4:D:351:THR:HA	1.30	1.08
1:A:173:GLN:HB2	1:A:459:ILE:HG23	1.23	1.07
1:A:295:LYS:HZ2	1:A:332:LEU:HA	1.18	1.07
1:A:296:LYS:HE2	1:A:299:LEU:HB2	1.33	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ALA:HA	1:A:523:ILE:HD11	1.31	1.07
2:B:79:ILE:HD11	2:B:84:PHE:HA	1.30	1.07
4:E:37:ARG:HG2	4:E:38:PRO:HD2	1.30	1.06
1:A:255:GLY:HA2	1:A:456:GLN:H	1.18	1.06
4:E:102:PRO:HB3	4:E:131:ALA:HB3	1.34	1.05
1:A:524:GLU:HG3	1:A:528:LYS:HD3	1.37	1.05
1:A:644:LYS:HD3	1:A:649:GLN:HG3	1.37	1.05
4:E:135:ALA:HB1	4:E:140:LEU:HD21	1.38	1.05
1:A:175:ILE:HD11	1:A:461:VAL:HG22	1.37	1.05
2:B:58:MET:HG3	2:B:60:ARG:H	1.15	1.04
3:C:92:VAL:HG11	3:C:100:GLU:HB2	1.06	1.04
1:A:338:ILE:HG21	1:A:348:LYS:HD2	1.36	1.04
1:A:564:ASN:HA	1:A:582:VAL:HG11	1.35	1.04
1:A:1:MET:O	1:A:2:SER:O	1.76	1.03
4:E:300:SER:HA	4:E:335:ARG:HG3	1.37	1.03
1:A:569:LYS:HG2	1:A:570:PRO:HD2	1.33	1.02
1:A:46:MET:HB2	1:A:690:HIS:HB2	1.38	1.02
1:A:207:LYS:HE2	1:A:453:GLN:HB3	1.41	1.02
4:D:142:LEU:HD11	4:D:165:ILE:HD11	1.41	1.02
1:A:708:ILE:HA	1:A:711:LYS:HE2	1.40	1.01
1:A:97:LEU:HD13	1:A:706:ILE:HG23	1.41	1.01
1:A:736:GLU:HA	1:A:740:ILE:HD11	1.41	1.01
4:E:61:LYS:HB3	4:E:65:LEU:HD23	1.41	1.01
4:E:120:THR:HB	4:E:367:PRO:HB3	1.40	1.00
4:D:34:ILE:HG22	4:D:68:LYS:H	1.23	1.00
4:E:151:ILE:HG23	4:E:297:ASN:HB3	1.40	1.00
3:C:54:LYS:HA	3:C:54:LYS:HE3	1.43	1.00
3:C:92:VAL:HG21	3:C:100:GLU:HG3	1.42	0.99
3:C:150:LEU:HD22	3:C:154:LEU:HD23	1.44	0.99
4:E:116:ARG:HH11	4:E:371:HIS:HA	1.25	0.99
3:C:86:ASN:HB3	3:C:91:LYS:HD3	1.43	0.98
1:A:130:LYS:HD3	1:A:132:LEU:HD11	1.45	0.98
4:D:357:ILE:HG12	4:D:370:VAL:HG23	1.45	0.97
1:A:9:ILE:HG22	1:A:20:PRO:HA	1.43	0.97
2:B:65:ASN:HB2	2:B:66:GLU:HG2	1.45	0.97
2:B:83:VAL:HA	2:B:86:THR:HG22	1.44	0.97
1:A:831:TRP:HE3	1:A:834:MET:HG2	1.28	0.96
1:A:103:LEU:HD22	1:A:690:HIS:HD2	1.28	0.96
1:A:272:LYS:HD3	1:A:431:LYS:HB3	1.45	0.96
1:A:314:PHE:CZ	1:A:362:GLY:HA2	2.01	0.96
1:A:292:MET:HE3	1:A:309:PRO:HB3	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:104:LEU:HB2	4:D:356:TRP:CH2	2.01	0.96
4:D:120:THR:HB	4:D:367:PRO:HB3	1.46	0.96
4:E:34:ILE:HB	4:E:54:VAL:HG11	1.44	0.96
1:A:94:MET:HE1	1:A:101:ALA:HB1	1.46	0.96
1:A:390:MET:HB3	1:A:392:LEU:CD2	1.95	0.96
1:A:811:ARG:HG2	1:A:815:ILE:HD11	1.45	0.95
1:A:358:VAL:HG22	1:A:430:ALA:HA	1.48	0.95
1:A:296:LYS:HD2	1:A:331:LEU:HD11	1.46	0.95
1:A:225:ALA:HA	1:A:341:LEU:HD23	1.47	0.95
1:A:418:ASN:H	1:A:421:GLN:HG2	1.26	0.95
1:A:817:CYS:HA	1:A:820:TYR:CE2	2.02	0.95
4:D:272:ALA:HB1	4:D:276:GLU:HG3	1.49	0.95
4:D:35:VAL:HG12	4:D:68:LYS:HB2	1.48	0.95
4:E:198:TYR:CZ	4:E:248:ILE:HG22	2.01	0.94
2:B:120:PHE:HE2	2:B:124:LEU:HD23	1.31	0.94
1:A:801:MET:HE3	3:C:57:PHE:HZ	1.31	0.94
1:A:799:TYR:CD1	3:C:166:VAL:HG12	2.03	0.94
1:A:128:PRO:HB2	1:A:132:LEU:HD21	1.49	0.93
4:D:153:LEU:HD21	4:D:274:ILE:HD12	1.49	0.93
4:E:140:LEU:HD13	4:E:343:GLY:CA	1.98	0.93
2:B:52:ARG:HD2	2:B:64:LYS:HG3	1.50	0.93
3:C:70:LEU:HG	3:C:91:LYS:HD2	1.47	0.93
1:A:107:LYS:CB	1:A:688:MET:HG3	1.98	0.93
1:A:247:GLY:N	1:A:269:LEU:HD11	1.84	0.93
1:A:97:LEU:HD13	1:A:706:ILE:CG2	1.97	0.93
2:B:120:PHE:CE2	2:B:124:LEU:HD23	2.02	0.93
3:C:67:LYS:HE3	3:C:101:MET:HB3	1.51	0.92
1:A:603:LEU:HG	1:A:648:PHE:CD1	2.04	0.92
4:D:39:ARG:HE	4:D:66:THR:HA	1.31	0.92
3:C:70:LEU:CG	3:C:91:LYS:HD2	2.00	0.92
4:D:37:ARG:HG2	4:D:38:PRO:HD2	1.51	0.92
4:D:297:ASN:HB2	4:D:329:ILE:HD13	1.49	0.92
4:E:34:ILE:HD12	4:E:67:LEU:HD13	1.51	0.92
3:C:42:LYS:HD2	3:C:47:LYS:CA	2.00	0.92
2:B:108:LEU:HD11	2:B:124:LEU:HD21	1.51	0.92
4:D:299:MET:HE2	4:D:304:THR:HB	1.49	0.92
2:B:51:LEU:HB3	2:B:68:LEU:HD11	1.52	0.91
1:A:390:MET:CG	1:A:618:LEU:HD22	2.00	0.91
4:D:189:LEU:HD23	4:D:209:VAL:HG13	1.48	0.91
1:A:475:LEU:HD13	1:A:595:TRP:CZ3	2.05	0.91
1:A:102:VAL:HG21	1:A:694:MET:HE1	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:TYR:CD2	1:A:199:ILE:HG21	2.06	0.91
4:E:300:SER:HA	4:E:335:ARG:CG	2.00	0.91
2:B:35:PHE:HD1	2:B:46:ILE:HD13	1.36	0.91
1:A:115:ILE:HG21	1:A:128:PRO:HD3	1.53	0.91
4:D:133:TYR:CZ	4:D:375:PHE:HB2	2.06	0.91
1:A:272:LYS:HB3	1:A:431:LYS:CG	2.00	0.90
1:A:272:LYS:HB3	1:A:431:LYS:HD2	1.54	0.90
1:A:51:MET:SD	1:A:63:LYS:HE3	2.12	0.90
1:A:825:PHE:CZ	1:A:829:LYS:HB3	2.06	0.90
1:A:377:PRO:HG2	1:A:398:LEU:HD22	1.53	0.90
3:C:159:GLU:HG2	3:C:162:LYS:HD3	1.53	0.90
4:D:185:LEU:HD11	4:D:261:LEU:CD2	2.00	0.90
1:A:618:LEU:HG	1:A:622:LEU:HD12	1.53	0.90
1:A:740:ILE:CG2	1:A:745:ALA:HB2	2.01	0.90
1:A:524:GLU:CG	1:A:528:LYS:HD3	2.02	0.90
1:A:236:LYS:HG2	1:A:241:ASP:HA	1.54	0.90
4:D:34:ILE:HG21	4:D:67:LEU:HB3	1.52	0.90
4:E:236:LEU:HD13	4:E:251:GLY:CA	2.02	0.90
1:A:14:ALA:HB3	1:A:15:PRO:HD3	1.53	0.90
1:A:578:HIS:CD2	1:A:592:ILE:HG12	2.06	0.90
1:A:232:PHE:CD2	1:A:287:ILE:HG12	2.07	0.89
4:D:35:VAL:HA	4:D:54:VAL:HG21	1.55	0.89
1:A:719:TYR:CE1	1:A:767:VAL:HB	2.07	0.89
4:D:287:ILE:HB	4:E:244:ASP:HB3	1.51	0.89
1:A:729:LEU:HD21	1:A:781:ARG:CB	2.03	0.89
3:C:92:VAL:HG11	3:C:100:GLU:CB	2.00	0.89
3:C:45:PHE:N	3:C:46:SER:HB2	1.88	0.89
3:C:123:ASP:HB3	3:C:126:THR:CG2	2.03	0.89
3:C:180:ILE:HD12	3:C:181:ASN:H	1.38	0.89
4:E:35:VAL:HG22	4:E:52:SER:HB2	1.53	0.89
1:A:193:ILE:HG21	1:A:219:GLU:CB	2.02	0.89
1:A:205:LYS:CG	1:A:257:THR:HG21	2.03	0.89
2:B:65:ASN:CB	2:B:66:GLU:HG2	2.02	0.89
3:C:152:HIS:CE1	3:C:160:LYS:HA	2.07	0.89
1:A:557:GLN:HG3	1:A:558:HIS:CD2	2.08	0.89
3:C:62:ARG:HD2	3:C:63:THR:N	1.88	0.89
3:C:140:GLU:HB3	3:C:180:ILE:HD11	1.50	0.89
1:A:272:LYS:HB3	1:A:431:LYS:HG2	1.53	0.88
1:A:445:ILE:HG12	1:A:449:LEU:CD1	2.03	0.88
1:A:225:ALA:HA	1:A:341:LEU:CD2	2.03	0.88
1:A:296:LYS:CD	1:A:331:LEU:HD11	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:HB3	1:A:100:PRO:HG2	1.56	0.88
1:A:173:GLN:HB2	1:A:459:ILE:CG2	2.03	0.88
1:A:546:THR:HG23	1:A:548:THR:H	1.35	0.88
4:D:35:VAL:CA	4:D:54:VAL:HG21	2.03	0.88
3:C:62:ARG:HB3	3:C:62:ARG:HH11	1.38	0.88
4:E:357:ILE:CG1	4:E:370:VAL:HG23	2.03	0.88
1:A:406:VAL:HG12	1:A:605:GLU:HB2	1.56	0.88
1:A:39:PHE:HB2	1:A:78:PHE:HB2	1.56	0.88
2:B:79:ILE:CG1	2:B:83:VAL:HG13	2.02	0.88
1:A:115:ILE:HG22	1:A:126:VAL:CG2	2.00	0.88
1:A:749:LEU:HD11	1:A:753:ILE:HD11	1.56	0.88
4:E:113:LYS:HB3	4:E:371:HIS:CD2	2.08	0.88
1:A:730:ASN:HB3	1:A:749:LEU:HD13	1.54	0.88
1:A:255:GLY:HA2	1:A:456:GLN:N	1.88	0.87
1:A:415:LYS:CB	4:D:333:PRO:HG2	2.04	0.87
3:C:83:ASN:HB2	3:C:84:PRO:HD3	1.56	0.87
3:C:150:LEU:HD22	3:C:154:LEU:CD2	2.04	0.87
3:C:152:HIS:HE1	3:C:160:LYS:HA	1.37	0.87
3:C:92:VAL:HG22	3:C:95:ASN:HA	1.55	0.87
1:A:578:HIS:CD2	1:A:591:ASN:HA	2.09	0.87
1:A:800:LEU:HG	3:C:162:LYS:CE	2.03	0.87
3:C:191:SER:HA	3:C:192:ILE:CG2	2.04	0.87
1:A:256:ALA:HA	1:A:456:GLN:HB2	1.55	0.87
1:A:296:LYS:HE2	1:A:299:LEU:CB	2.04	0.87
2:B:154:TYR:O	2:B:157:ILE:HG12	1.75	0.87
2:B:160:VAL:HG23	2:B:165:ASP:HB2	1.55	0.87
1:A:94:MET:CE	1:A:101:ALA:HB1	2.05	0.86
1:A:737:GLY:HA3	1:A:739:PHE:CD2	2.09	0.86
4:E:236:LEU:HD13	4:E:251:GLY:HA2	1.58	0.86
1:A:13:ALA:HB1	1:A:139:VAL:HG13	1.56	0.86
1:A:232:PHE:CG	1:A:287:ILE:HG21	2.10	0.86
1:A:404:PRO:HB3	1:A:606:THR:HB	1.57	0.86
1:A:272:LYS:HB3	1:A:431:LYS:CD	2.06	0.86
1:A:611:TYR:CD2	1:A:618:LEU:HD21	2.11	0.86
1:A:221:GLN:HE21	1:A:449:LEU:HD23	1.39	0.86
3:C:135:ARG:NH1	3:C:139:LYS:HB3	1.90	0.86
1:A:9:ILE:HD13	1:A:18:ARG:NH2	1.91	0.85
4:E:190:MET:CE	4:E:206:ARG:HA	2.06	0.85
1:A:78:PHE:HD2	1:A:98:HIS:HD2	1.22	0.85
1:A:418:ASN:N	1:A:421:GLN:HG2	1.90	0.85
1:A:612:GLN:O	1:A:619:LEU:HG	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:GLN:HE21	1:A:422:VAL:HG12	1.39	0.85
4:D:357:ILE:CG1	4:D:370:VAL:HG23	2.06	0.85
1:A:207:LYS:HD3	1:A:259:LYS:HB2	1.57	0.85
1:A:375:ALA:HB3	1:A:417:GLN:HE22	1.42	0.85
3:C:41:ILE:O	3:C:43:ILE:HG13	1.76	0.85
4:D:34:ILE:HB	4:D:54:VAL:HG11	1.59	0.85
4:D:299:MET:CE	4:D:304:THR:HB	2.05	0.85
1:A:495:MET:CE	1:A:708:ILE:HG21	2.06	0.85
1:A:833:TRP:NE1	2:B:71:MET:HG2	1.91	0.85
1:A:611:TYR:CB	1:A:622:LEU:HD13	2.02	0.85
1:A:9:ILE:CG2	1:A:20:PRO:HA	2.05	0.85
1:A:290:GLN:NE2	1:A:330:GLU:HB3	1.90	0.85
1:A:9:ILE:HG21	1:A:21:GLU:H	1.41	0.85
1:A:232:PHE:CD1	1:A:287:ILE:HG21	2.11	0.85
1:A:296:LYS:CG	1:A:331:LEU:HD11	2.07	0.85
1:A:506:GLU:HB3	1:A:508:ILE:HD11	1.59	0.85
2:B:35:PHE:CD1	2:B:46:ILE:HD13	2.12	0.85
3:C:92:VAL:HG23	3:C:93:LEU:H	1.42	0.85
3:C:191:SER:CA	3:C:192:ILE:HG22	2.05	0.85
4:D:154:ASP:CA	4:D:300:SER:HB3	2.05	0.85
4:D:299:MET:HE1	4:D:309:ILE:HD12	1.56	0.85
1:A:618:LEU:HG	1:A:622:LEU:CD1	2.05	0.84
1:A:811:ARG:HG2	1:A:815:ILE:CD1	2.05	0.84
4:D:189:LEU:HD23	4:D:209:VAL:CG1	2.06	0.84
1:A:99:GLU:HA	1:A:102:VAL:HG13	1.57	0.84
2:B:79:ILE:HD11	2:B:84:PHE:CA	2.05	0.84
1:A:335:ASP:O	1:A:338:ILE:HG22	1.78	0.84
3:C:140:GLU:HG2	3:C:180:ILE:HG12	1.59	0.84
1:A:736:GLU:HA	1:A:740:ILE:CD1	2.08	0.84
3:C:42:LYS:HE2	3:C:113:PRO:HG3	1.56	0.84
1:A:207:LYS:HD3	1:A:259:LYS:CB	2.06	0.84
2:B:137:ILE:HD13	2:B:141:TRP:HE1	1.43	0.84
1:A:303:LEU:HD22	1:A:305:ILE:CG1	2.08	0.84
4:E:79:TRP:CD2	4:E:118:LYS:HG2	2.13	0.83
1:A:329:GLU:O	1:A:332:LEU:HG	1.78	0.83
1:A:530:MET:HE1	4:D:351:THR:CA	2.08	0.83
3:C:90:LYS:HB2	3:C:111:PHE:HE2	1.42	0.83
4:D:35:VAL:HG12	4:D:68:LYS:CB	2.09	0.83
4:E:236:LEU:CD1	4:E:237:GLU:HG2	2.08	0.83
1:A:116:TYR:CD1	1:A:125:THR:HB	2.13	0.83
4:E:76:ILE:CG2	4:E:82:MET:HG2	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:MET:HE2	1:A:708:ILE:HG21	1.59	0.83
1:A:188:ASN:O	1:A:192:VAL:HG22	1.79	0.83
4:E:116:ARG:NH1	4:E:371:HIS:HA	1.93	0.83
4:E:133:TYR:CZ	4:E:375:PHE:HB2	2.13	0.83
1:A:223:ILE:HD12	1:A:224:GLN:N	1.94	0.83
3:C:135:ARG:HG3	3:C:138:ASP:H	1.44	0.83
4:D:104:LEU:HB2	4:D:356:TRP:HH2	1.42	0.83
1:A:111:ALA:HA	1:A:686:GLY:HA2	1.60	0.83
1:A:113:TRP:CE3	1:A:130:LYS:HE2	2.12	0.83
1:A:530:MET:CE	4:D:351:THR:HA	2.07	0.83
3:C:152:HIS:O	3:C:157:LEU:HB3	1.78	0.83
3:C:128:GLU:HB2	3:C:180:ILE:HG22	1.59	0.83
4:E:361:GLU:CB	4:E:369:ILE:HD13	2.07	0.83
1:A:253:HIS:HB2	1:A:455:ARG:CD	2.09	0.83
1:A:296:LYS:HB3	1:A:331:LEU:HD21	1.58	0.83
1:A:297:PRO:O	1:A:300:ILE:HG12	1.78	0.83
3:C:170:MET:HE1	3:C:186:VAL:HA	1.59	0.83
4:D:285:CYS:HB3	4:D:289:ILE:HD11	1.58	0.83
1:A:16:TYR:CZ	1:A:132:LEU:HB3	2.14	0.83
1:A:295:LYS:HG3	1:A:331:LEU:HD22	1.60	0.82
1:A:611:TYR:HD2	1:A:618:LEU:HD21	1.42	0.82
4:E:107:GLU:O	4:E:137:GLN:HG3	1.79	0.82
1:A:19:LYS:HD3	1:A:23:GLU:HB3	1.60	0.82
1:A:442:VAL:O	1:A:445:ILE:HG22	1.79	0.82
1:A:207:LYS:CD	1:A:259:LYS:HB2	2.09	0.82
3:C:57:PHE:HA	3:C:60:TYR:CD2	2.14	0.82
2:B:116:ILE:CG2	2:B:121:LEU:HD12	2.10	0.82
1:A:195:TYR:CZ	1:A:199:ILE:HD11	2.14	0.82
1:A:397:MET:O	1:A:401:LEU:HD23	1.80	0.82
4:E:36:GLY:O	4:E:52:SER:HA	1.79	0.82
4:E:79:TRP:CE2	4:E:118:LYS:HG2	2.14	0.82
1:A:535:ILE:HD12	1:A:557:GLN:NE2	1.95	0.82
4:D:153:LEU:CD2	4:D:274:ILE:HD12	2.08	0.82
4:E:8:LEU:HD12	4:E:90:PHE:HE1	1.43	0.82
1:A:749:LEU:O	1:A:753:ILE:HG12	1.80	0.82
1:A:800:LEU:O	1:A:803:VAL:HG12	1.79	0.82
3:C:82:THR:O	3:C:85:THR:HG22	1.79	0.82
1:A:16:TYR:CD1	1:A:134:VAL:HG23	2.15	0.82
1:A:115:ILE:HG21	1:A:128:PRO:CD	2.10	0.82
3:C:42:LYS:HA	3:C:43:ILE:CB	2.09	0.82
4:D:169:TYR:CD1	4:E:42:GLY:HA3	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:290:ARG:NH1	4:E:244:ASP:HB2	1.94	0.82
1:A:39:PHE:CB	1:A:100:PRO:HG2	2.10	0.82
1:A:291:ILE:HG13	1:A:296:LYS:HZ2	1.43	0.82
1:A:346:GLU:O	1:A:349:VAL:HG12	1.80	0.82
2:B:28:ILE:HD12	2:B:29:GLN:N	1.95	0.82
4:D:22:ALA:HB1	4:D:348:SER:HB3	1.59	0.82
4:E:106:THR:HG22	4:E:135:ALA:HB3	1.62	0.82
1:A:173:GLN:CB	1:A:459:ILE:HG23	2.08	0.82
1:A:740:ILE:HG21	1:A:745:ALA:HB2	1.62	0.82
3:C:80:LEU:HB2	3:C:121:ASN:OD1	1.80	0.82
2:B:97:PRO:O	2:B:100:VAL:HG12	1.80	0.81
1:A:73:ASN:H	1:A:76:GLN:HG2	1.43	0.81
1:A:144:ARG:HH22	1:A:199:ILE:HD13	1.44	0.81
1:A:445:ILE:HG23	1:A:449:LEU:HD12	1.63	0.81
1:A:551:LYS:HD2	1:A:555:TYR:HE2	1.45	0.81
4:E:140:LEU:HD13	4:E:343:GLY:HA3	1.61	0.81
1:A:19:LYS:HD3	1:A:23:GLU:CB	2.11	0.81
1:A:49:LYS:HD3	1:A:65:LEU:HD23	1.60	0.81
1:A:817:CYS:HA	1:A:820:TYR:CZ	2.16	0.81
4:E:35:VAL:HG12	4:E:68:LYS:HB3	1.62	0.81
1:A:72:LEU:HB3	1:A:76:GLN:HG2	1.63	0.81
1:A:364:MET:CG	1:A:382:VAL:HB	2.11	0.81
1:A:366:PHE:CD2	1:A:422:VAL:HG21	2.15	0.81
1:A:468:GLU:OE2	1:A:480:ILE:HD13	1.79	0.81
1:A:805:PHE:HA	1:A:808:MET:HE3	1.61	0.81
1:A:175:ILE:CD1	1:A:461:VAL:HG13	2.11	0.81
1:A:428:ALA:HA	1:A:431:LYS:HE2	1.63	0.81
1:A:605:GLU:O	1:A:608:VAL:HG12	1.81	0.81
1:A:644:LYS:CD	1:A:649:GLN:HG3	2.11	0.81
3:C:137:PHE:CD2	3:C:139:LYS:HB2	2.15	0.81
1:A:159:SER:HB3	1:A:195:TYR:CD2	2.16	0.81
1:A:424:ASN:HD21	1:A:602:PRO:HD2	1.45	0.81
1:A:787:THR:O	1:A:791:ARG:HD3	1.80	0.81
4:D:58:ALA:HB1	4:D:65:LEU:HD22	1.63	0.81
4:E:155:SER:HB3	4:E:160:THR:HG23	1.63	0.81
1:A:13:ALA:CB	1:A:139:VAL:HG22	2.11	0.81
1:A:727:ARG:NH1	1:A:745:ALA:HB1	1.96	0.81
3:C:113:PRO:O	3:C:116:GLN:HB3	1.80	0.81
1:A:232:PHE:CE1	1:A:287:ILE:HG21	2.16	0.80
3:C:90:LYS:HB2	3:C:111:PHE:CE2	2.16	0.80
4:D:209:VAL:HA	4:D:212:ILE:HD12	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:VAL:O	1:A:352:TYR:HB2	1.81	0.80
2:B:58:MET:HG3	2:B:60:ARG:N	1.96	0.80
1:A:472:PHE:CE1	1:A:591:ASN:HB3	2.16	0.80
1:A:493:HIS:HA	1:A:514:ASP:OD2	1.80	0.80
1:A:569:LYS:HD3	1:A:570:PRO:O	1.82	0.80
4:D:295:ALA:O	4:D:328:LYS:HB3	1.80	0.80
1:A:232:PHE:CD2	1:A:287:ILE:HG21	2.16	0.80
3:C:91:LYS:HE2	3:C:95:ASN:OD1	1.82	0.80
4:E:34:ILE:CB	4:E:54:VAL:HG11	2.11	0.80
1:A:805:PHE:HA	1:A:808:MET:CE	2.11	0.80
2:B:83:VAL:CA	2:B:86:THR:HG22	2.10	0.80
1:A:784:LYS:HD2	1:A:788:LEU:HD11	1.64	0.80
2:B:115:THR:HG21	2:B:154:TYR:CE2	2.17	0.80
2:B:125:LEU:HB3	2:B:132:PHE:CD1	2.17	0.80
3:C:98:ASN:HB3	3:C:99:GLU:HA	1.63	0.80
1:A:693:VAL:HA	1:A:696:GLN:HG3	1.63	0.80
3:C:72:GLN:HA	3:C:75:ASP:OD2	1.81	0.80
1:A:176:LEU:CD1	1:A:673:PHE:HA	2.12	0.80
3:C:67:LYS:CD	3:C:92:VAL:HG13	2.12	0.80
3:C:170:MET:CE	3:C:186:VAL:HG23	2.11	0.80
4:E:139:VAL:HG12	4:E:140:LEU:HD23	1.64	0.80
1:A:130:LYS:HG3	1:A:685:PRO:HG3	1.63	0.79
1:A:253:HIS:HB2	1:A:455:ARG:HD2	1.64	0.79
1:A:261:ALA:HB2	1:A:455:ARG:N	1.96	0.79
1:A:392:LEU:HD11	1:A:613:LYS:O	1.81	0.79
2:B:43:ASP:O	2:B:45:ILE:HG23	1.79	0.79
4:E:300:SER:HA	4:E:335:ARG:CD	2.13	0.79
1:A:89:GLU:O	1:A:117:THR:HG23	1.83	0.79
1:A:375:ALA:HB3	1:A:417:GLN:NE2	1.96	0.79
4:E:178:LEU:HD21	4:E:180:LEU:HB3	1.65	0.79
1:A:42:ASP:HB2	1:A:48:VAL:HG23	1.65	0.79
1:A:111:ALA:CA	1:A:686:GLY:HA2	2.12	0.79
1:A:217:THR:HB	1:A:218:LEU:O	1.81	0.79
2:B:70:ALA:O	2:B:73:LYS:HG2	1.82	0.79
1:A:283:ARG:HD2	1:A:289:TYR:CE2	2.18	0.79
1:A:385:LYS:O	1:A:389:LEU:HD12	1.83	0.79
1:A:611:TYR:HB3	1:A:622:LEU:CD1	2.03	0.79
2:B:61:LEU:HD22	2:B:62:ASN:H	1.47	0.79
3:C:57:PHE:CE2	3:C:69:THR:HG21	2.16	0.79
4:D:244:ASP:OD2	4:D:246:GLN:HG3	1.82	0.79
4:D:250:ILE:HG12	4:D:251:GLY:H	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TRP:C	1:A:132:LEU:HD13	2.02	0.79
1:A:256:ALA:N	1:A:456:GLN:HG3	1.98	0.79
4:E:34:ILE:HB	4:E:54:VAL:CG1	2.13	0.79
4:E:357:ILE:HG12	4:E:370:VAL:HG23	1.63	0.79
1:A:107:LYS:HB2	1:A:688:MET:HG3	1.64	0.79
1:A:568:PRO:HG2	1:A:577:ALA:HB3	1.65	0.79
1:A:644:LYS:HD3	1:A:649:GLN:CG	2.11	0.79
1:A:717:ILE:CG2	1:A:721:ASP:HB3	2.12	0.79
3:C:123:ASP:HB3	3:C:126:THR:HG22	1.64	0.79
1:A:47:TYR:CD2	1:A:100:PRO:HG3	2.18	0.79
1:A:535:ILE:HG23	1:A:553:LYS:HE2	1.63	0.79
3:C:148:ALA:HA	3:C:163:GLU:OE2	1.83	0.79
1:A:25:ILE:HD12	1:A:26:GLU:N	1.97	0.79
1:A:210:GLN:HG3	1:A:211:PRO:N	1.96	0.79
1:A:392:LEU:HD22	1:A:614:SER:HB3	1.65	0.79
3:C:92:VAL:N	3:C:95:ASN:HB3	1.98	0.79
3:C:127:TYR:HE2	3:C:187:LYS:HE2	1.47	0.79
4:D:321:ALA:HB1	4:D:322:PRO:HD2	1.65	0.78
4:E:237:GLU:O	4:E:249:THR:HG23	1.83	0.78
1:A:123:CYS:HG	1:A:153:PRO:HB3	1.47	0.78
1:A:287:ILE:HD12	1:A:288:PHE:N	1.98	0.78
1:A:789:MET:HE2	3:C:150:LEU:HD11	1.64	0.78
4:D:36:GLY:O	4:D:52:SER:HA	1.82	0.78
4:D:189:LEU:HA	4:D:192:ILE:HD11	1.65	0.78
1:A:272:LYS:CD	1:A:431:LYS:HB3	2.12	0.78
1:A:436:LYS:HD3	1:A:621:PHE:HB3	1.64	0.78
1:A:737:GLY:HA3	1:A:739:PHE:HD2	1.47	0.78
1:A:16:TYR:CE2	1:A:132:LEU:HG	2.19	0.78
1:A:462:LEU:HD13	1:A:463:ASP:N	1.98	0.78
4:E:189:LEU:HD12	4:E:189:LEU:O	1.84	0.78
4:E:236:LEU:HD12	4:E:237:GLU:HG2	1.66	0.78
1:A:91:MET:HE2	1:A:102:VAL:HA	1.66	0.78
4:D:124:PHE:CE2	4:D:362:TYR:HB2	2.19	0.78
1:A:47:TYR:CB	1:A:100:PRO:HG3	2.14	0.78
1:A:176:LEU:HD11	1:A:673:PHE:CD2	2.19	0.78
1:A:247:GLY:H	1:A:269:LEU:HD11	1.45	0.78
1:A:508:ILE:HG13	1:A:768:PHE:CZ	2.19	0.78
1:A:551:LYS:HG2	1:A:555:TYR:CE2	2.18	0.78
4:D:336:LYS:HE2	5:D:401:ADP:H5'2	1.65	0.78
4:E:97:ALA:HB1	4:E:99:GLU:OE1	1.83	0.78
4:E:336:LYS:HE2	5:E:401:ADP:H5'2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:GLU:O	1:A:480:ILE:HD12	1.83	0.78
4:E:180:LEU:HD12	4:E:181:ALA:H	1.49	0.78
1:A:79:PRO:HD2	1:A:98:HIS:NE2	1.99	0.78
1:A:795:LEU:HD23	3:C:187:LYS:HZ3	1.47	0.78
1:A:824:ALA:O	1:A:828:VAL:HG12	1.82	0.78
2:B:52:ARG:HD2	2:B:64:LYS:CG	2.14	0.78
4:D:39:ARG:HG2	4:D:66:THR:HG22	1.64	0.78
1:A:293:SER:HB3	1:A:327:ASP:HB2	1.65	0.77
3:C:62:ARG:HD2	3:C:63:THR:H	1.46	0.77
1:A:9:ILE:HG23	1:A:18:ARG:NH1	1.99	0.77
1:A:175:ILE:HD11	1:A:461:VAL:CG2	2.11	0.77
1:A:207:LYS:HD2	1:A:454:PRO:CD	2.06	0.77
1:A:436:LYS:HB3	1:A:621:PHE:CD1	2.18	0.77
4:E:164:PRO:HG2	4:E:174:ALA:HB1	1.66	0.77
1:A:207:LYS:CE	1:A:259:LYS:HB2	2.13	0.77
1:A:322:VAL:O	1:A:325:ILE:HG22	1.84	0.77
1:A:831:TRP:CE3	1:A:834:MET:HG2	2.17	0.77
3:C:134:LEU:HD21	3:C:150:LEU:HG	1.67	0.77
4:D:183:ARG:HG2	4:D:184:ASP:N	1.98	0.77
1:A:613:LYS:HD3	1:A:613:LYS:N	2.00	0.77
3:C:174:GLU:O	3:C:176:SER:HA	1.85	0.77
4:D:34:ILE:CB	4:D:54:VAL:HG11	2.15	0.77
1:A:5:ALA:HB1	1:A:18:ARG:NH1	2.00	0.77
1:A:62:VAL:HG12	1:A:70:LEU:O	1.85	0.77
1:A:727:ARG:NH2	1:A:749:LEU:HB2	2.00	0.77
4:D:332:PRO:HG2	4:D:335:ARG:CZ	2.15	0.77
1:A:175:ILE:HD12	1:A:175:ILE:O	1.84	0.77
2:B:108:LEU:CD2	2:B:116:ILE:HD13	2.07	0.77
4:D:142:LEU:HD21	4:D:165:ILE:CD1	2.09	0.77
1:A:158:ILE:HA	1:A:161:ASN:HD21	1.50	0.77
3:C:142:ASN:O	3:C:177:ASN:HB3	1.85	0.77
1:A:355:THR:O	1:A:358:VAL:HB	1.85	0.77
1:A:392:LEU:CD2	1:A:614:SER:HB3	2.13	0.77
1:A:392:LEU:HD11	1:A:613:LYS:C	2.05	0.77
1:A:795:LEU:HG	3:C:187:LYS:HD3	1.66	0.77
4:D:34:ILE:HG22	4:D:68:LYS:N	1.99	0.77
1:A:109:ARG:O	1:A:112:ALA:HB3	1.84	0.76
1:A:246:PHE:HA	1:A:269:LEU:CD1	2.15	0.76
1:A:801:MET:HE3	3:C:57:PHE:CZ	2.20	0.76
3:C:123:ASP:O	3:C:126:THR:HG23	1.85	0.76
4:D:142:LEU:CD2	4:D:165:ILE:HD13	2.10	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:233:SER:HB3	4:D:236:LEU:HG	1.66	0.76
4:E:365:ALA:CB	4:E:369:ILE:HD12	2.15	0.76
3:C:42:LYS:HD2	3:C:47:LYS:CB	2.16	0.76
4:E:269:MET:HG2	4:E:271:SER:OG	1.85	0.76
1:A:312:PHE:O	1:A:315:VAL:HG23	1.86	0.76
1:A:415:LYS:CG	4:D:333:PRO:HG2	2.15	0.76
1:A:694:MET:HE2	1:A:694:MET:HA	1.65	0.76
1:A:74:SER:O	1:A:77:VAL:HG22	1.83	0.76
1:A:40:ALA:HB1	1:A:72:LEU:CD2	2.16	0.76
1:A:107:LYS:CG	1:A:688:MET:HG3	2.16	0.76
1:A:246:PHE:CA	1:A:269:LEU:HD11	2.16	0.76
1:A:671:PRO:HB2	1:A:673:PHE:CE1	2.21	0.76
3:C:109:GLU:O	3:C:113:PRO:HD2	1.85	0.76
3:C:128:GLU:CB	3:C:180:ILE:HG22	2.15	0.76
1:A:62:VAL:HG11	1:A:72:LEU:HD13	1.68	0.76
1:A:314:PHE:CE2	1:A:362:GLY:HA2	2.20	0.76
1:A:464:ILE:HG12	1:A:465:ALA:N	1.98	0.76
3:C:92:VAL:CG2	3:C:95:ASN:HA	2.15	0.76
3:C:58:LEU:HD11	3:C:65:ASP:HB2	1.66	0.76
4:E:37:ARG:HG2	4:E:38:PRO:CD	2.12	0.76
4:E:149:THR:HG22	4:E:150:GLY:H	1.50	0.76
4:E:198:TYR:CE1	4:E:248:ILE:HG22	2.21	0.76
1:A:115:ILE:HG21	1:A:128:PRO:HG3	1.67	0.76
1:A:123:CYS:SG	1:A:153:PRO:HB3	2.26	0.76
3:C:67:LYS:HA	3:C:67:LYS:HE2	1.67	0.76
1:A:360:HIS:HB3	1:A:382:VAL:CG1	2.14	0.75
1:A:838:PHE:CE1	2:B:164:GLY:HA3	2.21	0.75
1:A:815:ILE:HG21	2:B:129:CYS:SG	2.26	0.75
3:C:67:LYS:O	3:C:70:LEU:HB2	1.86	0.75
4:D:287:ILE:HB	4:E:244:ASP:CB	2.16	0.75
1:A:253:HIS:O	1:A:260:LEU:HD22	1.87	0.75
1:A:255:GLY:CA	1:A:456:GLN:H	1.95	0.75
1:A:506:GLU:CB	1:A:508:ILE:HD11	2.16	0.75
3:C:180:ILE:O	3:C:183:GLU:HG3	1.86	0.75
4:E:140:LEU:O	4:E:342:GLY:HA3	1.86	0.75
1:A:46:MET:HA	1:A:46:MET:CE	2.17	0.75
1:A:64:THR:HG22	1:A:65:LEU:H	1.50	0.75
1:A:717:ILE:HG22	1:A:721:ASP:HB3	1.68	0.75
1:A:789:MET:CE	3:C:150:LEU:HD11	2.16	0.75
3:C:140:GLU:CG	3:C:180:ILE:HG12	2.17	0.75
1:A:166:MET:SD	1:A:457:TYR:HB2	2.27	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASN:ND2	1:A:600:LYS:HG2	2.02	0.75
1:A:825:PHE:HA	1:A:828:VAL:CG1	2.17	0.75
2:B:83:VAL:HA	2:B:86:THR:CG2	2.16	0.75
3:C:66:SER:CB	3:C:68:ILE:HG22	2.17	0.75
1:A:440:TRP:O	1:A:443:THR:HG22	1.87	0.75
1:A:800:LEU:HD11	3:C:162:LYS:HG2	1.69	0.75
1:A:833:TRP:CE2	2:B:71:MET:HG2	2.22	0.75
4:E:164:PRO:HG2	4:E:174:ALA:CB	2.16	0.75
3:C:74:GLY:HA3	3:C:112:LEU:HD11	1.68	0.75
1:A:122:PHE:CE1	1:A:673:PHE:HB2	2.22	0.75
1:A:130:LYS:CD	1:A:132:LEU:HD11	2.16	0.75
1:A:421:GLN:HG3	1:A:422:VAL:N	2.02	0.75
1:A:614:SER:N	1:A:619:LEU:HD11	2.00	0.75
4:D:11:ASP:HB3	4:D:18:LYS:HG2	1.68	0.75
4:E:236:LEU:HD22	4:E:251:GLY:C	2.08	0.75
1:A:14:ALA:CB	1:A:18:ARG:HD2	2.17	0.74
1:A:85:PHE:O	1:A:88:ILE:HB	1.87	0.74
1:A:232:PHE:CZ	1:A:287:ILE:HG21	2.23	0.74
1:A:303:LEU:HD22	1:A:305:ILE:HG13	1.66	0.74
4:D:59:GLN:O	4:D:62:ARG:HG3	1.87	0.74
4:E:47:MET:HG3	4:E:48:GLY:H	1.51	0.74
4:E:156:GLY:O	4:E:181:ALA:HB1	1.87	0.74
4:E:332:PRO:HG2	4:E:335:ARG:CZ	2.17	0.74
2:B:28:ILE:HG22	2:B:85:LEU:CD2	2.17	0.74
3:C:189:ILE:HG12	3:C:190:MET:N	2.03	0.74
4:E:223:PHE:CE1	4:E:259:GLU:HG2	2.22	0.74
1:A:387:GLY:HA2	1:A:397:MET:SD	2.28	0.74
3:C:137:PHE:HD2	3:C:139:LYS:HB2	1.50	0.74
1:A:142:ALA:O	1:A:146:LYS:HD2	1.88	0.74
1:A:390:MET:CB	1:A:392:LEU:HD23	2.10	0.74
1:A:436:LYS:HB3	1:A:621:PHE:HD1	1.53	0.74
1:A:167:LEU:HD21	1:A:258:GLY:HA3	1.69	0.74
3:C:57:PHE:HA	3:C:60:TYR:HD2	1.51	0.74
3:C:69:THR:HG22	3:C:72:GLN:HB2	1.69	0.74
4:E:39:ARG:HE	4:E:66:THR:HB	1.52	0.74
4:E:163:VAL:HG22	4:E:175:ILE:HG23	1.70	0.74
1:A:253:HIS:CB	1:A:458:PHE:HB3	2.17	0.74
3:C:180:ILE:HA	3:C:183:GLU:HG2	1.70	0.74
4:D:219:VAL:HG22	4:D:258:PRO:HB2	1.69	0.74
4:E:39:ARG:HE	4:E:66:THR:CB	2.01	0.74
1:A:253:HIS:CG	1:A:455:ARG:HD2	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:TYR:HA	1:A:364:MET:SD	2.28	0.74
3:C:92:VAL:H	3:C:95:ASN:HB3	1.49	0.74
4:D:158:GLY:HA2	4:D:183:ARG:HD2	1.70	0.74
4:E:365:ALA:HB3	4:E:369:ILE:HD12	1.68	0.74
1:A:159:SER:HB3	1:A:195:TYR:CG	2.22	0.73
1:A:232:PHE:CE2	1:A:287:ILE:HG21	2.24	0.73
1:A:778:GLU:O	1:A:781:ARG:HG3	1.87	0.73
2:B:70:ALA:HA	2:B:73:LYS:CE	2.18	0.73
3:C:135:ARG:CZ	3:C:137:PHE:HB3	2.17	0.73
3:C:71:SER:HB2	3:C:86:ASN:CG	2.08	0.73
4:E:34:ILE:CG1	4:E:54:VAL:HG11	2.18	0.73
4:E:178:LEU:HG	4:E:180:LEU:H	1.52	0.73
1:A:81:ASN:ND2	1:A:96:HIS:H	1.86	0.73
1:A:519:LEU:HD22	1:A:584:TYR:HB3	1.68	0.73
2:B:61:LEU:HD22	2:B:62:ASN:N	2.03	0.73
4:E:8:LEU:HD12	4:E:90:PHE:CE1	2.22	0.73
1:A:81:ASN:HD21	1:A:96:HIS:H	1.36	0.73
1:A:229:LEU:HD22	1:A:438:PHE:HE1	1.53	0.73
1:A:332:LEU:HD12	1:A:333:ALA:N	2.02	0.73
2:B:105:PHE:O	2:B:108:LEU:HB2	1.87	0.73
1:A:195:TYR:OH	1:A:199:ILE:HD11	1.88	0.73
1:A:205:LYS:HG2	1:A:257:THR:HG21	1.70	0.73
1:A:780:MET:O	1:A:783:GLU:HG3	1.88	0.73
3:C:142:ASN:H	3:C:177:ASN:N	1.86	0.73
4:D:287:ILE:HG12	4:D:288:ASP:N	2.02	0.73
1:A:246:PHE:HA	1:A:269:LEU:HD11	1.70	0.73
1:A:645:GLY:HA2	4:D:23:GLY:HA2	1.70	0.73
4:D:122:ILE:O	4:D:126:THR:HB	1.89	0.73
1:A:520:ALA:HA	1:A:523:ILE:CD1	2.16	0.73
3:C:50:GLN:NE2	3:C:112:LEU:HB2	2.03	0.73
4:D:306:TYR:O	4:D:309:ILE:HB	1.88	0.73
1:A:47:TYR:CG	1:A:100:PRO:HG3	2.24	0.73
1:A:841:LYS:HB3	1:A:842:PRO:HD3	1.69	0.73
3:C:156:THR:O	3:C:157:LEU:HD13	1.89	0.73
4:E:206:ARG:HG2	4:E:206:ARG:HH11	1.53	0.73
1:A:197:ALA:O	1:A:201:VAL:HG22	1.88	0.73
1:A:479:CYS:O	1:A:483:THR:HG23	1.89	0.73
1:A:485:GLU:OE1	1:A:523:ILE:HG23	1.89	0.73
1:A:513:ILE:HG22	1:A:514:ASP:H	1.52	0.73
1:A:755:VAL:HG11	1:A:773:LEU:HD21	1.69	0.73
3:C:47:LYS:HG3	3:C:109:GLU:OE2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:LYS:CE	3:C:101:MET:HB3	2.19	0.73
4:D:34:ILE:HB	4:D:54:VAL:CG1	2.19	0.73
4:E:153:LEU:HD11	4:E:274:ILE:CG2	2.19	0.73
1:A:546:THR:HG23	1:A:548:THR:N	2.03	0.73
4:E:190:MET:HE3	4:E:206:ARG:HG3	1.69	0.73
1:A:163:TYR:CE2	1:A:199:ILE:HG21	2.23	0.72
1:A:190:LYS:O	1:A:194:GLN:HG3	1.89	0.72
1:A:220:ASP:HA	1:A:223:ILE:CG1	2.19	0.72
1:A:279:LEU:HD23	1:A:279:LEU:H	1.53	0.72
1:A:351:ILE:HG12	1:A:437:MET:CE	2.19	0.72
1:A:245:ARG:HG3	1:A:285:TYR:CE1	2.24	0.72
1:A:295:LYS:CB	1:A:331:LEU:HB3	2.18	0.72
1:A:492:ASN:OD1	1:A:708:ILE:HD11	1.89	0.72
4:D:158:GLY:N	4:D:181:ALA:HB3	2.05	0.72
4:E:102:PRO:HB3	4:E:131:ALA:CB	2.18	0.72
4:D:346:LEU:O	4:D:349:LEU:HB2	1.90	0.72
1:A:800:LEU:CG	3:C:162:LYS:HE2	2.11	0.72
4:E:189:LEU:HG	4:E:209:VAL:HG13	1.69	0.72
1:A:207:LYS:CD	1:A:454:PRO:HD2	2.07	0.72
3:C:62:ARG:HD2	3:C:62:ARG:C	2.10	0.72
4:D:156:GLY:O	4:D:181:ALA:HB1	1.89	0.72
4:D:332:PRO:HG2	4:D:335:ARG:NE	2.04	0.72
1:A:46:MET:HB2	1:A:690:HIS:CB	2.19	0.72
1:A:167:LEU:HD22	1:A:257:THR:C	2.09	0.72
1:A:535:ILE:HG23	1:A:553:LYS:CE	2.19	0.72
3:C:51:ASP:O	3:C:54:LYS:HB3	1.90	0.72
1:A:5:ALA:HB1	1:A:18:ARG:CZ	2.19	0.72
1:A:14:ALA:HB1	1:A:18:ARG:CD	2.20	0.72
1:A:535:ILE:HD12	1:A:557:GLN:CD	2.09	0.72
1:A:833:TRP:HA	1:A:836:LEU:CD1	2.11	0.72
3:C:69:THR:HB	3:C:73:VAL:HG23	1.70	0.72
4:D:250:ILE:CG1	4:D:253:GLU:HB2	2.20	0.72
4:D:360:GLN:O	4:D:364:GLU:HG3	1.89	0.72
4:E:34:ILE:HD13	4:E:69:TYR:CZ	2.25	0.72
1:A:78:PHE:HB3	1:A:98:HIS:CD2	2.25	0.72
1:A:654:VAL:O	1:A:657:GLU:HB3	1.88	0.72
4:E:370:VAL:HG22	4:E:375:PHE:O	1.89	0.72
1:A:234:ASN:H	1:A:245:ARG:HG2	1.55	0.71
1:A:298:GLU:HG3	1:A:299:LEU:N	2.04	0.71
1:A:392:LEU:HD13	1:A:614:SER:HB2	1.72	0.71
1:A:736:GLU:O	1:A:740:ILE:HD12	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:295:ALA:O	4:E:328:LYS:HB3	1.90	0.71
1:A:14:ALA:HB1	1:A:18:ARG:HD2	1.70	0.71
1:A:514:ASP:HB3	1:A:517:MET:HE3	1.72	0.71
1:A:115:ILE:HG21	1:A:128:PRO:CG	2.20	0.71
1:A:290:GLN:HE21	1:A:330:GLU:HB3	1.53	0.71
1:A:351:ILE:HG12	1:A:437:MET:HE2	1.70	0.71
1:A:530:MET:HE2	4:D:351:THR:HG22	1.71	0.71
1:A:1:MET:O	1:A:2:SER:C	2.26	0.71
1:A:496:PHE:CG	1:A:514:ASP:HA	2.25	0.71
1:A:584:TYR:H	1:A:584:TYR:HD1	1.36	0.71
1:A:829:LYS:HD2	1:A:830:HIS:CD2	2.25	0.71
4:E:260:THR:HG23	4:E:266:PHE:HB2	1.72	0.71
1:A:520:ALA:CA	1:A:523:ILE:HD11	2.14	0.71
4:E:143:TYR:CE2	4:E:346:LEU:HB2	2.26	0.71
1:A:230:GLU:O	1:A:234:ASN:HB2	1.91	0.71
1:A:261:ALA:HB2	1:A:454:PRO:C	2.10	0.71
3:C:140:GLU:CB	3:C:180:ILE:HD11	2.19	0.71
4:E:334:GLU:HA	4:E:334:GLU:OE2	1.89	0.71
1:A:39:PHE:CD1	1:A:100:PRO:HB2	2.25	0.71
1:A:253:HIS:HB3	1:A:458:PHE:HB3	1.73	0.71
1:A:283:ARG:HB2	1:A:289:TYR:OH	1.91	0.71
1:A:415:LYS:HG3	1:A:416:GLY:N	2.06	0.71
1:A:524:GLU:HG3	1:A:528:LYS:CD	2.17	0.71
1:A:32:PHE:HB3	1:A:83:PRO:CG	2.18	0.71
1:A:131:TRP:O	1:A:132:LEU:HD13	1.90	0.71
3:C:108:PHE:CZ	3:C:112:LEU:HG	2.24	0.71
3:C:159:GLU:HG2	3:C:162:LYS:CD	2.21	0.71
1:A:291:ILE:HG13	1:A:296:LYS:NZ	2.06	0.71
1:A:515:PHE:HE1	1:A:711:LYS:HG2	1.55	0.71
1:A:784:LYS:HD2	1:A:788:LEU:CD1	2.21	0.71
2:B:58:MET:CG	2:B:60:ARG:H	1.97	0.71
3:C:68:ILE:O	3:C:91:LYS:HE3	1.91	0.71
4:E:27:PRO:HG3	4:E:340:TRP:CG	2.25	0.71
4:E:34:ILE:HG13	4:E:54:VAL:HG11	1.73	0.71
1:A:267:THR:HG21	1:A:438:PHE:HE2	1.56	0.71
3:C:55:GLU:O	3:C:59:LEU:HD13	1.91	0.71
1:A:79:PRO:HD2	1:A:98:HIS:HE2	1.56	0.70
3:C:170:MET:HE3	3:C:186:VAL:HG23	1.72	0.70
4:D:250:ILE:HG12	4:D:253:GLU:HB2	1.71	0.70
1:A:291:ILE:O	1:A:296:LYS:HD3	1.91	0.70
1:A:488:GLN:HG3	1:A:584:TYR:HE2	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ILE:HG13	1:A:768:PHE:CE2	2.26	0.70
1:A:822:ILE:HG12	2:B:132:PHE:CZ	2.26	0.70
3:C:47:LYS:HG3	3:C:109:GLU:CD	2.11	0.70
4:D:8:LEU:HD13	4:D:90:PHE:HE1	1.54	0.70
4:E:223:PHE:CD1	4:E:259:GLU:HG2	2.26	0.70
1:A:510:TRP:CE2	1:A:512:PHE:HB2	2.26	0.70
3:C:70:LEU:CB	3:C:91:LYS:HD2	2.21	0.70
4:E:362:TYR:HE1	4:E:367:PRO:HG3	1.56	0.70
1:A:78:PHE:CD2	1:A:98:HIS:HD2	2.07	0.70
1:A:176:LEU:HD11	1:A:673:PHE:HA	1.72	0.70
1:A:263:ALA:HB3	1:A:449:LEU:HD22	1.72	0.70
1:A:295:LYS:HG2	1:A:332:LEU:CA	2.21	0.70
3:C:45:PHE:H	3:C:46:SER:HB2	1.54	0.70
3:C:67:LYS:HD2	3:C:101:MET:CB	2.20	0.70
3:C:170:MET:HG3	3:C:182:TYR:CE1	2.27	0.70
3:C:179:CYS:O	3:C:183:GLU:HG2	1.91	0.70
4:E:134:VAL:O	4:E:375:PHE:HB3	1.90	0.70
3:C:46:SER:O	3:C:49:GLN:HG2	1.91	0.70
3:C:86:ASN:HB3	3:C:91:LYS:CD	2.21	0.70
4:D:39:ARG:NE	4:D:66:THR:HA	2.05	0.70
2:B:160:VAL:CG2	2:B:165:ASP:HB2	2.22	0.70
4:E:143:TYR:OH	4:E:349:LEU:HD11	1.91	0.70
1:A:345:SER:O	1:A:348:LYS:HB3	1.92	0.70
1:A:445:ILE:HG12	1:A:449:LEU:HD11	1.74	0.70
3:C:50:GLN:NE2	3:C:109:GLU:HA	2.07	0.70
3:C:57:PHE:HE2	3:C:69:THR:HG21	1.54	0.70
4:E:300:SER:CA	4:E:335:ARG:HG3	2.19	0.70
1:A:99:GLU:HA	1:A:102:VAL:CG1	2.20	0.70
1:A:103:LEU:HD22	1:A:690:HIS:CD2	2.20	0.70
1:A:475:LEU:HD22	1:A:595:TRP:CE3	2.26	0.70
1:A:569:LYS:HG2	1:A:570:PRO:CD	2.15	0.70
3:C:80:LEU:HD22	3:C:187:LYS:NZ	2.06	0.70
3:C:91:LYS:HG3	3:C:95:ASN:ND2	2.07	0.70
4:D:37:ARG:CG	4:D:38:PRO:HD2	2.21	0.70
4:D:326:LYS:C	4:D:327:ILE:HD12	2.12	0.70
4:E:33:SER:C	4:E:34:ILE:HG12	2.12	0.70
1:A:128:PRO:CB	1:A:132:LEU:HD21	2.19	0.70
1:A:220:ASP:HA	1:A:223:ILE:HG13	1.72	0.70
3:C:180:ILE:HD12	3:C:181:ASN:N	2.06	0.70
4:D:8:LEU:HD13	4:D:90:PHE:CE1	2.26	0.70
4:D:8:LEU:O	4:D:103:THR:HG23	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:357:ILE:HG13	4:E:370:VAL:HG23	1.74	0.70
1:A:443:THR:HA	1:A:446:ASN:HD22	1.55	0.69
1:A:822:ILE:CD1	2:B:132:PHE:HE2	2.05	0.69
3:C:91:LYS:HB2	3:C:95:ASN:HB3	1.73	0.69
4:D:185:LEU:CD1	4:D:261:LEU:HD21	2.11	0.69
4:D:220:ALA:HB1	4:D:226:GLU:HG3	1.74	0.69
4:E:34:ILE:CG2	4:E:67:LEU:HB3	2.22	0.69
4:D:143:TYR:CD2	4:D:346:LEU:HD13	2.27	0.69
4:E:35:VAL:HG12	4:E:68:LYS:CB	2.22	0.69
4:E:132:MET:O	4:E:357:ILE:HB	1.92	0.69
1:A:176:LEU:HD11	1:A:673:PHE:CG	2.27	0.69
1:A:296:LYS:HB3	1:A:331:LEU:CD2	2.22	0.69
1:A:485:GLU:HA	1:A:584:TYR:CE1	2.27	0.69
1:A:822:ILE:HD11	2:B:132:PHE:HE2	1.57	0.69
1:A:287:ILE:HD12	1:A:288:PHE:H	1.55	0.69
1:A:405:ARG:H	1:A:606:THR:HG21	1.57	0.69
1:A:90:ASP:HA	1:A:118:TYR:O	1.93	0.69
1:A:210:GLN:HG3	1:A:211:PRO:CD	2.23	0.69
1:A:583:HIS:C	1:A:585:ALA:HB3	2.13	0.69
1:A:800:LEU:CD1	3:C:162:LYS:HG2	2.23	0.69
3:C:45:PHE:O	3:C:48:GLU:HG2	1.91	0.69
1:A:293:SER:OG	1:A:328:SER:HA	1.91	0.69
4:D:61:LYS:O	4:D:64:ILE:HG22	1.92	0.69
2:B:108:LEU:HD21	2:B:124:LEU:HD23	1.75	0.69
3:C:111:PHE:O	3:C:115:LEU:HB3	1.92	0.69
4:D:212:ILE:CG2	4:D:216:LEU:HD12	2.20	0.69
1:A:103:LEU:HD11	1:A:107:LYS:HD3	1.75	0.69
1:A:272:LYS:HD3	1:A:431:LYS:CB	2.20	0.69
1:A:283:ARG:HD3	1:A:322:VAL:HG23	1.74	0.69
1:A:292:MET:CE	1:A:309:PRO:HB3	2.21	0.69
1:A:358:VAL:CG2	1:A:430:ALA:HA	2.20	0.69
1:A:567:LYS:HD3	1:A:578:HIS:O	1.93	0.69
1:A:760:TYR:HE2	1:A:762:PHE:CE1	2.11	0.69
4:E:310:ALA:HB1	4:E:329:ILE:HG21	1.73	0.69
1:A:380:THR:CG2	1:A:398:LEU:HD11	2.22	0.69
1:A:380:THR:OG1	1:A:398:LEU:HD11	1.93	0.69
4:D:34:ILE:CG2	4:D:67:LEU:HB3	2.22	0.69
1:A:235:ALA:HA	1:A:286:HIS:CE1	2.28	0.69
1:A:337:ALA:O	1:A:340:ILE:HG22	1.93	0.69
1:A:344:SER:O	1:A:347:GLU:HG3	1.92	0.69
1:A:404:PRO:HB2	1:A:414:THR:OG1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:HG11	1:A:414:THR:HG21	1.74	0.69
1:A:485:GLU:HG2	1:A:584:TYR:HE1	1.58	0.69
1:A:814:SER:HB2	2:B:104:ALA:O	1.92	0.69
4:D:116:ARG:HD3	4:D:370:VAL:HG13	1.75	0.69
