



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:45 am BST

PDB ID : 5FOA
Title : Crystal Structure of Human Complement C3b in complex with DAF (CCP2-4)
Authors : Forneris, F.; Wu, J.; Xue, X.; Gros, P.
Deposited on : 2015-11-18
Resolution : 4.19 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

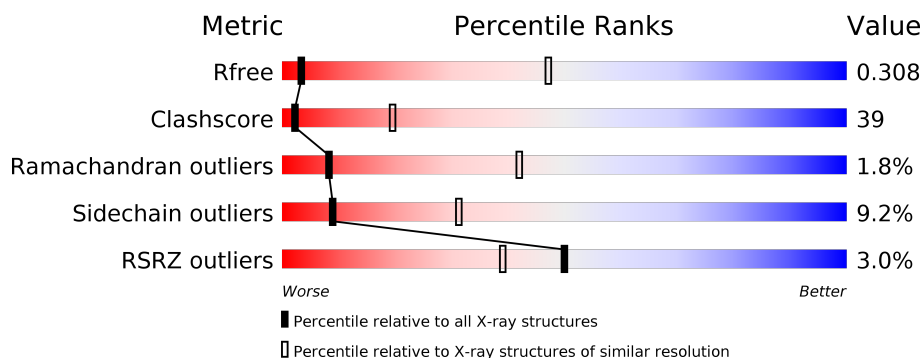
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.19 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	1034 (4.60-3.76)
Clashscore	141614	1030 (4.54-3.80)
Ramachandran outliers	138981	1006 (4.58-3.78)
Sidechain outliers	138945	1037 (4.60-3.76)
RSRZ outliers	127900	1056 (4.66-3.70)

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	645	<div> <div>3%</div> <div> <div>48%</div> <div>45%</div> <div>6%</div> </div> </div>
1	C	645	<div> <div>2%</div> <div> <div>52%</div> <div>41%</div> <div>5%</div> </div> </div>
2	B	915	<div> <div>3%</div> <div> <div>43%</div> <div>44%</div> <div>10%</div> </div> </div>
2	D	915	<div> <div>2%</div> <div> <div>43%</div> <div>44%</div> <div>10%</div> </div> </div>
3	E	194	<div> <div>6%</div> <div> <div>41%</div> <div>43%</div> <div>10%</div> </div> </div>
3	F	194	<div> <div>10%</div> <div> <div>41%</div> <div>40%</div> <div>14%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 27275 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 COMPLEMENT C3 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5002	3185	848	954	15			
1	C	642	Total	C	N	O	S	0	0	0
			5002	3185	848	954	15			

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	902	Total	C	N	O	S	0	0	0
			7177	4550	1205	1384	38			
2	D	902	Total	C	N	O	S	0	0	0
			7164	4543	1204	1380	37			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1013	GLU	GLN	SEE REMARK 999	UNP P01024
D	1013	GLU	GLN	SEE REMARK 999	UNP P01024

- Molecule 3 is a protein called DECAY ACCELERATING FACTOR, CD55.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	189	Total	C	N	O	S	0	0	0
			1465	920	249	283	13			
3	F	189	Total	C	N	O	S	0	0	0
			1465	920	249	283	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	95	GLY	-	expression tag	UNP P08174
E	96	SER	-	expression tag	UNP P08174

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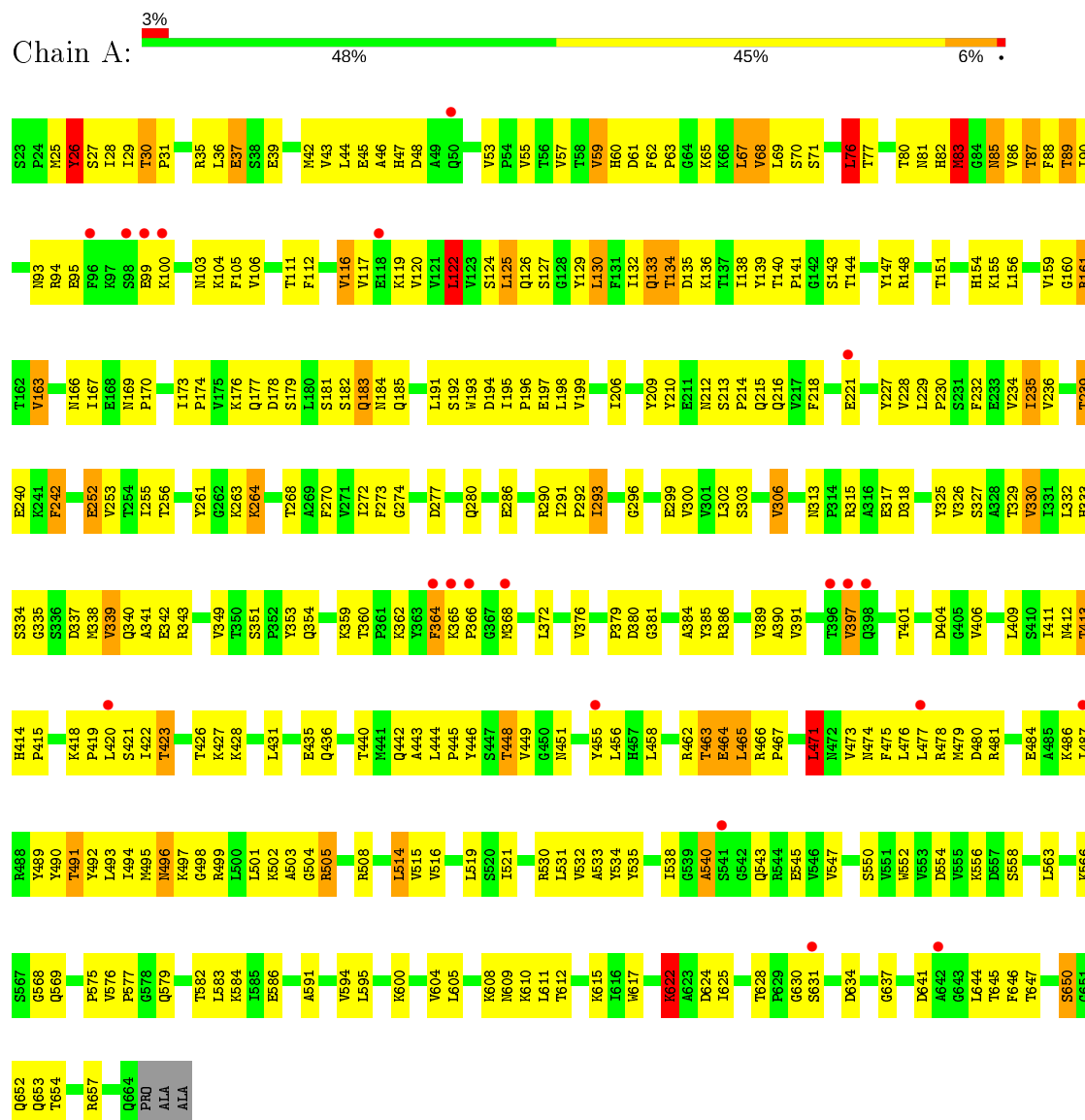
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Chain	Residue	Modelled	Actual	Comment	Reference
E	286	ALA	-	expression tag	UNP P08174
E	287	ALA	-	expression tag	UNP P08174
E	288	ALA	-	expression tag	UNP P08174
F	95	GLY	-	expression tag	UNP P08174
F	96	SER	-	expression tag	UNP P08174
F	286	ALA	-	expression tag	UNP P08174
F	287	ALA	-	expression tag	UNP P08174
F	288	ALA	-	expression tag	UNP P08174

3 Residue-property plots

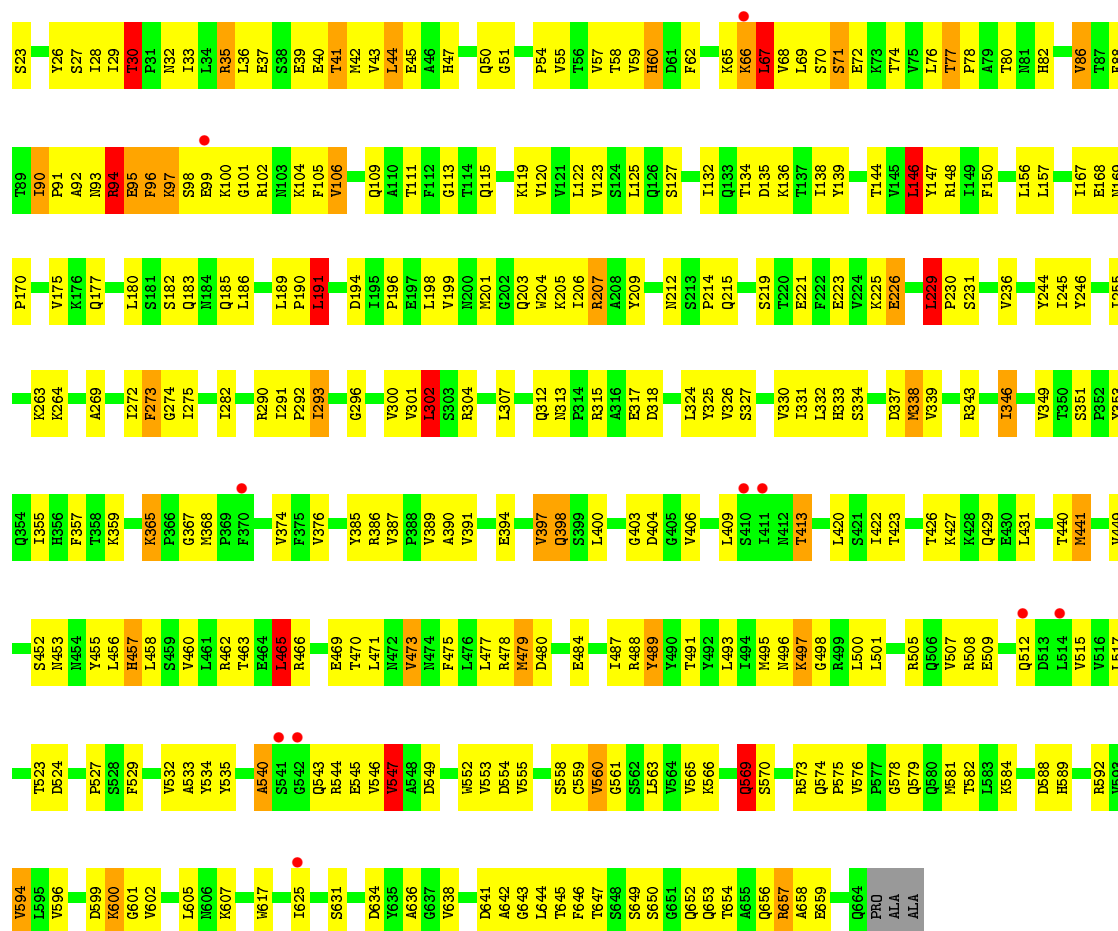
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: COMPLEMENT C3 BETA CHAIN

