



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:52 pm BST

PDB ID : 3K1B
Title : Structure of OmpF porin
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Center for Structures of Membrane Proteins (CSMP)
Deposited on : 2009-09-26
Resolution : 4.39 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

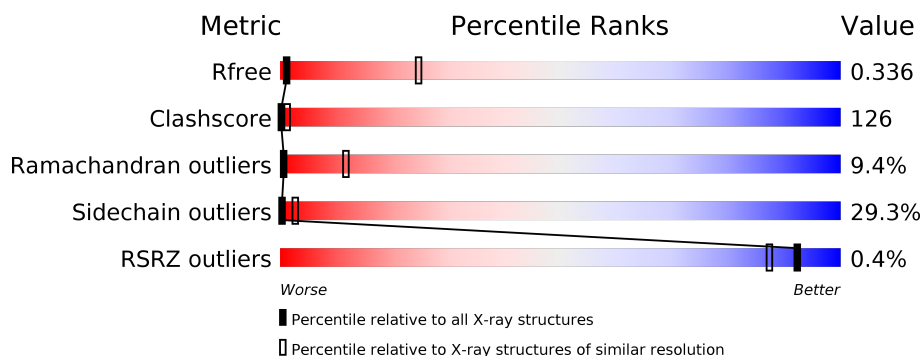
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.39 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1022 (4.92-3.80)
Clashscore	141614	1085 (4.92-3.80)
Ramachandran outliers	138981	1036 (4.92-3.80)
Sidechain outliers	138945	1019 (4.92-3.80)
RSRZ outliers	127900	1094 (5.06-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	340	<div> <div>16%</div> <div>51%</div> <div>27%</div> <div>6%</div> </div>
1	B	340	<div> <div>15%</div> <div>53%</div> <div>26%</div> <div>6%</div> </div>
1	C	340	<div> <div>19%</div> <div>54%</div> <div>22%</div> <div>5%</div> </div>
1	D	340	<div> <div>15%</div> <div>55%</div> <div>28%</div> <div>.</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10508 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

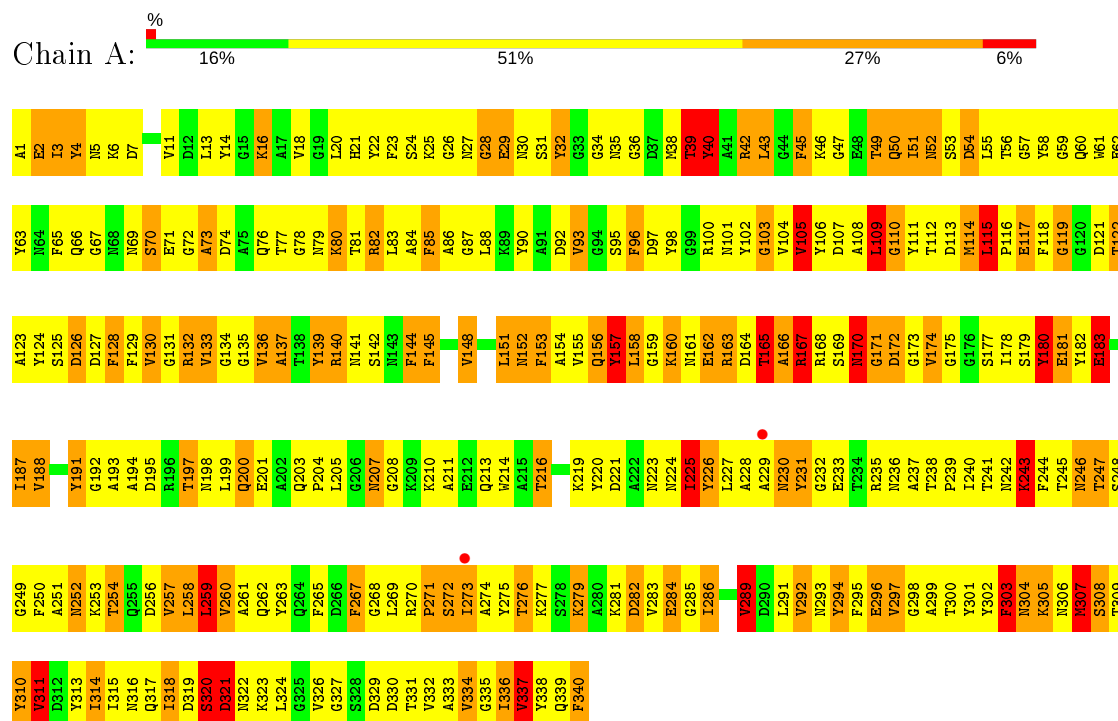
- Molecule 1 is a protein called Outer membrane protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	8	0	0
			2627	1654	438	532	3			
1	B	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	C	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	D	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			

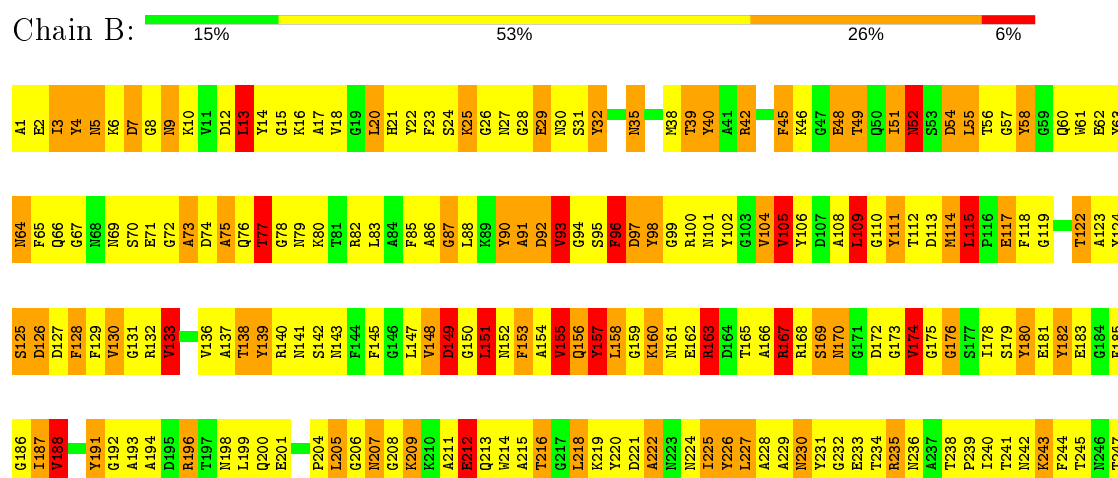
3 Residue-property plots

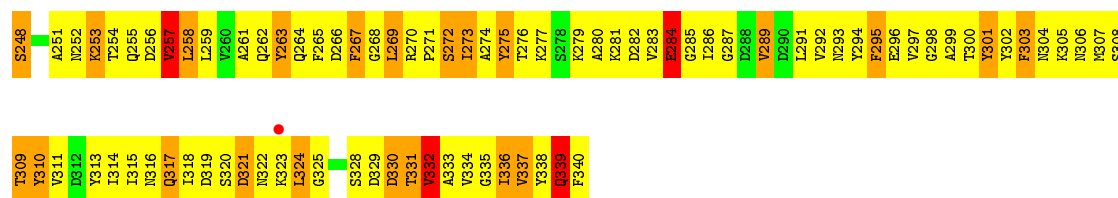
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Outer membrane protein F



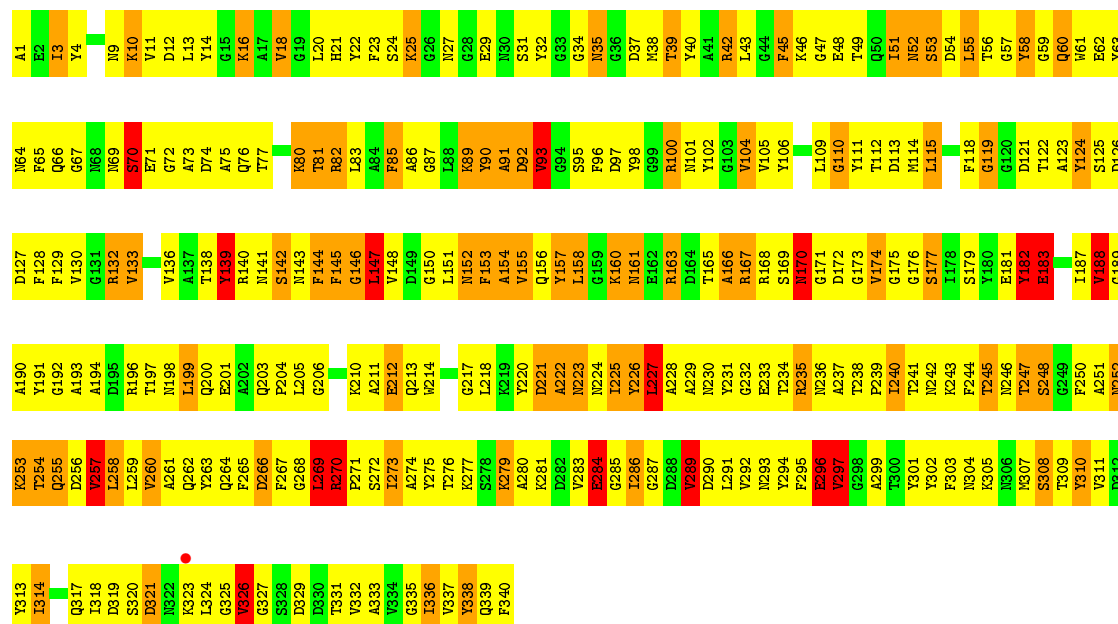
• Molecule 1: Outer membrane protein F





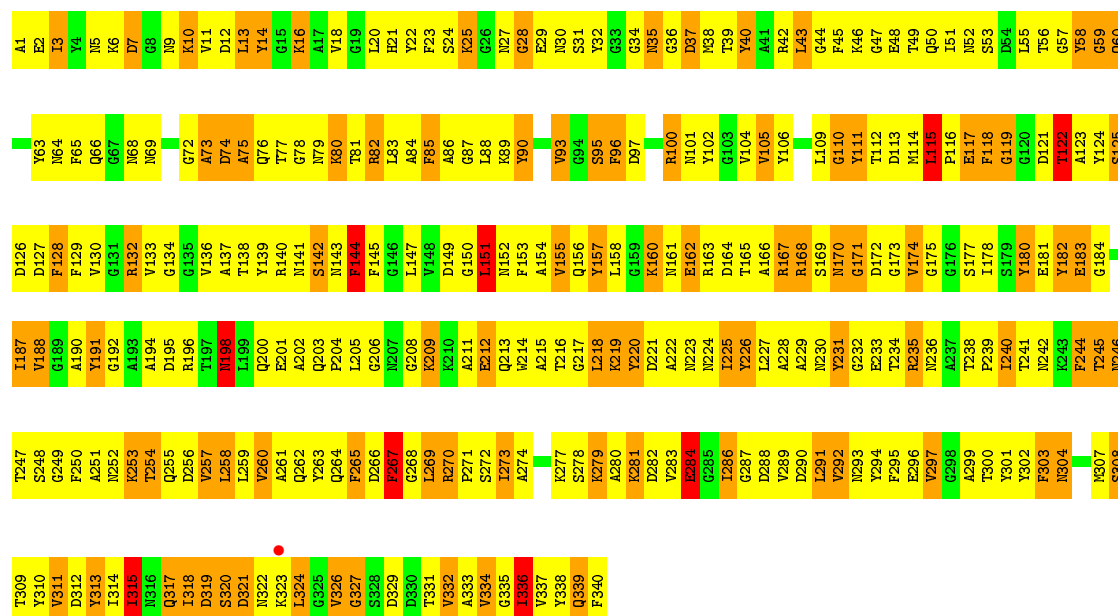
• Molecule 1: Outer membrane protein F

Chain C: 19% 54% 22% 5%



• Molecule 1: Outer membrane protein F

Chain D: 15% 55% 28%



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.53Å 215.53Å 137.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 4.39 49.23 – 4.39	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-4.39) 99.1 (49.23-4.39)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 4.45Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.264 , 0.329 0.273 , 0.336	Depositor DCC
R_{free} test set	1211 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	91.5	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 104.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.003 for -h,-k,l	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	10508	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.34	11/2683 (0.4%)	1.43	24/3628 (0.7%)
1	B	1.36	13/2683 (0.5%)	1.44	33/3628 (0.9%)
1	C	1.31	13/2683 (0.5%)	1.41	24/3628 (0.7%)
1	D	1.26	9/2683 (0.3%)	1.37	21/3628 (0.6%)
All	All	1.32	46/10732 (0.4%)	1.41	102/14512 (0.7%)

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	3
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	7

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	59	GLY	CA-C	9.52	1.67	1.51
1	B	157	TYR	CD1-CE1	9.44	1.53	1.39
1	A	311	VAL	CA-CB	-7.75	1.38	1.54
1	C	296	GLU	CG-CD	7.72	1.63	1.51
1	C	301	TYR	CD2-CE2	-7.41	1.28	1.39
1	B	157	TYR	CD2-CE2	7.40	1.50	1.39
1	B	157	TYR	CG-CD2	7.39	1.48	1.39
1	A	334	VAL	CA-CB	-7.07	1.39	1.54
1	C	157	TYR	CD1-CE1	7.04	1.50	1.39
1	B	157	TYR	CE1-CZ	6.84	1.47	1.38
1	D	168	ARG	CZ-NH1	6.73	1.41	1.33
1	B	263	TYR	CD1-CE1	-6.62	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	225	ILE	CA-CB	6.39	1.69	1.54
1	D	22	TYR	CD2-CE2	-6.31	1.29	1.39
1	D	326	VAL	CB-CG1	6.09	1.65	1.52
1	C	266	ASP	CB-CG	5.92	1.64	1.51
1	C	139	TYR	CD1-CE1	-5.91	1.30	1.39
1	B	263	TYR	CD2-CE2	-5.83	1.30	1.39
1	D	157	TYR	CD1-CE1	5.82	1.48	1.39
1	C	157	TYR	CE1-CZ	5.81	1.46	1.38
1	A	305	LYS	CD-CE	5.73	1.65	1.51
1	B	321	ASP	CB-CG	5.73	1.63	1.51
1	C	181	GLU	CG-CD	5.64	1.60	1.51
1	B	301	TYR	CD2-CE2	-5.63	1.30	1.39
1	B	257	VAL	CA-CB	-5.62	1.43	1.54
1	A	210	LYS	CD-CE	5.61	1.65	1.51
1	C	226	TYR	CE1-CZ	5.60	1.45	1.38
1	A	157	TYR	CG-CD2	5.54	1.46	1.39
1	A	3	ILE	CA-CB	-5.49	1.42	1.54
1	A	157	TYR	CE1-CZ	5.47	1.45	1.38
1	D	22	TYR	CD1-CE1	-5.47	1.31	1.39
1	B	191	TYR	CD1-CE1	-5.38	1.31	1.39
1	B	212	GLU	CG-CD	5.37	1.60	1.51
1	C	157	TYR	CG-CD1	5.34	1.46	1.39
1	B	332	VAL	CA-CB	-5.33	1.43	1.54
1	A	145	PHE	CB-CG	-5.31	1.42	1.51
1	A	157	TYR	CD1-CE1	5.30	1.47	1.39
1	D	157	TYR	CG-CD2	5.29	1.46	1.39
1	B	93	VAL	CA-CB	-5.28	1.43	1.54
1	C	183	GLU	CG-CD	5.26	1.59	1.51
1	C	257	VAL	CA-CB	-5.26	1.43	1.54
1	C	174	VAL	CB-CG2	-5.18	1.42	1.52
1	D	157	TYR	CD2-CE2	5.09	1.47	1.39
1	A	148	VAL	CB-CG1	5.05	1.63	1.52
1	A	289	VAL	CA-CB	-5.00	1.44	1.54
1	C	18	VAL	CA-CB	5.00	1.65	1.54

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	168	ARG	NE-CZ-NH1	-12.77	113.92	120.30
1	B	269	LEU	CA-CB-CG	-11.18	89.59	115.30
1	D	182	TYR	CA-CB-CG	-9.08	96.14	113.40
1	B	324	LEU	CB-CG-CD2	-9.06	95.59	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	VAL	CB-CA-C	-8.98	94.33	111.40
1	D	260	VAL	CB-CA-C	-8.76	94.76	111.40
1	B	155	VAL	CB-CA-C	-8.34	95.56	111.40
1	C	301	TYR	CB-CG-CD2	-8.02	116.19	121.00
1	D	218	LEU	CA-CB-CG	-7.67	97.65	115.30
1	A	132	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	B	227	LEU	CA-CB-CG	-7.56	97.91	115.30
1	B	133	VAL	CB-CA-C	-7.43	97.29	111.40
1	C	290	ASP	CB-CG-OD1	-7.38	111.66	118.30
1	A	132	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	C	227	LEU	CB-CG-CD1	-7.28	98.63	111.00
1	C	132	ARG	NE-CZ-NH1	-7.13	116.74	120.30
1	C	115	LEU	CA-CB-CG	-7.11	98.94	115.30
1	A	210	LYS	CD-CE-NZ	6.95	127.68	111.70
1	A	225	ILE	CG1-CB-CG2	-6.90	96.21	111.40
1	B	337	VAL	CB-CA-C	-6.90	98.30	111.40
1	C	158	LEU	CA-CB-CG	-6.80	99.67	115.30
1	B	42	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	A	259	LEU	CA-CB-CG	-6.69	99.91	115.30
1	A	165	THR	CB-CA-C	-6.67	93.59	111.60
1	D	324	LEU	CB-CG-CD2	-6.66	99.67	111.00
1	A	151	LEU	CB-CG-CD1	-6.64	99.71	111.00
1	C	297	VAL	CB-CA-C	-6.64	98.78	111.40
1	B	182	TYR	CB-CG-CD1	-6.60	117.04	121.00
1	B	115	LEU	CA-CB-CG	-6.57	100.19	115.30
1	B	92	ASP	CB-CG-OD1	-6.56	112.40	118.30
1	B	82	ARG	NE-CZ-NH2	6.53	123.57	120.30
1	D	269	LEU	CA-CB-CG	-6.51	100.32	115.30
1	B	207	ASN	N-CA-C	6.47	128.46	111.00
1	A	334	VAL	CB-CA-C	-6.42	99.21	111.40
1	C	289	VAL	CB-CA-C	-6.31	99.41	111.40
1	A	40	TYR	CB-CG-CD1	-6.29	117.23	121.00
1	D	151	LEU	CA-CB-CG	-6.20	101.05	115.30
1	A	39	THR	N-CA-CB	-6.16	98.60	110.30
1	D	182	TYR	N-CA-C	6.15	127.61	111.00
1	D	168	ARG	NH1-CZ-NH2	6.08	126.08	119.40
1	D	321	ASP	CB-CA-C	-6.06	98.28	110.40
1	B	77	THR	CB-CA-C	-6.05	95.26	111.60
1	B	109	LEU	CA-CB-CG	-6.05	101.39	115.30
1	B	182	TYR	CA-CB-CG	-6.02	101.97	113.40
1	A	43	LEU	CB-CG-CD1	-6.00	100.80	111.00
1	A	109	LEU	CA-CB-CG	-5.96	101.59	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	VAL	CB-CA-C	-5.89	100.21	111.40
1	D	174	VAL	CB-CA-C	-5.89	100.21	111.40
1	D	82	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	307	MET	CB-CG-SD	-5.82	94.94	112.40
1	B	55	LEU	CA-CB-CG	-5.78	102.01	115.30
1	B	87	GLY	N-CA-C	5.77	127.53	113.10
1	C	70	SER	CB-CA-C	-5.77	99.14	110.10
1	C	199	LEU	CA-CB-CG	5.77	128.57	115.30
1	C	269	LEU	CA-CB-CG	-5.71	102.18	115.30
1	A	303	PHE	CB-CG-CD1	-5.70	116.81	120.80
1	B	275	TYR	CB-CA-C	-5.65	99.10	110.40
1	A	337	VAL	CB-CA-C	-5.63	100.70	111.40
1	A	260	VAL	CB-CA-C	-5.62	100.72	111.40
1	D	43	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	B	151	LEU	CA-CB-CG	-5.61	102.41	115.30
1	B	209	LYS	CD-CE-NZ	5.59	124.57	111.70
1	B	332	VAL	CB-CA-C	-5.59	100.77	111.40
1	B	188	VAL	CB-CA-C	-5.59	100.78	111.40
1	C	268	GLY	N-CA-C	5.58	127.06	113.10
1	A	334	VAL	N-CA-C	-5.55	96.01	111.00
1	D	115	LEU	CA-CB-CG	-5.53	102.58	115.30
1	C	93	VAL	N-CA-C	-5.49	96.17	111.00
1	B	191	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	B	269	LEU	CB-CG-CD1	-5.48	101.69	111.00
1	C	326	VAL	CB-CA-C	-5.48	100.99	111.40
1	D	43	LEU	CA-CB-CG	-5.41	102.87	115.30
1	B	3	ILE	CB-CA-C	-5.33	100.93	111.60
1	C	321	ASP	CB-CA-C	-5.33	99.75	110.40
1	A	43	LEU	CA-CB-CG	-5.27	103.17	115.30
1	B	13	LEU	CA-CB-CG	5.27	127.42	115.30
1	C	270	ARG	C-N-CD	-5.21	109.13	120.60
1	B	309	THR	CB-CA-C	-5.21	97.54	111.60
1	A	156	GLN	N-CA-CB	-5.19	101.25	110.60
1	C	89	LYS	CB-CA-C	-5.19	100.02	110.40
1	C	182	TYR	CB-CG-CD1	-5.19	117.89	121.00
1	D	254	THR	CB-CA-C	-5.19	97.60	111.60
1	C	115	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	A	105	VAL	CB-CA-C	-5.15	101.61	111.40
1	A	207	ASN	CA-C-N	-5.14	105.93	116.20
1	D	164	ASP	C-N-CA	-5.13	108.86	121.70
1	B	148	VAL	CB-CA-C	-5.12	101.66	111.40
1	D	220	TYR	CB-CG-CD1	-5.11	117.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	C	93	VAL	CB-CA-C	-5.10	101.71	111.40
1	C	188	VAL	CB-CA-C	-5.09	101.72	111.40
1	D	326	VAL	N-CA-C	-5.09	97.26	111.00
1	D	313	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	A	180	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	B	174	VAL	N-CA-C	-5.08	97.28	111.00
1	B	216	THR	CB-CA-C	-5.07	97.92	111.60
1	C	155	VAL	CB-CA-C	-5.07	101.78	111.40
1	D	90	TYR	N-CA-C	5.05	124.64	111.00
1	A	340	PHE	N-CA-C	-5.05	97.37	111.00
1	C	210	LYS	CD-CE-NZ	-5.04	100.10	111.70
1	B	163	ARG	CG-CD-NE	-5.04	101.22	111.80
1	B	283	VAL	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ALA	Peptide
1	A	164	ASP	Peptide
1	A	321	ASP	Peptide
1	B	176	GLY	Peptide
1	C	255	GLN	Peptide
1	D	315	ILE	Peptide
1	D	336	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	2627	0	2442	772	0
1	B	2627	0	2443	693	5
1	C	2627	0	2444	650	2
1	D	2627	0	2444	608	1
All	All	10508	0	9773	2562	6

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 126.