1:A:793:GLN:HE22	3:C:156:THR:H	1.39	0.68
3:C:80:LEU:HD22	3:C:187:LYS:HZ3	1.57	0.68
1:A:99:GLU:CA	1:A:102:VAL:HG13	2.22	0.68
1:A:603:LEU:HG	1:A:648:PHE:CG	2.27	0.68
3:C:42:LYS:NZ	3:C:47:LYS:HB2	2.07	0.68
1:A:295:LYS:HB3	1:A:331:LEU:HD13	1.74	0.68
1:A:665:ASN:O	1:A:668:SER:HB2	1.93	0.68
1:A:750:LEU:O	1:A:753:ILE:HB	1.94	0.68
3:C:87:ALA:HB1	3:C:94:GLY:CA	2.24	0.68
3:C:148:ALA:HA	3:C:163:GLU:CD	2.13	0.68
4:E:180:LEU:HD12	4:E:181:ALA:N	2.08	0.68
1:A:478:LEU:HB2	1:A:590:TYR:CE1	2.27	0.68
2:B:52:ARG:HG2	2:B:68:LEU:CD2	2.23	0.68
4:D:39:ARG:CG	4:D:66:THR:HG22	2.24	0.68
1:A:113:TRP:CZ3	1:A:130:LYS:HE2	2.27	0.68
1:A:253:HIS:CB	1:A:455:ARG:HD2	2.23	0.68
1:A:269:LEU:O	1:A:269:LEU:HD13	1.93	0.68
1:A:383:ALA:O	1:A:386:ALA:HB3	1.93	0.68
3:C:66:SER:HB2	3:C:68:ILE:HG22	1.74	0.68
3:C:71:SER:O	3:C:75:ASP:HB3	1.93	0.68
4:D:282:ILE:HG22	4:D:290:ARG:HD3	1.75	0.68
1:A:21:GLU:HG2	1:A:22:LYS:N	2.07	0.68
1:A:528:LYS:HB2	1:A:529:PRO:HD2	1.75	0.68
2:B:28:ILE:HG22	2:B:85:LEU:HD21	1.75	0.68
4:D:158:GLY:CA	4:D:181:ALA:HB3	2.23	0.68
1:A:404:PRO:HB3	1:A:606:THR:CB	2.24	0.68
1:A:708:ILE:O	1:A:711:LYS:HB2	1.93	0.68
1:A:740:ILE:HG22	1:A:745:ALA:HB2	1.74	0.68
3:C:188:HIS:O	3:C:189:ILE:HG23	1.93	0.68
4:E:16:LEU:HB2	4:E:18:LYS:NZ	2.08	0.68
1:A:368:GLN:HG3	1:A:376:GLU:CB	2.23	0.68
1:A:423:THR:O	1:A:426:VAL:HG22	1.93	0.68
3:C:42:LYS:HD2	3:C:47:LYS:N	2.09	0.68
3:C:151:ARG:HD2	3:C:163:GLU:OE2	1.94	0.68
4:E:332:PRO:HG2	4:E:335:ARG:NE	2.09	0.68
1:A:116:TYR:CE1	1:A:125:THR:HB	2.29	0.68
1:A:295:LYS:HB3	1:A:331:LEU:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLU:OE1	1:A:373:GLU:HA	1.94	0.68
1:A:578:HIS:NE2	1:A:592:ILE:HG12	2.09	0.68
4:D:227:MET:SD	4:D:255:PHE:HE1	2.17	0.68
4:E:113:LYS:HB3	4:E:371:HIS:NE2	2.08	0.68
3:C:167:GLU:HA	3:C:182:TYR:HE1	1.57	0.68
4:D:299:MET:HE1	4:D:309:ILE:HG21	1.74	0.68
4:E:73:HIC:HA	4:E:183:ARG:HH12	1.59	0.68
4:E:233:SER:OG	4:E:236:LEU:HG	1.94	0.68
1:A:170:ARG:CZ	1:A:256:ALA:HB1	2.24	0.67
1:A:760:TYR:HE2	1:A:762:PHE:HE1	1.42	0.67
2:B:108:LEU:O	2:B:110:PRO:HD3	1.94	0.67
3:C:46:SER:H	3:C:49:GLN:H	1.40	0.67
3:C:68:ILE:HD11	3:C:95:ASN:O	1.94	0.67
4:D:212:ILE:HG23	4:D:216:LEU:CD1	2.18	0.67
1:A:701:GLY:O	1:A:704:GLU:HB3	1.93	0.67
1:A:793:GLN:NE2	3:C:156:THR:H	1.91	0.67
1:A:837:PHE:O	1:A:840:ILE:HG12	1.93	0.67
3:C:54:LYS:HE3	3:C:54:LYS:CA	2.11	0.67
3:C:167:GLU:HA	3:C:182:TYR:CE1	2.28	0.67
4:D:36:GLY:HA3	4:D:66:THR:O	1.94	0.67
4:E:190:MET:HE2	4:E:206:ARG:HA	1.75	0.67
1:A:515:PHE:CD1	1:A:711:LYS:HE3	2.29	0.67
1:A:88:ILE:HG22	1:A:105:ASN:OD1	1.94	0.67
1:A:417:GLN:HA	1:A:421:GLN:CD	2.14	0.67
1:A:418:ASN:H	1:A:421:GLN:CG	2.05	0.67
1:A:445:ILE:HG12	1:A:449:LEU:HD12	1.76	0.67
2:B:146:PRO:HG3	2:B:156:ASN:OD1	1.93	0.67
2:B:160:VAL:HG23	2:B:165:ASP:CB	2.25	0.67
3:C:62:ARG:HH11	3:C:62:ARG:CB	2.08	0.67
1:A:238:VAL:HA	1:A:281:SER:O	1.95	0.67
1:A:272:LYS:CB	1:A:431:LYS:HD2	2.24	0.67
1:A:364:MET:HG3	1:A:382:VAL:HB	1.74	0.67
1:A:9:ILE:HG21	1:A:21:GLU:N	2.10	0.67
1:A:12:GLU:C	1:A:15:PRO:HD2	2.14	0.67
1:A:17:LEU:HB3	1:A:152:PRO:CG	2.10	0.67
2:B:125:LEU:HD22	2:B:132:PHE:CE1	2.29	0.67
4:D:58:ALA:CB	4:D:65:LEU:HD22	2.25	0.67
4:D:257:CYS:HB3	4:D:258:PRO:HD3	1.76	0.67
1:A:81:ASN:OD1	1:A:95:THR:HG22	1.95	0.67
1:A:462:LEU:HD13	1:A:463:ASP:H	1.60	0.67
1:A:221:GLN:NE2	1:A:449:LEU:HD23	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:22:ALA:CB	4:D:348:SER:HB3	2.25	0.67
4:D:102:PRO:HB3	4:D:131:ALA:HB3	1.75	0.67
4:D:189:LEU:HD12	4:D:192:ILE:HD11	1.76	0.67
1:A:564:ASN:CA	1:A:582:VAL:HG11	2.19	0.67
1:A:729:LEU:CD2	1:A:781:ARG:HA	2.25	0.67
3:C:127:TYR:CE2	3:C:187:LYS:HG2	2.30	0.67
4:D:133:TYR:HB2	4:D:356:TRP:CE3	2.30	0.67
1:A:226:ASN:HB2	1:A:227:PRO:HD3	1.77	0.66
1:A:253:HIS:HA	1:A:458:PHE:CB	2.25	0.66
2:B:70:ALA:HA	2:B:73:LYS:CD	2.25	0.66
3:C:86:ASN:CB	3:C:91:LYS:HD3	2.24	0.66
4:E:143:TYR:HE2	4:E:346:LEU:HB2	1.60	0.66
1:A:13:ALA:HA	1:A:139:VAL:HG22	1.77	0.66
1:A:49:LYS:HD3	1:A:65:LEU:CD2	2.25	0.66
3:C:135:ARG:HD3	3:C:139:LYS:N	2.10	0.66
1:A:56:GLU:O	1:A:59:LYS:HD3	1.95	0.66
3:C:68:ILE:CD1	3:C:95:ASN:HB2	2.20	0.66
1:A:296:LYS:HB2	1:A:299:LEU:HD12	1.76	0.66
1:A:645:GLY:CA	4:D:23:GLY:HA2	2.25	0.66
1:A:719:TYR:OH	1:A:762:PHE:HA	1.96	0.66
3:C:127:TYR:CD2	3:C:187:LYS:HG2	2.30	0.66
4:D:142:LEU:HD11	4:D:165:ILE:CD1	2.20	0.66
4:D:287:ILE:CB	4:E:244:ASP:HB3	2.24	0.66
1:A:485:GLU:OE2	1:A:583:HIS:HB3	1.94	0.66
1:A:551:LYS:CD	1:A:555:TYR:HE2	2.08	0.66
1:A:557:GLN:O	1:A:561:LYS:HE2	1.94	0.66
3:C:135:ARG:HH11	3:C:141:GLY:H	1.42	0.66
3:C:91:LYS:HB2	3:C:95:ASN:CB	2.24	0.66
1:A:392:LEU:CD1	1:A:613:LYS:HB2	2.26	0.66
2:B:124:LEU:HA	2:B:128:GLN:OE1	1.95	0.66
3:C:127:TYR:O	3:C:130:PHE:HB3	1.95	0.66
4:D:357:ILE:HG12	4:D:370:VAL:CG2	2.21	0.66
1:A:5:ALA:HB1	1:A:18:ARG:NH2	2.11	0.66
1:A:39:PHE:CG	1:A:100:PRO:HG2	2.30	0.66
1:A:526:ILE:HD11	1:A:583:HIS:CE1	2.30	0.66
3:C:71:SER:HB2	3:C:91:LYS:HZ2	1.60	0.66
3:C:140:GLU:HB3	3:C:180:ILE:CD1	2.25	0.66
1:A:85:PHE:CD1	1:A:94:MET:HA	2.31	0.66
1:A:110:TYR:OH	1:A:128:PRO:HA	1.96	0.66
1:A:207:LYS:HE3	1:A:259:LYS:HB2	1.78	0.66
1:A:418:ASN:OD1	1:A:421:GLN:HB3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:LEU:HA	1:A:595:TRP:CZ3	2.30	0.66
1:A:651:VAL:O	1:A:654:VAL:HG22	1.96	0.66
1:A:836:LEU:O	1:A:840:ILE:HG23	1.96	0.66
2:B:96:ASP:HB2	2:B:97:PRO:HD2	1.77	0.66
4:D:236:LEU:HB2	4:D:251:GLY:HA3	1.76	0.66
1:A:207:LYS:HD3	1:A:259:LYS:HG3	1.78	0.66
1:A:256:ALA:CA	1:A:456:GLN:HB2	2.25	0.66
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.26	0.66
2:B:58:MET:HE3	2:B:60:ARG:HB2	1.77	0.66
4:D:328:LYS:HD3	4:D:330:ILE:HD11	1.77	0.66
1:A:256:ALA:H	1:A:456:GLN:HG3	1.60	0.65
3:C:135:ARG:HD3	3:C:140:GLU:H	1.61	0.65
4:D:116:ARG:HD3	4:D:370:VAL:CG1	2.27	0.65
1:A:13:ALA:HB2	1:A:139:VAL:HG22	1.78	0.65
1:A:118:TYR:CE2	1:A:153:PRO:HG3	2.31	0.65
1:A:205:LYS:CD	1:A:257:THR:HG21	2.25	0.65
3:C:58:LEU:CD1	3:C:65:ASP:HB2	2.25	0.65
1:A:380:THR:HG23	1:A:383:ALA:HB3	1.77	0.65
1:A:492:ASN:HB3	1:A:516:GLY:N	2.12	0.65
4:D:297:ASN:CB	4:D:329:ILE:HD13	2.25	0.65
4:E:32:PRO:HG3	4:E:59:GLN:NE2	2.12	0.65
1:A:12:GLU:O	1:A:15:PRO:HD2	1.96	0.65
1:A:104:TYR:CE1	1:A:108:GLU:HG3	2.30	0.65
1:A:253:HIS:HA	1:A:458:PHE:HB3	1.79	0.65
1:A:475:LEU:HD13	1:A:595:TRP:CE3	2.31	0.65
1:A:566:GLN:HG2	1:A:567:LYS:H	1.61	0.65
3:C:118:ILE:HG13	3:C:119:SER:OG	1.97	0.65
4:E:123:MET:HG3	4:E:132:MET:HE2	1.77	0.65
1:A:510:TRP:NE1	1:A:512:PHE:HB2	2.12	0.65
4:D:34:ILE:HA	4:D:68:LYS:O	1.97	0.65
1:A:5:ALA:HB1	1:A:18:ARG:HH12	1.61	0.65
1:A:173:GLN:O	1:A:459:ILE:HA	1.96	0.65
1:A:350:GLY:N	1:A:353:LYS:HG3	2.11	0.65
1:A:694:MET:CE	1:A:697:LEU:HD12	2.26	0.65
1:A:283:ARG:HD2	1:A:289:TYR:CD2	2.30	0.65
1:A:363:ASN:HB3	1:A:382:VAL:HG21	1.78	0.65
1:A:819:GLN:NE2	2:B:130:ASP:H	1.95	0.65
1:A:193:ILE:CG2	1:A:219:GLU:HB3	2.09	0.65
1:A:229:LEU:HD22	1:A:438:PHE:CE1	2.32	0.65
1:A:234:ASN:HD22	1:A:242:ASN:HD21	1.44	0.65
1:A:513:ILE:HG22	1:A:514:ASP:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:GLU:HA	1:A:527:GLU:HG2	1.79	0.65
4:D:42:GLY:O	4:D:43:VAL:HG12	1.97	0.65
4:D:101:HIS:O	4:D:129:VAL:HG12	1.96	0.65
4:D:134:VAL:O	4:D:375:PHE:HB3	1.95	0.65
4:E:153:LEU:HD11	4:E:274:ILE:HG21	1.78	0.65
1:A:27:ALA:HB1	1:A:87:LYS:HE2	1.79	0.65
1:A:261:ALA:HB3	1:A:455:ARG:NE	2.12	0.65
1:A:406:VAL:HG22	1:A:412:TYR:O	1.97	0.65
1:A:831:TRP:HE3	1:A:834:MET:CG	2.05	0.65
1:A:107:LYS:HA	1:A:688:MET:SD	2.37	0.65
1:A:799:TYR:HA	1:A:802:ARG:HH22	1.60	0.65
4:D:187:ASP:O	4:D:190:MET:HB2	1.97	0.65
4:D:341:ILE:O	4:D:344:SER:HB3	1.97	0.65
4:E:35:VAL:CG2	4:E:52:SER:HB2	2.25	0.65
1:A:39:PHE:CG	1:A:100:PRO:HB2	2.32	0.64
1:A:564:ASN:HA	1:A:582:VAL:CG1	2.19	0.64
3:C:150:LEU:O	3:C:154:LEU:HB2	1.95	0.64
3:C:170:MET:CE	3:C:186:VAL:HA	2.27	0.64
4:E:18:LYS:HD3	4:E:18:LYS:N	2.12	0.64
1:A:107:LYS:HD2	1:A:688:MET:CG	2.27	0.64
1:A:702:VAL:O	1:A:705:GLY:HA3	1.97	0.64
1:A:719:TYR:CZ	1:A:767:VAL:HB	2.32	0.64
3:C:68:ILE:HD12	3:C:95:ASN:CB	2.18	0.64
3:C:180:ILE:HA	3:C:183:GLU:CG	2.27	0.64
4:E:34:ILE:HD13	4:E:69:TYR:CE2	2.32	0.64
1:A:825:PHE:O	1:A:828:VAL:HG13	1.97	0.64
2:B:113:LYS:O	2:B:115:THR:HG23	1.97	0.64
1:A:238:VAL:N	1:A:282:GLU:HG3	2.12	0.64
1:A:255:GLY:HA3	1:A:259:LYS:HG2	1.79	0.64
1:A:811:ARG:CG	1:A:815:ILE:HD11	2.23	0.64
3:C:161:MET:O	3:C:165:GLU:HG2	1.98	0.64
1:A:39:PHE:HE1	1:A:49:LYS:CG	2.10	0.64
1:A:40:ALA:HB1	1:A:72:LEU:HD22	1.78	0.64
1:A:408:VAL:HG22	1:A:410:ASN:H	1.61	0.64
1:A:713:PHE:CD2	1:A:770:LYS:HD3	2.32	0.64
1:A:769:PHE:CD2	1:A:774:LEU:HD21	2.33	0.64
3:C:131:VAL:HG13	3:C:179:CYS:SG	2.37	0.64
4:D:189:LEU:CD2	4:D:209:VAL:HG13	2.26	0.64
4:E:102:PRO:CB	4:E:131:ALA:HB3	2.18	0.64
1:A:644:LYS:HG3	1:A:649:GLN:HA	1.80	0.64
1:A:787:THR:O	1:A:790:THR:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:THR:CG2	1:A:791:ARG:HD2	2.28	0.64
3:C:68:ILE:HG13	3:C:95:ASN:OD1	1.97	0.64
3:C:70:LEU:HD12	3:C:86:ASN:HD22	1.63	0.64
1:A:111:ALA:HA	1:A:686:GLY:CA	2.28	0.64
1:A:198:THR:O	1:A:201:VAL:HG23	1.98	0.64
1:A:407:LYS:HA	1:A:411:GLU:HA	1.79	0.64
1:A:551:LYS:HD2	1:A:555:TYR:CE2	2.31	0.64
3:C:131:VAL:HG13	3:C:179:CYS:HB2	1.78	0.64
4:D:65:LEU:HD13	4:D:67:LEU:HD21	1.78	0.64
4:D:218:TYR:O	4:D:255:PHE:HA	1.98	0.64
4:E:149:THR:HG22	4:E:150:GLY:N	2.12	0.64
1:A:99:GLU:O	1:A:102:VAL:HG22	1.98	0.64
1:A:207:LYS:HE2	1:A:453:GLN:CB	2.23	0.64
1:A:430:ALA:O	1:A:433:VAL:HG12	1.97	0.64
3:C:66:SER:HB3	3:C:68:ILE:HG22	1.80	0.64
4:E:178:LEU:CD2	4:E:180:LEU:HB3	2.27	0.64
4:E:294:TYR:CE1	4:E:321:ALA:HB2	2.33	0.64
1:A:40:ALA:HB1	1:A:72:LEU:HD21	1.80	0.64
1:A:295:LYS:HG2	1:A:332:LEU:N	2.12	0.64
3:C:131:VAL:CG1	3:C:179:CYS:HB2	2.27	0.64
1:A:261:ALA:HB3	1:A:455:ARG:CD	2.28	0.64
3:C:42:LYS:CE	3:C:113:PRO:HG3	2.28	0.64
1:A:93:MET:HA	1:A:93:MET:CE	2.28	0.63
1:A:271:GLU:OE1	1:A:274:ARG:HG2	1.97	0.63
3:C:67:LYS:HD3	3:C:92:VAL:HG13	1.78	0.63
4:D:91:TYR:O	4:D:95:ARG:HA	1.99	0.63
1:A:20:PRO:HD2	1:A:23:GLU:OE1	1.99	0.63
1:A:65:LEU:HD12	1:A:65:LEU:O	1.98	0.63
1:A:126:VAL:O	1:A:128:PRO:HD3	1.98	0.63
1:A:795:LEU:HD23	3:C:80:LEU:HD21	1.79	0.63
2:B:39:ASP:HA	2:B:50:ASP:OD2	1.98	0.63
1:A:19:LYS:CD	1:A:23:GLU:HB3	2.28	0.63
1:A:567:LYS:HG3	1:A:568:PRO:O	1.99	0.63
3:C:163:GLU:HG3	3:C:167:GLU:OE2	1.99	0.63
4:D:35:VAL:HG22	4:D:52:SER:HB2	1.80	0.63
4:E:310:ALA:HB1	4:E:329:ILE:CG2	2.28	0.63
1:A:47:TYR:HE2	1:A:78:PHE:CZ	2.17	0.63
1:A:406:VAL:HB	1:A:605:GLU:CD	2.18	0.63
1:A:793:GLN:NE2	3:C:157:LEU:H	1.96	0.63
1:A:837:PHE:HA	1:A:840:ILE:HG12	1.80	0.63
3:C:62:ARG:HB3	3:C:62:ARG:NH1	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:38:PRO:HD3	4:D:49:GLN:HE22	1.62	0.63
4:D:43:VAL:HG13	4:D:44:MET:N	2.14	0.63
4:E:104:LEU:HB2	4:E:356:TRP:CH2	2.32	0.63
2:B:61:LEU:HA	2:B:62:ASN:HB3	1.81	0.63
4:D:255:PHE:O	4:D:258:PRO:HD2	1.99	0.63
1:A:64:THR:HG22	1:A:65:LEU:N	2.14	0.63
1:A:224:GLN:HB3	1:A:340:ILE:CD1	2.28	0.63
3:C:87:ALA:HB1	3:C:94:GLY:HA3	1.81	0.63
3:C:91:LYS:HB2	3:C:95:ASN:CG	2.18	0.63
4:D:104:LEU:HB2	4:D:356:TRP:CZ3	2.33	0.63
1:A:360:HIS:C	1:A:382:VAL:HG11	2.19	0.63
1:A:526:ILE:HD11	1:A:583:HIS:HE1	1.62	0.63
3:C:91:LYS:HE2	3:C:95:ASN:CG	2.19	0.63
4:D:194:THR:HA	4:D:198:TYR:O	1.98	0.63
1:A:12:GLU:OE2	1:A:15:PRO:HG2	1.98	0.63
1:A:838:PHE:CD1	2:B:164:GLY:HA3	2.34	0.63
2:B:83:VAL:O	2:B:86:THR:HG22	1.99	0.63
1:A:144:ARG:HH22	1:A:199:ILE:CD1	2.10	0.63
1:A:415:LYS:HG3	1:A:416:GLY:H	1.62	0.63
1:A:475:LEU:HD22	1:A:595:TRP:HB3	1.81	0.63
1:A:588:VAL:HG11	1:A:590:TYR:CZ	2.34	0.63
1:A:797:ARG:CZ	1:A:797:ARG:HB2	2.29	0.63
2:B:147:ASP:HB3	2:B:152:VAL:HA	1.81	0.63
4:E:178:LEU:HG	4:E:180:LEU:N	2.14	0.63
1:A:47:TYR:HE2	1:A:78:PHE:CE1	2.17	0.62
1:A:349:VAL:HG22	1:A:353:LYS:HE3	1.81	0.62
2:B:102:THR:O	2:B:105:PHE:HB2	1.98	0.62
4:E:50:LYS:HG3	4:E:53:TYR:CE2	2.34	0.62
4:E:158:GLY:HA2	4:E:181:ALA:HB3	1.80	0.62
1:A:583:HIS:HB2	1:A:585:ALA:CB	2.29	0.62
1:A:833:TRP:HE1	2:B:71:MET:HG2	1.63	0.62
4:D:58:ALA:O	4:D:65:LEU:HD21	1.97	0.62
4:D:189:LEU:HA	4:D:192:ILE:CD1	2.28	0.62
4:E:120:THR:CB	4:E:367:PRO:HB3	2.23	0.62
1:A:207:LYS:HD3	1:A:259:LYS:CG	2.28	0.62
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.80	0.62
2:B:138:LYS:HA	2:B:141:TRP:HD1	1.63	0.62
3:C:70:LEU:HB3	3:C:91:LYS:HD2	1.80	0.62
4:E:43:VAL:HG13	4:E:44:MET:N	2.13	0.62
4:E:61:LYS:O	4:E:64:ILE:HG22	1.99	0.62
1:A:81:ASN:HD22	1:A:94:MET:HE3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASP:OD1	1:A:119:SER:HA	1.99	0.62
1:A:115:ILE:HD13	1:A:116:TYR:CE2	2.35	0.62
4:E:155:SER:HB3	4:E:160:THR:CG2	2.30	0.62
4:E:257:CYS:HB3	4:E:258:PRO:HD3	1.81	0.62
1:A:519:LEU:CD2	1:A:584:TYR:HB3	2.28	0.62
1:A:546:THR:HG23	1:A:547:ASP:N	2.13	0.62
3:C:128:GLU:HA	3:C:183:GLU:OE1	1.99	0.62
1:A:368:GLN:HG3	1:A:376:GLU:HB3	1.82	0.62
1:A:424:ASN:ND2	1:A:602:PRO:HD2	2.14	0.62
1:A:488:GLN:HG3	1:A:584:TYR:CE2	2.35	0.62
3:C:67:LYS:HD2	3:C:101:MET:HB2	1.80	0.62
4:D:111:ASN:ND2	4:D:115:ASN:HB3	2.14	0.62
4:E:16:LEU:HB2	4:E:18:LYS:HZ2	1.64	0.62
4:E:39:ARG:HE	4:E:66:THR:CA	2.13	0.62
1:A:107:LYS:HD2	1:A:688:MET:HB2	1.82	0.62
1:A:210:GLN:HG3	1:A:211:PRO:HD2	1.80	0.62
1:A:722:PHE:CE1	1:A:726:TYR:HD2	2.17	0.62
1:A:81:ASN:ND2	1:A:94:MET:HB3	2.15	0.62
1:A:364:MET:HG3	1:A:382:VAL:CG2	2.29	0.62
3:C:127:TYR:CE2	3:C:187:LYS:HE2	2.32	0.62
3:C:128:GLU:HG3	3:C:180:ILE:CG2	2.29	0.62
1:A:264:ASP:C	1:A:265:ILE:HD12	2.20	0.62
1:A:795:LEU:HD23	3:C:187:LYS:NZ	2.14	0.62
3:C:67:LYS:HD2	3:C:92:VAL:HG13	1.81	0.62
4:D:99:GLU:HA	4:D:128:ASN:O	2.00	0.62
1:A:779:GLU:O	1:A:782:ASP:HB2	1.99	0.61
2:B:27:GLN:O	2:B:30:GLU:HB3	2.00	0.61
2:B:81:PHE:O	2:B:84:PHE:HB3	1.99	0.61
1:A:98:HIS:O	1:A:101:ALA:HB3	1.99	0.61
1:A:176:LEU:HD12	1:A:673:PHE:HA	1.80	0.61
1:A:289:TYR:HA	1:A:292:MET:HE2	1.81	0.61
1:A:799:TYR:HE1	3:C:169:LEU:HD12	1.64	0.61
2:B:93:LYS:HG2	2:B:94:GLY:N	2.14	0.61
4:D:208:ILE:HG22	4:D:209:VAL:N	2.15	0.61
4:D:321:ALA:HB1	4:D:322:PRO:CD	2.30	0.61
4:D:334:GLU:HA	4:D:334:GLU:OE2	1.99	0.61
1:A:1:MET:C	1:A:2:SER:O	2.38	0.61
1:A:193:ILE:HD13	1:A:219:GLU:HB3	1.82	0.61
1:A:295:LYS:CG	1:A:331:LEU:HD22	2.28	0.61
1:A:729:LEU:HD22	1:A:781:ARG:HA	1.81	0.61
1:A:804:GLU:HB3	1:A:808:MET:CE	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:39:ARG:HE	4:D:66:THR:CA	2.09	0.61
4:D:299:MET:HE1	4:D:309:ILE:CG2	2.30	0.61
4:E:362:TYR:HE1	4:E:367:PRO:CG	2.13	0.61
1:A:42:ASP:CB	1:A:48:VAL:HG23	2.28	0.61
1:A:91:MET:HE1	1:A:105:ASN:HB3	1.82	0.61
1:A:166:MET:HE3	1:A:254:PHE:CB	2.30	0.61
1:A:639:LYS:NZ	4:D:4:GLU:HB3	2.14	0.61
3:C:70:LEU:HB3	3:C:91:LYS:HE3	1.82	0.61
4:D:250:ILE:HG12	4:D:251:GLY:N	2.14	0.61
4:E:210:ARG:HG2	4:E:210:ARG:HH11	1.65	0.61
1:A:166:MET:O	1:A:170:ARG:HA	2.01	0.61
1:A:715:SER:HB3	1:A:774:LEU:HD11	1.81	0.61
1:A:39:PHE:HD1	1:A:49:LYS:HA	1.66	0.61
1:A:220:ASP:O	1:A:223:ILE:HG13	2.01	0.61
1:A:607:VAL:HG12	1:A:611:TYR:CD1	2.36	0.61
4:D:299:MET:CE	4:D:309:ILE:HG21	2.31	0.61
1:A:59:LYS:HD3	1:A:59:LYS:O	2.01	0.61
1:A:167:LEU:HD23	1:A:167:LEU:N	2.14	0.61
1:A:348:LYS:O	1:A:351:ILE:HG22	2.00	0.61
1:A:789:MET:HE2	3:C:130:PHE:CZ	2.36	0.61
3:C:47:LYS:HG2	3:C:48:GLU:N	2.15	0.61
3:C:91:LYS:C	3:C:95:ASN:HB3	2.20	0.61
4:D:37:ARG:HG2	4:D:38:PRO:CD	2.30	0.61
4:E:180:LEU:HD21	4:E:261:LEU:HD23	1.83	0.61
1:A:703:LEU:O	1:A:706:ILE:HB	2.01	0.61
3:C:42:LYS:HG3	3:C:46:SER:HB3	1.83	0.61
4:D:158:GLY:HA3	4:D:183:ARG:NE	2.16	0.61
4:E:236:LEU:HD13	4:E:251:GLY:HA3	1.82	0.61
1:A:54:SER:O	1:A:60:VAL:HG13	2.00	0.61
1:A:161:ASN:HA	1:A:164:GLN:OE1	2.01	0.61
1:A:163:TYR:CE2	1:A:199:ILE:CG2	2.83	0.61
1:A:194:GLN:O	1:A:197:ALA:HB3	2.01	0.61
1:A:519:LEU:HD13	1:A:584:TYR:HB3	1.82	0.61
1:A:578:HIS:NE2	1:A:591:ASN:HA	2.16	0.61
2:B:96:ASP:HB2	2:B:100:VAL:HG11	1.82	0.61
3:C:47:LYS:HE3	3:C:109:GLU:OE2	2.01	0.61
1:A:154:HIS:CD2	1:A:156:PHE:HD2	2.18	0.61
1:A:360:HIS:O	1:A:382:VAL:HG11	2.01	0.61
1:A:474:SER:HA	1:A:595:TRP:HZ2	1.66	0.61
3:C:70:LEU:HD12	3:C:86:ASN:ND2	2.16	0.61
3:C:166:VAL:HG23	3:C:167:GLU:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:259:GLU:HG3	4:D:263:GLN:HG3	1.81	0.61
4:D:365:ALA:HB3	4:D:369:ILE:HB	1.82	0.61
1:A:154:HIS:NE2	1:A:156:PHE:HD2	1.99	0.60
1:A:832:PRO:O	1:A:836:LEU:HG	2.00	0.60
3:C:157:LEU:O	3:C:157:LEU:HD22	2.01	0.60
4:E:189:LEU:HD13	4:E:192:ILE:HD11	1.82	0.60
1:A:13:ALA:CA	1:A:139:VAL:HG22	2.31	0.60
1:A:406:VAL:HG11	1:A:414:THR:CG2	2.31	0.60
1:A:415:LYS:HB2	4:D:333:PRO:HG2	1.82	0.60
4:D:34:ILE:C	4:D:54:VAL:HG11	2.21	0.60
4:D:116:ARG:HD2	4:D:371:HIS:ND1	2.16	0.60
1:A:303:LEU:HD22	1:A:305:ILE:HG12	1.81	0.60
1:A:475:LEU:HA	1:A:595:TRP:CH2	2.36	0.60
1:A:717:ILE:HG22	1:A:718:LEU:N	2.16	0.60
2:B:96:ASP:OD1	2:B:101:ILE:HG13	2.00	0.60
4:D:144:ALA:HB2	4:D:342:GLY:H	1.67	0.60
4:D:160:THR:HB	4:D:178:LEU:HB3	1.82	0.60
4:E:136:ILE:HB	4:E:139:VAL:HB	1.83	0.60
1:A:91:MET:SD	1:A:106:LEU:HD11	2.41	0.60
1:A:115:ILE:O	1:A:126:VAL:HG22	2.01	0.60
1:A:149:GLN:HG2	1:A:150:GLU:N	2.15	0.60
1:A:428:ALA:HA	1:A:431:LYS:CE	2.32	0.60
2:B:108:LEU:HD21	2:B:124:LEU:CD2	2.31	0.60
2:B:147:ASP:HB2	2:B:151:ASN:O	2.02	0.60
3:C:116:GLN:HG2	3:C:117:ALA:HA	1.82	0.60
1:A:45:GLU:O	1:A:46:MET:HB2	1.99	0.60
4:D:200:PHE:HA	4:D:205:GLU:OE1	2.00	0.60
1:A:24:ARG:HH22	1:A:28:GLN:HB3	1.66	0.60
1:A:224:GLN:HB3	1:A:340:ILE:HD13	1.82	0.60
3:C:58:LEU:HD12	3:C:65:ASP:OD2	2.01	0.60
4:D:3:ASP:O	4:D:4:GLU:HB2	2.01	0.60
4:D:158:GLY:CA	4:D:183:ARG:HD2	2.31	0.60
1:A:360:HIS:CB	1:A:382:VAL:HG13	2.20	0.60
1:A:525:LEU:HD11	1:A:558:HIS:CE1	2.36	0.60
1:A:535:ILE:HD12	1:A:557:GLN:HE22	1.66	0.60
2:B:51:LEU:CB	2:B:68:LEU:HD11	2.30	0.60
2:B:137:ILE:CD1	2:B:141:TRP:HE1	2.12	0.60
4:D:133:TYR:OH	4:D:375:PHE:HB2	2.02	0.60
4:D:300:SER:HA	4:D:335:ARG:HG3	1.82	0.60
1:A:295:LYS:HG2	1:A:332:LEU:HA	1.82	0.60
1:A:424:ASN:HD21	1:A:600:LYS:HG2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:THR:C	1:A:452:LYS:HE2	2.22	0.60
1:A:814:SER:O	1:A:818:ILE:HG12	2.01	0.60
3:C:68:ILE:HD13	3:C:97:SER:O	2.02	0.60
4:E:35:VAL:HG22	4:E:52:SER:CB	2.27	0.60
4:E:236:LEU:HD12	4:E:237:GLU:CG	2.32	0.60
4:E:257:CYS:CB	4:E:258:PRO:HD3	2.31	0.60
1:A:56:GLU:HG2	1:A:57:ASN:HB2	1.84	0.60
1:A:166:MET:SD	1:A:254:PHE:HB2	2.42	0.60
1:A:368:GLN:HG3	1:A:376:GLU:HB2	1.84	0.60
4:E:103:THR:HG21	4:E:105:LEU:HD21	1.83	0.60
4:E:106:THR:HG22	4:E:140:LEU:HD11	1.83	0.60
4:E:106:THR:CG2	4:E:140:LEU:HD11	2.32	0.60
4:E:180:LEU:CD2	4:E:261:LEU:HD23	2.32	0.60
1:A:254:PHE:O	1:A:455:ARG:HB2	2.01	0.60
1:A:726:TYR:O	1:A:729:LEU:HG	2.02	0.60
2:B:52:ARG:HG2	2:B:68:LEU:HD22	1.82	0.60
3:C:162:LYS:HB3	3:C:162:LYS:HZ3	1.67	0.60
3:C:183:GLU:HG3	3:C:184:ALA:N	2.16	0.60
4:D:22:ALA:HB1	4:D:348:SER:CB	2.29	0.60
1:A:659:LEU:HD11	1:A:663:MET:HE3	1.84	0.59
1:A:729:LEU:N	1:A:729:LEU:HD23	2.16	0.59
1:A:793:GLN:OE1	3:C:156:THR:HG22	2.02	0.59
1:A:831:TRP:CD1	1:A:832:PRO:HD2	2.37	0.59
1:A:833:TRP:CA	1:A:836:LEU:HD12	2.14	0.59
4:D:171:LEU:HD13	4:D:285:CYS:SG	2.43	0.59
4:E:99:GLU:HA	4:E:128:ASN:O	2.02	0.59
1:A:22:LYS:O	1:A:25:ILE:HG13	2.02	0.59
1:A:32:PHE:CE2	1:A:82:PRO:HA	2.37	0.59
1:A:42:ASP:HB2	1:A:48:VAL:CG2	2.32	0.59
1:A:103:LEU:HD11	1:A:688:MET:HB2	1.83	0.59
1:A:296:LYS:HD2	1:A:331:LEU:CD1	2.29	0.59
1:A:484:ASN:HA	1:A:487:LEU:HD12	1.85	0.59
1:A:821:ASN:O	1:A:824:ALA:HB3	2.03	0.59
2:B:58:MET:N	2:B:59:GLY:HA2	2.17	0.59
4:D:18:LYS:HA	4:D:29:ALA:O	2.02	0.59
4:D:358:THR:OG1	4:D:361:GLU:HG3	2.03	0.59
4:E:196:ARG:NH2	4:E:251:GLY:H	2.00	0.59
4:E:299:MET:SD	4:E:304:THR:HB	2.42	0.59
1:A:45:GLU:O	1:A:690:HIS:HB2	2.01	0.59
1:A:295:LYS:NZ	1:A:332:LEU:HA	2.05	0.59
3:C:185:PHE:O	3:C:188:HIS:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:157:ASP:HA	5:D:401:ADP:H4'	1.83	0.59
1:A:232:PHE:O	1:A:285:TYR:HB3	2.01	0.59
1:A:252:ILE:O	1:A:458:PHE:HB2	2.01	0.59
1:A:495:MET:HE1	1:A:708:ILE:HG21	1.81	0.59
1:A:535:ILE:HD12	1:A:557:GLN:OE1	2.03	0.59
3:C:67:LYS:HE2	3:C:67:LYS:CA	2.27	0.59
3:C:131:VAL:HG11	3:C:180:ILE:N	2.18	0.59
4:D:210:ARG:HG2	4:D:210:ARG:HH11	1.67	0.59
1:A:16:TYR:HB2	1:A:134:VAL:CG2	2.32	0.59
1:A:195:TYR:O	1:A:198:THR:HG22	2.03	0.59
1:A:234:ASN:N	1:A:245:ARG:HG2	2.17	0.59
3:C:142:ASN:H	3:C:177:ASN:H	1.48	0.59
4:D:18:LYS:HD3	4:D:18:LYS:N	2.17	0.59
4:E:39:ARG:HE	4:E:66:THR:HA	1.67	0.59
4:E:133:TYR:HB2	4:E:356:TRP:CE3	2.38	0.59
4:E:133:TYR:OH	4:E:375:PHE:HB2	2.02	0.59
4:E:216:LEU:HD13	4:E:250:ILE:HG21	1.84	0.59
1:A:109:ARG:HB3	1:A:114:MET:HB2	1.85	0.59
1:A:261:ALA:HB3	1:A:455:ARG:HE	1.67	0.59
1:A:351:ILE:O	1:A:355:THR:HG23	2.03	0.59
1:A:515:PHE:CE1	1:A:711:LYS:HE3	2.38	0.59
2:B:46:ILE:HG12	2:B:79:ILE:O	2.02	0.59
1:A:130:LYS:CE	1:A:132:LEU:HD11	2.33	0.59
1:A:296:LYS:HG3	1:A:300:ILE:HG23	1.85	0.59
1:A:361:TYR:HE1	1:A:386:ALA:CB	2.15	0.59
1:A:656:ARG:HG2	1:A:656:ARG:HH11	1.68	0.59
3:C:98:ASN:HB3	3:C:99:GLU:CA	2.33	0.59
3:C:135:ARG:O	3:C:136:VAL:HG12	2.02	0.59
4:E:287:ILE:HA	4:E:290:ARG:CD	2.33	0.59
1:A:59:LYS:HD2	1:A:59:LYS:H	1.67	0.59
1:A:207:LYS:CD	1:A:259:LYS:CB	2.76	0.59
4:D:210:ARG:HG2	4:D:210:ARG:NH1	2.18	0.59
4:D:357:ILE:HA	4:D:361:GLU:OE2	2.02	0.59
1:A:175:ILE:CD1	1:A:461:VAL:HG22	2.23	0.59
1:A:419:VAL:HG13	1:A:420:GLN:N	2.18	0.59
1:A:694:MET:HA	1:A:694:MET:CE	2.30	0.59
2:B:164:GLY:O	2:B:165:ASP:HB3	2.02	0.59
3:C:42:LYS:CA	3:C:43:ILE:HB	2.20	0.59
3:C:86:ASN:O	3:C:91:LYS:HG2	2.03	0.59
3:C:91:LYS:O	3:C:94:GLY:HA2	2.03	0.59
3:C:190:MET:O	3:C:190:MET:HE3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:TYR:CE2	1:A:683:LYS:HB3	2.38	0.58
1:A:792:THR:HA	3:C:127:TYR:HE1	1.67	0.58
2:B:50:ASP:HA	2:B:53:ASP:OD2	2.03	0.58
3:C:142:ASN:HB3	3:C:179:CYS:SG	2.43	0.58
4:E:120:THR:HB	4:E:367:PRO:CB	2.26	0.58
4:E:250:ILE:CD1	4:E:253:GLU:HB2	2.33	0.58
1:A:349:VAL:HG13	1:A:350:GLY:N	2.18	0.58
1:A:727:ARG:HH11	1:A:745:ALA:HB1	1.68	0.58
1:A:814:SER:HA	2:B:104:ALA:HB1	1.85	0.58
2:B:35:PHE:CE1	2:B:46:ILE:HG23	2.38	0.58
4:D:8:LEU:HB2	4:D:103:THR:OG1	2.03	0.58
4:D:99:GLU:O	4:D:130:PRO:HG3	2.03	0.58
1:A:115:ILE:CG2	1:A:128:PRO:HG3	2.32	0.58
1:A:228:LEU:O	1:A:228:LEU:HD13	2.03	0.58
1:A:406:VAL:HB	1:A:605:GLU:OE1	2.02	0.58
1:A:816:PHE:CD2	1:A:820:TYR:HE2	2.21	0.58
3:C:42:LYS:HD2	3:C:47:LYS:HA	1.82	0.58
3:C:180:ILE:CA	3:C:183:GLU:HG2	2.32	0.58
4:D:153:LEU:HD21	4:D:274:ILE:CD1	2.26	0.58
4:E:34:ILE:HA	4:E:68:LYS:O	2.02	0.58
4:E:372:ARG:HG2	4:E:372:ARG:HH11	1.67	0.58
1:A:158:ILE:HA	1:A:161:ASN:ND2	2.18	0.58
1:A:175:ILE:HD12	1:A:461:VAL:HG13	1.82	0.58
1:A:220:ASP:CA	1:A:223:ILE:HG13	2.33	0.58
1:A:255:GLY:N	1:A:455:ARG:HA	2.18	0.58
1:A:421:GLN:HE21	1:A:422:VAL:CG1	2.14	0.58
3:C:42:LYS:HE2	3:C:113:PRO:CG	2.32	0.58
3:C:115:LEU:O	3:C:115:LEU:HD22	2.03	0.58
1:A:302:LEU:HD23	1:A:353:LYS:HE3	1.86	0.58
1:A:811:ARG:O	1:A:815:ILE:HG13	2.03	0.58
2:B:26:THR:O	2:B:27:GLN:HB2	2.02	0.58
4:D:218:TYR:O	4:D:258:PRO:HG2	2.02	0.58
4:E:180:LEU:CD1	4:E:184:ASP:HB2	2.33	0.58
1:A:81:ASN:HD21	1:A:95:THR:N	2.01	0.58
1:A:137:PRO:HA	1:A:140:VAL:HG23	1.85	0.58
1:A:154:HIS:HD2	1:A:156:PHE:H	1.51	0.58
1:A:289:TYR:HA	1:A:292:MET:CE	2.33	0.58
1:A:348:LYS:HA	1:A:351:ILE:HG22	1.85	0.58
1:A:377:PRO:CG	1:A:398:LEU:HD22	2.31	0.58
1:A:380:THR:CG2	1:A:383:ALA:HB3	2.33	0.58
1:A:618:LEU:HG	1:A:622:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:LEU:HD23	1:A:678:ILE:O	2.04	0.58
1:A:839:LYS:HE2	2:B:60:ARG:HH12	1.68	0.58
3:C:42:LYS:HG2	3:C:43:ILE:O	2.04	0.58
4:E:22:ALA:HB1	4:E:348:SER:HB2	1.84	0.58
4:E:47:MET:CG	4:E:48:GLY:H	2.15	0.58
4:E:238:LYS:HD3	4:E:254:ARG:NH1	2.17	0.58
1:A:256:ALA:H	1:A:259:LYS:HE2	1.69	0.58
2:B:167:LYS:HB3	2:B:168:ASP:C	2.24	0.58
3:C:128:GLU:HA	3:C:183:GLU:CD	2.24	0.58
3:C:135:ARG:CG	3:C:138:ASP:H	2.15	0.58
3:C:144:THR:HG23	3:C:145:VAL:N	2.18	0.58
4:D:43:VAL:HG22	4:D:44:MET:H	1.69	0.58
1:A:128:PRO:HG2	1:A:132:LEU:CD2	2.34	0.58
1:A:205:LYS:HG3	1:A:206:LYS:H	1.68	0.58
1:A:408:VAL:HG23	1:A:409:GLY:N	2.18	0.58
1:A:426:VAL:HG23	1:A:427:GLY:N	2.19	0.58
1:A:462:LEU:CD1	1:A:464:ILE:HG22	2.34	0.58
1:A:749:LEU:CD1	1:A:753:ILE:HD11	2.33	0.58
3:C:146:MET:O	3:C:149:GLU:HG3	2.04	0.58
4:E:210:ARG:HG2	4:E:210:ARG:NH1	2.18	0.58
1:A:12:GLU:CD	1:A:133:PRO:HG2	2.24	0.58
1:A:789:MET:HE3	3:C:130:PHE:CE1	2.39	0.58
2:B:29:GLN:O	2:B:32:LYS:HB3	2.04	0.58
4:D:148:THR:HG22	4:D:149:THR:N	2.16	0.58
1:A:170:ARG:HD2	1:A:256:ALA:O	2.02	0.58
1:A:304:LEU:O	1:A:305:ILE:HD13	2.04	0.58
4:D:26:ALA:HB1	4:D:27:PRO:HD2	1.85	0.58
4:D:236:LEU:O	4:D:251:GLY:HA3	2.04	0.58
4:D:299:MET:HE1	4:D:309:ILE:CD1	2.33	0.58
4:E:34:ILE:HG21	4:E:67:LEU:HB3	1.86	0.58
4:E:287:ILE:HA	4:E:290:ARG:NE	2.19	0.58
1:A:12:GLU:HG3	1:A:133:PRO:HB2	1.85	0.57
1:A:102:VAL:CG2	1:A:694:MET:HE1	2.31	0.57
1:A:246:PHE:HA	1:A:269:LEU:HD13	1.85	0.57
1:A:522:CYS:SG	1:A:583:HIS:HA	2.44	0.57
1:A:839:LYS:CE	2:B:60:ARG:HH12	2.16	0.57
4:D:107:GLU:O	4:D:137:GLN:HG3	2.04	0.57
4:D:326:LYS:O	4:D:327:ILE:HD12	2.03	0.57
4:E:300:SER:HB3	4:E:335:ARG:NE	2.18	0.57
4:E:336:LYS:CE	5:E:401:ADP:H5'2	2.34	0.57
1:A:2:SER:O	1:A:3:SER:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ASN:O	1:A:422:VAL:HG13	2.04	0.57
1:A:523:ILE:HD13	1:A:523:ILE:H	1.69	0.57
3:C:47:LYS:HG3	3:C:109:GLU:OE1	2.05	0.57
4:E:110:LEU:N	4:E:110:LEU:HD23	2.19	0.57
1:A:36:LYS:HD3	1:A:36:LYS:N	2.17	0.57
4:D:64:ILE:HG23	4:D:65:LEU:N	2.20	0.57
4:E:34:ILE:HB	4:E:54:VAL:HG21	1.87	0.57
1:A:205:LYS:HB3	1:A:257:THR:CG2	2.34	0.57
1:A:222:ILE:HD13	1:A:222:ILE:N	2.19	0.57
1:A:332:LEU:HD12	1:A:332:LEU:C	2.25	0.57
1:A:713:PHE:CE2	1:A:770:LYS:HG2	2.39	0.57
4:D:336:LYS:CE	5:D:401:ADP:H5'2	2.34	0.57
4:E:34:ILE:HG22	4:E:35:VAL:N	2.19	0.57
4:E:139:VAL:HG12	4:E:140:LEU:N	2.18	0.57
1:A:396:GLU:HG2	1:A:610:LEU:HD21	1.87	0.57
3:C:54:LYS:HZ1	3:C:73:VAL:CG2	2.17	0.57
4:E:5:THR:HG23	4:E:6:THR:O	2.04	0.57
4:E:365:ALA:HB3	4:E:369:ILE:HB	1.85	0.57
1:A:250:ILE:HG23	1:A:250:ILE:O	2.04	0.57
1:A:610:LEU:O	1:A:610:LEU:HD13	2.05	0.57
1:A:656:ARG:HG2	1:A:656:ARG:NH1	2.19	0.57
1:A:793:GLN:OE1	3:C:155:ALA:HB3	2.03	0.57
4:D:287:ILE:HG12	4:D:288:ASP:OD1	2.04	0.57
4:E:34:ILE:C	4:E:54:VAL:HG21	2.24	0.57
4:E:244:ASP:OD2	4:E:246:GLN:HG3	2.03	0.57
4:E:321:ALA:HB1	4:E:322:PRO:HD2	1.86	0.57
1:A:39:PHE:CE1	1:A:100:PRO:HB2	2.40	0.57
1:A:110:TYR:CZ	1:A:685:PRO:HA	2.39	0.57
1:A:514:ASP:HB3	1:A:517:MET:CE	2.34	0.57
3:C:67:LYS:HD2	3:C:101:MET:HB3	1.87	0.57
4:E:208:ILE:HD11	4:E:243:PRO:HG2	1.85	0.57
1:A:115:ILE:HD13	1:A:116:TYR:CD2	2.40	0.57
3:C:57:PHE:CD2	3:C:69:THR:HG21	2.39	0.57
4:D:37:ARG:H	4:D:66:THR:HG23	1.70	0.57
4:D:37:ARG:HG3	4:D:51:ASP:OD1	2.04	0.57
1:A:38:CYS:HB3	1:A:78:PHE:O	2.04	0.57
1:A:172:ASN:OD1	1:A:457:TYR:HA	2.05	0.57
1:A:292:MET:SD	1:A:315:VAL:HG11	2.45	0.57
1:A:464:ILE:HG12	1:A:465:ALA:H	1.70	0.57
1:A:567:LYS:HG3	1:A:568:PRO:N	2.18	0.57
1:A:617:LYS:N	1:A:617:LYS:HD3	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:MET:HE2	3:C:130:PHE:HZ	1.69	0.57
3:C:71:SER:HA	3:C:86:ASN:HD21	1.70	0.57
1:A:226:ASN:O	1:A:230:GLU:HG2	2.05	0.57
1:A:551:LYS:HG2	1:A:555:TYR:HE2	1.69	0.57
3:C:98:ASN:CB	3:C:99:GLU:HA	2.29	0.57
3:C:139:LYS:O	3:C:140:GLU:HB2	2.04	0.57
3:C:151:ARG:HG3	3:C:163:GLU:OE1	2.04	0.57
4:D:250:ILE:HD13	4:D:254:ARG:HG2	1.86	0.57
1:A:407:LYS:HG3	1:A:408:VAL:H	1.69	0.56
2:B:70:ALA:HA	2:B:73:LYS:HE3	1.84	0.56
2:B:134:GLN:O	2:B:137:ILE:HG22	2.04	0.56
4:D:352:PHE:O	4:D:355:MET:HG2	2.05	0.56
1:A:94:MET:HE2	1:A:96:HIS:O	2.05	0.56
1:A:143:TYR:HE2	1:A:151:ALA:CB	2.18	0.56
1:A:364:MET:SD	1:A:382:VAL:HB	2.44	0.56
1:A:533:PHE:O	1:A:537:GLU:HG3	2.05	0.56
1:A:790:THR:HG22	1:A:791:ARG:CD	2.34	0.56
1:A:19:LYS:HD3	1:A:23:GLU:HB2	1.84	0.56
1:A:290:GLN:O	1:A:331:LEU:HD12	2.05	0.56
1:A:349:VAL:C	1:A:353:LYS:HG3	2.26	0.56
1:A:422:VAL:HG23	1:A:423:THR:N	2.18	0.56
1:A:506:GLU:HB3	1:A:508:ILE:CD1	2.34	0.56
4:E:38:PRO:HD3	4:E:49:GLN:HE22	1.69	0.56
4:E:189:LEU:HG	4:E:209:VAL:CG1	2.34	0.56
3:C:135:ARG:HH11	3:C:139:LYS:HB3	1.69	0.56
4:E:238:LYS:HD3	4:E:254:ARG:HH12	1.70	0.56
4:E:309:ILE:HG23	4:E:310:ALA:N	2.21	0.56
1:A:485:GLU:HG2	1:A:584:TYR:CE1	2.39	0.56
1:A:515:PHE:CE1	1:A:711:LYS:HG2	2.39	0.56
1:A:607:VAL:O	1:A:611:TYR:HD1	1.89	0.56
1:A:811:ARG:HG2	1:A:815:ILE:CG1	2.36	0.56
2:B:124:LEU:HD12	2:B:125:LEU:N	2.21	0.56
3:C:76:VAL:HG12	3:C:77:LEU:N	2.19	0.56
3:C:128:GLU:HG3	3:C:180:ILE:HG21	1.86	0.56
4:D:31:PHE:HB2	4:D:32:PRO:HD2	1.87	0.56
4:E:194:THR:HA	4:E:198:TYR:O	2.05	0.56
1:A:789:MET:HE3	3:C:130:PHE:HE1	1.71	0.56
2:B:58:MET:CE	2:B:60:ARG:HB2	2.35	0.56
4:E:54:VAL:HG12	4:E:55:GLY:N	2.19	0.56
4:E:57:GLU:O	4:E:61:LYS:HB2	2.05	0.56
4:E:287:ILE:HA	4:E:290:ARG:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:MET:HG2	1:A:81:ASN:N	2.20	0.56
1:A:233:GLY:O	1:A:234:ASN:HB2	2.04	0.56
1:A:249:PHE:HD1	1:A:462:LEU:CD2	2.18	0.56
1:A:264:ASP:HA	1:A:446:ASN:OD1	2.06	0.56
4:D:37:ARG:O	4:D:66:THR:HG23	2.06	0.56
4:E:104:LEU:HB2	4:E:356:TRP:HH2	1.69	0.56
4:E:140:LEU:HD13	4:E:343:GLY:HA2	1.83	0.56
4:E:172:PRO:HA	4:E:175:ILE:CD1	2.35	0.56
1:A:170:ARG:NH2	1:A:256:ALA:HB1	2.21	0.56
1:A:305:ILE:HD12	1:A:312:PHE:CZ	2.40	0.56
1:A:553:LYS:NZ	4:D:351:THR:HG21	2.21	0.56
2:B:28:ILE:HG22	2:B:85:LEU:HD22	1.87	0.56
4:D:154:ASP:CB	4:D:300:SER:HB3	2.34	0.56
4:E:34:ILE:HG22	4:E:35:VAL:H	1.71	0.56
1:A:39:PHE:CD1	1:A:49:LYS:HA	2.41	0.56
1:A:238:VAL:HG23	1:A:282:GLU:OE2	2.06	0.56
1:A:245:ARG:CG	1:A:285:TYR:HE1	2.18	0.56
1:A:255:GLY:HA3	1:A:259:LYS:CG	2.35	0.56
1:A:396:GLU:CG	1:A:610:LEU:HD21	2.36	0.56
1:A:483:THR:O	1:A:487:LEU:HG	2.06	0.56
1:A:648:PHE:HA	1:A:649:GLN:NE2	2.21	0.56
1:A:755:VAL:HG23	1:A:760:TYR:HE1	1.71	0.56
1:A:822:ILE:O	1:A:825:PHE:HB3	2.04	0.56
4:E:47:MET:HG3	4:E:48:GLY:N	2.19	0.56
4:E:153:LEU:HD11	4:E:274:ILE:HG22	1.88	0.56
4:E:372:ARG:HG2	4:E:372:ARG:NH1	2.21	0.56
1:A:406:VAL:CG1	1:A:605:GLU:HB2	2.33	0.56
2:B:55:PHE:HA	2:B:58:MET:HB3	1.87	0.56
3:C:47:LYS:HA	3:C:50:GLN:OE1	2.06	0.56
4:D:34:ILE:CA	4:D:54:VAL:HG11	2.35	0.56
4:D:151:ILE:HD12	4:D:164:PRO:HG3	1.87	0.56
4:D:164:PRO:HG2	4:D:174:ALA:CB	2.35	0.56
4:E:285:CYS:HB3	4:E:289:ILE:HD11	1.87	0.56
1:A:16:TYR:HD2	1:A:115:ILE:HG13	1.71	0.55
1:A:246:PHE:C	1:A:269:LEU:HD11	2.27	0.55
1:A:497:VAL:HG12	1:A:501:GLU:OE1	2.06	0.55
1:A:684:THR:O	1:A:687:VAL:HG12	2.05	0.55
1:A:722:PHE:CZ	1:A:777:LEU:HD11	2.40	0.55
2:B:46:ILE:HG13	2:B:46:ILE:O	2.06	0.55
4:D:116:ARG:HH12	4:D:375:PHE:HA	1.72	0.55
4:E:78:ASN:O	4:E:82:MET:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:99:GLU:O	4:E:130:PRO:HG3	2.06	0.55
1:A:47:TYR:CE2	1:A:78:PHE:CE1	2.94	0.55
1:A:110:TYR:OH	1:A:685:PRO:HA	2.06	0.55
1:A:269:LEU:N	1:A:269:LEU:HD12	2.21	0.55
1:A:584:TYR:CD1	1:A:584:TYR:N	2.74	0.55
1:A:735:PRO:HB2	1:A:739:PHE:CD2	2.42	0.55
1:A:795:LEU:HD23	3:C:80:LEU:CD2	2.36	0.55
2:B:65:ASN:HB3	2:B:66:GLU:HG2	1.85	0.55
3:C:170:MET:HE1	3:C:186:VAL:HG23	1.87	0.55
1:A:170:ARG:NE	1:A:256:ALA:HB1	2.21	0.55
2:B:68:LEU:O	2:B:71:MET:HB2	2.06	0.55
2:B:79:ILE:O	2:B:79:ILE:HG23	2.06	0.55
3:C:183:GLU:HG3	3:C:184:ALA:H	1.71	0.55
4:D:220:ALA:CB	4:D:226:GLU:HG3	2.35	0.55
1:A:17:LEU:CD1	1:A:152:PRO:HB2	2.36	0.55
1:A:163:TYR:CZ	1:A:167:LEU:HD11	2.41	0.55
1:A:260:LEU:O	1:A:260:LEU:HD13	2.06	0.55
1:A:536:LEU:HA	1:A:550:PHE:CE1	2.41	0.55