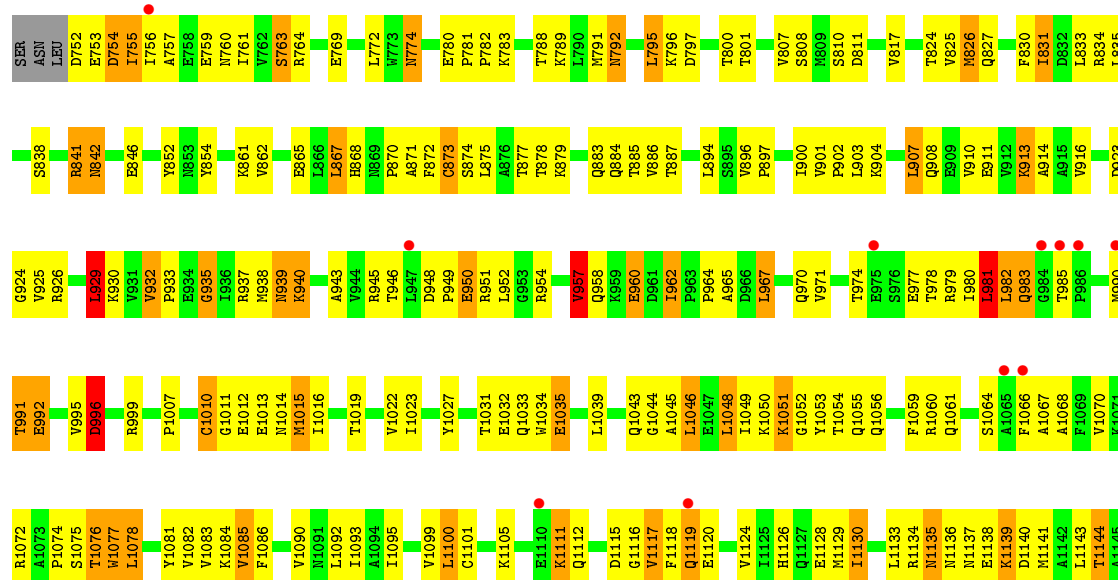
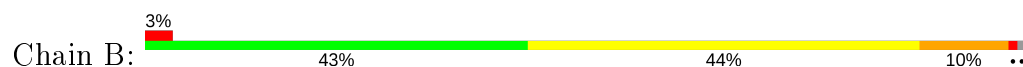


• Molecule 1: COMPLEMENT C3 BETA CHAIN



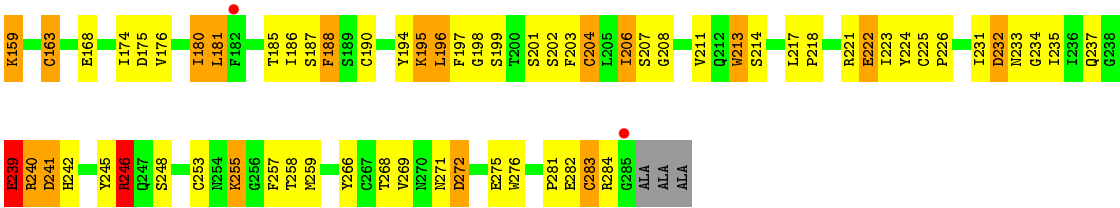


• Molecule 2: COMPLEMENT C3B ALPHA CHAIN









4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	117.43 Å 142.38 Å 323.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.39 – 4.19 110.39 – 4.19	Depositor EDS
% Data completeness (in resolution range)	95.5 (110.39-4.19) 89.6 (110.39-4.19)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 4.15 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.270 , 0.307 0.272 , 0.308	Depositor DCC
R_{free} test set	1955 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	124.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 115.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	27275	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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	0.58	2/5103 (0.0%)	0.90	16/6934 (0.2%)
1	C	0.63	5/5103 (0.1%)	0.95	21/6934 (0.3%)
2	B	0.71	16/7319 (0.2%)	1.07	55/9912 (0.6%)
2	D	0.71	10/7306 (0.1%)	1.09	49/9896 (0.5%)
3	E	0.82	5/1506 (0.3%)	1.07	11/2048 (0.5%)
3	F	0.68	1/1506 (0.1%)	1.00	11/2048 (0.5%)
All	All	0.68	39/27843 (0.1%)	1.02	163/37772 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	4
2	D	0	4
3	F	0	2
All	All	0	12

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1313	TRP	CE3-CZ3	-15.41	1.12	1.38
3	E	276	TRP	CB-CG	-9.69	1.32	1.50
2	D	813	LYS	CD-CE	-8.91	1.28	1.51
1	A	37	GLU	CG-CD	-8.84	1.38	1.51
3	E	158	CYS	CB-SG	-8.41	1.68	1.82
2	B	1358	CYS	CB-SG	-8.33	1.68	1.82
2	D	841	ARG	CB-CG	-7.26	1.32	1.52
1	C	67	LEU	CG-CD2	7.15	1.78	1.51
2	D	1036	LYS	CE-NZ	-6.97	1.31	1.49
2	D	1641	GLU	CD-OE2	6.70	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1506	CYS	CB-SG	-6.52	1.71	1.82
3	E	125	VAL	CB-CG2	-6.44	1.39	1.52
2	D	1249	VAL	CA-CB	6.25	1.67	1.54
1	C	569	GLN	CG-CD	-6.21	1.36	1.51
2	B	1313	TRP	CZ2-CH2	-6.20	1.25	1.37
3	E	283	CYS	CB-SG	-6.03	1.72	1.82
2	D	1550	VAL	CB-CG2	-5.99	1.40	1.52
1	C	66	LYS	CD-CE	-5.96	1.36	1.51
3	F	213	TRP	CB-CG	-5.96	1.39	1.50
2	B	1303	ARG	CB-CG	-5.89	1.36	1.52
2	D	1554	LEU	CG-CD1	-5.81	1.30	1.51
2	D	1036	LYS	CD-CE	-5.81	1.36	1.51
2	B	960	GLU	CB-CG	-5.78	1.41	1.52
2	B	1511	CYS	CB-SG	5.67	1.91	1.82
2	B	1035	GLU	CG-CD	-5.54	1.43	1.51
1	A	464	GLU	CD-OE2	-5.44	1.19	1.25
2	B	1580	GLN	CG-CD	-5.40	1.38	1.51
1	C	547	VAL	CB-CG1	-5.35	1.41	1.52
1	C	594	VAL	CB-CG2	-5.34	1.41	1.52
2	B	1292	LEU	CA-CB	5.34	1.66	1.53
2	B	1313	TRP	CB-CG	-5.31	1.40	1.50
2	D	813	LYS	CB-CG	-5.24	1.38	1.52
3	E	253	CYS	CB-SG	-5.24	1.73	1.81
2	B	1035	GLU	CB-CG	-5.23	1.42	1.52
2	B	960	GLU	CG-CD	-5.19	1.44	1.51
2	D	913	LYS	CE-NZ	-5.15	1.36	1.49
2	B	1111	LYS	CD-CE	-5.13	1.38	1.51
2	B	1580	GLN	CB-CG	-5.08	1.38	1.52
2	B	1591	ARG	CB-CG	-5.04	1.39	1.52