All (2562) 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:A:258:LEU:CD1	1:A:276:THR:HG23	1.28	1.58
1:A:313:TYR:CD1	1:A:332:VAL:CG2	1.86	1.58
1:A:114:MET:HE1	1:A:226:TYR:CE1	1.39	1.55
1:A:191:TYR:HD2	1:A:192:GLY:N	1.06	1.53
1:A:313:TYR:HD1	1:A:332:VAL:CG2	1.19	1.52
1:A:114:MET:CE	1:A:226:TYR:CE1	1.93	1.52
1:C:269:LEU:CD1	1:C:270:ARG:H	1.25	1.47
1:D:311:VAL:HG13	1:D:334:VAL:CG2	1.42	1.47
1:D:311:VAL:CG1	1:D:334:VAL:HG23	1.44	1.46
1:A:115:LEU:H	1:A:115:LEU:CD2	0.94	1.45
1:B:115:LEU:H	1:B:115:LEU:CD2	0.99	1.45
1:A:307:MET:CE	1:B:88:LEU:CD2	1.96	1.42
1:D:51:ILE:CD1	1:D:55:LEU:HD23	1.46	1.42
1:B:21:HIS:HD2	1:B:23:PHE:CE2	1.36	1.41
1:A:104:VAL:CG1	1:A:156:GLN:OE1	1.68	1.41
1:A:231:TYR:HD2	1:A:232:GLY:N	1.18	1.40
1:C:204:PRO:HG2	1:C:247:THR:CG2	1.50	1.39
1:A:51:ILE:CG1	1:A:55:LEU:HD23	1.54	1.38
1:D:229:ALA:HB2	1:D:259:LEU:CD2	1.49	1.38
1:A:294:TYR:CD2	1:A:314:ILE:HD12	1.59	1.37
1:A:211:ALA:HB1	1:A:235:ARG:O	1.19	1.36
1:A:170:ASN:O	1:A:170:ASN:ND2	1.56	1.36
1:A:4:TYR:CE1	1:C:1:ALA:HB1	1.59	1.35
1:A:20:LEU:CD2	1:A:117:GLU:OE1	1.75	1.35
1:D:104:VAL:CG1	1:D:156:GLN:OE1	1.73	1.35
1:D:144:PHE:O	1:D:144:PHE:CD2	1.80	1.34
1:A:51:ILE:CD1	1:A:55:LEU:HD23	1.58	1.34
1:A:51:ILE:CD1	1:A:55:LEU:CD2	2.04	1.33
1:B:21:HIS:CD2	1:B:23:PHE:HE2	1.45	1.33
1:D:132:ARG:HH11	1:D:132:ARG:CG	1.32	1.33
1:B:151:LEU:C	1:B:151:LEU:HD12	1.18	1.32
1:D:115:LEU:CD2	1:D:115:LEU:H	1.15	1.32
1:D:229:ALA:CB	1:D:259:LEU:CD2	2.08	1.31
1:A:191:TYR:CD2	1:A:192:GLY:N	1.96	1.30
1:A:90:TYR:O	1:A:93:VAL:HG23	1.26	1.30
1:B:276:THR:CG2	1:B:294:TYR:HE2	1.44	1.29
1:A:285:GLY:C	1:A:286:ILE:HD12	1.53	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ASP:O	1:C:194:ALA:HB1	1.24	1.29
1:C:269:LEU:HD12	1:C:270:ARG:N	0.96	1.28
1:A:258:LEU:O	1:A:259:LEU:HD23	1.15	1.28
1:C:45:PHE:O	1:C:45:PHE:HD1	1.16	1.28
1:D:104:VAL:HG13	1:D:156:GLN:OE1	1.15	1.27
1:A:20:LEU:HD21	1:A:117:GLU:OE1	1.21	1.27
1:B:258:LEU:O	1:B:259:LEU:HD23	1.30	1.27
1:A:285:GLY:O	1:A:286:ILE:HD12	1.21	1.27
1:A:114:MET:HE1	1:A:226:TYR:CD1	1.69	1.27
1:C:286:ILE:CD1	1:C:286:ILE:H	1.46	1.26
1:C:112:THR:HG23	1:C:230:ASN:OD1	1.34	1.26
1:C:269:LEU:CD1	1:C:270:ARG:N	1.87	1.26
1:A:313:TYR:CD1	1:A:332:VAL:HG22	1.59	1.26
1:B:87:GLY:O	1:B:88:LEU:HD23	1.13	1.26
1:B:115:LEU:HD12	1:B:119:GLY:CA	1.63	1.25
1:B:276:THR:CG2	1:B:294:TYR:CE2	2.18	1.25
1:A:172:ASP:O	1:A:194:ALA:CB	1.85	1.25
1:C:269:LEU:C	1:C:269:LEU:HD12	1.48	1.25
1:B:151:LEU:C	1:B:151:LEU:CD1	1.98	1.25
1:C:63:TYR:CD1	1:C:80:LYS:O	1.89	1.25
1:B:21:HIS:CD2	1:B:23:PHE:CE2	2.23	1.24
1:A:258:LEU:CD1	1:A:276:THR:CG2	2.16	1.24
1:A:294:TYR:CD2	1:A:314:ILE:CD1	2.20	1.23
1:D:279:LYS:HB2	1:D:279:LYS:NZ	1.24	1.23
1:A:1:ALA:HB3	1:B:4:TYR:CE1	1.73	1.23
1:A:337:VAL:CG1	1:A:337:VAL:O	1.74	1.23
1:B:229:ALA:CB	1:B:259:LEU:CD2	2.17	1.23
1:D:115:LEU:CD2	1:D:115:LEU:N	1.80	1.22
1:B:96:PHE:HD2	1:B:97:ASP:N	1.33	1.22
1:D:309:THR:CG2	1:D:336:ILE:HB	1.67	1.22
1:D:170:ASN:ND2	1:D:170:ASN:O	1.71	1.22
1:B:229:ALA:HB1	1:B:259:LEU:CD2	1.71	1.21
1:B:45:PHE:O	1:B:45:PHE:CD1	1.94	1.20
1:A:141:ASN:O	1:A:152:ASN:HB3	1.40	1.20
1:D:29:GLU:CG	1:D:30:ASN:N	2.01	1.20
1:B:151:LEU:HD12	1:B:152:ASN:N	1.56	1.20
1:C:174:VAL:HG12	1:C:175:GLY:N	1.56	1.20
1:D:144:PHE:O	1:D:144:PHE:HD2	0.91	1.20
1:C:172:ASP:O	1:C:194:ALA:CB	1.89	1.20
1:B:96:PHE:CD2	1:B:97:ASP:N	2.10	1.19
1:A:231:TYR:CD2	1:A:232:GLY:N	2.11	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:TRP:CZ2	1:C:65:PHE:CD1	2.29	1.19
1:D:315:ILE:N	1:D:315:ILE:HD12	1.48	1.19
1:B:313:TYR:CD1	1:B:332:VAL:HG23	1.77	1.19
1:A:111:TYR:CE2	1:A:219:LYS:HG2	1.77	1.18
1:B:45:PHE:O	1:B:45:PHE:HD1	1.22	1.18
1:C:286:ILE:N	1:C:286:ILE:HD12	1.47	1.18
1:B:115:LEU:CD1	1:B:119:GLY:HA3	1.72	1.18
1:A:262:GLN:OE1	1:A:270:ARG:NH1	1.76	1.18
1:B:242:ASN:O	1:B:242:ASN:OD1	1.62	1.18
1:B:276:THR:HG21	1:B:294:TYR:CE2	1.78	1.18
1:A:309:THR:CG2	1:A:336:ILE:HB	1.74	1.17
1:A:258:LEU:C	1:A:259:LEU:HD23	1.62	1.17
1:A:271:PRO:HA	1:A:299:ALA:CB	1.74	1.17
1:C:167:ARG:O	1:C:167:ARG:CG	1.91	1.17
1:A:258:LEU:O	1:A:259:LEU:CD2	1.92	1.17
1:C:338:TYR:CD2	1:C:339:GLN:N	2.13	1.16
1:D:51:ILE:CD1	1:D:55:LEU:CD2	2.22	1.16
1:A:267:PHE:HD1	1:A:267:PHE:N	1.42	1.16
1:B:105:VAL:O	1:B:105:VAL:CG1	1.89	1.16
1:D:96:PHE:CD2	1:D:97:ASP:N	2.14	1.16
1:B:143:ASN:OD1	1:B:150:GLY:N	1.79	1.15
1:B:113:ASP:C	1:B:114:MET:HG2	1.66	1.15
1:B:64:ASN:ND2	1:B:64:ASN:O	1.77	1.15
1:B:114:MET:HE1	1:B:226:TYR:CE1	1.81	1.15
1:D:226:TYR:O	1:D:227:LEU:HD23	1.47	1.15
1:D:29:GLU:HG3	1:D:30:ASN:N	1.37	1.15
1:A:275:TYR:O	1:A:276:THR:OG1	1.61	1.14
1:B:313:TYR:HD1	1:B:332:VAL:CG2	1.56	1.14
1:B:332:VAL:CG1	1:B:332:VAL:O	1.91	1.14
1:C:291:LEU:O	1:C:292:VAL:HG23	1.46	1.14
1:B:112:THR:HG21	1:B:230:ASN:HB2	1.18	1.14
1:C:204:PRO:HG2	1:C:247:THR:HG22	1.22	1.14
1:A:118:PHE:O	1:A:119:GLY:O	1.63	1.14
1:A:22:TYR:CD2	1:A:38:MET:HG3	1.82	1.14
1:A:45:PHE:O	1:A:45:PHE:HD1	1.29	1.14
1:C:307:MET:HG3	1:C:308:SER:H	1.12	1.13
1:A:69:ASN:HD21	1:A:77:THR:HB	0.97	1.13
1:C:27:ASN:OD1	1:C:27:ASN:O	1.65	1.13
1:A:313:TYR:CD1	1:A:332:VAL:HG23	1.63	1.13
1:A:307:MET:CE	1:B:88:LEU:HD21	1.64	1.13
1:B:113:ASP:O	1:B:114:MET:HG2	1.48	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HD13	1:A:276:THR:HG23	1.30	1.12
1:A:45:PHE:CD1	1:A:45:PHE:O	2.00	1.12
1:A:114:MET:O	1:A:115:LEU:O	1.66	1.12
1:B:180:TYR:C	1:B:180:TYR:HD2	1.47	1.12
1:A:307:MET:HE2	1:B:88:LEU:HD22	1.29	1.12
1:C:224:ASN:O	1:C:263:TYR:HD1	1.30	1.12
1:B:255:GLN:OE1	1:B:281:LYS:HE2	1.50	1.11
1:A:51:ILE:HG13	1:A:55:LEU:HD23	1.13	1.11
1:C:204:PRO:HG2	1:C:247:THR:HG21	1.25	1.11
1:A:172:ASP:O	1:A:194:ALA:HB1	1.39	1.11
1:B:87:GLY:C	1:B:88:LEU:HD23	1.70	1.11
1:A:187:ILE:CG2	1:A:187:ILE:O	1.99	1.11
1:A:114:MET:HE2	1:A:226:TYR:CZ	1.86	1.10
1:B:276:THR:HG21	1:B:294:TYR:HE2	0.99	1.10
1:A:141:ASN:OD1	1:A:153:PHE:HE1	1.32	1.10
1:A:129:PHE:HE2	1:A:193:ALA:N	1.48	1.10
1:B:115:LEU:N	1:B:115:LEU:HD23	0.97	1.10
1:D:203:GLN:HB3	1:D:204:PRO:HD2	1.34	1.10
1:A:211:ALA:CB	1:A:236:ASN:HB2	1.81	1.10
1:B:285:GLY:C	1:B:286:ILE:HD12	1.72	1.10
1:C:82:ARG:O	1:C:100:ARG:HD3	1.51	1.09
1:D:20:LEU:HD12	1:D:21:HIS:H	1.03	1.09
1:B:311:VAL:HG13	1:B:334:VAL:HG22	1.31	1.09
1:B:23:PHE:HA	1:B:35:ASN:HD21	1.04	1.09
1:A:104:VAL:HG13	1:A:156:GLN:OE1	0.91	1.09
1:A:113:ASP:O	1:A:114:MET:HG2	1.53	1.09
1:B:277:LYS:HD2	1:B:293:ASN:ND2	1.65	1.09
1:B:27:ASN:OD1	1:B:27:ASN:O	1.71	1.09
1:C:174:VAL:CG1	1:C:175:GLY:N	2.15	1.08
1:D:132:ARG:NH1	1:D:132:ARG:HG3	1.11	1.08
1:D:279:LYS:CB	1:D:279:LYS:NZ	2.10	1.08
1:A:115:LEU:N	1:A:115:LEU:HD22	1.67	1.08
1:A:258:LEU:HD12	1:A:276:THR:HG23	1.11	1.08
1:B:242:ASN:O	1:B:244:PHE:N	1.85	1.08
1:B:114:MET:CE	1:B:226:TYR:CE1	2.35	1.08
1:D:13:LEU:HD12	1:D:14:TYR:N	1.69	1.08
1:D:51:ILE:HD13	1:D:55:LEU:CD2	1.80	1.08
1:D:51:ILE:HD13	1:D:55:LEU:HD23	1.24	1.07
1:D:338:TYR:CD2	1:D:339:GLN:N	2.22	1.07
1:A:158:LEU:HD12	1:A:159:GLY:N	1.70	1.07
1:B:229:ALA:CB	1:B:259:LEU:HD22	1.85	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ILE:HD11	1:A:55:LEU:CD2	1.78	1.07
1:B:115:LEU:CD2	1:B:115:LEU:N	1.73	1.07
1:D:122:THR:HG21	1:D:256:ASP:OD2	1.53	1.07
1:A:293:ASN:HD22	1:A:317:GLN:HB3	1.14	1.07
1:A:276:THR:HB	1:A:294:TYR:HE1	1.18	1.07
1:D:144:PHE:HD2	1:D:144:PHE:C	1.58	1.07
1:D:271:PRO:HA	1:D:299:ALA:HB2	1.32	1.07
1:A:318:ILE:N	1:A:318:ILE:HD13	1.68	1.06
1:C:179:SER:HA	1:C:188:VAL:HG12	1.13	1.06
1:D:51:ILE:HD12	1:D:55:LEU:HD23	1.32	1.06
1:A:313:TYR:HD1	1:A:332:VAL:HG23	0.95	1.06
1:D:20:LEU:HD12	1:D:21:HIS:N	1.70	1.06
1:A:167:ARG:HH11	1:A:167:ARG:CG	1.68	1.06
1:A:114:MET:HE2	1:A:226:TYR:CE1	1.85	1.06
1:B:276:THR:CB	1:B:294:TYR:CE2	2.39	1.06
1:D:286:ILE:H	1:D:286:ILE:HD12	1.17	1.06
1:A:271:PRO:CA	1:A:299:ALA:HB2	1.86	1.06
1:B:87:GLY:O	1:B:88:LEU:CD2	2.03	1.06
1:A:129:PHE:CD2	1:A:192:GLY:HA3	1.90	1.05
1:B:276:THR:HB	1:B:294:TYR:CE2	1.90	1.05
1:B:180:TYR:CD2	1:B:180:TYR:C	2.24	1.05
1:B:69:ASN:HD21	1:B:77:THR:HB	1.21	1.05
1:D:309:THR:HG22	1:D:336:ILE:HA	1.38	1.05
1:B:205:LEU:HD11	1:B:247:THR:HG22	1.37	1.05
1:B:332:VAL:HG12	1:B:332:VAL:O	1.32	1.05
1:C:167:ARG:O	1:C:167:ARG:HG3	1.27	1.05
1:C:297:VAL:HG12	1:C:297:VAL:O	1.48	1.05
1:C:179:SER:CA	1:C:188:VAL:HG12	1.86	1.05
1:C:42:ARG:NH1	1:C:82:ARG:NH2	2.04	1.05
1:B:30:ASN:OD1	1:B:30:ASN:O	1.75	1.05
1:A:1:ALA:CB	1:B:4:TYR:CE1	2.38	1.05
1:A:158:LEU:C	1:A:158:LEU:HD12	1.73	1.05
1:B:167:ARG:HH11	1:B:167:ARG:HG3	1.15	1.05
1:D:115:LEU:N	1:D:115:LEU:HD23	1.01	1.04
1:C:45:PHE:O	1:C:45:PHE:CD1	2.08	1.04
1:D:286:ILE:H	1:D:286:ILE:CD1	1.71	1.04
1:A:165:THR:CG2	1:A:166:ALA:N	2.19	1.04
1:A:51:ILE:HD12	1:A:55:LEU:CD2	1.87	1.04
1:D:40:TYR:HE2	1:D:42:ARG:NH2	1.51	1.04
1:B:115:LEU:HD12	1:B:119:GLY:HA3	1.05	1.04
1:B:229:ALA:HB1	1:B:259:LEU:HD23	1.40	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:PHE:HD2	1:A:307:MET:HG2	1.21	1.04
1:D:229:ALA:HB2	1:D:259:LEU:HD22	1.33	1.04
1:D:274:ALA:HB3	1:D:296:GLU:HB3	1.35	1.04
1:B:125:SER:O	1:B:126:ASP:HB2	1.55	1.04
1:D:229:ALA:CB	1:D:259:LEU:HD21	1.84	1.04
1:A:127:ASP:O	1:A:128:PHE:CB	2.01	1.04
1:B:130:VAL:CG1	1:B:213:GLN:NE2	2.19	1.04
1:A:69:ASN:ND2	1:A:77:THR:HB	1.72	1.03
1:B:28:GLY:O	1:B:31:SER:N	1.89	1.03
1:C:309:THR:HG22	1:C:336:ILE:HA	1.37	1.03
1:D:187:ILE:HG13	1:D:218:LEU:HD21	1.36	1.03
1:B:20:LEU:HD21	1:B:117:GLU:OE1	1.56	1.03
1:D:315:ILE:N	1:D:315:ILE:CD1	2.21	1.03
1:D:40:TYR:CE2	1:D:42:ARG:NH2	2.25	1.03
1:B:112:THR:HG23	1:B:230:ASN:OD1	1.58	1.03
1:B:313:TYR:CD1	1:B:332:VAL:CG2	2.39	1.03
1:D:74:ASP:O	1:D:76:GLN:N	1.92	1.02
1:A:86:ALA:O	1:A:97:ASP:HB2	1.58	1.02
1:A:61:TRP:HZ2	1:C:65:PHE:CD1	1.69	1.02
1:C:241:THR:HG22	1:C:242:ASN:H	1.22	1.02
1:B:241:THR:HG22	1:B:242:ASN:N	1.63	1.02
1:A:4:TYR:CE1	1:C:1:ALA:CB	2.41	1.02
1:C:229:ALA:CB	1:C:259:LEU:CD2	2.38	1.02
1:D:229:ALA:CB	1:D:259:LEU:HD23	1.87	1.02
1:A:132:ARG:HH11	1:A:132:ARG:HG3	1.22	1.02
1:A:71:GLU:HG3	1:B:100:ARG:NH2	1.75	1.01
1:C:112:THR:CG2	1:C:230:ASN:OD1	2.07	1.01
1:B:114:MET:C	1:B:115:LEU:HD23	1.79	1.01
1:D:144:PHE:CD2	1:D:144:PHE:C	2.26	1.01
1:A:115:LEU:HD23	1:A:115:LEU:N	1.21	1.01
1:A:22:TYR:CD1	1:A:333:ALA:HB2	1.94	1.01
1:B:130:VAL:HG13	1:B:213:GLN:NE2	1.75	1.01
1:A:307:MET:HE1	1:B:87:GLY:O	1.60	1.01
1:B:311:VAL:HG13	1:B:334:VAL:CG2	1.90	1.01
1:B:64:ASN:C	1:B:64:ASN:HD22	1.59	1.01
1:C:289:VAL:CG1	1:C:323:LYS:HB2	1.91	1.01
1:A:127:ASP:OD1	1:A:239:PRO:HD3	1.61	1.01
1:B:101:ASN:OD1	1:B:102:TYR:N	1.93	1.01
1:B:285:GLY:O	1:B:286:ILE:HD12	1.58	1.01
1:A:1:ALA:CB	1:B:4:TYR:OH	2.07	1.01
1:A:258:LEU:HD12	1:A:276:THR:CG2	1.86	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:THR:HG22	1:C:39:THR:O	1.58	1.01
1:A:51:ILE:HG23	1:C:304:ASN:ND2	1.76	1.00
1:B:229:ALA:HB2	1:B:259:LEU:HD22	1.39	1.00
1:D:311:VAL:CG1	1:D:334:VAL:CG2	2.18	1.00
1:A:191:TYR:HD2	1:A:191:TYR:C	1.62	1.00
1:A:285:GLY:C	1:A:286:ILE:CD1	2.28	1.00
1:D:294:TYR:CD1	1:D:314:ILE:HD12	1.94	1.00
1:A:204:PRO:HG2	1:A:247:THR:HG22	1.43	1.00
1:D:105:VAL:CG1	1:D:105:VAL:O	2.09	1.00
1:B:306:ASN:OD1	1:C:9:ASN:HB2	1.59	1.00
1:B:338:TYR:O	1:B:339:GLN:HB3	1.62	1.00
1:A:241:THR:CG2	1:A:242:ASN:H	1.73	1.00
1:D:55:LEU:HD12	1:D:90:TYR:HD1	1.23	1.00
1:A:61:TRP:CZ2	1:C:65:PHE:CE1	2.49	1.00
1:B:105:VAL:O	1:B:105:VAL:HG13	1.18	1.00
1:A:294:TYR:HD2	1:A:314:ILE:HD12	0.87	1.00
1:A:211:ALA:HB2	1:A:236:ASN:HB2	1.00	0.99
1:A:129:PHE:CE2	1:A:193:ALA:N	2.29	0.99
1:A:309:THR:HG21	1:A:336:ILE:HB	1.43	0.99
1:C:104:VAL:HG11	1:C:176:GLY:CA	1.91	0.99
1:C:229:ALA:HB1	1:C:259:LEU:CD2	1.92	0.99
1:A:100:ARG:NH2	1:C:71:GLU:OE2	1.94	0.99
1:A:307:MET:HE2	1:B:88:LEU:CD2	1.79	0.99
1:B:294:TYR:CD1	1:B:314:ILE:HD12	1.97	0.99
1:C:277:LYS:HE2	1:C:279:LYS:HD2	1.40	0.99
1:C:224:ASN:O	1:C:263:TYR:CD1	2.14	0.99
1:B:23:PHE:HA	1:B:35:ASN:ND2	1.77	0.99
1:C:338:TYR:HD2	1:C:339:GLN:N	1.56	0.99
1:D:66:GLN:HG3	1:D:78:GLY:HA3	1.42	0.99
1:B:24:SER:H	1:B:35:ASN:ND2	1.60	0.99
1:B:51:ILE:O	1:B:52:ASN:HB3	1.61	0.99
1:D:132:ARG:NH1	1:D:132:ARG:CG	1.99	0.99
1:A:122:THR:HG23	1:A:256:ASP:OD2	1.61	0.99
1:A:24:SER:H	1:A:35:ASN:HD22	1.07	0.99
1:C:144:PHE:HD2	1:C:144:PHE:O	1.44	0.99
1:D:309:THR:HG21	1:D:336:ILE:HB	1.41	0.99
1:D:112:THR:HG23	1:D:230:ASN:OD1	1.63	0.98
1:C:163:ARG:HD2	1:C:168:ARG:O	1.64	0.98
1:D:299:ALA:O	1:D:310:TYR:HB2	1.62	0.98
1:B:302:TYR:O	1:B:303:PHE:C	1.98	0.98
1:C:167:ARG:HH11	1:C:167:ARG:HG3	1.27	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:ILE:N	1:C:286:ILE:CD1	2.09	0.98
1:A:289:VAL:CG1	1:A:323:LYS:HB2	1.94	0.98
1:D:124:TYR:HE2	1:D:238:THR:HG23	1.26	0.98
1:A:125:SER:O	1:A:126:ASP:HB2	1.57	0.98
1:A:211:ALA:HB2	1:A:236:ASN:CB	1.93	0.98
1:A:51:ILE:HD11	1:A:55:LEU:HD21	1.45	0.98
1:C:18:VAL:HG22	1:C:337:VAL:HG22	1.42	0.98
1:A:170:ASN:C	1:A:170:ASN:ND2	2.17	0.98
1:C:307:MET:O	1:C:308:SER:HB3	1.64	0.98
1:A:309:THR:HG22	1:A:336:ILE:HB	1.43	0.98
1:C:104:VAL:CG1	1:C:176:GLY:HA2	1.92	0.98
1:A:90:TYR:O	1:A:93:VAL:CG2	2.11	0.98
1:D:286:ILE:N	1:D:286:ILE:HD12	1.77	0.97
1:A:112:THR:HG23	1:A:230:ASN:OD1	1.61	0.97
1:A:127:ASP:O	1:A:128:PHE:HB2	1.17	0.97
1:A:241:THR:CG2	1:A:242:ASN:N	2.28	0.97
1:B:269:LEU:HG	1:B:270:ARG:N	1.79	0.97
1:C:307:MET:HG3	1:C:308:SER:N	1.75	0.97
1:A:318:ILE:HG21	1:A:322:ASN:HD22	1.29	0.97
1:D:111:TYR:CZ	1:D:188:VAL:CG2	2.48	0.97
1:D:229:ALA:HB1	1:D:259:LEU:HD21	1.43	0.97
1:A:211:ALA:CB	1:A:235:ARG:O	2.13	0.97
1:B:54:ASP:HB3	1:B:91:ALA:HB2	1.42	0.97
1:A:241:THR:HG23	1:A:242:ASN:H	1.27	0.97
1:D:111:TYR:CE2	1:D:188:VAL:CG2	2.48	0.97
1:B:180:TYR:CD2	1:B:181:GLU:N	2.33	0.96
1:A:141:ASN:OD1	1:A:153:PHE:CE1	2.19	0.96
1:A:1:ALA:CB	1:B:4:TYR:HE1	1.75	0.96
1:D:82:ARG:O	1:D:132:ARG:HD2	1.64	0.96
1:D:122:THR:CG2	1:D:256:ASP:OD2	2.13	0.96
1:A:170:ASN:C	1:A:170:ASN:HD22	1.69	0.96
1:A:284:GLU:OE2	1:A:284:GLU:N	1.98	0.96
1:C:104:VAL:HG11	1:C:176:GLY:HA2	0.98	0.96
1:C:51:ILE:CD1	1:C:55:LEU:HD23	1.94	0.96
1:D:13:LEU:HD12	1:D:13:LEU:C	1.84	0.96
1:A:231:TYR:HD2	1:A:231:TYR:C	1.67	0.96
1:A:276:THR:HB	1:A:294:TYR:CE1	1.99	0.96
1:D:51:ILE:HD12	1:D:55:LEU:CD2	1.90	0.96
1:B:127:ASP:O	1:B:128:PHE:HB2	1.63	0.96
1:D:311:VAL:HG13	1:D:334:VAL:HG22	1.48	0.96
1:A:307:MET:HE3	1:B:88:LEU:HD21	0.97	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ASP:HB2	1:C:90:TYR:HE1	1.29	0.96
1:A:180:TYR:HD2	1:A:180:TYR:C	1.68	0.95
1:D:180:TYR:HD2	1:D:181:GLU:N	1.63	0.95
1:D:196:ARG:NH2	1:D:250:PHE:HD1	1.63	0.95
1:D:229:ALA:HB1	1:D:259:LEU:CD2	1.95	0.95
1:A:130:VAL:CG1	1:A:213:GLN:NE2	2.29	0.95
1:A:141:ASN:CB	1:A:153:PHE:CE1	2.50	0.95
1:B:18:VAL:HG11	1:B:40:TYR:HE1	1.32	0.95
1:D:337:VAL:HG12	1:D:337:VAL:O	1.64	0.95
1:A:226:TYR:O	1:A:227:LEU:HD23	1.67	0.95
1:A:318:ILE:H	1:A:318:ILE:HD13	1.31	0.95
1:A:63:TYR:CD1	1:A:80:LYS:O	2.20	0.95
1:B:58:TYR:HD2	1:B:58:TYR:H	1.11	0.95
1:C:222:ALA:O	1:C:223:ASN:HB2	1.63	0.95
1:A:115:LEU:N	1:A:115:LEU:CD2	1.70	0.95
1:A:104:VAL:CG1	1:A:156:GLN:CD	2.35	0.94
1:A:231:TYR:CD2	1:A:231:TYR:C	2.38	0.94
1:D:96:PHE:HD2	1:D:97:ASP:N	1.65	0.94
1:A:24:SER:OG	1:A:331:THR:OG1	1.83	0.94
1:B:129:PHE:HE2	1:B:193:ALA:N	1.66	0.94
1:D:196:ARG:HH21	1:D:250:PHE:HD1	1.07	0.94
1:B:64:ASN:C	1:B:64:ASN:ND2	2.17	0.94
1:D:277:LYS:HB2	1:D:293:ASN:OD1	1.68	0.94
1:A:167:ARG:HH11	1:A:167:ARG:HG3	1.31	0.94
1:C:258:LEU:O	1:C:259:LEU:HD23	1.67	0.94
1:D:171:GLY:HA3	1:D:195:ASP:HB2	1.50	0.94
1:C:240:ILE:HD11	1:C:251:ALA:N	1.83	0.94
1:D:309:THR:CG2	1:D:336:ILE:CB	2.46	0.94
1:C:167:ARG:O	1:C:168:ARG:HD3	1.68	0.93
1:B:310:TYR:O	1:B:310:TYR:HD1	1.50	0.93
1:C:139:TYR:O	1:C:154:ALA:HB1	1.67	0.93
1:D:100:ARG:HH11	1:D:100:ARG:CG	1.82	0.93
1:D:83:LEU:HD21	1:D:102:TYR:CE2	2.04	0.93
1:A:104:VAL:HG13	1:A:156:GLN:CD	1.88	0.93
1:B:112:THR:HG21	1:B:230:ASN:CB	1.99	0.93
1:B:303:PHE:HB3	1:C:51:ILE:HG21	1.49	0.93
1:C:240:ILE:CD1	1:C:251:ALA:N	2.32	0.93
1:A:61:TRP:CZ2	1:C:65:PHE:HD1	1.79	0.93
1:D:318:ILE:CG2	1:D:319:ASP:N	2.29	0.93
1:D:60:GLN:HB3	1:D:85:PHE:CE2	2.03	0.93
1:B:241:THR:CG2	1:B:242:ASN:N	2.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:LYS:HE3	1:C:160:LYS:HA	1.46	0.93
1:C:169:SER:O	1:C:170:ASN:HB3	1.66	0.93
1:C:18:VAL:HG11	1:C:40:TYR:CZ	2.03	0.93
1:C:21:HIS:CD2	1:C:23:PHE:CZ	2.56	0.93
1:B:294:TYR:CE1	1:B:314:ILE:HD12	2.03	0.93
1:D:105:VAL:HG13	1:D:105:VAL:O	1.69	0.93
1:D:309:THR:HG22	1:D:336:ILE:CA	1.98	0.93
1:C:23:PHE:HA	1:C:35:ASN:HD22	1.30	0.93
1:A:309:THR:HG22	1:A:336:ILE:CB	1.97	0.93
1:D:314:ILE:C	1:D:315:ILE:HD12	1.88	0.93
1:D:20:LEU:CD1	1:D:21:HIS:H	1.81	0.92
1:C:241:THR:HG22	1:C:242:ASN:N	1.85	0.92
1:A:129:PHE:HE2	1:A:193:ALA:H	1.03	0.92
1:A:307:MET:HE3	1:B:88:LEU:CD2	1.73	0.92
1:B:180:TYR:HD2	1:B:181:GLU:N	1.67	0.92
1:A:180:TYR:HD2	1:A:181:GLU:N	1.67	0.92
1:A:22:TYR:HD1	1:A:333:ALA:HB2	1.34	0.92
1:B:15:GLY:N	1:B:340:PHE:CE2	2.38	0.92
1:B:241:THR:CG2	1:B:242:ASN:H	1.81	0.92
1:C:223:ASN:O	1:C:224:ASN:HB2	1.66	0.92
1:C:283:VAL:HG23	1:C:287:GLY:O	1.70	0.92
1:D:111:TYR:CZ	1:D:188:VAL:HG21	2.03	0.92
1:C:10:LYS:HG3	1:C:10:LYS:O	1.67	0.92
1:C:297:VAL:CG1	1:C:297:VAL:O	2.15	0.92
1:B:110:GLY:O	1:B:112:THR:N	2.02	0.92
1:D:24:SER:H	1:D:35:ASN:HD22	0.95	0.92
1:D:258:LEU:O	1:D:259:LEU:HD23	1.70	0.92
1:D:118:PHE:CD2	1:D:314:ILE:HG12	2.05	0.92
1:A:18:VAL:HB	1:A:40:TYR:CE1	2.04	0.91
1:B:20:LEU:HD12	1:B:21:HIS:H	1.34	0.91
1:B:309:THR:HG22	1:B:336:ILE:HA	1.51	0.91
1:C:204:PRO:CG	1:C:247:THR:CG2	2.46	0.91
1:C:60:GLN:HG2	1:C:61:TRP:N	1.85	0.91
1:D:104:VAL:HG12	1:D:156:GLN:OE1	1.69	0.91
1:A:165:THR:HG23	1:A:166:ALA:N	1.84	0.91
1:B:4:TYR:CE2	1:B:6:LYS:HB2	2.04	0.91
1:D:279:LYS:HZ3	1:D:279:LYS:HB2	1.12	0.91
1:A:268:GLY:O	1:A:301:TYR:HD2	1.53	0.91
1:A:22:TYR:HE2	1:A:38:MET:CE	1.83	0.91
1:B:112:THR:CG2	1:B:230:ASN:HB2	2.00	0.91
1:A:61:TRP:O	1:A:61:TRP:CE3	2.23	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:PHE:O	1:C:144:PHE:CD2	2.23	0.91
1:D:60:GLN:HG2	1:D:85:PHE:HE2	1.36	0.91
1:A:289:VAL:HG11	1:A:323:LYS:HB2	1.49	0.91
1:A:337:VAL:HG12	1:A:337:VAL:O	1.00	0.91
1:B:114:MET:HE1	1:B:226:TYR:HE1	1.27	0.91
1:A:85:PHE:HD2	1:A:101:ASN:HB2	1.36	0.91
1:A:322:ASN:C	1:A:322:ASN:OD1	2.06	0.91
1:C:274:ALA:HB3	1:C:296:GLU:HB3	1.53	0.91
1:D:307:MET:HG3	1:D:308:SER:H	1.36	0.91
1:D:318:ILE:HG23	1:D:319:ASP:H	1.34	0.91
1:A:1:ALA:HB3	1:B:4:TYR:CZ	2.05	0.90
1:D:223:ASN:O	1:D:224:ASN:HB2	1.68	0.90
1:A:51:ILE:CG2	1:C:304:ASN:ND2	2.33	0.90
1:A:100:ARG:HG2	1:A:134:GLY:HA2	1.51	0.90
1:B:241:THR:HG22	1:B:242:ASN:H	1.30	0.90
1:B:5:ASN:C	1:B:6:LYS:HG2	1.91	0.90
1:D:226:TYR:C	1:D:227:LEU:HD23	1.89	0.90
1:D:279:LYS:HZ3	1:D:279:LYS:CB	1.77	0.90
1:C:101:ASN:OD1	1:C:102:TYR:N	2.04	0.90
1:D:167:ARG:HG3	1:D:167:ARG:O	1.72	0.90
1:D:46:LYS:HD3	1:D:60:GLN:HE22	1.35	0.90
1:A:187:ILE:HG23	1:A:187:ILE:O	1.68	0.90
1:B:151:LEU:O	1:B:151:LEU:CG	2.17	0.90
1:B:58:TYR:CD2	1:B:58:TYR:O	2.25	0.90
1:C:51:ILE:HD12	1:C:55:LEU:HD23	1.49	0.90
1:D:96:PHE:C	1:D:96:PHE:CD2	2.45	0.90
1:B:14:TYR:C	1:B:340:PHE:HE2	1.75	0.90
1:B:277:LYS:CD	1:B:293:ASN:ND2	2.34	0.90
1:C:54:ASP:HB2	1:C:90:TYR:CE1	2.06	0.90
1:A:226:TYR:HE2	1:A:228:ALA:HB2	1.37	0.90
1:A:275:TYR:CD2	1:A:276:THR:N	2.40	0.90
1:A:311:VAL:HG12	1:A:311:VAL:O	1.71	0.90
1:B:269:LEU:HG	1:B:271:PRO:HD3	1.51	0.90
1:C:21:HIS:HD2	1:C:23:PHE:CZ	1.89	0.90
1:A:257:VAL:O	1:A:258:LEU:HD13	1.72	0.90
1:A:4:TYR:CD1	1:C:1:ALA:CB	2.55	0.90
1:C:18:VAL:HG11	1:C:40:TYR:CE1	2.07	0.90
1:D:55:LEU:CD1	1:D:90:TYR:HD1	1.84	0.89
1:A:153:PHE:HD1	1:A:153:PHE:H	1.17	0.89
1:C:18:VAL:CG2	1:C:337:VAL:HG22	2.03	0.89
1:A:115:LEU:HG	1:A:119:GLY:HA3	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:VAL:HG13	1:B:213:GLN:HE22	1.38	0.89
1:B:5:ASN:O	1:B:6:LYS:HG2	1.72	0.89
1:A:313:TYR:CG	1:A:332:VAL:HG22	2.08	0.89
1:C:223:ASN:HB3	1:C:225:ILE:HD11	1.53	0.89
1:C:269:LEU:HD11	1:C:270:ARG:H	1.36	0.89
1:B:90:TYR:HB3	1:B:93:VAL:HG23	1.52	0.88
1:A:102:TYR:O	1:A:103:GLY:O	1.89	0.88
1:C:42:ARG:HH12	1:C:82:ARG:NH2	1.71	0.88
1:D:24:SER:HB2	1:D:34:GLY:O	1.73	0.88
1:A:258:LEU:HD11	1:A:276:THR:HG23	1.56	0.88
1:A:22:TYR:HE2	1:A:38:MET:HE2	1.38	0.88
1:B:141:ASN:ND2	1:B:145:PHE:CD1	2.41	0.88
1:C:274:ALA:O	1:C:296:GLU:N	2.07	0.88
1:D:144:PHE:HB2	1:D:151:LEU:HD23	1.54	0.88
1:A:293:ASN:ND2	1:A:317:GLN:HB3	1.87	0.88
1:B:161:ASN:HB2	1:B:170:ASN:OD1	1.74	0.88
1:D:215:ALA:O	1:D:216:THR:CG2	2.21	0.88
1:B:151:LEU:O	1:B:151:LEU:HG	1.72	0.88
1:C:172:ASP:C	1:C:194:ALA:HB1	1.94	0.88
1:D:231:TYR:CD2	1:D:232:GLY:N	2.41	0.88
1:D:124:TYR:HE2	1:D:238:THR:CG2	1.87	0.88
1:A:129:PHE:CE2	1:A:192:GLY:HA3	2.09	0.88
1:A:51:ILE:HG21	1:C:303:PHE:HB3	1.56	0.88
1:B:151:LEU:O	1:B:151:LEU:CD1	2.20	0.88
1:D:187:ILE:CG1	1:D:218:LEU:HD21	2.04	0.87
1:A:187:ILE:O	1:A:187:ILE:HG22	1.74	0.87
1:A:271:PRO:HA	1:A:299:ALA:HB2	0.90	0.87
1:A:130:VAL:HG12	1:A:213:GLN:NE2	1.90	0.87
1:B:18:VAL:HG11	1:B:40:TYR:CE1	2.08	0.87
1:C:286:ILE:H	1:C:286:ILE:HD13	1.38	0.87
1:B:23:PHE:CA	1:B:35:ASN:HD21	1.87	0.87
1:B:125:SER:O	1:B:126:ASP:CB	2.19	0.87
1:C:141:ASN:HB3	1:C:153:PHE:CE1	2.10	0.87
1:A:336:ILE:HG13	1:A:337:VAL:N	1.90	0.87
1:B:111:TYR:CZ	1:B:188:VAL:HG21	2.10	0.87
1:B:98:TYR:HD2	1:B:98:TYR:C	1.77	0.87
1:A:281:LYS:O	1:A:282:ASP:HB2	1.74	0.86
1:C:45:PHE:C	1:C:45:PHE:HD1	1.77	0.86
1:D:6:LYS:O	1:D:7:ASP:HB2	1.74	0.86
1:B:71:GLU:HG3	1:C:100:ARG:NH2	1.88	0.86
1:C:310:TYR:HD1	1:C:310:TYR:O	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:ILE:HG22	1:C:319:ASP:H	1.39	0.86
1:A:276:THR:CB	1:A:294:TYR:HE1	1.88	0.86
1:A:275:TYR:C	1:A:276:THR:HG1	1.79	0.86
1:C:174:VAL:CG1	1:C:175:GLY:H	1.84	0.86
1:A:4:TYR:CD1	1:C:1:ALA:HB1	2.10	0.86
1:D:267:PHE:N	1:D:267:PHE:HD1	1.70	0.86
1:D:40:TYR:HE2	1:D:42:ARG:HH22	1.20	0.86
1:A:132:ARG:NH1	1:A:132:ARG:HG3	1.87	0.86
1:B:162:GLU:O	1:B:163:ARG:O	1.94	0.86
1:A:20:LEU:HD13	1:A:335:GLY:HA3	1.55	0.86
1:B:1:ALA:O	1:B:12:ASP:OD1	1.93	0.86
1:B:155:VAL:HG23	1:B:156:GLN:N	1.91	0.86
1:D:215:ALA:C	1:D:216:THR:HG23	1.95	0.86
1:A:326:VAL:O	1:A:326:VAL:HG12	1.73	0.86
1:C:144:PHE:O	1:C:145:PHE:HB2	1.76	0.86
1:C:229:ALA:HB2	1:C:259:LEU:HD22	1.58	0.86
1:B:98:TYR:HD2	1:B:99:GLY:N	1.73	0.86
1:A:114:MET:C	1:A:115:LEU:O	2.11	0.86
1:A:231:TYR:HD2	1:A:232:GLY:H	1.20	0.86
1:C:129:PHE:HE2	1:C:193:ALA:N	1.73	0.86
1:B:98:TYR:CD2	1:B:99:GLY:N	2.44	0.86
1:C:139:TYR:O	1:C:154:ALA:CB	2.23	0.86
1:B:112:THR:CG2	1:B:230:ASN:OD1	2.24	0.85
1:D:83:LEU:HD21	1:D:102:TYR:HE2	1.37	0.85
1:A:172:ASP:O	1:A:194:ALA:CA	2.23	0.85
1:C:229:ALA:HB2	1:C:259:LEU:CD2	2.05	0.85
1:A:237:ALA:O	1:A:238:THR:C	2.11	0.85
1:A:51:ILE:HD12	1:A:55:LEU:HD22	1.55	0.85
1:D:180:TYR:CD2	1:D:181:GLU:N	2.44	0.85
1:D:21:HIS:CD2	1:D:23:PHE:CE1	2.63	0.85
1:A:204:PRO:HG2	1:A:247:THR:CG2	2.06	0.85
1:A:307:MET:CE	1:B:88:LEU:HD23	2.06	0.85
1:B:274:ALA:HB3	1:B:296:GLU:OE1	1.76	0.85
1:D:111:TYR:CE2	1:D:188:VAL:HG23	2.10	0.85
1:B:167:ARG:O	1:B:167:ARG:HG3	1.73	0.85
1:B:87:GLY:C	1:B:88:LEU:CD2	2.44	0.85
1:A:100:ARG:CG	1:A:134:GLY:HA2	2.06	0.85
1:B:167:ARG:CG	1:B:167:ARG:HH11	1.89	0.85
1:A:180:TYR:CD2	1:A:180:TYR:C	2.46	0.85
1:A:51:ILE:HD13	1:C:303:PHE:HB3	1.59	0.85
1:B:269:LEU:CD2	1:B:271:PRO:HD3	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:MET:C	1:D:115:LEU:HD23	1.97	0.85
1:D:141:ASN:OD1	1:D:145:PHE:N	2.08	0.85
1:A:241:THR:HG22	1:A:242:ASN:N	1.89	0.85
1:B:151:LEU:O	1:B:151:LEU:HD12	1.75	0.85
1:D:180:TYR:HD2	1:D:180:TYR:C	1.80	0.85
1:C:85:PHE:HD2	1:C:101:ASN:HB2	1.42	0.84
1:A:303:PHE:HB2	1:A:307:MET:HB3	1.58	0.84
1:A:57:GLY:HA2	1:A:88:LEU:HD23	1.59	0.84
1:B:123:ALA:HA	1:B:130:VAL:HG23	1.58	0.84
1:C:286:ILE:H	1:C:286:ILE:HD12	1.13	0.84
1:B:101:ASN:CG	1:B:102:TYR:H	1.80	0.84
1:B:310:TYR:O	1:B:310:TYR:CD1	2.30	0.84
1:C:124:TYR:HD2	1:C:124:TYR:H	1.24	0.84
1:B:296:GLU:HB2	1:B:314:ILE:HD13	1.57	0.84
1:A:86:ALA:HB3	1:C:336:ILE:HG12	1.59	0.84
1:A:61:TRP:CD2	1:A:61:TRP:O	2.30	0.84
1:B:155:VAL:CG2	1:B:156:GLN:N	2.37	0.84
1:B:340:PHE:HE1	1:C:45:PHE:CD2	1.93	0.84
1:D:279:LYS:HE3	1:D:281:LYS:NZ	1.93	0.84
1:D:309:THR:HG22	1:D:336:ILE:CB	2.07	0.84
1:A:139:TYR:O	1:A:154:ALA:HB1	1.78	0.84
1:C:179:SER:HA	1:C:188:VAL:CG1	2.04	0.84
1:D:215:ALA:O	1:D:216:THR:HG23	1.78	0.84
1:D:111:TYR:CE2	1:D:219:LYS:HG2	2.13	0.84
1:A:22:TYR:CE2	1:A:38:MET:CE	2.60	0.84
1:A:336:ILE:HG13	1:A:337:VAL:H	1.40	0.84
1:D:170:ASN:C	1:D:170:ASN:HD22	1.78	0.84
1:C:204:PRO:CG	1:C:247:THR:HG21	2.07	0.84
1:D:112:THR:CG2	1:D:230:ASN:OD1	2.25	0.84
1:D:311:VAL:HG13	1:D:334:VAL:HG23	0.86	0.84
1:D:90:TYR:O	1:D:93:VAL:HG23	1.77	0.84
1:D:244:PHE:O	1:D:246:ASN:N	2.10	0.83
1:C:70:SER:OG	1:C:72:GLY:N	2.10	0.83
1:D:96:PHE:HD2	1:D:96:PHE:C	1.79	0.83
1:C:310:TYR:CD1	1:C:310:TYR:O	2.30	0.83
1:D:299:ALA:O	1:D:310:TYR:CB	2.26	0.83
1:C:204:PRO:CG	1:C:247:THR:HG22	2.08	0.83
1:A:58:TYR:HA	1:C:338:TYR:CD1	2.13	0.83
1:A:303:PHE:HE2	1:B:88:LEU:CD1	1.90	0.83
1:D:141:ASN:ND2	1:D:142:SER:H	1.75	0.83
1:D:82:ARG:O	1:D:132:ARG:CD	2.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:VAL:HG13	1:A:175:GLY:N	1.92	0.83
1:A:191:TYR:HE2	1:A:192:GLY:O	1.59	0.83
1:B:111:TYR:CZ	1:B:188:VAL:CG2	2.61	0.83
1:B:205:LEU:HD21	1:B:247:THR:HG21	1.61	0.83
1:A:289:VAL:HG21	1:A:324:LEU:HG	1.60	0.83
1:D:334:VAL:O	1:D:334:VAL:HG12	1.77	0.83
1:A:18:VAL:HG13	1:A:337:VAL:HG23	1.59	0.83
1:B:216:THR:O	1:B:230:ASN:ND2	2.10	0.83
1:C:18:VAL:HG22	1:C:337:VAL:CG2	2.09	0.83
1:D:267:PHE:N	1:D:267:PHE:CD1	2.46	0.83
1:D:60:GLN:CG	1:D:85:PHE:HE2	1.91	0.83
1:C:100:ARG:HG3	1:C:100:ARG:HH11	1.41	0.82
1:C:197:THR:O	1:C:200:GLN:HB2	1.79	0.82
1:A:114:MET:CE	1:A:226:TYR:CD1	2.45	0.82
1:A:114:MET:HE1	1:A:226:TYR:HE1	1.42	0.82
1:A:39:THR:O	1:A:39:THR:HG22	1.78	0.82
1:A:1:ALA:CB	1:B:4:TYR:CZ	2.61	0.82
1:A:51:ILE:HG13	1:A:55:LEU:CD2	2.04	0.82
1:A:51:ILE:O	1:A:52:ASN:HB3	1.78	0.82
1:B:4:TYR:HE2	1:B:6:LYS:HB2	1.43	0.82
1:C:220:TYR:CE1	1:C:222:ALA:HB3	2.15	0.82
1:A:241:THR:O	1:A:324:LEU:HB3	1.79	0.82
1:B:130:VAL:CG1	1:B:213:GLN:CD	2.48	0.82
1:C:144:PHE:HB3	1:C:148:VAL:HG23	1.62	0.82
1:C:141:ASN:O	1:C:152:ASN:HB3	1.79	0.82
1:A:303:PHE:CE2	1:B:88:LEU:HD13	2.15	0.82
1:C:173:GLY:HA2	1:C:194:ALA:HB2	1.62	0.82
1:C:291:LEU:O	1:C:292:VAL:CG2	2.27	0.82
1:D:208:GLY:HA3	1:D:236:ASN:ND2	1.95	0.82
1:D:55:LEU:HD12	1:D:90:TYR:CD1	2.14	0.82
1:A:1:ALA:HB3	1:B:4:TYR:HE1	1.31	0.82
1:A:315:ILE:HA	1:A:330:ASP:OD1	1.80	0.82
1:B:307:MET:HG3	1:B:308:SER:N	1.94	0.82
1:D:172:ASP:O	1:D:194:ALA:HB1	1.79	0.82
1:B:20:LEU:HD12	1:B:21:HIS:N	1.95	0.82
1:C:173:GLY:CA	1:C:194:ALA:HB2	2.10	0.82
1:D:104:VAL:CG1	1:D:156:GLN:CB	2.58	0.82
1:A:111:TYR:CD2	1:A:219:LYS:HG2	2.13	0.82
1:A:141:ASN:CG	1:A:153:PHE:HE1	1.82	0.82
1:A:313:TYR:CE1	1:A:332:VAL:HG23	2.15	0.82
1:B:183:GLU:HG3	1:B:183:GLU:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:THR:HG1	1:D:247:THR:HG1	0.95	0.81
1:D:294:TYR:CD1	1:D:314:ILE:CD1	2.62	0.81
1:A:172:ASP:H	1:A:195:ASP:HB2	1.43	0.81
1:A:1:ALA:HB1	1:B:4:TYR:OH	1.79	0.81
1:C:153:PHE:HD1	1:C:153:PHE:H	1.28	0.81
1:C:257:VAL:O	1:C:258:LEU:HD13	1.80	0.81
1:B:192:GLY:O	1:B:193:ALA:HB2	1.79	0.81
1:A:229:ALA:HB2	1:A:259:LEU:HD22	1.60	0.81
1:B:205:LEU:CD1	1:B:247:THR:HG22	2.08	0.81
1:C:234:THR:HB	1:C:237:ALA:HB3	1.61	0.81
1:A:284:GLU:O	1:A:286:ILE:HD13	1.79	0.81
1:B:274:ALA:CB	1:B:296:GLU:OE1	2.27	0.81
1:C:326:VAL:O	1:C:326:VAL:HG12	1.81	0.81
1:A:40:TYR:HD1	1:A:40:TYR:H	1.25	0.81
1:D:5:ASN:O	1:D:6:LYS:HD3	1.81	0.81
1:A:24:SER:H	1:A:35:ASN:ND2	1.77	0.81
1:D:111:TYR:OH	1:D:188:VAL:HG22	1.81	0.81
1:D:5:ASN:O	1:D:6:LYS:CD	2.29	0.81
1:B:255:GLN:OE1	1:B:281:LYS:CE	2.29	0.81
1:C:289:VAL:HG11	1:C:323:LYS:HB2	1.63	0.80
1:C:90:TYR:HD2	1:C:93:VAL:HG21	1.46	0.80
1:B:113:ASP:O	1:B:114:MET:CG	2.29	0.80
1:B:58:TYR:CD2	1:B:58:TYR:N	2.42	0.80
1:A:58:TYR:HA	1:C:338:TYR:HD1	1.44	0.80