1:A:439:LEU:O	1:A:439:LEU:HD13	2.07	0.55
1:A:475:LEU:HD22	1:A:595:TRP:CD2	2.41	0.55
1:A:607:VAL:HG12	1:A:611:TYR:CE1	2.41	0.55
1:A:659:LEU:HD11	1:A:663:MET:CE	2.37	0.55
1:A:694:MET:HE2	1:A:694:MET:CA	2.34	0.55
3:C:104:LYS:NZ	3:C:104:LYS:HB3	2.22	0.55
4:E:35:VAL:N	4:E:54:VAL:HG21	2.21	0.55
4:E:35:VAL:CA	4:E:54:VAL:HG21	2.36	0.55
1:A:128:PRO:HG2	1:A:132:LEU:HD23	1.87	0.55
1:A:245:ARG:HH22	1:A:274:ARG:HE	1.55	0.55
1:A:291:ILE:HG23	1:A:296:LYS:NZ	2.22	0.55
1:A:390:MET:O	1:A:615:ALA:HB2	2.07	0.55
1:A:565:PHE:CE2	1:A:579:PHE:CD2	2.95	0.55
1:A:583:HIS:HB2	1:A:585:ALA:HB3	1.88	0.55
2:B:39:ASP:HA	2:B:46:ILE:HG22	1.88	0.55
4:E:123:MET:HG3	4:E:132:MET:CE	2.36	0.55
4:E:123:MET:HA	4:E:123:MET:CE	2.37	0.55
1:A:104:TYR:CZ	1:A:108:GLU:HG3	2.41	0.55
1:A:107:LYS:HD2	1:A:688:MET:CB	2.36	0.55
4:D:34:ILE:HG21	4:D:67:LEU:CB	2.32	0.55
4:E:300:SER:HA	4:E:335:ARG:NE	2.21	0.55
1:A:143:TYR:HE2	1:A:151:ALA:HB3	1.72	0.55
1:A:392:LEU:HD22	1:A:614:SER:CB	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:VAL:O	1:A:429:LEU:HB3	2.07	0.55
1:A:474:SER:HA	1:A:595:TRP:CZ2	2.41	0.55
1:A:816:PHE:CD2	1:A:820:TYR:CE2	2.95	0.55
1:A:818:ILE:O	1:A:822:ILE:HG23	2.07	0.55
4:E:358:THR:OG1	4:E:361:GLU:HG3	2.07	0.55
1:A:167:LEU:HD13	1:A:257:THR:O	2.07	0.55
1:A:167:LEU:CD2	1:A:258:GLY:HA3	2.35	0.55
1:A:175:ILE:HD12	1:A:175:ILE:C	2.26	0.55
1:A:644:LYS:CG	1:A:649:GLN:HA	2.36	0.55
4:D:124:PHE:CD2	4:D:362:TYR:CG	2.95	0.55
4:E:8:LEU:HB2	4:E:103:THR:OG1	2.07	0.55
4:E:106:THR:HG21	4:E:140:LEU:CD1	2.37	0.55
1:A:32:PHE:CD2	1:A:83:PRO:HD3	2.41	0.55
1:A:166:MET:HE3	1:A:254:PHE:CG	2.42	0.55
4:E:208:ILE:O	4:E:212:ILE:HD12	2.07	0.55
1:A:249:PHE:CD1	1:A:462:LEU:HD23	2.42	0.54
1:A:283:ARG:HH22	1:A:325:ILE:CD1	2.20	0.54
4:E:36:GLY:HA2	4:E:66:THR:HG23	1.87	0.54
4:E:316:GLU:OE1	4:E:316:GLU:HA	2.07	0.54
1:A:338:ILE:O	1:A:341:LEU:HD12	2.07	0.54
1:A:835:ASN:O	1:A:839:LYS:HD3	2.08	0.54
2:B:82:THR:O	2:B:85:LEU:HB2	2.07	0.54
2:B:115:THR:HG21	2:B:154:TYR:CZ	2.42	0.54
4:E:158:GLY:CA	4:E:181:ALA:HB3	2.38	0.54
1:A:221:GLN:NE2	1:A:449:LEU:HA	2.22	0.54
1:A:780:MET:HA	1:A:783:GLU:CG	2.37	0.54
2:B:108:LEU:HD11	2:B:124:LEU:CD2	2.33	0.54
3:C:136:VAL:O	3:C:136:VAL:HG13	2.06	0.54
4:D:158:GLY:HA2	4:D:181:ALA:HB3	1.89	0.54
4:E:3:ASP:O	4:E:4:GLU:HG3	2.07	0.54
4:E:45:VAL:HG13	4:E:45:VAL:O	2.08	0.54
4:E:65:LEU:HD12	4:E:65:LEU:C	2.28	0.54
1:A:136:ASN:HB2	1:A:139:VAL:HG23	1.89	0.54
1:A:283:ARG:HB2	1:A:289:TYR:CZ	2.42	0.54
1:A:338:ILE:CG2	1:A:348:LYS:HD2	2.24	0.54
1:A:418:ASN:HB2	1:A:420:GLN:NE2	2.23	0.54
3:C:118:ILE:HG23	3:C:118:ILE:O	2.07	0.54
3:C:131:VAL:HG13	3:C:179:CYS:CB	2.38	0.54
4:D:121:GLN:HA	4:D:362:TYR:OH	2.07	0.54
4:E:148:THR:HG23	4:E:149:THR:N	2.22	0.54
4:E:182:GLY:HA2	4:E:185:LEU:HG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:193:LEU:HD22	4:E:198:TYR:HD2	1.73	0.54
1:A:253:HIS:CA	1:A:458:PHE:HB3	2.36	0.54
1:A:296:LYS:HG2	1:A:331:LEU:HD11	1.86	0.54
2:B:159:TYR:O	2:B:159:TYR:HD2	1.91	0.54
4:D:154:ASP:HA	4:D:300:SER:CB	2.22	0.54
4:D:261:LEU:N	4:D:261:LEU:HD23	2.22	0.54
4:E:37:ARG:H	4:E:66:THR:HG22	1.70	0.54
4:E:282:ILE:HA	4:E:285:CYS:SG	2.47	0.54
1:A:176:LEU:CD1	1:A:675:ARG:HH21	2.21	0.54
1:A:205:LYS:CB	1:A:257:THR:HG21	2.36	0.54
1:A:255:GLY:HA3	1:A:259:LYS:CE	2.38	0.54
1:A:645:GLY:N	4:D:23:GLY:HA2	2.21	0.54
1:A:722:PHE:HZ	1:A:777:LEU:HD11	1.73	0.54
4:E:157:ASP:OD1	5:E:401:ADP:H3'	2.08	0.54
4:E:172:PRO:HA	4:E:175:ILE:HD12	1.90	0.54
4:E:286:ASP:O	4:E:290:ARG:HG3	2.07	0.54
1:A:207:LYS:HZ3	1:A:453:GLN:CG	2.20	0.54
1:A:291:ILE:CG1	1:A:296:LYS:HZ2	2.18	0.54
1:A:308:ASN:OD1	1:A:310:PHE:HB3	2.08	0.54
1:A:365:LYS:HB2	1:A:378:ASP:HB3	1.89	0.54
1:A:715:SER:CB	1:A:774:LEU:HD11	2.37	0.54
3:C:42:LYS:HZ1	3:C:47:LYS:HB2	1.72	0.54
4:E:34:ILE:HG13	4:E:54:VAL:CG1	2.37	0.54
4:E:107:GLU:OE1	4:E:116:ARG:HG3	2.07	0.54
1:A:19:LYS:HG3	1:A:114:MET:HE2	1.90	0.54
1:A:407:LYS:O	1:A:408:VAL:HG12	2.07	0.54
1:A:500:GLN:O	1:A:504:LYS:HG2	2.08	0.54
1:A:694:MET:HE1	1:A:697:LEU:CD1	2.37	0.54
3:C:77:LEU:HD23	3:C:77:LEU:C	2.28	0.54
3:C:80:LEU:CD2	3:C:187:LYS:HZ3	2.21	0.54
3:C:106:ILE:HD13	3:C:106:ILE:C	2.27	0.54
4:D:121:GLN:HB2	4:D:362:TYR:OH	2.07	0.54
4:D:311:ASP:O	4:D:314:GLN:HB3	2.08	0.54
4:E:101:HIS:O	4:E:130:PRO:HD2	2.08	0.54
1:A:16:TYR:OH	1:A:132:LEU:HD12	2.08	0.54
1:A:236:LYS:HD3	1:A:236:LYS:C	2.28	0.54
1:A:287:ILE:HA	1:A:290:GLN:HG3	1.88	0.54
1:A:340:ILE:HG23	1:A:341:LEU:N	2.23	0.54
1:A:408:VAL:HG23	1:A:409:GLY:H	1.73	0.54
1:A:644:LYS:HZ2	1:A:649:GLN:HB3	1.73	0.54
1:A:645:GLY:O	1:A:646:SER:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:106:ILE:HA	3:C:109:GLU:CG	2.38	0.54
3:C:150:LEU:HD13	3:C:150:LEU:C	2.28	0.54
4:E:250:ILE:O	4:E:250:ILE:HG23	2.08	0.54
4:E:365:ALA:HB2	4:E:369:ILE:HD12	1.88	0.54
1:A:155:ILE:CD1	1:A:191:ARG:HB3	2.38	0.54
1:A:236:LYS:HA	1:A:241:ASP:O	2.07	0.54
1:A:364:MET:HG3	1:A:382:VAL:CB	2.37	0.54
2:B:52:ARG:NH1	2:B:64:LYS:HG2	2.22	0.54
4:D:211:ASP:OD1	4:D:215:LYS:HD2	2.08	0.54
4:E:34:ILE:HG23	4:E:67:LEU:HB3	1.90	0.54
1:A:433:VAL:HG13	1:A:434:TYR:N	2.22	0.53
1:A:455:ARG:C	1:A:456:GLN:HG2	2.15	0.53
1:A:554:LEU:O	1:A:557:GLN:HG2	2.08	0.53
1:A:723:LYS:NZ	1:A:723:LYS:HB3	2.23	0.53
1:A:524:GLU:OE2	1:A:528:LYS:HB3	2.08	0.53
1:A:205:LYS:CB	1:A:257:THR:CG2	2.86	0.53
1:A:526:ILE:HG22	1:A:533:PHE:CD1	2.43	0.53
1:A:535:ILE:HD13	1:A:553:LYS:HE2	1.90	0.53
1:A:600:LYS:HB3	1:A:600:LYS:NZ	2.22	0.53
3:C:54:LYS:HZ1	3:C:73:VAL:HG21	1.72	0.53
3:C:192:ILE:O	3:C:193:ASP:HB2	2.08	0.53
4:D:106:THR:HG22	4:D:140:LEU:HD11	1.90	0.53
1:A:332:LEU:HD12	1:A:333:ALA:CA	2.37	0.53
1:A:694:MET:HE1	1:A:697:LEU:HD12	1.91	0.53
1:A:804:GLU:HB3	1:A:808:MET:HE2	1.89	0.53
4:D:136:ILE:HB	4:D:139:VAL:HB	1.91	0.53
1:A:39:PHE:HZ	1:A:80:MET:HE1	1.72	0.53
1:A:103:LEU:CD1	1:A:107:LYS:HB2	2.39	0.53
1:A:249:PHE:CE2	1:A:251:ARG:HG2	2.44	0.53
1:A:380:THR:HG23	1:A:398:LEU:HD11	1.89	0.53
1:A:482:PHE:HZ	1:A:527:GLU:HB3	1.72	0.53
1:A:610:LEU:HD13	1:A:610:LEU:C	2.28	0.53
2:B:74:GLU:HG3	2:B:74:GLU:O	2.09	0.53
3:C:135:ARG:HD3	3:C:139:LYS:H	1.72	0.53
4:D:180:LEU:HD12	4:D:181:ALA:N	2.23	0.53
1:A:347:GLU:O	1:A:350:GLY:HA3	2.08	0.53
1:A:677:LEU:HG	1:A:696:GLN:OE1	2.09	0.53
1:A:801:MET:HG2	3:C:72:GLN:HB3	1.91	0.53
1:A:822:ILE:C	1:A:822:ILE:HD12	2.28	0.53
4:D:200:PHE:CD1	4:D:209:VAL:HG23	2.44	0.53
1:A:578:HIS:CD2	1:A:578:HIS:H	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:LYS:CG	1:A:649:GLN:HG3	2.39	0.53
4:D:157:ASP:HB2	5:D:401:ADP:PB	2.49	0.53
1:A:255:GLY:HA3	1:A:259:LYS:CD	2.38	0.53
1:A:405:ARG:H	1:A:606:THR:CG2	2.21	0.53
1:A:790:THR:HG22	1:A:791:ARG:HH11	1.73	0.53
3:C:134:LEU:CD2	3:C:150:LEU:HG	2.36	0.53
3:C:163:GLU:O	3:C:166:VAL:HG22	2.09	0.53
4:D:16:LEU:HD23	4:D:32:PRO:HA	1.89	0.53
1:A:176:LEU:HD13	1:A:675:ARG:NH2	2.24	0.53
1:A:272:LYS:O	1:A:275:VAL:HB	2.09	0.53
1:A:544:LYS:HD2	4:D:148:THR:OG1	2.08	0.53
2:B:81:PHE:HA	2:B:84:PHE:HB3	1.90	0.53
2:B:126:ILE:HG23	2:B:127:THR:N	2.24	0.53
3:C:71:SER:HB2	3:C:86:ASN:ND2	2.24	0.53
4:D:186:THR:HG21	4:D:206:ARG:CZ	2.39	0.53
1:A:79:PRO:HB2	1:A:96:HIS:CD2	2.44	0.53
1:A:559:LEU:HD12	1:A:560:GLY:N	2.24	0.53
2:B:83:VAL:C	2:B:86:THR:HG22	2.27	0.53
2:B:96:ASP:HB2	2:B:97:PRO:CD	2.39	0.53
2:B:97:PRO:HD2	2:B:100:VAL:HG11	1.90	0.53
2:B:108:LEU:HD21	2:B:120:PHE:HE2	1.74	0.53
4:D:143:TYR:CE2	4:D:346:LEU:HD13	2.43	0.53
4:D:169:TYR:CE1	4:E:42:GLY:HA3	2.44	0.53
1:A:220:ASP:O	1:A:224:GLN:HG3	2.09	0.52
1:A:238:VAL:HG12	1:A:239:ARG:N	2.24	0.52
1:A:312:PHE:O	1:A:316:SER:HB2	2.09	0.52
1:A:338:ILE:O	1:A:338:ILE:HD13	2.09	0.52
1:A:642:LYS:CG	1:A:643:LYS:H	2.21	0.52
3:C:106:ILE:HA	3:C:109:GLU:HG2	1.90	0.52
4:E:39:ARG:NE	4:E:66:THR:HA	2.24	0.52
4:E:42:GLY:O	4:E:43:VAL:HG12	2.08	0.52
4:E:105:LEU:O	4:E:134:VAL:HA	2.09	0.52
1:A:254:PHE:HB2	1:A:457:TYR:O	2.10	0.52
1:A:291:ILE:HG23	1:A:296:LYS:HZ2	1.74	0.52
1:A:600:LYS:C	1:A:602:PRO:HD3	2.29	0.52
1:A:765:THR:OG1	1:A:766:LYS:HG2	2.08	0.52
2:B:45:ILE:O	2:B:45:ILE:HG12	2.08	0.52
3:C:140:GLU:O	3:C:178:GLY:HA2	2.08	0.52
4:E:58:ALA:O	4:E:65:LEU:HD21	2.09	0.52
1:A:88:ILE:HD11	1:A:93:MET:HB3	1.92	0.52
1:A:175:ILE:O	1:A:461:VAL:HA	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LYS:HD2	4:D:148:THR:CB	2.38	0.52
2:B:160:VAL:CA	2:B:165:ASP:HB2	2.40	0.52
3:C:68:ILE:HG23	3:C:69:THR:N	2.25	0.52
3:C:140:GLU:CD	3:C:180:ILE:HG12	2.29	0.52
4:D:104:LEU:HD23	4:D:104:LEU:C	2.29	0.52
4:D:290:ARG:HH11	4:E:244:ASP:HB2	1.69	0.52
4:E:79:TRP:CZ2	4:E:118:LYS:HB3	2.44	0.52
1:A:205:LYS:HD3	1:A:257:THR:OG1	2.10	0.52
1:A:363:ASN:HB3	1:A:382:VAL:CG2	2.40	0.52
2:B:108:LEU:HD21	2:B:120:PHE:CE2	2.44	0.52
2:B:159:TYR:O	2:B:165:ASP:HA	2.08	0.52
4:D:335:ARG:NH2	4:D:338:SER:HB2	2.24	0.52
4:E:31:PHE:HB2	4:E:32:PRO:HD2	1.91	0.52
1:A:519:LEU:CD1	1:A:584:TYR:HB3	2.38	0.52
1:A:659:LEU:HD12	1:A:663:MET:HG2	1.92	0.52
1:A:805:PHE:CE1	3:C:53:PHE:CD1	2.98	0.52
2:B:58:MET:HE3	2:B:60:ARG:NE	2.25	0.52
3:C:67:LYS:CD	3:C:101:MET:HB3	2.40	0.52
4:D:53:TYR:O	4:D:54:VAL:HB	2.09	0.52
4:E:124:PHE:CE2	4:E:362:TYR:HB2	2.44	0.52
1:A:14:ALA:HB2	1:A:18:ARG:HD2	1.88	0.52
1:A:122:PHE:HE1	1:A:673:PHE:HB2	1.70	0.52
1:A:255:GLY:HA2	1:A:456:GLN:CG	2.39	0.52
1:A:283:ARG:HH22	1:A:325:ILE:HD13	1.74	0.52
1:A:287:ILE:O	1:A:291:ILE:HD13	2.08	0.52
1:A:729:LEU:HD21	1:A:781:ARG:CA	2.40	0.52
2:B:135:GLU:O	2:B:138:LYS:HB3	2.10	0.52
2:B:167:LYS:HB3	2:B:168:ASP:CA	2.38	0.52
4:E:206:ARG:HG2	4:E:206:ARG:NH1	2.23	0.52
4:E:370:VAL:HG22	4:E:375:PHE:C	2.30	0.52
1:A:5:ALA:HB1	1:A:18:ARG:HH22	1.74	0.52
1:A:228:LEU:HD13	1:A:228:LEU:C	2.30	0.52
1:A:617:LYS:O	1:A:621:PHE:HD2	1.92	0.52
1:A:760:TYR:CE2	1:A:762:PHE:CE1	2.96	0.52
1:A:818:ILE:HG21	2:B:125:LEU:HD21	1.92	0.52
1:A:833:TRP:CZ2	2:B:71:MET:HG2	2.44	0.52
4:D:61:LYS:HG2	4:D:64:ILE:HG21	1.92	0.52
4:D:120:THR:CB	4:D:367:PRO:HB3	2.31	0.52
4:E:336:LYS:HE2	5:E:401:ADP:C5'	2.38	0.52
1:A:73:ASN:O	1:A:77:VAL:HG13	2.10	0.52
1:A:91:MET:HE2	1:A:102:VAL:CA	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:CA	1:A:688:MET:HG3	2.39	0.52
2:B:48:LYS:NZ	2:B:69:ASP:HB3	2.25	0.52
2:B:137:ILE:HG23	2:B:138:LYS:N	2.24	0.52
4:D:180:LEU:HD21	4:D:261:LEU:HD22	1.92	0.52
4:E:58:ALA:HB1	4:E:65:LEU:CD2	2.40	0.52
1:A:228:LEU:HB2	1:A:337:ALA:HB1	1.90	0.52
1:A:361:TYR:CE1	1:A:386:ALA:CB	2.93	0.52
1:A:405:ARG:HG2	1:A:413:VAL:HG23	1.92	0.52
1:A:417:GLN:HG2	1:A:421:GLN:NE2	2.24	0.52
1:A:805:PHE:HA	1:A:808:MET:HE2	1.88	0.52
3:C:54:LYS:NZ	3:C:73:VAL:HG21	2.25	0.52
3:C:92:VAL:H	3:C:95:ASN:CB	2.19	0.52
4:E:299:MET:CE	4:E:309:ILE:HG12	2.40	0.52
1:A:85:PHE:HD1	1:A:94:MET:HA	1.75	0.52
1:A:107:LYS:CD	1:A:688:MET:HG3	2.40	0.52
1:A:268:TYR:C	1:A:269:LEU:HD12	2.30	0.52
1:A:643:LYS:O	1:A:644:LYS:HG2	2.10	0.52
3:C:41:ILE:HG12	3:C:42:LYS:N	2.25	0.52
4:D:169:TYR:CE1	4:E:42:GLY:CA	2.93	0.52
4:D:287:ILE:CG2	4:E:244:ASP:HB3	2.40	0.52
4:E:59:GLN:O	4:E:62:ARG:HG3	2.09	0.52
4:E:250:ILE:HD11	4:E:253:GLU:HB2	1.91	0.52
4:E:299:MET:SD	4:E:309:ILE:HG12	2.49	0.52
1:A:795:LEU:HD11	3:C:186:VAL:O	2.10	0.51
1:A:825:PHE:HA	1:A:828:VAL:HG13	1.92	0.51
2:B:124:LEU:HD12	2:B:124:LEU:C	2.30	0.51
3:C:44:GLU:O	3:C:48:GLU:HB3	2.10	0.51
4:D:10:CYS:HB2	4:D:19:ALA:HB2	1.92	0.51
4:D:17:VAL:O	4:D:30:VAL:HA	2.10	0.51
4:E:18:LYS:HG3	4:E:30:VAL:HG13	1.92	0.51
4:E:153:LEU:CD1	4:E:274:ILE:HG22	2.40	0.51
1:A:137:PRO:HA	1:A:140:VAL:CG2	2.40	0.51
1:A:230:GLU:HB2	1:A:234:ASN:ND2	2.25	0.51
1:A:530:MET:CE	4:D:351:THR:HG22	2.41	0.51
1:A:644:LYS:NZ	1:A:649:GLN:HB3	2.24	0.51
2:B:144:PHE:HA	2:B:145:SER:OG	2.10	0.51
4:D:164:PRO:HG2	4:D:174:ALA:HB1	1.92	0.51
4:E:178:LEU:HD13	4:E:271:SER:CB	2.40	0.51
1:A:249:PHE:HD1	1:A:462:LEU:HD22	1.74	0.51
1:A:639:LYS:HZ2	4:D:4:GLU:HB3	1.75	0.51
1:A:822:ILE:HG12	2:B:132:PHE:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:VAL:HG22	1:A:829:LYS:N	2.24	0.51
1:A:837:PHE:CA	1:A:840:ILE:HG12	2.40	0.51
1:A:564:ASN:O	1:A:582:VAL:HG12	2.09	0.51
3:C:83:ASN:CB	3:C:84:PRO:HD3	2.36	0.51
4:D:103:THR:HG22	4:D:105:LEU:HD23	1.92	0.51
4:D:236:LEU:HB2	4:D:251:GLY:CA	2.40	0.51
1:A:84:LYS:HD3	1:A:778:GLU:OE2	2.11	0.51
1:A:166:MET:HE3	1:A:258:GLY:HA2	1.93	0.51
1:A:531:GLY:O	1:A:535:ILE:HG13	2.10	0.51
1:A:582:VAL:HG13	1:A:582:VAL:O	2.10	0.51
3:C:54:LYS:NZ	3:C:73:VAL:HG11	2.25	0.51
4:D:141:SER:HA	4:D:338:SER:O	2.11	0.51
4:D:336:LYS:HE2	5:D:401:ADP:C5'	2.38	0.51
4:E:34:ILE:HG22	4:E:68:LYS:H	1.76	0.51
1:A:12:GLU:CG	1:A:133:PRO:HB2	2.41	0.51
1:A:47:TYR:HB3	1:A:100:PRO:HG3	1.90	0.51
1:A:88:ILE:HD13	1:A:93:MET:HB2	1.93	0.51
1:A:103:LEU:CD2	1:A:690:HIS:HD2	2.12	0.51
1:A:129:TYR:CZ	1:A:683:LYS:HB3	2.46	0.51
1:A:508:ILE:CD1	1:A:768:PHE:CE1	2.94	0.51
3:C:149:GLU:O	3:C:153:VAL:HG23	2.11	0.51
1:A:27:ALA:HB1	1:A:87:LYS:HG2	1.93	0.51
1:A:71:THR:HG23	1:A:71:THR:O	2.10	0.51
1:A:73:ASN:HB3	1:A:76:GLN:HB3	1.92	0.51
1:A:333:ALA:O	1:A:336:ASN:HB3	2.10	0.51
1:A:677:LEU:HD21	1:A:696:GLN:NE2	2.26	0.51
1:A:698:ARG:HG2	1:A:703:LEU:CD1	2.41	0.51
1:A:790:THR:HA	1:A:793:GLN:OE1	2.11	0.51
1:A:34:SER:HB2	1:A:779:GLU:OE1	2.10	0.51
1:A:249:PHE:CD2	1:A:251:ARG:HG2	2.46	0.51
1:A:600:LYS:CG	1:A:602:PRO:HD3	2.41	0.51
1:A:617:LYS:HD3	1:A:617:LYS:H	1.74	0.51
1:A:773:LEU:O	1:A:773:LEU:HD13	2.11	0.51
1:A:795:LEU:HD12	3:C:186:VAL:HG13	1.93	0.51
2:B:160:VAL:HA	2:B:165:ASP:HB2	1.93	0.51
4:D:69:TYR:HB2	4:D:72:GLU:HA	1.92	0.51
4:D:157:ASP:OD1	5:D:401:ADP:H3'	2.11	0.51
1:A:9:ILE:HA	1:A:18:ARG:CZ	2.41	0.51
1:A:332:LEU:HD12	1:A:333:ALA:HA	1.93	0.51
1:A:392:LEU:HD21	1:A:614:SER:HB3	1.93	0.51
1:A:484:ASN:O	1:A:487:LEU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:GLU:HG2	1:A:652:SER:OG	2.11	0.51
1:A:613:LYS:HD3	1:A:613:LYS:H	1.76	0.51
1:A:639:LYS:HZ2	1:A:639:LYS:HB3	1.75	0.51
4:D:103:THR:O	4:D:132:MET:HA	2.11	0.51
1:A:143:TYR:CE2	1:A:151:ALA:CB	2.94	0.51
1:A:237:THR:C	1:A:282:GLU:HG3	2.30	0.51
1:A:268:TYR:N	1:A:268:TYR:CD1	2.79	0.51
1:A:445:ILE:HG23	1:A:449:LEU:CD1	2.38	0.51
2:B:58:MET:HE3	2:B:60:ARG:NH1	2.26	0.51
2:B:100:VAL:O	2:B:103:GLY:HA3	2.10	0.51
2:B:147:ASP:OD1	2:B:152:VAL:HG22	2.11	0.51
2:B:161:ILE:O	2:B:164:GLY:HA2	2.10	0.51
3:C:170:MET:SD	3:C:186:VAL:HA	2.50	0.51
4:D:7:ALA:HB1	4:D:356:TRP:CH2	2.47	0.51
4:E:58:ALA:HA	4:E:65:LEU:CD2	2.40	0.51
1:A:283:ARG:NH2	1:A:325:ILE:HD13	2.27	0.50
2:B:71:MET:O	2:B:74:GLU:HG2	2.11	0.50
2:B:167:LYS:HB3	2:B:168:ASP:O	2.12	0.50
3:C:122:LYS:O	3:C:187:LYS:HE3	2.11	0.50
4:D:287:ILE:HG22	4:D:290:ARG:NH1	2.25	0.50
1:A:16:TYR:HH	1:A:113:TRP:HE3	1.59	0.50
1:A:128:PRO:HB3	1:A:130:LYS:NZ	2.26	0.50
1:A:176:LEU:O	1:A:177:ILE:HD13	2.11	0.50
1:A:790:THR:HG22	1:A:791:ARG:HD2	1.92	0.50
1:A:822:ILE:HD11	2:B:132:PHE:CE2	2.43	0.50
3:C:69:THR:HB	3:C:73:VAL:CG2	2.39	0.50
4:E:162:ASN:ND2	4:E:278:THR:HA	2.26	0.50
4:E:190:MET:CE	4:E:206:ARG:HG3	2.40	0.50
1:A:115:ILE:CD1	1:A:116:TYR:CD2	2.95	0.50
1:A:420:GLN:H	1:A:420:GLN:CD	2.14	0.50
1:A:564:ASN:CA	1:A:582:VAL:CG1	2.87	0.50
1:A:603:LEU:HB2	1:A:648:PHE:HB2	1.93	0.50
1:A:822:ILE:HG12	2:B:132:PHE:HZ	1.71	0.50
3:C:113:PRO:C	3:C:116:GLN:HB3	2.31	0.50
1:A:254:PHE:HB3	1:A:259:LYS:O	2.12	0.50
1:A:415:LYS:CD	4:D:333:PRO:HG2	2.41	0.50
1:A:791:ARG:O	1:A:794:ALA:HB3	2.11	0.50
2:B:55:PHE:CD2	2:B:62:ASN:HB2	2.47	0.50
3:C:105:LYS:HD3	3:C:106:ILE:HA	1.93	0.50
4:D:8:LEU:H	4:D:103:THR:HA	1.76	0.50
4:E:285:CYS:CB	4:E:289:ILE:HD11	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HG	1:A:143:TYR:OH	2.10	0.50
1:A:91:MET:CE	1:A:105:ASN:HB3	2.40	0.50
1:A:118:TYR:CD2	1:A:153:PRO:HG3	2.47	0.50
1:A:296:LYS:CB	1:A:331:LEU:HD11	2.42	0.50
1:A:551:LYS:CG	1:A:555:TYR:HE2	2.23	0.50
2:B:42:ARG:NH1	2:B:42:ARG:HG2	2.27	0.50
3:C:108:PHE:CE1	3:C:112:LEU:CD2	2.95	0.50
3:C:112:LEU:O	3:C:116:GLN:HB2	2.12	0.50
4:E:58:ALA:HB1	4:E:65:LEU:HD22	1.92	0.50
4:E:211:ASP:OD2	4:E:215:LYS:HE3	2.11	0.50
1:A:603:LEU:HD23	1:A:648:PHE:CD2	2.47	0.50
1:A:776:LEU:O	1:A:780:MET:HG3	2.12	0.50
3:C:68:ILE:HD13	3:C:97:SER:C	2.31	0.50
3:C:87:ALA:CB	3:C:94:GLY:HA3	2.41	0.50
4:D:58:ALA:HA	4:D:65:LEU:CD2	2.42	0.50
4:D:70:PRO:HG2	4:D:85:ILE:CD1	2.42	0.50
1:A:88:ILE:HD11	1:A:93:MET:CB	2.42	0.50
1:A:159:SER:CB	1:A:195:TYR:CG	2.93	0.50
1:A:166:MET:CE	1:A:254:PHE:CG	2.95	0.50
1:A:205:LYS:HZ2	1:A:257:THR:HG21	1.77	0.50
1:A:603:LEU:CD2	1:A:648:PHE:CD2	2.95	0.50
1:A:755:VAL:CG1	1:A:773:LEU:HD21	2.41	0.50
1:A:815:ILE:HD13	2:B:129:CYS:SG	2.52	0.50
4:E:240:TYR:O	4:E:247:VAL:HG13	2.12	0.50
4:E:294:TYR:CD1	4:E:327:ILE:CD1	2.95	0.50
1:A:46:MET:HA	1:A:46:MET:HE1	1.94	0.50
1:A:154:HIS:HE2	1:A:156:PHE:HD2	1.60	0.50
1:A:167:LEU:HD21	1:A:258:GLY:CA	2.39	0.50
1:A:232:PHE:HB3	1:A:434:TYR:OH	2.12	0.50
1:A:557:GLN:HG2	1:A:558:HIS:H	1.77	0.50
1:A:601:ASP:N	1:A:602:PRO:HD3	2.27	0.50
1:A:724:GLN:HG3	1:A:725:ARG:N	2.25	0.50
2:B:41:ASN:HB3	2:B:45:ILE:O	2.12	0.50
2:B:137:ILE:HD13	2:B:141:TRP:NE1	2.22	0.50
3:C:144:THR:HG23	3:C:145:VAL:H	1.75	0.50
4:D:10:CYS:HA	4:D:19:ALA:HA	1.94	0.50
4:D:279:TYR:HB2	4:D:320:LEU:HD13	1.93	0.50
4:D:335:ARG:HH21	4:D:338:SER:CB	2.25	0.50
4:E:45:VAL:O	4:E:45:VAL:HG22	2.11	0.50
1:A:17:LEU:HD13	1:A:152:PRO:HB2	1.94	0.50
1:A:292:MET:SD	1:A:309:PRO:HA	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:SER:O	1:A:647:SER:HB2	2.12	0.50
1:A:844:LEU:HD22	1:A:844:LEU:N	2.27	0.50
1:A:220:ASP:C	1:A:223:ILE:HG13	2.32	0.49
1:A:343:PHE:CE2	1:A:441:MET:SD	3.05	0.49
1:A:520:ALA:O	1:A:523:ILE:HG12	2.12	0.49
1:A:838:PHE:CE1	2:B:164:GLY:CA	2.95	0.49
1:A:839:LYS:HE2	2:B:60:ARG:NH1	2.26	0.49
4:D:107:GLU:HG3	4:D:111:ASN:HB2	1.94	0.49
4:E:89:THR:HG22	4:E:94:LEU:HD12	1.93	0.49
1:A:205:LYS:HD3	1:A:257:THR:CG2	2.43	0.49
1:A:296:LYS:N	1:A:297:PRO:HD3	2.27	0.49
1:A:512:PHE:HZ	1:A:711:LYS:O	1.94	0.49
1:A:544:LYS:HD2	4:D:148:THR:HB	1.93	0.49
1:A:755:VAL:CG2	1:A:760:TYR:CE1	2.95	0.49
2:B:70:ALA:HA	2:B:73:LYS:HD3	1.93	0.49
4:D:7:ALA:HB3	4:D:347:ALA:HB1	1.94	0.49
4:D:26:ALA:HB1	4:D:27:PRO:CD	2.42	0.49
4:D:140:LEU:HD13	4:D:343:GLY:N	2.27	0.49
1:A:207:LYS:CE	1:A:453:GLN:HB3	2.29	0.49
3:C:104:LYS:HB3	3:C:104:LYS:HZ1	1.76	0.49
1:A:185:LYS:O	1:A:189:THR:HG23	2.12	0.49
1:A:361:TYR:HE1	1:A:386:ALA:HB1	1.78	0.49
1:A:761:ARG:HG2	1:A:761:ARG:HH11	1.76	0.49
2:B:152:VAL:HG12	2:B:153:ASP:N	2.26	0.49
4:D:148:THR:HG22	4:D:149:THR:CB	2.43	0.49
4:D:255:PHE:C	4:D:258:PRO:HD2	2.33	0.49
4:E:38:PRO:CD	4:E:49:GLN:HE22	2.26	0.49
1:A:348:LYS:HG2	1:A:352:TYR:CE2	2.48	0.49
1:A:349:VAL:O	1:A:353:LYS:HG3	2.11	0.49
1:A:392:LEU:HD12	1:A:613:LYS:HB2	1.94	0.49
1:A:519:LEU:HD13	1:A:584:TYR:CG	2.47	0.49
1:A:730:ASN:HB3	1:A:749:LEU:CD1	2.36	0.49
1:A:789:MET:CE	3:C:130:PHE:CE1	2.95	0.49
1:A:792:THR:HA	3:C:127:TYR:CE1	2.47	0.49
3:C:127:TYR:HE2	3:C:187:LYS:CE	2.21	0.49
4:E:192:ILE:HG22	4:E:256:ARG:CZ	2.42	0.49
4:E:193:LEU:HD22	4:E:198:TYR:CD2	2.48	0.49
1:A:176:LEU:HD11	1:A:673:PHE:CA	2.41	0.49
1:A:234:ASN:ND2	1:A:242:ASN:HD21	2.10	0.49
1:A:361:TYR:CE1	1:A:386:ALA:HB1	2.48	0.49
2:B:122:GLU:HG3	2:B:137:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:188:HIS:NE2	3:C:192:ILE:HA	2.27	0.49
4:E:190:MET:HE1	4:E:206:ARG:HA	1.90	0.49
1:A:30:ARG:HB2	1:A:31:PRO:HD2	1.95	0.49
1:A:155:ILE:HD12	1:A:191:ARG:HB3	1.95	0.49
1:A:287:ILE:CD1	1:A:288:PHE:CD2	2.96	0.49
1:A:607:VAL:CG1	1:A:611:TYR:CE1	2.95	0.49
1:A:612:GLN:HB3	1:A:623:PHE:CZ	2.48	0.49
1:A:760:TYR:HA	1:A:768:PHE:O	2.12	0.49
1:A:799:TYR:CE2	3:C:170:MET:CE	2.95	0.49
1:A:801:MET:HE1	3:C:72:GLN:NE2	2.28	0.49
1:A:825:PHE:CE1	1:A:829:LYS:HB3	2.47	0.49
3:C:135:ARG:HE	3:C:135:ARG:C	2.16	0.49
4:D:69:TYR:N	4:D:69:TYR:CD1	2.81	0.49
4:E:49:GLN:C	4:E:50:LYS:HD3	2.33	0.49
1:A:348:LYS:HG2	1:A:352:TYR:HE2	1.76	0.49
1:A:375:ALA:CB	1:A:417:GLN:HE22	2.19	0.49
1:A:508:ILE:CG1	1:A:768:PHE:CZ	2.94	0.49
2:B:154:TYR:CD1	2:B:155:LYS:N	2.81	0.49
3:C:45:PHE:CA	3:C:46:SER:HB2	2.42	0.49
3:C:142:ASN:N	3:C:176:SER:HB3	2.27	0.49
3:C:189:ILE:HG12	3:C:190:MET:H	1.75	0.49
4:D:143:TYR:CE2	4:D:346:LEU:CD1	2.96	0.49
4:E:34:ILE:HB	4:E:54:VAL:CG2	2.43	0.49
4:E:106:THR:HG21	4:E:140:LEU:HD12	1.93	0.49
1:A:151:ALA:HB1	1:A:152:PRO:HD2	1.94	0.49
1:A:300:ILE:O	1:A:303:LEU:HB3	2.13	0.49
1:A:441:MET:O	1:A:444:ARG:HB2	2.13	0.49
1:A:722:PHE:CE1	1:A:777:LEU:CD1	2.96	0.49
3:C:56:ALA:O	3:C:59:LEU:HB2	2.13	0.49
4:E:26:ALA:HB1	4:E:27:PRO:HD2	1.94	0.49
4:E:94:LEU:HB3	4:E:96:VAL:HG13	1.95	0.49
4:E:143:TYR:HD1	4:E:143:TYR:O	1.96	0.49
1:A:279:LEU:H	1:A:279:LEU:CD2	2.24	0.49
1:A:295:LYS:HB3	1:A:331:LEU:CB	2.41	0.49
4:D:151:ILE:HA	4:D:164:PRO:HA	1.95	0.49
4:D:194:THR:HG23	4:D:198:TYR:O	2.13	0.49
4:D:294:TYR:CD2	4:D:325:MET:HG2	2.48	0.49
1:A:287:ILE:HD12	1:A:288:PHE:CD2	2.47	0.48
1:A:312:PHE:CD1	1:A:312:PHE:N	2.81	0.48
1:A:557:GLN:O	1:A:561:LYS:HG3	2.13	0.48
1:A:697:LEU:HB3	1:A:703:LEU:HG	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:LYS:HZ1	3:C:73:VAL:CG1	2.25	0.48
4:D:339:VAL:O	4:D:342:GLY:HA3	2.13	0.48
1:A:16:TYR:CD1	1:A:16:TYR:N	2.79	0.48
1:A:30:ARG:HB2	1:A:31:PRO:CD	2.42	0.48
1:A:319:GLU:HG3	1:A:321:THR:H	1.78	0.48
1:A:722:PHE:CZ	1:A:777:LEU:CD1	2.96	0.48
3:C:71:SER:HB2	3:C:86:ASN:OD1	2.13	0.48
3:C:144:THR:HG23	3:C:145:VAL:HG13	1.95	0.48
4:E:219:VAL:HG22	4:E:258:PRO:HB2	1.95	0.48
4:E:275:HIS:HB3	4:E:313:MET:HE1	1.95	0.48
1:A:129:TYR:CD2	1:A:683:LYS:HB3	2.48	0.48
1:A:130:LYS:HE2	1:A:132:LEU:HD11	1.94	0.48
1:A:205:LYS:HG3	1:A:206:LYS:N	2.28	0.48
1:A:275:VAL:HG12	1:A:276:THR:N	2.27	0.48
1:A:351:ILE:HG12	1:A:437:MET:HE3	1.93	0.48
1:A:372:GLU:H	1:A:372:GLU:HG2	1.43	0.48
1:A:485:GLU:HB3	1:A:523:ILE:CG2	2.43	0.48
2:B:108:LEU:CD2	2:B:120:PHE:CE2	2.95	0.48
2:B:147:ASP:CB	2:B:152:VAL:HA	2.44	0.48
4:D:189:LEU:O	4:D:192:ILE:HG12	2.12	0.48
4:E:238:LYS:O	4:E:250:ILE:HG22	2.13	0.48
1:A:39:PHE:CE1	1:A:49:LYS:CG	2.95	0.48
1:A:98:HIS:O	1:A:102:VAL:HG13	2.14	0.48
1:A:176:LEU:HD13	1:A:675:ARG:HH21	1.76	0.48
1:A:268:TYR:O	1:A:269:LEU:HD12	2.13	0.48
1:A:348:LYS:CA	1:A:351:ILE:HG22	2.43	0.48
1:A:519:LEU:HD13	1:A:584:TYR:CB	2.43	0.48
1:A:557:GLN:HG2	1:A:558:HIS:N	2.28	0.48
1:A:722:PHE:CE1	1:A:726:TYR:CD2	2.98	0.48
2:B:81:PHE:CA	2:B:84:PHE:HB3	2.43	0.48
2:B:120:PHE:CZ	2:B:124:LEU:HB3	2.48	0.48
3:C:122:LYS:HB3	3:C:127:TYR:CZ	2.48	0.48
4:D:362:TYR:CE1	4:D:367:PRO:HG3	2.47	0.48
1:A:16:TYR:CG	1:A:134:VAL:HG23	2.48	0.48
1:A:81:ASN:CG	1:A:96:HIS:H	2.16	0.48
1:A:166:MET:CG	1:A:457:TYR:HB2	2.43	0.48
1:A:228:LEU:HD23	1:A:337:ALA:HB3	1.94	0.48
1:A:240:ASN:HD22	1:A:241:ASP:N	2.11	0.48
1:A:249:PHE:CD1	1:A:462:LEU:CD2	2.96	0.48
2:B:160:VAL:HA	2:B:165:ASP:HA	1.95	0.48
3:C:90:LYS:HG3	3:C:90:LYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:143:GLY:N	3:C:176:SER:HB3	2.28	0.48
4:D:7:ALA:HA	4:D:102:PRO:O	2.13	0.48
4:E:32:PRO:HG2	4:E:55:GLY:O	2.14	0.48
4:E:58:ALA:CA	4:E:65:LEU:CD2	2.91	0.48
1:A:14:ALA:HB1	1:A:18:ARG:HB2	1.94	0.48
1:A:19:LYS:CG	1:A:114:MET:HE2	2.43	0.48
1:A:170:ARG:HB3	1:A:457:TYR:OH	2.14	0.48
1:A:319:GLU:CD	1:A:320:VAL:H	2.17	0.48
1:A:713:PHE:HE2	1:A:770:LYS:HG2	1.79	0.48
4:E:16:LEU:HD23	4:E:32:PRO:HA	1.95	0.48
4:E:223:PHE:CD1	4:E:259:GLU:CG	2.96	0.48
4:E:229:THR:HG22	4:E:233:SER:HB3	1.95	0.48
1:A:286:HIS:O	1:A:290:GLN:HG3	2.13	0.48
1:A:582:VAL:HA	1:A:587:THR:HA	1.95	0.48
2:B:85:LEU:O	2:B:88:PHE:HB2	2.14	0.48
3:C:127:TYR:CE2	3:C:187:LYS:CG	2.96	0.48
4:D:20:GLY:HA3	4:D:340:TRP:HZ2	1.78	0.48
4:D:153:LEU:HD11	4:D:160:THR:CG2	2.43	0.48
4:E:103:THR:CG2	4:E:105:LEU:HD21	2.42	0.48
1:A:176:LEU:HD11	1:A:673:PHE:CB	2.44	0.48
1:A:367:LYS:HD3	1:A:378:ASP:OD2	2.13	0.48
1:A:704:GLU:O	1:A:707:ARG:HB3	2.12	0.48
3:C:51:ASP:OD2	3:C:105:LYS:HE3	2.13	0.48
3:C:92:VAL:HG23	3:C:93:LEU:N	2.19	0.48
3:C:157:LEU:HD22	3:C:157:LEU:C	2.34	0.48
4:D:106:THR:HG22	4:D:140:LEU:CD1	2.43	0.48
4:D:107:GLU:HG2	4:D:108:ALA:N	2.28	0.48
4:E:73:HIC:HD2	4:E:183:ARG:NH1	2.29	0.48
1:A:789:MET:HB3	3:C:155:ALA:HB2	1.95	0.48
1:A:799:TYR:CE1	3:C:169:LEU:HD12	2.46	0.48
3:C:146:MET:N	3:C:147:GLY:HA3	2.28	0.48
3:C:162:LYS:HB3	3:C:162:LYS:NZ	2.28	0.48
4:D:115:ASN:O	4:D:119:MET:HG3	2.13	0.48
4:E:66:THR:C	4:E:67:LEU:HD23	2.33	0.48
4:E:262:PHE:O	4:E:273:GLY:HA3	2.14	0.48
1:A:159:SER:CB	1:A:195:TYR:CD2	2.93	0.48
1:A:472:PHE:CE1	1:A:591:ASN:CB	2.93	0.48
1:A:729:LEU:HD21	1:A:781:ARG:HA	1.93	0.48
1:A:790:THR:HG22	1:A:791:ARG:HD3	1.96	0.48
4:D:58:ALA:HB1	4:D:65:LEU:CD2	2.40	0.48
4:D:157:ASP:OD1	5:D:401:ADP:C3'	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:335:ARG:HD3	4:D:335:ARG:HA	1.51	0.48
4:E:314:GLN:NE2	4:E:327:ILE:HB	2.28	0.48
1:A:7:MET:HB2	1:A:8:ALA:H	1.21	0.47
1:A:250:ILE:C	1:A:250:ILE:HD13	2.35	0.47
1:A:515:PHE:CD1	1:A:711:LYS:CE	2.97	0.47
1:A:544:LYS:CD	4:D:148:THR:HB	2.44	0.47
1:A:600:LYS:HG2	1:A:602:PRO:CD	2.43	0.47
3:C:162:LYS:HA	3:C:165:GLU:CD	2.34	0.47
4:D:85:ILE:HG22	4:D:86:TRP:N	2.27	0.47
4:D:357:ILE:HD13	4:D:357:ILE:N	2.28	0.47
4:E:58:ALA:CB	4:E:65:LEU:HD22	2.44	0.47
4:E:198:TYR:CE2	4:E:248:ILE:HG22	2.46	0.47
4:E:240:TYR:HB3	4:E:248:ILE:HG13	1.96	0.47
1:A:39:PHE:CZ	1:A:80:MET:CE	2.96	0.47
1:A:46:MET:HA	1:A:46:MET:HE2	1.95	0.47
1:A:805:PHE:CE2	1:A:809:MET:SD	3.07	0.47
4:E:294:TYR:CE1	4:E:321:ALA:CB	2.97	0.47
4:E:347:ALA:HA	4:E:356:TRP:CZ2	2.49	0.47
1:A:253:HIS:HB2	1:A:455:ARG:CG	2.44	0.47
1:A:790:THR:CG2	1:A:791:ARG:HH11	2.26	0.47
1:A:805:PHE:O	1:A:809:MET:HG3	2.14	0.47
1:A:39:PHE:HE1	1:A:49:LYS:HG2	1.78	0.47
1:A:328:SER:O	1:A:331:LEU:HB3	2.15	0.47
1:A:808:MET:HB3	3:C:60:TYR:OH	2.14	0.47
1:A:837:PHE:CE2	1:A:838:PHE:CE1	3.02	0.47
3:C:42:LYS:HD2	3:C:47:LYS:HB3	1.96	0.47
4:D:35:VAL:HG12	4:D:68:LYS:HB3	1.93	0.47
4:D:66:THR:O	4:D:67:LEU:HD23	2.14	0.47
4:D:373:LYS:HA	4:D:373:LYS:HD2	1.67	0.47
4:E:285:CYS:SG	4:E:293:LEU:HD11	2.53	0.47
4:E:362:TYR:CE1	4:E:367:PRO:HG3	2.44	0.47
1:A:9:ILE:HD13	1:A:18:ARG:HH22	1.74	0.47
1:A:9:ILE:HA	1:A:18:ARG:NE	2.30	0.47
1:A:135:TYR:N	1:A:135:TYR:CD1	2.82	0.47
1:A:295:LYS:HB3	1:A:331:LEU:CD1	2.42	0.47
1:A:361:TYR:HE1	1:A:386:ALA:HB2	1.79	0.47
1:A:445:ILE:CG2	1:A:449:LEU:HD12	2.38	0.47
1:A:526:ILE:CG2	1:A:533:PHE:CD1	2.98	0.47
1:A:773:LEU:HD13	1:A:773:LEU:C	2.35	0.47
1:A:783:GLU:O	1:A:787:THR:HG23	2.14	0.47
3:C:105:LYS:O	3:C:108:PHE:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:158:GLY:HA3	4:D:183:ARG:CD	2.45	0.47
4:D:194:THR:HG23	4:D:199:SER:HA	1.96	0.47
4:E:236:LEU:HD22	4:E:252:ASN:HA	1.96	0.47
1:A:103:LEU:HD12	1:A:107:LYS:HB2	1.96	0.47
1:A:312:PHE:HB2	1:A:315:VAL:CG2	2.45	0.47
1:A:396:GLU:HG2	1:A:610:LEU:CD2	2.44	0.47
1:A:726:TYR:HD1	1:A:726:TYR:HA	1.35	0.47
1:A:825:PHE:CE1	2:B:161:ILE:CG2	2.97	0.47
2:B:47:ASP:O	2:B:50:ASP:HB2	2.14	0.47
4:D:121:GLN:HA	4:D:362:TYR:CZ	2.49	0.47
4:E:335:ARG:HD3	4:E:335:ARG:HA	1.65	0.47
1:A:19:LYS:CG	1:A:114:MET:CE	2.93	0.47
1:A:27:ALA:CB	1:A:87:LYS:HG2	2.45	0.47
1:A:103:LEU:HD11	1:A:688:MET:CB	2.44	0.47
1:A:107:LYS:HA	1:A:688:MET:HG3	1.97	0.47
1:A:110:TYR:CE1	1:A:128:PRO:HA	2.49	0.47
1:A:167:LEU:HD22	1:A:258:GLY:N	2.30	0.47
1:A:210:GLN:CG	1:A:211:PRO:HD2	2.45	0.47
1:A:226:ASN:CB	1:A:227:PRO:HD3	2.42	0.47
1:A:234:ASN:H	1:A:245:ARG:CG	2.27	0.47
1:A:259:LYS:H	1:A:259:LYS:HD3	1.79	0.47
1:A:350:GLY:H	1:A:353:LYS:HG3	1.78	0.47
1:A:566:GLN:HG2	1:A:567:LYS:N	2.29	0.47
1:A:603:LEU:HG	1:A:648:PHE:CE1	2.46	0.47
1:A:603:LEU:CG	1:A:648:PHE:CG	2.97	0.47
1:A:678:ILE:O	1:A:678:ILE:HG23	2.15	0.47
1:A:763:GLY:HA3	1:A:766:LYS:O	2.15	0.47
1:A:808:MET:SD	3:C:57:PHE:CE1	3.08	0.47
2:B:63:VAL:CG1	2:B:67:GLU:HB2	2.45	0.47
3:C:70:LEU:HB3	3:C:91:LYS:CD	2.44	0.47
3:C:85:THR:O	3:C:89:VAL:HB	2.15	0.47
3:C:89:VAL:O	3:C:90:LYS:HB2	2.14	0.47
3:C:90:LYS:CD	3:C:111:PHE:HZ	2.28	0.47
3:C:135:ARG:CD	3:C:140:GLU:H	2.27	0.47
3:C:156:THR:C	3:C:157:LEU:HD13	2.34	0.47
4:D:35:VAL:HA	4:D:54:VAL:CG2	2.35	0.47
4:D:35:VAL:C	4:D:54:VAL:HG21	2.35	0.47
4:E:65:LEU:HD13	4:E:67:LEU:HD23	1.95	0.47
1:A:17:LEU:HD12	1:A:152:PRO:CB	2.45	0.47
1:A:88:ILE:CD1	1:A:93:MET:HB2	2.44	0.47
1:A:189:THR:HA	1:A:192:VAL:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:TYR:HE2	4:D:337:TYR:CD2	2.33	0.47
3:C:70:LEU:O	3:C:73:VAL:HB	2.15	0.47
4:E:159:VAL:HG22	4:E:160:THR:N	2.30	0.47
1:A:167:LEU:CD2	1:A:258:GLY:CA	2.93	0.47
1:A:246:PHE:CA	1:A:269:LEU:CD1	2.82	0.47
1:A:485:GLU:HA	1:A:584:TYR:CZ	2.49	0.47
1:A:541:MET:CE	4:D:345:ILE:HG23	2.44	0.47
1:A:659:LEU:CD1	1:A:663:MET:HE2	2.45	0.47
1:A:673:PHE:CD1	1:A:673:PHE:N	2.82	0.47
1:A:831:TRP:CE3	1:A:834:MET:CE	2.97	0.47
2:B:69:ASP:O	2:B:72:MET:HB2	2.14	0.47
2:B:81:PHE:HA	2:B:84:PHE:CB	2.45	0.47
4:D:133:TYR:CE2	4:D:375:PHE:HB2	2.46	0.47
4:E:218:TYR:O	4:E:255:PHE:HA	2.14	0.47
1:A:24:ARG:HH11	1:A:27:ALA:HB3	1.80	0.47
1:A:117:THR:HB	1:A:124:VAL:CG2	2.45	0.47
1:A:139:VAL:HG12	1:A:143:TYR:CE1	2.50	0.47
1:A:236:LYS:HD3	1:A:237:THR:O	2.14	0.47
1:A:245:ARG:CD	1:A:285:TYR:HE1	2.28	0.47
1:A:388:TYR:C	1:A:388:TYR:CD2	2.88	0.47
1:A:408:VAL:HG22	1:A:410:ASN:O	2.13	0.47
1:A:415:LYS:HE3	4:D:333:PRO:CG	2.45	0.47
1:A:651:VAL:O	1:A:655:PHE:HD1	1.98	0.47
1:A:755:VAL:CG2	1:A:760:TYR:HE1	2.27	0.47
1:A:789:MET:HE1	3:C:150:LEU:HD21	1.96	0.47
3:C:51:ASP:CG	3:C:105:LYS:HE3	2.36	0.47
3:C:69:THR:CB	3:C:73:VAL:HG23	2.41	0.47
3:C:87:ALA:CB	3:C:94:GLY:CA	2.93	0.47
3:C:122:LYS:HB3	3:C:127:TYR:CE2	2.50	0.47
3:C:167:GLU:O	3:C:170:MET:HB2	2.15	0.47
4:D:230:ALA:HA	4:D:233:SER:HB2	1.96	0.47
4:D:314:GLN:OE1	4:D:314:GLN:HA	2.15	0.47
4:E:54:VAL:HA	4:E:58:ALA:HB2	1.97	0.47
1:A:80:MET:HG2	1:A:81:ASN:H	1.80	0.46
1:A:254:PHE:HD1	1:A:458:PHE:HA	1.79	0.46
1:A:525:LEU:HD11	1:A:558:HIS:ND1	2.29	0.46
1:A:558:HIS:O	1:A:561:LYS:HB2	2.15	0.46
1:A:583:HIS:CB	1:A:585:ALA:HB3	2.45	0.46
1:A:801:MET:CE	3:C:57:PHE:CZ	2.95	0.46
2:B:58:MET:HG3	2:B:59:GLY:N	2.30	0.46
2:B:58:MET:HE3	2:B:60:ARG:HH11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:294:TYR:HD1	4:E:327:ILE:HD12	1.80	0.46
1:A:14:ALA:HB3	1:A:15:PRO:CD	2.37	0.46
1:A:80:MET:CG	1:A:81:ASN:N	2.78	0.46
1:A:118:TYR:OH	1:A:148:ARG:HD3	2.16	0.46
1:A:193:ILE:HG22	1:A:194:GLN:N	2.26	0.46
1:A:392:LEU:HD11	1:A:613:LYS:HB2	1.95	0.46
1:A:417:GLN:HG2	1:A:422:VAL:CG1	2.45	0.46
1:A:451:THR:OG1	1:A:452:LYS:N	2.45	0.46
1:A:708:ILE:HA	1:A:711:LYS:CE	2.29	0.46
3:C:73:VAL:HG12	3:C:108:PHE:CZ	2.50	0.46
4:D:104:LEU:HD23	4:D:105:LEU:N	2.30	0.46
1:A:295:LYS:C	1:A:297:PRO:HD3	2.36	0.46
1:A:408:VAL:CG2	1:A:410:ASN:H	2.27	0.46
1:A:498:LEU:O	1:A:501:GLU:HB2	2.15	0.46
1:A:578:HIS:HD2	1:A:591:ASN:HA	1.71	0.46
1:A:613:LYS:C	1:A:619:LEU:HD11	2.34	0.46
2:B:81:PHE:C	2:B:84:PHE:HB3	2.36	0.46
3:C:183:GLU:HA	3:C:186:VAL:HG12	1.97	0.46
4:E:294:TYR:HE1	4:E:321:ALA:HB2	1.76	0.46
1:A:130:LYS:HD3	1:A:132:LEU:CD1	2.32	0.46
1:A:408:VAL:CG2	1:A:409:GLY:N	2.78	0.46
2:B:108:LEU:CD2	2:B:120:PHE:HE2	2.28	0.46
4:D:134:VAL:HG12	4:D:375:PHE:OXT	2.15	0.46
1:A:9:ILE:HA	1:A:18:ARG:HD3	1.97	0.46
1:A:220:ASP:HA	1:A:223:ILE:HG12	1.97	0.46
2:B:82:THR:HG23	2:B:83:VAL:H	1.80	0.46
4:E:370:VAL:CG1	4:E:371:HIS:N	2.78	0.46
1:A:122:PHE:HE1	1:A:673:PHE:CB	2.27	0.46
1:A:129:TYR:OH	1:A:678:ILE:HG13	2.14	0.46
1:A:264:ASP:O	1:A:265:ILE:HD12	2.16	0.46
1:A:309:PRO:HB2	1:A:320:VAL:HG13	1.97	0.46
1:A:537:GLU:HA	1:A:540:CYS:SG	2.56	0.46
1:A:642:LYS:HG3	1:A:643:LYS:H	1.79	0.46
