



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:40 PM BST

PDB ID : 3IZQ
EMDB ID: : EMD-1811
Title : Structure of the Dom34-Hbs1-GDPNP complex bound to a translating ribosome
Authors : Becker, T.; Armache, J.-P.; Jarasch, A.; Anger, A.M.; Villa, E.; Sieber, H.; Abdel Motaal, B.; Mielke, T.; Berninghausen, O.; Beckmann, R.
Deposited on : 2010-11-30
Resolution : 9.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

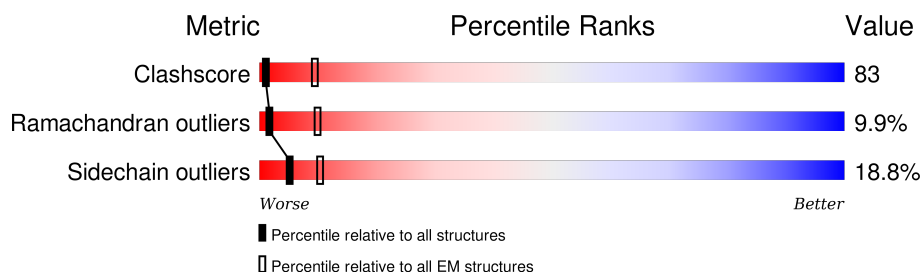
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.50 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	386	
2	1	611	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7183 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 Protein DOM34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	386	Total	C	N	O	S	0	0
			3097	1996	483	603	15		

- Molecule 2 is a protein called Elongation factor 1 alpha-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	516	Total	C	N	O	S	0	0
			4086	2589	692	789	16		

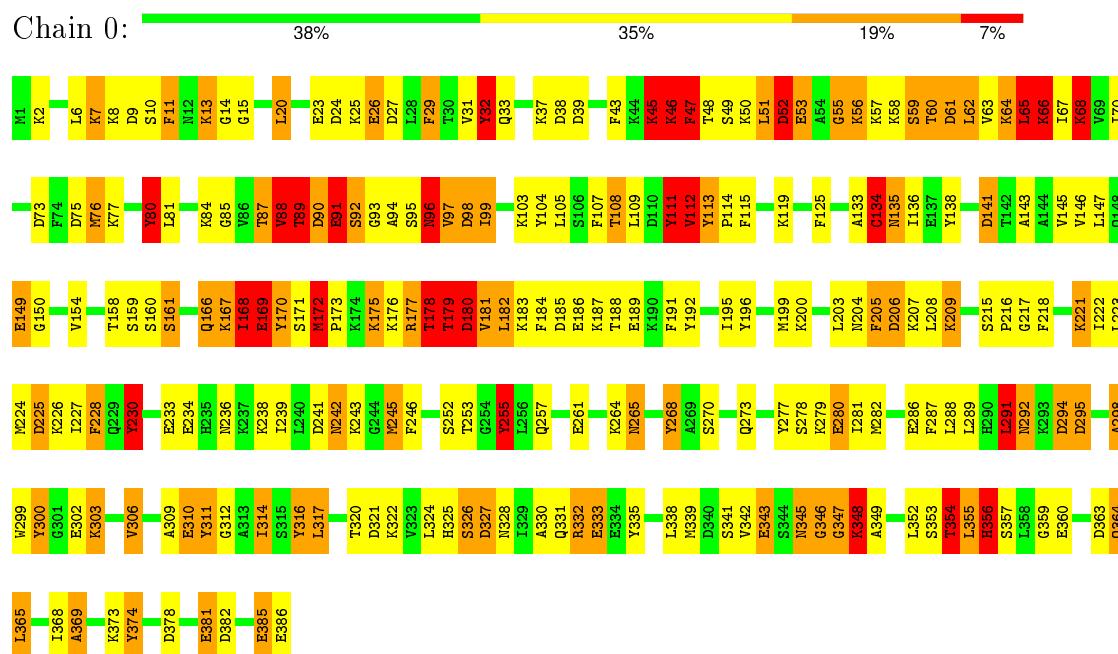
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	32	GLU	ASP	ENGINEERED MUTATION	UNP P32769

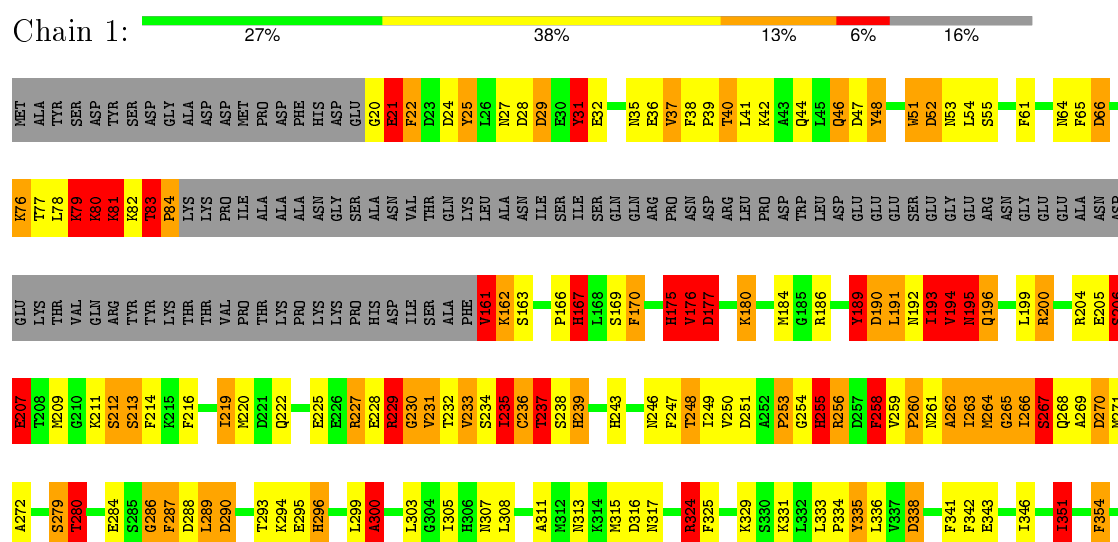
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Protein DOM34



• Molecule 2: Elongation factor 1 alpha-like protein






4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2500	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	39000	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	0	1.63	35/3149 (1.1%)	2.13	143/4230 (3.4%)
2	1	1.44	15/4162 (0.4%)	2.06	171/5618 (3.0%)
All	All	1.52	50/7311 (0.7%)	2.09	314/9848 (3.2%)

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	0	6	22
2	1	4	26
All	All	10	48

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	168	ILE	CG1-CD1	17.39	2.70	1.50
1	0	99	ILE	CG1-CD1	12.90	2.39	1.50
1	0	91	GLU	CG-CD	9.53	1.66	1.51
2	1	235	ILE	N-CA	-8.54	1.29	1.46
1	0	65	LEU	CA-CB	8.46	1.73	1.53
1	0	341	SER	CA-CB	8.31	1.65	1.52
1	0	91	GLU	CB-CG	8.23	1.67	1.52
1	0	356	HIS	CA-CB	7.75	1.71	1.53
1	0	346	GLY	CA-C	7.69	1.64	1.51
1	0	112	VAL	CA-CB	7.53	1.70	1.54
1	0	215	SER	CA-CB	7.25	1.63	1.52
1	0	347	GLY	CA-C	7.21	1.63	1.51
2	1	537	ARG	NE-CZ	6.93	1.42	1.33
1	0	47	PHE	C-N	6.85	1.49	1.34
1	0	161	SER	CA-CB	6.77	1.63	1.52
1	0	111	TYR	CG-CD1	6.46	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	243	HIS	CB-CG	6.32	1.61	1.50
1	0	23	GLU	CD-OE1	-6.31	1.18	1.25
2	1	267	SER	CA-C	-6.18	1.36	1.52
1	0	316	TYR	CG-CD1	6.18	1.47	1.39
1	0	64	LYS	C-N	6.17	1.48	1.34
1	0	347	GLY	N-CA	6.16	1.55	1.46
1	0	65	LEU	CG-CD2	6.13	1.74	1.51
1	0	32	TYR	CB-CG	6.11	1.60	1.51
2	1	517	ARG	CD-NE	6.10	1.56	1.46
1	0	357	SER	CA-CB	6.08	1.62	1.52
1	0	278	SER	CA-CB	6.02	1.61	1.52
2	1	189	TYR	CB-CG	-5.94	1.42	1.51
1	0	113	TYR	C-N	5.91	1.45	1.34
1	0	302	GLU	CB-CG	5.67	1.62	1.52
2	1	342	PHE	CG-CD1	5.62	1.47	1.38
2	1	295	GLU	CD-OE2	-5.59	1.19	1.25
2	1	235	ILE	CA-CB	-5.58	1.42	1.54
1	0	180	ASP	CA-CB	5.54	1.66	1.53
1	0	346	GLY	N-CA	5.54	1.54	1.46
1	0	114	PRO	N-CD	5.54	1.55	1.47
2	1	588	ARG	NE-CZ	5.52	1.40	1.33
1	0	11	PHE	CA-CB	5.50	1.66	1.53
2	1	36	GLU	CG-CD	5.47	1.60	1.51
1	0	159	SER	CA-CB	5.41	1.61	1.52
2	1	518	PRO	N-CA	-5.41	1.38	1.47
1	0	385	GLU	CB-CG	5.39	1.62	1.52
1	0	299	TRP	NE1-CE2	5.39	1.44	1.37
1	0	333	GLU	CB-CG	5.30	1.62	1.52
1	0	65	LEU	CA-C	-5.22	1.39	1.52
1	0	270	SER	CA-CB	5.17	1.60	1.52
2	1	372	TYR	CE1-CZ	5.10	1.45	1.38
2	1	338	ASP	CA-CB	5.08	1.65	1.53
2	1	324	ARG	CG-CD	5.07	1.64	1.51
1	0	216	PRO	N-CD	-5.06	1.40	1.47