1:C:90:TYR:O	1:C:92:ASP:N	2.14	0.80
1:B:267:PHE:H	1:B:267:PHE:HD1	1.29	0.80
1:B:30:ASN:CG	1:B:30:ASN:O	2.17	0.80
1:A:274:ALA:HB3	1:A:296:GLU:OE1	1.80	0.80
1:A:275:TYR:HD2	1:A:276:THR:N	1.78	0.80
1:C:338:TYR:C	1:C:338:TYR:CD2	2.53	0.80
1:A:65:PHE:CD1	1:B:61:TRP:HZ2	2.00	0.80
1:C:70:SER:HG	1:C:72:GLY:H	1.30	0.80
1:D:294:TYR:CE1	1:D:314:ILE:CD1	2.64	0.80
1:A:141:ASN:HB3	1:A:153:PHE:CE1	2.16	0.80
1:B:300:THR:HG21	1:B:302:TYR:CE1	2.16	0.80
1:C:182:TYR:HD1	1:C:183:GLU:N	1.80	0.80
1:C:289:VAL:HG13	1:C:323:LYS:HB2	1.61	0.80
1:A:70:SER:OG	1:A:71:GLU:N	2.11	0.80
1:B:222:ALA:O	1:B:225:ILE:HG13	1.80	0.80
1:C:18:VAL:CG1	1:C:40:TYR:CE1	2.64	0.80
1:B:229:ALA:HB1	1:B:258:LEU:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLY:O	1:A:301:TYR:CD2	2.34	0.80
1:C:172:ASP:C	1:C:194:ALA:CB	2.48	0.80
1:A:191:TYR:CD2	1:A:191:TYR:C	2.40	0.79
1:A:82:ARG:NH1	1:A:82:ARG:HG2	1.97	0.79
1:B:21:HIS:HD2	1:B:23:PHE:CZ	1.99	0.79
1:B:5:ASN:OD1	1:B:5:ASN:C	2.18	0.79
1:B:66:GLN:HG3	1:B:78:GLY:HA3	1.63	0.79
1:C:223:ASN:CB	1:C:225:ILE:CD1	2.60	0.79
1:A:129:PHE:CE2	1:A:192:GLY:CA	2.66	0.79
1:D:29:GLU:CG	1:D:30:ASN:H	1.96	0.79
1:D:118:PHE:HD2	1:D:314:ILE:HG12	1.43	0.79
1:A:114:MET:CE	1:A:226:TYR:CZ	2.50	0.79
1:D:338:TYR:O	1:D:339:GLN:HB3	1.82	0.79
1:D:60:GLN:HG2	1:D:85:PHE:CE2	2.18	0.79
1:A:161:ASN:O	1:A:169:SER:HB3	1.80	0.79
1:A:85:PHE:CD2	1:A:101:ASN:HB2	2.17	0.79
1:B:258:LEU:O	1:B:259:LEU:CD2	2.24	0.79
1:D:24:SER:H	1:D:35:ASN:ND2	1.78	0.79
1:A:114:MET:H	1:A:115:LEU:HD23	1.45	0.79
1:A:259:LEU:N	1:A:259:LEU:HD23	1.83	0.79
1:A:262:GLN:HG2	1:A:272:SER:HB2	1.64	0.79
1:C:274:ALA:CB	1:C:296:GLU:OE1	2.31	0.79
1:A:112:THR:CG2	1:A:230:ASN:OD1	2.29	0.79
1:B:158:LEU:HD12	1:B:159:GLY:N	1.98	0.79
1:B:226:TYR:O	1:B:227:LEU:HD23	1.82	0.79
1:B:231:TYR:CD1	1:B:232:GLY:N	2.50	0.79
1:B:24:SER:N	1:B:35:ASN:ND2	2.30	0.79
1:D:51:ILE:HD12	1:D:55:LEU:CG	2.12	0.79
1:A:122:THR:CG2	1:A:256:ASP:OD2	2.30	0.78
1:A:71:GLU:CG	1:B:100:ARG:NH2	2.46	0.78
1:D:267:PHE:H	1:D:267:PHE:HD1	1.31	0.78
1:D:124:TYR:CE2	1:D:238:THR:HG23	2.15	0.78
1:D:318:ILE:HG22	1:D:319:ASP:N	1.99	0.78
1:A:125:SER:O	1:A:126:ASP:CB	2.31	0.78
1:A:303:PHE:CD2	1:A:307:MET:HG2	2.13	0.78
1:A:86:ALA:HB1	1:C:336:ILE:CG1	2.13	0.78
1:B:240:ILE:CG2	1:B:291:LEU:CD2	2.62	0.78
1:B:258:LEU:C	1:B:259:LEU:HD23	2.04	0.78
1:A:102:TYR:CD1	1:A:106:TYR:CD2	2.72	0.78
1:D:100:ARG:HH11	1:D:100:ARG:HG3	1.46	0.78
1:D:279:LYS:HZ2	1:D:279:LYS:HB2	0.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:THR:HG22	1:A:166:ALA:N	1.93	0.78
1:B:221:ASP:O	1:B:222:ALA:CB	2.32	0.78
1:A:69:ASN:HD21	1:A:77:THR:CB	1.90	0.77
1:B:300:THR:CG2	1:B:302:TYR:CE1	2.67	0.77
1:B:90:TYR:O	1:B:92:ASP:N	2.17	0.77
1:C:318:ILE:HG13	1:C:326:VAL:HG11	1.66	0.77
1:C:331:THR:HG22	1:C:332:VAL:N	1.96	0.77
1:A:191:TYR:CE2	1:A:192:GLY:O	2.37	0.77
1:A:267:PHE:CZ	1:A:269:LEU:HD12	2.18	0.77
1:B:269:LEU:HG	1:B:270:ARG:H	1.48	0.77
1:C:255:GLN:C	1:C:256:ASP:OD1	2.22	0.77
1:A:141:ASN:HB3	1:A:153:PHE:CD1	2.20	0.77
1:A:285:GLY:O	1:A:286:ILE:CD1	2.17	0.77
1:A:59:GLY:N	1:C:338:TYR:CD1	2.53	0.77
1:D:109:LEU:O	1:D:110:GLY:C	2.23	0.77
1:D:231:TYR:CD2	1:D:231:TYR:C	2.56	0.77
1:D:313:TYR:CD1	1:D:332:VAL:HG22	2.19	0.77
1:B:130:VAL:HG11	1:B:213:GLN:NE2	1.99	0.77
1:C:179:SER:CB	1:C:188:VAL:CG1	2.63	0.77
1:A:51:ILE:CG1	1:A:55:LEU:CD2	2.46	0.77
1:D:265:PHE:HB2	1:D:269:LEU:O	1.85	0.77
1:D:51:ILE:CB	1:D:55:LEU:HD23	2.14	0.77
1:A:121:ASP:OD1	1:A:294:TYR:OH	2.03	0.77
1:B:263:TYR:O	1:B:270:ARG:HA	1.84	0.77
1:A:174:VAL:CG1	1:A:175:GLY:N	2.46	0.77
1:B:238:THR:O	1:B:238:THR:HG22	1.84	0.77
1:D:121:ASP:O	1:D:123:ALA:N	2.18	0.77
1:A:114:MET:O	1:A:115:LEU:C	2.21	0.76
1:A:20:LEU:CD1	1:A:335:GLY:HA3	2.13	0.76
1:D:104:VAL:HG11	1:D:156:GLN:HB3	1.66	0.76
1:D:180:TYR:C	1:D:180:TYR:CD2	2.59	0.76
1:C:263:TYR:O	1:C:270:ARG:HA	1.86	0.76
1:A:326:VAL:O	1:A:326:VAL:CG1	2.33	0.76
1:C:229:ALA:CB	1:C:259:LEU:HD23	2.14	0.76
1:D:226:TYR:HE2	1:D:228:ALA:HB2	1.51	0.76
1:B:16:LYS:HB3	1:B:339:GLN:CB	2.16	0.76
1:B:242:ASN:HB3	1:B:247:THR:HB	1.66	0.76
1:B:229:ALA:HB2	1:B:259:LEU:CD2	2.01	0.76
1:C:48:GLU:O	1:C:48:GLU:HG2	1.81	0.76
1:D:128:PHE:O	1:D:133:VAL:HG21	1.86	0.76
1:D:24:SER:N	1:D:35:ASN:HD22	1.79	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:TYR:CE2	1:A:314:ILE:HD11	2.20	0.76
1:A:58:TYR:CA	1:C:338:TYR:HD1	1.97	0.76
1:B:240:ILE:CG2	1:B:291:LEU:HD22	2.15	0.76
1:A:294:TYR:CE2	1:A:314:ILE:CD1	2.69	0.76
1:C:179:SER:CB	1:C:188:VAL:HG12	2.14	0.76
1:D:273:ILE:HD11	1:D:297:VAL:CG2	2.16	0.76
1:A:88:LEU:HD11	1:C:303:PHE:HE2	1.50	0.76
1:B:307:MET:HG3	1:B:308:SER:H	1.50	0.76
1:D:271:PRO:HA	1:D:299:ALA:CB	2.15	0.76
1:A:307:MET:HE1	1:B:88:LEU:CD2	2.12	0.76
1:A:242:ASN:O	1:A:244:PHE:N	2.18	0.75
1:B:114:MET:HE2	1:B:226:TYR:CE1	2.21	0.75
1:D:144:PHE:HB2	1:D:151:LEU:CD2	2.16	0.75
1:D:315:ILE:H	1:D:315:ILE:HD12	1.48	0.75
1:A:307:MET:CE	1:B:87:GLY:O	2.33	0.75
1:B:129:PHE:HE2	1:B:193:ALA:H	1.32	0.75
1:B:221:ASP:O	1:B:222:ALA:HB2	1.86	0.75
1:B:339:GLN:HG3	1:B:339:GLN:O	1.85	0.75
1:C:85:PHE:CE2	1:C:101:ASN:ND2	2.54	0.75
1:C:314:ILE:HG22	1:C:314:ILE:O	1.85	0.75
1:B:4:TYR:C	1:B:4:TYR:HD2	1.89	0.75
1:D:236:ASN:OD1	1:D:252:ASN:HA	1.86	0.75
1:B:185:PHE:CE2	1:B:220:TYR:CE1	2.75	0.75
1:B:236:ASN:OD1	1:B:252:ASN:HA	1.85	0.75
1:C:241:THR:CG2	1:C:242:ASN:H	1.99	0.75
1:A:167:ARG:NH1	1:A:167:ARG:CG	2.41	0.75
1:A:167:ARG:HG2	1:A:167:ARG:HH11	1.49	0.75
1:A:22:TYR:CE1	1:A:333:ALA:HB2	2.21	0.75
1:C:240:ILE:HD11	1:C:250:PHE:C	2.06	0.75
1:C:274:ALA:HB3	1:C:296:GLU:OE1	1.85	0.75
1:A:318:ILE:N	1:A:318:ILE:CD1	2.42	0.75
1:A:104:VAL:HG12	1:A:156:GLN:OE1	1.84	0.75
1:A:167:ARG:HG2	1:A:167:ARG:O	1.87	0.75
1:A:129:PHE:HD2	1:A:192:GLY:HA3	1.49	0.74
1:B:269:LEU:CG	1:B:271:PRO:HD3	2.16	0.74
1:B:65:PHE:CD2	1:C:61:TRP:CZ2	2.74	0.74
1:B:72:GLY:O	1:B:74:ASP:N	2.20	0.74
1:A:86:ALA:CB	1:C:336:ILE:CG1	2.64	0.74
1:D:303:PHE:HB2	1:D:307:MET:HB3	1.69	0.74
1:A:61:TRP:CZ2	1:A:63:TYR:HB2	2.21	0.74
1:B:296:GLU:HB2	1:B:314:ILE:CD1	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ALA:O	1:C:225:ILE:HD12	1.87	0.74
1:A:258:LEU:HD11	1:A:276:THR:CG2	2.10	0.74
1:B:124:TYR:O	1:B:131:GLY:HA3	1.87	0.74
1:B:23:PHE:CA	1:B:35:ASN:ND2	2.45	0.74
1:C:182:TYR:CD1	1:C:182:TYR:C	2.57	0.74
1:D:29:GLU:HG3	1:D:30:ASN:CA	2.18	0.74
1:C:51:ILE:HD12	1:C:55:LEU:CD2	2.17	0.74
1:D:205:LEU:HG	1:D:247:THR:HG22	1.70	0.74
1:B:167:ARG:NH1	1:B:167:ARG:HG3	1.97	0.74
1:B:338:TYR:O	1:B:339:GLN:CB	2.33	0.74
1:C:223:ASN:HB2	1:C:225:ILE:CD1	2.18	0.74
1:C:203:GLN:HB3	1:C:248:SER:O	1.88	0.74
1:A:61:TRP:HZ2	1:C:65:PHE:CE1	1.99	0.74
1:C:174:VAL:HG13	1:C:175:GLY:H	1.53	0.74
1:D:174:VAL:CG1	1:D:175:GLY:N	2.50	0.74
1:A:226:TYR:C	1:A:227:LEU:HD23	2.07	0.74
1:A:22:TYR:CE2	1:A:38:MET:HE3	2.22	0.74
1:A:263:TYR:O	1:A:271:PRO:HD2	1.87	0.74
1:C:11:VAL:HG12	1:C:12:ASP:N	2.01	0.74
1:C:32:TYR:CE2	1:C:314:ILE:HG13	2.23	0.74
1:A:113:ASP:C	1:A:114:MET:HG2	2.07	0.74
1:B:141:ASN:HB3	1:B:153:PHE:CE1	2.23	0.74
1:C:139:TYR:CE1	1:C:140:ARG:O	2.41	0.74
1:C:286:ILE:CG2	1:C:323:LYS:HB3	2.17	0.74
1:D:124:TYR:CE2	1:D:238:THR:CG2	2.71	0.74
1:D:28:GLY:O	1:D:31:SER:OG	2.06	0.74
1:A:336:ILE:CG1	1:A:337:VAL:N	2.51	0.74
1:A:153:PHE:N	1:A:153:PHE:HD1	1.84	0.73
1:A:170:ASN:CG	1:A:170:ASN:O	2.25	0.73
1:A:319:ASP:O	1:A:321:ASP:N	2.21	0.73
1:B:111:TYR:CZ	1:B:219:LYS:HE2	2.23	0.73
1:B:310:TYR:C	1:B:310:TYR:CD1	2.59	0.73
1:B:336:ILE:CD1	1:C:87:GLY:HA2	2.17	0.73
1:A:4:TYR:CD1	1:C:1:ALA:HB3	2.23	0.73
1:A:336:ILE:HD11	1:B:87:GLY:N	2.03	0.73
1:C:104:VAL:N	1:C:156:GLN:OE1	2.20	0.73
1:C:32:TYR:CD2	1:C:314:ILE:HG13	2.23	0.73
1:A:86:ALA:CB	1:C:336:ILE:HG12	2.18	0.73
1:C:90:TYR:CD2	1:C:93:VAL:HG21	2.22	0.73
1:D:303:PHE:HD2	1:D:307:MET:HG2	1.53	0.73
1:D:34:GLY:O	1:D:35:ASN:HB2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:SER:N	1:A:35:ASN:HD22	1.83	0.73
1:B:310:TYR:C	1:B:310:TYR:HD1	1.91	0.73
1:A:65:PHE:CE1	1:B:61:TRP:HZ2	2.07	0.73
1:C:229:ALA:HB1	1:C:259:LEU:HD23	1.66	0.73
1:C:90:TYR:O	1:C:91:ALA:C	2.24	0.73
1:D:51:ILE:CG1	1:D:55:LEU:HD23	2.17	0.73
1:B:1:ALA:HB2	1:C:4:TYR:CE2	2.23	0.73
1:A:4:TYR:HE1	1:C:1:ALA:HB1	1.45	0.73
1:C:21:HIS:CD2	1:C:23:PHE:CE2	2.77	0.73
1:D:205:LEU:HD23	1:D:284:GLU:HG3	1.69	0.73
1:D:258:LEU:CD2	1:D:258:LEU:N	2.51	0.73
1:A:232:GLY:O	1:A:256:ASP:HB2	1.87	0.73
1:B:126:ASP:OD2	1:B:168:ARG:NH1	2.21	0.73
1:B:96:PHE:HD2	1:B:96:PHE:C	1.91	0.73
1:C:223:ASN:CB	1:C:225:ILE:HD11	2.19	0.73
1:D:182:TYR:CD2	1:D:182:TYR:O	2.41	0.73
1:A:161:ASN:O	1:A:169:SER:CB	2.37	0.73
1:B:98:TYR:CD2	1:B:98:TYR:C	2.54	0.73
1:C:132:ARG:HG3	1:C:132:ARG:NH1	2.02	0.73
1:D:300:THR:HA	1:D:310:TYR:HB3	1.70	0.73
1:B:16:LYS:HB3	1:B:339:GLN:HB3	1.69	0.73
1:B:51:ILE:HB	1:B:55:LEU:O	1.88	0.73
1:C:82:ARG:O	1:C:100:ARG:CD	2.33	0.73
1:B:160:LYS:NZ	1:B:162:GLU:OE2	2.17	0.73
1:C:229:ALA:HB1	1:C:259:LEU:HD21	1.70	0.73
1:D:231:TYR:HD2	1:D:231:TYR:C	1.91	0.73
1:D:52:ASN:OD1	1:D:53:SER:N	2.22	0.73
1:A:292:VAL:O	1:A:292:VAL:HG12	1.88	0.73
1:B:174:VAL:HG13	1:B:175:GLY:N	2.02	0.72
1:B:4:TYR:CD2	1:B:4:TYR:C	2.57	0.72
1:C:105:VAL:HG23	1:C:129:PHE:HB3	1.69	0.72
1:D:66:GLN:HG3	1:D:78:GLY:CA	2.18	0.72
1:B:240:ILE:HG22	1:B:291:LEU:HD22	1.71	0.72
1:C:223:ASN:O	1:C:224:ASN:CB	2.36	0.72
1:C:23:PHE:HA	1:C:35:ASN:ND2	2.04	0.72
1:D:29:GLU:HG2	1:D:30:ASN:H	1.54	0.72
1:D:60:GLN:HB3	1:D:85:PHE:HE2	1.54	0.72
1:C:21:HIS:HD2	1:C:23:PHE:CE2	2.07	0.72
1:A:182:TYR:CG	1:A:182:TYR:O	2.36	0.72
1:B:15:GLY:N	1:B:340:PHE:HE2	1.81	0.72
1:A:167:ARG:HG3	1:A:167:ARG:NH1	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:LEU:HD11	1:C:102:TYR:HE2	1.55	0.72
1:C:125:SER:O	1:C:126:ASP:C	2.22	0.72
1:C:284:GLU:H	1:C:284:GLU:CD	1.91	0.72
1:C:58:TYR:HE2	1:C:89:LYS:HE3	1.55	0.72
1:A:61:TRP:CH2	1:C:65:PHE:CE1	2.76	0.72
1:D:167:ARG:HG3	1:D:167:ARG:HH11	1.55	0.72
1:D:229:ALA:HB2	1:D:259:LEU:HD23	1.50	0.72
1:A:132:ARG:NH1	1:A:132:ARG:CG	2.50	0.72
1:D:172:ASP:O	1:D:194:ALA:CB	2.37	0.72
1:D:263:TYR:O	1:D:270:ARG:HA	1.88	0.72
1:A:16:LYS:HB3	1:A:339:GLN:HB3	1.70	0.72
1:D:240:ILE:HG21	1:D:251:ALA:HB2	1.70	0.72
1:D:29:GLU:HG2	1:D:30:ASN:N	1.99	0.72
1:A:82:ARG:HH11	1:A:82:ARG:HG2	1.54	0.71
1:B:229:ALA:HB1	1:B:259:LEU:HD21	1.72	0.71
1:B:69:ASN:ND2	1:B:77:THR:HB	2.03	0.71
1:D:255:GLN:O	1:D:278:SER:HA	1.89	0.71
1:B:315:ILE:O	1:B:315:ILE:HG22	1.89	0.71
1:C:230:ASN:HB2	1:C:258:LEU:HB2	1.71	0.71
1:A:279:LYS:NZ	1:A:279:LYS:CB	2.53	0.71
1:A:309:THR:HG22	1:A:336:ILE:CA	2.20	0.71
1:B:141:ASN:ND2	1:B:145:PHE:CE1	2.58	0.71
1:C:308:SER:O	1:C:309:THR:HG23	1.90	0.71
1:B:196:ARG:HA	1:B:200:GLN:OE1	1.90	0.71
1:B:226:TYR:HE2	1:B:228:ALA:HB2	1.53	0.71
1:B:28:GLY:O	1:B:29:GLU:C	2.23	0.71
1:D:303:PHE:O	1:D:304:ASN:CB	2.38	0.71
1:D:48:GLU:HG3	1:D:56:THR:CG2	2.20	0.71
1:A:139:TYR:O	1:A:154:ALA:CB	2.38	0.71
1:A:86:ALA:HB1	1:C:336:ILE:HG13	1.70	0.71
1:B:141:ASN:OD1	1:B:153:PHE:HE1	1.73	0.71
1:D:239:PRO:HA	1:D:250:PHE:HD2	1.54	0.71
1:A:104:VAL:HG11	1:A:156:GLN:CB	2.21	0.71
1:A:18:VAL:HG22	1:A:337:VAL:HG22	1.72	0.71
1:B:141:ASN:CG	1:B:153:PHE:HE1	1.94	0.71
1:D:144:PHE:CB	1:D:151:LEU:HD23	2.21	0.71
1:D:51:ILE:HD13	1:D:55:LEU:HD21	1.70	0.71
1:D:60:GLN:CB	1:D:85:PHE:HE2	2.04	0.71
1:D:337:VAL:O	1:D:337:VAL:CG1	2.38	0.71
1:C:25:LYS:NZ	1:C:25:LYS:HB2	2.05	0.71
1:C:308:SER:O	1:C:309:THR:CG2	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ASN:CB	1:C:153:PHE:CE1	2.74	0.71
1:D:21:HIS:HD2	1:D:23:PHE:CE1	2.08	0.71
1:C:283:VAL:O	1:C:286:ILE:HD13	1.90	0.70
1:B:336:ILE:HD11	1:C:87:GLY:N	2.06	0.70
1:D:231:TYR:HD2	1:D:232:GLY:N	1.87	0.70
1:D:310:TYR:O	1:D:310:TYR:CD1	2.44	0.70
1:B:129:PHE:CE2	1:B:193:ALA:N	2.56	0.70
1:C:338:TYR:HD2	1:C:338:TYR:C	1.91	0.70
1:B:340:PHE:CE1	1:C:45:PHE:CD2	2.78	0.70
1:D:273:ILE:CD1	1:D:297:VAL:HG23	2.20	0.70
1:B:315:ILE:HA	1:B:330:ASP:OD2	1.91	0.70
1:C:303:PHE:HD2	1:C:307:MET:HG2	1.54	0.70
1:C:45:PHE:CD1	1:C:45:PHE:C	2.52	0.70
1:D:158:LEU:HB3	1:D:173:GLY:HA3	1.73	0.70
1:D:18:VAL:O	1:D:18:VAL:HG12	1.89	0.70
1:A:18:VAL:HB	1:A:40:TYR:HE1	1.50	0.70
1:A:51:ILE:HD13	1:C:303:PHE:CB	2.22	0.70
1:D:174:VAL:HG12	1:D:175:GLY:N	2.05	0.70
1:A:11:VAL:CG2	1:C:340:PHE:HB2	2.22	0.70
1:B:18:VAL:CG1	1:B:40:TYR:CE1	2.75	0.70
1:B:277:LYS:CE	1:B:293:ASN:ND2	2.55	0.70
1:B:70:SER:O	1:B:75:ALA:HB2	1.91	0.70
1:C:262:GLN:OE1	1:C:270:ARG:NH1	2.25	0.70
1:A:309:THR:CG2	1:A:336:ILE:CB	2.58	0.70
1:B:129:PHE:CD2	1:B:192:GLY:HA3	2.26	0.70
1:C:100:ARG:HG2	1:C:133:VAL:O	1.92	0.70
1:D:239:PRO:HA	1:D:250:PHE:CD2	2.26	0.70
1:A:51:ILE:HG23	1:C:304:ASN:HD21	1.57	0.70
1:B:123:ALA:HA	1:B:130:VAL:CG2	2.21	0.70
1:A:303:PHE:CE2	1:B:88:LEU:CD1	2.71	0.70
1:C:100:ARG:HG3	1:C:100:ARG:NH1	2.06	0.70
1:D:25:LYS:HE2	1:D:329:ASP:OD1	1.91	0.70
1:C:63:TYR:CD1	1:C:80:LYS:C	2.65	0.70
1:D:24:SER:OG	1:D:331:THR:OG1	2.09	0.70
1:D:48:GLU:CD	1:D:56:THR:CG2	2.60	0.70
1:B:224:ASN:O	1:B:263:TYR:CD1	2.44	0.70
1:A:336:ILE:CD1	1:B:87:GLY:HA2	2.22	0.70
1:B:71:GLU:HG3	1:C:100:ARG:HH21	1.54	0.70
1:C:214:TRP:CH2	1:C:231:TYR:HE2	2.10	0.70
1:D:105:VAL:O	1:D:105:VAL:HG12	1.90	0.70
1:C:58:TYR:CE2	1:C:89:LYS:HE3	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:HIS:CD2	1:A:23:PHE:CE2	2.79	0.69
1:C:115:LEU:HD12	1:C:119:GLY:CA	2.21	0.69
1:C:303:PHE:HB2	1:C:307:MET:HB3	1.73	0.69
1:D:104:VAL:CG1	1:D:156:GLN:HB3	2.19	0.69
1:D:294:TYR:CE1	1:D:314:ILE:HD12	2.27	0.69
1:D:311:VAL:HG11	1:D:334:VAL:HG23	1.65	0.69
1:A:274:ALA:O	1:A:296:GLU:N	2.23	0.69
1:A:320:SER:O	1:A:322:ASN:N	2.26	0.69
1:B:240:ILE:HG21	1:B:291:LEU:HD21	1.75	0.69
1:A:156:GLN:N	1:A:175:GLY:O	2.23	0.69
1:B:191:TYR:CD1	1:B:192:GLY:N	2.60	0.69
1:C:167:ARG:HH11	1:C:167:ARG:CG	2.01	0.69
1:D:56:THR:HB	1:D:89:LYS:HB2	1.74	0.69
1:B:18:VAL:CG1	1:B:40:TYR:HE1	2.05	0.69
1:C:240:ILE:HD12	1:C:251:ALA:HB2	1.74	0.69
1:C:307:MET:O	1:C:308:SER:CB	2.39	0.69
1:A:316:ASN:N	1:A:330:ASP:OD1	2.25	0.69
1:C:170:ASN:ND2	1:C:170:ASN:O	2.26	0.69
1:D:86:ALA:O	1:D:97:ASP:HB2	1.92	0.69
1:C:96:PHE:HD1	1:C:138:THR:O	1.75	0.69
1:A:267:PHE:CD1	1:A:267:PHE:N	2.19	0.69
1:A:313:TYR:CB	1:A:332:VAL:HG22	2.23	0.69
1:B:113:ASP:C	1:B:114:MET:CG	2.53	0.69
1:B:318:ILE:HG22	1:B:319:ASP:N	2.07	0.69
1:C:124:TYR:CD2	1:C:124:TYR:N	2.54	0.69
1:D:27:ASN:O	1:D:29:GLU:N	2.25	0.69
1:D:307:MET:O	1:D:308:SER:HB3	1.90	0.69
1:A:113:ASP:C	1:A:114:MET:CG	2.60	0.69
1:B:274:ALA:HB3	1:B:296:GLU:HB3	1.74	0.69
1:C:240:ILE:CD1	1:C:251:ALA:HB2	2.23	0.69
1:A:123:ALA:HA	1:A:130:VAL:CG2	2.23	0.68
1:A:223:ASN:O	1:A:224:ASN:HB2	1.92	0.68
1:A:303:PHE:HE2	1:B:88:LEU:HD11	1.56	0.68
1:A:319:ASP:O	1:A:320:SER:C	2.31	0.68
1:B:165:THR:HG22	1:B:166:ALA:N	2.08	0.68
1:B:295:PHE:N	1:B:295:PHE:CD1	2.59	0.68
1:C:141:ASN:CG	1:C:153:PHE:HE1	1.97	0.68
1:D:100:ARG:NH1	1:D:100:ARG:CG	2.51	0.68
1:B:18:VAL:HG22	1:B:337:VAL:HG13	1.76	0.68
1:B:296:GLU:CB	1:B:314:ILE:HD13	2.23	0.68
1:D:104:VAL:HG11	1:D:156:GLN:CB	2.21	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:LEU:O	1:D:259:LEU:CD2	2.40	0.68
1:B:158:LEU:C	1:B:158:LEU:HD12	2.13	0.68
1:C:130:VAL:HG13	1:C:213:GLN:NE2	2.09	0.68
1:D:308:SER:O	1:D:309:THR:HG23	1.93	0.68
1:A:163:ARG:N	1:A:169:SER:OG	2.21	0.68
1:A:55:LEU:HG	1:A:56:THR:N	2.08	0.68
1:C:196:ARG:NH2	1:C:250:PHE:HB2	2.09	0.68
1:A:309:THR:HG22	1:A:336:ILE:HA	1.75	0.68
1:D:203:GLN:HB3	1:D:204:PRO:CD	2.19	0.68
1:A:20:LEU:HD22	1:A:117:GLU:OE1	1.87	0.68
1:A:130:VAL:HG12	1:A:213:GLN:CD	2.13	0.68
1:A:39:THR:O	1:A:67:GLY:N	2.27	0.68
1:A:66:GLN:HG3	1:A:78:GLY:O	1.94	0.68
1:B:229:ALA:CB	1:B:259:LEU:HD23	2.04	0.68
1:B:309:THR:HG22	1:B:336:ILE:HB	1.76	0.68
1:C:182:TYR:CD1	1:C:183:GLU:N	2.62	0.68
1:C:206:GLY:CA	1:C:250:PHE:O	2.42	0.68
1:A:58:TYR:C	1:C:338:TYR:HD1	1.97	0.68
1:B:220:TYR:N	1:B:227:LEU:O	2.20	0.68
1:D:238:THR:OG1	1:D:254:THR:HG21	1.94	0.68
1:D:258:LEU:HD23	1:D:258:LEU:N	2.09	0.68
1:D:279:LYS:CB	1:D:279:LYS:HZ2	1.86	0.68
1:A:3:ILE:O	1:A:3:ILE:HG13	1.90	0.68
1:B:243:LYS:H	1:B:243:LYS:HD2	1.57	0.68
1:C:273:ILE:O	1:C:273:ILE:HG22	1.94	0.68
1:D:60:GLN:CB	1:D:85:PHE:CE2	2.76	0.68
1:A:114:MET:N	1:A:115:LEU:HD23	2.09	0.68
1:A:152:ASN:N	1:A:152:ASN:HD22	1.92	0.68
1:A:137:ALA:O	1:A:156:GLN:HA	1.94	0.68
1:A:313:TYR:CD1	1:A:332:VAL:HG21	2.17	0.68
1:C:25:LYS:HZ2	1:C:25:LYS:HB2	1.59	0.68
1:B:214:TRP:HE1	1:B:233:GLU:HB2	1.59	0.67
1:B:337:VAL:HG12	1:B:338:TYR:O	1.94	0.67
1:D:215:ALA:O	1:D:216:THR:HG22	1.94	0.67
1:A:313:TYR:CE1	1:A:332:VAL:CG2	2.68	0.67
1:B:295:PHE:N	1:B:295:PHE:HD1	1.91	0.67
1:B:90:TYR:HB3	1:B:93:VAL:CG2	2.23	0.67
1:C:165:THR:O	1:C:166:ALA:C	2.30	0.67
1:C:222:ALA:O	1:C:225:ILE:CD1	2.42	0.67
1:A:104:VAL:HG11	1:A:156:GLN:HB3	1.74	0.67
1:B:139:TYR:CD2	1:B:139:TYR:C	2.67	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:TYR:HE1	1:C:140:ARG:O	1.77	0.67
1:C:338:TYR:HD2	1:C:339:GLN:CA	2.08	0.67
1:A:113:ASP:O	1:A:114:MET:CG	2.39	0.67
1:A:167:ARG:O	1:A:167:ARG:CG	2.41	0.67
1:A:61:TRP:HZ2	1:C:65:PHE:HD1	1.15	0.67
1:B:115:LEU:HD12	1:B:119:GLY:HA2	1.71	0.67
1:C:3:ILE:HD11	1:C:13:LEU:HB2	1.75	0.67
1:D:315:ILE:H	1:D:315:ILE:CD1	2.02	0.67
1:A:245:THR:OG1	1:A:247:THR:OG1	2.12	0.67
1:C:69:ASN:HD21	1:C:77:THR:HB	1.60	0.67
1:A:118:PHE:O	1:A:119:GLY:C	2.33	0.67
1:A:129:PHE:HE2	1:A:192:GLY:C	1.97	0.67
1:C:136:VAL:HG12	1:C:158:LEU:CD1	2.25	0.67
1:C:267:PHE:CZ	1:C:269:LEU:HB3	2.29	0.67
1:C:37:ASP:OD1	1:C:38:MET:N	2.28	0.67
1:C:63:TYR:CE1	1:C:80:LYS:O	2.48	0.67
1:D:118:PHE:CZ	1:D:333:ALA:HB2	2.28	0.67
1:A:141:ASN:CG	1:A:153:PHE:CE1	2.65	0.67
1:A:172:ASP:O	1:A:194:ALA:HA	1.93	0.67
1:A:122:THR:OG1	1:A:258:LEU:HD21	1.95	0.67
1:A:293:ASN:HB3	1:A:317:GLN:HB2	1.76	0.67
1:B:309:THR:HG22	1:B:336:ILE:CA	2.24	0.67
1:A:104:VAL:HG12	1:A:156:GLN:CD	2.15	0.67
1:C:63:TYR:HD1	1:C:80:LYS:O	1.72	0.67
1:D:13:LEU:HD12	1:D:14:TYR:H	1.60	0.67
1:B:277:LYS:CD	1:B:293:ASN:HD21	2.07	0.67
1:C:226:TYR:O	1:C:227:LEU:HD23	1.95	0.67
1:C:24:SER:OG	1:C:331:THR:OG1	2.12	0.67
1:C:31:SER:HA	1:C:329:ASP:HB2	1.77	0.67
1:C:65:PHE:HD2	1:C:65:PHE:N	1.91	0.67
1:D:118:PHE:O	1:D:119:GLY:O	2.12	0.67
1:A:39:THR:O	1:A:67:GLY:CA	2.43	0.66
1:B:28:GLY:O	1:B:30:ASN:N	2.28	0.66
1:C:13:LEU:HD12	1:C:14:TYR:H	1.60	0.66
1:C:318:ILE:HG22	1:C:319:ASP:N	2.08	0.66
1:A:208:GLY:HA3	1:A:236:ASN:HD22	1.60	0.66
1:A:279:LYS:HB2	1:A:279:LYS:HZ2	1.60	0.66
1:A:289:VAL:HG13	1:A:323:LYS:HB2	1.75	0.66
1:B:185:PHE:HE2	1:B:220:TYR:CE1	2.12	0.66
1:B:240:ILE:HG21	1:B:291:LEU:CD2	2.26	0.66
1:D:104:VAL:CG1	1:D:156:GLN:HB2	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:VAL:O	1:A:292:VAL:CG1	2.38	0.66
1:A:296:GLU:HG2	1:A:297:VAL:N	2.09	0.66
1:B:174:VAL:CG1	1:B:175:GLY:N	2.59	0.66
1:B:9:ASN:O	1:B:9:ASN:CG	2.33	0.66
1:B:303:PHE:HB2	1:B:307:MET:HB3	1.75	0.66
1:D:18:VAL:HG22	1:D:337:VAL:HG22	1.78	0.66
1:C:310:TYR:CD1	1:C:310:TYR:C	2.69	0.66
1:C:294:TYR:CD1	1:C:314:ILE:HD12	2.31	0.66
1:C:46:LYS:HA	1:C:60:GLN:HB2	1.77	0.66
1:D:119:GLY:HA2	1:D:294:TYR:OH	1.96	0.66
1:D:24:SER:CB	1:D:34:GLY:O	2.43	0.66
1:A:124:TYR:O	1:A:131:GLY:HA3	1.95	0.66
1:D:273:ILE:HD11	1:D:297:VAL:HG23	1.77	0.66
1:A:229:ALA:HB2	1:A:259:LEU:CD2	2.26	0.66
1:C:10:LYS:CG	1:C:10:LYS:O	2.44	0.66
1:C:144:PHE:CD1	1:C:151:LEU:HD23	2.30	0.66
1:D:112:THR:O	1:D:114:MET:N	2.28	0.66
1:A:322:ASN:OD1	1:A:323:LYS:N	2.28	0.66
1:D:257:VAL:C	1:D:258:LEU:HD22	2.16	0.66
1:D:310:TYR:C	1:D:310:TYR:CD1	2.69	0.66
1:A:229:ALA:CB	1:A:259:LEU:CD2	2.74	0.66
1:D:111:TYR:OH	1:D:188:VAL:CG2	2.41	0.66
1:B:141:ASN:CB	1:B:153:PHE:CE1	2.79	0.66
1:C:70:SER:OG	1:C:71:GLU:N	2.18	0.66
1:C:217:GLY:HA3	1:C:230:ASN:ND2	2.11	0.65
1:C:96:PHE:CD1	1:C:138:THR:O	2.49	0.65
1:D:182:TYR:CE2	1:D:183:GLU:HB3	2.30	0.65
1:A:42:ARG:NH1	1:A:82:ARG:NH2	2.44	0.65
1:D:205:LEU:HD22	1:D:284:GLU:HG2	1.77	0.65
1:D:51:ILE:HB	1:D:55:LEU:HD23	1.77	0.65
1:B:58:TYR:HE2	1:B:87:GLY:C	2.00	0.65
1:C:13:LEU:HD12	1:C:14:TYR:N	2.11	0.65
1:D:205:LEU:CD2	1:D:284:GLU:HG3	2.27	0.65
1:D:303:PHE:O	1:D:304:ASN:CG	2.35	0.65
1:D:48:GLU:CG	1:D:56:THR:CG2	2.74	0.65
1:A:208:GLY:HA3	1:A:236:ASN:ND2	2.12	0.65
1:A:242:ASN:O	1:A:246:ASN:N	2.29	0.65
1:B:158:LEU:HD11	1:B:170:ASN:ND2	2.12	0.65
1:B:111:TYR:OH	1:B:188:VAL:HG22	1.97	0.65
1:D:224:ASN:ND2	1:D:264:GLN:O	2.30	0.65
1:A:340:PHE:HE1	1:B:45:PHE:CE2	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:GLU:CG	1:B:183:GLU:O	2.44	0.65
1:B:310:TYR:CE1	1:B:335:GLY:HA3	2.31	0.65
1:C:172:ASP:O	1:C:194:ALA:HB2	1.88	0.65
1:A:39:THR:O	1:A:39:THR:CG2	2.45	0.65
1:C:198:ASN:C	1:C:200:GLN:N	2.49	0.65
1:C:240:ILE:HD13	1:C:251:ALA:N	2.11	0.65
1:A:50:GLN:HA	1:A:56:THR:HA	1.78	0.65
1:A:82:ARG:HG3	1:A:132:ARG:HH21	1.62	0.65
1:B:165:THR:CG2	1:B:166:ALA:N	2.59	0.65
1:B:285:GLY:C	1:B:286:ILE:CD1	2.60	0.65
1:C:236:ASN:OD1	1:C:252:ASN:HA	1.97	0.65
1:D:130:VAL:HG13	1:D:213:GLN:CD	2.17	0.65
1:D:20:LEU:CD1	1:D:21:HIS:N	2.49	0.65
1:D:273:ILE:CD1	1:D:297:VAL:CG2	2.75	0.65
1:A:203:GLN:HA	1:A:203:GLN:NE2	2.11	0.65
1:A:300:THR:HA	1:A:310:TYR:HB3	1.79	0.65
1:B:220:TYR:HB3	1:B:227:LEU:HB2	1.77	0.65
1:B:340:PHE:CB	1:C:11:VAL:HG21	2.26	0.65
1:B:54:ASP:HB3	1:B:91:ALA:CB	2.21	0.65
1:A:105:VAL:HB	1:A:129:PHE:O	1.97	0.65
1:A:144:PHE:O	1:A:145:PHE:HB2	1.96	0.65
1:B:148:VAL:O	1:B:148:VAL:HG12	1.94	0.65
1:B:293:ASN:OD1	1:B:317:GLN:HB3	1.97	0.65
1:C:182:TYR:HD1	1:C:182:TYR:C	1.99	0.65
1:D:158:LEU:HG	1:D:158:LEU:O	1.96	0.65
1:B:336:ILE:HD11	1:C:87:GLY:HA2	1.78	0.65
1:B:5:ASN:O	1:B:6:LYS:CG	2.44	0.65
1:C:48:GLU:HG3	1:C:56:THR:HG23	1.78	0.65
1:D:314:ILE:HG22	1:D:314:ILE:O	1.96	0.65
1:A:115:LEU:HD23	1:A:115:LEU:H	0.48	0.64
1:A:14:TYR:OH	1:A:62:GLU:HB2	1.97	0.64
1:A:57:GLY:HA2	1:A:88:LEU:CD2	2.27	0.64
1:B:281:LYS:O	1:B:282:ASP:HB2	1.97	0.64
1:B:2:GLU:OE2	1:B:5:ASN:HB2	1.98	0.64
1:C:232:GLY:O	1:C:256:ASP:HB2	1.97	0.64
1:A:22:TYR:CE2	1:A:38:MET:HE2	2.25	0.64
1:A:86:ALA:O	1:A:97:ASP:CB	2.39	0.64
1:B:276:THR:HG22	1:B:294:TYR:CE2	2.24	0.64
1:B:49:THR:N	1:B:57:GLY:O	2.27	0.64
1:C:331:THR:CG2	1:C:332:VAL:N	2.61	0.64
1:D:102:TYR:H	1:D:102:TYR:HD2	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:SER:HB2	1:A:188:VAL:HG13	1.80	0.64
1:A:40:TYR:N	1:A:40:TYR:HD1	1.89	0.64
1:A:43:LEU:HG	1:A:43:LEU:O	1.92	0.64
1:B:54:ASP:O	1:B:90:TYR:HA	1.98	0.64
1:C:27:ASN:OD1	1:C:27:ASN:C	2.35	0.64
1:D:307:MET:HG3	1:D:308:SER:N	2.09	0.64
1:A:71:GLU:HG3	1:B:100:ARG:HH22	1.59	0.64
1:D:51:ILE:HB	1:D:55:LEU:HB3	1.79	0.64
1:C:285:GLY:C	1:C:286:ILE:HD12	2.14	0.64
1:C:338:TYR:CD2	1:C:339:GLN:CA	2.80	0.64
1:A:157:TYR:HA	1:A:173:GLY:O	1.97	0.64
1:A:22:TYR:CD2	1:A:38:MET:CG	2.73	0.64
1:A:70:SER:HG	1:A:72:GLY:H	1.46	0.64
1:B:242:ASN:ND2	1:B:245:THR:OG1	2.29	0.64
1:C:211:ALA:C	1:C:212:GLU:CG	2.66	0.64
1:D:27:ASN:C	1:D:29:GLU:H	2.01	0.64
1:A:338:TYR:CD2	1:A:339:GLN:N	2.66	0.64
1:B:273:ILE:HD11	1:B:297:VAL:HG22	1.80	0.64
1:B:32:TYR:CD2	1:B:32:TYR:C	2.71	0.64
1:B:58:TYR:HD2	1:B:58:TYR:O	1.77	0.64
1:B:91:ALA:C	1:B:92:ASP:OD1	2.36	0.64
1:C:308:SER:C	1:C:309:THR:HG23	2.18	0.64
1:C:45:PHE:O	1:C:60:GLN:HG3	1.97	0.64
1:A:80:LYS:HD2	1:C:71:GLU:HB3	1.79	0.64
1:A:102:TYR:C	1:A:103:GLY:O	2.37	0.64
1:A:152:ASN:N	1:A:152:ASN:ND2	2.46	0.64
1:C:179:SER:HB2	1:C:188:VAL:CG1	2.27	0.64
1:C:198:ASN:C	1:C:200:GLN:H	2.01	0.64
1:C:263:TYR:CE2	1:C:265:PHE:CE1	2.86	0.64
1:C:270:ARG:HD2	1:C:302:TYR:HE2	1.63	0.64
1:D:129:PHE:CE2	1:D:192:GLY:HA3	2.33	0.64
1:A:283:VAL:HB	1:A:286:ILE:HB	1.80	0.64
1:B:22:TYR:O	1:B:23:PHE:CD2	2.50	0.64
1:B:205:LEU:HA	1:B:284:GLU:OE2	1.97	0.64
1:C:145:PHE:C	1:C:147:LEU:H	2.01	0.64
1:A:26:GLY:C	1:A:28:GLY:H	2.01	0.63
1:B:309:THR:CG2	1:B:336:ILE:HB	2.28	0.63
1:B:4:TYR:HD2	1:B:5:ASN:N	1.95	0.63
1:D:165:THR:HG22	1:D:166:ALA:N	2.13	0.63
1:C:191:TYR:CD1	1:C:192:GLY:N	2.65	0.63
1:D:102:TYR:N	1:D:102:TYR:CD2	2.65	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:GLU:CD	1:D:56:THR:HG21	2.18	0.63
1:D:104:VAL:HG12	1:D:156:GLN:HB2	1.81	0.63
1:A:104:VAL:CG1	1:A:156:GLN:CB	2.75	0.63
1:A:308:SER:O	1:A:309:THR:HG23	1.98	0.63
1:C:141:ASN:CB	1:C:153:PHE:HE1	2.11	0.63
1:D:74:ASP:O	1:D:75:ALA:C	2.35	0.63
1:A:18:VAL:HG13	1:A:337:VAL:CG2	2.29	0.63
1:B:1:ALA:HB1	1:C:4:TYR:CD1	2.33	0.63
1:C:54:ASP:CB	1:C:90:TYR:CE1	2.81	0.63
1:D:205:LEU:HD22	1:D:284:GLU:CG	2.28	0.63
1:A:229:ALA:HB1	1:A:259:LEU:HD21	1.79	0.63
1:A:51:ILE:HG22	1:C:304:ASN:ND2	2.14	0.63
1:B:240:ILE:HG22	1:B:291:LEU:CD2	2.28	0.63
1:C:289:VAL:HG21	1:C:324:LEU:HG	1.81	0.63
1:B:72:GLY:O	1:B:73:ALA:C	2.36	0.63
1:C:65:PHE:N	1:C:65:PHE:CD2	2.60	0.63
1:A:114:MET:H	1:A:115:LEU:CD2	2.11	0.63
1:B:1:ALA:HB1	1:C:4:TYR:CE1	2.34	0.63
1:B:257:VAL:O	1:B:258:LEU:HD13	1.99	0.63
1:B:6:LYS:O	1:B:8:GLY:N	2.32	0.63
1:C:139:TYR:CD1	1:C:140:ARG:N	2.67	0.63
1:C:136:VAL:HG12	1:C:158:LEU:HD12	1.81	0.63
1:C:264:GLN:HG3	1:C:264:GLN:O	1.98	0.63
1:B:129:PHE:CE2	1:B:192:GLY:HA3	2.34	0.62
1:A:172:ASP:N	1:A:195:ASP:HB2	2.14	0.62
1:A:45:PHE:CD1	1:A:45:PHE:C	2.72	0.62
1:B:274:ALA:O	1:B:295:PHE:HA	1.99	0.62
1:C:125:SER:O	1:C:126:ASP:HB2	1.99	0.62
1:C:167:ARG:O	1:C:167:ARG:HG2	1.95	0.62
1:C:206:GLY:H	1:C:284:GLU:CD	2.03	0.62
1:C:16:LYS:HB3	1:C:339:GLN:HB3	1.80	0.62
1:D:127:ASP:O	1:D:128:PHE:HB2	1.99	0.62
1:D:263:TYR:O	1:D:271:PRO:HD2	2.00	0.62
1:A:171:GLY:C	1:A:172:ASP:OD1	2.38	0.62
1:A:267:PHE:H	1:A:267:PHE:HD1	0.72	0.62
1:B:304:ASN:ND2	1:C:51:ILE:HG23	2.14	0.62
1:D:122:THR:HG22	1:D:256:ASP:OD2	2.00	0.62
1:D:270:ARG:HB3	1:D:302:TYR:HE2	1.64	0.62
1:D:311:VAL:HG11	1:D:334:VAL:CG2	2.22	0.62
1:A:223:ASN:O	1:A:224:ASN:CB	2.47	0.62
1:A:49:THR:O	1:A:49:THR:OG1	2.10	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:PHE:CE2	1:B:220:TYR:CD1	2.87	0.62
1:A:307:MET:HE1	1:B:88:LEU:HD23	1.75	0.62
1:C:260:VAL:HG12	1:C:261:ALA:N	2.15	0.62
1:C:284:GLU:O	1:C:286:ILE:CD1	2.47	0.62
1:D:85:PHE:HD2	1:D:85:PHE:N	1.96	0.62
1:A:179:SER:CB	1:A:188:VAL:HG13	2.30	0.62
1:B:140:ARG:HG2	1:B:154:ALA:HB2	1.81	0.62
1:B:270:ARG:HG2	1:B:270:ARG:O	1.98	0.62
1:B:309:THR:HG22	1:B:336:ILE:CB	2.29	0.62
1:B:340:PHE:HB3	1:C:11:VAL:HG21	1.81	0.62
1:C:161:ASN:HB2	1:C:170:ASN:HD21	1.64	0.62
1:C:235:ARG:O	1:C:236:ASN:C	2.38	0.62
1:D:40:TYR:CD2	1:D:42:ARG:NH2	2.67	0.62
1:A:1:ALA:HB1	1:B:4:TYR:CE1	2.31	0.62
1:A:20:LEU:HD21	1:A:117:GLU:CD	2.16	0.62
1:C:214:TRP:CH2	1:C:231:TYR:CE2	2.86	0.62
1:A:165:THR:HG23	1:A:166:ALA:H	1.64	0.62
1:C:60:GLN:CG	1:C:61:TRP:N	2.60	0.62
1:D:257:VAL:C	1:D:258:LEU:CD2	2.68	0.62
1:D:297:VAL:O	1:D:313:TYR:HB3	2.00	0.62
1:A:273:ILE:O	1:A:273:ILE:HG22	1.98	0.62
1:A:334:VAL:HG12	1:A:334:VAL:O	1.88	0.62
1:A:88:LEU:HD11	1:C:303:PHE:CE2	2.34	0.62
1:D:102:TYR:CD1	1:D:106:TYR:CE2	2.87	0.62
1:D:134:GLY:O	1:D:136:VAL:HG13	2.00	0.62
1:A:39:THR:HG22	1:A:67:GLY:HA3	1.81	0.62
1:B:163:ARG:NH1	1:B:163:ARG:HG2	2.15	0.62
1:D:270:ARG:HG2	1:D:270:ARG:O	1.99	0.62
1:A:251:ALA:O	1:A:252:ASN:C	2.37	0.61
1:A:293:ASN:HB3	1:A:317:GLN:CB	2.29	0.61
1:A:22:TYR:CD1	1:A:333:ALA:CB	2.77	0.61
1:B:259:LEU:HB2	1:B:275:TYR:HB3	1.81	0.61
1:B:83:LEU:HD22	1:B:85:PHE:HE2	1.65	0.61
1:A:87:GLY:N	1:C:336:ILE:HD11	2.15	0.61
1:D:111:TYR:CZ	1:D:219:LYS:HG2	2.35	0.61
1:D:3:ILE:HD11	1:D:11:VAL:HG12	1.82	0.61
1:B:42:ARG:HE	1:B:64:ASN:HB2	1.65	0.61
1:C:145:PHE:O	1:C:147:LEU:N	2.28	0.61
1:D:295:PHE:O	1:D:315:ILE:HD13	1.99	0.61
1:B:155:VAL:O	1:B:155:VAL:HG22	1.94	0.61
1:B:336:ILE:HD11	1:C:87:GLY:CA	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:TYR:HA	1:D:173:GLY:O	1.99	0.61
1:A:197:THR:O	1:A:200:GLN:HB2	2.01	0.61
1:A:260:VAL:HG12	1:A:261:ALA:N	2.13	0.61
1:C:274:ALA:HB3	1:C:296:GLU:CB	2.29	0.61
1:D:106:TYR:HB2	1:D:130:VAL:O	1.99	0.61
1:B:276:THR:HB	1:B:294:TYR:CD2	2.33	0.61
1:A:65:PHE:CZ	1:B:61:TRP:CZ2	2.87	0.61
1:B:63:TYR:CD2	1:B:65:PHE:CE1	2.88	0.61
1:B:21:HIS:HD1	1:C:98:TYR:HH	1.46	0.61