1:A:723:LYS:HB3	1:A:723:LYS:HZ3	1.81	0.46
4:E:65:LEU:HD13	4:E:67:LEU:CD2	2.45	0.46
4:E:321:ALA:HB1	4:E:322:PRO:CD	2.45	0.46
1:A:51:MET:O	1:A:62:VAL:HG23	2.16	0.46
1:A:475:LEU:HD22	1:A:595:TRP:CG	2.50	0.46
1:A:488:GLN:CB	1:A:584:TYR:CE2	2.98	0.46
1:A:680:ASN:OD1	1:A:687:VAL:HG11	2.16	0.46
1:A:819:GLN:OE1	2:B:130:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:LEU:C	3:C:70:LEU:HD13	2.36	0.46
4:D:90:PHE:CD2	4:D:98:PRO:HG3	2.51	0.46
4:D:180:LEU:HD12	4:D:181:ALA:H	1.80	0.46
4:E:116:ARG:HD3	4:E:370:VAL:HG13	1.98	0.46
1:A:99:GLU:HG2	1:A:100:PRO:N	2.31	0.46
1:A:255:GLY:CA	1:A:259:LYS:HG2	2.45	0.46
1:A:412:TYR:N	1:A:412:TYR:HD1	2.14	0.46
1:A:559:LEU:C	1:A:561:LYS:H	2.18	0.46
1:A:588:VAL:HG12	1:A:590:TYR:CE2	2.50	0.46
1:A:793:GLN:HE22	3:C:155:ALA:N	2.14	0.46
1:A:802:ARG:O	1:A:805:PHE:HB3	2.15	0.46
1:A:804:GLU:HB3	1:A:808:MET:HE1	1.97	0.46
1:A:805:PHE:O	1:A:808:MET:HB2	2.16	0.46
1:A:837:PHE:C	1:A:840:ILE:HG12	2.36	0.46
4:D:34:ILE:O	4:D:54:VAL:HG11	2.16	0.46
4:D:351:THR:OG1	4:D:352:PHE:CD1	2.68	0.46
1:A:408:VAL:CG1	1:A:412:TYR:CE1	2.99	0.46
1:A:614:SER:C	1:A:619:LEU:HD11	2.36	0.46
3:C:57:PHE:CD1	3:C:60:TYR:HE2	2.34	0.46
3:C:106:ILE:HG23	3:C:107:GLU:N	2.30	0.46
4:D:45:VAL:O	4:D:45:VAL:HG13	2.16	0.46
4:D:262:PHE:C	4:D:264:PRO:HD3	2.36	0.46
4:E:335:ARG:O	4:E:338:SER:HB3	2.16	0.46
1:A:22:LYS:HA	1:A:25:ILE:HG13	1.97	0.46
1:A:24:ARG:HA	1:A:24:ARG:HD2	1.72	0.46
1:A:60:VAL:HG12	1:A:61:THR:N	2.31	0.46
1:A:95:THR:CG2	1:A:96:HIS:ND1	2.79	0.46
1:A:261:ALA:HB1	1:A:453:GLN:O	2.16	0.46
1:A:755:VAL:HG21	1:A:760:TYR:CE1	2.51	0.46
1:A:761:ARG:HG2	1:A:761:ARG:NH1	2.31	0.46
4:D:298:VAL:HA	4:D:330:ILE:O	2.15	0.46
4:D:362:TYR:HE1	4:D:367:PRO:HG3	1.79	0.46
4:E:294:TYR:CD2	4:E:325:MET:SD	3.10	0.46
1:A:210:GLN:CG	1:A:212:GLY:N	2.79	0.45
1:A:535:ILE:CG2	1:A:553:LYS:HE2	2.39	0.45
1:A:541:MET:HE2	4:D:345:ILE:HG23	1.98	0.45
4:D:278:THR:O	4:D:282:ILE:HG13	2.15	0.45
4:E:181:ALA:O	4:E:185:LEU:HG	2.16	0.45
1:A:9:ILE:HA	1:A:18:ARG:CD	2.46	0.45
1:A:48:VAL:HG12	1:A:49:LYS:O	2.16	0.45
1:A:88:ILE:CD1	1:A:93:MET:CB	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:CD	1:A:688:MET:CG	2.94	0.45
1:A:260:LEU:HD13	1:A:261:ALA:C	2.36	0.45
1:A:644:LYS:HG2	1:A:649:GLN:HG3	1.98	0.45
1:A:825:PHE:CE1	2:B:161:ILE:HG21	2.51	0.45
2:B:122:GLU:HG3	2:B:137:ILE:CD1	2.46	0.45
3:C:162:LYS:O	3:C:165:GLU:HG2	2.16	0.45
4:D:164:PRO:HG3	4:D:281:SER:OG	2.16	0.45
4:E:34:ILE:CD1	4:E:69:TYR:CZ	2.98	0.45
4:E:140:LEU:HB3	4:E:343:GLY:N	2.32	0.45
4:E:244:ASP:CG	4:E:246:GLN:H	2.19	0.45
1:A:16:TYR:CG	1:A:134:VAL:CG2	2.99	0.45
1:A:130:LYS:HG3	1:A:685:PRO:CG	2.42	0.45
1:A:292:MET:HB2	1:A:309:PRO:HG3	1.98	0.45
1:A:396:GLU:CG	1:A:610:LEU:CD2	2.94	0.45
1:A:452:LYS:N	1:A:452:LYS:CD	2.79	0.45
1:A:557:GLN:CG	1:A:558:HIS:N	2.80	0.45
1:A:574:LYS:HB2	1:A:574:LYS:HE3	1.56	0.45
3:C:157:LEU:HB2	3:C:158:GLY:O	2.16	0.45
4:D:107:GLU:HG3	4:D:111:ASN:CB	2.46	0.45
1:A:36:LYS:HB3	1:A:51:MET:HB3	1.98	0.45
1:A:113:TRP:CE3	1:A:130:LYS:CE	2.95	0.45
1:A:160:ASP:HA	1:A:195:TYR:OH	2.17	0.45
1:A:253:HIS:HE2	1:A:264:ASP:CG	2.19	0.45
1:A:595:TRP:N	1:A:595:TRP:CD1	2.85	0.45
1:A:760:TYR:CD1	1:A:760:TYR:N	2.84	0.45
2:B:27:GLN:C	2:B:30:GLU:HB3	2.37	0.45
2:B:125:LEU:HB3	2:B:132:PHE:HD1	1.74	0.45
2:B:147:ASP:HA	2:B:148:VAL:HG23	1.98	0.45
4:D:153:LEU:HD13	4:D:162:ASN:ND2	2.31	0.45
4:E:346:LEU:HA	4:E:349:LEU:HG	1.99	0.45
1:A:16:TYR:HE2	1:A:132:LEU:HG	1.78	0.45
1:A:116:TYR:HB3	1:A:153:PRO:HG2	1.98	0.45
1:A:279:LEU:HD23	1:A:279:LEU:N	2.26	0.45
1:A:615:ALA:O	1:A:619:LEU:HD13	2.16	0.45
1:A:671:PRO:HB2	1:A:673:PHE:HE1	1.73	0.45
1:A:716:ARG:O	1:A:717:ILE:HG13	2.17	0.45
3:C:67:LYS:CD	3:C:92:VAL:CG1	2.92	0.45
3:C:73:VAL:CG1	3:C:108:PHE:CZ	2.99	0.45
3:C:83:ASN:HB2	3:C:84:PRO:CD	2.38	0.45
3:C:105:LYS:CD	3:C:106:ILE:N	2.79	0.45
4:D:58:ALA:CA	4:D:65:LEU:CD2	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:MET:HA	1:A:93:MET:HE1	1.96	0.45
1:A:295:LYS:HB2	1:A:328:SER:O	2.16	0.45
1:A:510:TRP:CZ2	1:A:512:PHE:HB2	2.51	0.45
1:A:717:ILE:HG22	1:A:718:LEU:O	2.16	0.45
1:A:805:PHE:CE1	3:C:53:PHE:HD1	2.34	0.45
1:A:825:PHE:CD1	2:B:161:ILE:HG21	2.51	0.45
4:E:17:VAL:C	4:E:18:LYS:HD3	2.37	0.45
4:E:191:LYS:HD2	4:E:191:LYS:HA	1.57	0.45
1:A:53:GLN:NE2	1:A:53:GLN:HA	2.31	0.45
1:A:62:VAL:HG22	1:A:63:LYS:N	2.32	0.45
1:A:81:ASN:OD1	1:A:96:HIS:HB2	2.17	0.45
1:A:110:TYR:CE2	1:A:686:GLY:N	2.84	0.45
1:A:205:LYS:HD3	1:A:257:THR:HG21	1.97	0.45
1:A:221:GLN:HG2	1:A:449:LEU:CD2	2.46	0.45
1:A:526:ILE:CD1	1:A:583:HIS:HE1	2.28	0.45
1:A:583:HIS:CB	1:A:585:ALA:CB	2.94	0.45
1:A:738:GLN:HG2	1:A:738:GLN:O	2.16	0.45
1:A:833:TRP:CZ2	2:B:71:MET:CE	2.99	0.45
1:A:836:LEU:HA	1:A:839:LYS:CG	2.47	0.45
4:E:236:LEU:HD22	4:E:252:ASN:N	2.32	0.45
4:E:236:LEU:HD22	4:E:251:GLY:O	2.17	0.45
1:A:39:PHE:HZ	1:A:80:MET:CE	2.30	0.45
1:A:314:PHE:CE2	1:A:362:GLY:CA	2.97	0.45
1:A:392:LEU:HD22	1:A:392:LEU:N	2.30	0.45
1:A:462:LEU:CD1	1:A:464:ILE:CG2	2.94	0.45
1:A:499:GLU:O	1:A:503:TYR:HD1	2.00	0.45
1:A:528:LYS:HB2	1:A:529:PRO:CD	2.46	0.45
1:A:727:ARG:HH12	1:A:745:ALA:HB1	1.77	0.45
1:A:757:ARG:NH1	1:A:757:ARG:HG2	2.31	0.45
2:B:58:MET:CE	2:B:60:ARG:CB	2.95	0.45
2:B:146:PRO:HD3	2:B:157:ILE:HG22	1.99	0.45
3:C:46:SER:N	3:C:49:GLN:H	2.12	0.45
3:C:67:LYS:HD2	3:C:92:VAL:CG1	2.47	0.45
3:C:122:LYS:HD2	3:C:122:LYS:HA	1.86	0.45
4:D:299:MET:CE	4:D:309:ILE:CG2	2.94	0.45
4:D:370:VAL:HG12	4:D:371:HIS:N	2.32	0.45
4:E:16:LEU:HB2	4:E:18:LYS:HZ3	1.82	0.45
4:E:106:THR:HA	4:E:135:ALA:H	1.82	0.45
4:E:129:VAL:O	4:E:129:VAL:HG23	2.14	0.45
4:E:287:ILE:HG12	4:E:288:ASP:OD1	2.16	0.45
4:E:329:ILE:O	4:E:329:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ALA:HA	1:A:139:VAL:CG2	2.45	0.45
1:A:27:ALA:CB	1:A:87:LYS:HE2	2.47	0.45
1:A:136:ASN:HA	1:A:137:PRO:HD3	1.69	0.45
1:A:277:PHE:CG	1:A:278:GLN:N	2.84	0.45
1:A:795:LEU:HA	3:C:80:LEU:HD21	1.99	0.45
1:A:799:TYR:CE2	3:C:170:MET:HE3	2.52	0.45
3:C:135:ARG:HD3	3:C:140:GLU:N	2.28	0.45
4:E:211:ASP:CG	4:E:215:LYS:HE3	2.38	0.45
4:E:221:LEU:HD12	4:E:221:LEU:HA	1.85	0.45
1:A:17:LEU:HD22	1:A:17:LEU:N	2.31	0.45
1:A:254:PHE:N	1:A:254:PHE:CD1	2.84	0.45
1:A:296:LYS:HB3	1:A:331:LEU:HD11	1.99	0.45
1:A:472:PHE:HZ	1:A:591:ASN:OD1	2.00	0.45
1:A:482:PHE:CE1	1:A:526:ILE:HB	2.52	0.45
1:A:648:PHE:CG	1:A:649:GLN:N	2.83	0.45
2:B:58:MET:HE3	2:B:60:ARG:CB	2.46	0.45
3:C:58:LEU:HG	3:C:64:GLY:C	2.38	0.45
4:D:36:GLY:N	4:D:54:VAL:CG2	2.80	0.45
4:E:39:ARG:NE	4:E:66:THR:HB	2.28	0.45
1:A:85:PHE:HE1	1:A:93:MET:O	2.00	0.44
1:A:155:ILE:HD12	1:A:191:ARG:CG	2.47	0.44
1:A:210:GLN:HG3	1:A:212:GLY:N	2.32	0.44
1:A:237:THR:HG22	1:A:274:ARG:NH2	2.32	0.44
1:A:245:ARG:CG	1:A:285:TYR:CE1	2.94	0.44
1:A:260:LEU:O	1:A:453:GLN:CB	2.65	0.44
1:A:322:VAL:HG12	1:A:323:ALA:N	2.31	0.44
1:A:358:VAL:HG22	1:A:430:ALA:CA	2.33	0.44
1:A:508:ILE:HD13	1:A:508:ILE:N	2.32	0.44
1:A:748:LYS:HE3	1:A:748:LYS:HB2	1.68	0.44
3:C:70:LEU:HB3	3:C:91:LYS:CE	2.45	0.44
3:C:134:LEU:H	3:C:134:LEU:HD12	1.82	0.44
4:D:192:ILE:HG22	4:D:256:ARG:NH1	2.32	0.44
4:D:341:ILE:HG22	4:D:345:ILE:HD11	1.99	0.44
4:E:35:VAL:CA	4:E:54:VAL:CG2	2.95	0.44
1:A:91:MET:CE	1:A:102:VAL:HA	2.40	0.44
1:A:219:GLU:CD	1:A:219:GLU:H	2.13	0.44
1:A:245:ARG:HA	1:A:245:ARG:HE	1.82	0.44
1:A:295:LYS:HB3	1:A:331:LEU:CG	2.47	0.44
1:A:648:PHE:CD1	1:A:649:GLN:NE2	2.85	0.44
3:C:54:LYS:HZ1	3:C:73:VAL:HG11	1.82	0.44
4:D:24:ASP:HB2	4:D:340:TRP:HH2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:38:PRO:CD	4:D:49:GLN:HE22	2.28	0.44
4:E:34:ILE:HG21	4:E:67:LEU:CB	2.46	0.44
4:E:162:ASN:HD22	4:E:278:THR:HA	1.82	0.44
1:A:16:TYR:CZ	1:A:132:LEU:HG	2.51	0.44
1:A:19:LYS:N	1:A:114:MET:CE	2.81	0.44
1:A:41:VAL:HG23	1:A:78:PHE:CE1	2.53	0.44
1:A:167:LEU:O	1:A:170:ARG:HG2	2.17	0.44
1:A:301:ASP:O	1:A:304:LEU:HD23	2.18	0.44
1:A:698:ARG:CG	1:A:703:LEU:CD1	2.95	0.44
1:A:730:ASN:CB	1:A:749:LEU:HD13	2.36	0.44
1:A:805:PHE:CE1	3:C:53:PHE:CE1	3.06	0.44
2:B:51:LEU:CD1	2:B:71:MET:CE	2.95	0.44
2:B:52:ARG:CZ	2:B:64:LYS:HG2	2.47	0.44
4:D:169:TYR:CE1	4:E:42:GLY:HA2	2.52	0.44
4:D:332:PRO:HA	4:D:333:PRO:HD3	1.71	0.44
1:A:47:TYR:N	1:A:47:TYR:CD1	2.85	0.44
1:A:107:LYS:HA	1:A:688:MET:CG	2.46	0.44
1:A:187:VAL:O	1:A:190:LYS:HB2	2.18	0.44
1:A:245:ARG:NH1	1:A:274:ARG:HD2	2.33	0.44
1:A:283:ARG:NE	1:A:322:VAL:HG21	2.32	0.44
1:A:412:TYR:N	1:A:412:TYR:CD1	2.85	0.44
1:A:526:ILE:HG22	1:A:533:PHE:HD1	1.82	0.44
3:C:140:GLU:OE1	3:C:180:ILE:HG12	2.18	0.44
4:D:158:GLY:CA	4:D:183:ARG:CD	2.95	0.44
4:D:180:LEU:HD21	4:D:261:LEU:HA	1.99	0.44
4:D:335:ARG:HH21	4:D:338:SER:HB2	1.81	0.44
4:D:370:VAL:CG1	4:D:371:HIS:N	2.81	0.44
4:E:65:LEU:CD1	4:E:67:LEU:CD2	2.95	0.44
1:A:235:ALA:HA	1:A:286:HIS:ND1	2.32	0.44
1:A:253:HIS:CD2	1:A:253:HIS:N	2.86	0.44
1:A:260:LEU:O	1:A:453:GLN:HB3	2.17	0.44
1:A:642:LYS:CG	1:A:643:LYS:N	2.80	0.44
1:A:802:ARG:CZ	1:A:802:ARG:HB2	2.47	0.44
2:B:97:PRO:HD2	2:B:100:VAL:CG1	2.48	0.44
3:C:131:VAL:HG21	3:C:179:CYS:O	2.17	0.44
3:C:180:ILE:CD1	3:C:181:ASN:N	2.79	0.44
4:D:223:PHE:CD1	4:D:259:GLU:HG2	2.53	0.44
4:D:223:PHE:HB2	4:D:259:GLU:OE2	2.17	0.44
4:D:251:GLY:CA	4:D:254:ARG:HG3	2.24	0.44
4:E:108:ALA:HB1	4:E:109:PRO:HD2	1.98	0.44
1:A:205:LYS:CG	1:A:206:LYS:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:THR:CG2	1:A:437:MET:CE	2.95	0.44
1:A:445:ILE:HG23	1:A:446:ASN:N	2.33	0.44
1:A:789:MET:CE	3:C:130:PHE:CZ	3.01	0.44
1:A:802:ARG:NH2	1:A:802:ARG:HB3	2.33	0.44
2:B:51:LEU:HD12	2:B:68:LEU:CD1	2.48	0.44
2:B:166:ALA:O	2:B:167:LYS:HD3	2.18	0.44
3:C:163:GLU:HG3	3:C:163:GLU:O	2.15	0.44
4:D:27:PRO:HG3	4:D:340:TRP:CG	2.52	0.44
4:D:70:PRO:HG3	4:D:81:ASP:HB3	1.99	0.44
4:D:280:ASN:O	4:D:284:LYS:HG3	2.16	0.44
4:E:36:GLY:HA3	4:E:66:THR:O	2.18	0.44
4:E:53:TYR:HD1	4:E:53:TYR:HA	1.42	0.44
1:A:16:TYR:CD1	1:A:134:VAL:CG2	2.96	0.44
1:A:81:ASN:HD22	1:A:94:MET:CE	2.29	0.44
1:A:245:ARG:HA	1:A:245:ARG:NE	2.33	0.44
1:A:496:PHE:CD1	1:A:514:ASP:HA	2.53	0.44
1:A:517:MET:HE3	1:A:517:MET:HB2	1.63	0.44
1:A:642:LYS:HG3	1:A:643:LYS:N	2.32	0.44
1:A:735:PRO:O	1:A:739:PHE:HB2	2.17	0.44
2:B:154:TYR:HD1	2:B:155:LYS:N	2.15	0.44
4:D:39:ARG:HD2	4:D:65:LEU:O	2.18	0.44
4:E:8:LEU:HD11	4:E:96:VAL:HG21	2.00	0.44
4:E:261:LEU:HB3	4:E:274:ILE:HD11	2.00	0.44
1:A:70:LEU:N	1:A:70:LEU:HD12	2.33	0.44
1:A:246:PHE:N	1:A:246:PHE:CD1	2.85	0.44
1:A:283:ARG:CD	1:A:322:VAL:HG23	2.45	0.44
1:A:368:GLN:CG	1:A:376:GLU:HB3	2.48	0.44
1:A:693:VAL:O	1:A:696:GLN:HB2	2.18	0.44
1:A:778:GLU:OE1	1:A:778:GLU:HA	2.18	0.44
1:A:790:THR:HG23	1:A:791:ARG:HD2	1.98	0.44
4:E:282:ILE:HG12	4:E:293:LEU:HD13	1.99	0.44
1:A:16:TYR:CZ	1:A:132:LEU:CB	2.94	0.44
1:A:32:PHE:HD2	1:A:83:PRO:HD3	1.83	0.44
1:A:33:ASP:CG	1:A:35:LYS:H	2.21	0.44
1:A:175:ILE:HD11	1:A:461:VAL:HG13	1.97	0.44
1:A:380:THR:O	1:A:380:THR:HG22	2.17	0.44
1:A:406:VAL:HB	1:A:605:GLU:OE2	2.17	0.44
1:A:519:LEU:HD22	1:A:584:TYR:CB	2.43	0.44
1:A:536:LEU:CD1	1:A:596:LEU:CD2	2.95	0.44
1:A:603:LEU:HD22	1:A:603:LEU:HA	1.76	0.44
1:A:700:ASN:HB3	1:A:702:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:ILE:HG13	1:A:823:ARG:N	2.32	0.44
1:A:825:PHE:CD1	1:A:828:VAL:HG13	2.53	0.44
2:B:58:MET:CE	2:B:60:ARG:HH11	2.30	0.44
2:B:88:PHE:HD2	2:B:91:LYS:HE2	1.82	0.44
1:A:22:LYS:HA	1:A:25:ILE:CG1	2.48	0.43
1:A:99:GLU:OE1	1:A:694:MET:HG3	2.17	0.43
1:A:325:ILE:CG1	1:A:326:ASP:N	2.81	0.43
1:A:415:LYS:HB2	1:A:415:LYS:HE2	1.40	0.43
1:A:418:ASN:CB	1:A:420:GLN:HE22	2.31	0.43
1:A:463:ASP:C	1:A:464:ILE:HG22	2.38	0.43
1:A:693:VAL:CA	1:A:696:GLN:HG3	2.42	0.43
2:B:115:THR:CG2	2:B:154:TYR:CE2	2.96	0.43
2:B:137:ILE:CD1	2:B:141:TRP:NE1	2.79	0.43
4:D:50:LYS:HG3	4:D:53:TYR:CE2	2.53	0.43
4:D:53:TYR:HD1	4:D:53:TYR:HA	1.57	0.43
4:E:347:ALA:O	4:E:356:TRP:HZ2	2.01	0.43
1:A:117:THR:CG2	1:A:118:TYR:N	2.81	0.43
1:A:210:GLN:HE21	1:A:211:PRO:HD2	1.83	0.43
1:A:262:SER:CB	1:A:455:ARG:HH21	2.31	0.43
1:A:283:ARG:HD3	1:A:322:VAL:CG2	2.46	0.43
1:A:792:THR:HG1	3:C:127:TYR:HE1	1.64	0.43
2:B:68:LEU:HD12	2:B:71:MET:HE1	1.99	0.43
3:C:142:ASN:C	3:C:177:ASN:H	2.21	0.43
4:E:236:LEU:HD12	4:E:237:GLU:N	2.34	0.43
4:E:342:GLY:HA2	4:E:345:ILE:HD12	2.01	0.43
1:A:17:LEU:N	1:A:17:LEU:CD2	2.80	0.43
1:A:155:ILE:CD1	1:A:191:ARG:CB	2.96	0.43
1:A:198:THR:CG2	1:A:199:ILE:N	2.81	0.43
1:A:255:GLY:CA	1:A:455:ARG:HA	2.48	0.43
1:A:380:THR:CB	1:A:398:LEU:HD11	2.49	0.43
1:A:452:LYS:H	1:A:452:LYS:HD2	1.84	0.43
1:A:588:VAL:CG1	1:A:589:ASP:N	2.80	0.43
1:A:592:ILE:O	1:A:595:TRP:CD1	2.71	0.43
1:A:796:CYS:O	1:A:799:TYR:HB3	2.19	0.43
1:A:822:ILE:CD1	2:B:132:PHE:CE2	2.94	0.43
2:B:98:GLU:HB3	2:B:99:ASP:H	1.50	0.43
4:E:8:LEU:CD1	4:E:90:PHE:CE1	2.97	0.43
1:A:16:TYR:HB3	1:A:115:ILE:HD11	2.00	0.43
1:A:139:VAL:O	1:A:142:ALA:HB3	2.18	0.43
1:A:439:LEU:HD13	1:A:439:LEU:C	2.39	0.43
2:B:55:PHE:CG	2:B:62:ASN:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:78:ASN:O	4:D:82:MET:HB2	2.18	0.43
4:D:335:ARG:HD2	4:D:338:SER:HB3	1.99	0.43
4:E:158:GLY:CA	4:E:181:ALA:CB	2.96	0.43
4:E:164:PRO:CG	4:E:174:ALA:HB1	2.44	0.43
1:A:214:MET:O	1:A:215:GLN:HG3	2.18	0.43
1:A:348:LYS:HA	1:A:351:ILE:CG2	2.47	0.43
1:A:370:GLN:HG2	1:A:373:GLU:O	2.18	0.43
1:A:406:VAL:CG1	1:A:414:THR:CG2	2.95	0.43
1:A:452:LYS:HE2	1:A:452:LYS:N	2.34	0.43
1:A:551:LYS:CG	1:A:555:TYR:CE2	2.94	0.43
1:A:724:GLN:CG	1:A:725:ARG:N	2.81	0.43
1:A:795:LEU:CA	3:C:80:LEU:HD21	2.49	0.43
3:C:140:GLU:CB	3:C:180:ILE:CD1	2.93	0.43
4:D:44:MET:HG3	4:D:46:GLY:O	2.18	0.43
4:D:189:LEU:HD23	4:D:209:VAL:HG12	1.98	0.43
4:E:103:THR:CG2	4:E:105:LEU:CD2	2.96	0.43
4:E:369:ILE:CG2	4:E:370:VAL:N	2.81	0.43
1:A:93:MET:CE	1:A:93:MET:CA	2.95	0.43
1:A:128:PRO:CG	1:A:132:LEU:HD21	2.48	0.43
1:A:820:TYR:HE1	1:A:821:ASN:HD21	1.67	0.43
3:C:67:LYS:H	3:C:103:ALA:H	1.67	0.43
4:D:31:PHE:HB2	4:D:32:PRO:CD	2.48	0.43
1:A:31:PRO:O	1:A:32:PHE:HB2	2.19	0.43
1:A:407:LYS:CG	1:A:408:VAL:H	2.32	0.43
1:A:524:GLU:HA	1:A:527:GLU:CG	2.47	0.43
1:A:592:ILE:O	1:A:592:ILE:HG22	2.19	0.43
1:A:726:TYR:N	1:A:726:TYR:CD1	2.82	0.43
1:A:793:GLN:HE22	3:C:156:THR:N	2.11	0.43
1:A:795:LEU:CD1	3:C:186:VAL:HG22	2.49	0.43
1:A:835:ASN:O	1:A:839:LYS:HG2	2.18	0.43
3:C:112:LEU:HD22	3:C:112:LEU:HA	1.53	0.43
4:D:272:ALA:HB3	4:D:277:THR:HG23	2.00	0.43
4:E:158:GLY:N	4:E:181:ALA:CB	2.81	0.43
1:A:81:ASN:HA	1:A:82:PRO:HD3	1.66	0.43
1:A:103:LEU:CD1	1:A:688:MET:CB	2.97	0.43
1:A:176:LEU:CD1	1:A:673:PHE:CD2	2.96	0.43
1:A:348:LYS:C	1:A:351:ILE:HG22	2.38	0.43
1:A:408:VAL:HG11	1:A:412:TYR:CE1	2.54	0.43
1:A:476:GLU:H	1:A:476:GLU:CD	2.21	0.43
1:A:790:THR:CG2	1:A:791:ARG:N	2.81	0.43
1:A:831:TRP:CE3	1:A:834:MET:SD	3.12	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:ILE:CG2	2:B:127:THR:N	2.82	0.43
4:D:236:LEU:HB2	4:D:251:GLY:C	2.39	0.43
4:D:242:LEU:HG	4:D:246:GLN:O	2.18	0.43
4:E:94:LEU:HD23	4:E:94:LEU:HA	1.96	0.43
4:E:272:ALA:HB1	4:E:276:GLU:HB2	2.01	0.43
1:A:99:GLU:O	1:A:102:VAL:N	2.51	0.43
1:A:154:HIS:O	1:A:157:SER:HB2	2.19	0.43
1:A:163:TYR:CE2	1:A:167:LEU:HD11	2.54	0.43
1:A:338:ILE:CG2	1:A:339:ASP:N	2.82	0.43
1:A:358:VAL:HG23	1:A:433:VAL:HG11	2.01	0.43
1:A:406:VAL:O	1:A:411:GLU:HB3	2.19	0.43
1:A:529:PRO:HG3	4:D:4:GLU:OE2	2.19	0.43
1:A:550:PHE:CE2	1:A:554:LEU:HD11	2.53	0.43
1:A:636:GLY:HA2	1:A:637:SER:HA	1.74	0.43
1:A:698:ARG:HG2	1:A:703:LEU:HD13	2.01	0.43
1:A:800:LEU:CG	3:C:162:LYS:HG2	2.49	0.43
1:A:825:PHE:CA	1:A:828:VAL:CG1	2.94	0.43
2:B:51:LEU:HD12	2:B:68:LEU:HD11	2.00	0.43
2:B:124:LEU:O	2:B:128:GLN:HB3	2.19	0.43
3:C:108:PHE:CZ	3:C:112:LEU:CG	2.99	0.43
3:C:118:ILE:HA	3:C:119:SER:OG	2.18	0.43
4:D:143:TYR:O	4:D:143:TYR:HD1	2.02	0.43
4:D:153:LEU:HD13	4:D:162:ASN:HD22	1.84	0.43
1:A:30:ARG:HH21	1:A:30:ARG:HD2	1.72	0.43
1:A:39:PHE:HA	1:A:49:LYS:HA	2.00	0.43
1:A:147:LYS:HG2	1:A:149:GLN:OE1	2.19	0.43
1:A:222:ILE:CD1	1:A:449:LEU:HD21	2.49	0.43
1:A:239:ARG:NH2	1:A:470:PHE:HA	2.34	0.43
1:A:415:LYS:CE	4:D:333:PRO:HG2	2.48	0.43
1:A:418:ASN:CG	1:A:420:GLN:HE22	2.22	0.43
1:A:433:VAL:CG1	1:A:434:TYR:N	2.82	0.43
1:A:588:VAL:CG1	1:A:590:TYR:CE2	3.01	0.43
2:B:55:PHE:CA	2:B:58:MET:HB3	2.48	0.43
3:C:108:PHE:CE1	3:C:112:LEU:HD23	2.53	0.43
3:C:134:LEU:HD21	3:C:150:LEU:CG	2.44	0.43
3:C:134:LEU:O	3:C:136:VAL:HB	2.19	0.43
3:C:135:ARG:HG2	3:C:138:ASP:HA	2.00	0.43
4:D:65:LEU:H	4:D:65:LEU:HG	1.54	0.43
4:D:262:PHE:CB	4:D:312:ARG:HH21	2.31	0.43
4:E:183:ARG:CG	4:E:184:ASP:N	2.82	0.43
1:A:16:TYR:CB	1:A:134:VAL:CG2	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ARG:HG3	1:A:470:PHE:CE2	2.54	0.42
1:A:462:LEU:HD11	1:A:464:ILE:HG22	2.00	0.42
1:A:736:GLU:HG2	1:A:737:GLY:H	1.84	0.42
2:B:170:GLU:OE2	2:B:170:GLU:HA	2.18	0.42
3:C:57:PHE:CD1	3:C:60:TYR:CE2	3.07	0.42
4:D:309:ILE:CG2	4:D:310:ALA:N	2.82	0.42
4:E:287:ILE:CG1	4:E:288:ASP:N	2.82	0.42
4:E:309:ILE:CG2	4:E:310:ALA:N	2.81	0.42
1:A:19:LYS:NZ	1:A:112:ALA:HB1	2.34	0.42
1:A:19:LYS:HA	1:A:114:MET:HE1	2.01	0.42
1:A:76:GLN:O	1:A:78:PHE:CE1	2.72	0.42
1:A:279:LEU:CD2	1:A:279:LEU:N	2.82	0.42
1:A:339:ASP:O	1:A:342:GLY:HA2	2.19	0.42
1:A:401:LEU:N	1:A:401:LEU:CD2	2.82	0.42
1:A:413:VAL:O	1:A:413:VAL:HG13	2.17	0.42
1:A:452:LYS:N	1:A:452:LYS:HD2	2.34	0.42
1:A:820:TYR:CE1	1:A:821:ASN:ND2	2.88	0.42
1:A:836:LEU:O	1:A:839:LYS:HG2	2.19	0.42
2:B:25:GLN:HE21	2:B:29:GLN:CD	2.22	0.42
2:B:58:MET:HE3	2:B:60:ARG:HE	1.83	0.42
2:B:118:LYS:HE3	2:B:141:TRP:CZ3	2.54	0.42
3:C:122:LYS:C	3:C:187:LYS:HE2	2.39	0.42
3:C:131:VAL:HG12	3:C:132:GLU:N	2.33	0.42
3:C:145:VAL:CG2	3:C:146:MET:N	2.82	0.42
4:D:152:VAL:O	4:D:162:ASN:HA	2.19	0.42
1:A:488:GLN:CG	1:A:584:TYR:HE2	2.28	0.42
2:B:160:VAL:O	2:B:165:ASP:HA	2.20	0.42
4:E:349:LEU:HB3	4:E:352:PHE:HB2	2.01	0.42
1:A:39:PHE:CG	1:A:100:PRO:CG	3.02	0.42
1:A:87:LYS:N	1:A:87:LYS:HD3	2.35	0.42
1:A:295:LYS:HB2	1:A:331:LEU:HB3	1.98	0.42
1:A:369:LYS:HB3	1:A:369:LYS:HE2	1.92	0.42
1:A:407:LYS:CG	1:A:408:VAL:N	2.82	0.42
2:B:42:ARG:HA	2:B:43:ASP:HA	1.77	0.42
2:B:144:PHE:CG	2:B:144:PHE:O	2.72	0.42
2:B:160:VAL:HA	2:B:165:ASP:CB	2.50	0.42
3:C:135:ARG:HH11	3:C:141:GLY:N	2.11	0.42
3:C:170:MET:SD	3:C:185:PHE:HB3	2.59	0.42
4:D:297:ASN:N	4:D:297:ASN:HD22	2.18	0.42
4:D:369:ILE:CG2	4:D:370:VAL:N	2.82	0.42
1:A:188:ASN:HD22	1:A:188:ASN:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ILE:CG2	1:A:306:SER:N	2.82	0.42
1:A:312:PHE:HA	1:A:313:PRO:HD3	1.89	0.42
1:A:380:THR:CG2	1:A:398:LEU:CD1	2.97	0.42
1:A:415:LYS:HE3	4:D:333:PRO:HG3	2.01	0.42
1:A:475:LEU:N	1:A:595:TRP:CZ2	2.87	0.42
1:A:734:ILE:HA	1:A:735:PRO:HD3	1.70	0.42
1:A:789:MET:HE1	3:C:150:LEU:HD11	1.95	0.42
1:A:820:TYR:O	1:A:823:ARG:HB3	2.19	0.42
2:B:152:VAL:CG1	2:B:153:ASP:N	2.82	0.42
3:C:159:GLU:CG	3:C:162:LYS:HG3	2.50	0.42
3:C:170:MET:SD	3:C:186:VAL:CA	3.08	0.42
3:C:190:MET:HE3	3:C:190:MET:C	2.40	0.42
4:D:279:TYR:HB2	4:D:320:LEU:CD1	2.48	0.42
4:E:152:VAL:CG1	4:E:153:LEU:N	2.83	0.42
4:E:170:ALA:O	4:E:172:PRO:HD3	2.19	0.42
4:E:300:SER:O	4:E:304:THR:CG2	2.67	0.42
4:E:300:SER:O	4:E:304:THR:HG23	2.18	0.42
1:A:6:GLU:O	1:A:7:MET:HB2	2.20	0.42
1:A:406:VAL:HG12	1:A:605:GLU:CB	2.38	0.42
1:A:478:LEU:O	1:A:478:LEU:HD12	2.18	0.42
1:A:506:GLU:CB	1:A:508:ILE:CD1	2.94	0.42
1:A:573:GLY:N	1:A:574:LYS:HA	2.33	0.42
1:A:671:PRO:HB2	1:A:673:PHE:CZ	2.53	0.42
1:A:717:ILE:CG2	1:A:718:LEU:N	2.82	0.42
2:B:74:GLU:O	2:B:75:ALA:HB2	2.19	0.42
2:B:137:ILE:CG2	2:B:138:LYS:N	2.82	0.42
3:C:95:ASN:N	3:C:96:PRO:HD3	2.34	0.42
3:C:108:PHE:CZ	3:C:112:LEU:CD2	3.02	0.42
4:D:21:PHE:CZ	4:D:96:VAL:HG11	2.55	0.42
4:D:64:ILE:CG2	4:D:65:LEU:N	2.82	0.42
4:D:65:LEU:HD13	4:D:67:LEU:CD2	2.48	0.42
4:D:286:ASP:O	4:D:290:ARG:HG3	2.20	0.42
4:E:242:LEU:HB2	4:E:244:ASP:OD1	2.20	0.42
4:E:332:PRO:HD2	4:E:335:ARG:HG2	2.01	0.42
1:A:80:MET:CG	1:A:81:ASN:H	2.33	0.42
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.76	0.42
1:A:151:ALA:HB1	1:A:152:PRO:CD	2.49	0.42
1:A:172:ASN:HB3	1:A:458:PHE:O	2.19	0.42
1:A:207:LYS:HZ3	1:A:453:GLN:HG2	1.84	0.42
1:A:210:GLN:HG3	1:A:212:GLY:H	1.85	0.42
1:A:287:ILE:H	1:A:287:ILE:HG13	1.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLU:OE2	1:A:319:GLU:HA	2.19	0.42
1:A:475:LEU:CD2	1:A:595:TRP:HB3	2.48	0.42
1:A:608:VAL:O	1:A:612:GLN:HG3	2.20	0.42
1:A:697:LEU:O	1:A:700:ASN:HB2	2.19	0.42
1:A:787:THR:HB	1:A:791:ARG:NH1	2.35	0.42
1:A:788:LEU:CD1	1:A:788:LEU:N	2.83	0.42
1:A:811:ARG:NH1	2:B:120:PHE:CZ	2.87	0.42
3:C:115:LEU:HD13	3:C:115:LEU:C	2.39	0.42
4:E:134:VAL:HB	4:E:375:PHE:OXT	2.20	0.42
4:E:236:LEU:O	4:E:251:GLY:HA2	2.19	0.42
4:E:357:ILE:N	4:E:357:ILE:HD13	2.35	0.42
1:A:144:ARG:NH2	1:A:198:THR:HG23	2.34	0.42
1:A:170:ARG:O	1:A:457:TYR:CZ	2.73	0.42
1:A:177:ILE:HD13	1:A:177:ILE:HA	1.86	0.42
1:A:188:ASN:HD22	1:A:188:ASN:H	1.67	0.42
1:A:230:GLU:HB2	1:A:234:ASN:CG	2.40	0.42
1:A:249:PHE:CD2	1:A:251:ARG:CG	3.02	0.42
1:A:458:PHE:CD1	1:A:458:PHE:C	2.93	0.42
1:A:755:VAL:HG23	1:A:760:TYR:CE1	2.52	0.42
1:A:801:MET:O	1:A:804:GLU:HB2	2.19	0.42
1:A:804:GLU:C	1:A:808:MET:HE2	2.40	0.42
1:A:811:ARG:HG2	1:A:815:ILE:HG13	2.01	0.42
3:C:85:THR:CG2	3:C:86:ASN:N	2.82	0.42
3:C:183:GLU:O	3:C:187:LYS:HB2	2.19	0.42
3:C:187:LYS:HD2	3:C:187:LYS:HA	1.48	0.42
4:D:99:GLU:HG2	4:D:100:GLU:HG2	2.02	0.42
4:D:155:SER:O	4:D:301:GLY:HA3	2.20	0.42
4:D:275:HIS:CG	4:D:276:GLU:N	2.87	0.42
4:D:316:GLU:HA	4:D:316:GLU:OE1	2.19	0.42
4:D:357:ILE:HA	4:D:357:ILE:HD12	1.85	0.42
4:D:357:ILE:CG2	4:D:358:THR:N	2.83	0.42
4:D:357:ILE:HG13	4:D:370:VAL:HG23	1.96	0.42
1:A:232:PHE:CG	1:A:287:ILE:CG2	2.94	0.42
1:A:340:ILE:CG2	1:A:341:LEU:N	2.83	0.42
1:A:349:VAL:CG1	1:A:350:GLY:N	2.82	0.42
1:A:600:LYS:HG2	1:A:602:PRO:HD3	2.01	0.42
2:B:61:LEU:CD2	2:B:62:ASN:N	2.80	0.42
2:B:157:ILE:O	2:B:160:VAL:HG13	2.19	0.42
4:D:202:THR:OG1	4:D:205:GLU:HG3	2.18	0.42
4:D:335:ARG:O	4:D:338:SER:HB3	2.20	0.42
4:E:150:GLY:HA3	4:E:296:ASN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:193:LEU:HD23	4:E:193:LEU:HA	1.71	0.42
1:A:41:VAL:HB	1:A:76:GLN:NE2	2.35	0.42
1:A:81:ASN:HB2	1:A:94:MET:HE3	2.02	0.42
1:A:113:TRP:CZ3	1:A:132:LEU:HD12	2.54	0.42
1:A:155:ILE:HG21	1:A:192:VAL:HG13	2.01	0.42
1:A:261:ALA:H	1:A:455:ARG:HB3	1.85	0.42
1:A:289:TYR:CD1	1:A:320:VAL:O	2.73	0.42
1:A:419:VAL:CG1	1:A:420:GLN:N	2.83	0.42
1:A:796:CYS:O	1:A:800:LEU:HD23	2.20	0.42
3:C:57:PHE:HA	3:C:60:TYR:CE2	2.52	0.42
3:C:88:GLU:CG	3:C:89:VAL:N	2.83	0.42
3:C:92:VAL:HG22	3:C:95:ASN:CA	2.37	0.42
3:C:182:TYR:CD2	3:C:182:TYR:C	2.94	0.42
4:D:113:LYS:HB3	4:D:371:HIS:CD2	2.55	0.42
4:D:371:HIS:CD2	4:D:372:ARG:HH11	2.38	0.42
4:E:67:LEU:HD23	4:E:67:LEU:N	2.35	0.42
4:E:120:THR:HA	4:E:132:MET:HE1	2.02	0.42
4:E:190:MET:CE	4:E:206:ARG:CG	2.98	0.42
1:A:2:SER:O	1:A:3:SER:CB	2.68	0.41
1:A:76:GLN:O	1:A:76:GLN:HG3	2.20	0.41
1:A:111:ALA:N	1:A:686:GLY:HA2	2.35	0.41
2:B:157:ILE:CG1	2:B:158:CYS:N	2.82	0.41
2:B:160:VAL:HG13	2:B:161:ILE:N	2.35	0.41
3:C:120:ASN:HD22	3:C:120:ASN:HA	1.41	0.41
3:C:170:MET:SD	3:C:186:VAL:HB	2.60	0.41
1:A:103:LEU:HD11	1:A:107:LYS:CD	2.45	0.41
1:A:170:ARG:HB3	1:A:457:TYR:CZ	2.55	0.41
1:A:388:TYR:C	1:A:388:TYR:HD2	2.24	0.41
1:A:406:VAL:CG1	1:A:414:THR:HG23	2.49	0.41
1:A:486:LYS:HB3	1:A:486:LYS:HE3	1.93	0.41
1:A:802:ARG:CZ	1:A:802:ARG:CB	2.99	0.41
1:A:844:LEU:N	1:A:844:LEU:CD2	2.84	0.41
2:B:39:ASP:C	2:B:41:ASN:H	2.23	0.41
2:B:60:ARG:HB2	2:B:60:ARG:HE	1.48	0.41
3:C:42:LYS:HZ3	3:C:113:PRO:CG	2.34	0.41
3:C:68:ILE:CG2	3:C:69:THR:N	2.83	0.41
3:C:123:ASP:O	3:C:127:TYR:CD2	2.73	0.41
4:D:117:GLU:HG2	4:D:367:PRO:HB2	2.02	0.41
4:D:140:LEU:HD22	4:D:343:GLY:HA2	2.02	0.41
4:D:227:MET:O	4:D:230:ALA:HB3	2.19	0.41
1:A:295:LYS:O	1:A:295:LYS:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:PHE:CZ	1:A:527:GLU:HB3	2.54	0.41
3:C:192:ILE:O	3:C:192:ILE:HG23	2.20	0.41
4:D:97:ALA:HA	4:D:98:PRO:HD3	1.67	0.41
4:D:207:GLU:HA	4:D:207:GLU:OE2	2.20	0.41
4:E:132:MET:HE2	4:E:132:MET:HB2	1.89	0.41
4:E:143:TYR:CD2	4:E:346:LEU:HB2	2.54	0.41
4:E:317:ILE:HD13	4:E:317:ILE:HA	1.70	0.41
1:A:125:THR:O	1:A:125:THR:HG23	2.19	0.41
1:A:245:ARG:NH2	1:A:274:ARG:HE	2.17	0.41
1:A:351:ILE:CG1	1:A:437:MET:CE	2.95	0.41
1:A:364:MET:SD	1:A:382:VAL:HG11	2.60	0.41
1:A:445:ILE:CG2	1:A:446:ASN:N	2.83	0.41
1:A:462:LEU:HD11	1:A:464:ILE:CG2	2.50	0.41
1:A:475:LEU:HD22	1:A:595:TRP:CB	2.48	0.41
3:C:106:ILE:HD13	3:C:106:ILE:O	2.20	0.41
4:D:183:ARG:HG2	4:D:184:ASP:H	1.77	0.41
1:A:47:TYR:CD1	1:A:99:GLU:CD	2.92	0.41
1:A:89:GLU:HA	1:A:109:ARG:NH1	2.35	0.41
1:A:171:ASP:HA	1:A:457:TYR:CD1	2.55	0.41
1:A:260:LEU:HD13	1:A:260:LEU:C	2.40	0.41
1:A:306:SER:O	1:A:307:THR:HG23	2.21	0.41
1:A:367:LYS:HG2	1:A:378:ASP:HB2	2.01	0.41
1:A:645:GLY:HA2	4:D:23:GLY:CA	2.43	0.41
1:A:819:GLN:HE22	2:B:130:ASP:H	1.66	0.41
1:A:839:LYS:O	1:A:842:PRO:HD2	2.19	0.41
2:B:55:PHE:O	2:B:58:MET:HB3	2.19	0.41
2:B:88:PHE:CD2	2:B:91:LYS:HE2	2.56	0.41
3:C:43:ILE:HG22	3:C:45:PHE:H	1.84	0.41
3:C:98:ASN:CB	3:C:99:GLU:CA	2.92	0.41
3:C:130:PHE:C	3:C:130:PHE:CD1	2.92	0.41
3:C:131:VAL:CG1	3:C:179:CYS:CB	2.96	0.41
3:C:180:ILE:CA	3:C:183:GLU:CG	2.95	0.41
4:D:200:PHE:CD1	4:D:209:VAL:CG2	3.03	0.41
4:D:349:LEU:HD23	4:D:349:LEU:HA	1.80	0.41
4:E:106:THR:CG2	4:E:140:LEU:CD1	2.96	0.41
4:E:294:TYR:HD1	4:E:327:ILE:CD1	2.32	0.41
1:A:78:PHE:HD2	1:A:98:HIS:CD2	2.15	0.41
1:A:199:ILE:HA	1:A:202:THR:OG1	2.20	0.41
1:A:235:ALA:HB3	1:A:245:ARG:HH11	1.86	0.41
1:A:351:ILE:HG23	1:A:352:TYR:N	2.35	0.41
1:A:429:LEU:O	1:A:429:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ILE:CG2	1:A:514:ASP:N	2.82	0.41
1:A:524:GLU:CA	1:A:527:GLU:HG2	2.48	0.41
1:A:599:ASN:OD1	1:A:650:THR:HB	2.21	0.41
1:A:800:LEU:HD21	3:C:162:LYS:HB3	2.02	0.41
1:A:836:LEU:HA	1:A:839:LYS:HG3	2.02	0.41
2:B:116:ILE:HG22	2:B:117:LYS:O	2.20	0.41
3:C:70:LEU:CD1	3:C:71:SER:N	2.84	0.41
4:E:37:ARG:H	4:E:66:THR:CG2	2.34	0.41
4:E:357:ILE:CG2	4:E:358:THR:N	2.83	0.41
1:A:283:ARG:CD	1:A:322:VAL:CG2	2.98	0.41
1:A:364:MET:SD	1:A:382:VAL:CB	3.08	0.41
1:A:404:PRO:CB	1:A:606:THR:HB	2.41	0.41
1:A:504:LYS:HA	1:A:504:LYS:HD2	1.90	0.41
1:A:578:HIS:NE2	1:A:591:ASN:CA	2.81	0.41
1:A:618:LEU:CG	1:A:622:LEU:HD11	2.49	0.41
2:B:124:LEU:C	2:B:124:LEU:CD1	2.89	0.41
4:D:69:TYR:HB2	4:D:72:GLU:CA	2.50	0.41
4:D:82:MET:HE2	4:D:86:TRP:CE2	2.56	0.41
4:E:120:THR:HG23	4:E:132:MET:SD	2.60	0.41
4:E:189:LEU:HD12	4:E:189:LEU:C	2.40	0.41
4:E:299:MET:CE	4:E:309:ILE:CG1	2.98	0.41
1:A:231:ALA:O	1:A:286:HIS:HB2	2.21	0.41
1:A:236:LYS:CG	1:A:241:ASP:HA	2.36	0.41
1:A:305:ILE:HG22	1:A:306:SER:N	2.36	0.41
1:A:519:LEU:CD1	1:A:584:TYR:CB	2.98	0.41
2:B:51:LEU:CD1	2:B:68:LEU:HD11	2.50	0.41
2:B:159:TYR:C	2:B:159:TYR:CD2	2.94	0.41
3:C:137:PHE:CD2	3:C:137:PHE:O	2.74	0.41
4:D:33:SER:O	4:D:69:TYR:CD2	2.74	0.41
4:D:50:LYS:CG	4:D:53:TYR:CE2	3.03	0.41
4:D:107:GLU:HG2	4:D:108:ALA:O	2.20	0.41
4:D:285:CYS:CB	4:D:289:ILE:HD11	2.41	0.41
4:D:372:ARG:O	4:D:373:LYS:HB2	2.20	0.41
4:E:47:MET:CG	4:E:48:GLY:N	2.82	0.41
4:E:143:TYR:CZ	4:E:345:ILE:HG21	2.56	0.41
4:E:148:THR:CG2	4:E:149:THR:N	2.82	0.41
4:E:282:ILE:HG12	4:E:293:LEU:CD1	2.50	0.41
1:A:147:LYS:HB3	1:A:150:GLU:HG3	2.03	0.41
1:A:174:SER:HA	1:A:460:GLY:H	1.86	0.41
1:A:254:PHE:C	1:A:455:ARG:HA	2.40	0.41
1:A:261:ALA:CB	1:A:455:ARG:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:SER:HB3	1:A:451:THR:H	1.86	0.41
1:A:311:ASP:HB2	1:A:312:PHE:CE1	2.56	0.41
1:A:343:PHE:CD1	1:A:444:ARG:NH2	2.89	0.41
1:A:368:GLN:CG	1:A:376:GLU:CB	2.95	0.41
1:A:485:GLU:HB3	1:A:523:ILE:HG21	2.03	0.41
1:A:506:GLU:HB2	1:A:508:ILE:HD11	1.98	0.41
1:A:537:GLU:O	1:A:540:CYS:HB2	2.20	0.41
1:A:544:LYS:HE2	1:A:544:LYS:HB2	1.87	0.41
1:A:694:MET:CE	1:A:697:LEU:CD1	2.95	0.41
1:A:762:PHE:CD1	1:A:762:PHE:N	2.89	0.41
1:A:784:LYS:O	1:A:788:LEU:HD13	2.21	0.41
1:A:795:LEU:CD2	3:C:80:LEU:HD21	2.48	0.41
1:A:805:PHE:CD1	3:C:53:PHE:HE1	2.38	0.41
1:A:822:ILE:CG1	1:A:823:ARG:N	2.83	0.41
2:B:42:ARG:HH11	2:B:42:ARG:CG	2.34	0.41
2:B:55:PHE:O	2:B:59:GLY:HA2	2.21	0.41
2:B:159:TYR:CE2	2:B:165:ASP:O	2.74	0.41
2:B:169:GLN:O	2:B:169:GLN:HG2	2.20	0.41
3:C:43:ILE:CG2	3:C:44:GLU:N	2.83	0.41
3:C:70:LEU:HB3	3:C:71:SER:H	1.62	0.41
4:D:143:TYR:HD2	4:D:346:LEU:HD13	1.80	0.41
4:D:170:ALA:O	4:D:172:PRO:HD3	2.21	0.41
4:D:219:VAL:HG12	4:D:220:ALA:N	2.36	0.41
4:D:251:GLY:HA2	4:D:254:ARG:CG	2.23	0.41
4:E:171:LEU:HA	4:E:172:PRO:HD3	1.85	0.41
4:E:189:LEU:HA	4:E:192:ILE:HG12	2.03	0.41
4:E:244:ASP:CG	4:E:246:GLN:HE21	2.24	0.41
4:E:299:MET:O	4:E:332:PRO:HD2	2.21	0.41
4:E:365:ALA:HB3	4:E:369:ILE:CD1	2.46	0.41
1:A:25:ILE:HD12	1:A:26:GLU:H	1.78	0.41
1:A:137:PRO:O	1:A:141:THR:HG23	2.21	0.41
1:A:205:LYS:HB3	1:A:257:THR:HG23	2.02	0.41
1:A:265:ILE:N	1:A:265:ILE:CD1	2.85	0.41
1:A:338:ILE:HA	1:A:341:LEU:CD1	2.50	0.41
3:C:90:LYS:CB	3:C:111:PHE:CE2	2.95	0.41
3:C:148:ALA:HB1	3:C:163:GLU:HG2	2.01	0.41
4:D:210:ARG:HH11	4:D:210:ARG:CG	2.34	0.41
4:E:149:THR:CG2	4:E:150:GLY:N	2.82	0.41
4:E:150:GLY:CA	4:E:296:ASN:HB2	2.50	0.41
4:E:312:ARG:O	4:E:312:ARG:HG3	2.20	0.41
1:A:32:PHE:CD2	1:A:83:PRO:CD	3.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:TYR:CE1	1:A:108:GLU:CG	3.03	0.40
1:A:161:ASN:O	1:A:165:PHE:CD2	2.74	0.40
1:A:173:GLN:C	1:A:459:ILE:HG23	2.41	0.40
1:A:277:PHE:CZ	1:A:278:GLN:O	2.75	0.40
1:A:474:SER:CA	1:A:595:TRP:CZ2	3.04	0.40
2:B:140:MET:SD	2:B:145:SER:HB3	2.61	0.40
3:C:166:VAL:CG2	3:C:167:GLU:N	2.84	0.40
4:D:37:ARG:HH11	4:D:37:ARG:HD3	1.75	0.40
4:D:288:ASP:HA	4:E:243:PRO:HB2	2.03	0.40
1:A:102:VAL:CG2	1:A:103:LEU:N	2.84	0.40
1:A:183:ALA:HB3	1:A:185:LYS:H	1.87	0.40
1:A:626:TYR:CG	1:A:627:ALA:N	2.89	0.40
1:A:644:LYS:C	1:A:646:SER:H	2.23	0.40
3:C:54:LYS:HE2	3:C:65:ASP:OD2	2.20	0.40
4:E:165:ILE:N	4:E:165:ILE:HD12	2.36	0.40
4:E:297:ASN:OD1	4:E:329:ILE:HD11	2.21	0.40
4:E:332:PRO:HA	4:E:333:PRO:HD3	1.81	0.40
1:A:115:ILE:CD1	1:A:116:TYR:CE2	3.04	0.40
1:A:234:ASN:N	1:A:245:ARG:CG	2.83	0.40
1:A:234:ASN:O	1:A:235:ALA:HB2	2.21	0.40
1:A:351:ILE:CD1	1:A:437:MET:CE	2.99	0.40
2:B:58:MET:HE3	2:B:60:ARG:CZ	2.50	0.40
3:C:53:PHE:CE2	3:C:73:VAL:O	2.75	0.40
3:C:128:GLU:CG	3:C:180:ILE:CG2	2.99	0.40
4:D:140:LEU:HD23	4:D:140:LEU:HA	1.85	0.40
4:D:233:SER:HB3	4:D:236:LEU:CG	2.45	0.40
1:A:16:TYR:HB2	1:A:134:VAL:HG22	2.02	0.40
1:A:72:LEU:HB3	1:A:76:GLN:CG	2.43	0.40
1:A:159:SER:HB3	1:A:195:TYR:CE2	2.55	0.40
1:A:245:ARG:HG2	1:A:245:ARG:H	1.56	0.40
1:A:292:MET:SD	1:A:309:PRO:HB3	2.62	0.40
1:A:398:LEU:HD23	1:A:398:LEU:HA	1.87	0.40
4:E:8:LEU:HD23	4:E:8:LEU:HA	1.92	0.40
4:E:148:THR:O	4:E:165:ILE:HG22	2.21	0.40
1:A:38:CYS:HB3	1:A:39:PHE:H	1.54	0.40
1:A:116:TYR:CE1	1:A:125:THR:CB	3.02	0.40
1:A:192:VAL:O	1:A:195:TYR:HB3	2.22	0.40
1:A:446:ASN:HA	1:A:449:LEU:HB2	2.03	0.40
1:A:789:MET:HG3	3:C:130:PHE:CZ	2.57	0.40
4:D:36:GLY:H	4:D:52:SER:HB2	1.86	0.40
4:E:49:GLN:O	4:E:50:LYS:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:142:LEU:HD21	4:E:165:ILE:HG12	2.03	0.40
4:E:143:TYR:CE2	4:E:346:LEU:CB	3.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	843/845 (100%)	776 (92%)	42 (5%)	25 (3%)	4	30
2	B	144/146 (99%)	116 (81%)	17 (12%)	11 (8%)	1	14
3	C	151/153 (99%)	121 (80%)	15 (10%)	15 (10%)	0	10
4	D	372/375 (99%)	338 (91%)	24 (6%)	10 (3%)	5	33
4	E	372/375 (99%)	343 (92%)	18 (5%)	11 (3%)	4	30
All	All	1882/1894 (99%)	1694 (90%)	116 (6%)	72 (4%)	5	26