All (314) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	65	LEU	CB-CG-CD2	18.11	141.79	111.00
1	0	11	PHE	CB-CG-CD1	17.04	132.73	120.80
2	1	372	TYR	CB-CG-CD2	-15.99	111.41	121.00
1	0	11	PHE	CB-CG-CD2	-14.97	110.32	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	11	PHE	N-CA-CB	13.84	135.51	110.60
2	1	235	ILE	CG1-CB-CG2	12.85	139.67	111.40
2	1	248	THR	N-CA-CB	12.76	134.55	110.30
1	0	180	ASP	N-CA-CB	12.48	133.06	110.60
1	0	27	ASP	CB-CG-OD1	12.36	129.42	118.30
2	1	390	LYS	O-C-N	-11.77	103.87	122.70
2	1	79	LYS	CB-CA-C	-11.76	86.88	110.40
1	0	180	ASP	CA-CB-CG	11.62	138.97	113.40
1	0	277	TYR	CB-CG-CD2	-11.60	114.04	121.00
2	1	258	PHE	CB-CG-CD1	11.31	128.72	120.80
1	0	255	TYR	CB-CG-CD1	-11.25	114.25	121.00
1	0	356	HIS	CA-CB-CG	11.09	132.46	113.60
1	0	356	HIS	CB-CA-C	-11.02	88.36	110.40
2	1	236	CYS	CB-CA-C	10.82	132.04	110.40
1	0	89	THR	CB-CA-C	10.75	140.62	111.60
2	1	369	ARG	NE-CZ-NH1	10.75	125.67	120.30
2	1	79	LYS	N-CA-CB	-10.73	91.29	110.60
1	0	268	TYR	CB-CG-CD1	-10.56	114.67	121.00
1	0	295	ASP	CB-CG-OD1	-10.40	108.94	118.30
2	1	455	GLN	CB-CA-C	10.40	131.20	110.40
1	0	45	LYS	O-C-N	-10.38	106.10	122.70
2	1	79	LYS	C-N-CA	10.19	147.18	121.70
1	0	218	PHE	CB-CG-CD1	-10.16	113.69	120.80
2	1	518	PRO	CA-N-CD	-10.13	97.31	111.50
1	0	10	SER	O-C-N	-10.00	106.70	122.70
2	1	79	LYS	O-C-N	-9.90	106.86	122.70
2	1	79	LYS	N-CA-C	9.84	137.57	111.00
1	0	292	ASN	CB-CA-C	9.79	129.98	110.40
2	1	500	ILE	O-C-N	-9.63	107.29	122.70
1	0	47	PHE	CA-C-N	-9.55	96.19	117.20
1	0	65	LEU	N-CA-CB	9.31	129.02	110.40
1	0	45	LYS	C-N-CA	9.19	144.66	121.70
1	0	91	GLU	CB-CG-CD	9.15	138.91	114.20
2	1	360	TYR	CB-CG-CD1	-9.13	115.52	121.00
2	1	195	ASN	CA-C-N	9.13	137.28	117.20
2	1	466	ASP	C-N-CA	9.07	144.37	121.70
2	1	195	ASN	O-C-N	-9.03	108.25	122.70
2	1	296	HIS	CA-CB-CG	9.01	128.92	113.60
2	1	287	PHE	CB-CG-CD2	-8.95	114.53	120.80
1	0	347	GLY	N-CA-C	8.92	135.40	113.10
2	1	258	PHE	CB-CG-CD2	-8.90	114.57	120.80
2	1	83	THR	CA-C-N	8.84	141.84	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	241	ASP	CB-CG-OD2	8.82	126.24	118.30
1	0	88	VAL	C-N-CA	8.76	143.60	121.70
1	0	27	ASP	CB-CG-OD2	-8.60	110.56	118.30
2	1	364	TYR	CB-CG-CD2	-8.58	115.85	121.00
2	1	364	TYR	CB-CG-CD1	8.51	126.11	121.00
1	0	32	TYR	CG-CD2-CE2	-8.48	114.52	121.30
2	1	390	LYS	CB-CA-C	8.45	127.31	110.40
2	1	170	PHE	CB-CG-CD1	-8.45	114.89	120.80
1	0	91	GLU	N-CA-CB	8.40	125.72	110.60
2	1	290	ASP	CB-CG-OD1	8.34	125.80	118.30
1	0	311	TYR	CG-CD2-CE2	8.32	127.96	121.30
2	1	82	LYS	C-N-CA	8.25	142.33	121.70
2	1	79	LYS	CA-C-N	8.14	135.11	117.20
2	1	29	ASP	CB-CG-OD1	8.12	125.61	118.30
2	1	83	THR	N-CA-C	8.04	132.72	111.00
2	1	386	PHE	CB-CG-CD2	8.04	126.43	120.80
2	1	195	ASN	N-CA-C	7.98	132.56	111.00
2	1	189	TYR	CB-CG-CD1	7.92	125.75	121.00
2	1	517	ARG	C-N-CD	-7.85	103.33	120.60
1	0	68	LYS	C-N-CA	-7.85	102.08	121.70
1	0	39	ASP	CB-CG-OD2	7.84	125.36	118.30
1	0	228	PHE	CB-CG-CD2	7.82	126.28	120.80
2	1	588	ARG	CB-CG-CD	7.82	131.93	111.60
1	0	306	VAL	CA-CB-CG2	-7.79	99.22	110.90
1	0	311	TYR	CZ-CE2-CD2	-7.76	112.81	119.80
2	1	235	ILE	CB-CG1-CD1	7.72	135.52	113.90
1	0	218	PHE	CB-CG-CD2	7.71	126.20	120.80
1	0	88	VAL	O-C-N	7.71	135.04	122.70
2	1	190	ASP	CB-CG-OD1	-7.69	111.38	118.30
1	0	125	PHE	CB-CG-CD2	-7.69	115.42	120.80
2	1	354	PHE	N-CA-CB	-7.68	96.77	110.60
1	0	113	TYR	CB-CA-C	-7.66	95.09	110.40
1	0	277	TYR	CB-CG-CD1	7.64	125.58	121.00
2	1	24	ASP	CB-CG-OD1	-7.61	111.45	118.30
1	0	11	PHE	CB-CA-C	-7.57	95.25	110.40
1	0	245	MET	CG-SD-CE	-7.57	88.09	100.20
2	1	36	GLU	O-C-N	-7.54	110.64	122.70
1	0	346	GLY	N-CA-C	7.50	131.85	113.10
1	0	91	GLU	CA-CB-CG	7.48	129.85	113.40
2	1	81	LYS	N-CA-C	7.39	130.96	111.00
2	1	262	ALA	N-CA-C	7.34	130.82	111.00
1	0	343	GLU	CB-CA-C	-7.31	95.78	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	230	TYR	CB-CG-CD2	-7.21	116.67	121.00
1	0	80	TYR	CA-CB-CG	7.21	127.10	113.40
2	1	392	ASN	N-CA-CB	-7.20	97.64	110.60
1	0	298	ALA	CB-CA-C	7.18	120.88	110.10
2	1	52	ASP	CB-CG-OD1	-7.18	111.83	118.30
1	0	76	MET	CG-SD-CE	-7.17	88.73	100.20
2	1	418	LEU	C-N-CA	7.16	139.59	121.70
2	1	338	ASP	CB-CG-OD1	7.13	124.72	118.30
1	0	228	PHE	CB-CG-CD1	-7.12	115.81	120.80
2	1	390	LYS	C-N-CA	7.08	139.41	121.70
2	1	83	THR	O-C-N	-7.08	107.64	121.10
1	0	112	VAL	CB-CA-C	7.07	124.83	111.40
1	0	45	LYS	CA-C-N	7.06	132.73	117.20
1	0	80	TYR	CB-CG-CD2	-7.06	116.77	121.00
1	0	90	ASP	N-CA-CB	7.05	123.28	110.60
1	0	335	TYR	CB-CG-CD1	7.03	125.22	121.00
2	1	386	PHE	CB-CG-CD1	-7.01	115.89	120.80
2	1	52	ASP	CB-CG-OD2	6.98	124.58	118.30
2	1	441	SER	N-CA-CB	6.96	120.94	110.50
1	0	94	ALA	O-C-N	-6.96	111.57	122.70
1	0	255	TYR	CD1-CE1-CZ	-6.95	113.54	119.80
1	0	158	THR	N-CA-CB	6.95	123.51	110.30
1	0	10	SER	CA-C-N	6.92	132.44	117.20
2	1	189	TYR	CB-CG-CD2	-6.91	116.85	121.00
2	1	193	ILE	C-N-CA	6.90	138.95	121.70
1	0	46	LYS	N-CA-CB	6.88	122.98	110.60
1	0	89	THR	N-CA-C	-6.87	92.45	111.00
1	0	180	ASP	CB-CG-OD2	-6.86	112.13	118.30
2	1	65	PHE	CB-CG-CD2	-6.86	116.00	120.80
2	1	270	ASP	CB-CA-C	-6.84	96.71	110.40
2	1	390	LYS	N-CA-CB	-6.77	98.41	110.60
2	1	264	MET	C-N-CA	6.75	136.48	122.30
2	1	371	TRP	CB-CG-CD2	-6.73	117.85	126.60
2	1	473	PHE	CB-CA-C	-6.70	97.00	110.40
2	1	256	ARG	NE-CZ-NH2	-6.69	116.95	120.30
2	1	266	ILE	CA-CB-CG1	6.68	123.69	111.00
2	1	266	ILE	CB-CA-C	-6.64	98.32	111.60
2	1	80	LYS	N-CA-C	6.63	128.91	111.00
2	1	180	LYS	CB-CA-C	6.60	123.60	110.40
2	1	258	PHE	N-CA-CB	6.60	122.49	110.60
2	1	248	THR	CA-CB-CG2	6.58	121.61	112.40
1	0	108	THR	CA-CB-CG2	-6.57	103.20	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	167	HIS	CB-CA-C	6.55	123.49	110.40
2	1	40	THR	O-C-N	-6.54	112.23	122.70
2	1	311	ALA	N-CA-CB	-6.53	100.95	110.10
2	1	396	ASN	C-N-CA	6.48	137.91	121.70
1	0	230	TYR	CB-CG-CD1	6.47	124.89	121.00
2	1	268	GLN	C-N-CA	6.47	137.86	121.70
1	0	56	LYS	N-CA-CB	6.46	122.23	110.60
1	0	280	GLU	OE1-CD-OE2	-6.44	115.57	123.30
2	1	369	ARG	NH1-CZ-NH2	-6.44	112.31	119.40
2	1	473	PHE	CB-CG-CD1	-6.44	116.29	120.80
1	0	112	VAL	N-CA-CB	6.42	125.63	111.50
1	0	161	SER	CB-CA-C	-6.41	97.91	110.10
2	1	369	ARG	O-C-N	-6.41	112.44	122.70
2	1	406	LEU	CA-CB-CG	6.39	130.00	115.30
2	1	519	LEU	N-CA-CB	-6.38	97.63	110.40
1	0	180	ASP	CB-CG-OD1	6.38	124.05	118.30
2	1	486	ILE	N-CA-C	-6.38	93.79	111.00
1	0	52	ASP	N-CA-CB	6.37	122.07	110.60
1	0	75	ASP	CB-CG-OD1	6.36	124.02	118.30
1	0	332	ARG	NE-CZ-NH1	-6.36	117.12	120.30
2	1	229	ARG	NE-CZ-NH2	-6.35	117.12	120.30
2	1	235	ILE	CA-CB-CG2	-6.34	98.21	110.90
2	1	341	PHE	CB-CG-CD2	-6.30	116.39	120.80
1	0	88	VAL	CA-C-N	-6.25	103.45	117.20
2	1	586	ASN	C-N-CA	6.25	137.32	121.70
2	1	167	HIS	C-N-CA	6.24	137.29	121.70
1	0	265	ASN	CB-CA-C	6.22	122.85	110.40
2	1	227	ARG	CD-NE-CZ	6.22	132.31	123.60
2	1	397	LYS	N-CA-CB	6.17	121.71	110.60
2	1	486	ILE	CA-CB-CG1	6.16	122.70	111.00
2	1	78	LEU	C-N-CA	6.15	137.06	121.70
1	0	345	ASN	C-N-CA	6.14	135.20	122.30
1	0	335	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	0	66	LYS	N-CA-CB	6.12	121.61	110.60
1	0	11	PHE	CA-CB-CG	6.11	128.56	113.90
2	1	186	ARG	CD-NE-CZ	6.07	132.10	123.60
2	1	196	GLN	N-CA-CB	6.07	121.53	110.60
1	0	112	VAL	CA-CB-CG2	6.06	119.98	110.90
1	0	65	LEU	N-CA-C	6.05	127.34	111.00
2	1	280	THR	O-C-N	-6.05	113.02	122.70
2	1	227	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	0	291	LEU	CA-C-N	-6.04	103.91	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	516	ASN	N-CA-C	-6.03	94.72	111.00
1	0	179	THR	O-C-N	-6.02	113.06	122.70
1	0	310	GLU	CB-CA-C	-6.01	98.37	110.40
1	0	294	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	0	311	TYR	CB-CG-CD1	5.99	124.60	121.00
1	0	66	LYS	CA-CB-CG	5.99	126.58	113.40
1	0	314	ILE	O-C-N	-5.96	113.17	122.70
2	1	372	TYR	CB-CG-CD1	5.94	124.57	121.00
1	0	135	ASN	N-CA-CB	5.94	121.29	110.60
1	0	215	SER	N-CA-CB	5.93	119.39	110.50
2	1	418	LEU	N-CA-C	-5.92	95.01	111.00
1	0	143	ALA	CB-CA-C	5.92	118.98	110.10
1	0	38	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	0	125	PHE	CB-CG-CD1	5.90	124.93	120.80
2	1	61	PHE	CB-CG-CD1	5.89	124.92	120.80
2	1	207	GLU	OE1-CD-OE2	5.86	130.33	123.30
2	1	587	ASP	CB-CG-OD1	-5.85	113.03	118.30
2	1	279	SER	N-CA-CB	5.85	119.28	110.50
2	1	48	TYR	CG-CD1-CE1	5.83	125.96	121.30
2	1	161	VAL	C-N-CA	5.83	136.26	121.70
1	0	65	LEU	CA-CB-CG	5.81	128.67	115.30
2	1	503	ALA	N-CA-C	5.81	126.69	111.00
1	0	268	TYR	CG-CD2-CE2	-5.81	116.65	121.30
2	1	587	ASP	CB-CG-OD2	5.80	123.52	118.30
1	0	90	ASP	CB-CA-C	5.78	121.96	110.40
1	0	39	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	0	65	LEU	CD1-CG-CD2	-5.78	93.17	110.50
2	1	377	LEU	O-C-N	-5.77	113.46	122.70
1	0	172	MET	CB-CA-C	5.77	121.94	110.40
2	1	419	ALA	N-CA-C	-5.77	95.43	111.00
2	1	28	ASP	CB-CA-C	5.76	121.93	110.40
2	1	466	ASP	O-C-N	-5.75	113.50	122.70
2	1	46	GLN	C-N-CA	5.75	136.06	121.70
1	0	225	ASP	CB-CG-OD1	5.74	123.47	118.30
1	0	90	ASP	C-N-CA	5.73	136.02	121.70
1	0	369	ALA	O-C-N	-5.73	113.54	122.70
2	1	253	PRO	N-CA-C	5.71	126.95	112.10
1	0	268	TYR	CG-CD1-CE1	-5.70	116.74	121.30
1	0	374	TYR	CZ-CE2-CD2	5.68	124.92	119.80
2	1	161	VAL	N-CA-C	5.68	126.34	111.00
2	1	76	LYS	N-CA-CB	5.67	120.81	110.60
1	0	299	TRP	CD1-NE1-CE2	-5.66	103.90	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	455	GLN	CA-CB-CG	-5.64	101.00	113.40
1	0	268	TYR	CD1-CG-CD2	5.62	124.08	117.90
2	1	419	ALA	CB-CA-C	-5.59	101.71	110.10
1	0	75	ASP	N-CA-CB	5.58	120.64	110.60
2	1	22	PHE	CB-CG-CD1	5.58	124.71	120.80
1	0	53	GLU	N-CA-CB	5.57	120.63	110.60
2	1	406	LEU	CB-CG-CD2	5.54	120.43	111.00
2	1	381	LEU	CB-CG-CD1	5.54	120.42	111.00
2	1	587	ASP	CA-C-N	5.54	129.39	117.20
1	0	225	ASP	CB-CA-C	-5.53	99.34	110.40
2	1	61	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	0	99	ILE	CB-CG1-CD1	5.52	129.36	113.90
2	1	177	ASP	CB-CG-OD1	-5.51	113.34	118.30
2	1	169	SER	O-C-N	-5.50	113.90	122.70
2	1	516	ASN	C-N-CA	-5.50	107.95	121.70
1	0	311	TYR	CB-CG-CD2	-5.50	117.70	121.00
2	1	300	ALA	N-CA-CB	5.49	117.79	110.10
2	1	341	PHE	CB-CG-CD1	5.49	124.64	120.80
1	0	92	SER	N-CA-CB	5.48	118.72	110.50
1	0	29	PHE	CA-CB-CG	5.48	127.04	113.90
2	1	588	ARG	N-CA-CB	5.46	120.42	110.60
2	1	417	ASP	N-CA-CB	5.45	120.42	110.60
2	1	184	MET	CG-SD-CE	-5.44	91.50	100.20
2	1	455	GLN	O-C-N	-5.42	114.03	122.70
1	0	330	ALA	C-N-CA	5.41	135.23	121.70
2	1	235	ILE	CA-CB-CG1	5.41	121.28	111.00
2	1	504	GLN	CA-CB-CG	5.39	125.27	113.40
2	1	286	GLY	C-N-CA	5.39	135.18	121.70
2	1	465	THR	N-CA-CB	5.39	120.54	110.30
1	0	89	THR	CA-C-N	5.38	129.04	117.20
2	1	250	VAL	N-CA-C	-5.37	96.49	111.00
2	1	237	THR	OG1-CB-CG2	-5.37	97.65	110.00
1	0	354	THR	N-CA-C	5.37	125.49	111.00
1	0	233	GLU	CB-CA-C	-5.36	99.67	110.40
2	1	268	GLN	CA-C-N	-5.36	105.40	117.20
1	0	354	THR	CA-CB-CG2	-5.35	104.91	112.40
1	0	277	TYR	CG-CD2-CE2	-5.34	117.03	121.30
1	0	303	LYS	CA-CB-CG	5.33	125.14	113.40
1	0	26	GLU	O-C-N	-5.33	114.18	122.70
2	1	251	ASP	CB-CG-OD1	5.33	123.09	118.30
1	0	287	PHE	CB-CG-CD1	-5.32	117.08	120.80
1	0	80	TYR	CB-CA-C	5.31	121.02	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	111	TYR	CB-CG-CD2	-5.31	117.82	121.00
2	1	84	PRO	N-CA-C	5.30	125.89	112.10
2	1	194	VAL	O-C-N	-5.30	114.22	122.70
2	1	354	PHE	CB-CG-CD1	-5.30	117.09	120.80
1	0	149	GLU	CB-CA-C	-5.30	99.80	110.40
1	0	277	TYR	CZ-CE2-CD2	5.30	124.57	119.80
2	1	200	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	0	180	ASP	CA-C-O	-5.30	108.98	120.10
1	0	242	ASN	CB-CG-OD1	-5.29	111.01	121.60
1	0	2	LYS	CB-CA-C	5.29	120.98	110.40
2	1	36	GLU	CB-CA-C	-5.29	99.82	110.40
2	1	266	ILE	C-N-CA	5.29	134.92	121.70
2	1	473	PHE	N-CA-CB	5.28	120.11	110.60
2	1	176	VAL	CA-CB-CG1	5.28	118.81	110.90
2	1	335	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	0	291	LEU	CB-CG-CD1	5.27	119.95	111.00
1	0	289	LEU	CB-CG-CD1	-5.25	102.07	111.00
2	1	519	LEU	CB-CG-CD2	5.25	119.93	111.00
2	1	40	THR	C-N-CA	5.25	134.82	121.70
1	0	246	PHE	CB-CG-CD2	-5.24	117.13	120.80
1	0	134	CYS	N-CA-C	5.24	125.14	111.00
2	1	290	ASP	N-CA-CB	-5.23	101.18	110.60
2	1	41	LEU	C-N-CA	5.22	134.75	121.70
2	1	371	TRP	CB-CG-CD1	5.21	133.78	127.00
2	1	290	ASP	O-C-N	-5.20	114.37	123.20
2	1	251	ASP	CB-CG-OD2	5.18	122.96	118.30
1	0	66	LYS	CB-CA-C	5.17	120.75	110.40
2	1	466	ASP	CA-C-N	5.17	128.57	117.20
1	0	57	LYS	CB-CG-CD	5.16	125.01	111.60
1	0	277	TYR	CB-CA-C	-5.15	100.10	110.40
2	1	325	PHE	CB-CG-CD2	-5.15	117.20	120.80
2	1	515	MET	C-N-CA	5.13	134.53	121.70
1	0	32	TYR	CB-CG-CD2	-5.12	117.93	121.00
2	1	253	PRO	N-CD-CG	5.12	110.88	103.20
2	1	25	TYR	CG-CD2-CE2	-5.12	117.21	121.30
2	1	250	VAL	CA-CB-CG1	-5.12	103.23	110.90
1	0	224	MET	CA-CB-CG	5.11	121.99	113.30
1	0	365	LEU	CB-CG-CD2	5.10	119.67	111.00
2	1	461	ASN	C-N-CA	5.10	134.45	121.70
2	1	254	GLY	C-N-CA	5.10	134.45	121.70
2	1	51	TRP	N-CA-CB	-5.10	101.42	110.60
2	1	329	LYS	CA-CB-CG	5.09	124.61	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	47	PHE	O-C-N	-5.09	114.56	122.70
2	1	288	ASP	CB-CG-OD2	5.09	122.88	118.30
1	0	7	LYS	N-CA-CB	-5.08	101.45	110.60
2	1	516	ASN	N-CA-CB	5.07	119.72	110.60
1	0	64	LYS	O-C-N	5.07	130.80	122.70
2	1	79	LYS	CA-CB-CG	5.05	124.51	113.40
2	1	441	SER	CA-C-O	-5.05	109.50	120.10
2	1	418	LEU	CA-C-N	-5.04	106.10	117.20
1	0	134	CYS	O-C-N	-5.04	114.64	122.70
1	0	255	TYR	CB-CG-CD2	5.03	124.02	121.00
2	1	351	ILE	CA-CB-CG1	5.03	120.55	111.00
2	1	501	HIS	N-CA-C	5.03	124.58	111.00
2	1	369	ARG	CA-C-O	5.01	130.62	120.10
1	0	300	TYR	CG-CD1-CE1	-5.00	117.30	121.30
2	1	48	TYR	CB-CG-CD2	5.00	124.00	121.00
2	1	251	ASP	OD1-CG-OD2	-5.00	113.80	123.30

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	11	PHE	CA
1	0	56	LYS	CA
1	0	65	LEU	CA
1	0	90	ASP	CA
1	0	91	GLU	CA
1	0	112	VAL	CA
2	1	161	VAL	CA
2	1	235	ILE	CB
2	1	576	ARG	CA
2	1	586	ASN	CA

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	111	TYR	Sidechain
1	0	112	VAL	Mainchain
1	0	113	TYR	Sidechain
1	0	14	GLY	Peptide
1	0	230	TYR	Sidechain
1	0	255	TYR	Sidechain
1	0	268	TYR	Sidechain
1	0	311	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	0	32	TYR	Sidechain
1	0	332	ARG	Sidechain
1	0	353	SER	Peptide
1	0	354	THR	Peptide
1	0	356	HIS	Sidechain
1	0	381	GLU	Peptide
1	0	47	PHE	Mainchain
1	0	48	THR	Peptide
1	0	51	LEU	Peptide
1	0	55	GLY	Peptide
1	0	66	LYS	Mainchain
1	0	68	LYS	Mainchain
1	0	80	TYR	Sidechain
1	0	91	GLU	Peptide
2	1	175	HIS	Sidechain
2	1	177	ASP	Sidechain
2	1	189	TYR	Sidechain
2	1	194	VAL	Mainchain
2	1	20	GLY	Peptide
2	1	200	ARG	Sidechain
2	1	21	GLU	Peptide
2	1	229	ARG	Sidechain
2	1	230	GLY	Peptide
2	1	265	GLY	Peptide
2	1	287	PHE	Sidechain
2	1	31	TYR	Sidechain
2	1	324	ARG	Sidechain
2	1	354	PHE	Sidechain
2	1	360	TYR	Sidechain
2	1	363	GLU	Peptide
2	1	392	ASN	Peptide
2	1	394	GLY	Peptide
2	1	396	ASN	Peptide
2	1	500	ILE	Mainchain
2	1	517	ARG	Peptide
2	1	76	LYS	Peptide
2	1	79	LYS	Peptide
2	1	81	LYS	Mainchain,Peptide
2	1	83	THR	Peptide

5.2 Too-close contacts ⓘ

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	0	3097	0	3156	613	0
2	1	4086	0	4068	688	0
All	All	7183	0	7224	1200	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 83.