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1554	LEU	CB-CG-CD1	-12.82	89.20	111.00
1	A	83	MET	CG-SD-CE	-12.34	80.46	100.20
2	D	1649	LEU	CB-CG-CD2	-12.30	90.09	111.00
2	B	1292	LEU	CA-CB-CG	12.19	143.33	115.30
2	B	1300	LEU	CB-CG-CD1	-11.78	90.98	111.00
2	B	1292	LEU	CB-CG-CD1	11.53	130.60	111.00
2	B	1292	LEU	CD1-CG-CD2	-10.99	77.54	110.50
2	B	1303	ARG	NE-CZ-NH1	-10.85	114.88	120.30
1	A	364	PHE	CB-CG-CD2	-10.77	113.26	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	143	LEU	CB-CG-CD1	-10.53	93.09	111.00
2	D	1554	LEU	CB-CG-CD2	10.50	128.85	111.00
1	A	364	PHE	CB-CG-CD1	10.08	127.86	120.80
3	E	146	LEU	CA-CB-CG	9.91	138.09	115.30
2	D	1639	ASP	CB-CG-OD2	-9.82	109.46	118.30
3	E	143	LEU	CB-CG-CD2	9.57	127.27	111.00
2	D	796	LYS	CD-CE-NZ	-9.48	89.89	111.70
2	D	813	LYS	CD-CE-NZ	-9.42	90.04	111.70
1	C	94	ARG	NE-CZ-NH2	-9.37	115.61	120.30
3	E	143	LEU	CA-CB-CG	9.28	136.65	115.30
3	E	246	ARG	NE-CZ-NH1	9.16	124.88	120.30
2	B	1076	THR	CA-CB-CG2	-9.16	99.58	112.40
1	C	229	LEU	CA-CB-CG	9.14	136.33	115.30
2	B	1291	GLU	N-CA-C	-9.06	86.53	111.00
2	D	1037	PHE	CB-CG-CD2	-8.85	114.60	120.80
2	B	1300	LEU	CB-CG-CD2	8.80	125.97	111.00
2	D	1037	PHE	CB-CG-CD1	8.75	126.92	120.80
2	B	867	LEU	CB-CG-CD2	-8.72	96.18	111.00
2	D	1148	LEU	CA-CB-CG	8.63	135.15	115.30
2	D	813	LYS	CB-CG-CD	-8.57	89.31	111.60
1	A	83	MET	CA-CB-CG	-8.56	98.75	113.30
2	D	1243	LEU	CB-CG-CD2	-8.39	96.73	111.00
2	B	981	LEU	CB-CG-CD1	-8.34	96.83	111.00
3	F	181	LEU	CA-CB-CG	-8.17	96.51	115.30
1	C	67	LEU	CB-CG-CD1	-8.11	97.22	111.00
2	B	1646	CYS	CA-CB-SG	8.05	128.49	114.00
2	B	1497	LYS	CD-CE-NZ	-7.96	93.40	111.70
2	B	1092	LEU	CB-CG-CD2	-7.94	97.50	111.00
2	D	1508	ASP	CB-CG-OD1	7.87	125.38	118.30
2	D	1511	CYS	CA-CB-SG	7.86	128.15	114.00
1	C	67	LEU	CA-CB-CG	7.82	133.28	115.30
2	D	841	ARG	NE-CZ-NH1	-7.72	116.44	120.30
3	E	130	ARG	C-N-CD	-7.71	103.63	120.60
2	B	1202	LEU	CA-CB-CG	7.56	132.68	115.30
1	C	191	LEU	CA-CB-CG	7.49	132.53	115.30
2	B	1303	ARG	CG-CD-NE	-7.49	96.08	111.80
2	B	1207	LEU	CB-CG-CD1	-7.46	98.31	111.00
3	E	205	LEU	CA-CB-CG	7.40	132.33	115.30
2	D	1505	LEU	CA-CB-CG	-7.38	98.33	115.30
2	B	1294	LEU	CA-CB-CG	7.33	132.15	115.30
3	F	130	ARG	C-N-CD	-7.32	104.50	120.60
1	C	146	LEU	CB-CG-CD1	-7.29	98.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	761	ILE	CG1-CB-CG2	-7.07	95.85	111.40
1	A	76	LEU	CA-CB-CG	7.05	131.52	115.30
2	B	873	CYS	CA-CB-SG	-7.02	101.36	114.00
2	D	894	LEU	CA-CB-CG	-6.97	99.27	115.30
2	D	1582	ARG	NE-CZ-NH1	-6.96	116.82	120.30
2	D	1356	LEU	CA-CB-CG	6.92	131.22	115.30
1	C	465	LEU	CB-CG-CD1	-6.89	99.29	111.00
2	B	1292	LEU	CB-CG-CD2	6.87	122.68	111.00
2	B	1143	LEU	CB-CG-CD1	6.80	122.55	111.00
2	B	1506	CYS	CA-CB-SG	6.79	126.21	114.00
2	B	795	LEU	CA-CB-CG	6.78	130.90	115.30
3	F	246	ARG	NE-CZ-NH1	6.75	123.67	120.30
3	E	276	TRP	CA-CB-CG	-6.74	100.89	113.70
2	D	1176	LEU	CB-CG-CD1	6.73	122.45	111.00
2	D	1342	LEU	CA-CB-CG	6.68	130.67	115.30
2	B	1010	CYS	CA-CB-SG	6.66	125.98	114.00
2	B	1407	MET	CG-SD-CE	-6.64	89.58	100.20
3	E	136	GLU	C-N-CD	-6.64	105.99	120.60
2	D	1519	PHE	CB-CG-CD1	-6.52	116.24	120.80
1	C	479	MET	CG-SD-CE	-6.43	89.90	100.20
1	C	657	ARG	CG-CD-NE	6.35	125.14	111.80
2	B	1243	LEU	CB-CG-CD2	-6.34	100.21	111.00
2	D	1436	LYS	CD-CE-NZ	-6.31	97.20	111.70
2	D	1554	LEU	CD1-CG-CD2	-6.29	91.64	110.50
1	C	574	GLN	C-N-CD	6.28	141.58	128.40
2	B	1607	LEU	CA-CB-CG	6.26	129.69	115.30
3	E	170	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	D	1175	PHE	CB-CG-CD1	-6.15	116.49	120.80
1	A	471	LEU	CA-CB-CG	6.15	129.44	115.30
1	C	44	LEU	CB-CG-CD2	-6.13	100.58	111.00
3	F	269	VAL	CG1-CB-CG2	6.11	120.67	110.90
2	D	795	LEU	CA-CB-CG	6.07	129.26	115.30
2	B	967	LEU	CB-CG-CD2	6.05	121.28	111.00
2	B	1238	LEU	CB-CG-CD1	-6.03	100.74	111.00
2	B	1637	CYS	CA-CB-SG	6.03	124.85	114.00
1	C	30	THR	C-N-CD	5.99	140.97	128.40
2	D	1107	LEU	CA-CB-CG	5.95	128.99	115.30
2	B	913	LYS	CD-CE-NZ	-5.94	98.03	111.70
1	C	304	ARG	CG-CD-NE	-5.92	99.36	111.80
2	D	1298	LEU	CB-CG-CD1	-5.89	100.99	111.00
2	D	1202	LEU	CA-CB-CG	5.89	128.84	115.30
1	A	264	LYS	CD-CE-NZ	-5.86	98.23	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1065	ALA	N-CA-C	-5.84	95.22	111.00
2	B	996	ASP	CB-CG-OD1	5.83	123.54	118.30
2	B	867	LEU	CB-CG-CD1	5.82	120.89	111.00
3	E	172	GLY	N-CA-C	-5.79	98.61	113.10
2	D	1258	GLU	CA-CB-CG	5.79	126.15	113.40
1	C	302	LEU	CA-CB-CG	5.78	128.59	115.30
2	B	754	ASP	CB-CG-OD1	5.78	123.50	118.30
1	C	207	ARG	NE-CZ-NH1	-5.77	117.41	120.30
2	B	1632	PRO	CA-C-O	-5.76	106.39	120.20
2	B	1144	THR	CA-CB-CG2	-5.75	104.35	112.40
2	B	1015	MET	CA-CB-CG	5.75	123.07	113.30
2	D	1060	ARG	CA-CB-CG	5.75	126.04	113.40
2	B	1158	CYS	CA-CB-SG	5.71	124.28	114.00
1	C	273	PHE	CB-CG-CD2	-5.70	116.81	120.80
2	B	1287	PRO	N-CA-CB	5.70	110.13	103.30
1	A	26	TYR	CB-CG-CD1	5.63	124.38	121.00
2	D	778	LEU	CB-CG-CD2	-5.60	101.49	111.00
2	D	1497	LYS	CD-CE-NZ	5.55	124.47	111.70
1	C	489	TYR	CB-CG-CD2	-5.55	117.67	121.00
2	B	1100	LEU	CB-CG-CD2	-5.53	101.61	111.00
1	A	161	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	122	LEU	CA-CB-CG	5.52	128.00	115.30
2	B	1610	ASP	CB-CG-OD1	-5.52	113.33	118.30
2	B	1176	LEU	CB-CG-CD1	5.51	120.37	111.00
2	B	1119	GLN	CA-C-N	5.50	129.31	117.20
1	A	48	ASP	CB-CG-OD2	5.49	123.24	118.30
3	F	136	GLU	C-N-CD	-5.48	108.54	120.60
2	B	1549	LEU	CB-CG-CD1	5.48	120.31	111.00
2	D	1240	LEU	CB-CG-CD2	-5.47	101.70	111.00
2	D	1092	LEU	CA-CB-CG	-5.46	102.75	115.30
1	A	505	ARG	NE-CZ-NH2	5.45	123.03	120.30
2	B	1300	LEU	CA-CB-CG	5.44	127.81	115.30
1	C	94	ARG	CD-NE-CZ	5.42	131.19	123.60
2	B	1139	LYS	CD-CE-NZ	-5.40	99.27	111.70
1	C	559	CYS	N-CA-C	-5.39	96.45	111.00
2	B	1535	LYS	CB-CG-CD	5.38	125.60	111.60
2	B	1171	LYS	CA-CB-CG	5.38	125.23	113.40
1	C	207	ARG	CB-CG-CD	-5.38	97.62	111.60
2	D	1106	TRP	CA-CB-CG	-5.37	103.50	113.70
3	F	139	LEU	CB-CG-CD2	-5.36	101.89	111.00
2	D	1039	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	514	LEU	CA-CB-CG	5.33	127.57	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1497	LYS	CA-CB-CG	5.33	125.12	113.40
2	B	1046	LEU	CA-CB-CG	5.31	127.51	115.30
3	F	134	ARG	CG-CD-NE	-5.30	100.67	111.80
2	B	1580	GLN	CA-CB-CG	-5.22	101.92	113.40
3	F	239	GLU	CG-CD-OE1	5.22	128.73	118.30
2	D	813	LYS	N-CA-CB	-5.18	101.27	110.60
2	B	929	LEU	CA-CB-CG	5.17	127.20	115.30
2	D	764	ARG	NE-CZ-NH1	-5.17	117.71	120.30
3	F	204	CYS	CA-CB-SG	5.17	123.30	114.00
3	F	241	ASP	CB-CG-OD2	5.15	122.94	118.30
2	B	1078	LEU	CB-CG-CD1	-5.15	102.24	111.00
2	D	1328	GLU	CA-CB-CG	5.15	124.73	113.40
1	A	48	ASP	CB-CG-OD1	-5.15	113.67	118.30
2	D	979	ARG	CG-CD-NE	-5.14	101.01	111.80
3	F	241	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	A	339	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	C	94	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	B	1535	LYS	CD-CE-NZ	5.12	123.47	111.70
2	D	1078	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	26	TYR	CB-CG-CD2	-5.10	117.94	121.00
2	B	1519	PHE	CB-CG-CD2	-5.08	117.24	120.80
2	D	1648	ASP	CB-CG-OD1	5.07	122.87	118.30
2	B	1292	LEU	N-CA-C	-5.06	97.34	111.00
2	D	1425	VAL	CG1-CB-CG2	5.05	118.98	110.90
2	B	1077	TRP	CA-CB-CG	-5.03	104.14	113.70
2	D	947	LEU	CB-CG-CD1	-5.03	102.46	111.00
2	D	1615	LYS	C-N-CD	5.02	138.95	128.40
2	D	1591	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	GLN	Mainchain
1	A	622	LYS	Mainchain
2	B	1292	LEU	Mainchain
2	B	1311	ILE	Mainchain
2	B	1632	PRO	Mainchain
2	B	841	ARG	Mainchain
2	D	1063	SER	Mainchain
2	D	1414	ASP	Mainchain
2	D	1507	ARG	Mainchain

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Mol	Chain	Res	Type	Group
2	D	949	PRO	Mainchain
3	F	232	ASP	Mainchain
3	F	240	ARG	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5002	0	5058	352	2
1	C	5002	0	5058	343	1
2	B	7177	0	7086	567	2
2	D	7164	0	7066	667	1
3	E	1465	0	1389	153	1
3	F	1465	0	1389	142	0
All	All	27275	0	27046	2109	4

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 39.