1:D:24:SER:HB2	1:D:35:ASN:HB2	1.83	0.61
1:D:294:TYR:CE1	1:D:314:ILE:HD11	2.36	0.61
1:D:74:ASP:C	1:D:76:GLN:H	2.03	0.61
1:C:132:ARG:HH11	1:C:132:ARG:HG3	1.64	0.61
1:C:240:ILE:CD1	1:C:251:ALA:CA	2.78	0.61
1:D:144:PHE:CE2	1:D:145:PHE:HD2	2.19	0.61
1:D:302:TYR:C	1:D:304:ASN:H	2.03	0.61
1:C:37:ASP:C	1:C:38:MET:HG2	2.21	0.61
1:B:128:PHE:O	1:B:133:VAL:HG11	2.01	0.61
1:B:90:TYR:O	1:B:91:ALA:C	2.39	0.61
1:D:13:LEU:CD1	1:D:13:LEU:C	2.52	0.61
1:D:143:ASN:HB3	1:D:149:ASP:HA	1.83	0.61
1:A:22:TYR:HE1	1:A:118:PHE:CZ	2.19	0.61
1:A:61:TRP:CG	1:A:61:TRP:O	2.52	0.61
1:A:71:GLU:HB3	1:B:80:LYS:HD2	1.82	0.61
1:C:16:LYS:HB3	1:C:339:GLN:CB	2.30	0.61
1:C:105:VAL:HA	1:C:190:ALA:HB3	1.83	0.61
1:A:65:PHE:CE1	1:B:61:TRP:CZ2	2.89	0.61
1:B:338:TYR:CD2	1:B:339:GLN:N	2.68	0.61
1:B:340:PHE:CE1	1:C:45:PHE:CE2	2.89	0.61
1:D:117:GLU:HG3	1:D:118:PHE:CD1	2.36	0.61
1:D:143:ASN:OD1	1:D:150:GLY:N	2.34	0.61
1:D:338:TYR:CG	1:D:339:GLN:N	2.68	0.61
1:A:300:THR:HG21	1:A:302:TYR:CE1	2.36	0.60
1:A:13:LEU:HD11	1:A:43:LEU:HD11	1.81	0.60
1:B:90:TYR:O	1:B:93:VAL:HG23	2.00	0.60
1:C:112:THR:HG21	1:C:230:ASN:HB2	1.82	0.60
1:A:100:ARG:HG3	1:C:67:GLY:O	2.01	0.60
1:B:219:LYS:O	1:B:219:LYS:HG3	1.99	0.60
1:C:179:SER:HB2	1:C:188:VAL:HG11	1.83	0.60
1:D:205:LEU:CD2	1:D:284:GLU:CG	2.79	0.60
1:D:254:THR:HA	1:D:279:LYS:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:TYR:O	1:D:339:GLN:CB	2.49	0.60
1:D:48:GLU:HG3	1:D:57:GLY:O	2.02	0.60
1:A:129:PHE:HE2	1:A:192:GLY:CA	2.12	0.60
1:B:242:ASN:CG	1:B:242:ASN:O	2.39	0.60
1:B:9:ASN:HB2	1:B:49:THR:HB	1.83	0.60
1:C:193:ALA:HB1	1:C:211:ALA:O	2.01	0.60
1:D:141:ASN:ND2	1:D:142:SER:N	2.48	0.60
1:A:35:ASN:C	1:A:35:ASN:OD1	2.39	0.60
1:A:40:TYR:N	1:A:40:TYR:CD1	2.67	0.60
1:A:71:GLU:CD	1:B:132:ARG:HH21	2.05	0.60
1:C:169:SER:O	1:C:170:ASN:CB	2.42	0.60
1:D:313:TYR:CE1	1:D:332:VAL:HG22	2.37	0.60
1:B:340:PHE:HB3	1:C:11:VAL:CG2	2.30	0.60
1:C:24:SER:HB2	1:C:34:GLY:O	2.01	0.60
1:D:40:TYR:N	1:D:40:TYR:CD1	2.67	0.60
1:B:301:TYR:C	1:B:301:TYR:CD2	2.72	0.60
1:C:118:PHE:O	1:C:119:GLY:O	2.20	0.60
1:C:160:LYS:CA	1:C:160:LYS:HE3	2.19	0.60
1:C:231:TYR:CD2	1:C:231:TYR:C	2.74	0.60
1:C:214:TRP:HH2	1:C:231:TYR:HE2	1.47	0.60
1:D:30:ASN:O	1:D:30:ASN:OD1	2.19	0.60
1:A:157:TYR:N	1:A:157:TYR:CD2	2.70	0.60
1:A:158:LEU:C	1:A:158:LEU:CD1	2.52	0.60
1:A:11:VAL:HG22	1:C:340:PHE:HB2	1.83	0.60
1:B:224:ASN:O	1:B:263:TYR:HD1	1.82	0.60
1:C:11:VAL:CG1	1:C:12:ASP:N	2.65	0.60
1:C:77:THR:HG22	1:C:77:THR:O	2.01	0.60
1:D:48:GLU:HG3	1:D:56:THR:HG22	1.83	0.60
1:D:87:GLY:O	1:D:88:LEU:HD23	2.02	0.60
1:B:262:GLN:OE1	1:B:270:ARG:NH1	2.35	0.60
1:A:141:ASN:O	1:A:152:ASN:CB	2.33	0.60
1:B:111:TYR:CE2	1:B:219:LYS:HE2	2.37	0.60
1:B:226:TYR:O	1:B:227:LEU:CD2	2.48	0.60
1:C:3:ILE:CD1	1:C:13:LEU:HB2	2.31	0.60
1:A:102:TYR:O	1:A:103:GLY:C	2.37	0.59
1:C:167:ARG:HD2	1:C:239:PRO:CB	2.31	0.59
1:A:205:LEU:O	1:A:250:PHE:O	2.19	0.59
1:C:144:PHE:O	1:C:145:PHE:CB	2.49	0.59
1:C:45:PHE:HE1	1:C:60:GLN:HA	1.67	0.59
1:D:127:ASP:O	1:D:127:ASP:OD1	2.20	0.59
1:A:22:TYR:CE1	1:A:118:PHE:CE1	2.91	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TYR:CE1	1:A:118:PHE:CZ	2.91	0.59
1:A:158:LEU:HD12	1:A:159:GLY:H	1.65	0.59
1:A:63:TYR:CE1	1:A:80:LYS:O	2.55	0.59
1:D:104:VAL:CG1	1:D:156:GLN:CD	2.67	0.59
1:D:167:ARG:HH11	1:D:167:ARG:CG	2.16	0.59
1:D:203:GLN:CB	1:D:204:PRO:HD2	2.13	0.59
1:D:262:GLN:HG2	1:D:272:SER:HB2	1.84	0.59
1:D:49:THR:O	1:D:49:THR:HG23	2.01	0.59
1:A:180:TYR:CD2	1:A:181:GLU:N	2.58	0.59
1:A:254:THR:HB	1:A:279:LYS:O	2.03	0.59
1:A:28:GLY:O	1:A:31:SER:N	2.28	0.59
1:B:233:GLU:HG2	1:B:254:THR:O	2.02	0.59
1:B:269:LEU:CD2	1:B:271:PRO:CD	2.80	0.59
1:B:45:PHE:C	1:B:45:PHE:CD1	2.74	0.59
1:B:71:GLU:CG	1:C:100:ARG:NH2	2.63	0.59
1:B:71:GLU:CG	1:C:100:ARG:HH21	2.16	0.59
1:C:303:PHE:CD2	1:C:307:MET:HG2	2.37	0.59
1:D:257:VAL:HG23	1:D:277:LYS:O	2.02	0.59
1:B:259:LEU:HB2	1:B:275:TYR:CB	2.32	0.59
1:B:5:ASN:O	1:B:6:LYS:HE2	2.03	0.59
1:C:109:LEU:O	1:C:111:TYR:N	2.36	0.59
1:C:153:PHE:N	1:C:153:PHE:HD1	1.99	0.59
1:B:111:TYR:OH	1:B:188:VAL:CG2	2.51	0.59
1:B:27:ASN:OD1	1:B:27:ASN:C	2.35	0.59
1:B:334:VAL:HG12	1:B:334:VAL:O	2.03	0.59
1:B:6:LYS:C	1:B:8:GLY:N	2.54	0.59
1:C:115:LEU:HD12	1:C:119:GLY:HA3	1.83	0.59
1:C:141:ASN:HB3	1:C:153:PHE:CD1	2.38	0.59
1:D:196:ARG:NH2	1:D:250:PHE:CD1	2.54	0.59
1:D:278:SER:HB3	1:D:292:VAL:HG23	1.85	0.59
1:A:274:ALA:CB	1:A:296:GLU:OE1	2.50	0.59
1:B:16:LYS:HB3	1:B:339:GLN:HB2	1.85	0.59
1:C:18:VAL:HG11	1:C:40:TYR:OH	2.02	0.59
1:D:211:ALA:HB2	1:D:236:ASN:O	2.02	0.59
1:D:74:ASP:C	1:D:76:GLN:N	2.57	0.59
1:A:279:LYS:HB2	1:A:279:LYS:NZ	2.16	0.59
1:B:101:ASN:CG	1:B:102:TYR:N	2.44	0.59
1:B:58:TYR:CD2	1:B:58:TYR:C	2.60	0.59
1:A:182:TYR:O	1:A:183:GLU:HB3	2.02	0.59
1:A:65:PHE:CE2	1:B:61:TRP:CZ2	2.91	0.59
1:A:71:GLU:OE2	1:B:132:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:TYR:HA	1:B:173:GLY:O	2.03	0.59
1:A:51:ILE:HG22	1:C:304:ASN:HD22	1.67	0.59
1:B:338:TYR:CZ	1:C:47:GLY:HA3	2.38	0.59
1:D:114:MET:O	1:D:115:LEU:O	2.21	0.59
1:A:130:VAL:O	1:A:130:VAL:CG2	2.51	0.58
1:A:132:ARG:NH2	1:C:71:GLU:OE1	2.36	0.58
1:A:284:GLU:O	1:A:286:ILE:CD1	2.50	0.58
1:C:132:ARG:HH11	1:C:132:ARG:CG	2.14	0.58
1:A:259:LEU:HB2	1:A:275:TYR:HB3	1.85	0.58
1:A:71:GLU:OE1	1:B:132:ARG:NH2	2.36	0.58
1:B:165:THR:CG2	1:B:166:ALA:H	2.16	0.58
1:C:144:PHE:HB3	1:C:148:VAL:CG2	2.33	0.58
1:D:90:TYR:C	1:D:90:TYR:CD2	2.75	0.58
1:B:108:ALA:O	1:B:109:LEU:C	2.41	0.58
1:D:5:ASN:O	1:D:6:LYS:CE	2.52	0.58
1:A:23:PHE:HB2	1:A:332:VAL:O	2.04	0.58
1:B:216:THR:OG1	1:B:216:THR:O	2.21	0.58
1:C:174:VAL:HG12	1:C:175:GLY:CA	2.33	0.58
1:D:122:THR:HG21	1:D:256:ASP:CG	2.22	0.58
1:D:290:ASP:HB2	1:D:318:ILE:HD11	1.85	0.58
1:A:129:PHE:CE2	1:A:192:GLY:C	2.74	0.58
1:B:230:ASN:O	1:B:257:VAL:HA	2.03	0.58
1:C:24:SER:HB3	1:C:31:SER:HB3	1.85	0.58
1:A:314:ILE:HB	1:A:331:THR:O	2.03	0.58
1:B:24:SER:OG	1:B:331:THR:OG1	2.17	0.58
1:B:277:LYS:CE	1:B:293:ASN:HD21	2.15	0.58
1:C:24:SER:HB2	1:C:35:ASN:HB2	1.85	0.58
1:D:85:PHE:CE1	1:D:101:ASN:ND2	2.71	0.58
1:D:167:ARG:O	1:D:167:ARG:CG	2.48	0.58
1:D:187:ILE:HG13	1:D:218:LEU:CD2	2.23	0.58
1:A:320:SER:C	1:A:322:ASN:H	2.05	0.58
1:B:111:TYR:H	1:B:111:TYR:HD1	1.52	0.58
1:B:162:GLU:O	1:B:163:ARG:C	2.42	0.58
1:B:274:ALA:HB2	1:B:296:GLU:OE1	2.02	0.58
1:D:314:ILE:CA	1:D:315:ILE:HD12	2.34	0.58
1:A:136:VAL:HG21	1:A:156:GLN:NE2	2.18	0.58
1:A:21:HIS:HD2	1:A:23:PHE:CZ	2.21	0.58
1:A:293:ASN:C	1:A:317:GLN:HB2	2.24	0.58
1:C:167:ARG:O	1:C:167:ARG:NH1	2.32	0.58
1:C:191:TYR:CG	1:C:192:GLY:N	2.71	0.58
1:C:214:TRP:HH2	1:C:231:TYR:CE2	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ASP:O	1:C:76:GLN:N	2.37	0.58
1:D:253:LYS:HE3	1:D:254:THR:O	2.03	0.58
1:D:47:GLY:O	1:D:58:TYR:HA	2.04	0.58
1:D:85:PHE:CD2	1:D:85:PHE:N	2.69	0.58
1:C:163:ARG:HG2	1:C:163:ARG:NH1	2.19	0.58
1:A:21:HIS:ND1	1:A:36:GLY:O	2.36	0.58
1:B:185:PHE:HE2	1:B:220:TYR:HE1	1.50	0.58
1:C:257:VAL:C	1:C:258:LEU:HD13	2.23	0.58
1:D:165:THR:HG22	1:D:167:ARG:H	1.68	0.58
1:A:128:PHE:CE1	1:A:170:ASN:HB2	2.39	0.57
1:A:308:SER:O	1:A:309:THR:CG2	2.52	0.57
1:B:110:GLY:O	1:B:111:TYR:C	2.41	0.57
1:D:200:GLN:O	1:D:201:GLU:C	2.42	0.57
1:A:152:ASN:H	1:A:152:ASN:HD22	1.49	0.57
1:A:267:PHE:CZ	1:A:269:LEU:CD1	2.87	0.57
1:B:321:ASP:OD1	1:D:282:ASP:HA	2.03	0.57
1:C:182:TYR:CE1	1:C:183:GLU:HB3	2.39	0.57
1:D:102:TYR:HD1	1:D:106:TYR:CD2	2.22	0.57
1:D:111:TYR:CE2	1:D:188:VAL:HG21	2.31	0.57
1:D:72:GLY:O	1:D:73:ALA:C	2.42	0.57
1:A:18:VAL:CB	1:A:40:TYR:CE1	2.82	0.57
1:B:64:ASN:O	1:B:79:ASN:HA	2.05	0.57
1:C:105:VAL:HA	1:C:190:ALA:CB	2.33	0.57
1:C:234:THR:OG1	1:C:254:THR:HG23	2.05	0.57
1:D:313:TYR:CB	1:D:332:VAL:HG13	2.33	0.57
1:A:151:LEU:HD23	1:A:151:LEU:O	2.05	0.57
1:C:206:GLY:HA2	1:C:250:PHE:O	2.03	0.57
1:D:96:PHE:HA	1:D:138:THR:O	2.04	0.57
1:A:141:ASN:HB2	1:A:153:PHE:CE1	2.39	0.57
1:B:205:LEU:HD11	1:B:247:THR:CG2	2.25	0.57
1:B:234:THR:C	1:B:235:ARG:HD3	2.25	0.57
1:B:276:THR:CB	1:B:294:TYR:CZ	2.88	0.57
1:B:48:GLU:HG3	1:B:56:THR:CG2	2.34	0.57
1:A:98:TYR:HE2	1:C:20:LEU:O	1.88	0.57
1:D:100:ARG:HG2	1:D:100:ARG:NH1	2.19	0.57
1:D:211:ALA:CB	1:D:236:ASN:O	2.52	0.57
1:D:303:PHE:O	1:D:304:ASN:HB3	2.04	0.57
1:A:100:ARG:HG3	1:A:134:GLY:HA2	1.85	0.57
1:A:1:ALA:O	1:A:3:ILE:HG22	2.04	0.57
1:A:4:TYR:HE2	1:A:6:LYS:H	1.51	0.57
1:B:300:THR:HG22	1:B:302:TYR:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:THR:CB	1:C:237:ALA:HB3	2.34	0.57
1:C:51:ILE:HD11	1:C:55:LEU:HD23	1.81	0.57
1:A:129:PHE:CD2	1:A:192:GLY:CA	2.76	0.57
1:B:180:TYR:CE2	1:B:182:TYR:HB2	2.39	0.57
1:B:276:THR:HB	1:B:294:TYR:CZ	2.38	0.57
1:B:302:TYR:O	1:B:303:PHE:O	2.22	0.57
1:B:293:ASN:OD1	1:B:317:GLN:CB	2.51	0.57
1:D:315:ILE:O	1:D:317:GLN:NE2	2.37	0.57
1:A:216:THR:O	1:A:230:ASN:HA	2.05	0.57
1:A:226:TYR:CE2	1:A:228:ALA:HB2	2.29	0.57
1:B:66:GLN:CG	1:B:78:GLY:HA3	2.35	0.57
1:A:18:VAL:CB	1:A:40:TYR:HE1	2.16	0.57
1:B:115:LEU:CG	1:B:119:GLY:HA3	2.34	0.57
1:C:155:VAL:O	1:C:155:VAL:CG1	2.50	0.57
1:C:313:TYR:CD1	1:C:332:VAL:HG23	2.39	0.57
1:D:265:PHE:HB3	1:D:267:PHE:HE1	1.69	0.57
1:D:301:TYR:N	1:D:309:THR:O	2.36	0.57
1:A:129:PHE:CZ	1:A:174:VAL:O	2.57	0.56
1:A:314:ILE:HG22	1:A:314:ILE:O	2.04	0.56
1:C:179:SER:CB	1:C:188:VAL:HG11	2.35	0.56
1:D:48:GLU:CG	1:D:56:THR:HG23	2.35	0.56
1:D:64:ASN:ND2	1:D:78:GLY:O	2.38	0.56
1:A:115:LEU:HG	1:A:119:GLY:CA	2.31	0.56
1:A:114:MET:SD	1:A:226:TYR:CE1	2.99	0.56
1:A:267:PHE:HZ	1:A:269:LEU:HD12	1.66	0.56
1:B:294:TYR:CD1	1:B:314:ILE:HG23	2.40	0.56
1:C:129:PHE:HE2	1:C:193:ALA:H	1.51	0.56
1:C:258:LEU:HD11	1:C:276:THR:HG23	1.85	0.56
1:B:141:ASN:HB3	1:B:153:PHE:CD1	2.40	0.56
1:B:180:TYR:HE2	1:B:182:TYR:HB2	1.69	0.56
1:C:127:ASP:O	1:C:128:PHE:HB2	2.05	0.56
1:C:270:ARG:N	1:C:271:PRO:CD	2.67	0.56
1:C:274:ALA:HB2	1:C:296:GLU:OE1	2.05	0.56
1:A:200:GLN:HE21	1:A:250:PHE:HZ	1.53	0.56
1:B:226:TYR:CE2	1:B:228:ALA:HB2	2.38	0.56
1:C:45:PHE:CE1	1:C:60:GLN:HA	2.40	0.56
1:D:177:SER:C	1:D:178:ILE:HG13	2.25	0.56
1:A:141:ASN:CB	1:A:153:PHE:HE1	2.02	0.56
1:A:21:HIS:HD2	1:A:23:PHE:CE2	2.22	0.56
1:C:3:ILE:HD13	1:C:13:LEU:HB3	1.88	0.56
1:D:100:ARG:HH11	1:D:100:ARG:HG2	1.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:PRO:O	1:D:271:PRO:HG2	2.05	0.56
1:B:2:GLU:OE2	1:B:5:ASN:CB	2.53	0.56
1:C:140:ARG:HA	1:C:154:ALA:HB2	1.88	0.56
1:D:55:LEU:CD1	1:D:90:TYR:CD1	2.76	0.56
1:A:245:THR:O	1:A:246:ASN:C	2.39	0.56
1:B:311:VAL:HG13	1:B:334:VAL:HG23	1.85	0.56
1:C:90:TYR:HB3	1:C:93:VAL:HB	1.88	0.56
1:D:32:TYR:CE2	1:D:314:ILE:HG13	2.40	0.56
1:D:48:GLU:HA	1:D:57:GLY:O	2.06	0.56
1:A:118:PHE:C	1:A:119:GLY:O	2.40	0.56
1:A:11:VAL:HG21	1:C:340:PHE:HB2	1.86	0.56
1:A:240:ILE:HG22	1:A:291:LEU:HD22	1.88	0.56
1:A:40:TYR:HE2	1:A:42:ARG:NH2	2.04	0.56
1:A:65:PHE:CZ	1:B:61:TRP:CH2	2.93	0.56
1:B:4:TYR:CD2	1:B:5:ASN:N	2.73	0.56
1:C:18:VAL:HG12	1:C:40:TYR:CE1	2.40	0.56
1:C:129:PHE:CE2	1:C:193:ALA:N	2.65	0.56
1:D:205:LEU:HA	1:D:284:GLU:HG3	1.86	0.56
1:A:201:GLU:OE1	1:A:208:GLY:O	2.23	0.56
1:A:279:LYS:CB	1:A:279:LYS:HZ3	2.18	0.56
1:B:162:GLU:C	1:B:163:ARG:O	2.42	0.56
1:B:167:ARG:HD2	1:B:239:PRO:CB	2.36	0.56
1:B:187:ILE:CG2	1:B:187:ILE:O	2.54	0.56
1:D:309:THR:CG2	1:D:336:ILE:HA	2.25	0.56
1:B:143:ASN:O	1:B:147:LEU:N	2.39	0.56
1:B:234:THR:O	1:B:235:ARG:HD3	2.05	0.56
1:D:151:LEU:O	1:D:151:LEU:HG	1.93	0.56
1:D:313:TYR:HA	1:D:332:VAL:HG13	1.88	0.56
1:D:66:GLN:NE2	1:D:68:ASN:HD21	2.04	0.56
1:A:82:ARG:CG	1:A:132:ARG:HH21	2.19	0.56
1:B:276:THR:HG22	1:B:294:TYR:HE2	1.52	0.56
1:C:271:PRO:HA	1:C:299:ALA:HB2	1.88	0.56
1:C:60:GLN:HE21	1:C:85:PHE:HE1	1.54	0.56
1:D:205:LEU:HG	1:D:247:THR:CG2	2.36	0.56
1:A:109:LEU:O	1:A:110:GLY:C	2.43	0.55
1:B:206:GLY:N	1:B:284:GLU:OE2	2.38	0.55
1:B:6:LYS:C	1:B:8:GLY:H	2.08	0.55
1:C:179:SER:CA	1:C:188:VAL:CG1	2.70	0.55
1:C:231:TYR:CD2	1:C:232:GLY:N	2.74	0.55
1:D:51:ILE:HD12	1:D:55:LEU:HG	1.88	0.55
1:B:214:TRP:O	1:B:215:ALA:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ASP:N	1:C:114:MET:HG2	2.20	0.55
1:C:142:SER:O	1:C:143:ASN:C	2.44	0.55
1:C:326:VAL:HG12	1:C:327:GLY:O	2.05	0.55
1:A:11:VAL:HG11	1:C:340:PHE:CD2	2.41	0.55
1:A:127:ASP:OD1	1:A:239:PRO:CD	2.44	0.55
1:A:250:PHE:N	1:A:250:PHE:CD1	2.73	0.55
1:A:307:MET:HG3	1:A:308:SER:N	2.21	0.55
1:B:301:TYR:CD2	1:B:302:TYR:N	2.75	0.55
1:B:313:TYR:CE1	1:B:332:VAL:HG23	2.37	0.55
1:C:139:TYR:CD1	1:C:139:TYR:C	2.76	0.55
1:C:74:ASP:C	1:C:76:GLN:N	2.58	0.55
1:D:226:TYR:HE2	1:D:228:ALA:CB	2.18	0.55
1:A:40:TYR:CE2	1:A:42:ARG:NH2	2.74	0.55
1:A:58:TYR:C	1:C:338:TYR:CD1	2.78	0.55
1:A:200:GLN:NE2	1:A:250:PHE:CZ	2.75	0.55
1:A:271:PRO:CA	1:A:299:ALA:CB	2.66	0.55
1:B:264:GLN:HA	1:B:270:ARG:HB2	1.89	0.55
1:B:14:TYR:CA	1:B:340:PHE:HE2	2.18	0.55
1:A:166:ALA:O	1:A:168:ARG:N	2.39	0.55
1:C:115:LEU:HD22	1:C:296:GLU:OE2	2.07	0.55
1:D:191:TYR:HD1	1:D:213:GLN:O	1.89	0.55
1:A:130:VAL:O	1:A:130:VAL:HG23	2.06	0.55
1:B:96:PHE:C	1:B:96:PHE:CD2	2.64	0.55
1:C:153:PHE:N	1:C:153:PHE:CD1	2.72	0.55
1:C:339:GLN:HG3	1:C:339:GLN:O	2.07	0.55
1:D:40:TYR:N	1:D:40:TYR:HD1	2.04	0.55
1:A:104:VAL:N	1:A:156:GLN:OE1	2.39	0.55
1:A:219:LYS:HA	1:A:227:LEU:O	2.07	0.55
1:A:86:ALA:CB	1:C:336:ILE:HG13	2.33	0.55
1:D:13:LEU:HG	1:D:13:LEU:O	2.07	0.55
1:D:111:TYR:CD2	1:D:219:LYS:HG2	2.42	0.55
1:D:52:ASN:CG	1:D:53:SER:H	2.10	0.55
1:A:22:TYR:HD2	1:A:38:MET:HG3	1.63	0.54
1:A:85:PHE:CE2	1:A:101:ASN:ND2	2.76	0.54
1:C:85:PHE:CD2	1:C:101:ASN:ND2	2.76	0.54
1:C:24:SER:HB3	1:C:31:SER:CB	2.37	0.54
1:C:69:ASN:ND2	1:C:77:THR:H	2.05	0.54
1:D:270:ARG:HD2	1:D:302:TYR:OH	2.07	0.54
1:D:313:TYR:CD1	1:D:332:VAL:HG13	2.42	0.54
1:D:58:TYR:HE2	1:D:87:GLY:C	2.10	0.54
1:A:242:ASN:C	1:A:244:PHE:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:TYR:C	1:B:340:PHE:CE2	2.65	0.54
1:C:198:ASN:O	1:C:200:GLN:N	2.40	0.54
1:A:105:VAL:O	1:A:105:VAL:HG13	2.07	0.54
1:A:284:GLU:C	1:A:286:ILE:HD13	2.26	0.54
1:A:318:ILE:HG13	1:A:326:VAL:HG12	1.88	0.54
1:C:144:PHE:HB2	1:C:151:LEU:HD23	1.88	0.54
1:C:167:ARG:HD2	1:C:239:PRO:HB3	1.90	0.54
1:C:20:LEU:HB3	1:C:38:MET:HB2	1.90	0.54
1:D:86:ALA:O	1:D:97:ASP:CB	2.55	0.54
1:A:249:GLY:C	1:A:250:PHE:CD1	2.81	0.54
1:A:1:ALA:O	1:A:3:ILE:CG2	2.55	0.54
1:B:4:TYR:CE2	1:B:6:LYS:CB	2.86	0.54
1:C:220:TYR:HE1	1:C:222:ALA:HB3	1.66	0.54
1:D:144:PHE:CE2	1:D:145:PHE:HB2	2.42	0.54
1:D:167:ARG:NH1	1:D:167:ARG:CG	2.68	0.54
1:D:155:VAL:O	1:D:155:VAL:CG1	2.54	0.54
1:D:137:ALA:O	1:D:156:GLN:HA	2.07	0.54
1:A:155:VAL:CG2	1:A:156:GLN:N	2.71	0.54
1:A:39:THR:O	1:A:67:GLY:HA3	2.06	0.54
1:B:141:ASN:OD1	1:B:153:PHE:CE1	2.59	0.54
1:C:42:ARG:NH1	1:C:82:ARG:HH21	1.96	0.54
1:B:1:ALA:HB2	1:C:4:TYR:CD2	2.43	0.54
1:D:1:ALA:HB2	1:D:340:PHE:C	2.28	0.54
1:D:223:ASN:O	1:D:224:ASN:CB	2.41	0.54
1:D:115:LEU:HD12	1:D:296:GLU:HG3	1.89	0.54
1:A:296:GLU:HG2	1:A:297:VAL:H	1.72	0.54
1:B:235:ARG:HD3	1:B:235:ARG:N	2.19	0.54
1:B:271:PRO:HA	1:B:299:ALA:CB	2.37	0.54
1:C:51:ILE:O	1:C:52:ASN:HB3	2.08	0.54
1:D:157:TYR:CD2	1:D:157:TYR:N	2.75	0.54
1:D:163:ARG:HD2	1:D:168:ARG:O	2.08	0.54
1:D:280:ALA:O	1:D:288:ASP:HA	2.07	0.54
1:D:302:TYR:C	1:D:304:ASN:N	2.61	0.54
1:A:4:TYR:CD2	1:A:5:ASN:N	2.76	0.54
1:B:109:LEU:HD11	1:B:122:THR:HB	1.90	0.54
1:B:167:ARG:HD2	1:B:239:PRO:HB2	1.90	0.54
1:B:277:LYS:HE3	1:B:293:ASN:HD21	1.72	0.54
1:A:65:PHE:CG	1:B:61:TRP:CZ2	2.95	0.54
1:C:90:TYR:CD2	1:C:93:VAL:CG2	2.90	0.54
1:A:223:ASN:N	1:A:223:ASN:HD22	2.06	0.54
1:A:242:ASN:C	1:A:244:PHE:N	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:CD1	1:B:119:GLY:CA	2.50	0.54
1:B:265:PHE:HB2	1:B:269:LEU:O	2.08	0.54
1:A:336:ILE:HD11	1:B:87:GLY:CA	2.37	0.54
1:C:240:ILE:HD13	1:C:251:ALA:H	1.70	0.54
1:C:263:TYR:CD2	1:C:265:PHE:CZ	2.95	0.54
1:D:102:TYR:CD1	1:D:106:TYR:CD2	2.96	0.54
1:A:26:GLY:O	1:A:28:GLY:N	2.41	0.54
1:A:318:ILE:HG13	1:A:326:VAL:CG1	2.38	0.54
1:B:48:GLU:HA	1:B:58:TYR:HA	1.90	0.54
1:C:325:GLY:O	1:C:326:VAL:C	2.44	0.54
1:C:74:ASP:O	1:C:75:ALA:C	2.41	0.54
1:D:266:ASP:C	1:D:268:GLY:H	2.09	0.54
1:A:136:VAL:HG23	1:A:137:ALA:N	2.23	0.53
1:A:24:SER:O	1:A:25:LYS:C	2.45	0.53
1:A:311:VAL:CG2	1:A:334:VAL:HG22	2.38	0.53
1:B:208:GLY:HA3	1:B:236:ASN:ND2	2.23	0.53
1:B:65:PHE:CE2	1:C:61:TRP:CZ2	2.96	0.53
1:C:114:MET:O	1:C:115:LEU:C	2.44	0.53
1:D:14:TYR:CE2	1:D:44:GLY:C	2.82	0.53
1:A:293:ASN:ND2	1:A:317:GLN:CB	2.66	0.53
1:A:65:PHE:CD1	1:B:61:TRP:CZ2	2.89	0.53
1:A:96:PHE:O	1:A:97:ASP:HB3	2.07	0.53
1:B:63:TYR:HE2	1:B:79:ASN:HB3	1.73	0.53
1:C:85:PHE:CD2	1:C:101:ASN:HB2	2.33	0.53
1:C:251:ALA:O	1:C:252:ASN:C	2.47	0.53
1:C:23:PHE:CA	1:C:35:ASN:HD22	2.15	0.53
1:B:268:GLY:O	1:B:301:TYR:HD2	1.92	0.53
1:C:37:ASP:O	1:C:38:MET:HG2	2.07	0.53
1:B:87:GLY:C	1:B:88:LEU:CG	2.77	0.53
1:C:226:TYR:C	1:C:227:LEU:HD23	2.29	0.53
1:D:208:GLY:HA3	1:D:236:ASN:HD22	1.72	0.53
1:B:4:TYR:HE2	1:B:6:LYS:CB	2.19	0.53
1:C:223:ASN:CB	1:C:225:ILE:HD12	2.37	0.53
1:C:286:ILE:HG21	1:C:323:LYS:HB3	1.91	0.53
1:D:279:LYS:HE3	1:D:281:LYS:HZ3	1.70	0.53
1:A:108:ALA:O	1:A:109:LEU:C	2.46	0.53
1:B:196:ARG:HD3	1:B:208:GLY:O	2.08	0.53
1:B:204:PRO:HD2	1:B:248:SER:O	2.09	0.53
1:D:100:ARG:HA	1:D:134:GLY:HA2	1.89	0.53
1:D:114:MET:O	1:D:115:LEU:C	2.46	0.53
1:D:160:LYS:CB	1:D:172:ASP:OD1	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ASN:HD22	1:D:317:GLN:HB3	1.73	0.53
1:A:114:MET:C	1:A:115:LEU:HD23	2.17	0.53
1:A:82:ARG:HH11	1:A:82:ARG:CG	2.21	0.53
1:A:62:GLU:OE2	1:A:82:ARG:NH2	2.41	0.53
1:B:205:LEU:HD21	1:B:247:THR:CG2	2.36	0.53
1:D:127:ASP:O	1:D:127:ASP:CG	2.45	0.53
1:D:182:TYR:CZ	1:D:183:GLU:HB3	2.44	0.53
1:A:16:LYS:HG2	1:A:42:ARG:HB2	1.91	0.53
1:A:51:ILE:CG2	1:C:304:ASN:HD22	2.15	0.53
1:A:72:GLY:O	1:A:74:ASP:N	2.42	0.53
1:B:273:ILE:HG23	1:B:274:ALA:N	2.23	0.53
1:A:163:ARG:NH1	1:C:70:SER:H	2.07	0.53
1:D:27:ASN:C	1:D:29:GLU:N	2.62	0.53
1:D:48:GLU:HG2	1:D:49:THR:N	2.24	0.53
1:A:226:TYR:C	1:A:226:TYR:CD2	2.82	0.53
1:B:118:PHE:CZ	1:B:333:ALA:HB2	2.43	0.53
1:B:25:LYS:O	1:B:27:ASN:N	2.42	0.53
1:C:74:ASP:C	1:C:76:GLN:H	2.10	0.53
1:D:208:GLY:HA3	1:D:236:ASN:HD21	1.73	0.53
1:D:273:ILE:HD13	1:D:297:VAL:HG23	1.89	0.53
1:A:172:ASP:C	1:A:194:ALA:HB1	2.24	0.53
1:B:85:PHE:CD2	1:B:101:ASN:HB2	2.44	0.53
1:B:265:PHE:N	1:B:269:LEU:O	2.38	0.53
1:B:18:VAL:O	1:B:39:THR:HA	2.09	0.53
1:B:54:ASP:HB2	1:B:90:TYR:CE1	2.44	0.53
1:C:18:VAL:CG1	1:C:40:TYR:CZ	2.82	0.53
1:C:283:VAL:CG2	1:C:287:GLY:O	2.52	0.53
1:D:115:LEU:H	1:D:115:LEU:HD23	0.44	0.53
1:D:232:GLY:C	1:D:233:GLU:HG3	2.29	0.53
1:A:136:VAL:CG2	1:A:156:GLN:HE21	2.23	0.52
1:B:251:ALA:O	1:B:252:ASN:C	2.47	0.52
1:B:300:THR:HG21	1:B:302:TYR:HE1	1.69	0.52
1:D:165:THR:CG2	1:D:166:ALA:N	2.72	0.52
1:D:158:LEU:HB3	1:D:173:GLY:CA	2.39	0.52
1:D:278:SER:HB3	1:D:292:VAL:CG2	2.38	0.52
1:A:100:ARG:HG2	1:A:134:GLY:CA	2.31	0.52
1:A:83:LEU:HD23	1:A:101:ASN:HA	1.91	0.52
1:A:23:PHE:O	1:A:24:SER:OG	2.22	0.52
1:A:279:LYS:HB3	1:A:279:LYS:HZ3	1.72	0.52
1:A:301:TYR:O	1:A:308:SER:HA	2.09	0.52
1:C:182:TYR:O	1:C:183:GLU:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LEU:HD11	1:C:299:ALA:HB1	1.92	0.52
1:C:294:TYR:CD1	1:C:314:ILE:CD1	2.92	0.52
1:C:318:ILE:CG2	1:C:319:ASP:H	2.17	0.52
1:D:25:LYS:HE2	1:D:329:ASP:CG	2.30	0.52
1:D:266:ASP:C	1:D:268:GLY:N	2.63	0.52
1:D:318:ILE:HG23	1:D:319:ASP:N	1.98	0.52
1:A:161:ASN:HB2	1:A:170:ASN:OD1	2.09	0.52
1:A:214:TRP:CE2	1:A:233:GLU:HB2	2.44	0.52
1:A:313:TYR:HB2	1:A:332:VAL:HG22	1.90	0.52
1:B:48:GLU:OE1	1:B:56:THR:HG21	2.08	0.52
1:B:5:ASN:HA	1:B:10:LYS:HA	1.91	0.52
1:C:58:TYR:O	1:C:58:TYR:HD1	1.92	0.52
1:A:340:PHE:CE1	1:B:45:PHE:CE2	2.97	0.52
1:A:226:TYR:C	1:A:226:TYR:HD2	2.13	0.52
1:B:267:PHE:CD1	1:B:267:PHE:N	2.73	0.52
1:C:114:MET:HE1	1:C:226:TYR:CE1	2.45	0.52
1:C:82:ARG:HG2	1:C:82:ARG:HH11	1.74	0.52
1:D:12:ASP:HB3	1:D:46:LYS:O	2.08	0.52
1:D:58:TYR:CE2	1:D:87:GLY:C	2.83	0.52
1:A:214:TRP:CZ2	1:A:233:GLU:HB2	2.44	0.52
1:A:116:PRO:O	1:A:310:TYR:CE2	2.63	0.52
1:B:212:GLU:H	1:B:235:ARG:HB2	1.75	0.52
1:A:197:THR:O	1:A:200:GLN:N	2.43	0.52
1:A:26:GLY:C	1:A:28:GLY:N	2.63	0.52
1:B:172:ASP:O	1:B:194:ALA:HA	2.10	0.52
1:C:64:ASN:ND2	1:C:80:LYS:HE2	2.24	0.52
1:D:182:TYR:CD2	1:D:182:TYR:C	2.77	0.52
1:A:331:THR:CG2	1:A:332:VAL:N	2.71	0.52
1:B:104:VAL:HG21	1:B:176:GLY:HA2	1.92	0.52
1:C:193:ALA:HB2	1:C:212:GLU:HB3	1.91	0.52
1:D:319:ASP:CG	1:D:320:SER:N	2.61	0.52
1:B:269:LEU:HD21	1:B:271:PRO:HD3	1.91	0.52
1:C:318:ILE:HG13	1:C:326:VAL:CG1	2.39	0.52
1:B:1:ALA:CB	1:C:4:TYR:CD2	2.93	0.52
1:D:104:VAL:N	1:D:156:GLN:OE1	2.43	0.52
1:B:186:GLY:HA3	1:B:219:LYS:HE3	1.92	0.52
1:C:196:ARG:NH2	1:C:250:PHE:CD1	2.78	0.52
1:D:244:PHE:C	1:D:246:ASN:H	2.12	0.52
1:D:286:ILE:CG2	1:D:323:LYS:HB3	2.39	0.52
1:A:163:ARG:NH1	1:C:70:SER:N	2.58	0.51
1:A:286:ILE:CD1	1:A:286:ILE:N	2.71	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:ILE:CD1	1:C:251:ALA:CB	2.88	0.51
1:C:242:ASN:ND2	1:C:245:THR:OG1	2.43	0.51
1:C:203:GLN:CB	1:C:248:SER:O	2.58	0.51
1:A:102:TYR:CE1	1:A:106:TYR:CE2	2.99	0.51
1:C:310:TYR:C	1:C:310:TYR:HD1	2.05	0.51
1:D:32:TYR:CD2	1:D:32:TYR:C	2.83	0.51
1:B:291:LEU:C	1:B:292:VAL:CG2	2.79	0.51
1:B:294:TYR:CE1	1:B:314:ILE:CD1	2.87	0.51
1:B:63:TYR:CE2	1:B:79:ASN:HB3	2.45	0.51
1:D:160:LYS:HD3	1:D:162:GLU:OE2	2.11	0.51
1:A:22:TYR:CE1	1:A:333:ALA:CB	2.91	0.51
1:A:320:SER:C	1:A:322:ASN:N	2.64	0.51
1:A:45:PHE:C	1:A:45:PHE:HD1	2.07	0.51
1:A:56:THR:O	1:A:88:LEU:HA	2.10	0.51
1:B:14:TYR:HA	1:B:340:PHE:CE2	2.46	0.51
1:D:31:SER:HA	1:D:329:ASP:H	1.74	0.51
1:A:82:ARG:CG	1:A:132:ARG:NH2	2.73	0.51
1:A:139:TYR:CD1	1:A:140:ARG:N	2.79	0.51
1:A:163:ARG:HG3	1:A:169:SER:OG	2.11	0.51
1:B:148:VAL:O	1:B:149:ASP:C	2.49	0.51
1:B:167:ARG:CG	1:B:167:ARG:O	2.55	0.51
1:B:169:SER:O	1:B:170:ASN:HB3	2.09	0.51
1:B:273:ILE:HD12	1:B:296:GLU:O	2.10	0.51
1:B:48:GLU:HG3	1:B:56:THR:HG22	1.93	0.51
1:B:5:ASN:O	1:B:5:ASN:OD1	2.27	0.51
1:C:152:ASN:N	1:C:152:ASN:ND2	2.58	0.51
1:C:167:ARG:HD2	1:C:239:PRO:HB2	1.92	0.51
1:D:18:VAL:HG11	1:D:40:TYR:CE1	2.45	0.51
1:A:272:SER:N	1:A:298:GLY:O	2.42	0.51
1:A:293:ASN:CB	1:A:317:GLN:HB2	2.40	0.51
1:B:302:TYR:O	1:B:304:ASN:N	2.43	0.51
1:C:3:ILE:HD13	1:C:13:LEU:CB	2.40	0.51
1:C:296:GLU:HG2	1:C:297:VAL:N	2.26	0.51
1:D:104:VAL:HG12	1:D:156:GLN:CD	2.30	0.51
1:D:3:ILE:HD13	1:D:13:LEU:HB3	1.92	0.51
1:D:241:THR:HG22	1:D:242:ASN:N	2.25	0.51
1:A:113:ASP:OD1	1:A:113:ASP:C	2.49	0.51
1:B:229:ALA:CB	1:B:258:LEU:O	2.55	0.51
1:B:318:ILE:CG2	1:B:319:ASP:N	2.73	0.51
1:B:332:VAL:HG13	1:B:332:VAL:O	1.97	0.51
1:B:54:ASP:O	1:B:90:TYR:HD1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ASP:O	1:A:194:ALA:HB2	1.99	0.51
1:A:21:HIS:CE1	1:A:36:GLY:C	2.85	0.51
1:A:237:ALA:O	1:A:239:PRO:HD3	2.11	0.51
1:A:245:THR:O	1:A:246:ASN:O	2.28	0.51
1:B:138:THR:OG1	1:B:156:GLN:NE2	2.42	0.51
1:B:167:ARG:CG	1:B:167:ARG:NH1	2.55	0.51
1:B:284:GLU:O	1:B:286:ILE:HD13	2.10	0.51
1:C:144:PHE:CD2	1:C:144:PHE:C	2.84	0.51
1:C:309:THR:HG22	1:C:336:ILE:CA	2.26	0.51
1:D:109:LEU:O	1:D:110:GLY:O	2.29	0.51
1:D:265:PHE:HB3	1:D:267:PHE:CE1	2.46	0.51
1:D:313:TYR:CZ	1:D:315:ILE:HG13	2.46	0.51
1:D:76:GLN:O	1:D:79:ASN:HB2	2.11	0.51
1:B:9:ASN:HA	1:B:49:THR:HA	1.92	0.51
1:C:205:LEU:HA	1:C:284:GLU:HG3	1.92	0.51
1:C:196:ARG:HH22	1:C:250:PHE:HB2	1.74	0.51
1:C:123:ALA:HB1	1:C:130:VAL:O	2.11	0.51
1:C:161:ASN:HB2	1:C:170:ASN:ND2	2.26	0.51
1:A:105:VAL:O	1:A:105:VAL:CG1	2.50	0.50
1:A:153:PHE:N	1:A:153:PHE:CD1	2.54	0.50
1:B:114:MET:CE	1:B:226:TYR:CD1	2.92	0.50
1:B:275:TYR:HE1	1:B:295:PHE:CE1	2.29	0.50
1:A:65:PHE:CD2	1:B:61:TRP:CZ2	2.99	0.50
1:D:90:TYR:HD2	1:D:93:VAL:HG23	1.76	0.50
1:A:170:ASN:ND2	1:A:171:GLY:O	2.44	0.50
1:B:296:GLU:CG	1:B:314:ILE:HD13	2.42	0.50
1:D:102:TYR:N	1:D:102:TYR:HD2	2.07	0.50
1:A:139:TYR:O	1:A:154:ALA:CA	2.60	0.50
1:B:24:SER:H	1:B:35:ASN:CG	2.14	0.50
1:B:231:TYR:HA	1:B:256:ASP:O	2.11	0.50
1:B:263:TYR:HD1	1:B:264:GLN:H	1.58	0.50
1:C:85:PHE:HE2	1:C:101:ASN:ND2	2.10	0.50
1:C:160:LYS:CE	1:C:160:LYS:CA	2.88	0.50
1:C:211:ALA:C	1:C:212:GLU:HG3	2.30	0.50
1:C:25:LYS:NZ	1:C:25:LYS:CB	2.71	0.50
1:C:263:TYR:CD1	1:C:264:GLN:N	2.78	0.50
1:C:307:MET:CG	1:C:308:SER:N	2.51	0.50
1:D:293:ASN:O	1:D:317:GLN:N	2.44	0.50
1:B:338:TYR:CG	1:B:339:GLN:N	2.79	0.50
1:A:61:TRP:CH2	1:C:65:PHE:HE1	2.26	0.50
1:D:87:GLY:HA3	1:D:97:ASP:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ALA:HA	1:D:258:LEU:O	2.12	0.50
1:D:204:PRO:HG2	1:D:248:SER:O	2.11	0.50
1:D:307:MET:CG	1:D:308:SER:H	2.16	0.50
1:A:167:ARG:HG2	1:A:167:ARG:NH1	2.17	0.50
1:A:1:ALA:HB1	1:B:4:TYR:CZ	2.40	0.50
1:B:137:ALA:O	1:B:156:GLN:HA	2.11	0.50
1:B:179:SER:CB	1:B:188:VAL:HG13	2.42	0.50
1:A:66:GLN:CG	1:A:78:GLY:O	2.58	0.50
1:A:65:PHE:CE2	1:B:61:TRP:CH2	3.00	0.50
1:D:239:PRO:HB3	1:D:250:PHE:HE2	1.77	0.50
1:D:280:ALA:HB2	1:D:291:LEU:HD11	1.94	0.50
1:D:85:PHE:HE1	1:D:101:ASN:ND2	2.09	0.50
1:B:106:TYR:CD2	1:B:106:TYR:O	2.64	0.50
1:B:123:ALA:CA	1:B:130:VAL:HG23	2.37	0.50
1:B:143:ASN:OD1	1:B:149:ASP:HA	2.12	0.50
1:B:231:TYR:HD1	1:B:232:GLY:H	1.58	0.50
1:B:2:GLU:CD	1:B:5:ASN:HB2	2.32	0.50
1:B:63:TYR:CD2	1:B:64:ASN:N	2.80	0.50
1:C:136:VAL:CG1	1:C:158:LEU:CD1	2.90	0.50
1:C:262:GLN:HG2	1:C:272:SER:HB2	1.92	0.50
1:B:1:ALA:CB	1:C:4:TYR:CE2	2.93	0.50
1:D:160:LYS:HA	1:D:171:GLY:O	2.12	0.50
1:A:123:ALA:HA	1:A:130:VAL:HG21	1.94	0.50
1:A:71:GLU:CD	1:B:100:ARG:HH21	2.15	0.50
1:B:242:ASN:C	1:B:244:PHE:H	2.12	0.50
1:C:309:THR:CG2	1:C:336:ILE:HA	2.25	0.50
1:D:229:ALA:CA	1:D:259:LEU:HD23	2.40	0.50
1:A:319:ASP:O	1:A:322:ASN:N	2.45	0.49
1:B:205:LEU:CA	1:B:284:GLU:OE2	2.59	0.49
1:B:76:GLN:O	1:B:77:THR:C	2.47	0.49
1:D:1:ALA:HB2	1:D:340:PHE:OXT	2.12	0.49
1:A:179:SER:CB	1:A:188:VAL:CG1	2.90	0.49
1:A:20:LEU:CD1	1:A:335:GLY:CA	2.87	0.49
1:A:322:ASN:O	1:A:322:ASN:OD1	2.28	0.49
1:B:193:ALA:HB2	1:B:212:GLU:HB3	1.94	0.49
1:C:144:PHE:CD1	1:C:151:LEU:CD2	2.95	0.49
1:C:222:ALA:O	1:C:223:ASN:CB	2.47	0.49
1:D:268:GLY:O	1:D:302:TYR:HD2	1.95	0.49
1:D:312:ASP:O	1:D:332:VAL:HG12	2.12	0.49
1:A:211:ALA:CB	1:A:236:ASN:CB	2.71	0.49
1:A:315:ILE:CA	1:A:330:ASP:OD1	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LYS:HA	1:B:227:LEU:O	2.12	0.49
1:B:231:TYR:C	1:B:231:TYR:CD1	2.79	0.49
1:C:141:ASN:OD1	1:C:153:PHE:HE1	1.94	0.49
1:C:242:ASN:CG	1:C:245:THR:OG1	2.51	0.49
1:D:115:LEU:CB	1:D:116:PRO:CD	2.90	0.49
1:D:21:HIS:ND1	1:D:37:ASP:HA	2.27	0.49
1:D:301:TYR:CD1	1:D:303:PHE:CE1	3.01	0.49
1:A:58:TYR:HA	1:C:338:TYR:CE1	2.47	0.49
1:B:215:ALA:C	1:B:216:THR:CG2	2.79	0.49
1:C:165:THR:HB	1:C:168:ARG:HG2	1.94	0.49
1:C:196:ARG:NH2	1:C:250:PHE:HD1	2.11	0.49
1:C:274:ALA:HB3	1:C:296:GLU:CD	2.33	0.49
1:C:83:LEU:HD11	1:C:102:TYR:CE2	2.43	0.49
1:A:52:ASN:C	1:A:52:ASN:OD1	2.50	0.49
1:B:139:TYR:HB3	1:B:155:VAL:HG13	1.95	0.49
1:B:226:TYR:HD2	1:B:227:LEU:N	2.10	0.49
1:B:119:GLY:HA2	1:B:294:TYR:OH	2.13	0.49
1:D:211:ALA:C	1:D:212:GLU:HG3	2.33	0.49
1:D:242:ASN:ND2	1:D:245:THR:OG1	2.45	0.49
1:A:132:ARG:HH11	1:A:132:ARG:CG	1.94	0.49
1:A:83:LEU:O	1:A:84:ALA:HB2	2.11	0.49
1:B:179:SER:HB2	1:B:188:VAL:HG13	1.95	0.49
1:B:297:VAL:HG12	1:B:298:GLY:N	2.26	0.49
1:B:308:SER:O	1:B:309:THR:HG23	2.12	0.49
1:A:334:VAL:CG1	1:A:335:GLY:N	2.65	0.49
1:A:55:LEU:HG	1:A:56:THR:H	1.76	0.49
1:C:100:ARG:CG	1:C:133:VAL:O	2.59	0.49
1:A:88:LEU:CD1	1:C:303:PHE:HE2	2.21	0.49
1:C:42:ARG:NH1	1:C:82:ARG:CZ	2.72	0.49
1:D:198:ASN:O	1:D:202:ALA:N	2.35	0.49
1:A:132:ARG:NH2	1:C:71:GLU:OE2	2.46	0.49
1:A:151:LEU:HA	1:A:179:SER:O	2.13	0.49
1:B:313:TYR:HE2	1:B:315:ILE:HG13	1.75	0.49
1:C:217:GLY:HA3	1:C:230:ASN:HD21	1.78	0.49
1:C:80:LYS:N	1:C:80:LYS:HD3	2.28	0.49
1:A:21:HIS:ND1	1:A:36:GLY:C	2.66	0.49
1:A:259:LEU:O	1:A:260:VAL:HG22	2.13	0.49
1:C:145:PHE:C	1:C:147:LEU:N	2.64	0.49
1:C:160:LYS:CE	1:C:160:LYS:HA	2.31	0.49
1:C:289:VAL:HG11	1:C:323:LYS:CB	2.41	0.49
1:C:314:ILE:HA	1:C:314:ILE:HD13	1.69	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ALA:O	1:C:97:ASP:HA	2.12	0.49