All (1200) 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)
1:0:170:TYR:CD1	1:0:187:LYS:HE3	1.35	1.60
1:0:45:LYS:HE2	1:0:47:PHE:CD2	1.35	1.60
1:0:170:TYR:CG	1:0:187:LYS:HE3	1.33	1.60
1:0:173:PRO:CB	1:0:184:PHE:CE2	1.76	1.59
1:0:314:ILE:HD12	1:0:342:VAL:CG1	1.34	1.58
1:0:314:ILE:CD1	1:0:342:VAL:HG11	1.22	1.56
1:0:65:LEU:CD2	1:0:65:LEU:CG	1.74	1.55
1:0:177:ARG:CD	2:1:458:GLN:NE2	1.68	1.54
2:1:426:GLU:CG	2:1:589:LEU:HD13	1.37	1.53
1:0:205:PHE:CZ	1:0:239:ILE:HG12	1.44	1.52
2:1:426:GLU:HG3	2:1:589:LEU:CD1	1.40	1.50
1:0:176:LYS:HD2	1:0:181:VAL:CG1	1.34	1.50
1:0:175:LYS:HD2	2:1:232:THR:CG2	1.07	1.49
1:0:175:LYS:CD	2:1:232:THR:HG22	1.03	1.49
1:0:173:PRO:HB2	1:0:184:PHE:CE2	0.98	1.49
1:0:170:TYR:CD1	1:0:187:LYS:CE	1.96	1.48
1:0:175:LYS:NZ	2:1:232:THR:HB	1.23	1.47
1:0:173:PRO:CB	1:0:184:PHE:CD2	1.99	1.46
1:0:176:LYS:NZ	1:0:183:LYS:HD3	1.29	1.45
1:0:205:PHE:CE2	1:0:239:ILE:HG13	1.52	1.45
1:0:177:ARG:HD2	2:1:458:GLN:NE2	1.21	1.44
1:0:45:LYS:CE	1:0:47:PHE:HD2	1.31	1.44
1:0:205:PHE:CZ	1:0:239:ILE:CG1	2.01	1.44
1:0:45:LYS:CE	1:0:47:PHE:CD2	1.99	1.43
2:1:31:TYR:CE2	2:1:32:GLU:HG3	1.52	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:45:LYS:HZ3	1:0:63:VAL:C	1.22	1.42
1:0:171:SER:N	1:0:187:LYS:HE2	1.28	1.41
1:0:175:LYS:NZ	2:1:232:THR:CB	1.84	1.40
1:0:184:PHE:CE1	2:1:230:GLY:O	1.75	1.39
1:0:64:LYS:O	1:0:99:ILE:CD1	1.69	1.37
2:1:426:GLU:CG	2:1:589:LEU:CD1	1.91	1.37
1:0:175:LYS:HZ3	2:1:232:THR:CB	1.37	1.36
1:0:170:TYR:HB2	1:0:187:LYS:NZ	1.40	1.35
1:0:32:TYR:O	1:0:325:HIS:CE1	1.78	1.35
1:0:173:PRO:HB2	1:0:184:PHE:CD2	1.59	1.33
1:0:322:LYS:NZ	1:0:363:ASP:HB2	1.41	1.32
1:0:45:LYS:CD	1:0:63:VAL:O	1.78	1.30
1:0:176:LYS:CD	1:0:181:VAL:HG11	1.61	1.29
1:0:67:ILE:HD11	1:0:105:LEU:CD2	1.62	1.28
1:0:322:LYS:NZ	1:0:363:ASP:CB	1.96	1.28
1:0:181:VAL:O	1:0:183:LYS:N	1.67	1.27
1:0:322:LYS:HZ1	1:0:363:ASP:CB	1.46	1.27
2:1:426:GLU:CD	2:1:589:LEU:CD1	2.03	1.26
1:0:170:TYR:CD1	1:0:187:LYS:CD	2.17	1.25
1:0:96:ASN:O	1:0:99:ILE:HG13	1.36	1.25
1:0:45:LYS:HD3	1:0:63:VAL:O	1.17	1.24
1:0:170:TYR:CD2	1:0:191:PHE:CD1	2.26	1.24
1:0:200:LYS:HD3	1:0:236:ASN:ND2	1.51	1.24
1:0:47:PHE:CE2	1:0:63:VAL:HB	1.71	1.23
1:0:386:GLU:OE1	2:1:541:LEU:HB3	1.36	1.23
1:0:182:LEU:HD23	1:0:182:LEU:O	1.40	1.22
1:0:170:TYR:CB	1:0:187:LYS:HE3	1.69	1.21
1:0:386:GLU:OE2	2:1:541:LEU:HD22	1.40	1.21
1:0:170:TYR:HB2	1:0:187:LYS:CE	1.68	1.21
1:0:317:LEU:CD1	1:0:339:MET:HG2	1.72	1.20
1:0:200:LYS:CD	1:0:236:ASN:HD21	1.55	1.19
1:0:60:THR:HG23	1:0:61:ASP:N	1.54	1.19
1:0:386:GLU:OE1	2:1:541:LEU:O	1.61	1.19
1:0:173:PRO:HB3	1:0:184:PHE:CD2	1.65	1.18
1:0:322:LYS:O	1:0:326:SER:HB3	1.44	1.18
1:0:170:TYR:HD1	1:0:187:LYS:CD	1.53	1.18
1:0:177:ARG:HH11	2:1:458:GLN:NE2	1.38	1.18
1:0:205:PHE:CG	1:0:238:LYS:O	1.98	1.17
2:1:426:GLU:CD	2:1:589:LEU:HD13	1.63	1.17
1:0:205:PHE:CE1	1:0:245:MET:CE	2.28	1.17
1:0:348:LYS:HD2	1:0:348:LYS:N	1.51	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:322:LYS:HE2	1:0:363:ASP:OD2	0.99	1.17
1:0:64:LYS:C	1:0:99:ILE:HD11	1.63	1.16
1:0:67:ILE:HD11	1:0:105:LEU:CG	1.74	1.16
1:0:175:LYS:HG3	2:1:234:SER:O	1.44	1.16
1:0:322:LYS:CE	1:0:363:ASP:OD2	1.92	1.16
1:0:182:LEU:CD2	1:0:186:GLU:HG2	1.73	1.16
1:0:192:TYR:CB	1:0:230:TYR:OH	1.93	1.16
1:0:43:PHE:CE2	1:0:67:ILE:HD12	1.79	1.16
1:0:314:ILE:CG1	1:0:342:VAL:HG11	1.77	1.14
1:0:175:LYS:NZ	2:1:232:THR:CG2	2.10	1.14
1:0:205:PHE:CD1	1:0:245:MET:CE	2.31	1.14
1:0:314:ILE:CD1	1:0:342:VAL:CG1	2.06	1.13
1:0:175:LYS:HZ2	2:1:232:THR:CG2	1.59	1.13
2:1:426:GLU:CG	2:1:589:LEU:HD11	1.77	1.13
1:0:192:TYR:CD1	1:0:226:LYS:HG3	1.85	1.12
1:0:192:TYR:HB2	1:0:230:TYR:OH	1.47	1.12
1:0:181:VAL:HG22	1:0:183:LYS:HG3	1.29	1.12
1:0:312:GLY:N	1:0:345:ASN:HB3	1.39	1.12
1:0:43:PHE:O	1:0:64:LYS:HB2	1.46	1.12
2:1:248:THR:CB	2:1:454:SER:HA	1.80	1.11
1:0:205:PHE:CE1	1:0:245:MET:HE1	1.83	1.11
2:1:248:THR:N	2:1:454:SER:OG	1.84	1.11
2:1:31:TYR:CE2	2:1:32:GLU:CG	2.33	1.11
1:0:176:LYS:NZ	1:0:183:LYS:CD	2.14	1.11
1:0:170:TYR:CB	1:0:187:LYS:CE	2.25	1.10
1:0:175:LYS:CG	2:1:234:SER:O	1.97	1.10
1:0:167:LYS:O	1:0:167:LYS:HG2	1.51	1.10
1:0:60:THR:HG23	1:0:61:ASP:H	0.96	1.10
1:0:175:LYS:HZ2	2:1:232:THR:HG21	1.09	1.10
1:0:317:LEU:HD13	1:0:339:MET:HG2	1.18	1.09
1:0:195:ILE:HG21	1:0:223:LEU:HD11	1.32	1.09
1:0:314:ILE:CG1	1:0:342:VAL:CG1	2.29	1.09
1:0:176:LYS:HZ3	1:0:183:LYS:CD	1.65	1.09
1:0:171:SER:O	1:0:187:LYS:CD	2.00	1.09
1:0:200:LYS:HD3	1:0:236:ASN:HD21	0.94	1.08
1:0:171:SER:O	1:0:187:LYS:HG3	1.51	1.08
1:0:47:PHE:CE2	1:0:63:VAL:CB	2.36	1.08
1:0:177:ARG:HD3	2:1:458:GLN:NE2	1.68	1.08
1:0:386:GLU:CD	2:1:541:LEU:HD22	1.72	1.08
1:0:47:PHE:CE2	1:0:63:VAL:CG1	2.37	1.07
1:0:310:GLU:O	1:0:345:ASN:OD1	1.70	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:248:THR:HB	2:1:454:SER:CA	1.83	1.07
1:0:45:LYS:CE	1:0:47:PHE:CE2	2.36	1.07
1:0:45:LYS:NZ	1:0:63:VAL:C	2.08	1.07
2:1:491:LEU:HD13	2:1:500:ILE:HG21	1.31	1.07
2:1:580:LEU:HD12	2:1:606:ILE:HD13	1.14	1.06
1:0:177:ARG:NH1	2:1:458:GLN:NE2	2.02	1.06
1:0:171:SER:N	1:0:187:LYS:CE	2.17	1.06
1:0:47:PHE:CZ	1:0:63:VAL:HG11	1.91	1.06
2:1:556:ILE:HA	2:1:564:ARG:HA	1.31	1.06
1:0:67:ILE:HD11	1:0:105:LEU:HD23	1.31	1.05
2:1:426:GLU:OE2	2:1:589:LEU:HD12	1.56	1.05
2:1:410:PRO:HB3	2:1:416:ASN:HA	1.35	1.05
2:1:426:GLU:OE2	2:1:589:LEU:CD1	2.03	1.05
2:1:459:SER:HB2	2:1:477:LYS:NZ	1.69	1.05
1:0:45:LYS:HE2	1:0:47:PHE:CE2	1.91	1.05
1:0:314:ILE:HD12	1:0:342:VAL:CB	1.87	1.05
1:0:85:GLY:O	1:0:104:TYR:CD2	2.08	1.05
1:0:205:PHE:CE2	1:0:239:ILE:CG1	2.27	1.04
1:0:45:LYS:CE	1:0:63:VAL:O	2.04	1.04
2:1:571:LEU:HD12	2:1:577:TRP:HB3	1.39	1.04
1:0:171:SER:O	1:0:187:LYS:CG	2.05	1.03
2:1:454:SER:HB3	2:1:456:GLN:NE2	1.70	1.03
1:0:184:PHE:HE1	2:1:230:GLY:O	1.19	1.03
2:1:459:SER:CB	2:1:477:LYS:HZ3	1.69	1.03
1:0:65:LEU:CD1	1:0:65:LEU:CD2	2.35	1.03
2:1:397:LYS:HB2	2:1:428:GLY:H	1.23	1.03
1:0:386:GLU:OE1	2:1:541:LEU:CB	2.06	1.03
1:0:181:VAL:HG21	1:0:183:LYS:HD2	1.09	1.02
2:1:527:LEU:HG	2:1:592:VAL:HG11	1.41	1.02
1:0:322:LYS:HE2	1:0:363:ASP:CG	1.80	1.02
2:1:542:ILE:HG21	2:1:566:PHE:HD2	1.20	1.02
1:0:175:LYS:CE	2:1:232:THR:CG2	2.37	1.01
1:0:45:LYS:HE3	1:0:47:PHE:CD2	1.93	1.01
1:0:348:LYS:HZ3	1:0:348:LYS:HA	1.20	1.01
1:0:181:VAL:HG21	1:0:183:LYS:CD	1.89	1.01
1:0:179:THR:O	2:1:233:VAL:HG22	1.60	1.01
1:0:309:ALA:O	1:0:345:ASN:HB2	1.59	1.00
2:1:235:ILE:HG21	2:1:237:THR:HG23	1.41	1.00
1:0:205:PHE:CD1	1:0:245:MET:HE2	1.94	1.00
1:0:45:LYS:HZ1	1:0:47:PHE:HE2	1.06	1.00
1:0:93:GLY:O	1:0:97:VAL:HG23	1.62	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:205:PHE:HB3	1:0:242:ASN:ND2	1.76	1.00
1:0:171:SER:O	1:0:187:LYS:HD2	1.61	0.99
1:0:99:ILE:CD1	1:0:99:ILE:CG1	2.39	0.99
1:0:208:LEU:C	1:0:209:LYS:HE2	1.83	0.99
1:0:171:SER:H	1:0:187:LYS:CE	1.74	0.99
1:0:47:PHE:HE2	1:0:63:VAL:CG1	1.73	0.99
1:0:45:LYS:HZ1	1:0:63:VAL:HG12	1.27	0.99
2:1:493:ALA:HB2	2:1:500:ILE:HD11	1.45	0.99
1:0:170:TYR:CG	1:0:187:LYS:CE	2.28	0.98
1:0:43:PHE:O	1:0:64:LYS:CB	2.09	0.98
1:0:181:VAL:CG2	1:0:183:LYS:HD2	1.92	0.98
1:0:43:PHE:HE2	1:0:67:ILE:HD12	1.15	0.98
1:0:199:MET:HG3	1:0:203:LEU:HD23	1.41	0.98
1:0:32:TYR:O	1:0:325:HIS:HE1	1.43	0.98
2:1:556:ILE:HG12	2:1:564:ARG:HG3	1.45	0.98
1:0:176:LYS:HZ2	1:0:183:LYS:HD3	1.20	0.98
2:1:491:LEU:HD22	2:1:500:ILE:HD13	1.46	0.97
1:0:176:LYS:HD2	1:0:181:VAL:HG12	1.46	0.97
1:0:192:TYR:HB3	1:0:230:TYR:OH	1.65	0.97
1:0:45:LYS:NZ	1:0:63:VAL:O	1.94	0.97
1:0:181:VAL:C	1:0:183:LYS:H	1.67	0.97
1:0:322:LYS:H	1:0:354:THR:HG21	1.26	0.97
2:1:459:SER:CB	2:1:477:LYS:NZ	2.26	0.97
1:0:64:LYS:C	1:0:99:ILE:CD1	2.27	0.96
1:0:170:TYR:HD1	1:0:187:LYS:HD3	1.28	0.96
2:1:446:ILE:HG22	2:1:479:ARG:HB3	1.42	0.96
1:0:205:PHE:HE2	1:0:239:ILE:HG13	1.22	0.96
1:0:182:LEU:HD21	1:0:186:GLU:HG2	1.41	0.96
2:1:489:GLY:C	2:1:579:PRO:HG2	1.86	0.96
1:0:205:PHE:CD1	1:0:245:MET:HE1	1.96	0.96
1:0:205:PHE:CD2	1:0:238:LYS:O	2.18	0.95
2:1:459:SER:HA	2:1:477:LYS:HZ1	1.30	0.95
2:1:411:SER:HB2	2:1:414:THR:HG22	1.49	0.95
1:0:45:LYS:NZ	1:0:47:PHE:HE2	1.65	0.95
2:1:402:LEU:HD13	2:1:581:LEU:CD1	1.97	0.95
2:1:583:ALA:HB3	2:1:605:LYS:HE3	1.49	0.95
1:0:175:LYS:CE	2:1:232:THR:HB	1.96	0.94
1:0:43:PHE:CZ	1:0:105:LEU:HD21	2.02	0.94
1:0:309:ALA:O	1:0:345:ASN:CB	2.15	0.94
2:1:454:SER:HB3	2:1:456:GLN:HE22	1.23	0.94
1:0:60:THR:CG2	1:0:61:ASP:H	1.79	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:267:SER:H	2:1:473:PHE:HB2	1.30	0.94
1:0:67:ILE:HD11	1:0:105:LEU:HG	1.46	0.94
1:0:170:TYR:HD1	1:0:187:LYS:CE	1.50	0.94
2:1:459:SER:HA	2:1:477:LYS:NZ	1.82	0.94
1:0:45:LYS:NZ	1:0:63:VAL:HG12	1.82	0.93
1:0:309:ALA:HB1	1:0:342:VAL:N	1.82	0.93
1:0:60:THR:CG2	1:0:61:ASP:N	2.30	0.93
1:0:173:PRO:CB	1:0:184:PHE:CZ	2.51	0.93
2:1:526:ILE:HG23	2:1:528:PHE:HE1	1.34	0.93
1:0:85:GLY:N	1:0:104:TYR:CZ	2.37	0.93
1:0:170:TYR:CD1	1:0:191:PHE:HB2	2.03	0.93
1:0:176:LYS:CD	1:0:181:VAL:CG1	2.30	0.93
1:0:175:LYS:CE	2:1:232:THR:HG22	1.97	0.93
1:0:317:LEU:CD1	1:0:339:MET:CG	2.47	0.92
1:0:199:MET:CG	1:0:203:LEU:HD23	1.99	0.92
2:1:564:ARG:HD2	2:1:564:ARG:H	1.30	0.92
2:1:235:ILE:HG12	2:1:237:THR:O	1.70	0.92
1:0:205:PHE:CE1	1:0:245:MET:HE2	2.01	0.92
1:0:312:GLY:H	1:0:345:ASN:HB3	1.34	0.91
2:1:418:LEU:HB3	2:1:481:ALA:HB3	1.52	0.91
2:1:402:LEU:CD1	2:1:581:LEU:HD11	1.99	0.91
2:1:452:VAL:HG12	2:1:453:GLY:H	1.31	0.91
1:0:67:ILE:CD1	1:0:105:LEU:HG	2.01	0.91
1:0:64:LYS:O	1:0:99:ILE:HD11	0.74	0.91
2:1:401:PHE:CD2	2:1:493:ALA:HA	2.04	0.91
1:0:170:TYR:HB2	1:0:187:LYS:HZ1	1.12	0.90
2:1:528:PHE:HB2	2:1:593:VAL:CG2	2.00	0.90
1:0:312:GLY:O	1:0:346:GLY:HA3	1.70	0.90
1:0:326:SER:O	1:0:327:ASP:HB2	1.70	0.90
1:0:59:SER:O	1:0:60:THR:HB	1.69	0.90
2:1:508:LEU:HD21	2:1:604:GLY:HA3	1.51	0.90
1:0:205:PHE:HE1	1:0:245:MET:CE	1.78	0.90
2:1:545:ILE:HG13	2:1:557:ARG:HA	1.51	0.90
1:0:199:MET:HG3	1:0:203:LEU:CD2	2.00	0.89
1:0:70:ILE:HD12	1:0:104:TYR:HE2	1.36	0.89
1:0:173:PRO:CG	1:0:184:PHE:CE2	2.56	0.89
2:1:235:ILE:HG21	2:1:237:THR:CG2	2.03	0.89
2:1:556:ILE:HA	2:1:564:ARG:CA	2.01	0.89
1:0:85:GLY:C	1:0:104:TYR:CE2	2.47	0.89
1:0:195:ILE:HG21	1:0:223:LEU:CD1	2.02	0.89
1:0:348:LYS:N	1:0:348:LYS:CD	2.33	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:45:LYS:HG2	1:0:46:LYS:H	1.36	0.88
1:0:173:PRO:HB3	1:0:184:PHE:CG	2.07	0.88
2:1:511:THR:HA	2:1:564:ARG:CB	2.03	0.88
2:1:459:SER:HB2	2:1:477:LYS:CE	2.02	0.88
1:0:45:LYS:NZ	1:0:47:PHE:CE2	2.42	0.88
1:0:168:ILE:HG22	1:0:169:GLU:N	1.88	0.88
1:0:175:LYS:CE	2:1:232:THR:CB	2.52	0.88
2:1:402:LEU:HD13	2:1:581:LEU:HD11	1.56	0.88
2:1:31:TYR:CZ	2:1:32:GLU:CG	2.55	0.88
1:0:170:TYR:CD1	1:0:187:LYS:HD3	2.03	0.88
1:0:67:ILE:CD1	1:0:105:LEU:HD23	2.03	0.88
1:0:322:LYS:HZ1	1:0:363:ASP:HB2	0.97	0.88
1:0:205:PHE:HD1	1:0:245:MET:CE	1.83	0.87
1:0:348:LYS:HD2	1:0:348:LYS:H	1.37	0.87
1:0:85:GLY:O	1:0:104:TYR:CE2	2.27	0.87
1:0:205:PHE:HZ	1:0:239:ILE:HG12	0.73	0.87
1:0:322:LYS:HZ3	1:0:363:ASP:HB2	1.34	0.87
2:1:512:THR:HG22	2:1:555:LYS:H	1.37	0.87
1:0:175:LYS:CD	2:1:232:THR:CG2	1.89	0.87
2:1:491:LEU:HD22	2:1:500:ILE:CD1	2.04	0.87
1:0:170:TYR:CB	1:0:187:LYS:NZ	2.33	0.87
1:0:342:VAL:O	1:0:346:GLY:N	2.08	0.87
1:0:177:ARG:HD3	2:1:458:GLN:CD	1.95	0.86
2:1:540:ARG:NH2	2:1:541:LEU:HA	1.90	0.86
1:0:84:LYS:HB3	1:0:104:TYR:OH	1.75	0.86
1:0:67:ILE:CD1	1:0:105:LEU:CG	2.52	0.86
1:0:205:PHE:HZ	1:0:239:ILE:CG1	1.60	0.86
2:1:544:PHE:CE2	2:1:555:LYS:HD3	2.09	0.86
1:0:43:PHE:CE2	1:0:67:ILE:CD1	2.56	0.86
2:1:559:LEU:HD23	2:1:560:GLY:N	1.91	0.86
2:1:409:ILE:HD13	2:1:410:PRO:N	1.91	0.86
2:1:511:THR:CB	2:1:564:ARG:HG2	2.04	0.86
2:1:31:TYR:CZ	2:1:32:GLU:HG3	2.11	0.86
2:1:514:ASP:HA	2:1:553:LYS:CD	2.06	0.86
2:1:527:LEU:CG	2:1:592:VAL:HG11	2.05	0.86
2:1:426:GLU:HG3	2:1:589:LEU:HD13	0.92	0.85
1:0:47:PHE:HZ	1:0:63:VAL:HG11	1.40	0.85
1:0:200:LYS:CE	1:0:236:ASN:HD21	1.90	0.85
1:0:173:PRO:CG	1:0:184:PHE:CZ	2.60	0.85
1:0:47:PHE:CE2	1:0:63:VAL:HG11	2.09	0.85
1:0:182:LEU:CD2	1:0:186:GLU:CG	2.54	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:420:LEU:HD23	2:1:421:VAL:N	1.91	0.84
2:1:526:ILE:HD11	2:1:533:GLU:HG2	1.57	0.84
1:0:45:LYS:HE3	1:0:47:PHE:HD2	1.34	0.84
2:1:534:GLN:HE22	2:1:571:LEU:HD13	1.41	0.84
2:1:459:SER:CA	2:1:477:LYS:NZ	2.40	0.84
2:1:580:LEU:HD12	2:1:606:ILE:CD1	2.04	0.84
2:1:510:LEU:HD11	2:1:602:ALA:HB3	1.58	0.84
2:1:542:ILE:HG21	2:1:566:PHE:CD2	2.10	0.84
1:0:65:LEU:CG	1:0:99:ILE:HG21	2.07	0.83
1:0:181:VAL:HG22	1:0:183:LYS:CG	2.07	0.83
1:0:65:LEU:HD23	1:0:87:THR:CG2	2.08	0.83
1:0:386:GLU:OE2	2:1:541:LEU:CD2	2.26	0.83
2:1:556:ILE:HG12	2:1:564:ARG:CG	2.08	0.83
1:0:192:TYR:CE1	1:0:226:LYS:HG3	2.14	0.83
1:0:314:ILE:CG1	1:0:342:VAL:HG13	2.08	0.83
1:0:43:PHE:CZ	1:0:67:ILE:CD1	2.61	0.83
2:1:526:ILE:HG23	2:1:528:PHE:CE1	2.14	0.83
2:1:512:THR:HG21	2:1:552:SER:O	1.78	0.83
2:1:510:LEU:O	2:1:564:ARG:HB2	1.78	0.83
1:0:65:LEU:HD12	1:0:99:ILE:HD13	1.59	0.82
2:1:544:PHE:CE1	2:1:551:ALA:HA	2.13	0.82
1:0:65:LEU:HD23	1:0:87:THR:HG21	1.62	0.82
2:1:495:VAL:C	2:1:498:SER:HB2	2.00	0.82
1:0:192:TYR:CD1	1:0:226:LYS:CG	2.62	0.82
2:1:31:TYR:CD2	2:1:32:GLU:HG3	2.14	0.82
1:0:322:LYS:HZ1	1:0:363:ASP:HB3	1.43	0.82
2:1:508:LEU:HD23	2:1:509:GLU:N	1.95	0.82
1:0:171:SER:CA	1:0:187:LYS:HE2	2.09	0.82
2:1:575:LYS:HD2	2:1:577:TRP:CH2	2.14	0.82