All (2109) 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:C:67:LEU:CG	1:C:67:LEU:CD2	1.78	1.61
1:C:32:ASN:HD21	1:C:657:ARG:HD3	1.11	1.16
1:A:466:ARG:HG3	1:A:556:LYS:HD3	1.28	1.15
2:D:978:THR:HG22	2:D:1346:THR:HG22	1.31	1.10
3:F:157:PHE:O	3:F:159:LYS:NZ	1.84	1.09
3:F:135:ARG:HH21	3:F:141:PRO:HD3	0.92	1.07
2:D:1559:ASP:OD1	2:D:1591:ARG:NH2	1.87	1.07
2:B:1300:LEU:HD11	2:B:1303:ARG:HG2	1.33	1.06
2:D:758:GLU:HA	2:D:913:LYS:HZ3	1.21	1.04
3:E:246:ARG:NH1	3:E:246:ARG:O	1.87	1.04
2:D:947:LEU:HD11	2:D:1342:LEU:HB3	1.38	1.04
3:F:135:ARG:NH2	3:F:141:PRO:HD3	1.73	1.03
2:B:1076:THR:HG21	2:B:1111:LYS:HE2	1.09	1.03
1:C:62:PHE:O	1:C:104:LYS:NZ	1.92	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1140:ASP:O	2:D:1144:THR:OG1	1.78	1.02
2:B:1015:MET:SD	2:B:1056:GLN:NE2	2.34	1.01
2:D:766:GLU:HB3	2:D:796:LYS:HZ1	1.26	1.00
2:B:945:ARG:NH1	2:B:960:GLU:OE2	1.94	1.00
1:C:508:ARG:NH1	1:C:512:GLN:O	1.93	1.00
1:A:44:LEU:HD11	1:A:86:VAL:HG22	1.42	1.00
2:B:1202:LEU:HD13	2:B:1207:LEU:HD11	1.42	1.00
2:B:1517:ASN:ND2	2:B:1521:GLN:OE1	1.95	1.00
1:C:94:ARG:HE	1:C:94:ARG:HA	1.26	0.99
3:E:246:ARG:C	3:E:246:ARG:HH11	1.66	0.98
2:B:1202:LEU:HD11	2:B:1243:LEU:HD21	1.46	0.97
2:B:971:VAL:HG22	2:B:1351:LYS:HD2	1.42	0.97
1:C:560:VAL:HG22	2:D:813:LYS:HZ1	1.26	0.97
1:A:406:VAL:HG11	1:A:462:ARG:HH11	1.30	0.96
1:C:578:GLY:H	2:D:795:LEU:HD11	1.29	0.96
3:E:239:GLU:O	3:E:240:ARG:NH1	1.98	0.96
3:F:180:ILE:HD11	3:F:213:TRP:CZ2	2.00	0.96
1:C:28:ILE:HD11	1:C:42:MET:HG3	1.46	0.96
1:C:138:ILE:HG22	1:C:223:GLU:HB3	1.45	0.95
2:B:1129:MET:O	2:B:1270:GLN:NE2	1.98	0.95
2:D:1577:GLN:H	2:D:1580:GLN:HE21	1.02	0.95
2:D:1105:LYS:HG2	2:D:1106:TRP:CD1	2.01	0.95
2:D:810:SER:HB3	2:D:813:LYS:HB3	1.47	0.94
2:B:1635:ASP:HA	2:B:1638:GLN:HE22	1.31	0.94
1:A:181:SER:HB3	3:E:246:ARG:HE	1.30	0.94
1:C:508:ARG:HG3	1:C:508:ARG:HH11	1.32	0.93
2:D:1369:PRO:HA	2:D:1384:MET:HG2	1.50	0.93
1:A:406:VAL:HG11	1:A:462:ARG:NH1	1.83	0.93
1:C:496:ASN:HB3	1:C:501:LEU:HG	1.47	0.93
1:C:32:ASN:ND2	1:C:657:ARG:HD3	1.81	0.93
2:B:1013:GLU:O	2:B:1016:ILE:HG13	1.68	0.93
2:B:1076:THR:HG21	2:B:1111:LYS:CE	1.99	0.92
2:B:1610:ASP:N	2:B:1610:ASP:OD1	1.99	0.92
2:D:1506:CYS:SG	2:D:1511:CYS:HB2	2.10	0.92
2:D:1149:ILE:HD13	2:D:1194:TYR:HE2	1.33	0.92
1:C:523:THR:HB	1:C:560:VAL:HG23	1.52	0.91
2:D:757:ALA:O	2:D:913:LYS:NZ	2.04	0.91
2:B:1366:THR:OG1	2:B:1387:GLU:OE2	1.89	0.90
2:D:1101:CYS:SG	2:D:1161:GLN:NE2	2.44	0.90
2:D:1202:LEU:HD11	2:D:1243:LEU:HD21	1.53	0.90
2:B:951:ARG:HH21	2:B:1339:GLN:HG3	1.33	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1298:LEU:O	2:B:1303:ARG:NH2	2.04	0.90
2:D:1258:GLU:HA	2:D:1260:ARG:NH1	1.87	0.90
1:C:66:LYS:NZ	3:E:145:CYS:O	2.05	0.89
2:D:1202:LEU:HD13	2:D:1207:LEU:HD13	1.54	0.89
3:E:260:ILE:HD12	3:E:284:ARG:HD3	1.55	0.89
2:D:1105:LYS:HE3	2:D:1106:TRP:HE1	1.36	0.89
1:C:349:VAL:HG12	1:C:351:SER:H	1.38	0.88
2:B:1512:ARG:NH1	2:B:1609:SER:O	2.05	0.88
2:B:1554:LEU:HD13	2:B:1591:ARG:HH12	1.37	0.88
1:A:418:LYS:HD2	1:A:419:PRO:HD2	1.54	0.88
3:E:170:ARG:HG3	3:E:170:ARG:HH11	1.38	0.88
1:C:207:ARG:NH1	1:C:219:SER:OG	2.05	0.88
2:B:841:ARG:NH1	2:B:902:PRO:O	2.06	0.87
1:C:98:SER:O	1:C:101:GLY:N	2.08	0.87
3:F:135:ARG:HH21	3:F:141:PRO:CD	1.83	0.87
2:B:1295:ASP:OD1	2:B:1310:ARG:NE	2.07	0.87
1:C:50:GLN:HE21	1:C:51:GLY:H	1.16	0.86
2:D:1033:GLN:HB3	2:D:1036:LYS:NZ	1.90	0.86
2:D:1298:LEU:HB3	2:D:1332:VAL:HG22	1.55	0.86
2:B:1136:ASN:HA	2:B:1139:LYS:HZ1	1.41	0.86
1:C:93:ASN:OD1	1:C:94:ARG:N	2.08	0.86
1:A:568:GLY:O	3:F:271:ASN:ND2	2.07	0.86
3:E:135:ARG:NH2	3:E:137:PRO:HA	1.90	0.86
1:C:69:LEU:HD21	1:C:91:PRO:HD2	1.58	0.86
2:D:856:GLN:HA	2:D:891:LYS:HE2	1.58	0.86
1:A:103:ASN:ND2	2:B:1035:GLU:OE2	2.08	0.85
2:B:1300:LEU:CD1	2:B:1303:ARG:HG2	2.06	0.85
2:D:867:LEU:HD11	2:D:913:LYS:HE2	1.57	0.85
2:D:764:ARG:NH1	2:D:923:ASP:OD1	2.09	0.85
2:B:1060:ARG:NH2	2:B:1064:SER:OG	2.10	0.84
2:D:1152:GLN:NE2	2:D:1198:GLN:OE1	2.11	0.83
2:D:755:ILE:HG21	2:D:863:ARG:HD3	1.58	0.83
1:A:264:LYS:HB3	1:A:296:GLY:HA3	1.61	0.83
3:F:233:ASN:ND2	3:F:283:CYS:O	2.11	0.83
1:C:594:VAL:HG13	2:D:807:VAL:HG13	1.58	0.83
2:D:832:ASP:OD2	2:D:834:ARG:NH2	2.12	0.83
1:A:181:SER:CB	3:E:246:ARG:HH21	1.91	0.83
2:D:1106:TRP:CD1	2:D:1106:TRP:N	2.44	0.83
2:D:883:GLN:OE1	2:D:883:GLN:N	2.12	0.83
1:A:229:LEU:O	2:B:834:ARG:NH2	2.10	0.83
2:D:1577:GLN:OE1	2:D:1580:GLN:NE2	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1190:ALA:HA	2:D:1220:TRP:HZ3	1.42	0.82
2:B:985:THR:OG1	2:B:1339:GLN:O	1.96	0.82
3:F:135:ARG:NH2	3:F:139:LEU:O	2.12	0.82
1:A:349:VAL:HG12	1:A:351:SER:H	1.42	0.82
2:B:1635:ASP:HA	2:B:1638:GLN:NE2	1.95	0.82
1:C:560:VAL:HG22	2:D:813:LYS:NZ	1.93	0.82
1:A:134:THR:HG1	1:A:139:TYR:HH	1.26	0.82
3:E:146:LEU:HG	3:E:150:LYS:HB2	1.61	0.82
2:D:1492:PHE:H	2:D:1492:PHE:HD1	1.24	0.82
2:D:755:ILE:HG22	2:D:756:ILE:H	1.44	0.81
2:B:865:GLU:OE1	2:B:883:GLN:NE2	2.13	0.81
2:B:862:VAL:HG12	2:B:916:VAL:HG12	1.61	0.81
2:B:1118:PHE:H	2:B:1144:THR:HG22	1.45	0.81
2:D:1105:LYS:HG2	2:D:1106:TRP:HD1	1.42	0.81
2:D:871:ALA:O	2:D:903:LEU:N	2.13	0.81
1:C:423:THR:HG23	1:C:440:THR:HG22	1.61	0.81
2:D:1106:TRP:N	2:D:1106:TRP:HD1	1.77	0.81
3:E:223:ILE:HD11	3:E:269:VAL:HG22	1.63	0.81
2:B:1572:GLY:O	2:B:1574:ASP:N	2.13	0.81
1:C:535:TYR:CZ	1:C:547:VAL:HG11	2.15	0.81
2:B:1311:ILE:O	2:B:1313:TRP:HZ3	1.64	0.81
2:D:826:MET:HG2	2:D:827:GLN:H	1.46	0.81
1:C:385:TYR:CE1	1:C:386:ARG:HG3	2.15	0.80
2:D:759:GLU:HG2	2:D:760:ASN:H	1.45	0.80
3:E:109:LEU:HB2	3:E:114:ILE:HG12	1.63	0.80
1:C:264:LYS:HB3	1:C:296:GLY:HA3	1.64	0.80
2:B:983:GLN:OE1	2:B:983:GLN:N	2.15	0.80
2:D:1158:CYS:HA	2:D:1161:GLN:NE2	1.95	0.80
2:D:978:THR:OG1	2:D:1324:THR:HG23	1.82	0.80
3:F:136:GLU:HB2	3:F:159:LYS:CE	2.12	0.79
2:D:766:GLU:HB3	2:D:796:LYS:NZ	1.95	0.79
2:B:1300:LEU:HD23	2:B:1324:THR:HG21	1.64	0.79
1:C:168:GLU:HG3	1:C:205:LYS:HB3	1.62	0.79
2:D:1550:VAL:HG21	2:D:1581:GLN:NE2	1.96	0.79
2:B:1313:TRP:N	2:B:1313:TRP:CE3	2.50	0.79
1:A:486:LYS:HZ3	1:A:538:ILE:HG12	1.48	0.79
2:D:1397:ASP:HB3	2:D:1450:LYS:HE2	1.64	0.79
2:D:1505:LEU:HD13	2:D:1585:ILE:HD11	1.65	0.79
3:F:136:GLU:HB2	3:F:159:LYS:HE2	1.63	0.78
3:F:223:ILE:HD13	3:F:272:ASP:HA	1.65	0.78
3:F:224:TYR:CE1	3:F:242:HIS:HB3	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:VAL:HG21	1:A:411:ILE:HD11	1.63	0.78