1:D:144:PHE:CE2	1:D:145:PHE:CD2	3.00	0.49
1:D:307:MET:O	1:D:308:SER:CB	2.60	0.49
1:A:24:SER:CB	1:A:331:THR:OG1	2.61	0.49
1:A:306:ASN:HD21	1:B:9:ASN:ND2	2.10	0.49
1:C:115:LEU:N	1:C:115:LEU:HD23	2.18	0.49
1:C:235:ARG:O	1:C:237:ALA:HB2	2.12	0.49
1:D:117:GLU:HG2	1:D:333:ALA:CB	2.43	0.49
1:A:4:TYR:C	1:A:4:TYR:CD2	2.86	0.48
1:B:215:ALA:C	1:B:216:THR:HG23	2.34	0.48
1:C:153:PHE:O	1:C:154:ALA:CB	2.60	0.48
1:A:214:TRP:HZ2	1:A:233:GLU:OE2	1.96	0.48
1:B:118:PHE:O	1:B:119:GLY:O	2.30	0.48
1:B:63:TYR:CD2	1:B:65:PHE:CD1	3.01	0.48
1:A:18:VAL:HB	1:A:40:TYR:CD1	2.45	0.48
1:A:220:TYR:O	1:A:220:TYR:CG	2.64	0.48
1:A:240:ILE:HD13	1:A:251:ALA:HB2	1.95	0.48
1:C:139:TYR:HD1	1:C:140:ARG:N	2.10	0.48
1:C:144:PHE:HD1	1:C:151:LEU:HD23	1.78	0.48
1:D:132:ARG:NH1	1:D:132:ARG:CB	2.75	0.48
1:D:144:PHE:CD2	1:D:145:PHE:HB2	2.47	0.48
1:A:277:LYS:HA	1:A:292:VAL:O	2.12	0.48
1:A:61:TRP:CZ2	1:C:65:PHE:HE1	2.25	0.48
1:B:291:LEU:C	1:B:292:VAL:HG23	2.32	0.48
1:B:304:ASN:ND2	1:C:51:ILE:CG2	2.77	0.48
1:A:124:TYR:HB2	1:A:127:ASP:HB2	1.93	0.48
1:A:166:ALA:C	1:A:168:ARG:H	2.16	0.48
1:A:171:GLY:HA3	1:A:195:ASP:HB2	1.94	0.48
1:A:281:LYS:O	1:A:282:ASP:CB	2.51	0.48
1:B:110:GLY:C	1:B:112:THR:H	2.15	0.48
1:B:276:THR:HG21	1:B:294:TYR:CZ	2.40	0.48
1:C:139:TYR:O	1:C:154:ALA:CA	2.61	0.48
1:C:153:PHE:O	1:C:154:ALA:HB2	2.12	0.48
1:C:167:ARG:HG3	1:C:167:ARG:NH1	2.06	0.48
1:C:172:ASP:C	1:C:194:ALA:HB2	2.29	0.48
1:C:284:GLU:O	1:C:286:ILE:HD11	2.13	0.48
1:D:212:GLU:O	1:D:234:THR:HA	2.13	0.48
1:D:264:GLN:NE2	1:D:268:GLY:HA2	2.28	0.48
1:D:273:ILE:HG23	1:D:274:ALA:N	2.27	0.48
1:A:24:SER:OG	1:A:331:THR:CB	2.60	0.48
1:B:86:ALA:O	1:B:97:ASP:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ARG:HH11	1:C:163:ARG:CG	2.26	0.48
1:C:309:THR:HB	1:C:335:GLY:O	2.14	0.48
1:C:48:GLU:HA	1:C:57:GLY:O	2.13	0.48
1:D:304:ASN:OD1	1:D:307:MET:N	2.37	0.48
1:A:111:TYR:CZ	1:A:188:VAL:CG2	2.97	0.48
1:A:4:TYR:OH	1:A:6:LYS:HB2	2.14	0.48
1:D:10:LYS:O	1:D:47:GLY:HA2	2.13	0.48
1:B:271:PRO:HA	1:B:299:ALA:HB2	1.93	0.48
1:C:136:VAL:HG12	1:C:158:LEU:HD13	1.96	0.48
1:C:217:GLY:CA	1:C:230:ASN:ND2	2.76	0.48
1:C:275:TYR:CE1	1:C:295:PHE:CE1	3.02	0.48
1:A:259:LEU:O	1:A:260:VAL:CG2	2.62	0.48
1:A:295:PHE:N	1:A:295:PHE:HD1	2.10	0.48
1:B:313:TYR:CE2	1:B:315:ILE:HG13	2.48	0.48
1:C:251:ALA:O	1:C:253:LYS:N	2.46	0.48
1:C:52:ASN:OD1	1:C:53:SER:N	2.47	0.48
1:C:60:GLN:HG2	1:C:61:TRP:H	1.72	0.48
1:D:18:VAL:CG1	1:D:40:TYR:CE1	2.96	0.48
1:D:112:THR:HG21	1:D:230:ASN:OD1	2.12	0.48
1:C:3:ILE:CD1	1:C:13:LEU:CB	2.91	0.48
1:D:118:PHE:HZ	1:D:333:ALA:HB2	1.79	0.48
1:A:105:VAL:HG12	1:A:106:TYR:N	2.24	0.47
1:A:82:ARG:HG2	1:A:132:ARG:NH2	2.29	0.47
1:B:264:GLN:OE1	1:B:270:ARG:NE	2.44	0.47
1:B:306:ASN:CG	1:C:9:ASN:HB2	2.33	0.47
1:D:121:ASP:C	1:D:123:ALA:H	2.16	0.47
1:D:16:LYS:HG2	1:D:42:ARG:HB2	1.96	0.47
1:D:340:PHE:CD1	1:D:340:PHE:N	2.82	0.47
1:D:36:GLY:O	1:D:37:ASP:C	2.52	0.47
1:A:192:GLY:O	1:A:193:ALA:HB2	2.14	0.47
1:A:295:PHE:N	1:A:295:PHE:CD1	2.80	0.47
1:A:88:LEU:CD1	1:C:303:PHE:CE2	2.97	0.47
1:B:112:THR:CG2	1:B:230:ASN:CG	2.81	0.47
1:C:332:VAL:CG1	1:C:333:ALA:N	2.76	0.47
1:D:124:TYR:CD2	1:D:239:PRO:HD2	2.50	0.47
1:D:273:ILE:HD11	1:D:297:VAL:HG22	1.95	0.47
1:D:37:ASP:OD1	1:D:38:MET:N	2.48	0.47
1:A:116:PRO:O	1:A:117:GLU:HB2	2.14	0.47
1:A:104:VAL:HG11	1:A:156:GLN:HB2	1.94	0.47
1:A:242:ASN:O	1:A:243:LYS:C	2.50	0.47
1:B:322:ASN:OD1	1:B:325:GLY:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ASP:HB2	1:B:90:TYR:HE1	1.79	0.47
1:D:48:GLU:CD	1:D:56:THR:HG23	2.33	0.47
1:A:109:LEU:HD13	1:A:122:THR:HB	1.95	0.47
1:A:71:GLU:CD	1:B:132:ARG:NH2	2.68	0.47
1:B:110:GLY:C	1:B:112:THR:N	2.67	0.47
1:B:130:VAL:HG13	1:B:213:GLN:CD	2.25	0.47
1:C:229:ALA:HA	1:C:258:LEU:O	2.14	0.47
1:D:253:LYS:HD2	1:D:254:THR:H	1.80	0.47
1:D:130:VAL:HG13	1:D:213:GLN:NE2	2.29	0.47
1:D:161:ASN:H	1:D:170:ASN:ND2	2.13	0.47
1:D:160:LYS:HB3	1:D:172:ASP:OD1	2.14	0.47
1:A:161:ASN:ND2	1:A:163:ARG:NH2	2.63	0.47
1:A:22:TYR:CE1	1:A:118:PHE:HE1	2.33	0.47
1:A:76:GLN:HE22	1:B:79:ASN:HB2	1.79	0.47
1:B:115:LEU:H	1:B:115:LEU:HD23	0.56	0.47
1:B:303:PHE:HB3	1:C:51:ILE:HD13	1.96	0.47
1:C:11:VAL:CG1	1:C:12:ASP:H	2.28	0.47
1:A:7:ASP:OD2	1:C:305:LYS:NZ	2.47	0.47
1:D:84:ALA:O	1:D:100:ARG:N	2.43	0.47
1:A:130:VAL:CG1	1:A:213:GLN:HE22	2.18	0.47
1:A:141:ASN:CB	1:A:153:PHE:CD1	2.90	0.47
1:A:270:ARG:HD2	1:A:302:TYR:CE2	2.49	0.47
1:B:104:VAL:HG11	1:B:176:GLY:HA2	1.96	0.47
1:B:112:THR:CG2	1:B:230:ASN:CB	2.75	0.47
1:C:313:TYR:CD1	1:C:332:VAL:CG2	2.97	0.47
1:A:258:LEU:O	1:A:259:LEU:HD21	2.04	0.47
1:A:51:ILE:HD13	1:C:303:PHE:CG	2.50	0.47
1:B:118:PHE:C	1:B:119:GLY:O	2.52	0.47
1:B:48:GLU:HG2	1:B:48:GLU:O	2.14	0.47
1:B:63:TYR:CE2	1:B:65:PHE:CD1	3.03	0.47
1:D:111:TYR:HE2	1:D:188:VAL:HG23	1.75	0.47
1:D:83:LEU:HD21	1:D:102:TYR:CD2	2.48	0.47
1:B:188:VAL:O	1:B:216:THR:HA	2.15	0.47
1:C:223:ASN:HB2	1:C:225:ILE:HD12	1.95	0.47
1:C:293:ASN:HD22	1:C:317:GLN:HB3	1.80	0.47
1:D:184:GLY:O	1:D:221:ASP:N	2.44	0.47
1:D:48:GLU:CG	1:D:49:THR:N	2.77	0.47
1:D:114:MET:HE3	1:D:270:ARG:HH12	1.79	0.47
1:A:284:GLU:CD	1:A:284:GLU:H	2.09	0.47
1:A:77:THR:O	1:A:77:THR:HG22	2.14	0.47
1:B:241:THR:HG23	1:B:242:ASN:H	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ASN:HA	1:C:264:GLN:HB3	1.97	0.47
1:A:132:ARG:NH2	1:C:71:GLU:CD	2.68	0.47
1:D:117:GLU:HG3	1:D:118:PHE:CE1	2.49	0.47
1:D:118:PHE:CD2	1:D:314:ILE:CG1	2.90	0.47
1:A:289:VAL:HG21	1:A:324:LEU:CG	2.36	0.46
1:B:104:VAL:N	1:B:156:GLN:OE1	2.48	0.46
1:B:111:TYR:CE2	1:B:188:VAL:CG2	2.98	0.46
1:B:196:ARG:CA	1:B:200:GLN:OE1	2.60	0.46
1:D:139:TYR:HB3	1:D:155:VAL:HG12	1.97	0.46
1:D:130:VAL:CG1	1:D:213:GLN:CD	2.83	0.46
1:A:72:GLY:O	1:A:73:ALA:C	2.54	0.46
1:B:262:GLN:HE21	1:B:272:SER:HB2	1.80	0.46
1:B:259:LEU:O	1:B:274:ALA:HA	2.15	0.46
1:C:106:TYR:O	1:C:110:GLY:N	2.42	0.46
1:C:144:PHE:HD1	1:C:151:LEU:CD2	2.29	0.46
1:C:92:ASP:O	1:C:93:VAL:C	2.53	0.46
1:D:2:GLU:OE2	1:D:5:ASN:HB2	2.15	0.46
1:A:22:TYR:CE1	1:A:118:PHE:HZ	2.33	0.46
1:A:155:VAL:HG22	1:A:156:GLN:N	2.28	0.46
1:A:207:ASN:O	1:A:252:ASN:OD1	2.32	0.46
1:A:260:VAL:CG1	1:A:261:ALA:N	2.78	0.46
1:A:57:GLY:HA3	1:C:307:MET:SD	2.55	0.46
1:B:65:PHE:CE2	1:C:61:TRP:CH2	3.04	0.46
1:B:58:TYR:CE2	1:B:87:GLY:C	2.86	0.46
1:C:39:THR:O	1:C:39:THR:CG2	2.31	0.46
1:D:116:PRO:HB2	1:D:312:ASP:HB2	1.97	0.46
1:D:264:GLN:HE21	1:D:268:GLY:HA2	1.80	0.46
1:A:129:PHE:CE2	1:A:174:VAL:O	2.69	0.46
1:B:263:TYR:CD1	1:B:264:GLN:N	2.84	0.46
1:C:113:ASP:C	1:C:114:MET:HG2	2.35	0.46
1:C:58:TYR:C	1:C:58:TYR:HD1	2.18	0.46
1:D:25:LYS:O	1:D:25:LYS:HG3	2.14	0.46
1:D:313:TYR:CA	1:D:332:VAL:HG13	2.45	0.46
1:D:318:ILE:HD13	1:D:318:ILE:HA	1.55	0.46
1:A:136:VAL:O	1:A:137:ALA:HB2	2.16	0.46
1:A:274:ALA:HB3	1:A:296:GLU:HB3	1.97	0.46
1:A:24:SER:CB	1:A:331:THR:HG1	2.19	0.46
1:B:25:LYS:HB2	1:B:25:LYS:NZ	2.30	0.46
1:B:262:GLN:HG2	1:B:272:SER:HB2	1.97	0.46
1:C:223:ASN:HB3	1:C:225:ILE:CD1	2.24	0.46
1:C:63:TYR:CE1	1:C:80:LYS:C	2.87	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ARG:HH11	1:D:154:ALA:HB2	1.80	0.46
1:D:301:TYR:CD1	1:D:303:PHE:HE1	2.33	0.46
1:D:30:ASN:O	1:D:30:ASN:CG	2.53	0.46
1:A:160:LYS:HD3	1:A:162:GLU:OE2	2.14	0.46
1:A:229:ALA:CB	1:A:259:LEU:HD21	2.39	0.46
1:C:126:ASP:OD2	1:C:168:ARG:NH1	2.48	0.46
1:C:156:GLN:N	1:C:175:GLY:O	2.47	0.46
1:A:136:VAL:HG21	1:A:156:GLN:HE21	1.79	0.46
1:C:226:TYR:O	1:C:261:ALA:HA	2.15	0.46
1:C:269:LEU:HG	1:C:271:PRO:HD3	1.97	0.46
1:C:273:ILE:HD12	1:C:296:GLU:O	2.16	0.46
1:D:14:TYR:HE2	1:D:45:PHE:N	2.14	0.46
1:D:309:THR:HG22	1:D:335:GLY:O	2.15	0.46
1:D:43:LEU:HA	1:D:43:LEU:HD12	1.61	0.46
1:D:90:TYR:HD2	1:D:93:VAL:CG2	2.29	0.46
1:A:32:TYR:C	1:A:32:TYR:CD2	2.87	0.46
1:D:313:TYR:CD1	1:D:314:ILE:N	2.84	0.46
1:A:179:SER:HB2	1:A:188:VAL:CG1	2.45	0.46
1:A:90:TYR:C	1:A:90:TYR:CD1	2.87	0.46
1:B:131:GLY:O	1:B:133:VAL:HG22	2.15	0.46
1:C:87:GLY:HA3	1:C:96:PHE:O	2.16	0.46
1:D:127:ASP:C	1:D:127:ASP:OD1	2.53	0.46
1:D:30:ASN:HD21	1:D:327:GLY:HA2	1.81	0.46
1:B:242:ASN:O	1:B:243:LYS:C	2.51	0.46
1:B:15:GLY:HA3	1:B:42:ARG:O	2.15	0.46
1:B:51:ILE:O	1:B:52:ASN:CB	2.42	0.46
1:C:177:SER:HA	1:C:189:GLY:O	2.16	0.46
1:C:262:GLN:HG2	1:C:272:SER:CB	2.46	0.46
1:D:95:SER:O	1:D:139:TYR:HD1	1.98	0.46
1:D:37:ASP:OD2	1:D:68:ASN:HA	2.15	0.46
1:D:72:GLY:O	1:D:73:ALA:O	2.34	0.46
1:A:238:THR:HG21	1:A:291:LEU:HD12	1.98	0.45
1:A:29:GLU:CG	1:A:29:GLU:O	2.63	0.45
1:A:319:ASP:C	1:A:321:ASP:N	2.68	0.45
1:B:220:TYR:CD2	1:B:220:TYR:C	2.89	0.45
1:B:269:LEU:HA	1:B:269:LEU:HD12	1.25	0.45
1:B:257:VAL:HG23	1:B:277:LYS:HB3	1.98	0.45
1:C:234:THR:HB	1:C:237:ALA:CB	2.40	0.45
1:B:3:ILE:HG22	1:C:4:TYR:HB2	1.98	0.45
1:D:222:ALA:O	1:D:223:ASN:HB2	2.16	0.45
1:D:274:ALA:O	1:D:295:PHE:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:THR:HG23	1:D:336:ILE:HB	1.84	0.45
1:D:59:GLY:O	1:D:60:GLN:HB2	2.16	0.45
1:A:140:ARG:HG3	1:A:154:ALA:HB2	1.97	0.45
1:A:104:VAL:CG1	1:A:156:GLN:HB3	2.40	0.45
1:A:203:GLN:HA	1:A:203:GLN:HE21	1.79	0.45
1:B:191:TYR:C	1:B:191:TYR:CD1	2.84	0.45
1:B:294:TYR:HD1	1:B:314:ILE:HG23	1.80	0.45
1:B:95:SER:O	1:B:96:PHE:CB	2.64	0.45
1:A:58:TYR:CA	1:C:338:TYR:CD1	2.82	0.45
1:D:30:ASN:O	1:D:329:ASP:HB2	2.16	0.45
1:A:337:VAL:HG13	1:A:337:VAL:O	1.97	0.45
1:B:293:ASN:HB3	1:B:317:GLN:HB3	1.98	0.45
1:C:123:ALA:O	1:C:124:TYR:O	2.35	0.45
1:D:129:PHE:CD2	1:D:192:GLY:HA3	2.52	0.45
1:D:51:ILE:HB	1:D:55:LEU:CD2	2.46	0.45
1:A:97:ASP:O	1:A:137:ALA:HB1	2.15	0.45
1:A:310:TYR:HE1	1:A:335:GLY:HA3	1.82	0.45
1:B:111:TYR:CE1	1:B:188:VAL:HG21	2.49	0.45
1:B:130:VAL:HG12	1:B:213:GLN:CD	2.33	0.45
1:B:269:LEU:HD23	1:B:271:PRO:CD	2.46	0.45
1:B:336:ILE:HG13	1:B:337:VAL:N	2.31	0.45
1:C:277:LYS:HE2	1:C:279:LYS:CD	2.29	0.45
1:C:308:SER:C	1:C:309:THR:CG2	2.81	0.45
1:C:60:GLN:CG	1:C:61:TRP:H	2.28	0.45
1:B:13:LEU:HD12	1:B:14:TYR:N	2.32	0.45
1:B:196:ARG:HG3	1:B:196:ARG:H	1.46	0.45
1:C:112:THR:CG2	1:C:230:ASN:CG	2.82	0.45
1:C:227:LEU:N	1:C:227:LEU:HD23	2.31	0.45
1:C:43:LEU:HD12	1:C:43:LEU:HA	1.82	0.45
1:D:283:VAL:O	1:D:286:ILE:HD13	2.17	0.45
1:A:303:PHE:O	1:A:304:ASN:CB	2.62	0.45
1:A:74:ASP:C	1:A:76:GLN:H	2.20	0.45
1:A:63:TYR:HD1	1:A:81:THR:HG1	1.63	0.45
1:A:86:ALA:HB3	1:C:336:ILE:CG1	2.33	0.45
1:A:96:PHE:CG	1:A:97:ASP:N	2.85	0.45
1:B:16:LYS:HB2	1:B:17:ALA:H	1.61	0.45
1:B:187:ILE:HG23	1:B:187:ILE:O	2.16	0.45
1:B:268:GLY:O	1:B:301:TYR:HA	2.16	0.45
1:B:273:ILE:HA	1:B:273:ILE:HD12	1.77	0.45
1:B:313:TYR:CD1	1:B:332:VAL:HG21	2.43	0.45
1:B:52:ASN:OD1	1:B:52:ASN:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:TYR:CG	1:C:232:GLY:N	2.84	0.45
1:C:24:SER:OG	1:C:331:THR:HA	2.16	0.45
1:C:85:PHE:CD1	1:C:85:PHE:C	2.90	0.45
1:D:205:LEU:O	1:D:250:PHE:N	2.44	0.45
1:D:253:LYS:HD2	1:D:253:LYS:HA	1.54	0.45
1:D:253:LYS:O	1:D:280:ALA:HA	2.16	0.45
1:D:338:TYR:HD2	1:D:339:GLN:N	2.01	0.45
1:A:130:VAL:HG11	1:A:213:GLN:NE2	2.26	0.45
1:A:22:TYR:HD1	1:A:333:ALA:CB	2.17	0.45
1:A:24:SER:O	1:A:26:GLY:O	2.34	0.45
1:C:58:TYR:CD1	1:C:58:TYR:C	2.88	0.45
1:A:109:LEU:HD23	1:A:109:LEU:HA	1.47	0.45
1:A:60:GLN:HG2	1:A:61:TRP:N	2.32	0.45
1:A:79:ASN:HB2	1:C:76:GLN:NE2	2.31	0.45
1:B:142:SER:HG	1:B:152:ASN:CG	2.18	0.45
1:B:272:SER:OG	1:B:272:SER:O	2.34	0.45
1:B:318:ILE:HA	1:B:318:ILE:HD13	1.79	0.45
1:B:60:GLN:HG3	1:B:61:TRP:N	2.31	0.45
1:A:263:TYR:O	1:A:270:ARG:HA	2.17	0.45
1:A:16:LYS:H	1:A:42:ARG:HB2	1.81	0.45
1:A:74:ASP:C	1:A:76:GLN:N	2.70	0.45
1:B:262:GLN:CG	1:B:272:SER:HB2	2.47	0.45
1:B:3:ILE:HG13	1:B:4:TYR:N	2.31	0.45
1:B:6:LYS:O	1:B:7:ASP:C	2.54	0.45
1:D:307:MET:CG	1:D:308:SER:N	2.71	0.45
1:D:69:ASN:ND2	1:D:74:ASP:O	2.50	0.45
1:A:114:MET:CE	1:A:226:TYR:HE1	2.00	0.45
1:A:20:LEU:HD12	1:A:21:HIS:H	1.81	0.45
1:B:129:PHE:CE2	1:B:192:GLY:CA	3.00	0.45
1:B:22:TYR:C	1:B:23:PHE:CD2	2.90	0.45
1:B:243:LYS:N	1:B:243:LYS:HD2	2.30	0.45
1:A:340:PHE:CE1	1:B:45:PHE:CD2	3.05	0.45
1:B:63:TYR:CE2	1:B:65:PHE:CE1	3.04	0.45
1:C:163:ARG:HH11	1:C:163:ARG:HG2	1.82	0.45
1:C:18:VAL:HG23	1:C:337:VAL:HG22	1.95	0.45
1:D:281:LYS:HA	1:D:288:ASP:OD1	2.17	0.45
1:D:313:TYR:HB2	1:D:332:VAL:HG13	1.97	0.45
1:D:34:GLY:O	1:D:35:ASN:CB	2.53	0.45
1:D:58:TYR:HD2	1:D:58:TYR:N	2.16	0.45
1:A:23:PHE:C	1:A:24:SER:HG	2.16	0.44
1:A:54:ASP:N	1:A:54:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:TYR:CE2	1:B:140:ARG:O	2.70	0.44
1:C:130:VAL:HG13	1:C:213:GLN:CD	2.37	0.44
1:C:235:ARG:HD3	1:C:235:ARG:HA	1.77	0.44
1:D:83:LEU:HD23	1:D:101:ASN:HA	1.99	0.44
1:D:293:ASN:C	1:D:317:GLN:HB2	2.38	0.44
1:D:30:ASN:ND2	1:D:327:GLY:HA2	2.32	0.44
1:B:22:TYR:CE1	1:B:38:MET:HG3	2.53	0.44
1:C:14:TYR:OH	1:C:62:GLU:HG3	2.17	0.44
1:C:92:ASP:O	1:C:93:VAL:O	2.35	0.44
1:D:63:TYR:CD1	1:D:80:LYS:O	2.70	0.44
1:A:128:PHE:HB3	1:A:129:PHE:H	1.61	0.44
1:A:294:TYR:HA	1:A:317:GLN:HG2	1.98	0.44
1:A:4:TYR:CE2	1:A:6:LYS:N	2.74	0.44
1:C:104:VAL:HG22	1:C:156:GLN:OE1	2.17	0.44
1:C:146:GLY:O	1:C:147:LEU:C	2.56	0.44
1:C:167:ARG:NH1	1:C:168:ARG:HD3	2.32	0.44
1:D:114:MET:CE	1:D:270:ARG:HH12	2.30	0.44
1:A:106:TYR:O	1:A:108:ALA:N	2.50	0.44
1:A:172:ASP:N	1:A:172:ASP:OD1	2.42	0.44
1:A:291:LEU:O	1:A:292:VAL:HG23	2.18	0.44
1:B:124:TYR:HB2	1:B:127:ASP:HB2	1.98	0.44
1:B:62:GLU:HB3	1:B:83:LEU:HB2	2.00	0.44
1:C:23:PHE:O	1:C:332:VAL:N	2.37	0.44
1:C:255:GLN:O	1:C:256:ASP:OD1	2.35	0.44
1:C:24:SER:OG	1:C:331:THR:CB	2.65	0.44
1:C:82:ARG:NH1	1:C:82:ARG:HG2	2.32	0.44
1:D:111:TYR:HE2	1:D:217:GLY:O	2.00	0.44
1:D:167:ARG:HG3	1:D:167:ARG:NH1	2.27	0.44
1:D:219:LYS:HA	1:D:227:LEU:O	2.17	0.44
1:D:5:ASN:O	1:D:6:LYS:HE2	2.18	0.44
1:A:225:ILE:HD13	1:A:225:ILE:HG23	1.71	0.44
1:B:111:TYR:CE2	1:B:219:LYS:HG2	2.53	0.44
1:B:227:LEU:CD2	1:B:261:ALA:HA	2.48	0.44
1:C:115:LEU:HA	1:C:115:LEU:HD23	1.44	0.44
1:C:203:GLN:HG2	1:C:203:GLN:H	1.56	0.44
1:D:104:VAL:HG12	1:D:156:GLN:CB	2.40	0.44
1:D:150:GLY:O	1:D:181:GLU:HG3	2.17	0.44
1:D:45:PHE:O	1:D:60:GLN:HA	2.17	0.44
1:A:13:LEU:HD21	1:B:13:LEU:HD22	1.99	0.44
1:A:251:ALA:O	1:A:252:ASN:O	2.36	0.44
1:A:338:TYR:CG	1:A:339:GLN:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASN:OD1	1:A:36:GLY:N	2.51	0.44
1:B:157:TYR:CD2	1:B:157:TYR:N	2.85	0.44
1:B:294:TYR:HD1	1:B:314:ILE:HD12	1.68	0.44
1:C:114:MET:HB3	1:C:262:GLN:HE22	1.82	0.44
1:C:160:LYS:HA	1:C:172:ASP:OD1	2.17	0.44
1:C:55:LEU:HD12	1:C:90:TYR:CD1	2.53	0.44
1:D:20:LEU:CG	1:D:21:HIS:N	2.81	0.44
1:B:98:TYR:HA	1:B:136:VAL:O	2.18	0.44
1:B:211:ALA:HA	1:B:235:ARG:O	2.17	0.44
1:B:233:GLU:HG2	1:B:255:GLN:HG2	2.00	0.44
1:C:275:TYR:HE1	1:C:295:PHE:CE1	2.36	0.44
1:D:219:LYS:CG	1:D:219:LYS:O	2.66	0.44
1:D:301:TYR:O	1:D:308:SER:HB2	2.17	0.44
1:D:313:TYR:CD1	1:D:313:TYR:C	2.87	0.44
1:D:319:ASP:CG	1:D:321:ASP:H	2.20	0.44
1:D:36:GLY:O	1:D:37:ASP:O	2.36	0.44
1:A:95:SER:O	1:A:139:TYR:HD1	2.00	0.44
1:A:139:TYR:O	1:A:154:ALA:HA	2.18	0.44
1:A:307:MET:CE	1:B:57:GLY:HA3	2.48	0.44
1:B:227:LEU:HD21	1:B:261:ALA:HA	1.99	0.44
1:C:167:ARG:CG	1:C:167:ARG:NH1	2.69	0.44
1:C:192:GLY:O	1:C:193:ALA:HB2	2.18	0.44
1:A:310:TYR:HD1	1:A:310:TYR:O	2.01	0.44
1:A:306:ASN:ND2	1:A:339:GLN:O	2.41	0.44
1:C:109:LEU:C	1:C:111:TYR:H	2.21	0.44
1:C:129:PHE:CE2	1:C:192:GLY:HA3	2.53	0.44
1:C:22:TYR:CB	1:C:35:ASN:HA	2.48	0.44
1:C:112:THR:HG21	1:C:230:ASN:OD1	2.11	0.44
1:D:218:LEU:HD23	1:D:218:LEU:HA	1.33	0.44
1:D:219:LYS:O	1:D:219:LYS:HG3	2.18	0.44
1:D:266:ASP:O	1:D:268:GLY:N	2.51	0.44
1:D:273:ILE:CG2	1:D:274:ALA:N	2.80	0.44
1:A:275:TYR:C	1:A:276:THR:OG1	2.38	0.43
1:B:122:THR:CG2	1:B:256:ASP:OD2	2.66	0.43
1:B:262:GLN:HG2	1:B:272:SER:HA	1.99	0.43
1:D:125:SER:O	1:D:127:ASP:N	2.51	0.43
1:D:245:THR:HG1	1:D:247:THR:CB	2.21	0.43
1:D:5:ASN:C	1:D:6:LYS:HG2	2.38	0.43
1:A:115:LEU:CG	1:A:119:GLY:HA3	2.35	0.43
1:A:11:VAL:HG21	1:C:340:PHE:CD2	2.52	0.43
1:A:289:VAL:HG21	1:A:324:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:VAL:HG23	1:A:334:VAL:HG22	1.98	0.43
1:B:196:ARG:HB3	1:B:200:GLN:OE1	2.18	0.43
1:B:54:ASP:O	1:B:90:TYR:CD1	2.71	0.43
1:D:323:LYS:HD2	1:D:323:LYS:HA	1.64	0.43
1:D:66:GLN:NE2	1:D:68:ASN:ND2	2.66	0.43
1:A:182:TYR:CD1	1:A:182:TYR:C	2.88	0.43
1:A:240:ILE:CG2	1:A:291:LEU:HD22	2.49	0.43
1:B:185:PHE:CE2	1:B:220:TYR:HE1	2.26	0.43
1:B:282:ASP:O	1:B:284:GLU:N	2.51	0.43
1:B:316:ASN:HD22	1:B:329:ASP:N	2.16	0.43
1:C:14:TYR:HA	1:C:340:PHE:CE2	2.53	0.43
1:D:212:GLU:OE1	1:D:235:ARG:HB2	2.19	0.43
1:A:104:VAL:CG1	1:A:156:GLN:HB2	2.48	0.43
1:A:294:TYR:HD1	1:A:294:TYR:O	2.01	0.43
1:B:208:GLY:HA3	1:B:236:ASN:HD22	1.83	0.43
1:B:263:TYR:HD1	1:B:264:GLN:N	2.15	0.43
1:B:285:GLY:O	1:B:286:ILE:CD1	2.48	0.43
1:C:45:PHE:O	1:C:60:GLN:CG	2.65	0.43
1:C:49:THR:HG23	1:C:49:THR:O	2.18	0.43
1:D:240:ILE:HG12	1:D:240:ILE:O	2.14	0.43
1:D:45:PHE:O	1:D:45:PHE:CD1	2.71	0.43
1:A:178:ILE:CG2	1:A:179:SER:N	2.78	0.43
1:A:69:ASN:HD22	1:A:77:THR:H	1.65	0.43
1:D:161:ASN:H	1:D:170:ASN:HD21	1.66	0.43
1:D:129:PHE:HB2	1:D:213:GLN:OE1	2.19	0.43
1:A:69:ASN:ND2	1:A:77:THR:CB	2.63	0.43
1:B:139:TYR:HD2	1:B:139:TYR:C	2.16	0.43
1:B:22:TYR:O	1:B:23:PHE:HD2	1.97	0.43
1:B:78:GLY:O	1:B:79:ASN:C	2.51	0.43
1:C:115:LEU:HD12	1:C:119:GLY:N	2.32	0.43
1:C:163:ARG:CG	1:C:163:ARG:NH1	2.78	0.43
1:C:163:ARG:CD	1:C:168:ARG:O	2.52	0.43
1:D:260:VAL:HG12	1:D:261:ALA:N	2.33	0.43
1:D:286:ILE:HG23	1:D:323:LYS:HB3	2.00	0.43
1:D:58:TYR:H	1:D:58:TYR:HD2	1.67	0.43
1:A:102:TYR:CD1	1:A:106:TYR:HD2	2.30	0.43
1:B:167:ARG:C	1:B:168:ARG:HG2	2.39	0.43
1:B:22:TYR:N	1:B:22:TYR:CD1	2.86	0.43
1:A:6:LYS:O	1:A:7:ASP:HB2	2.17	0.43
1:C:60:GLN:NE2	1:C:85:PHE:CE1	2.80	0.43
1:D:124:TYR:CE2	1:D:238:THR:HG22	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ALA:O	1:D:191:TYR:HB2	2.18	0.43
1:D:273:ILE:CD1	1:D:297:VAL:HG22	2.48	0.43
1:D:274:ALA:HB3	1:D:296:GLU:OE1	2.18	0.43
1:D:291:LEU:C	1:D:292:VAL:HG22	2.39	0.43
1:D:24:SER:OG	1:D:331:THR:HG23	2.18	0.43
1:A:104:VAL:O	1:A:105:VAL:C	2.57	0.43
1:B:104:VAL:HG21	1:B:176:GLY:CA	2.49	0.43
1:B:242:ASN:CB	1:B:247:THR:HB	2.45	0.43
1:B:122:THR:HG21	1:B:256:ASP:OD2	2.19	0.43
1:B:277:LYS:HE3	1:B:293:ASN:ND2	2.31	0.43
1:B:318:ILE:HG23	1:B:318:ILE:HD12	1.60	0.43
1:A:188:VAL:O	1:A:216:THR:HA	2.19	0.43
1:A:294:TYR:O	1:A:294:TYR:CD1	2.72	0.43
1:B:318:ILE:HG22	1:B:319:ASP:H	1.82	0.43
1:C:13:LEU:HD12	1:C:13:LEU:HA	1.56	0.43
1:C:176:GLY:O	1:C:190:ALA:HA	2.19	0.43
1:C:303:PHE:HA	1:C:303:PHE:HD1	1.68	0.43
1:B:1:ALA:CB	1:C:4:TYR:CG	3.02	0.43
1:D:264:GLN:O	1:D:264:GLN:HG3	2.18	0.43
1:D:206:GLY:N	1:D:284:GLU:OE2	2.50	0.43
1:D:314:ILE:HA	1:D:314:ILE:HD13	1.84	0.43
1:D:318:ILE:HG23	1:D:318:ILE:HD12	1.70	0.43
1:A:225:ILE:HG21	1:A:225:ILE:HD12	1.78	0.42
1:A:112:THR:HG21	1:A:230:ASN:HB2	2.00	0.42
1:C:205:LEU:HA	1:C:284:GLU:CG	2.49	0.42
1:C:269:LEU:HA	1:C:269:LEU:HD13	1.55	0.42
1:C:311:VAL:HA	1:C:333:ALA:O	2.19	0.42
1:D:125:SER:C	1:D:127:ASP:N	2.68	0.42
1:D:151:LEU:O	1:D:151:LEU:CG	2.62	0.42
1:D:209:LYS:HE3	1:D:209:LYS:HB3	1.42	0.42
1:A:226:TYR:HD2	1:A:227:LEU:N	2.17	0.42
1:A:237:ALA:O	1:A:239:PRO:N	2.52	0.42
1:A:74:ASP:OD1	1:A:74:ASP:N	2.30	0.42
1:C:211:ALA:C	1:C:212:GLU:HG2	2.38	0.42
1:C:267:PHE:CZ	1:C:269:LEU:CB	3.01	0.42
1:C:296:GLU:HB2	1:C:314:ILE:HD13	2.00	0.42
1:A:203:GLN:HB3	1:A:204:PRO:CD	2.49	0.42
1:A:2:GLU:OE2	1:A:5:ASN:ND2	2.42	0.42
1:A:85:PHE:C	1:A:85:PHE:CD1	2.92	0.42
1:B:196:ARG:CD	1:B:208:GLY:O	2.67	0.42
1:B:20:LEU:HA	1:B:20:LEU:HD13	1.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:THR:HG22	1:B:39:THR:O	2.11	0.42
1:D:338:TYR:CD2	1:D:339:GLN:CA	3.00	0.42
1:A:340:PHE:HE1	1:B:45:PHE:CZ	2.38	0.42
1:A:47:GLY:O	1:A:58:TYR:HB2	2.20	0.42
1:B:114:MET:CA	1:B:115:LEU:HD23	2.47	0.42
1:B:163:ARG:HH11	1:B:163:ARG:HG2	1.84	0.42
1:B:51:ILE:HD13	1:B:51:ILE:HG21	1.84	0.42
1:D:154:ALA:HB3	1:D:177:SER:OG	2.20	0.42
1:D:229:ALA:HA	1:D:259:LEU:HD23	2.01	0.42
1:D:58:TYR:CE2	1:D:87:GLY:HA3	2.54	0.42
1:A:22:TYR:CZ	1:A:118:PHE:HE1	2.37	0.42
1:A:334:VAL:HG13	1:A:335:GLY:N	2.34	0.42
1:B:180:TYR:HD2	1:B:180:TYR:O	1.96	0.42
1:B:255:GLN:C	1:B:256:ASP:OD1	2.58	0.42
1:B:277:LYS:HA	1:B:292:VAL:O	2.18	0.42
1:C:105:VAL:O	1:C:106:TYR:C	2.57	0.42
1:D:156:GLN:O	1:D:175:GLY:N	2.53	0.42
1:D:183:GLU:HG2	1:D:183:GLU:O	2.19	0.42
1:D:21:HIS:CD2	1:D:23:PHE:CZ	3.07	0.42
1:A:21:HIS:CD2	1:A:23:PHE:CZ	3.03	0.42
1:A:277:LYS:HB2	1:A:293:ASN:OD1	2.19	0.42
1:A:303:PHE:O	1:A:304:ASN:HB3	2.20	0.42
1:B:139:TYR:HE2	1:B:141:ASN:HB2	1.85	0.42
1:B:186:GLY:O	1:B:218:LEU:HA	2.20	0.42
1:B:280:ALA:HB2	1:B:291:LEU:HD11	2.01	0.42
1:B:22:TYR:CD1	1:B:38:MET:HG3	2.54	0.42
1:C:198:ASN:HA	1:C:201:GLU:HG2	2.02	0.42
1:D:205:LEU:O	1:D:249:GLY:HA3	2.19	0.42
1:D:270:ARG:HA	1:D:271:PRO:HD2	1.76	0.42
1:D:277:LYS:CB	1:D:293:ASN:OD1	2.53	0.42
1:D:82:ARG:O	1:D:132:ARG:HD3	2.11	0.42
1:A:226:TYR:HE2	1:A:228:ALA:CB	2.21	0.42
1:A:336:ILE:CD1	1:B:87:GLY:CA	2.92	0.42
1:A:52:ASN:CG	1:A:53:SER:N	2.71	0.42
1:B:166:ALA:C	1:B:168:ARG:H	2.23	0.42
1:B:182:TYR:C	1:B:182:TYR:CD1	2.87	0.42
1:C:111:TYR:O	1:C:228:ALA:CB	2.68	0.42
1:C:24:SER:O	1:C:25:LYS:C	2.58	0.42
1:A:51:ILE:CD1	1:C:303:PHE:HB3	2.39	0.42
1:C:85:PHE:HD1	1:C:85:PHE:C	2.23	0.42
1:D:231:TYR:HA	1:D:256:ASP:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ASN:O	1:D:6:LYS:CG	2.68	0.42
1:A:111:TYR:CD2	1:A:219:LYS:CG	2.95	0.42
1:A:237:ALA:O	1:A:238:THR:O	2.35	0.42
1:A:34:GLY:O	1:A:35:ASN:HB2	2.20	0.42
1:B:257:VAL:C	1:B:258:LEU:HD13	2.40	0.42
1:B:324:LEU:HD23	1:B:324:LEU:N	2.27	0.42
1:C:61:TRP:HE1	1:C:81:THR:CG2	2.33	0.42
1:D:300:THR:HA	1:D:310:TYR:CB	2.44	0.42
1:D:9:ASN:HA	1:D:48:GLU:O	2.20	0.42
1:A:303:PHE:CB	1:A:307:MET:HB3	2.41	0.42
1:A:31:SER:HA	1:A:329:ASP:H	1.85	0.42
1:B:128:PHE:O	1:B:133:VAL:CG1	2.66	0.42
1:C:191:TYR:CE1	1:C:192:GLY:O	2.72	0.42
1:C:294:TYR:C	1:C:294:TYR:CD1	2.94	0.42
1:D:24:SER:OG	1:D:331:THR:CB	2.68	0.42
1:B:127:ASP:O	1:B:129:PHE:N	2.53	0.42
1:B:182:TYR:HD1	1:B:182:TYR:HA	1.59	0.42
1:A:65:PHE:CD1	1:B:63:TYR:CD1	3.08	0.42
1:B:95:SER:O	1:B:96:PHE:HB2	2.20	0.42
1:A:168:ARG:HD3	1:C:70:SER:HB2	2.01	0.42
1:D:170:ASN:C	1:D:170:ASN:ND2	2.49	0.42
1:B:141:ASN:CG	1:B:153:PHE:CE1	2.83	0.41
1:C:235:ARG:CZ	1:C:253:LYS:HD3	2.49	0.41
1:D:227:LEU:HD23	1:D:227:LEU:N	2.24	0.41
1:A:318:ILE:CG1	1:A:326:VAL:HG12	2.50	0.41
1:C:140:ARG:HG2	1:C:154:ALA:CB	2.50	0.41
1:D:160:LYS:HB2	1:D:160:LYS:HE2	1.29	0.41
1:D:232:GLY:O	1:D:233:GLU:HG3	2.20	0.41
1:A:22:TYR:OH	1:A:118:PHE:HE1	2.02	0.41
1:A:171:GLY:HA3	1:A:195:ASP:CB	2.50	0.41
1:A:85:PHE:HD1	1:A:85:PHE:O	2.02	0.41
1:B:201:GLU:OE1	1:B:208:GLY:O	2.37	0.41
1:B:251:ALA:O	1:B:253:LYS:N	2.53	0.41
1:B:296:GLU:CG	1:B:314:ILE:CD1	2.98	0.41
1:C:25:LYS:HG3	1:C:25:LYS:O	2.19	0.41
1:C:260:VAL:HG12	1:C:261:ALA:H	1.85	0.41
1:C:280:ALA:HB2	1:C:291:LEU:HD12	2.03	0.41
1:C:52:ASN:OD1	1:C:54:ASP:N	2.53	0.41
1:D:141:ASN:OD1	1:D:145:PHE:CA	2.67	0.41
1:D:190:ALA:O	1:D:191:TYR:CB	2.68	0.41
1:D:265:PHE:HD1	1:D:265:PHE:HA	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:VAL:HG13	1:A:175:GLY:H	1.76	0.41
1:B:148:VAL:CG1	1:B:148:VAL:O	2.57	0.41
1:B:178:ILE:CG2	1:B:179:SER:N	2.83	0.41
1:B:205:LEU:CG	1:B:247:THR:HG22	2.49	0.41
1:C:105:VAL:HG23	1:C:129:PHE:CB	2.46	0.41
1:C:240:ILE:HD11	1:C:251:ALA:CA	2.44	0.41
1:D:121:ASP:C	1:D:123:ALA:N	2.74	0.41
1:D:3:ILE:CD1	1:D:13:LEU:HB3	2.50	0.41
1:A:20:LEU:HD12	1:A:21:HIS:N	2.35	0.41
1:A:42:ARG:HD3	1:A:42:ARG:HA	1.36	0.41
1:B:132:ARG:C	1:B:133:VAL:HG22	2.41	0.41
1:B:275:TYR:CG	1:B:276:THR:N	2.87	0.41
1:B:307:MET:CG	1:B:308:SER:N	2.71	0.41
1:B:94:GLY:HA3	1:B:140:ARG:O	2.20	0.41
1:C:11:VAL:HG12	1:C:12:ASP:H	1.76	0.41
1:D:241:THR:O	1:D:324:LEU:HD22	2.21	0.41
1:B:106:TYR:C	1:B:108:ALA:N	2.71	0.41
1:B:129:PHE:HB2	1:B:213:GLN:OE1	2.21	0.41
1:A:336:ILE:CD1	1:B:87:GLY:N	2.80	0.41
1:C:153:PHE:HA	1:C:177:SER:O	2.21	0.41
1:C:130:VAL:CG1	1:C:213:GLN:NE2	2.80	0.41
1:C:48:GLU:HG3	1:C:56:THR:CG2	2.48	0.41
1:D:125:SER:O	1:D:126:ASP:C	2.58	0.41
1:D:293:ASN:ND2	1:D:317:GLN:HB3	2.34	0.41
1:D:303:PHE:CD2	1:D:307:MET:HG2	2.42	0.41
1:A:240:ILE:CD1	1:A:251:ALA:HB2	2.50	0.41
1:B:158:LEU:CD1	1:B:170:ASN:ND2	2.82	0.41
1:B:336:ILE:CG1	1:B:337:VAL:N	2.81	0.41
1:C:140:ARG:HG2	1:C:154:ALA:HB2	2.02	0.41
1:C:155:VAL:O	1:C:155:VAL:HG12	2.21	0.41
1:B:265:PHE:CD2	1:B:267:PHE:HE1	2.39	0.41
1:B:293:ASN:CG	1:B:317:GLN:HB3	2.40	0.41
1:D:123:ALA:HA	1:D:130:VAL:HG23	2.02	0.41
1:D:100:ARG:HH12	1:D:133:VAL:CA	2.34	0.41
1:D:191:TYR:HB2	1:D:214:TRP:CB	2.51	0.41
1:A:203:GLN:CA	1:A:203:GLN:NE2	2.83	0.41
1:B:265:PHE:HB3	1:B:267:PHE:CE1	2.56	0.41
1:B:289:VAL:HG21	1:B:324:LEU:HG	2.02	0.41
1:C:221:ASP:OD1	1:C:221:ASP:C	2.60	0.41
1:C:48:GLU:CG	1:C:48:GLU:O	2.58	0.41
1:B:321:ASP:HB3	1:D:287:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:LEU:CD1	1:D:296:GLU:HG3	2.51	0.41
1:D:65:PHE:HA	1:D:79:ASN:OD1	2.20	0.41
1:A:114:MET:HE2	1:A:226:TYR:CE2	2.50	0.41
1:A:22:TYR:HE1	1:A:118:PHE:HZ	1.67	0.41
1:B:28:GLY:C	1:B:30:ASN:N	2.73	0.41
1:C:294:TYR:CG	1:C:314:ILE:HD12	2.56	0.41
1:C:12:ASP:O	1:C:45:PHE:HA	2.20	0.41
1:D:144:PHE:N	1:D:151:LEU:O	2.51	0.41
1:D:172:ASP:H	1:D:195:ASP:HB2	1.86	0.41
1:D:205:LEU:HA	1:D:284:GLU:CG	2.51	0.41
1:D:322:ASN:OD1	1:D:326:VAL:HG23	2.21	0.41
1:D:313:TYR:HB2	1:D:332:VAL:CG1	2.51	0.41
1:D:334:VAL:O	1:D:334:VAL:CG1	2.45	0.41
1:A:161:ASN:O	1:A:169:SER:OG	2.39	0.41
1:A:277:LYS:HE3	1:A:279:LYS:HD2	2.03	0.41
1:C:238:THR:HA	1:C:239:PRO:HD2	1.82	0.41
1:B:338:TYR:HB3	1:C:59:GLY:HA3	2.04	0.41
1:C:90:TYR:HA	1:C:90:TYR:HD1	1.60	0.41
1:D:241:THR:CG2	1:D:242:ASN:N	2.84	0.41
1:A:317:GLN:N	1:A:317:GLN:NE2	2.69	0.40
1:B:104:VAL:HG22	1:B:104:VAL:H	1.64	0.40
1:C:112:THR:HG21	1:C:230:ASN:CB	2.51	0.40
1:C:111:TYR:CZ	1:C:188:VAL:CG2	3.04	0.40
1:C:255:GLN:HE22	1:C:281:LYS:NZ	2.19	0.40
1:C:275:TYR:CD2	1:C:275:TYR:C	2.94	0.40
1:C:326:VAL:CG1	1:C:327:GLY:O	2.69	0.40
1:C:42:ARG:HH12	1:C:82:ARG:HH22	1.59	0.40
1:B:1:ALA:CB	1:C:4:TYR:CZ	3.04	0.40
1:D:14:TYR:CD2	1:D:44:GLY:O	2.73	0.40
1:D:20:LEU:HD21	1:D:117:GLU:OE2	2.21	0.40
1:D:235:ARG:HD3	1:D:252:ASN:O	2.21	0.40
1:D:269:LEU:HG	1:D:271:PRO:HD3	2.03	0.40
1:A:104:VAL:CG2	1:A:105:VAL:N	2.79	0.40
1:A:165:THR:HG22	1:A:166:ALA:C	2.41	0.40
1:A:314:ILE:O	1:A:330:ASP:OD1	2.40	0.40
1:B:14:TYR:CA	1:B:340:PHE:CE2	2.99	0.40
1:B:316:ASN:HB3	1:B:328:SER:O	2.21	0.40
1:D:184:GLY:O	1:D:220:TYR:HA	2.21	0.40
1:A:165:THR:O	1:A:165:THR:HG22	1.99	0.40
1:A:32:TYR:CG	1:A:32:TYR:O	2.72	0.40
1:A:50:GLN:HG3	1:A:50:GLN:H	1.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LEU:O	1:B:109:LEU:HD23	2.21	0.40
1:B:76:GLN:O	1:B:78:GLY:N	2.54	0.40
1:C:111:TYR:CZ	1:C:188:VAL:HG21	2.56	0.40
1:C:165:THR:O	1:C:166:ALA:O	2.40	0.40
1:C:169:SER:HB3	1:C:170:ASN:H	1.43	0.40
1:C:198:ASN:O	1:C:201:GLU:N	2.54	0.40
1:C:241:THR:HG23	1:C:247:THR:O	2.20	0.40
1:C:256:ASP:C	1:C:257:VAL:CG2	2.82	0.40
1:A:340:PHE:HE1	1:B:45:PHE:CD2	2.39	0.40
1:B:129:PHE:CZ	1:B:174:VAL:O	2.75	0.40
1:B:139:TYR:CE2	1:B:141:ASN:HB2	2.56	0.40
1:C:106:TYR:O	1:C:109:LEU:N	2.55	0.40
1:C:14:TYR:CD1	1:C:14:TYR:C	2.94	0.40
1:C:233:GLU:HG2	1:C:255:GLN:HG2	2.04	0.40
1:C:323:LYS:HD3	1:C:323:LYS:HA	1.73	0.40
1:A:200:GLN:HG2	1:A:250:PHE:CE1	2.57	0.40
1:B:166:ALA:C	1:B:168:ARG:N	2.75	0.40
1:B:21:HIS:ND1	1:C:98:TYR:OH	2.38	0.40
1:B:3:ILE:HD13	1:B:13:LEU:HD23	2.03	0.40
1:B:39:THR:HG22	1:B:67:GLY:HA3	2.02	0.40
1:C:147:LEU:HD22	1:C:147:LEU:HA	1.43	0.40
1:C:308:SER:O	1:C:309:THR:HG22	2.17	0.40
1:D:161:ASN:N	1:D:170:ASN:HD21	2.20	0.40
1:D:239:PRO:CA	1:D:250:PHE:HD2	2.27	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LYS:CB	1:B:6:LYS:NZ[5_555]	1.70	0.50
1:B:6:LYS:C	1:B:6:LYS:NZ[5_555]	1.91	0.29
1:B:6:LYS:CA	1:B:6:LYS:NZ[5_555]	1.96	0.24
1:C:287:GLY:CA	1:D:321:ASP:OD1[2_565]	1.97	0.23
1:B:287:GLY:CA	1:C:321:ASP:OD1[3_455]	2.07	0.13
1:B:6:LYS:CD	1:B:6:LYS:CD[5_555]	2.09	0.11