2:1:437:THR:HG22	2:1:493:ALA:O	1.80	0.82
2:1:445:CYS:SG	2:1:478:LEU:HB3	2.20	0.81
2:1:491:LEU:HD13	2:1:500:ILE:CG2	2.08	0.81
1:0:185:ASP:O	1:0:188:THR:HG22	1.79	0.81
2:1:397:LYS:CG	2:1:399:ASP:HB2	2.10	0.81
1:0:13:LYS:HE3	1:0:13:LYS:N	1.95	0.81
1:0:65:LEU:HB2	1:0:105:LEU:HD23	1.59	0.81
1:0:43:PHE:HZ	1:0:105:LEU:CD2	1.93	0.81
1:0:187:LYS:O	1:0:187:LYS:HD3	1.81	0.81
1:0:173:PRO:HB2	1:0:184:PHE:HE2	1.00	0.81
1:0:322:LYS:CE	1:0:363:ASP:CG	2.44	0.81
2:1:540:ARG:HE	2:1:542:ILE:H	1.24	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:571:LEU:HD11	2:1:578:ILE:CG2	2.11	0.81
1:0:314:ILE:HG13	1:0:342:VAL:HG13	1.63	0.81
2:1:439:TYR:CD1	2:1:499:SER:HB2	2.15	0.81
2:1:541:LEU:HD13	2:1:549:ASN:O	1.80	0.81
1:0:309:ALA:CA	1:0:342:VAL:HA	2.08	0.81
1:0:322:LYS:O	1:0:326:SER:CB	2.28	0.81
2:1:495:VAL:O	2:1:498:SER:HB2	1.80	0.81
1:0:65:LEU:CG	1:0:105:LEU:HD22	2.11	0.80
2:1:446:ILE:CG2	2:1:479:ARG:HB3	2.11	0.80
1:0:43:PHE:HZ	1:0:67:ILE:HD11	1.45	0.80
2:1:578:ILE:HD12	2:1:579:PRO:HD2	1.62	0.80
1:0:386:GLU:CD	2:1:541:LEU:O	2.19	0.80
2:1:411:SER:HB2	2:1:414:THR:CG2	2.11	0.80
2:1:410:PRO:CB	2:1:416:ASN:HA	2.12	0.80
1:0:170:TYR:CD2	1:0:191:PHE:HD1	1.99	0.80
1:0:177:ARG:CD	2:1:458:GLN:CD	2.49	0.80
2:1:234:SER:HB3	2:1:235:ILE:HD13	1.62	0.80
2:1:505:CYS:SG	2:1:568:GLU:HG2	2.21	0.80
1:0:314:ILE:HB	1:0:342:VAL:CG1	2.12	0.80
1:0:65:LEU:HG	1:0:99:ILE:HG21	1.64	0.80
2:1:264:MET:HA	2:1:588:ARG:HG3	1.61	0.80
1:0:386:GLU:HA	2:1:548:GLY:O	1.80	0.80
2:1:397:LYS:HD3	2:1:399:ASP:HB2	1.62	0.80
1:0:93:GLY:O	1:0:97:VAL:CG2	2.30	0.80
1:0:314:ILE:CB	1:0:342:VAL:CG1	2.60	0.80
1:0:170:TYR:CG	1:0:191:PHE:CD1	2.69	0.79
1:0:175:LYS:CD	2:1:234:SER:O	2.29	0.79
2:1:514:ASP:HA	2:1:553:LYS:HG3	1.63	0.79
1:0:167:LYS:O	1:0:167:LYS:CG	2.30	0.79
2:1:556:ILE:CA	2:1:564:ARG:HA	2.12	0.79
2:1:425:LEU:HD22	2:1:470:LYS:HA	1.61	0.79
1:0:205:PHE:CD2	1:0:238:LYS:C	2.56	0.79
1:0:60:THR:O	1:0:61:ASP:CB	2.30	0.79
1:0:177:ARG:NE	2:1:458:GLN:NE2	2.31	0.79
2:1:510:LEU:HD23	2:1:511:THR:N	1.98	0.79
2:1:489:GLY:O	2:1:579:PRO:HG2	1.83	0.78
2:1:542:ILE:HG23	2:1:566:PHE:HB3	1.65	0.78
2:1:425:LEU:HD11	2:1:429:SER:HA	1.64	0.78
2:1:532:LYS:NZ	2:1:578:ILE:HD13	1.99	0.78
2:1:459:SER:CA	2:1:477:LYS:HZ1	1.97	0.78
1:0:196:TYR:CB	1:0:230:TYR:HD2	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:489:GLY:O	2:1:579:PRO:HB2	1.83	0.78
2:1:491:LEU:CD1	2:1:500:ILE:HG21	2.13	0.78
1:0:180:ASP:HB3	2:1:233:VAL:O	1.84	0.78
1:0:317:LEU:HD13	1:0:339:MET:CG	2.07	0.78
1:0:177:ARG:CZ	2:1:458:GLN:NE2	2.47	0.78
2:1:507:VAL:HG11	2:1:566:PHE:CZ	2.19	0.78
1:0:43:PHE:CZ	1:0:67:ILE:HD11	2.19	0.77
1:0:196:TYR:HB2	1:0:230:TYR:HD2	1.49	0.77
1:0:177:ARG:O	2:1:235:ILE:HD12	1.84	0.77
2:1:405:VAL:HG13	2:1:488:ASN:HA	1.65	0.77
1:0:65:LEU:HD22	1:0:105:LEU:HD22	1.65	0.77
1:0:175:LYS:HG3	2:1:235:ILE:HA	1.67	0.77
2:1:438:ILE:HD13	2:1:486:ILE:HD12	1.65	0.77
2:1:420:LEU:HD21	2:1:475:THR:HG23	1.66	0.77
1:0:181:VAL:CG2	1:0:183:LYS:CD	2.55	0.77
2:1:31:TYR:CZ	2:1:32:GLU:HG2	2.20	0.77
1:0:326:SER:O	1:0:327:ASP:CB	2.31	0.77
1:0:182:LEU:HD23	1:0:186:GLU:HG2	1.65	0.76
2:1:583:ALA:CB	2:1:605:LYS:HG3	2.14	0.76
2:1:534:GLN:OE1	2:1:573:GLU:HB2	1.85	0.76
2:1:510:LEU:HD12	2:1:594:LEU:HD22	1.66	0.76
2:1:397:LYS:HB2	2:1:428:GLY:N	2.00	0.76
1:0:168:ILE:CG2	1:0:169:GLU:N	2.49	0.76
1:0:322:LYS:CE	1:0:363:ASP:CB	2.63	0.76
1:0:255:TYR:CE1	2:1:535:PRO:HD3	2.21	0.76
1:0:176:LYS:C	2:1:235:ILE:HG23	2.06	0.76
1:0:43:PHE:CZ	1:0:67:ILE:HD12	2.20	0.76
2:1:511:THR:HA	2:1:564:ARG:HB3	1.67	0.76
1:0:154:VAL:HG23	1:0:168:ILE:CD1	2.15	0.76
1:0:208:LEU:O	1:0:209:LYS:HE2	1.85	0.76
1:0:171:SER:H	1:0:187:LYS:HE2	0.93	0.76
1:0:176:LYS:HZ3	1:0:183:LYS:HD3	0.93	0.76
1:0:175:LYS:HD3	2:1:232:THR:HG22	1.57	0.76
1:0:348:LYS:CA	1:0:348:LYS:HZ3	1.98	0.76
1:0:65:LEU:CA	1:0:99:ILE:CD1	2.64	0.75
1:0:176:LYS:HD2	1:0:181:VAL:HG11	0.76	0.75
2:1:534:GLN:HG3	2:1:573:GLU:CD	2.05	0.75
1:0:322:LYS:NZ	1:0:363:ASP:CG	2.40	0.75
2:1:512:THR:CG2	2:1:555:LYS:H	1.99	0.75
2:1:439:TYR:HB2	2:1:499:SER:O	1.86	0.75
2:1:514:ASP:OD1	2:1:553:LYS:HD2	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:65:LEU:CA	1:0:99:ILE:HD13	2.16	0.75
2:1:409:ILE:HD13	2:1:410:PRO:CD	2.17	0.75
2:1:401:PHE:CE1	2:1:430:ILE:HD11	2.21	0.75
2:1:402:LEU:HD13	2:1:581:LEU:HD12	1.68	0.75
1:0:309:ALA:HA	1:0:342:VAL:HA	1.67	0.75
2:1:583:ALA:HB3	2:1:605:LYS:CE	2.17	0.75
2:1:193:ILE:HG22	2:1:194:VAL:H	1.51	0.74
1:0:168:ILE:O	1:0:169:GLU:HB3	1.85	0.74
1:0:84:LYS:C	1:0:104:TYR:OH	2.25	0.74
1:0:314:ILE:HD12	1:0:342:VAL:CG2	2.16	0.74
1:0:65:LEU:CD2	1:0:105:LEU:HD22	2.18	0.74
1:0:90:ASP:HA	1:0:96:ASN:HB2	1.68	0.74
1:0:168:ILE:CG2	1:0:169:GLU:H	1.99	0.74
1:0:181:VAL:HG13	1:0:183:LYS:HB2	1.69	0.74
2:1:511:THR:HB	2:1:564:ARG:HG2	1.68	0.74
2:1:397:LYS:CD	2:1:399:ASP:HB2	2.16	0.74
1:0:181:VAL:CG2	1:0:183:LYS:HG3	2.14	0.74
1:0:365:LEU:HD22	2:1:520:LEU:HD12	1.68	0.74
1:0:386:GLU:CA	2:1:548:GLY:O	2.35	0.74
2:1:267:SER:N	2:1:473:PHE:HB2	2.03	0.73
2:1:538:ILE:HG13	2:1:540:ARG:HH12	1.51	0.73
1:0:45:LYS:HZ1	1:0:63:VAL:CG1	2.01	0.73
1:0:65:LEU:CD2	1:0:65:LEU:HD11	2.16	0.73
1:0:314:ILE:CD1	1:0:342:VAL:HG21	2.19	0.73
2:1:583:ALA:HB2	2:1:605:LYS:HG3	1.68	0.73
1:0:66:LYS:C	1:0:88:VAL:CG2	2.56	0.73
2:1:539:LYS:O	2:1:540:ARG:HD3	1.88	0.73
1:0:209:LYS:N	1:0:209:LYS:HE2	2.03	0.73
2:1:248:THR:HB	2:1:454:SER:HA	0.87	0.73
1:0:170:TYR:CG	1:0:191:PHE:HD1	2.06	0.73
2:1:414:THR:C	2:1:419:ALA:HA	2.08	0.73
2:1:247:PHE:C	2:1:454:SER:OG	2.27	0.73
1:0:61:ASP:O	1:0:62:LEU:HB2	1.88	0.73
2:1:514:ASP:HA	2:1:553:LYS:CG	2.17	0.73
1:0:43:PHE:CZ	1:0:105:LEU:CD2	2.69	0.73
1:0:47:PHE:HE2	1:0:63:VAL:HG12	1.53	0.73
2:1:528:PHE:HB2	2:1:593:VAL:HG22	1.70	0.73
1:0:170:TYR:CD2	1:0:191:PHE:CE1	2.77	0.72
1:0:170:TYR:CD1	1:0:187:LYS:HD2	2.20	0.72
1:0:170:TYR:CE2	1:0:191:PHE:CD1	2.77	0.72
2:1:418:LEU:CB	2:1:481:ALA:HB3	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:190:ASP:O	2:1:193:ILE:HG23	1.89	0.72
2:1:405:VAL:HG23	2:1:421:VAL:HG13	1.70	0.72
2:1:538:ILE:CG1	2:1:540:ARG:HH12	2.02	0.72
1:0:181:VAL:HG13	1:0:181:VAL:O	1.88	0.72
2:1:408:ILE:HG13	2:1:417:ASP:CG	2.10	0.72
1:0:255:TYR:CD1	2:1:535:PRO:HD3	2.24	0.72
1:0:291:LEU:HD13	1:0:298:ALA:O	1.90	0.72
1:0:312:GLY:N	1:0:345:ASN:CB	2.35	0.72
2:1:404:SER:HB3	2:1:589:LEU:HD11	1.71	0.72
1:0:261:GLU:OE1	2:1:597:ASP:OD1	2.06	0.72
2:1:544:PHE:CZ	2:1:555:LYS:HD3	2.25	0.72
2:1:513:PHE:O	2:1:553:LYS:HG3	1.90	0.71
2:1:489:GLY:O	2:1:579:PRO:CG	2.39	0.71
1:0:205:PHE:HD2	1:0:238:LYS:HG2	1.55	0.71
1:0:173:PRO:HG3	1:0:184:PHE:CZ	2.25	0.71
2:1:426:GLU:HG2	2:1:589:LEU:HD11	1.71	0.71
1:0:182:LEU:CD2	1:0:182:LEU:O	2.30	0.71
1:0:65:LEU:CB	1:0:99:ILE:HD13	2.20	0.71
2:1:542:ILE:CG2	2:1:566:PHE:HB3	2.21	0.71
1:0:386:GLU:OE1	2:1:541:LEU:C	2.28	0.71
1:0:154:VAL:HG23	1:0:168:ILE:HD12	1.71	0.71
1:0:205:PHE:CB	1:0:238:LYS:O	2.39	0.71
1:0:85:GLY:CA	1:0:104:TYR:CE2	2.74	0.71
1:0:65:LEU:CD2	1:0:99:ILE:CG2	2.69	0.70
1:0:322:LYS:HZ3	1:0:363:ASP:CB	1.92	0.70
1:0:70:ILE:HD12	1:0:104:TYR:CE2	2.23	0.70
1:0:346:GLY:HA3	1:0:373:LYS:HZ3	1.54	0.70
2:1:552:SER:HB3	2:1:555:LYS:CE	2.21	0.70
1:0:168:ILE:CG1	1:0:168:ILE:CD1	2.70	0.70
2:1:489:GLY:C	2:1:579:PRO:CG	2.60	0.70
2:1:459:SER:HB2	2:1:477:LYS:HE2	1.72	0.70
1:0:184:PHE:HE1	2:1:230:GLY:C	1.93	0.70
1:0:176:LYS:NZ	1:0:183:LYS:CE	2.55	0.70
1:0:314:ILE:HD12	1:0:342:VAL:HG11	0.70	0.70
2:1:491:LEU:CD2	2:1:500:ILE:HD13	2.21	0.70
1:0:175:LYS:HD2	2:1:232:THR:HG21	1.57	0.70
1:0:205:PHE:C	1:0:206:ASP:OD1	2.30	0.70
2:1:406:LEU:HG	2:1:531:VAL:CG2	2.22	0.69
2:1:527:LEU:CD2	2:1:592:VAL:HG11	2.22	0.69
1:0:168:ILE:HD13	1:0:195:ILE:HG13	1.74	0.69
1:0:386:GLU:OE1	2:1:541:LEU:HD22	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:175:LYS:CD	2:1:232:THR:HG21	2.15	0.69
2:1:401:PHE:HD2	2:1:493:ALA:HA	1.58	0.69
2:1:510:LEU:CD1	2:1:594:LEU:HD22	2.22	0.69
2:1:493:ALA:HB2	2:1:500:ILE:CD1	2.20	0.69
1:0:59:SER:O	1:0:60:THR:CB	2.38	0.69
1:0:175:LYS:NZ	2:1:232:THR:HG21	1.88	0.69
2:1:436:LEU:HD13	2:1:447:VAL:HG23	1.72	0.69
1:0:97:VAL:O	1:0:98:ASP:CB	2.41	0.69
2:1:402:LEU:CD1	2:1:581:LEU:CD1	2.66	0.69
2:1:495:VAL:CA	2:1:498:SER:HB2	2.24	0.68
2:1:418:LEU:HA	2:1:478:LEU:HB2	1.73	0.68
2:1:532:LYS:CD	2:1:578:ILE:HD13	2.23	0.68
2:1:540:ARG:NH1	2:1:568:GLU:H	1.92	0.68
2:1:510:LEU:HD21	2:1:602:ALA:CB	2.22	0.68
2:1:418:LEU:HD13	2:1:478:LEU:HD12	1.75	0.68
2:1:528:PHE:CE2	2:1:533:GLU:HG3	2.27	0.68
1:0:47:PHE:CZ	1:0:63:VAL:CG1	2.66	0.68
1:0:65:LEU:CD1	1:0:99:ILE:HD13	2.23	0.68
2:1:571:LEU:CD1	2:1:577:TRP:HB3	2.22	0.68
2:1:426:GLU:CD	2:1:589:LEU:HD12	2.00	0.68
2:1:408:ILE:HD11	2:1:417:ASP:HB2	1.75	0.68
2:1:527:LEU:HG	2:1:592:VAL:CG1	2.21	0.68
1:0:314:ILE:HB	1:0:342:VAL:HG12	1.75	0.68
2:1:397:LYS:HG2	2:1:399:ASP:OD2	1.93	0.68
1:0:65:LEU:CD2	1:0:99:ILE:HG21	2.24	0.67
2:1:510:LEU:HD11	2:1:602:ALA:CB	2.24	0.67
1:0:200:LYS:NZ	1:0:236:ASN:OD1	2.27	0.67
2:1:408:ILE:CG1	2:1:417:ASP:HB2	2.23	0.67
2:1:542:ILE:HG22	2:1:566:PHE:O	1.94	0.67
1:0:45:LYS:HZ3	1:0:64:LYS:N	1.90	0.67
2:1:438:ILE:HD11	2:1:490:ASP:OD2	1.95	0.67
2:1:540:ARG:CZ	2:1:567:VAL:HA	2.25	0.67
2:1:544:PHE:HE1	2:1:551:ALA:HA	1.59	0.67
1:0:180:ASP:HB3	2:1:233:VAL:HA	1.76	0.67
2:1:235:ILE:H	2:1:235:ILE:CD1	2.07	0.67
2:1:544:PHE:CE2	2:1:555:LYS:HB3	2.30	0.67
1:0:181:VAL:CG2	1:0:183:LYS:CG	2.72	0.67
1:0:176:LYS:CE	1:0:181:VAL:HG11	2.25	0.67
2:1:452:VAL:HG12	2:1:453:GLY:N	2.07	0.67
2:1:434:GLU:O	2:1:446:ILE:HD12	1.95	0.66
1:0:90:ASP:CG	1:0:91:GLU:HA	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:508:LEU:HD21	2:1:604:GLY:CA	2.25	0.66
1:0:13:LYS:HE3	1:0:13:LYS:CA	2.25	0.66
2:1:489:GLY:O	2:1:579:PRO:CB	2.43	0.66
2:1:540:ARG:CZ	2:1:541:LEU:HA	2.26	0.66
2:1:167:HIS:O	2:1:454:SER:HB2	1.95	0.66
2:1:532:LYS:HE2	2:1:534:GLN:NE2	2.10	0.66
2:1:248:THR:CA	2:1:454:SER:OG	2.43	0.66
2:1:545:ILE:O	2:1:563:GLN:HB2	1.94	0.66
2:1:408:ILE:HG13	2:1:417:ASP:CB	2.25	0.66
1:0:209:LYS:O	1:0:245:MET:HB2	1.95	0.66
2:1:540:ARG:HG2	2:1:541:LEU:N	2.10	0.66
1:0:97:VAL:O	1:0:98:ASP:HB2	1.96	0.66
1:0:175:LYS:HZ3	2:1:232:THR:HB	0.55	0.66
2:1:408:ILE:CD1	2:1:417:ASP:HB2	2.25	0.66
1:0:385:GLU:O	2:1:548:GLY:O	2.12	0.66
1:0:84:LYS:CB	1:0:104:TYR:OH	2.44	0.66
1:0:168:ILE:HG22	1:0:169:GLU:H	1.55	0.65
2:1:540:ARG:CZ	2:1:568:GLU:H	2.09	0.65
1:0:67:ILE:CG1	1:0:105:LEU:HD23	2.26	0.65
1:0:386:GLU:CD	2:1:541:LEU:CD2	2.59	0.65
1:0:45:LYS:NZ	1:0:65:LEU:HD12	2.12	0.65
2:1:571:LEU:HD12	2:1:577:TRP:CB	2.20	0.65
2:1:526:ILE:CG2	2:1:595:ARG:HG2	2.26	0.65
2:1:408:ILE:HG13	2:1:417:ASP:HB2	1.76	0.65
1:0:346:GLY:HA3	1:0:373:LYS:NZ	2.12	0.65
1:0:386:GLU:OE1	2:1:541:LEU:CD2	2.44	0.65
1:0:314:ILE:CD1	1:0:342:VAL:CG2	2.75	0.65
2:1:557:ARG:HD3	2:1:561:SER:O	1.97	0.65
2:1:266:ILE:HA	2:1:473:PHE:CD1	2.32	0.65
2:1:238:SER:H	2:1:455:GLN:HG2	1.61	0.65
1:0:348:LYS:HA	1:0:348:LYS:NZ	2.05	0.65
2:1:406:LEU:HD13	2:1:473:PHE:CE1	2.32	0.64
1:0:85:GLY:N	1:0:104:TYR:OH	2.29	0.64
1:0:96:ASN:O	1:0:99:ILE:CG1	2.30	0.64
2:1:402:LEU:CD2	2:1:500:ILE:HG12	2.28	0.64
2:1:529:ILE:HG23	2:1:530:GLY:N	2.13	0.64
2:1:595:ARG:HB2	2:1:599:ARG:O	1.96	0.64
1:0:204:ASN:ND2	1:0:238:LYS:NZ	2.45	0.64
1:0:204:ASN:ND2	1:0:206:ASP:OD2	2.30	0.64
2:1:510:LEU:HD21	2:1:602:ALA:HB1	1.78	0.64
2:1:266:ILE:HG22	2:1:473:PHE:CZ	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:417:ASP:N	2:1:419:ALA:HB2	2.13	0.64
2:1:489:GLY:CA	2:1:579:PRO:HG2	2.28	0.64
2:1:449:LYS:HB3	2:1:477:LYS:HD2	1.80	0.64
1:0:65:LEU:HA	1:0:99:ILE:CD1	2.28	0.64
1:0:192:TYR:O	1:0:230:TYR:HE2	1.80	0.64
1:0:47:PHE:CD2	1:0:63:VAL:HB	2.31	0.63
2:1:417:ASP:HA	2:1:419:ALA:HB3	1.79	0.63
1:0:314:ILE:HD11	1:0:342:VAL:HG21	1.80	0.63
2:1:402:LEU:HD22	2:1:491:LEU:CD1	2.28	0.63
1:0:170:TYR:CE1	1:0:187:LYS:CD	2.79	0.63
1:0:65:LEU:HD21	1:0:99:ILE:CG2	2.28	0.63
2:1:507:VAL:HG11	2:1:566:PHE:CE2	2.34	0.63
1:0:64:LYS:C	1:0:99:ILE:HD13	2.17	0.63
2:1:493:ALA:CB	2:1:500:ILE:HD11	2.27	0.63
1:0:65:LEU:CB	1:0:99:ILE:CD1	2.76	0.63
1:0:192:TYR:HB3	1:0:230:TYR:CZ	2.34	0.63
1:0:200:LYS:CD	1:0:236:ASN:ND2	2.32	0.63
2:1:535:PRO:HD2	2:1:573:GLU:OE2	1.99	0.63
1:0:322:LYS:N	1:0:354:THR:HG21	2.07	0.63
1:0:252:SER:OG	2:1:597:ASP:OD1	2.10	0.63
2:1:410:PRO:HB3	2:1:416:ASN:CA	2.21	0.63
2:1:436:LEU:HD13	2:1:447:VAL:CG2	2.29	0.62
1:0:65:LEU:CD1	1:0:105:LEU:HD22	2.28	0.62
2:1:418:LEU:HD22	2:1:418:LEU:N	2.13	0.62
2:1:405:VAL:HG23	2:1:421:VAL:CG1	2.28	0.62
1:0:45:LYS:NZ	1:0:63:VAL:CG1	2.58	0.62
1:0:60:THR:O	1:0:61:ASP:HB2	1.98	0.62
1:0:65:LEU:CG	1:0:99:ILE:HD13	2.29	0.62
1:0:175:LYS:HG3	2:1:234:SER:C	2.18	0.62
1:0:45:LYS:HE2	1:0:47:PHE:HD2	0.81	0.62
1:0:182:LEU:HD21	1:0:186:GLU:CG	2.23	0.62
2:1:510:LEU:CG	2:1:602:ALA:HB1	2.29	0.62
2:1:556:ILE:HG22	2:1:557:ARG:N	2.14	0.62
2:1:526:ILE:HD11	2:1:533:GLU:CG	2.28	0.62
1:0:205:PHE:HB3	1:0:242:ASN:HD21	1.63	0.62
2:1:508:LEU:O	2:1:567:VAL:HG22	1.99	0.62
1:0:314:ILE:CB	1:0:342:VAL:HG11	2.27	0.62
2:1:583:ALA:HB3	2:1:605:LYS:CD	2.29	0.62
2:1:571:LEU:HB2	2:1:577:TRP:CD1	2.35	0.62
2:1:401:PHE:HE1	2:1:430:ILE:HD11	1.64	0.62
1:0:65:LEU:CG	1:0:105:LEU:CD2	2.78	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:555:LYS:O	2:1:564:ARG:HB3	2.00	0.62