1:A:486:LYS:NZ	1:A:538:ILE:HG12	1.97	0.78
3:E:225:CYS:HB3	3:E:276:TRP:CZ2	2.19	0.78
2:D:1517:ASN:HD21	2:D:1521:GLN:HB2	1.49	0.78
2:D:1577:GLN:H	2:D:1580:GLN:NE2	1.79	0.78
2:B:1303:ARG:HH12	2:B:1306:LYS:HA	1.48	0.78
2:B:980:ILE:HD11	2:B:1322:GLU:HB2	1.63	0.78
1:A:496:ASN:HD22	1:A:501:LEU:HD22	1.47	0.78
1:C:205:LYS:HE2	1:C:207:ARG:HD3	1.65	0.78
2:D:1506:CYS:CB	2:D:1511:CYS:HB2	2.13	0.78
2:D:962:ILE:HG13	2:D:1330:PHE:O	1.82	0.78
2:D:756:ILE:HD13	2:D:761:ILE:HG13	1.64	0.78
2:B:1240:LEU:HD13	2:B:1249:VAL:HG22	1.66	0.77
1:C:207:ARG:HH11	1:C:219:SER:HG	1.32	0.77
1:A:53:VAL:HB	1:A:76:LEU:HD22	1.64	0.77
1:C:59:VAL:HG23	1:C:106:VAL:HG21	1.66	0.77
3:E:237:GLN:HB3	3:E:250:THR:HG23	1.65	0.77
2:B:1238:LEU:HD11	2:B:1277:GLN:HE21	1.47	0.77
1:C:578:GLY:H	2:D:795:LEU:CD1	1.98	0.77
3:F:135:ARG:HG3	3:F:135:ARG:HH11	1.49	0.77
3:F:233:ASN:ND2	3:F:283:CYS:HB3	2.00	0.77
1:A:28:ILE:HG23	1:A:647:THR:OG1	1.85	0.77
2:B:1111:LYS:NZ	2:B:1119:GLN:O	2.16	0.77
1:C:578:GLY:N	2:D:795:LEU:HD11	2.00	0.77
1:C:28:ILE:HD11	1:C:42:MET:CG	2.15	0.77
2:B:1146:PHE:O	2:B:1149:ILE:HG13	1.85	0.77
2:B:763:SER:HB2	2:B:926:ARG:HB2	1.67	0.77
3:E:240:ARG:HB2	3:E:243:TYR:CZ	2.20	0.77
2:B:1303:ARG:HH12	2:B:1306:LYS:CA	1.98	0.76
2:D:1104:VAL:HG13	2:D:1151:LEU:HD11	1.66	0.76
1:C:496:ASN:OD1	1:C:497:LYS:HG3	1.85	0.76
1:A:286:GLU:HG3	1:A:306:VAL:HG23	1.65	0.76
1:A:558:SER:O	1:A:617:TRP:NE1	2.17	0.76
2:B:1014:ASN:HB2	2:B:1055:GLN:NE2	1.99	0.76
1:C:312:GLN:OE1	1:C:312:GLN:N	2.17	0.76
1:C:576:VAL:N	1:C:579:GLN:OE1	2.17	0.76
1:C:66:LYS:HG2	3:E:147:GLN:HG3	1.67	0.76
2:D:1551:LYS:HE3	2:D:1562:ILE:CD1	2.16	0.76
2:D:1300:LEU:HD12	2:D:1303:ARG:H	1.49	0.76
1:A:230:PRO:HG3	1:A:604:VAL:HG11	1.67	0.76
1:C:291:ILE:HD13	1:C:300:VAL:HB	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1233:THR:HG21	2:B:1256:LEU:HD11	1.67	0.76
1:C:290:ARG:NH1	2:D:1400:MET:SD	2.59	0.76
1:C:535:TYR:CE1	1:C:547:VAL:HG11	2.21	0.76
1:C:136:LYS:NZ	1:C:138:ILE:O	2.17	0.76
2:B:1494:HIS:HD2	2:B:1495:PRO:HD2	1.50	0.75
2:D:1145:ALA:HA	2:D:1148:LEU:HG	1.67	0.75
2:B:1303:ARG:NH1	2:B:1307:ILE:HG12	2.01	0.75
1:C:67:LEU:HD13	3:E:144:THR:HG21	1.67	0.75
2:B:967:LEU:HD22	2:B:1348:TYR:CD2	2.21	0.75
2:B:1303:ARG:NH1	2:B:1305:SER:O	2.20	0.75
1:C:331:ILE:HG12	1:C:338:MET:HB3	1.66	0.75
1:A:45:GLU:OE2	1:A:83:MET:HE1	1.87	0.75
1:C:214:PRO:HB2	2:D:1316:ALA:HB3	1.68	0.75
1:A:471:LEU:HB3	1:A:521:ILE:HD11	1.68	0.75
2:D:1355:GLN:N	2:D:1356:LEU:HB3	2.02	0.75
3:E:141:PRO:HA	3:E:157:PHE:CD2	2.22	0.75
1:A:291:ILE:HD13	1:A:300:VAL:HB	1.68	0.74
1:A:44:LEU:HD23	1:A:55:VAL:HG21	1.69	0.74
1:C:67:LEU:HD12	1:C:68:VAL:H	1.52	0.74
1:A:181:SER:HB3	3:E:246:ARG:NE	2.01	0.74
1:C:69:LEU:HD21	1:C:90:ILE:HA	1.69	0.74
1:A:364:PHE:HE2	1:A:366:PRO:HA	1.52	0.74
1:C:496:ASN:ND2	1:C:524:ASP:O	2.20	0.74
2:D:1597:GLU:HG3	2:D:1600:LYS:HG3	1.67	0.74
1:A:136:LYS:NZ	1:A:138:ILE:O	2.20	0.74
2:B:1311:ILE:O	2:B:1313:TRP:CZ3	2.41	0.74
1:C:473:VAL:HG13	1:C:517:LEU:HB3	1.70	0.74
1:C:69:LEU:CD2	1:C:90:ILE:HA	2.18	0.74
1:A:650:SER:OG	1:A:652:GLN:NE2	2.20	0.74
2:B:1292:LEU:HD22	2:B:1338:GLY:HA2	1.70	0.74
2:D:1107:LEU:HD11	2:D:1147:VAL:HG13	1.69	0.73
1:C:67:LEU:HG	1:C:67:LEU:CD2	2.12	0.73
2:D:1284:LYS:NZ	2:D:1285:ASP:OD1	2.20	0.73
3:F:239:GLU:CD	3:F:240:ARG:H	1.92	0.73
2:B:1136:ASN:HD22	2:B:1139:LYS:NZ	1.87	0.73
2:B:763:SER:OG	2:B:911:GLU:OE2	2.06	0.73
2:D:1436:LYS:NZ	2:D:1439:SER:O	2.21	0.73
2:D:1631:TRP:CD1	2:D:1649:LEU:HD21	2.22	0.73
1:A:111:THR:HG22	1:A:116:VAL:HG23	1.70	0.73
2:B:1019:THR:HG1	2:B:1081:TYR:HH	1.34	0.73
1:A:181:SER:HB3	3:E:246:ARG:HH21	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1313:TRP:HE3	2:B:1313:TRP:N	1.84	0.73
2:B:935:GLY:HA3	2:B:1349:HIS:ND1	2.04	0.73
1:C:508:ARG:NH1	1:C:508:ARG:HG3	2.03	0.73
1:A:37:GLU:OE2	1:A:161:ARG:NH1	2.22	0.73
2:D:1255:TRP:HA	2:D:1258:GLU:OE2	1.89	0.73
2:B:1240:LEU:CD1	2:B:1249:VAL:HG22	2.19	0.72
1:A:36:LEU:HD12	1:A:37:GLU:HG2	1.70	0.72
2:B:1507:ARG:HB2	2:B:1612:TRP:CZ2	2.24	0.72
3:F:157:PHE:C	3:F:159:LYS:NZ	2.43	0.72
1:A:449:VAL:HG21	1:A:545:GLU:HG3	1.71	0.72
1:A:466:ARG:CG	1:A:556:LYS:HD3	2.14	0.72
3:E:135:ARG:HH22	3:E:137:PRO:HA	1.54	0.72
1:A:36:LEU:HD21	1:A:125:LEU:HA	1.72	0.72
1:A:530:ARG:NH1	1:A:624:ASP:OD2	2.21	0.72
2:B:1111:LYS:HE3	2:B:1119:GLN:O	1.89	0.72
2:D:1197:ALA:HB2	2:D:1202:LEU:HD21	1.72	0.72
1:A:313:ASN:OD1	1:A:315:ARG:N	2.22	0.72
1:A:431:LEU:HD11	1:A:436:GLN:CD	2.09	0.72
1:C:313:ASN:ND2	1:C:315:ARG:O	2.23	0.72
1:C:93:ASN:ND2	1:C:95:GLU:OE1	2.21	0.72
1:C:94:ARG:CA	1:C:94:ARG:HE	2.02	0.72
2:D:1113:LYS:HB2	2:D:1117:VAL:HG22	1.72	0.72
3:F:195:LYS:HD2	3:F:196:LEU:H	1.55	0.72
2:D:1551:LYS:HE3	2:D:1562:ILE:HD11	1.71	0.72
2:D:937:ARG:HH21	2:D:1349:HIS:HE1	1.37	0.72
2:D:1633:GLU:HB2	2:D:1636:GLU:OE1	1.89	0.72
2:D:1035:GLU:HA	2:D:1039:LEU:CD1	2.19	0.72
1:C:561:GLY:HA3	2:D:813:LYS:HE2	1.72	0.72
2:D:1060:ARG:HD3	2:D:1066:PHE:CZ	2.24	0.72
2:B:1497:LYS:HZ3	2:B:1502:LEU:HA	1.54	0.72
2:D:1367:ILE:HD11	2:D:1386:LEU:HD13	1.71	0.72
2:D:1574:ASP:OD2	2:D:1620:TYR:OH	2.05	0.72
1:A:25:MET:SD	1:A:652:GLN:NE2	2.63	0.71
1:A:423:THR:HG22	1:A:440:THR:HG23	1.71	0.71
3:E:195:LYS:HE3	3:E:197:PHE:HE1	1.55	0.71
3:E:273:GLU:HG3	3:E:275:GLU:OE2	1.90	0.71
3:F:113:TYR:HA	3:F:116:GLN:HG2	1.72	0.71
2:D:1303:ARG:NH2	3:F:239:GLU:OE1	2.22	0.71
1:A:122:LEU:HD11	1:A:657:ARG:HB3	1.72	0.71
2:B:1298:LEU:HB3	2:B:1332:VAL:HG22	1.72	0.71
2:B:958:GLN:NE2	2:B:1334:ALA:HB3	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1405:ILE:HG12	2:D:1477:VAL:HG22	1.72	0.71
2:B:1249:VAL:HB	2:B:1250:PRO:HD3	1.72	0.71
2:D:1149:ILE:HD13	2:D:1194:TYR:CE2	2.23	0.71
2:B:1554:LEU:HD13	2:B:1591:ARG:NH1	2.05	0.71
2:B:780:GLU:N	2:B:780:GLU:OE1	2.24	0.71
2:D:1161:GLN:N	2:D:1161:GLN:OE1	2.23	0.71
3:E:224:TYR:CD2	3:E:242:HIS:HB3	2.25	0.71
2:D:1512:ARG:CZ	2:D:1621:ILE:HD13	2.21	0.71
2:B:1117:VAL:HA	2:B:1144:THR:HG21	1.73	0.71
2:B:1174:ASP:HA	2:B:1201:ARG:HH22	1.55	0.71
2:B:1544:VAL:HG22	2:B:1569:ILE:HB	1.73	0.71
3:E:146:LEU:HD13	3:E:148:ASN:H	1.56	0.71
2:D:1249:VAL:CG2	2:D:1250:PRO:HD3	2.19	0.71
1:A:652:GLN:N	1:A:652:GLN:OE1	2.22	0.71
2:B:1140:ASP:O	2:B:1144:THR:OG1	2.07	0.71
2:B:873:CYS:HB3	2:B:901:VAL:HG13	1.72	0.71
3:E:170:ARG:CG	3:E:170:ARG:HH11	2.02	0.71
3:E:226:PRO:N	3:E:276:TRP:HH2	1.89	0.71