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	SER
1	A	46	MET
1	A	215	GLN
1	A	269	LEU
1	A	307	THR
1	A	367	LYS
1	A	369	LYS
1	A	380	THR
1	A	453	GLN
1	A	614	SER
2	B	39	ASP

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Mol	Chain	Res	Type
2	B	62	ASN
2	B	75	ALA
2	B	111	GLU
2	B	167	LYS
3	C	46	SER
3	C	62	ARG
3	C	67	LYS
3	C	94	GLY
3	C	116	GLN
3	C	136	VAL
3	C	157	LEU
4	D	43	VAL
4	D	97	ALA
4	D	373	LYS
4	E	3	ASP
4	E	4	GLU
4	E	43	VAL
4	E	44	MET
1	A	262	SER
1	A	408	VAL
1	A	642	LYS
1	A	705	GLY
2	B	44	GLY
2	B	65	ASN
2	B	165	ASP
3	C	43	ILE
3	C	90	LYS
3	C	189	ILE
4	D	3	ASP
4	D	238	LYS
1	A	19	LYS
1	A	205	LYS
1	A	280	SER
1	A	344	SER
1	A	425	SER
1	A	646	SER
2	B	98	GLU
3	C	70	LEU
3	C	192	ILE
4	D	4	GLU
4	D	44	MET
4	D	158	GLY