1:0:45:LYS:HG2	1:0:46:LYS:N	2.11	0.62
1:0:175:LYS:HG3	2:1:235:ILE:CA	2.29	0.62
1:0:253:THR:HG21	2:1:526:ILE:HD12	1.82	0.62
2:1:526:ILE:HG23	2:1:595:ARG:HG2	1.82	0.62
1:0:65:LEU:HB2	1:0:105:LEU:CD2	2.29	0.61
2:1:405:VAL:HG12	2:1:490:ASP:O	2.00	0.61
2:1:540:ARG:NH2	2:1:567:VAL:HG12	2.14	0.61
2:1:556:ILE:CG1	2:1:564:ARG:HG3	2.27	0.61
2:1:402:LEU:HD22	2:1:491:LEU:HD11	1.81	0.61
2:1:456:GLN:O	2:1:457:GLY:C	2.37	0.61
2:1:508:LEU:HG	2:1:605:LYS:O	1.99	0.61
2:1:510:LEU:CD2	2:1:602:ALA:HB1	2.30	0.61
2:1:540:ARG:HE	2:1:542:ILE:N	1.95	0.61
1:0:43:PHE:HZ	1:0:105:LEU:CG	2.13	0.61
1:0:196:TYR:HB2	1:0:230:TYR:CD2	2.33	0.61
2:1:434:GLU:HG2	2:1:435:SER:N	2.15	0.61
2:1:571:LEU:HD11	2:1:578:ILE:HG22	1.81	0.61
2:1:495:VAL:HA	2:1:498:SER:HB2	1.83	0.61
2:1:410:PRO:HG3	2:1:416:ASN:ND2	2.15	0.61
2:1:418:LEU:HD11	2:1:486:ILE:CD1	2.29	0.61
2:1:397:LYS:HE2	2:1:399:ASP:OD2	2.00	0.61
1:0:65:LEU:HD21	1:0:65:LEU:HD11	1.81	0.61
2:1:433:GLY:O	2:1:446:ILE:HD11	2.01	0.61
1:0:187:LYS:C	1:0:187:LYS:HD3	2.21	0.60
2:1:511:THR:OG1	2:1:564:ARG:HG2	2.01	0.60
2:1:574:VAL:O	2:1:577:TRP:HA	2.00	0.60
2:1:426:GLU:HG3	2:1:589:LEU:CG	2.24	0.60
2:1:592:VAL:HG12	2:1:593:VAL:N	2.16	0.60
2:1:535:PRO:HB2	2:1:572:ILE:HG21	1.83	0.60
2:1:404:SER:HB3	2:1:589:LEU:CD1	2.30	0.60
2:1:411:SER:CB	2:1:414:THR:HG22	2.26	0.60
2:1:418:LEU:HG	2:1:481:ALA:HB1	1.82	0.60
1:0:84:LYS:HB3	1:0:104:TYR:CE1	2.37	0.60
1:0:170:TYR:CE1	1:0:191:PHE:HB2	2.36	0.60
2:1:534:GLN:NE2	2:1:571:LEU:HD22	2.15	0.60
2:1:540:ARG:HH21	2:1:541:LEU:HA	1.66	0.60
2:1:418:LEU:HG	2:1:481:ALA:CB	2.32	0.60
1:0:205:PHE:HB3	1:0:242:ASN:HD22	1.65	0.60
2:1:432:PRO:CG	2:1:450:ILE:HG22	2.32	0.60
2:1:574:VAL:HG12	2:1:575:LYS:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:453:GLY:O	2:1:454:SER:C	2.40	0.59
2:1:553:LYS:HG2	2:1:554:LYS:HG2	1.84	0.59
1:0:175:LYS:HE2	2:1:232:THR:O	2.03	0.59
2:1:238:SER:C	2:1:455:GLN:HE21	2.05	0.59
2:1:542:ILE:HG23	2:1:543:SER:N	2.18	0.59
1:0:96:ASN:C	1:0:99:ILE:HG13	2.21	0.59
1:0:182:LEU:HA	1:0:185:ASP:OD2	2.01	0.59
2:1:414:THR:HG23	2:1:419:ALA:CA	2.33	0.59
2:1:494:SER:O	2:1:498:SER:HA	2.02	0.59
1:0:203:LEU:HD12	1:0:208:LEU:CD1	2.32	0.59
1:0:322:LYS:NZ	1:0:360:GLU:HA	2.17	0.59
2:1:397:LYS:HG2	2:1:399:ASP:HB2	1.84	0.59
1:0:65:LEU:HA	1:0:99:ILE:HD13	1.82	0.59
2:1:525:PHE:HD1	2:1:596:LYS:HA	1.67	0.59
1:0:182:LEU:HG	1:0:185:ASP:OD2	2.02	0.59
1:0:61:ASP:O	1:0:62:LEU:CB	2.51	0.58
1:0:192:TYR:HB2	1:0:230:TYR:HH	1.65	0.58
1:0:204:ASN:O	1:0:206:ASP:N	2.30	0.58
2:1:583:ALA:HB3	2:1:605:LYS:HG3	1.85	0.58
1:0:60:THR:O	1:0:61:ASP:HB3	2.03	0.58
2:1:258:PHE:HA	2:1:261:ASN:HD22	1.69	0.58
1:0:209:LYS:CA	1:0:209:LYS:HE2	2.33	0.58
2:1:538:ILE:O	2:1:538:ILE:HG23	2.03	0.58
1:0:95:SER:C	1:0:97:VAL:H	2.05	0.58
2:1:423:GLY:O	2:1:473:PHE:CD1	2.56	0.58
1:0:200:LYS:CE	1:0:236:ASN:ND2	2.64	0.58
1:0:180:ASP:CG	2:1:233:VAL:HG23	2.24	0.58
2:1:581:LEU:CD2	2:1:582:THR:H	2.16	0.58
1:0:45:LYS:HZ2	1:0:65:LEU:HD12	1.68	0.58
1:0:65:LEU:HD13	1:0:105:LEU:HD22	1.85	0.58
1:0:314:ILE:HD12	1:0:342:VAL:HG21	1.83	0.58
2:1:418:LEU:HD21	2:1:486:ILE:HD13	1.84	0.58
1:0:84:LYS:HB3	1:0:104:TYR:CZ	2.37	0.58
2:1:402:LEU:CA	2:1:491:LEU:HD21	2.34	0.58
1:0:61:ASP:OD2	1:0:63:VAL:HG22	2.03	0.58
1:0:180:ASP:HB3	2:1:233:VAL:CA	2.34	0.58
1:0:253:THR:HG21	2:1:526:ILE:CD1	2.34	0.58
2:1:175:HIS:H	2:1:175:HIS:CD2	2.21	0.58
2:1:235:ILE:H	2:1:235:ILE:HD13	1.69	0.58
2:1:418:LEU:HD13	2:1:478:LEU:CD1	2.34	0.58
1:0:386:GLU:HB2	2:1:549:ASN:O	1.90	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:167:LYS:NZ	1:0:167:LYS:O	2.30	0.58
1:0:96:ASN:OD1	1:0:99:ILE:HD12	2.04	0.57
2:1:495:VAL:HA	2:1:498:SER:CB	2.34	0.57
2:1:529:ILE:HG23	2:1:530:GLY:H	1.69	0.57
1:0:352:LEU:O	1:0:354:THR:HG23	2.03	0.57
1:0:252:SER:CB	2:1:597:ASP:OD1	2.51	0.57
2:1:510:LEU:HD23	2:1:510:LEU:C	2.24	0.57
2:1:235:ILE:CG2	2:1:237:THR:HG23	2.27	0.57
1:0:154:VAL:HG23	1:0:168:ILE:HD11	1.84	0.57
1:0:338:LEU:HD23	1:0:368:ILE:HD11	1.86	0.57
2:1:235:ILE:HG22	2:1:237:THR:H	1.70	0.57
2:1:406:LEU:O	2:1:531:VAL:HG21	2.04	0.57
2:1:408:ILE:HG23	2:1:408:ILE:O	2.04	0.57
2:1:534:GLN:HG2	2:1:535:PRO:N	2.19	0.57
1:0:204:ASN:HA	1:0:238:LYS:HE3	1.85	0.57
1:0:322:LYS:HZ3	1:0:363:ASP:CG	2.05	0.57
2:1:510:LEU:HG	2:1:602:ALA:HB1	1.86	0.57
2:1:430:ILE:HG22	2:1:431:GLN:N	2.19	0.57
2:1:553:LYS:O	2:1:555:LYS:HG3	2.04	0.57
2:1:266:ILE:HB	2:1:473:PHE:CG	2.40	0.57
1:0:257:GLN:NE2	2:1:535:PRO:HB3	2.19	0.57
2:1:581:LEU:HD22	2:1:582:THR:H	1.69	0.57
2:1:557:ARG:HB3	2:1:561:SER:O	2.05	0.57
1:0:65:LEU:CD2	1:0:65:LEU:HG	2.17	0.57
2:1:405:VAL:O	2:1:405:VAL:HG13	2.05	0.57
2:1:406:LEU:HG	2:1:531:VAL:HG23	1.87	0.57
1:0:175:LYS:HZ2	2:1:232:THR:CB	1.80	0.56
2:1:526:ILE:CD1	2:1:533:GLU:HG2	2.31	0.56
2:1:540:ARG:NH2	2:1:567:VAL:HA	2.19	0.56
2:1:510:LEU:HD23	2:1:511:THR:C	2.25	0.56
1:0:310:GLU:C	1:0:345:ASN:OD1	2.43	0.56
2:1:527:LEU:HD23	2:1:527:LEU:C	2.25	0.56
1:0:208:LEU:O	1:0:209:LYS:CE	2.52	0.56
1:0:322:LYS:HZ1	1:0:360:GLU:HA	1.69	0.56
1:0:47:PHE:HE2	1:0:63:VAL:CB	1.96	0.56
2:1:532:LYS:HZ2	2:1:578:ILE:HD13	1.71	0.56
2:1:454:SER:CB	2:1:456:GLN:NE2	2.58	0.56
2:1:552:SER:HB3	2:1:555:LYS:HD2	1.88	0.56
1:0:43:PHE:HE2	1:0:67:ILE:CD1	2.00	0.56
2:1:401:PHE:CE1	2:1:403:PHE:HB2	2.41	0.56
1:0:347:GLY:C	1:0:348:LYS:HD2	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:564:ARG:H	2:1:564:ARG:CD	2.05	0.56
1:0:65:LEU:CG	1:0:99:ILE:CG2	2.82	0.56
2:1:418:LEU:CG	2:1:481:ALA:HB3	2.35	0.56
1:0:90:ASP:CA	1:0:91:GLU:HG2	2.35	0.55
2:1:265:GLY:HA2	2:1:406:LEU:HD12	1.87	0.55
2:1:438:ILE:O	2:1:438:ILE:HG23	2.05	0.55
1:0:181:VAL:C	1:0:183:LYS:N	2.34	0.55
2:1:544:PHE:HE1	2:1:551:ALA:CB	2.20	0.55
1:0:66:LYS:O	1:0:88:VAL:HG23	2.05	0.55
2:1:514:ASP:HA	2:1:553:LYS:HD2	1.83	0.55
2:1:544:PHE:HE2	2:1:555:LYS:HD3	1.69	0.55
1:0:65:LEU:CD2	1:0:87:THR:CG2	2.84	0.55
2:1:552:SER:HB3	2:1:555:LYS:NZ	2.22	0.55
1:0:160:SER:C	1:0:356:HIS:HA	2.27	0.55
1:0:45:LYS:HZ3	1:0:63:VAL:CA	2.14	0.55
2:1:443:GLN:HG3	2:1:444:SER:H	1.72	0.55
1:0:184:PHE:CZ	2:1:230:GLY:O	2.51	0.55
2:1:414:THR:HG23	2:1:419:ALA:HA	1.89	0.55
2:1:572:ILE:HG23	2:1:573:GLU:N	2.21	0.55
1:0:177:ARG:NH2	2:1:455:GLN:HE22	2.03	0.55
2:1:523:THR:HG23	2:1:525:PHE:CE2	2.41	0.55
1:0:65:LEU:CB	1:0:105:LEU:CD2	2.84	0.55
1:0:178:THR:OG1	1:0:179:THR:N	2.40	0.55
1:0:317:LEU:HD12	1:0:339:MET:HG2	1.83	0.55
1:0:322:LYS:H	1:0:354:THR:CG2	2.10	0.55
1:0:252:SER:HB3	2:1:597:ASP:OD1	2.07	0.55
1:0:65:LEU:HD13	1:0:105:LEU:CD2	2.37	0.54
2:1:418:LEU:HB3	2:1:481:ALA:CB	2.34	0.54
2:1:406:LEU:C	2:1:531:VAL:HG21	2.27	0.54
2:1:544:PHE:HE1	2:1:551:ALA:CA	2.20	0.54
1:0:43:PHE:HZ	1:0:67:ILE:CD1	2.09	0.54
2:1:399:ASP:HB3	2:1:400:PRO:HD2	1.89	0.54
2:1:432:PRO:HG2	2:1:450:ILE:HG22	1.89	0.54
1:0:65:LEU:N	1:0:99:ILE:HD13	2.22	0.54
2:1:581:LEU:HD22	2:1:582:THR:N	2.23	0.54
1:0:85:GLY:C	1:0:104:TYR:CD2	2.76	0.54
1:0:111:TYR:O	1:0:112:VAL:CB	2.55	0.54
2:1:540:ARG:HD2	2:1:568:GLU:HB2	1.89	0.54
1:0:171:SER:OG	1:0:187:LYS:CG	2.56	0.54
2:1:459:SER:CA	2:1:477:LYS:HZ3	2.10	0.54
2:1:426:GLU:OE1	2:1:426:GLU:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:581:LEU:HD22	2:1:582:THR:HG22	1.89	0.54
2:1:545:ILE:HG23	2:1:546:ASP:N	2.23	0.54
1:0:66:LYS:C	1:0:88:VAL:HG22	2.27	0.54
2:1:417:ASP:O	2:1:418:LEU:HB2	2.08	0.54
1:0:348:LYS:CB	1:0:348:LYS:NZ	2.71	0.54
1:0:264:LYS:HA	1:0:281:ILE:HG23	1.89	0.54
1:0:170:TYR:O	1:0:172:MET:HG3	2.07	0.53
1:0:189:GLU:HA	1:0:192:TYR:HD2	1.73	0.53
2:1:407:GLU:C	2:1:488:ASN:HD21	2.11	0.53
2:1:401:PHE:O	2:1:402:LEU:HD23	2.07	0.53
2:1:511:THR:HA	2:1:564:ARG:HB2	1.86	0.53
2:1:416:ASN:C	2:1:419:ALA:HB2	2.28	0.53
1:0:180:ASP:O	1:0:181:VAL:C	2.46	0.53
2:1:406:LEU:HD13	2:1:473:PHE:HE1	1.71	0.53
2:1:535:PRO:HG2	2:1:573:GLU:HG3	1.90	0.53
1:0:346:GLY:CA	1:0:373:LYS:NZ	2.71	0.53
2:1:402:LEU:HA	2:1:491:LEU:HD21	1.91	0.53
1:0:205:PHE:CD2	1:0:238:LYS:HG2	2.39	0.53
2:1:580:LEU:N	2:1:580:LEU:HD23	2.22	0.53
1:0:184:PHE:CZ	2:1:231:VAL:O	2.62	0.53
1:0:175:LYS:HD3	2:1:232:THR:O	2.08	0.53
1:0:343:GLU:HA	1:0:346:GLY:C	2.28	0.53
2:1:426:GLU:HG3	2:1:589:LEU:HD11	1.50	0.53
2:1:443:GLN:HG3	2:1:444:SER:N	2.23	0.53
2:1:455:GLN:CD	2:1:455:GLN:C	2.67	0.53
1:0:320:THR:HB	1:0:354:THR:HG21	1.90	0.53
1:0:170:TYR:CE1	1:0:187:LYS:HD2	2.42	0.53
2:1:529:ILE:HD13	2:1:529:ILE:C	2.28	0.53
1:0:204:ASN:OD1	1:0:206:ASP:HB2	2.08	0.53
1:0:200:LYS:NZ	1:0:236:ASN:HD21	2.07	0.53
1:0:338:LEU:HD23	1:0:368:ILE:CD1	2.39	0.53
1:0:355:LEU:H	1:0:355:LEU:HD22	1.74	0.53
1:0:37:LYS:H	1:0:37:LYS:HD2	1.73	0.53
2:1:514:ASP:CG	2:1:553:LYS:HD2	2.29	0.53
2:1:239:HIS:CB	2:1:455:GLN:O	2.57	0.53
1:0:312:GLY:O	1:0:346:GLY:CA	2.49	0.52
1:0:217:GLY:HA2	2:1:255:HIS:CE1	2.43	0.52
2:1:166:PRO:HA	2:1:167:HIS:HB2	1.90	0.52
2:1:495:VAL:HA	2:1:498:SER:OG	2.09	0.52
1:0:206:ASP:CG	1:0:238:LYS:HZ1	2.13	0.52
1:0:176:LYS:NZ	1:0:181:VAL:HG11	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:196:TYR:OH	1:0:234:GLU:OE1	2.16	0.52
1:0:314:ILE:HB	1:0:346:GLY:O	2.09	0.52
1:0:292:ASN:HA	2:1:518:PRO:HB2	1.91	0.52
1:0:90:ASP:N	1:0:91:GLU:HG2	2.24	0.52
2:1:409:ILE:CG2	2:1:420:LEU:HB3	2.40	0.52
1:0:195:ILE:CG2	1:0:223:LEU:HD11	2.23	0.52
1:0:177:ARG:O	2:1:235:ILE:CD1	2.54	0.52
2:1:454:SER:CB	2:1:456:GLN:HE22	2.07	0.52
2:1:510:LEU:HD23	2:1:511:THR:CA	2.40	0.52
1:0:255:TYR:CE2	2:1:573:GLU:OE2	2.63	0.52
1:0:309:ALA:O	1:0:345:ASN:CG	2.47	0.52
1:0:207:LYS:O	1:0:209:LYS:HE3	2.09	0.52
1:0:68:LYS:O	1:0:85:GLY:HA3	2.09	0.52
1:0:66:LYS:C	1:0:88:VAL:HG23	2.30	0.51
2:1:571:LEU:CD1	2:1:578:ILE:HB	2.40	0.51
2:1:263:ILE:CD1	2:1:264:MET:HG2	2.41	0.51
2:1:401:PHE:CZ	2:1:403:PHE:CB	2.94	0.51
2:1:545:ILE:HA	2:1:563:GLN:O	2.11	0.51
2:1:400:PRO:HG3	2:1:497:TYR:CG	2.46	0.51
2:1:450:ILE:O	2:1:450:ILE:HG23	2.09	0.51
2:1:532:LYS:HZ3	2:1:578:ILE:HD13	1.75	0.51
2:1:426:GLU:HG3	2:1:589:LEU:CD2	2.40	0.51
1:0:386:GLU:OE1	2:1:541:LEU:CA	2.58	0.51
2:1:499:SER:O	2:1:500:ILE:HB	2.11	0.51
1:0:47:PHE:CZ	1:0:63:VAL:CB	2.89	0.51
1:0:89:THR:HB	1:0:91:GLU:OE2	2.10	0.51
2:1:397:LYS:O	2:1:428:GLY:HA2	2.11	0.51
2:1:504:GLN:HG3	2:1:577:TRP:CD2	2.46	0.51
2:1:574:VAL:HG12	2:1:575:LYS:N	2.24	0.51
1:0:192:TYR:CD1	1:0:226:LYS:CD	2.94	0.51
1:0:160:SER:HA	1:0:356:HIS:CD2	2.46	0.51
2:1:269:ALA:HB3	2:1:305:ILE:HD13	1.92	0.51
2:1:556:ILE:HG23	2:1:564:ARG:HG3	1.93	0.51
2:1:266:ILE:HG22	2:1:473:PHE:CE1	2.46	0.51
2:1:541:LEU:C	2:1:541:LEU:HD23	2.32	0.51
1:0:65:LEU:HD21	1:0:99:ILE:HG23	1.92	0.50
1:0:291:LEU:HD11	2:1:520:LEU:HD23	1.93	0.50
1:0:356:HIS:HB2	1:0:359:GLY:H	1.75	0.50
1:0:206:ASP:OD2	1:0:238:LYS:NZ	2.45	0.50
2:1:190:ASP:H	2:1:193:ILE:HG23	1.77	0.50
1:0:178:THR:O	1:0:180:ASP:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:544:PHE:CZ	2:1:555:LYS:CD	2.94	0.50
1:0:184:PHE:HZ	2:1:231:VAL:O	1.94	0.50
2:1:410:PRO:HD3	2:1:416:ASN:OD1	2.12	0.50
1:0:292:ASN:O	2:1:518:PRO:HD2	2.12	0.50
1:0:171:SER:C	1:0:187:LYS:HE2	2.32	0.50
1:0:317:LEU:CD1	1:0:339:MET:HA	2.42	0.50
1:0:348:LYS:CA	1:0:348:LYS:NZ	2.70	0.50
1:0:33:GLN:HA	1:0:325:HIS:CG	2.47	0.50
2:1:269:ALA:O	2:1:305:ILE:HG23	2.12	0.50
1:0:45:LYS:HE2	1:0:63:VAL:HB	1.93	0.50
2:1:405:VAL:HG13	2:1:489:GLY:H	1.77	0.50
1:0:208:LEU:C	1:0:209:LYS:CE	2.70	0.50
2:1:507:VAL:CG1	2:1:566:PHE:CE2	2.95	0.50
2:1:453:GLY:O	2:1:454:SER:O	2.30	0.50
2:1:544:PHE:CZ	2:1:555:LYS:CB	2.95	0.50
1:0:176:LYS:O	2:1:235:ILE:HG23	2.11	0.50
2:1:401:PHE:CE1	2:1:430:ILE:CG1	2.95	0.50
1:0:85:GLY:N	1:0:104:TYR:CE2	2.75	0.50
2:1:514:ASP:OD1	2:1:554:LYS:HE2	2.12	0.50
2:1:544:PHE:CE2	2:1:555:LYS:CB	2.94	0.50
1:0:176:LYS:C	2:1:235:ILE:CG2	2.77	0.49
2:1:545:ILE:CG1	2:1:557:ARG:HA	2.34	0.49
1:0:170:TYR:CG	1:0:191:PHE:HB2	2.47	0.49
1:0:177:ARG:O	1:0:178:THR:O	2.30	0.49
2:1:267:SER:HA	2:1:473:PHE:H	1.77	0.49
2:1:439:TYR:CE1	2:1:499:SER:HB2	2.48	0.49
2:1:522:GLY:HA2	2:1:537:ARG:HE	1.75	0.49
1:0:45:LYS:NZ	1:0:63:VAL:CB	2.75	0.49
1:0:176:LYS:HZ3	1:0:183:LYS:CE	2.23	0.49
2:1:489:GLY:HA3	2:1:579:PRO:HG2	1.95	0.49
2:1:401:PHE:CZ	2:1:403:PHE:HB2	2.47	0.49
2:1:491:LEU:HD13	2:1:500:ILE:HD13	1.95	0.49
2:1:369:ARG:HB3	2:1:369:ARG:HH11	1.76	0.49
1:0:90:ASP:CA	1:0:96:ASN:HB2	2.39	0.49
1:0:181:VAL:CG1	1:0:181:VAL:O	2.59	0.49
2:1:238:SER:N	2:1:455:GLN:HG2	2.26	0.49
2:1:426:GLU:OE2	2:1:589:LEU:HD11	2.05	0.49
2:1:535:PRO:O	2:1:572:ILE:HG22	2.12	0.49
1:0:205:PHE:O	1:0:206:ASP:OD1	2.30	0.49
2:1:193:ILE:HG22	2:1:194:VAL:N	2.24	0.49
2:1:397:LYS:HG2	2:1:399:ASP:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:534:GLN:HG3	2:1:573:GLU:CG	2.42	0.49
2:1:290:ASP:OD2	2:1:599:ARG:CZ	2.59	0.49
2:1:583:ALA:HB3	2:1:605:LYS:CG	2.43	0.49
1:0:171:SER:OG	1:0:187:LYS:HG3	2.12	0.49
1:0:89:THR:C	1:0:91:GLU:HG2	2.33	0.49
2:1:588:ARG:O	2:1:588:ARG:HG2	2.13	0.49
1:0:205:PHE:CZ	1:0:239:ILE:CB	2.92	0.49
2:1:264:MET:HG3	2:1:529:ILE:O	2.13	0.49
2:1:170:PHE:CE2	2:1:249:ILE:HG12	2.48	0.49
1:0:300:TYR:HA	1:0:369:ALA:HA	1.95	0.49
2:1:417:ASP:HA	2:1:419:ALA:CB	2.42	0.48
2:1:527:LEU:HD23	2:1:528:PHE:N	2.28	0.48
2:1:589:LEU:HD12	2:1:589:LEU:N	2.27	0.48
1:0:306:VAL:HG23	1:0:338:LEU:HD21	1.86	0.48
1:0:160:SER:HA	1:0:356:HIS:CG	2.47	0.48
2:1:420:LEU:HD23	2:1:420:LEU:C	2.34	0.48