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	338/340 (99%)	255 (75%)	47 (14%)	36 (11%)	0	8
1	B	338/340 (99%)	270 (80%)	41 (12%)	27 (8%)	1	14
1	C	338/340 (99%)	255 (75%)	53 (16%)	30 (9%)	1	12
1	D	338/340 (99%)	256 (76%)	48 (14%)	34 (10%)	0	10
All	All	1352/1360 (99%)	1036 (77%)	189 (14%)	127 (9%)	0	12

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	52	ASN
1	A	73	ALA
1	A	115	LEU
1	A	119	GLY
1	A	126	ASP
1	A	135	GLY
1	A	166	ALA
1	A	276	THR
1	A	304	ASN
1	A	320	SER
1	A	321	ASP
1	A	327	GLY
1	B	39	THR
1	B	52	ASN
1	B	73	ALA
1	B	75	ALA
1	B	91	ALA
1	B	111	TYR
1	B	163	ARG
1	B	222	ALA
1	B	243	LYS

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Mol	Chain	Res	Type
1	C	91	ALA
1	C	110	GLY
1	C	154	ALA
1	C	170	ASN
1	C	183	GLU
1	C	244	PHE
1	C	252	ASN
1	C	284	GLU
1	C	308	SER
1	C	326	VAL
1	D	7	ASP
1	D	60	GLN
1	D	73	ALA
1	D	75	ALA
1	D	113	ASP
1	D	119	GLY
1	D	122	THR
1	D	245	THR
1	D	265	PHE
1	D	304	ASN
1	D	339	GLN
1	A	103	GLY
1	A	107	ASP
1	A	109	LEU
1	A	110	GLY
1	A	117	GLU
1	A	163	ARG
1	A	167	ARG
1	A	170	ASN
1	A	200	GLN
1	A	243	LYS
1	A	252	ASN
1	A	282	ASP
1	B	7	ASP
1	B	26	GLY
1	B	29	GLU
1	B	170	ASN
1	B	303	PHE
1	B	339	GLN
1	C	39	THR
1	C	124	TYR
1	C	146	GLY