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Mol	Chain	Res	Type
4	D	181	ALA
4	E	41	GLN
4	E	54	VAL
1	A	624	SER
2	B	27	GLN
2	B	169	GLN
3	C	97	SER
3	C	154	LEU
4	E	181	ALA
4	E	323	SER
4	E	374	CYS
1	A	296	LYS
1	A	457	TYR
1	A	601	ASP
3	C	152	HIS
4	E	238	LYS
4	D	54	VAL
4	E	158	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	738/738 (100%)	566 (77%)	172 (23%)	1 5
2	B	125/125 (100%)	86 (69%)	39 (31%)	0 2
3	C	131/131 (100%)	76 (58%)	55 (42%)	0 0
4	D	317/317 (100%)	255 (80%)	62 (20%)	1 9
4	E	317/317 (100%)	261 (82%)	56 (18%)	2 11
All	All	1628/1628 (100%)	1244 (76%)	384 (24%)	3 5

All (384) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	4	ASP
1	A	9	ILE
1	A	17	LEU
1	A	18	ARG
1	A	19	LYS
1	A	21	GLU
1	A	24	ARG
1	A	26	GLU
1	A	28	GLN
1	A	29	ASN
1	A	33	ASP
1	A	35	LYS
1	A	36	LYS
1	A	41	VAL
1	A	43	ASP
1	A	45	GLU
1	A	46	MET
1	A	49	LYS
1	A	51	MET
1	A	54	SER
1	A	55	ARG
1	A	57	ASN
1	A	59	LYS
1	A	69	THR
1	A	71	THR
1	A	74	SER
1	A	76	GLN
1	A	86	ASP
1	A	87	LYS
1	A	91	MET
1	A	95	THR
1	A	102	VAL
1	A	106	LEU
1	A	115	ILE
1	A	130	LYS
1	A	132	LEU
1	A	138	GLU
1	A	144	ARG
1	A	147	LYS
1	A	159	SER
1	A	176	LEU
1	A	190	LYS