2:1:401:PHE:CE2	2:1:493:ALA:HA	2.45	0.48
1:0:65:LEU:HD23	1:0:87:THR:HG23	1.93	0.48
1:0:178:THR:HG23	1:0:181:VAL:H	1.77	0.48
1:0:199:MET:HG2	1:0:203:LEU:HD23	1.91	0.48
2:1:454:SER:O	2:1:456:GLN:OE1	2.31	0.48
2:1:438:ILE:HD12	2:1:486:ILE:HG13	1.94	0.48
1:0:317:LEU:HD12	1:0:339:MET:HA	1.94	0.48
2:1:439:TYR:N	2:1:440:PRO:HD2	2.29	0.48
1:0:196:TYR:CB	1:0:230:TYR:CD2	2.87	0.48
2:1:239:HIS:HB3	2:1:455:GLN:O	2.13	0.48
1:0:203:LEU:HD12	1:0:208:LEU:HD13	1.95	0.48
1:0:181:VAL:O	1:0:182:LEU:C	2.46	0.48
2:1:235:ILE:HG22	2:1:236:CYS:N	2.29	0.48
2:1:411:SER:HB2	2:1:414:THR:O	2.14	0.48
1:0:171:SER:O	1:0:187:LYS:CE	2.61	0.48
1:0:91:GLU:H	1:0:93:GLY:H	1.62	0.48
1:0:205:PHE:HD2	1:0:238:LYS:CG	2.22	0.48
2:1:552:SER:HB3	2:1:555:LYS:CD	2.42	0.48
1:0:364:GLN:O	1:0:365:LEU:HD23	2.13	0.48
1:0:204:ASN:ND2	1:0:238:LYS:HZ1	2.11	0.48
2:1:31:TYR:OH	2:1:32:GLU:HG2	2.14	0.48
1:0:338:LEU:CD2	1:0:368:ILE:HD11	2.44	0.48
1:0:150:GLY:CA	1:0:172:MET:HG2	2.44	0.48
2:1:491:LEU:HD23	2:1:492:ALA:N	2.29	0.48
1:0:13:LYS:HA	1:0:13:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:21:GLU:HG2	2:1:22:PHE:H	1.79	0.47
1:0:63:VAL:CG1	1:0:99:ILE:HG12	2.43	0.47
2:1:508:LEU:HD23	2:1:509:GLU:C	2.35	0.47
2:1:194:VAL:O	2:1:196:GLN:CB	2.62	0.47
2:1:425:LEU:HD23	2:1:425:LEU:C	2.34	0.47
1:0:67:ILE:HD13	1:0:105:LEU:HG	1.91	0.47
1:0:96:ASN:ND2	1:0:99:ILE:HB	2.30	0.47
2:1:238:SER:O	2:1:455:GLN:HG3	2.14	0.47
1:0:348:LYS:O	1:0:349:ALA:HB2	2.15	0.47
2:1:438:ILE:HG21	2:1:486:ILE:CD1	2.44	0.47
2:1:507:VAL:CG1	2:1:566:PHE:CZ	2.95	0.47
2:1:300:ALA:HA	2:1:305:ILE:HD12	1.97	0.47
1:0:181:VAL:HG11	1:0:183:LYS:HD3	1.96	0.47
2:1:451:GLN:NE2	2:1:455:GLN:HA	2.30	0.47
2:1:532:LYS:HD3	2:1:578:ILE:HD13	1.94	0.47
1:0:180:ASP:HB3	2:1:233:VAL:C	2.35	0.47
2:1:235:ILE:CG2	2:1:237:THR:CG2	2.85	0.47
2:1:280:THR:HA	2:1:324:ARG:NH2	2.30	0.47
2:1:271:MET:HA	2:1:307:ASN:O	2.15	0.47
2:1:235:ILE:CG1	2:1:237:THR:O	2.51	0.46
2:1:578:ILE:CD1	2:1:579:PRO:HD2	2.40	0.46
2:1:404:SER:HB3	2:1:589:LEU:CG	2.44	0.46
2:1:397:LYS:HD3	2:1:399:ASP:CB	2.40	0.46
1:0:88:VAL:O	1:0:91:GLU:HG3	2.16	0.46
2:1:437:THR:HG21	2:1:498:SER:OG	2.15	0.46
1:0:199:MET:HE2	1:0:227:ILE:HG12	1.97	0.46
2:1:417:ASP:CA	2:1:419:ALA:CB	2.93	0.46
2:1:525:PHE:CD1	2:1:596:LYS:HA	2.48	0.46
1:0:175:LYS:CD	2:1:232:THR:CB	2.78	0.46
1:0:177:ARG:CZ	2:1:455:GLN:HE22	2.29	0.46
2:1:526:ILE:CG2	2:1:595:ARG:CG	2.94	0.46
2:1:541:LEU:HD21	2:1:543:SER:O	2.15	0.46
1:0:180:ASP:CB	2:1:233:VAL:O	2.59	0.46
2:1:410:PRO:CA	2:1:416:ASN:HA	2.46	0.46
2:1:405:VAL:HG13	2:1:489:GLY:N	2.31	0.46
2:1:272:ALA:O	2:1:308:LEU:HD12	2.15	0.46
1:0:145:VAL:HG11	1:0:195:ILE:HD11	1.96	0.46
1:0:206:ASP:OD1	1:0:206:ASP:N	2.48	0.46
2:1:439:TYR:CD1	2:1:499:SER:CB	2.95	0.46
2:1:528:PHE:CE2	2:1:533:GLU:CG	2.95	0.46
2:1:239:HIS:HB2	2:1:455:GLN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:437:THR:HG21	2:1:498:SER:HG	1.81	0.46
2:1:167:HIS:HA	2:1:246:ASN:O	2.16	0.46
1:0:66:LYS:O	1:0:88:VAL:CG2	2.63	0.46
2:1:418:LEU:CG	2:1:481:ALA:CB	2.93	0.46
2:1:264:MET:HE1	2:1:588:ARG:HA	1.97	0.46
2:1:420:LEU:HD23	2:1:421:VAL:C	2.37	0.45
1:0:43:PHE:CD2	1:0:107:PHE:HB2	2.51	0.45
2:1:526:ILE:O	2:1:526:ILE:HG23	2.16	0.45
1:0:386:GLU:CB	2:1:549:ASN:O	2.63	0.45
2:1:512:THR:HG23	2:1:554:LYS:N	2.31	0.45
2:1:256:ARG:HH11	2:1:296:HIS:CE1	2.34	0.45
2:1:415:SER:N	2:1:419:ALA:HA	2.31	0.45
2:1:425:LEU:HD21	2:1:427:SER:C	2.37	0.45
2:1:544:PHE:O	2:1:563:GLN:HB3	2.17	0.45
2:1:229:ARG:HG3	2:1:229:ARG:HH11	1.81	0.45
1:0:177:ARG:HA	2:1:235:ILE:HG13	1.98	0.45
2:1:401:PHE:CE1	2:1:430:ILE:CD1	2.94	0.45
2:1:528:PHE:CE1	2:1:595:ARG:HD2	2.51	0.45
1:0:386:GLU:N	2:1:548:GLY:HA3	2.32	0.45
1:0:43:PHE:HZ	1:0:105:LEU:HG	1.79	0.45
2:1:409:ILE:HD13	2:1:410:PRO:HD2	1.97	0.45
2:1:586:ASN:CG	2:1:587:ASP:H	2.19	0.45
2:1:405:VAL:HG13	2:1:488:ASN:CA	2.42	0.45
2:1:403:PHE:N	2:1:491:LEU:HD21	2.32	0.45
2:1:526:ILE:CG2	2:1:528:PHE:CE1	2.95	0.45
1:0:386:GLU:OE1	2:1:541:LEU:CG	2.63	0.45
2:1:259:VAL:HG11	2:1:296:HIS:CD2	2.52	0.45
1:0:175:LYS:CD	2:1:232:THR:O	2.64	0.45
1:0:176:LYS:HZ2	1:0:183:LYS:CD	2.01	0.45
2:1:403:PHE:H	2:1:491:LEU:CD2	2.29	0.45
2:1:581:LEU:CD2	2:1:582:THR:N	2.80	0.45
1:0:322:LYS:CE	1:0:363:ASP:HB3	2.46	0.45
1:0:288:LEU:O	1:0:292:ASN:HB2	2.17	0.45
2:1:308:LEU:HB3	2:1:346:ILE:HD12	1.99	0.45
2:1:266:ILE:CA	2:1:473:PHE:HB2	2.47	0.45
2:1:405:VAL:CG1	2:1:488:ASN:HA	2.42	0.45
2:1:264:MET:O	2:1:588:ARG:HD2	2.17	0.45
1:0:204:ASN:HD22	1:0:238:LYS:NZ	2.15	0.45
1:0:205:PHE:HD1	1:0:245:MET:HE2	1.54	0.45
2:1:259:VAL:HG13	2:1:260:PRO:CD	2.46	0.45
1:0:192:TYR:O	1:0:230:TYR:CE2	2.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:177:ARG:HD3	2:1:458:GLN:CG	2.47	0.45
2:1:426:GLU:O	2:1:470:LYS:HD2	2.17	0.45
1:0:170:TYR:CE2	1:0:191:PHE:CG	3.05	0.44
1:0:192:TYR:HE1	1:0:222:ILE:HG22	1.82	0.44
2:1:436:LEU:CD1	2:1:447:VAL:CG2	2.95	0.44
2:1:397:LYS:CB	2:1:399:ASP:HB2	2.47	0.44
2:1:303:LEU:HD22	2:1:305:ILE:HG13	1.98	0.44
1:0:171:SER:OG	1:0:187:LYS:HG2	2.17	0.44
1:0:170:TYR:C	1:0:187:LYS:CE	2.83	0.44
2:1:415:SER:C	2:1:419:ALA:HB2	2.38	0.44
1:0:177:ARG:HH22	2:1:455:GLN:HE22	1.65	0.44
2:1:404:SER:CB	2:1:589:LEU:HD11	2.46	0.44
1:0:228:PHE:CE1	1:0:243:LYS:HG2	2.53	0.44
2:1:503:ALA:HB3	2:1:609:ILE:HD11	1.99	0.44
1:0:154:VAL:CG2	1:0:168:ILE:HD11	2.47	0.44
2:1:578:ILE:HG13	2:1:579:PRO:N	2.32	0.44
2:1:526:ILE:HG22	2:1:595:ARG:O	2.17	0.44
2:1:528:PHE:CZ	2:1:533:GLU:HG3	2.51	0.44
2:1:333:LEU:HD23	2:1:336:LEU:HD12	2.00	0.44
1:0:89:THR:CB	1:0:91:GLU:OE2	2.65	0.44
2:1:235:ILE:HB	2:1:237:THR:O	2.17	0.44
2:1:532:LYS:CD	2:1:578:ILE:CD1	2.95	0.44
2:1:425:LEU:HD22	2:1:470:LYS:CA	2.39	0.44
2:1:370:GLN:CD	2:1:370:GLN:H	2.20	0.44
2:1:266:ILE:HA	2:1:473:PHE:HB2	1.99	0.44
2:1:418:LEU:CB	2:1:481:ALA:CB	2.93	0.44
2:1:592:VAL:CG1	2:1:593:VAL:N	2.80	0.44
1:0:253:THR:CG2	2:1:526:ILE:CD1	2.95	0.44
2:1:396:ASN:HD22	2:1:469:ILE:HD12	1.82	0.44
2:1:289:LEU:HD12	2:1:294:LYS:HE3	1.99	0.44
2:1:425:LEU:HD22	2:1:470:LYS:HB2	1.99	0.44
2:1:527:LEU:CD2	2:1:592:VAL:CG1	2.95	0.44
2:1:510:LEU:CD1	2:1:602:ALA:HB3	2.39	0.44
2:1:390:LYS:HB2	2:1:392:ASN:HA	1.99	0.44
1:0:170:TYR:H	1:0:170:TYR:HD2	1.65	0.44
1:0:65:LEU:HB2	1:0:67:ILE:HG13	1.99	0.44
1:0:97:VAL:O	1:0:98:ASP:CG	2.55	0.44
2:1:532:LYS:HE2	2:1:534:GLN:HB2	1.99	0.44
2:1:534:GLN:HE22	2:1:571:LEU:CD1	2.23	0.44
2:1:403:PHE:O	2:1:491:LEU:HD23	2.16	0.44
1:0:200:LYS:NZ	1:0:236:ASN:ND2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:204:ARG:HH12	2:1:213:SER:HA	1.82	0.44
1:0:180:ASP:CG	1:0:184:PHE:HB3	2.39	0.44
1:0:195:ILE:HG23	1:0:196:TYR:N	2.32	0.44
2:1:418:LEU:HB2	2:1:481:ALA:C	2.39	0.44
2:1:401:PHE:CZ	2:1:403:PHE:HB3	2.53	0.44
2:1:597:ASP:HB3	2:1:598:GLY:H	1.58	0.44
2:1:247:PHE:C	2:1:454:SER:HG	2.20	0.44
1:0:20:LEU:HD21	1:0:115:PHE:CE1	2.53	0.44
2:1:571:LEU:CD1	2:1:578:ILE:HG22	2.48	0.43
2:1:510:LEU:CG	2:1:602:ALA:CB	2.95	0.43
1:0:45:LYS:HZ3	1:0:63:VAL:CB	2.30	0.43
2:1:438:ILE:HG21	2:1:486:ILE:HD12	1.99	0.43
2:1:390:LYS:HG2	2:1:390:LYS:H	1.51	0.43
1:0:188:THR:HG23	1:0:189:GLU:N	2.33	0.43
2:1:237:THR:HA	2:1:455:GLN:HG2	2.00	0.43
2:1:406:LEU:O	2:1:488:ASN:CG	2.57	0.43
2:1:571:LEU:HD11	2:1:578:ILE:CB	2.47	0.43
2:1:574:VAL:O	2:1:577:TRP:CG	2.71	0.43
2:1:540:ARG:CZ	2:1:567:VAL:CA	2.94	0.43
2:1:527:LEU:HD21	2:1:592:VAL:HG11	1.99	0.43
2:1:538:ILE:HG12	2:1:540:ARG:HH12	1.78	0.43
2:1:399:ASP:HB3	2:1:400:PRO:CD	2.49	0.43
1:0:321:ASP:HA	1:0:324:LEU:HB2	1.99	0.43
1:0:45:LYS:NZ	1:0:64:LYS:N	2.60	0.43
2:1:410:PRO:HB3	2:1:416:ASN:CG	2.39	0.43
2:1:403:PHE:N	2:1:491:LEU:CD2	2.82	0.43
2:1:426:GLU:OE2	2:1:588:ARG:HD3	2.18	0.43
1:0:386:GLU:N	2:1:548:GLY:C	2.68	0.43
2:1:196:GLN:HG2	2:1:199:LEU:HB2	2.00	0.43
1:0:66:LYS:HG3	1:0:88:VAL:HG23	2.00	0.43
2:1:438:ILE:HD11	2:1:490:ASP:CB	2.48	0.43
2:1:190:ASP:HB2	2:1:196:GLN:HB2	2.00	0.43
2:1:408:ILE:CD1	2:1:417:ASP:CB	2.95	0.43
2:1:410:PRO:HA	2:1:415:SER:O	2.18	0.43
2:1:504:GLN:HG3	2:1:577:TRP:CE2	2.53	0.43
1:0:205:PHE:CZ	1:0:239:ILE:HA	2.53	0.43
2:1:587:ASP:O	2:1:591:ARG:N	2.51	0.43
2:1:313:ASN:HA	2:1:351:ILE:HD12	2.01	0.43
2:1:540:ARG:HD3	2:1:568:GLU:HB3	2.01	0.43
1:0:96:ASN:O	1:0:97:VAL:C	2.54	0.43
1:0:205:PHE:CE1	1:0:239:ILE:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:504:GLN:HB3	2:1:611:GLN:OXT	2.19	0.42
2:1:571:LEU:HD11	2:1:578:ILE:HB	2.00	0.42
2:1:510:LEU:CD1	2:1:602:ALA:CB	2.95	0.42
2:1:417:ASP:OD2	2:1:486:ILE:HB	2.20	0.42
2:1:418:LEU:N	2:1:418:LEU:CD2	2.81	0.42
2:1:526:ILE:CD1	2:1:533:GLU:CG	2.95	0.42
2:1:583:ALA:CB	2:1:605:LYS:CG	2.94	0.42
2:1:511:THR:O	2:1:602:ALA:HB1	2.19	0.42
2:1:409:ILE:HG22	2:1:420:LEU:HB3	2.01	0.42
1:0:292:ASN:O	2:1:518:PRO:CD	2.68	0.42
2:1:448:ASP:HB3	2:1:477:LYS:HB2	2.00	0.42
1:0:192:TYR:C	1:0:230:TYR:HE2	2.22	0.42
2:1:262:ALA:O	2:1:265:GLY:C	2.58	0.42
2:1:493:ALA:HB2	2:1:500:ILE:CG1	2.48	0.42
2:1:540:ARG:HH22	2:1:567:VAL:HG12	1.84	0.42
2:1:193:ILE:CG2	2:1:194:VAL:H	2.17	0.42
2:1:51:TRP:CG	2:1:52:ASP:N	2.86	0.42
2:1:191:LEU:HD13	2:1:191:LEU:H	1.84	0.42
1:0:257:GLN:CD	2:1:535:PRO:HB3	2.40	0.42
2:1:572:ILE:CG2	2:1:573:GLU:N	2.83	0.42
2:1:532:LYS:HD3	2:1:578:ILE:CD1	2.49	0.42
2:1:491:LEU:HG	2:1:589:LEU:HD21	2.01	0.42
1:0:141:ASP:HB2	1:0:209:LYS:HB2	2.00	0.42
2:1:51:TRP:HE1	2:1:55:SER:HB2	1.84	0.42
1:0:65:LEU:CG	1:0:99:ILE:CD1	2.96	0.42
1:0:221:LYS:NZ	1:0:225:ASP:OD1	2.52	0.42
2:1:219:ILE:HD13	2:1:219:ILE:HG21	1.88	0.42
2:1:574:VAL:CG1	2:1:575:LYS:N	2.82	0.42
2:1:263:ILE:HD12	2:1:264:MET:HG2	2.01	0.42
2:1:542:ILE:CG2	2:1:543:SER:N	2.82	0.42
2:1:544:PHE:CE2	2:1:555:LYS:CD	2.94	0.42
2:1:511:THR:OG1	2:1:556:ILE:HG12	2.20	0.42
1:0:43:PHE:O	1:0:64:LYS:CA	2.65	0.42
1:0:182:LEU:CD2	1:0:185:ASP:OD1	2.68	0.42
2:1:445:CYS:SG	2:1:480:LYS:N	2.93	0.42
2:1:528:PHE:C	2:1:592:VAL:HG13	2.40	0.42
2:1:438:ILE:HG22	2:1:443:GLN:O	2.19	0.42
1:0:33:GLN:HA	1:0:325:HIS:CD2	2.55	0.42
2:1:51:TRP:HE1	2:1:55:SER:CB	2.33	0.42
2:1:206:SER:O	2:1:222:GLN:HB3	2.20	0.42
2:1:437:THR:O	2:1:437:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:589:LEU:N	2:1:589:LEU:CD1	2.82	0.42
2:1:510:LEU:HD21	2:1:602:ALA:HB2	1.99	0.42
2:1:545:ILE:CG2	2:1:546:ASP:N	2.82	0.42
2:1:194:VAL:O	2:1:196:GLN:HB2	2.19	0.42
1:0:95:SER:C	1:0:97:VAL:N	2.73	0.41
2:1:402:LEU:HD21	2:1:500:ILE:HG12	2.02	0.41
2:1:580:LEU:N	2:1:580:LEU:CD2	2.83	0.41
2:1:259:VAL:HG13	2:1:260:PRO:HD2	2.02	0.41
1:0:133:ALA:HA	1:0:135:ASN:HB2	2.02	0.41
2:1:451:GLN:O	2:1:474:VAL:HA	2.18	0.41
2:1:175:HIS:HB3	2:1:286:GLY:HA2	2.01	0.41
2:1:441:SER:HB3	2:1:485:ASP:O	2.20	0.41
1:0:65:LEU:CB	1:0:99:ILE:HD12	2.49	0.41
1:0:195:ILE:HD13	1:0:223:LEU:HD21	2.01	0.41
2:1:529:ILE:HG12	2:1:592:VAL:HG22	2.02	0.41
1:0:31:VAL:HG11	1:0:109:LEU:HD21	2.02	0.41
1:0:80:TYR:CE1	1:0:108:THR:HG21	2.55	0.41
2:1:405:VAL:CG2	2:1:421:VAL:HG13	2.45	0.41
2:1:574:VAL:O	2:1:577:TRP:CD1	2.73	0.41
1:0:346:GLY:CA	1:0:373:LYS:HZ1	2.34	0.41
2:1:491:LEU:CD2	2:1:492:ALA:N	2.83	0.41
2:1:518:PRO:HG3	2:1:552:SER:HA	2.02	0.41
2:1:555:LYS:O	2:1:564:ARG:HA	2.20	0.41
2:1:556:ILE:CG2	2:1:557:ARG:N	2.82	0.41
1:0:85:GLY:O	1:0:104:TYR:CG	2.70	0.41
2:1:204:ARG:NH1	2:1:213:SER:HA	2.35	0.41
1:0:65:LEU:HD12	1:0:99:ILE:CD1	2.41	0.41
2:1:237:THR:OG1	2:1:455:GLN:CD	2.58	0.41
2:1:417:ASP:CA	2:1:419:ALA:HB2	2.50	0.41
2:1:523:THR:O	2:1:538:ILE:HG22	2.21	0.41
2:1:435:SER:C	2:1:436:LEU:HD12	2.40	0.41
2:1:473:PHE:CG	2:1:474:VAL:N	2.85	0.41
2:1:573:GLU:HB3	2:1:574:VAL:HG23	2.02	0.41
2:1:495:VAL:HG12	2:1:495:VAL:O	2.20	0.41
2:1:248:THR:HA	2:1:454:SER:OG	2.20	0.41
2:1:545:ILE:HG13	2:1:557:ARG:CA	2.36	0.41
1:0:324:LEU:HD23	1:0:324:LEU:HA	1.93	0.41
1:0:170:TYR:CD2	1:0:170:TYR:N	2.87	0.41
1:0:168:ILE:HG23	1:0:169:GLU:H	1.83	0.41
2:1:529:ILE:CG2	2:1:530:GLY:N	2.81	0.41
2:1:593:VAL:HG23	2:1:593:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:540:ARG:CG	2:1:541:LEU:N	2.82	0.41
2:1:596:LYS:HD3	2:1:597:ASP:H	1.85	0.41
1:0:73:ASP:OD2	1:0:84:LYS:NZ	2.51	0.41
2:1:534:GLN:CG	2:1:535:PRO:N	2.84	0.41
2:1:403:PHE:CZ	2:1:404:SER:O	2.74	0.41
1:0:97:VAL:HG13	1:0:98:ASP:OD1	2.21	0.41
1:0:177:ARG:NH1	2:1:455:GLN:HE22	2.19	0.41
2:1:430:ILE:CG2	2:1:431:GLN:N	2.83	0.41
2:1:557:ARG:CB	2:1:563:GLN:H	2.34	0.41
2:1:459:SER:HB2	2:1:477:LYS:HZ1	1.74	0.41
1:0:47:PHE:C	1:0:47:PHE:CD1	2.94	0.41
2:1:161:VAL:HG23	2:1:162:LYS:H	1.84	0.41
2:1:415:SER:O	2:1:419:ALA:CB	2.69	0.40
2:1:583:ALA:HA	2:1:590:GLY:HA3	2.04	0.40
1:0:188:THR:CG2	1:0:189:GLU:N	2.84	0.40
2:1:434:GLU:C	2:1:446:ILE:HD12	2.42	0.40
1:0:322:LYS:HE2	1:0:363:ASP:CB	2.39	0.40
2:1:397:LYS:HG2	2:1:399:ASP:CG	2.42	0.40
1:0:168:ILE:O	1:0:169:GLU:CB	2.58	0.40
1:0:343:GLU:HG2	1:0:347:GLY:O	2.21	0.40
1:0:177:ARG:NH1	2:1:237:THR:HG1	2.19	0.40
1:0:90:ASP:N	1:0:91:GLU:OE2	2.55	0.40
1:0:168:ILE:CD1	1:0:195:ILE:HG13	2.48	0.40
2:1:445:CYS:SG	2:1:479:ARG:N	2.95	0.40
2:1:571:LEU:HB2	2:1:577:TRP:HD1	1.84	0.40
1:0:339:MET:O	1:0:343:GLU:HG3	2.21	0.40
2:1:528:PHE:HE1	2:1:595:ARG:HG2	1.85	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	0	384/386 (100%)	302 (79%)	46 (12%)	36 (9%)	1	16
2	1	512/611 (84%)	410 (80%)	49 (10%)	53 (10%)	1	12
All	All	896/997 (90%)	712 (80%)	95 (11%)	89 (10%)	2	14