1:A:26:TYR:HE2	1:A:53:VAL:HG11	1.55	0.70
2:B:1101:CYS:O	2:B:1105:LYS:HG3	1.91	0.70
2:D:1003:LEU:HD11	2:D:1276:PHE:HE2	1.56	0.70
2:D:1067:ALA:HB2	2:D:1074:PRO:HA	1.72	0.70
2:D:1574:ASP:OD2	2:D:1582:ARG:NH1	2.24	0.70
2:B:964:PRO:HB3	2:B:1327:ASN:OD1	1.90	0.70
1:C:29:ILE:HA	1:C:645:THR:O	1.90	0.70
2:D:1507:ARG:HE	2:D:1510:LEU:HD23	1.56	0.70
3:F:246:ARG:CG	3:F:246:ARG:HH11	2.03	0.70
1:C:659:GLU:OE1	1:C:659:GLU:N	2.24	0.70
2:D:1311:ILE:HD11	2:D:1318:LEU:HD23	1.71	0.70
2:D:758:GLU:HA	2:D:913:LYS:NZ	2.04	0.70
2:D:934:GLU:N	2:D:934:GLU:OE1	2.22	0.70
3:E:133:TYR:HB3	3:E:158:CYS:HB3	1.72	0.70
2:B:1111:LYS:CE	2:B:1119:GLN:O	2.40	0.70
1:C:99:GLU:CB	1:C:102:ARG:HB2	2.22	0.70
2:D:1498:GLU:C	2:D:1500:GLY:H	1.94	0.70
1:A:481:ARG:HA	1:A:484:GLU:OE1	1.92	0.70
2:B:1118:PHE:H	2:B:1144:THR:CG2	2.04	0.70
1:C:390:ALA:HB2	1:C:398:GLN:OE1	1.90	0.69
2:D:1485:LEU:HD12	2:D:1486:GLU:H	1.56	0.69
2:D:776:GLU:HG3	2:D:791:MET:SD	2.31	0.69
2:D:935:GLY:HA2	2:D:1353:LYS:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:TYR:HE1	1:A:634:ASP:HA	1.57	0.69
1:C:458:LEU:HD11	1:C:533:ALA:HB3	1.73	0.69
2:D:1149:ILE:HA	2:D:1152:GLN:NE2	2.07	0.69
2:D:987:VAL:HG22	2:D:988:ALA:H	1.57	0.69
2:D:1151:LEU:HG	2:D:1165:LEU:HD11	1.74	0.69
2:D:904:LYS:O	2:D:908:GLN:NE2	2.24	0.69
2:B:1078:LEU:HD11	2:B:1124:VAL:HG23	1.75	0.69
2:D:1544:VAL:HG23	2:D:1570:LYS:HD3	1.74	0.69
2:D:768:PRO:HD3	2:D:796:LYS:HZ2	1.56	0.69
2:B:938:MET:HB3	2:B:940:LYS:HZ2	1.57	0.69
1:A:125:LEU:HD22	1:A:215:GLN:HE22	1.56	0.69
1:A:647:THR:HG22	1:A:653:GLN:OE1	1.93	0.69
2:B:990:MET:O	2:B:1282:TYR:OH	2.11	0.69
1:C:183:GLN:N	1:C:183:GLN:OE1	2.21	0.69
1:A:141:PRO:HA	1:A:195:ILE:HD12	1.75	0.69
2:B:1050:LYS:O	2:B:1054:THR:HG23	1.92	0.69
2:B:1387:GLU:OE1	2:B:1387:GLU:N	2.25	0.69
2:B:1472:ILE:HD11	2:B:1494:HIS:NE2	2.08	0.69
3:E:143:LEU:HD12	3:E:143:LEU:C	2.13	0.69
2:B:800:THR:OG1	2:B:801:THR:N	2.25	0.69
1:A:647:THR:HG22	1:A:653:GLN:NE2	2.07	0.69
2:D:1496:GLU:OE1	2:D:1496:GLU:N	2.23	0.69
2:D:948:ASP:OD2	2:D:951:ARG:NH1	2.26	0.69
2:B:1396:GLN:C	2:B:1453:HIS:HD2	1.97	0.69
1:A:83:MET:HE2	1:A:505:ARG:HH11	1.57	0.69
2:B:1202:LEU:CD1	2:B:1243:LEU:HD21	2.22	0.69
2:B:1300:LEU:HD12	2:B:1300:LEU:O	1.92	0.69
2:D:1552:VAL:HG12	2:D:1561:TYR:CD1	2.28	0.69
2:B:1202:LEU:HA	2:B:1206:LEU:HD11	1.74	0.68
1:C:646:PHE:H	1:C:654:THR:CG2	2.05	0.68
2:D:1105:LYS:HE3	2:D:1106:TRP:NE1	2.08	0.68
1:A:476:LEU:HD13	1:A:514:LEU:HD12	1.75	0.68
1:C:201:MET:HE1	1:C:226:GLU:H	1.55	0.68
2:D:1631:TRP:HD1	2:D:1649:LEU:HD21	1.56	0.68
3:E:106:SER:OG	3:E:156:GLU:HG2	1.92	0.68
1:A:181:SER:HB2	3:E:246:ARG:HH21	1.58	0.68
3:F:246:ARG:HG2	3:F:246:ARG:HH11	1.58	0.68
1:A:494:ILE:HD13	1:A:531:LEU:HD13	1.74	0.68
2:B:1641:GLU:N	2:B:1641:GLU:OE1	2.27	0.68
1:A:471:LEU:CD1	1:A:519:LEU:HB3	2.23	0.68
2:B:1067:ALA:HB2	2:B:1074:PRO:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1544:VAL:HG13	2:B:1570:LYS:HB3	1.73	0.68
2:B:877:THR:HG23	2:B:879:LYS:H	1.57	0.68
1:A:215:GLN:HG2	1:A:216:GLN:N	2.07	0.68
2:D:1128:GLU:CD	2:D:1267:GLY:HA3	2.14	0.68
2:D:1066:PHE:HB2	2:D:1078:LEU:HD11	1.76	0.68
2:B:1076:THR:CG2	2:B:1111:LYS:HE2	2.04	0.68
2:B:1126:HIS:O	2:B:1129:MET:HG2	1.92	0.68
2:B:1299:GLN:HA	2:B:1303:ARG:NH2	2.09	0.68
2:B:1640:GLU:O	2:B:1643:GLN:HG2	1.93	0.68
2:B:913:LYS:HD2	2:B:923:ASP:O	1.94	0.68
1:C:246:TYR:OH	1:C:317:GLU:OE2	2.08	0.68
2:B:1105:LYS:HG2	2:B:1162:VAL:HG22	1.75	0.68
2:B:1494:HIS:ND1	2:B:1497:LYS:HB3	2.09	0.68
2:D:949:PRO:O	2:D:950:GLU:HB2	1.94	0.68
2:B:1174:ASP:OD1	2:B:1175:PHE:N	2.27	0.68
2:D:1035:GLU:HA	2:D:1039:LEU:HD12	1.76	0.68
1:A:234:VAL:HG13	1:A:341:ALA:HB2	1.75	0.68
2:B:1554:LEU:HD12	2:B:1555:SER:N	2.09	0.68
2:B:1586:SER:HB2	2:B:1622:ILE:HG12	1.76	0.68
1:C:94:ARG:NE	1:C:94:ARG:HA	2.04	0.67
2:D:1148:LEU:HD12	2:D:1149:ILE:N	2.09	0.67
2:D:855:ARG:HG2	2:D:858:GLN:HB3	1.76	0.67
1:A:130:LEU:HD11	1:A:151:THR:HG22	1.75	0.67
1:C:231:SER:HB3	2:D:834:ARG:NH2	2.09	0.67
3:F:136:GLU:HB2	3:F:159:LYS:NZ	2.09	0.67
1:C:98:SER:O	1:C:100:LYS:HA	1.95	0.67
2:D:1435:ASP:OD1	2:D:1435:ASP:N	2.25	0.67
3:E:276:TRP:N	3:E:276:TRP:CE3	2.62	0.67
2:D:979:ARG:NH1	2:D:1323:GLU:OE2	2.26	0.67
2:D:1417:ASP:O	2:D:1421:LEU:HG	1.94	0.67
2:D:1492:PHE:N	2:D:1492:PHE:HD1	1.92	0.67
2:B:1263:GLY:HA3	2:B:1272:THR:HG22	1.77	0.67
2:D:1574:ASP:CG	2:D:1582:ARG:HH12	1.98	0.67
1:A:471:LEU:CD1	1:A:473:VAL:HG23	2.25	0.67
1:A:464:GLU:HB3	1:A:556:LYS:HE3	1.75	0.67
2:B:1650:GLY:O	2:B:1653:THR:HG22	1.94	0.67
2:B:991:THR:HG22	2:B:1282:TYR:HE2	1.59	0.67
2:D:1436:LYS:HB3	2:D:1441:ARG:HE	1.60	0.67
1:A:566:LYS:HE3	1:A:584:LYS:HD2	1.75	0.67
1:A:193:TRP:CZ3	1:A:195:ILE:HG22	2.30	0.67
1:C:138:ILE:HD11	1:C:602:VAL:HG13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:983:GLN:HB3	2:D:1341:THR:OG1	1.95	0.67
2:D:1659:PHE:HZ	2:D:1662:PRO:HA	1.60	0.67
1:A:141:PRO:HA	1:A:195:ILE:CD1	2.26	0.66
3:E:229:PRO:HG2	3:E:280:PRO:HG2	1.75	0.66
3:F:107:ALA:HB2	3:F:158:CYS:SG	2.35	0.66
2:B:1202:LEU:CD1	2:B:1207:LEU:HD11	2.24	0.66
2:D:906:GLY:O	2:D:931:VAL:HG22	1.95	0.66
3:F:186:ILE:HG13	3:F:188:PHE:HE1	1.60	0.66
2:D:1118:PHE:H	2:D:1144:THR:HG23	1.60	0.66
2:B:1149:ILE:HA	2:B:1152:GLN:HE22	1.61	0.66
2:D:1311:ILE:HD13	2:D:1320:ARG:HH21	1.61	0.66
2:D:872:PHE:HD1	2:D:902:PRO:HA	1.60	0.66
2:B:867:LEU:HD21	2:B:911:GLU:HB3	1.78	0.66
1:C:201:MET:CE	1:C:225:LYS:HA	2.25	0.66
2:B:1010:CYS:HA	2:B:1059:PHE:CZ	2.30	0.66
2:B:1172:ALA:O	2:B:1176:LEU:HD13	1.95	0.66
2:B:1357:THR:HA	2:B:1359:ASN:N	2.10	0.66
1:C:397:VAL:CG1	1:C:409:LEU:HD22	2.25	0.66
1:C:479:MET:HE1	1:C:487:ILE:CD1	2.26	0.66
2:D:1225:LYS:HE3	2:D:1227:LEU:HD11	1.78	0.66
2:D:886:VAL:HG21	2:D:894:LEU:HD23	1.78	0.66
1:C:168:GLU:CG	1:C:205:LYS:HB3	2.25	0.66
1:C:59:VAL:HG23	1:C:106:VAL:CG2	2.26	0.66
1:C:97:LYS:HG2	2:D:1314:GLU:HB3	1.78	0.66
1:A:471:LEU:HD11	1:A:519:LEU:HB3	1.76	0.65
1:C:29:ILE:HB	1:C:43:VAL:CG1	2.26	0.65
2:D:1077:TRP:CZ2	2:D:1130:ILE:HA	2.31	0.65
2:D:1498:GLU:O	2:D:1500:GLY:N	2.29	0.65
1:A:376:VAL:HG13	1:A:384:ALA:HB3	1.78	0.65
2:D:985:THR:CG2	2:D:987:VAL:HG12	2.26	0.65
2:D:1508:ASP:CG	2:D:1509:GLU:H	1.98	0.65
2:D:1550:VAL:HG21	2:D:1581:GLN:HE22	1.62	0.65
1:A:129:TYR:HA	1:A:218:PHE:HE2	1.61	0.65
2:B:1203:LYS:HA	2:B:1207:LEU:HD22	1.78	0.65
2:B:1652:PHE:CE1	2:B:1656:MET:HE3	2.30	0.65
1:C:245:ILE:H	1:C:245:ILE:HD12	1.61	0.65