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Mol	Chain	Res	Type
1	A	191	ARG
1	A	192	VAL
1	A	198	THR
1	A	199	ILE
1	A	201	VAL
1	A	206	LYS
1	A	207	LYS
1	A	210	GLN
1	A	217	THR
1	A	219	GLU
1	A	236	LYS
1	A	240	ASN
1	A	245	ARG
1	A	250	ILE
1	A	253	HIS
1	A	257	THR
1	A	259	LYS
1	A	260	LEU
1	A	262	SER
1	A	264	ASP
1	A	266	GLU
1	A	268	TYR
1	A	269	LEU
1	A	271	GLU
1	A	279	LEU
1	A	295	LYS
1	A	301	ASP
1	A	307	THR
1	A	315	VAL
1	A	327	ASP
1	A	328	SER
1	A	330	GLU
1	A	338	ILE
1	A	340	ILE
1	A	341	LEU
1	A	344	SER
1	A	345	SER
1	A	351	ILE
1	A	364	MET
1	A	365	LYS
1	A	367	LYS
1	A	369	LYS

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Mol	Chain	Res	Type
1	A	370	GLN
1	A	372	GLU
1	A	374	GLN
1	A	376	GLU
1	A	388	TYR
1	A	390	MET
1	A	397	MET
1	A	399	LYS
1	A	401	LEU
1	A	403	CYS
1	A	408	VAL
1	A	411	GLU
1	A	412	TYR
1	A	415	LYS
1	A	418	ASN
1	A	420	GLN
1	A	431	LYS
1	A	449	LEU
1	A	452	LYS
1	A	453	GLN
1	A	455	ARG
1	A	456	GLN
1	A	459	ILE
1	A	462	LEU
1	A	464	ILE
1	A	468	GLU
1	A	471	ASP
1	A	475	LEU
1	A	488	GLN
1	A	500	GLN
1	A	508	ILE
1	A	517	MET
1	A	518	ASP
1	A	523	ILE
1	A	526	ILE
1	A	536	LEU
1	A	544	LYS
1	A	551	LYS
1	A	567	LYS
1	A	574	LYS
1	A	582	VAL
1	A	584	TYR

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Mol	Chain	Res	Type
1	A	591	ASN
1	A	601	ASP
1	A	603	LEU
1	A	608	VAL
1	A	613	LYS
1	A	616	LEU
1	A	617	LYS
1	A	634	SER
1	A	637	SER
1	A	642	LYS
1	A	643	LYS
1	A	644	LYS
1	A	646	SER
1	A	651	VAL
1	A	652	SER
1	A	659	LEU
1	A	667	ARG
1	A	675	ARG
1	A	677	LEU
1	A	683	LYS
1	A	707	ARG
1	A	710	ARG
1	A	711	LYS
1	A	724	GLN
1	A	727	ARG
1	A	740	ILE
1	A	742	SER
1	A	746	SER
1	A	748	LYS
1	A	767	VAL
1	A	770	LYS
1	A	781	ARG
1	A	783	GLU
1	A	789	MET
1	A	790	THR
1	A	797	ARG
1	A	801	MET
1	A	807	LYS
1	A	827	ASN
1	A	828	VAL
1	A	829	LYS
1	A	836	LEU

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Mol	Chain	Res	Type
1	A	839	LYS
1	A	841	LYS
1	A	845	LYS
2	B	25	GLN
2	B	31	PHE
2	B	32	LYS
2	B	36	THR
2	B	40	GLN
2	B	45	ILE
2	B	47	ASP
2	B	48	LYS
2	B	51	LEU
2	B	58	MET
2	B	60	ARG
2	B	61	LEU
2	B	62	ASN
2	B	63	VAL
2	B	71	MET
2	B	73	LYS
2	B	82	THR
2	B	83	VAL
2	B	90	GLU
2	B	91	LYS
2	B	92	LEU
2	B	93	LYS
2	B	106	LYS
2	B	108	LEU
2	B	113	LYS
2	B	118	LYS
2	B	119	GLN
2	B	124	LEU
2	B	128	GLN
2	B	131	ARG
2	B	135	GLU
2	B	136	GLU
2	B	137	ILE
2	B	140	MET
2	B	155	LYS
2	B	159	TYR
2	B	165	ASP
2	B	167	LYS
2	B	168	ASP

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Mol	Chain	Res	Type
3	C	41	ILE
3	C	45	PHE
3	C	46	SER
3	C	47	LYS
3	C	48	GLU
3	C	50	GLN
3	C	52	GLU
3	C	54	LYS
3	C	57	PHE
3	C	58	LEU
3	C	62	ARG
3	C	67	LYS
3	C	68	ILE
3	C	75	ASP
3	C	76	VAL
3	C	77	LEU
3	C	78	ARG
3	C	80	LEU
3	C	90	LYS
3	C	91	LYS
3	C	92	VAL
3	C	95	ASN
3	C	104	LYS
3	C	105	LYS
3	C	106	ILE
3	C	112	LEU
3	C	115	LEU
3	C	120	ASN
3	C	122	LYS
3	C	124	GLN
3	C	126	THR
3	C	128	GLU
3	C	129	ASP
3	C	130	PHE
3	C	131	VAL
3	C	132	GLU
3	C	135	ARG
3	C	136	VAL
3	C	138	ASP
3	C	142	ASN
3	C	144	THR
3	C	149	GLU

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Mol	Chain	Res	Type
3	C	151	ARG
3	C	156	THR
3	C	157	LEU
3	C	160	LYS
3	C	163	GLU
3	C	164	GLU
3	C	174	GLU
3	C	179	CYS
3	C	180	ILE
3	C	183	GLU
3	C	187	LYS
3	C	189	ILE
3	C	190	MET
4	D	1	ASP
4	D	10	CYS
4	D	18	LYS
4	D	28	ARG
4	D	34	ILE
4	D	35	VAL
4	D	37	ARG
4	D	43	VAL
4	D	47	MET
4	D	49	GLN
4	D	51	ASP
4	D	56	ASP
4	D	57	GLU
4	D	59	GLN
4	D	61	LYS
4	D	65	LEU
4	D	66	THR
4	D	68	LYS
4	D	69	TYR
4	D	85	ILE
4	D	107	GLU
4	D	113	LYS
4	D	118	LYS
4	D	121	GLN
4	D	129	VAL
4	D	134	VAL
4	D	139	VAL
4	D	142	LEU
4	D	143	TYR

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Mol	Chain	Res	Type
4	D	145	SER
4	D	147	ARG
4	D	148	THR
4	D	149	THR
4	D	167	GLU
4	D	171	LEU
4	D	180	LEU
4	D	183	ARG
4	D	186	THR
4	D	196	ARG
4	D	208	ILE
4	D	232	SER
4	D	233	SER
4	D	236	LEU
4	D	244	ASP
4	D	250	ILE
4	D	256	ARG
4	D	267	ILE
4	D	286	ASP
4	D	287	ILE
4	D	309	ILE
4	D	312	ARG
4	D	315	LYS
4	D	335	ARG
4	D	349	LEU
4	D	350	SER
4	D	354	GLN
4	D	357	ILE
4	D	369	ILE
4	D	370	VAL
4	D	372	ARG
4	D	373	LYS
4	D	374	CYS
4	E	8	LEU
4	E	18	LYS
4	E	34	ILE
4	E	49	GLN
4	E	51	ASP
4	E	56	ASP
4	E	57	GLU
4	E	60	SER
4	E	61	LYS

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Mol	Chain	Res	Type
4	E	68	LYS
4	E	82	MET
4	E	95	ARG
4	E	103	THR
4	E	104	LEU
4	E	113	LYS
4	E	132	MET
4	E	139	VAL
4	E	141	SER
4	E	143	TYR
4	E	145	SER
4	E	147	ARG
4	E	151	ILE
4	E	157	ASP
4	E	167	GLU
4	E	176	MET
4	E	189	LEU
4	E	191	LYS
4	E	196	ARG
4	E	199	SER
4	E	208	ILE
4	E	232	SER
4	E	236	LEU
4	E	238	LYS
4	E	239	SER
4	E	244	ASP
4	E	248	ILE
4	E	250	ILE
4	E	257	CYS
4	E	269	MET
4	E	274	ILE
4	E	285	CYS
4	E	286	ASP
4	E	287	ILE
4	E	297	ASN
4	E	300	SER
4	E	312	ARG
4	E	315	LYS
4	E	323	SER
4	E	324	THR
4	E	329	ILE
4	E	335	ARG

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Mol	Chain	Res	Type
4	E	346	LEU
4	E	350	SER
4	E	370	VAL
4	E	372	ARG
4	E	373	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	53	GLN
1	A	76	GLN
1	A	98	HIS
1	A	105	ASN
1	A	161	ASN
1	A	188	ASN
1	A	210	GLN
1	A	221	GLN
1	A	240	ASN
1	A	242	ASN
1	A	286	HIS
1	A	360	HIS
1	A	370	GLN
1	A	393	ASN
1	A	421	GLN
1	A	424	ASN
1	A	453	GLN
1	A	456	GLN
1	A	488	GLN
1	A	557	GLN
1	A	558	HIS
1	A	583	HIS
1	A	649	GLN
1	A	665	ASN
1	A	670	HIS
1	A	672	HIS
1	A	690	HIS
1	A	793	GLN
1	A	819	GLN
1	A	821	ASN
1	A	827	ASN
1	A	835	ASN

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Mol	Chain	Res	Type
2	B	25	GLN
2	B	27	GLN
2	B	29	GLN
2	B	62	ASN
2	B	65	ASN
2	B	119	GLN
2	B	139	ASN
3	C	72	GLN
3	C	86	ASN
3	C	120	ASN
3	C	142	ASN
3	C	152	HIS
3	C	177	ASN
4	D	49	GLN
4	D	92	ASN
4	D	121	GLN
4	D	246	GLN
4	D	297	ASN
4	D	353	GLN
4	D	360	GLN
4	E	59	GLN
4	E	92	ASN
4	E	162	ASN
4	E	246	GLN
4	E	353	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	HIC	D	73	4	8,11,12	1.06	0	6,14,16	1.12	1 (16%)
4	HIC	E	73	4	8,11,12	1.07	0	6,14,16	1.17	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HIC	D	73	4	-	2/5/6/8	0/1/1/1
4	HIC	E	73	4	-	2/5/6/8	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	73	HIC	CG-CD2-NE2	2.18	110.14	107.78
4	D	73	HIC	CG-CD2-NE2	2.07	110.02	107.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	73	HIC	O-C-CA-CB
4	D	73	HIC	CA-CB-CG-ND1
4	E	73	HIC	O-C-CA-CB
4	E	73	HIC	CA-CB-CG-ND1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	73	HIC	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ADP	D	401	-	24,29,29	1.24	3 (12%)	29,45,45	1.38	4 (13%)
5	ADP	E	401	-	24,29,29	1.25	3 (12%)	29,45,45	1.38	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	D	401	-	-	0/12/32/32	0/3/3/3
5	ADP	E	401	-	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	401	ADP	C2-N1	3.02	1.39	1.33
5	D	401	ADP	C2-N1	2.93	1.39	1.33
5	D	401	ADP	C2'-C1'	-2.10	1.50	1.53
5	E	401	ADP	C2'-C1'	-2.05	1.50	1.53
5	D	401	ADP	C8-N7	-2.05	1.31	1.34
5	E	401	ADP	C8-N7	-2.00	1.31	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	401	ADP	C4-C5-N7	3.92	113.48	109.40
5	D	401	ADP	C4-C5-N7	3.88	113.44	109.40
5	D	401	ADP	C2-N1-C6	2.28	122.65	118.75
5	E	401	ADP	C2-N1-C6	2.25	122.61	118.75
5	D	401	ADP	N3-C2-N1	-2.23	125.19	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	401	ADP	N3-C2-N1	-2.20	125.24	128.68
5	D	401	ADP	O3B-PB-O2B	2.20	116.04	107.64
5	E	401	ADP	O3B-PB-O2B	2.18	115.98	107.64

There are no chirality outliers.