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Mol	Chain	Res	Type
1	C	150	GLY
1	C	166	ALA
1	C	171	GLY
1	C	177	SER
1	C	223	ASN
1	D	28	GLY
1	D	35	ASN
1	D	37	ASP
1	D	74	ASP
1	D	111	TYR
1	D	118	PHE
1	D	144	PHE
1	D	183	GLU
1	D	244	PHE
1	D	284	GLU
1	D	308	SER
1	D	327	GLY
1	A	27	ASN
1	A	128	PHE
1	A	337	VAL
1	B	96	PHE
1	B	97	ASP
1	B	117	GLU
1	B	149	ASP
1	B	167	ARG
1	B	284	GLU
1	C	145	PHE
1	C	199	LEU
1	C	222	ALA
1	D	50	GLN
1	D	117	GLU
1	D	171	GLY
1	D	303	PHE
1	A	177	SER
1	A	183	GLU
1	A	221	ASP
1	A	303	PHE
1	B	77	THR
1	B	114	MET
1	B	126	ASP
1	C	52	ASN
1	C	70	SER

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Mol	Chain	Res	Type
1	C	73	ALA
1	C	93	VAL
1	C	119	GLY
1	C	147	LEU
1	C	245	THR
1	D	110	GLY
1	D	191	TYR
1	D	198	ASN
1	D	267	PHE
1	B	128	PHE
1	C	35	ASN
1	C	144	PHE
1	D	39	THR
1	D	115	LEU
1	D	128	PHE
1	A	114	MET
1	A	171	GLY
1	B	51	ILE
1	B	105	VAL
1	A	28	GLY
1	A	286	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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	263/263 (100%)	174 (66%)	89 (34%)	0	2
1	B	263/263 (100%)	184 (70%)	79 (30%)	0	2
1	C	263/263 (100%)	192 (73%)	71 (27%)	0	3
1	D	263/263 (100%)	194 (74%)	69 (26%)	0	4
All	All	1052/1052 (100%)	744 (71%)	308 (29%)	0	3