1:C:488:ARG:NH1	1:C:508:ARG:O	2.29	0.65
1:C:573:ARG:HE	1:C:579:GLN:NE2	1.94	0.65
2:D:1033:GLN:HB3	2:D:1036:LYS:HZ2	1.61	0.65
2:D:1215:LYS:O	2:D:1216:ASP:OD1	2.14	0.65
2:D:1363:LEU:HD21	2:D:1477:VAL:HG12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1604:MET:HA	2:B:1627:TRP:O	1.97	0.65
1:C:177:GLN:O	3:F:240:ARG:NH2	2.29	0.65
1:C:205:LYS:HE3	1:C:219:SER:HB3	1.77	0.65
1:A:140:THR:HG23	1:A:227:TYR:CE2	2.32	0.65
1:C:404:ASP:OD1	1:C:406:VAL:HG12	1.96	0.65
2:D:934:GLU:HG2	2:D:1352:ALA:C	2.17	0.65
2:B:1060:ARG:HG3	2:B:1060:ARG:HH11	1.62	0.65
2:B:1525:ASP:N	2:B:1525:ASP:OD1	2.17	0.65
2:D:1506:CYS:SG	2:D:1511:CYS:CB	2.84	0.65
3:E:205:LEU:HD12	3:E:212:GLN:O	1.97	0.65
3:F:246:ARG:CB	3:F:246:ARG:HH11	2.09	0.65
1:A:313:ASN:ND2	1:A:318:ASP:OD2	2.29	0.65
2:D:1102:GLY:O	2:D:1106:TRP:CD1	2.50	0.65
2:D:755:ILE:HG22	2:D:756:ILE:N	2.11	0.65
2:D:950:GLU:N	2:D:953:GLY:O	2.27	0.64
2:D:756:ILE:HB	3:F:134:ARG:HH22	1.62	0.64
3:F:272:ASP:N	3:F:272:ASP:OD1	2.30	0.64
1:A:196:PRO:HD2	1:A:199:VAL:HG21	1.78	0.64
1:A:446:TYR:CE1	1:A:634:ASP:HA	2.32	0.64
1:A:93:ASN:OD1	1:A:94:ARG:N	2.31	0.64
2:B:937:ARG:NH1	2:B:1347:MET:HE1	2.12	0.64
2:B:1607:LEU:HD23	2:B:1608:SER:H	1.60	0.64
1:C:487:ILE:O	1:C:508:ARG:HD3	1.98	0.64
2:D:1326:GLU:OE1	2:D:1328:GLU:HB2	1.98	0.64
3:E:110:LYS:HD3	3:E:128:GLU:HB3	1.78	0.64
3:F:135:ARG:HG3	3:F:135:ARG:NH1	2.12	0.64
1:A:35:ARG:HD3	1:A:154:HIS:NE2	2.11	0.64
2:B:1066:PHE:CE1	2:B:1082:VAL:HG11	2.32	0.64
1:A:166:ASN:HD21	1:A:174:PRO:HG3	1.62	0.64
2:D:880:ARG:CZ	2:D:1471:LEU:HG	2.27	0.64
1:A:197:GLU:OE1	1:A:198:LEU:HD12	1.98	0.64
2:B:1356:LEU:HD13	2:B:1357:THR:H	1.61	0.64
2:B:962:ILE:HG13	2:B:1330:PHE:O	1.97	0.64
1:A:239:THR:OG1	1:A:252:GLU:HG2	1.98	0.64
1:A:274:GLY:HA3	1:A:325:TYR:CZ	2.32	0.64
2:D:766:GLU:CB	2:D:796:LYS:HZ1	2.08	0.64
2:D:905:THR:HA	2:D:931:VAL:HG23	1.79	0.64
3:E:223:ILE:HG13	3:E:223:ILE:O	1.98	0.64
1:C:625:ILE:HD12	1:C:643:GLY:HA3	1.80	0.64
2:B:1392:TYR:CD1	2:B:1398:ALA:HB2	2.32	0.64
2:B:938:MET:CB	2:B:940:LYS:HZ2	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1249:VAL:HG22	2:D:1250:PRO:HD3	1.79	0.64
1:A:216:GLN:HE21	1:A:218:PHE:HE1	1.46	0.64
1:A:466:ARG:HG3	1:A:556:LYS:CD	2.16	0.64
2:B:940:LYS:HD3	2:B:940:LYS:N	2.13	0.64
2:B:991:THR:HG22	2:B:1282:TYR:CE2	2.34	0.64
1:C:207:ARG:NH1	1:C:219:SER:HG	1.92	0.64
1:C:302:LEU:HD21	1:C:307:LEU:HB2	1.79	0.64
2:D:1423:ASN:ND2	2:D:1423:ASN:O	2.26	0.64
2:D:971:VAL:HG12	2:D:1349:HIS:HB2	1.80	0.64
1:A:404:ASP:OD1	1:A:406:VAL:HG12	1.97	0.63
2:B:761:ILE:HD12	2:B:761:ILE:O	1.97	0.63
2:D:1291:GLU:OE2	2:D:1337:LYS:HB3	1.99	0.63
2:D:1368:LYS:HB2	2:D:1385:ILE:HD11	1.80	0.63
2:B:1411:PHE:CZ	2:B:1465:GLN:HB3	2.33	0.63
2:B:1516:GLU:OE1	2:B:1624:LYS:HG2	1.98	0.63
2:D:1552:VAL:HG12	2:D:1561:TYR:HD1	1.63	0.63
2:B:1405:ILE:HG12	2:B:1477:VAL:HG22	1.80	0.63
3:E:146:LEU:CD1	3:E:150:LYS:HB2	2.29	0.63
3:E:195:LYS:HE3	3:E:197:PHE:CE1	2.34	0.63
1:A:456:LEU:HB2	1:A:535:TYR:HE2	1.63	0.63
2:B:1188:THR:HA	2:B:1191:ILE:HD11	1.80	0.63
2:D:1292:LEU:HB2	2:D:1313:TRP:HB2	1.79	0.63
1:C:205:LYS:CE	1:C:219:SER:HB3	2.28	0.63
2:D:1604:MET:HA	2:D:1627:TRP:O	1.99	0.63
1:C:148:ARG:HG3	2:D:773:TRP:CZ2	2.33	0.63
1:A:83:MET:CE	1:A:505:ARG:HH11	2.11	0.63
2:D:1066:PHE:CB	2:D:1078:LEU:HD11	2.29	0.63
2:D:853:ASN:HD22	2:D:888:ILE:HG23	1.62	0.63
2:B:1503:ASN:ND2	2:B:1589:LYS:HE3	2.14	0.63
2:D:1148:LEU:O	2:D:1152:GLN:HG2	1.99	0.63
3:F:121:VAL:HA	3:F:145:CYS:SG	2.39	0.63
3:F:222:GLU:OE2	3:F:224:TYR:OH	2.13	0.63
1:C:600:LYS:NZ	2:D:822:GLU:OE2	2.23	0.63
3:F:199:SER:OG	3:F:201:SER:O	2.15	0.63
1:C:69:LEU:HD21	1:C:91:PRO:CD	2.28	0.62
2:D:763:SER:HB3	2:D:926:ARG:HB2	1.80	0.62
1:A:45:GLU:OE2	1:A:491:THR:HG21	1.98	0.62
2:B:1174:ASP:OD1	2:B:1175:PHE:CD2	2.53	0.62
2:B:1187:TYR:HD1	2:B:1232:ALA:HB2	1.65	0.62
2:B:761:ILE:HG21	2:B:913:LYS:HE3	1.81	0.62
2:D:1310:ARG:HD2	2:D:1312:HIS:NE2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:SER:CB	3:E:246:ARG:NH2	2.63	0.62
3:F:259:MET:SD	3:F:281:PRO:HB2	2.39	0.62
2:B:871:ALA:O	2:B:903:LEU:N	2.28	0.62
2:B:945:ARG:HD2	2:B:960:GLU:CD	2.20	0.62
1:C:566:LYS:HB2	1:C:584:LYS:HE2	1.81	0.62
2:D:1108:ILE:HD11	2:D:1151:LEU:HD21	1.81	0.62
2:D:996:ASP:OD1	2:D:1036:LYS:HE2	1.98	0.62
2:B:1136:ASN:HA	2:B:1139:LYS:NZ	2.14	0.62
2:D:1089:ALA:HA	2:D:1092:LEU:HD13	1.79	0.62
2:D:1313:TRP:CZ3	2:D:1318:LEU:HD11	2.34	0.62
2:D:1420:GLN:O	2:D:1423:ASN:ND2	2.31	0.62
2:D:1528:THR:OG1	2:D:1529:LEU:N	2.32	0.62
1:A:647:THR:HG22	1:A:653:GLN:CD	2.20	0.62
2:D:1496:GLU:O	2:D:1498:GLU:N	2.32	0.62
2:D:1492:PHE:HE2	2:D:1500:GLY:O	1.82	0.62
2:D:756:ILE:HD11	2:D:760:ASN:OD1	2.00	0.62
2:B:1436:LYS:O	2:B:1441:ARG:NH2	2.33	0.62
2:B:1532:ARG:NH2	2:B:1629:GLU:OE2	2.31	0.62
2:D:957:VAL:HG21	2:D:1335:GLU:HA	1.82	0.62
2:B:1082:VAL:O	2:B:1086:PHE:HD1	1.82	0.62
1:C:120:VAL:O	1:C:656:GLN:NE2	2.30	0.62
2:D:1291:GLU:OE2	2:D:1338:GLY:N	2.33	0.62
2:D:1659:PHE:HE2	2:D:1662:PRO:HD3	1.63	0.62
3:E:163:CYS:HB2	3:E:180:ILE:O	2.00	0.62
3:F:232:ASP:O	3:F:233:ASN:OD1	2.18	0.62
2:B:1144:THR:O	2:B:1148:LEU:HB2	1.98	0.62
2:B:1189:VAL:HG11	2:B:1213:THR:HG21	1.82	0.62
2:D:1210:PHE:CE1	2:D:1220:TRP:HH2	2.18	0.62
2:D:886:VAL:HG21	2:D:894:LEU:CD2	2.29	0.62
2:D:987:VAL:HG22	2:D:988:ALA:N	2.15	0.62
3:E:145:CYS:HB2	3:E:151:TRP:CZ3	2.35	0.62
3:E:141:PRO:HA	3:E:157:PHE:HD2	1.63	0.62
1:A:502:LYS:NZ	1:A:503:ALA:O	2.30	0.62
2:B:1312:HIS:C	2:B:1313:TRP:CE3	2.73	0.62
1:C:146:LEU:HD13	2:D:773:TRP:CD2	2.34	0.62
2:D:800:THR:HG22	2:D:801:THR:H	1.64	0.62
1:A:376:VAL:CG1	1:A:401:THR:HG21	2.30	0.61
2:B:1303:ARG:NH1	2:B:1306:LYS:HA	2.13	0.61
2:B:1538:GLU:O	2:B:1541:VAL:HG12	2.00	0.61
1:C:479:MET:HE1	1:C:487:ILE:HD11	1.82	0.61
3:E:130:ARG:NH1	3:E:130:ARG:HG3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLY:C	1:A:161:ARG:HG2	2.19	0.61
2:B:945:ARG:HD2	2:B:960:GLU:OE1	1.99	0.61
2:D:985:THR:HG22	2:D:987:VAL:HG12	1.82	0.61
1:A:155:LYS:HG2	1:A:499:ARG:HE	1.64	0.61
1:A:364:PHE:CE2	1:A:366:PRO:HA	2.32	0.61
2:B:983:GLN:HG2	2:B:1341:THR:HB	1.81	0.61
2:D:1214:ALA:HB2	2:D:1220:TRP:HE1	1.65	0.61
2:D:1643:GLN:HG3	2:D:1644:LYS:HD2	1.82	0.61
1:A:134:THR:OG1	1:A:139:TYR:OH	2.07	0.61
1:A:317:GLU:H	1:A:317:GLU:CD	2.03	0.61
1:A:148:ARG:CZ	1:A:594:VAL:HB	2.30	0.61
2:D:1060:ARG:HH11	2:D:1060:ARG:HG3	1.65	0.61