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	15	GLY
1	0	46	LYS
1	0	51	LEU
1	0	52	ASP
1	0	56	LYS
1	0	60	THR
1	0	61	ASP
1	0	62	LEU
1	0	89	THR
1	0	92	SER
1	0	103	LYS
1	0	136	ILE
1	0	178	THR
1	0	180	ASP
1	0	181	VAL
1	0	182	LEU
1	0	327	ASP
1	0	328	ASN
1	0	382	ASP
2	1	38	PHE
2	1	42	LYS
2	1	44	GLN
2	1	46	GLN
2	1	48	TYR
2	1	79	LYS
2	1	80	LYS
2	1	81	LYS
2	1	83	THR
2	1	175	HIS
2	1	176	VAL
2	1	189	TYR
2	1	195	ASN
2	1	206	SER
2	1	207	GLU
2	1	211	LYS

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Mol	Chain	Res	Type
2	1	213	SER
2	1	231	VAL
2	1	253	PRO
2	1	255	HIS
2	1	300	ALA
2	1	390	LYS
2	1	415	SER
2	1	546	ASP
1	0	9	ASP
1	0	55	GLY
1	0	96	ASN
1	0	134	CYS
1	0	168	ILE
1	0	169	GLU
1	0	179	THR
1	0	205	PHE
2	1	21	GLU
2	1	25	TYR
2	1	27	ASN
2	1	37	VAL
2	1	40	THR
2	1	66	ASP
2	1	167	HIS
2	1	212	SER
2	1	229	ARG
2	1	258	PHE
2	1	363	GLU
2	1	452	VAL
2	1	453	GLY
2	1	454	SER
2	1	457	GLY
2	1	465	THR
2	1	500	ILE
2	1	596	LYS
1	0	6	LEU
1	0	331	GLN
1	0	364	GLN
2	1	54	LEU
2	1	216	PHE
2	1	396	ASN
2	1	577	TRP
1	0	98	ASP