There are no torsion outliers.

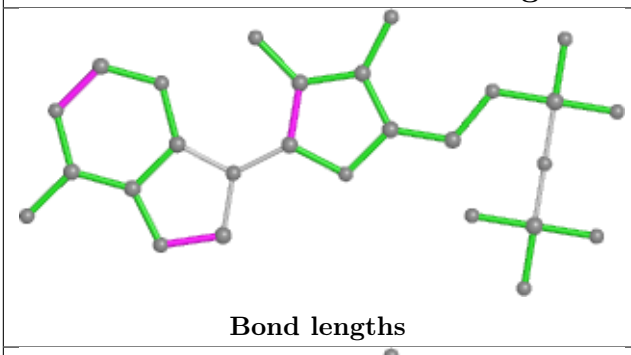
There are no ring outliers.

2 monomers are involved in 11 short contacts:

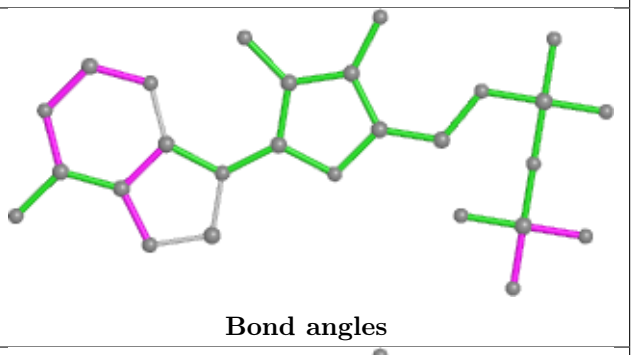
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	401	ADP	7	0
5	E	401	ADP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

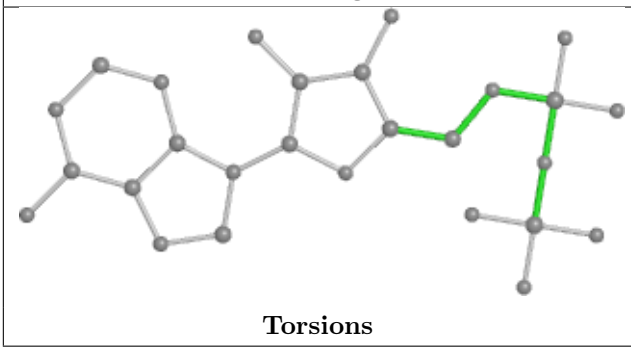
Ligand ADP D 401



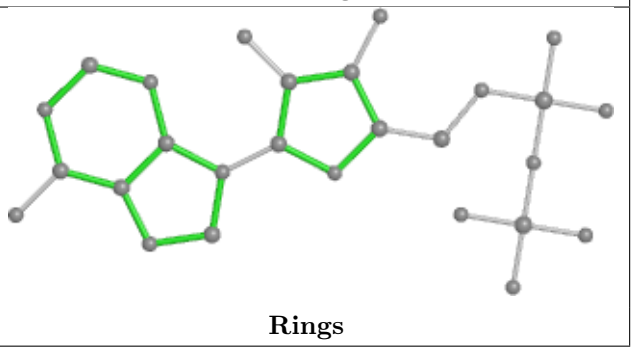
Bond lengths



Bond angles

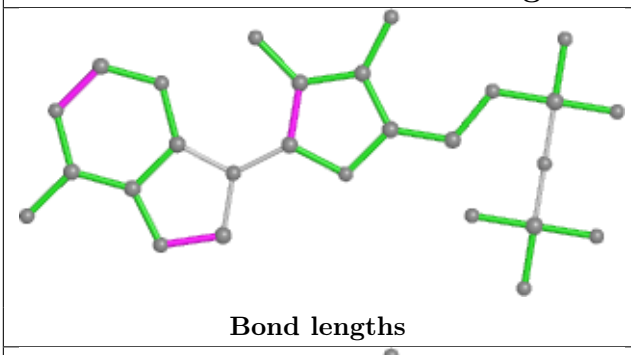


Torsions

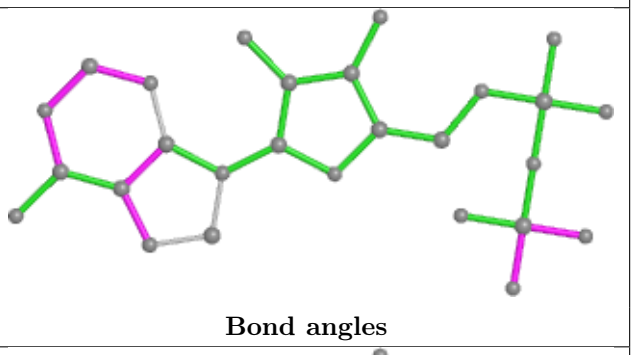


Rings

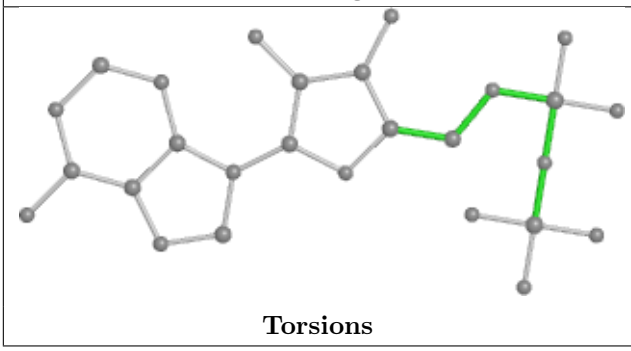
Ligand ADP E 401



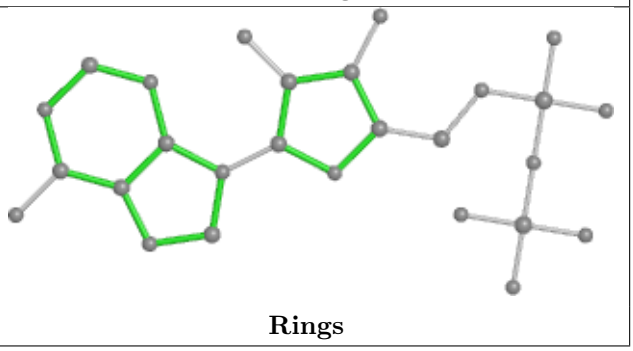
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

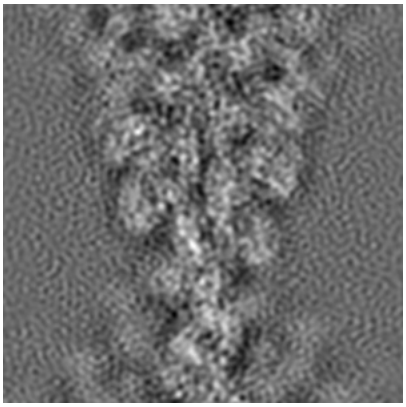
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6664. These allow visual inspection of the internal detail of the map and identification of artifacts.

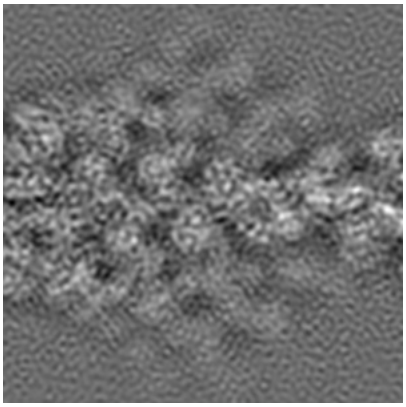
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

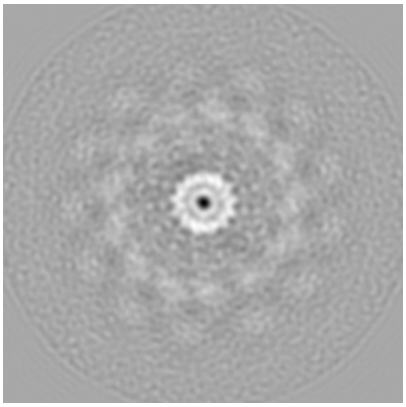
6.1.1 Primary map



X



Y

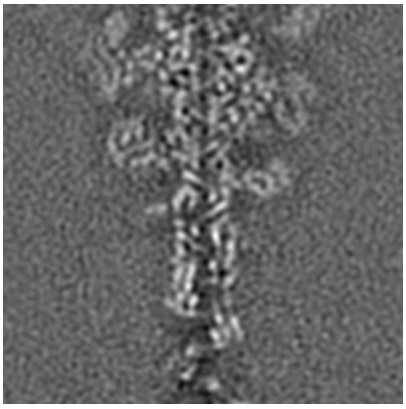


Z

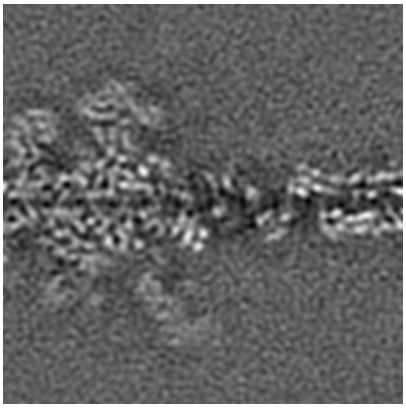
The images above show the map projected in three orthogonal directions.

6.2 Central slices

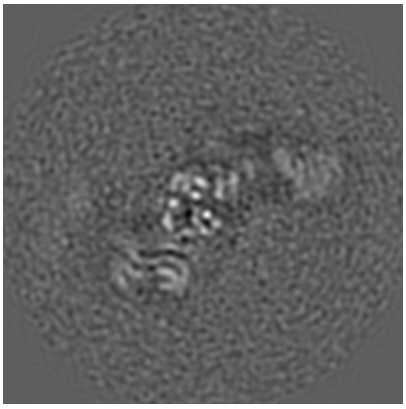
6.2.1 Primary map



X Index: 125



Y Index: 125

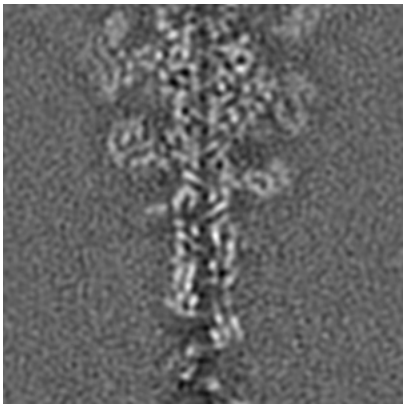


Z Index: 125

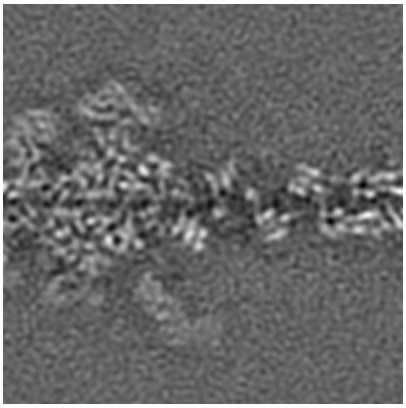
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

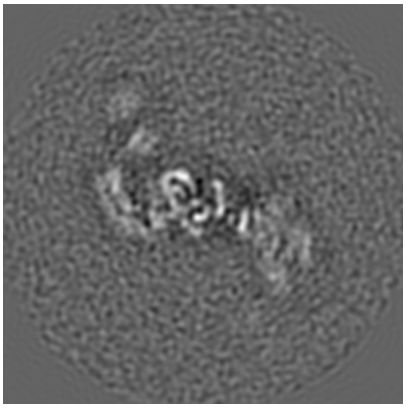
6.3.1 Primary map



X Index: 125



Y Index: 126



Z Index: 33

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 1.52. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

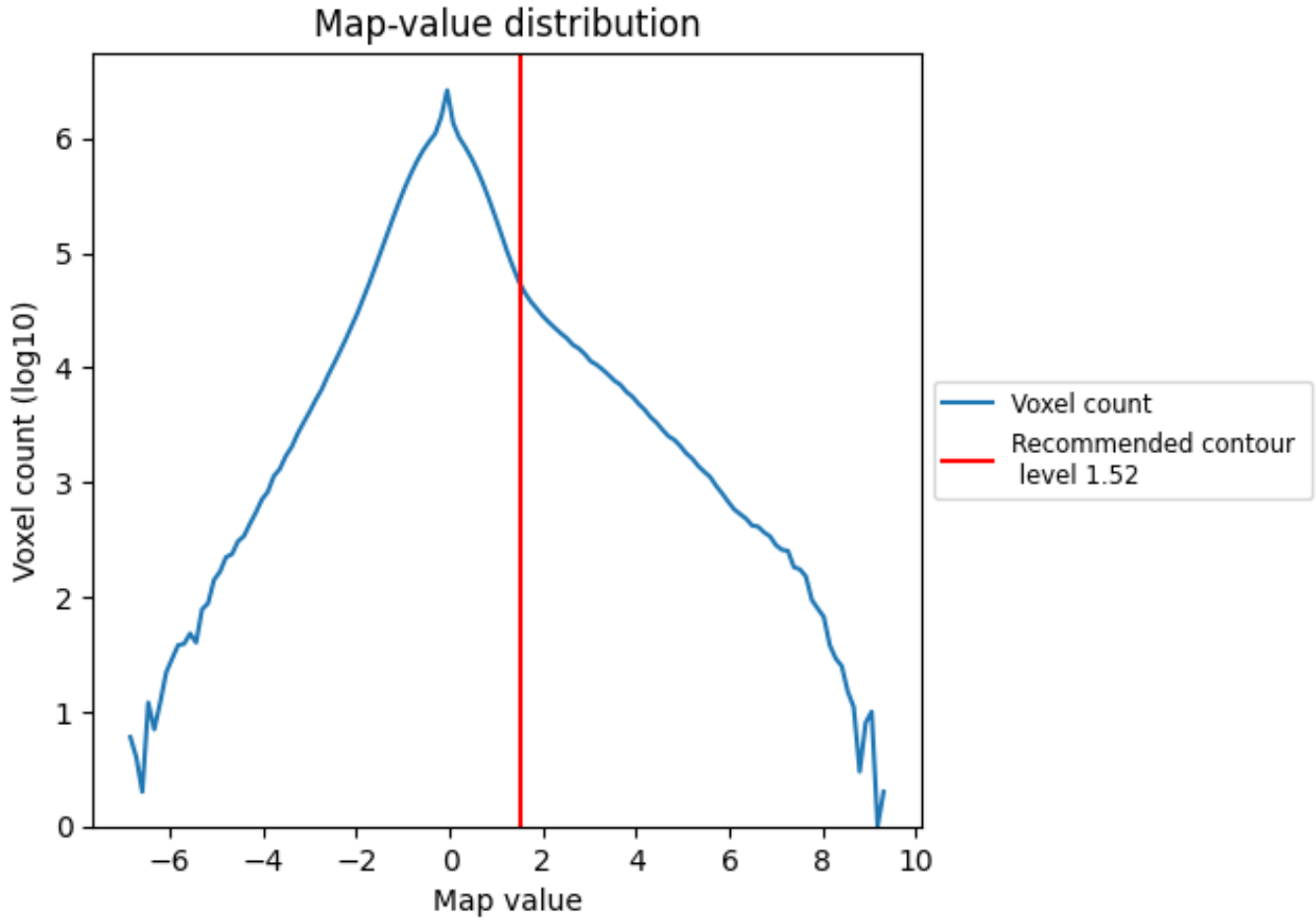
6.5 Mask visualisation (i)

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

7 Map analysis

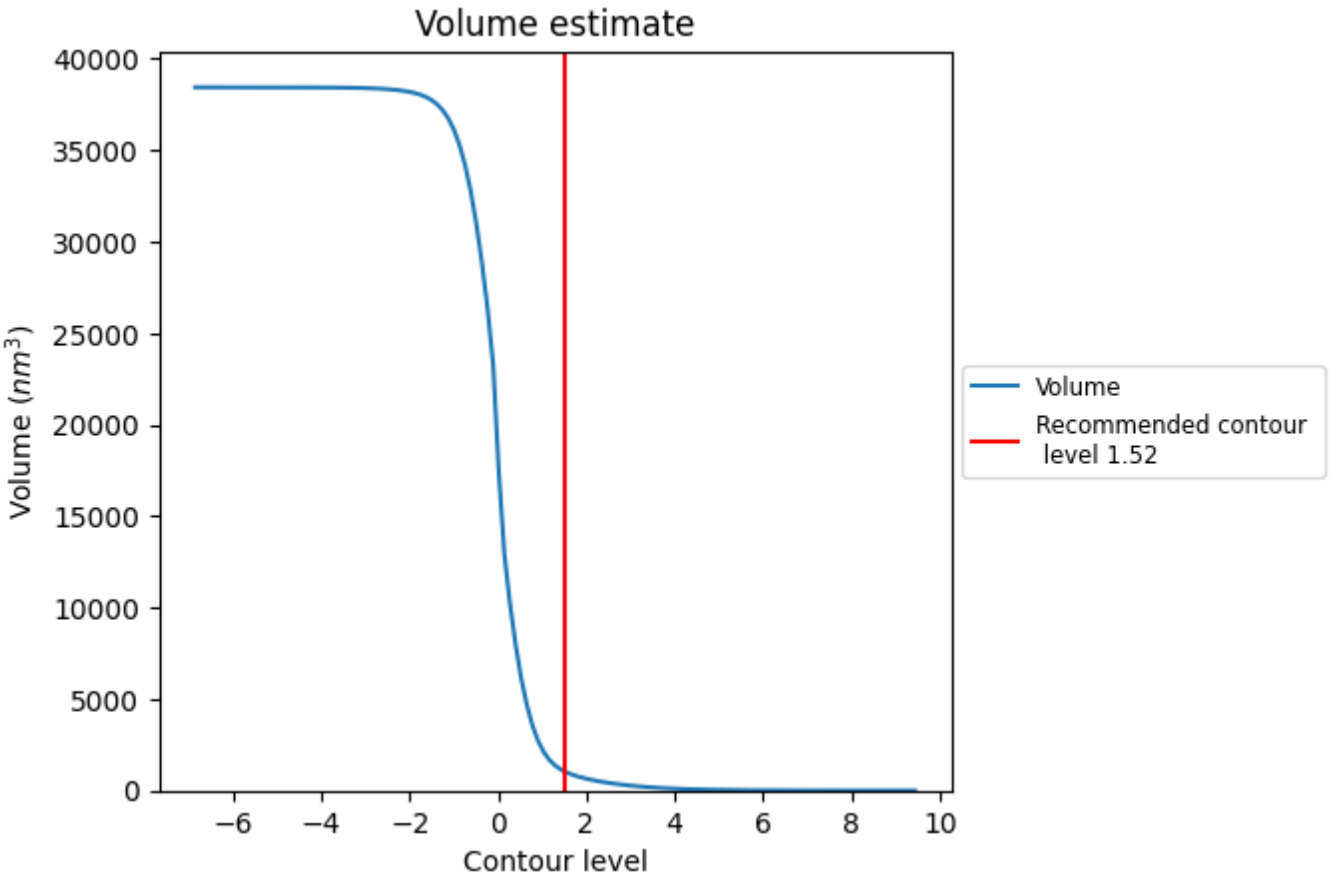
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

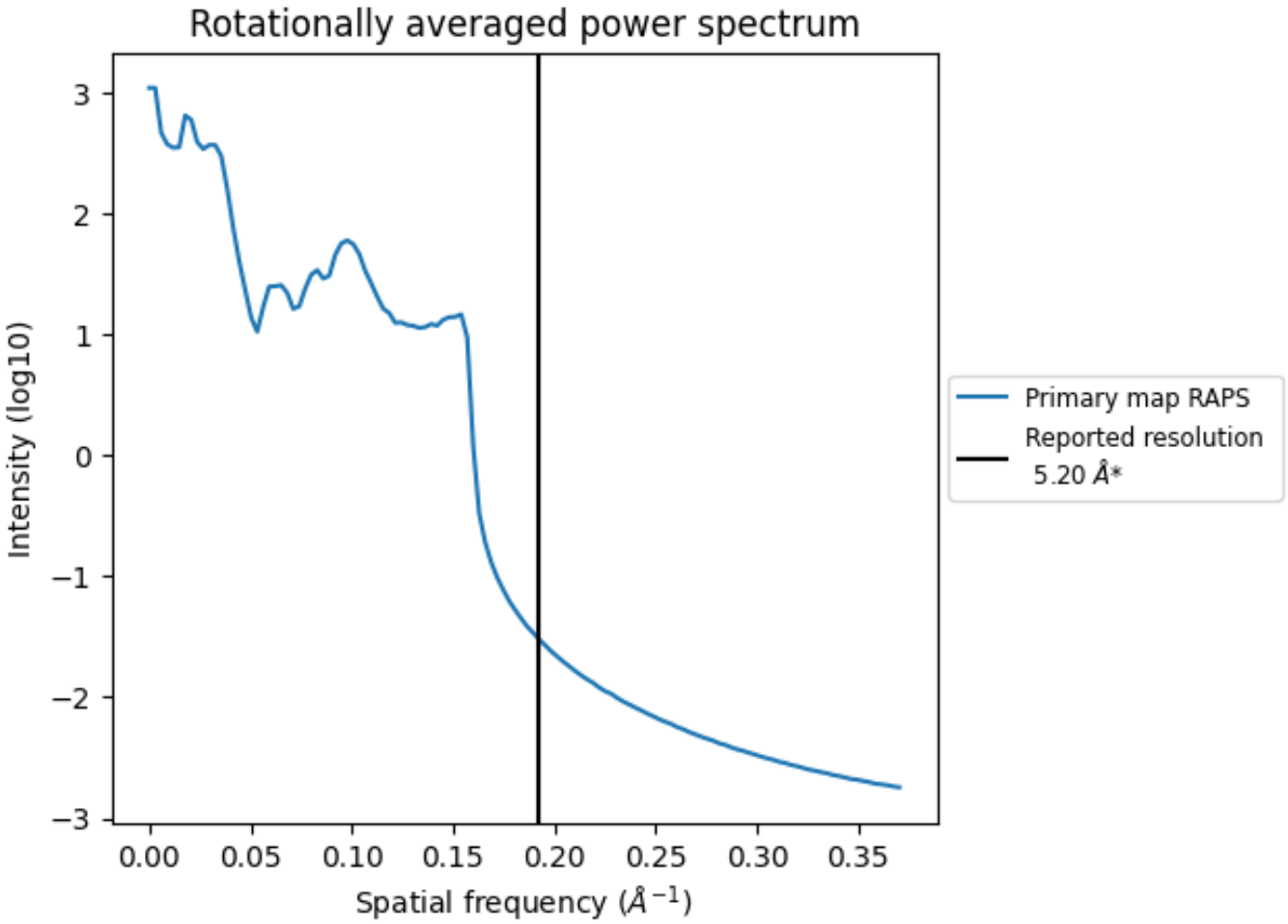
7.2 Volume estimate



The volume at the recommended contour level is 1033 nm^3; this corresponds to an approximate mass of 933 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 0.192 Å^{-1}

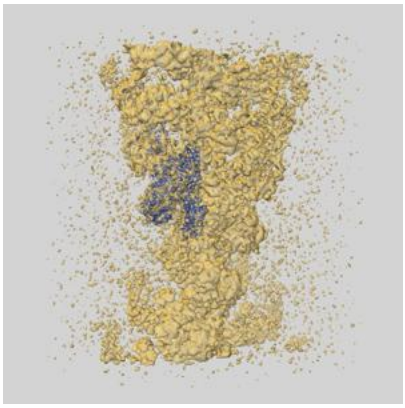
8 Fourier-Shell correlation (i)

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

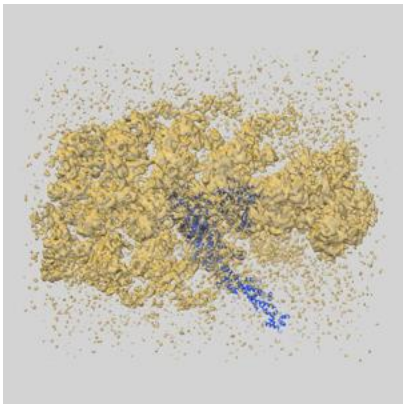
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6664 and PDB model 5H53. Per-residue inclusion information can be found in section 3 on page 5.

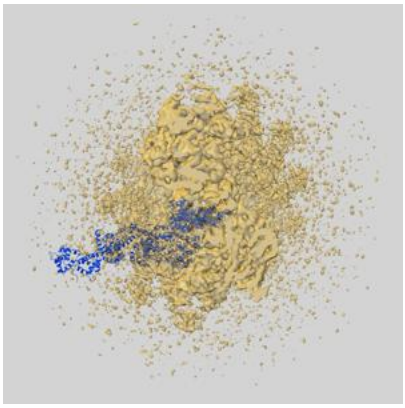
9.1 Map-model overlay



X



Y



Z

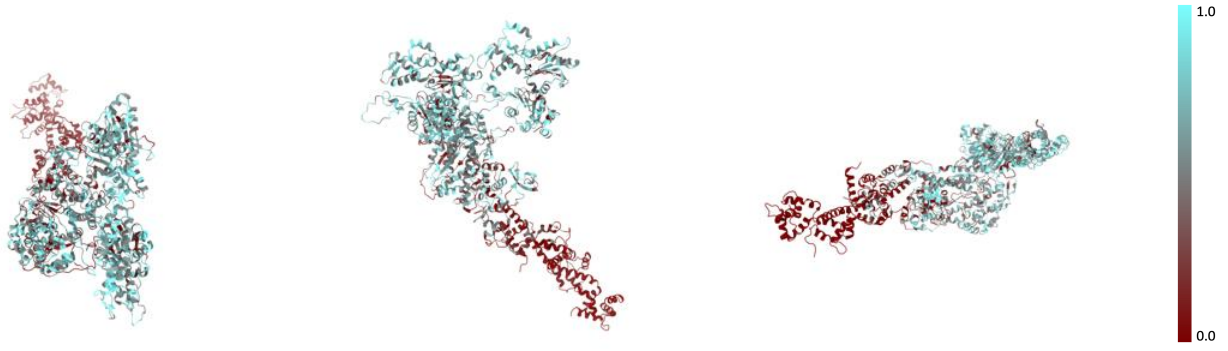
The images above show the 3D surface view of the map at the recommended contour level 1.52 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

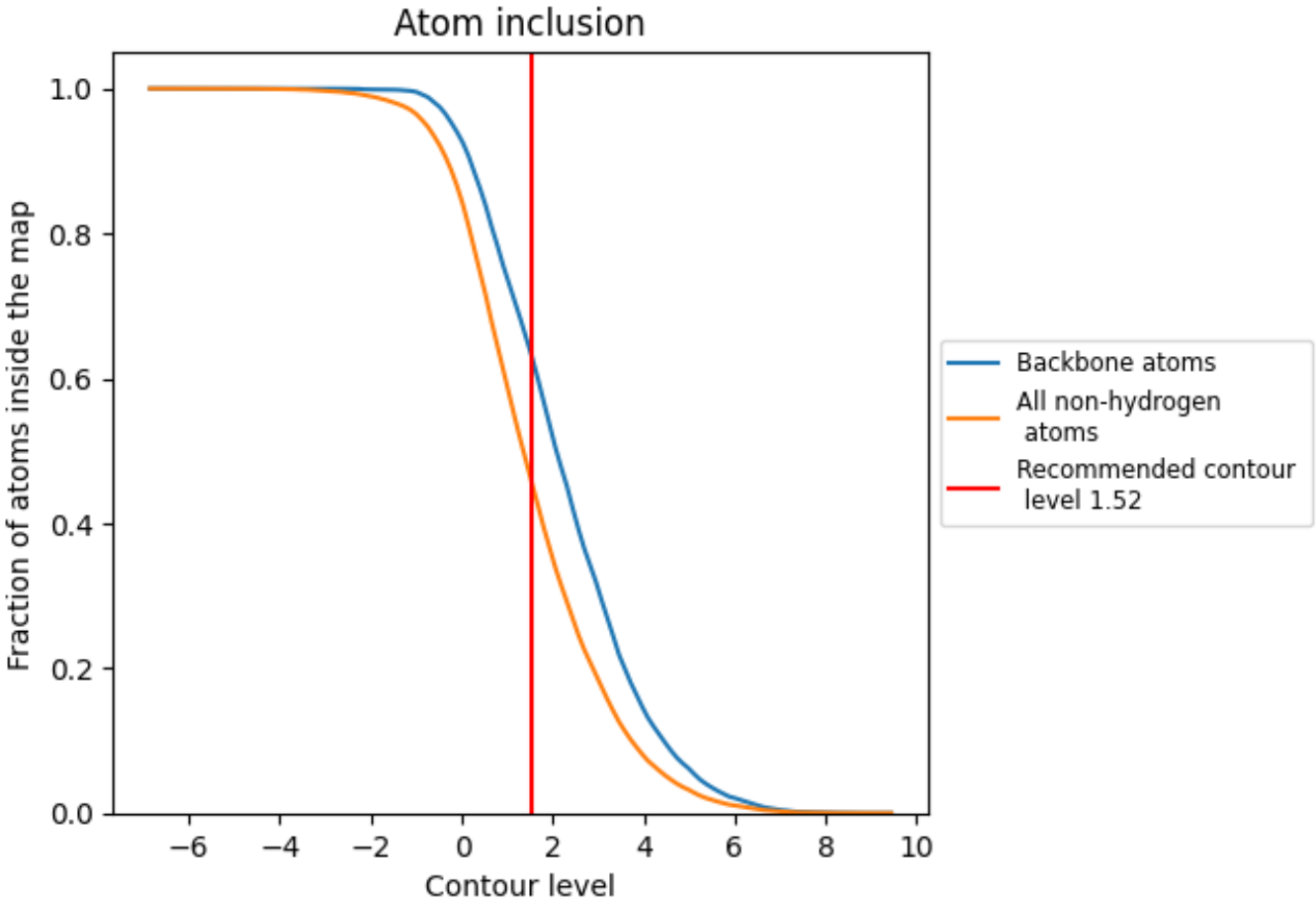
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.52).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 46% 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 (1.52) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4592	0.1140
A	0.4602	0.1190
B	0.0000	0.0200
C	0.1040	0.0340
D	0.6207	0.1430
E	0.6224	0.1450