All (308) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	4	TYR
1	A	16	LYS
1	A	30	ASN
1	A	32	TYR
1	A	39	THR
1	A	40	TYR
1	A	42	ARG
1	A	45	PHE
1	A	46	LYS
1	A	49	THR
1	A	50	GLN
1	A	51	ILE
1	A	54	ASP
1	A	70	SER
1	A	80	LYS
1	A	82	ARG
1	A	85	PHE
1	A	92	ASP
1	A	93	VAL
1	A	96	PHE
1	A	105	VAL
1	A	115	LEU
1	A	122	THR
1	A	130	VAL
1	A	133	VAL
1	A	136	VAL
1	A	139	TYR
1	A	140	ARG
1	A	142	SER
1	A	144	PHE
1	A	148	VAL
1	A	152	ASN
1	A	153	PHE
1	A	157	TYR
1	A	158	LEU
1	A	160	LYS
1	A	162	GLU
1	A	165	THR
1	A	167	ARG
1	A	170	ASN
1	A	172	ASP
1	A	174	VAL

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Mol	Chain	Res	Type
1	A	180	TYR
1	A	181	GLU
1	A	183	GLU
1	A	187	ILE
1	A	188	VAL
1	A	191	TYR
1	A	197	THR
1	A	198	ASN
1	A	199	LEU
1	A	216	THR
1	A	225	ILE
1	A	226	TYR
1	A	230	ASN
1	A	231	TYR
1	A	243	LYS
1	A	246	ASN
1	A	247	THR
1	A	248	SER
1	A	253	LYS
1	A	254	THR
1	A	257	VAL
1	A	258	LEU
1	A	259	LEU
1	A	265	PHE
1	A	267	PHE
1	A	271	PRO
1	A	272	SER
1	A	273	ILE
1	A	279	LYS
1	A	284	GLU
1	A	289	VAL
1	A	292	VAL
1	A	294	TYR
1	A	296	GLU
1	A	297	VAL
1	A	305	LYS
1	A	307	MET
1	A	308	SER
1	A	310	TYR
1	A	311	VAL
1	A	314	ILE
1	A	318	ILE

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Mol	Chain	Res	Type
1	A	320	SER
1	A	321	ASP
1	A	336	ILE
1	A	337	VAL
1	B	4	TYR
1	B	5	ASN
1	B	9	ASN
1	B	13	LEU
1	B	20	LEU
1	B	25	LYS
1	B	32	TYR
1	B	35	ASN
1	B	40	TYR
1	B	45	PHE
1	B	46	LYS
1	B	48	GLU
1	B	49	THR
1	B	52	ASN
1	B	54	ASP
1	B	58	TYR
1	B	64	ASN
1	B	90	TYR
1	B	93	VAL
1	B	96	PHE
1	B	98	TYR
1	B	104	VAL
1	B	105	VAL
1	B	109	LEU
1	B	115	LEU
1	B	122	THR
1	B	125	SER
1	B	130	VAL
1	B	133	VAL
1	B	138	THR
1	B	139	TYR
1	B	149	ASP
1	B	151	LEU
1	B	153	PHE
1	B	155	VAL
1	B	156	GLN
1	B	157	TYR
1	B	158	LEU

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Mol	Chain	Res	Type
1	B	160	LYS
1	B	167	ARG
1	B	169	SER
1	B	174	VAL
1	B	180	TYR
1	B	187	ILE
1	B	188	VAL
1	B	196	ARG
1	B	198	ASN
1	B	199	LEU
1	B	205	LEU
1	B	207	ASN
1	B	209	LYS
1	B	212	GLU
1	B	218	LEU
1	B	225	ILE
1	B	226	TYR
1	B	230	ASN
1	B	235	ARG
1	B	248	SER
1	B	253	LYS
1	B	257	VAL
1	B	258	LEU
1	B	266	ASP
1	B	267	PHE
1	B	272	SER
1	B	273	ILE
1	B	279	LYS
1	B	284	GLU
1	B	289	VAL
1	B	295	PHE
1	B	305	LYS
1	B	310	TYR
1	B	317	GLN
1	B	320	SER
1	B	323	LYS
1	B	330	ASP
1	B	331	THR
1	B	332	VAL
1	B	336	ILE
1	B	339	GLN
1	C	3	ILE

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Mol	Chain	Res	Type
1	C	10	LYS
1	C	16	LYS
1	C	25	LYS
1	C	29	GLU
1	C	42	ARG
1	C	45	PHE
1	C	51	ILE
1	C	53	SER
1	C	55	LEU
1	C	58	TYR
1	C	60	GLN
1	C	66	GLN
1	C	70	SER
1	C	80	LYS
1	C	81	THR
1	C	82	ARG
1	C	85	PHE
1	C	90	TYR
1	C	92	ASP
1	C	95	SER
1	C	100	ARG
1	C	104	VAL
1	C	121	ASP
1	C	122	THR
1	C	133	VAL
1	C	139	TYR
1	C	142	SER
1	C	147	LEU
1	C	152	ASN
1	C	153	PHE
1	C	157	TYR
1	C	160	LYS
1	C	161	ASN
1	C	163	ARG
1	C	167	ARG
1	C	170	ASN
1	C	182	TYR
1	C	183	GLU
1	C	187	ILE
1	C	188	VAL
1	C	212	GLU
1	C	218	LEU

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Mol	Chain	Res	Type
1	C	221	ASP
1	C	225	ILE
1	C	227	LEU
1	C	235	ARG
1	C	240	ILE
1	C	243	LYS
1	C	246	ASN
1	C	247	THR
1	C	248	SER
1	C	253	LYS
1	C	254	THR
1	C	257	VAL
1	C	258	LEU
1	C	266	ASP
1	C	269	LEU
1	C	270	ARG
1	C	273	ILE
1	C	279	LYS
1	C	284	GLU
1	C	286	ILE
1	C	289	VAL
1	C	296	GLU
1	C	297	VAL
1	C	310	TYR
1	C	314	ILE
1	C	320	SER
1	C	336	ILE
1	C	338	TYR
1	D	3	ILE
1	D	10	LYS
1	D	13	LEU
1	D	14	TYR
1	D	16	LYS
1	D	25	LYS
1	D	40	TYR
1	D	58	TYR
1	D	77	THR
1	D	80	LYS
1	D	81	THR
1	D	85	PHE
1	D	93	VAL
1	D	95	SER

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Mol	Chain	Res	Type
1	D	96	PHE
1	D	100	ARG
1	D	105	VAL
1	D	115	LEU
1	D	122	THR
1	D	125	SER
1	D	132	ARG
1	D	142	SER
1	D	144	PHE
1	D	147	LEU
1	D	151	LEU
1	D	152	ASN
1	D	153	PHE
1	D	155	VAL
1	D	160	LYS
1	D	162	GLU
1	D	167	ARG
1	D	169	SER
1	D	170	ASN
1	D	180	TYR
1	D	187	ILE
1	D	188	VAL
1	D	198	ASN
1	D	209	LYS
1	D	212	GLU
1	D	219	LYS
1	D	225	ILE
1	D	226	TYR
1	D	231	TYR
1	D	235	ARG
1	D	240	ILE
1	D	246	ASN
1	D	253	LYS
1	D	257	VAL
1	D	258	LEU
1	D	267	PHE
1	D	270	ARG
1	D	273	ILE
1	D	279	LYS
1	D	281	LYS
1	D	284	GLU
1	D	286	ILE

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Mol	Chain	Res	Type
1	D	289	VAL
1	D	291	LEU
1	D	292	VAL
1	D	297	VAL
1	D	311	VAL
1	D	315	ILE
1	D	317	GLN
1	D	318	ILE
1	D	319	ASP
1	D	320	SER
1	D	332	VAL
1	D	334	VAL
1	D	336	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	35	ASN
1	A	60	GLN
1	A	69	ASN
1	A	141	ASN
1	A	152	ASN
1	A	161	ASN
1	A	203	GLN
1	A	223	ASN
1	A	246	ASN
1	A	252	ASN
1	A	293	ASN
1	A	306	ASN
1	A	317	GLN
1	A	339	GLN
1	B	21	HIS
1	B	35	ASN
1	B	60	GLN
1	B	66	GLN
1	B	69	ASN
1	B	246	ASN
1	B	316	ASN
1	C	35	ASN
1	C	64	ASN
1	C	66	GLN

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Mol	Chain	Res	Type
1	C	69	ASN
1	C	76	GLN
1	C	152	ASN
1	C	170	ASN
1	C	255	GLN
1	D	9	ASN
1	D	21	HIS
1	D	35	ASN
1	D	60	GLN
1	D	66	GLN
1	D	101	ASN
1	D	255	GLN
1	D	264	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	339/340 (99%)	-0.29	2 (0%) 89 84	71, 125, 137, 149	0
1	B	340/340 (100%)	-0.39	1 (0%) 94 90	99, 122, 134, 139	0
1	C	340/340 (100%)	-0.40	1 (0%) 94 90	101, 124, 138, 146	0
1	D	340/340 (100%)	-0.25	1 (0%) 94 90	118, 135, 147, 157	0
All	All	1359/1360 (99%)	-0.33	5 (0%) 92 87	71, 126, 142, 157	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	323	LYS	2.5
1	A	273	ILE	2.4
1	B	323	LYS	2.2
1	D	323	LYS	2.2
1	A	229	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.