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Mol	Chain	Res	Type
1	0	348	LYS
2	1	47	ASP
2	1	194	VAL
2	1	267	SER
2	1	503	ALA
1	0	138	TYR
2	1	39	PRO
1	0	49	SER
1	0	166	GLN
2	1	53	ASN
2	1	193	ILE
1	0	97	VAL

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	0	348/348 (100%)	280 (80%)	68 (20%)	2	12
2	1	456/538 (85%)	373 (82%)	83 (18%)	2	15
All	All	804/886 (91%)	653 (81%)	151 (19%)	5	13

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	7	LYS
1	0	8	LYS
1	0	11	PHE
1	0	13	LYS
1	0	20	LEU
1	0	24	ASP
1	0	25	LYS
1	0	26	GLU
1	0	29	PHE
1	0	45	LYS
1	0	46	LYS

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Mol	Chain	Res	Type
1	0	50	LYS
1	0	52	ASP
1	0	53	GLU
1	0	58	LYS
1	0	59	SER
1	0	65	LEU
1	0	66	LYS
1	0	68	LYS
1	0	76	MET
1	0	77	LYS
1	0	80	TYR
1	0	81	LEU
1	0	87	THR
1	0	88	VAL
1	0	89	THR
1	0	91	GLU
1	0	96	ASN
1	0	112	VAL
1	0	119	LYS
1	0	134	CYS
1	0	141	ASP
1	0	146	VAL
1	0	147	LEU
1	0	149	GLU
1	0	161	SER
1	0	166	GLN
1	0	167	LYS
1	0	169	GLU
1	0	170	TYR
1	0	172	MET
1	0	175	LYS
1	0	177	ARG
1	0	178	THR
1	0	180	ASP
1	0	206	ASP
1	0	209	LYS
1	0	221	LYS
1	0	265	ASN
1	0	273	GLN
1	0	279	LYS
1	0	280	GLU
1	0	282	MET

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Mol	Chain	Res	Type
1	0	286	GLU
1	0	291	LEU
1	0	294	ASP
1	0	295	ASP
1	0	303	LYS
1	0	316	TYR
1	0	317	LEU
1	0	326	SER
1	0	333	GLU
1	0	348	LYS
1	0	354	THR
1	0	355	LEU
1	0	374	TYR
1	0	378	ASP
1	0	381	GLU
2	1	21	GLU
2	1	29	ASP
2	1	31	TYR
2	1	35	ASN
2	1	37	VAL
2	1	64	ASN
2	1	66	ASP
2	1	77	THR
2	1	80	LYS
2	1	84	PRO
2	1	161	VAL
2	1	162	LYS
2	1	163	SER
2	1	167	HIS
2	1	175	HIS
2	1	176	VAL
2	1	177	ASP
2	1	180	LYS
2	1	189	TYR
2	1	191	LEU
2	1	192	ASN
2	1	195	ASN
2	1	205	GLU
2	1	206	SER
2	1	207	GLU
2	1	209	MET
2	1	212	SER

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Mol	Chain	Res	Type
2	1	214	PHE
2	1	219	ILE
2	1	220	MET
2	1	225	GLU
2	1	227	ARG
2	1	228	GLU
2	1	233	VAL
2	1	235	ILE
2	1	237	THR
2	1	239	HIS
2	1	255	HIS
2	1	258	PHE
2	1	260	PRO
2	1	263	ILE
2	1	270	ASP
2	1	279	SER
2	1	280	THR
2	1	284	GLU
2	1	289	LEU
2	1	293	THR
2	1	299	LEU
2	1	315	MET
2	1	316	ASP
2	1	317	ASN
2	1	331	LYS
2	1	334	PRO
2	1	335	TYR
2	1	338	ASP
2	1	343	GLU
2	1	351	ILE
2	1	357	GLU
2	1	359	VAL
2	1	361	LYS
2	1	368	VAL
2	1	369	ARG
2	1	370	GLN
2	1	382	GLU
2	1	390	LYS
2	1	393	GLU
2	1	409	ILE
2	1	422	SER
2	1	454	SER

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Mol	Chain	Res	Type
2	1	459	SER
2	1	465	THR
2	1	483	PRO
2	1	486	ILE
2	1	491	LEU
2	1	518	PRO
2	1	529	ILE
2	1	540	ARG
2	1	564	ARG
2	1	581	LEU
2	1	588	ARG
2	1	596	LYS
2	1	601	ILE
2	1	609	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	204	ASN
1	0	242	ASN
2	1	192	ASN
2	1	195	ASN
2	1	261	ASN
2	1	396	ASN
2	1	451	GLN
2	1	488	ASN
2	1	504	GLN
2	1	534	GLN
2	1	558	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.