1:A:167:ILE:HG12	1:A:176:LYS:HB3	1.83	0.61
2:B:1469:VAL:HG13	2:B:1472:ILE:HG22	1.81	0.61
2:D:1202:LEU:CD1	2:D:1243:LEU:HD21	2.27	0.61
2:D:937:ARG:HH21	2:D:1349:HIS:CE1	2.17	0.61
1:A:181:SER:HB3	3:E:246:ARG:NH2	2.14	0.61
2:B:1554:LEU:CD1	2:B:1591:ARG:HH12	2.11	0.61
1:C:449:VAL:HG21	1:C:545:GLU:HG3	1.83	0.61
1:C:646:PHE:H	1:C:654:THR:HG21	1.65	0.61
2:D:1301:PRO:HD2	2:D:1328:GLU:OE2	2.01	0.61
2:D:756:ILE:HD12	3:F:134:ARG:HH22	1.65	0.61
1:A:647:THR:HG22	1:A:653:GLN:HE22	1.64	0.61
1:A:76:LEU:HG	1:A:82:HIS:HA	1.83	0.61
2:B:1548:ARG:HD2	2:B:1566:GLU:OE2	2.01	0.61
2:B:1643:GLN:HG3	2:B:1644:LYS:N	2.16	0.61
2:B:780:GLU:OE2	2:B:789:LYS:HD3	2.00	0.61
1:C:487:ILE:H	1:C:487:ILE:HD12	1.65	0.61
2:D:997:ALA:H	2:D:1036:LYS:HE2	1.66	0.61
1:A:125:LEU:H	1:A:125:LEU:CD1	2.12	0.61
1:A:622:LYS:HD2	1:A:622:LYS:O	2.01	0.61
2:B:1496:GLU:HG2	2:B:1497:LYS:H	1.65	0.61
1:C:135:ASP:HB3	1:C:146:LEU:HD11	1.82	0.61
2:D:1507:ARG:O	2:D:1508:ASP:OD1	2.18	0.61
3:F:157:PHE:C	3:F:159:LYS:HZ1	2.05	0.61
1:A:42:MET:HB3	1:A:86:VAL:HG23	1.83	0.60
2:B:1138:GLU:HG3	2:B:1188:THR:HG21	1.83	0.60
1:C:479:MET:HG3	1:C:480:ASP:OD1	2.01	0.60
1:A:591:ALA:HB2	2:B:810:SER:HB2	1.82	0.60
2:B:1576:VAL:CA	2:B:1580:GLN:HE22	2.15	0.60
2:D:1131:GLY:O	2:D:1228:TYR:HE1	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:LEU:CD1	1:C:67:LEU:CD2	2.71	0.60
3:E:146:LEU:CG	3:E:150:LYS:HB2	2.30	0.60
1:C:599:ASP:OD1	2:D:800:THR:HG21	2.01	0.60
2:D:1061:GLN:HG3	2:D:1062:PRO:HD2	1.83	0.60
2:D:1397:ASP:CB	2:D:1450:LYS:HE2	2.32	0.60
2:D:759:GLU:HG2	2:D:760:ASN:N	2.16	0.60
3:F:109:LEU:HB2	3:F:114:ILE:HG12	1.81	0.60
2:B:1202:LEU:O	2:B:1202:LEU:HD12	2.01	0.60
2:B:904:LYS:HG3	2:B:908:GLN:OE1	2.00	0.60
1:C:365:LYS:NZ	1:C:457:HIS:HA	2.16	0.60
1:C:477:LEU:HD11	1:C:479:MET:HE2	1.82	0.60
2:D:778:LEU:HG	2:D:787:SER:HB3	1.82	0.60
1:A:364:PHE:CE1	1:A:420:LEU:HG	2.36	0.60
2:D:1148:LEU:HD11	2:D:1195:ALA:HB1	1.83	0.60
2:D:1187:TYR:HD1	2:D:1232:ALA:HB2	1.67	0.60
2:D:1487:GLU:OE1	2:D:1487:GLU:N	2.35	0.60
3:E:226:PRO:O	3:E:276:TRP:CZ2	2.54	0.60
1:A:83:MET:HG3	1:A:505:ARG:HD2	1.81	0.60
2:B:1136:ASN:O	2:B:1185:ARG:NH1	2.35	0.60
2:D:1013:GLU:O	2:D:1016:ILE:HG22	2.01	0.60
1:A:36:LEU:CD2	1:A:125:LEU:HA	2.31	0.60
1:A:133:GLN:HG3	1:A:133:GLN:O	2.02	0.60
2:B:1382:ASN:OD1	2:B:1383:THR:N	2.34	0.60
2:B:1543:TYR:HB2	2:B:1545:TYR:CZ	2.36	0.60
2:B:872:PHE:CD1	2:B:902:PRO:HA	2.37	0.60
2:D:947:LEU:HD12	2:D:947:LEU:N	2.17	0.60
2:D:990:MET:N	2:D:991:THR:HA	2.17	0.60
2:B:1274:MET:SD	2:B:1277:GLN:NE2	2.75	0.60
2:B:1303:ARG:HH12	2:B:1307:ILE:N	1.99	0.60
2:B:1317:SER:OG	2:B:1320:ARG:NH2	2.35	0.60
2:D:1217:LYS:HG3	2:D:1248:PHE:CE2	2.37	0.60
2:D:1241:LEU:HD21	2:D:1285:ASP:HB2	1.83	0.60
2:D:1610:ASP:HA	2:D:1621:ILE:HD11	1.83	0.60
3:E:106:SER:O	3:E:130:ARG:N	2.30	0.60
3:F:233:ASN:ND2	3:F:257:PHE:CD2	2.69	0.60
2:B:1429:ILE:HD11	2:B:1433:GLU:HG3	1.83	0.60
2:D:1130:ILE:HD12	2:D:1133:LEU:HB2	1.84	0.60
2:D:1233:THR:HG22	2:D:1256:LEU:HD11	1.84	0.60
2:D:1652:PHE:CZ	2:D:1656:MET:HE2	2.36	0.60
2:D:899:VAL:HG23	2:D:1473:GLN:HE21	1.67	0.60
2:D:987:VAL:CG2	2:D:988:ALA:H	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:186:ILE:HD13	3:F:213:TRP:CH2	2.35	0.60
1:A:62:PHE:CE2	2:B:1039:LEU:HD11	2.36	0.59
1:C:465:LEU:CD1	1:C:555:VAL:HG22	2.32	0.59
1:C:558:SER:O	1:C:617:TRP:NE1	2.26	0.59
2:D:1104:VAL:O	2:D:1108:ILE:HG12	2.02	0.59
2:D:1128:GLU:OE2	2:D:1267:GLY:HA3	2.01	0.59
2:D:1600:LYS:HD2	2:D:1633:GLU:OE2	2.02	0.59
1:A:105:PHE:HE2	1:A:122:LEU:HG	1.67	0.59
2:B:1078:LEU:HD21	2:B:1124:VAL:HG21	1.84	0.59
2:B:1171:LYS:O	2:B:1174:ASP:OD1	2.20	0.59
2:B:1197:ALA:HA	2:B:1202:LEU:HG	1.83	0.59
2:B:1636:GLU:OE2	2:B:1642:ASN:ND2	2.35	0.59
2:B:872:PHE:HD1	2:B:902:PRO:HA	1.66	0.59
1:C:484:GLU:OE1	1:C:484:GLU:N	2.32	0.59
2:D:756:ILE:CG1	3:F:134:ARG:HH22	2.15	0.59
2:B:1240:LEU:HA	2:B:1243:LEU:HB2	1.85	0.59
1:C:196:PRO:HD2	1:C:199:VAL:HG21	1.83	0.59
1:A:227:TYR:OH	2:B:769:GLU:OE1	2.18	0.59
1:C:455:TYR:HB2	1:C:478:ARG:HB3	1.84	0.59
3:F:180:ILE:HD11	3:F:213:TRP:CH2	2.36	0.59
2:D:1185:ARG:O	2:D:1189:VAL:HG22	2.02	0.59
2:D:1240:LEU:HD23	2:D:1249:VAL:HG12	1.83	0.59
2:D:1392:TYR:CD1	2:D:1398:ALA:HB2	2.37	0.59
2:B:1117:VAL:HG22	2:B:1144:THR:HG21	1.83	0.59
2:B:1214:ALA:HB2	2:B:1220:TRP:CE2	2.38	0.59
2:B:1607:LEU:CD2	2:B:1608:SER:H	2.15	0.59
1:A:611:LEU:HG	2:B:817:VAL:HG21	1.83	0.59
1:C:100:LYS:HD3	2:D:1313:TRP:CZ2	2.37	0.59
2:D:1149:ILE:CD1	2:D:1194:TYR:HE2	2.12	0.59
2:D:1128:GLU:OE1	2:D:1267:GLY:HA3	2.03	0.59
2:B:1007:PRO:HB2	2:B:1055:GLN:NE2	2.18	0.59
2:B:1075:SER:HB3	2:B:1078:LEU:HD12	1.84	0.59
2:B:982:LEU:HD21	2:B:1296:VAL:HG21	1.82	0.59
1:C:357:PHE:CE1	1:C:441:MET:HE1	2.38	0.59
2:D:1506:CYS:HB3	2:D:1511:CYS:HB2	1.82	0.59
2:D:761:ILE:HG22	2:D:762:VAL:N	2.18	0.59
2:D:877:THR:HG23	2:D:879:LYS:H	1.68	0.59
1:A:471:LEU:HD13	1:A:473:VAL:HG23	1.85	0.59
2:D:877:THR:OG1	2:D:878:THR:N	2.34	0.59
2:D:1515:GLU:HA	2:D:1589:LYS:NZ	2.18	0.59
2:D:755:ILE:CG2	2:D:756:ILE:H	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1582:ARG:HD2	2:B:1620:TYR:HE1	1.68	0.59
2:D:1397:ASP:OD1	2:D:1453:HIS:ND1	2.36	0.59
3:E:107:ALA:C	3:E:130:ARG:NH1	2.55	0.59
3:E:113:TYR:CD1	3:E:125:VAL:HG12	2.38	0.59
3:E:171:ASN:ND2	3:E:194:TYR:CZ	2.69	0.59
1:A:81:ASN:O	1:A:82:HIS:CG	2.56	0.58
2:D:1562:ILE:O	2:D:1562:ILE:HG13	2.02	0.58
2:D:1148:LEU:HD11	2:D:1195:ALA:CB	2.32	0.58
2:D:1253:VAL:HA	2:D:1256:LEU:HD22	1.85	0.58
1:A:140:THR:O	1:A:195:ILE:HD11	2.03	0.58
1:A:389:VAL:HG12	1:A:426:THR:HG22	1.85	0.58
2:B:1015:MET:HG2	2:B:1056:GLN:HE22	1.69	0.58
1:C:28:ILE:HD12	1:C:29:ILE:H	1.68	0.58
1:C:449:VAL:O	1:C:452:SER:OG	2.22	0.58
2:D:1311:ILE:HD11	2:D:1318:LEU:HA	1.85	0.58
1:A:628:THR:CG2	1:A:641:ASP:HB3	2.33	0.58
2:B:1130:ILE:HG13	2:B:1133:LEU:HB2	1.84	0.58
1:A:340:GLN:OE1	1:A:340:GLN:HA	2.04	0.58
2:B:971:VAL:HB	2:B:1349:HIS:NE2	2.18	0.58
2:B:1587:PRO:HG2	2:B:1590:CYS:SG	2.44	0.58
2:B:1639:ASP:HB3	2:B:1641:GLU:OE1	2.04	0.58
1:C:28:ILE:HD12	1:C:29:ILE:N	2.18	0.58
2:D:937:ARG:NH2	2:D:1349:HIS:HE1	2.00	0.58
2:D:756:ILE:CD1	3:F:134:ARG:HH12	2.16	0.58
2:B:1112:GLN:HA	2:B:1112:GLN:OE1	2.03	0.58
2:B:1631:TRP:CD1	2:B:1649:LEU:HD13	2.38	0.58
1:C:135:ASP:OD1	1:C:139:TYR:OH	2.17	0.58
1:C:30:THR:HG23	1:C:645:THR:OG1	2.03	0.58
2:D:757:ALA:O	2:D:761:ILE:HD13	2.03	0.58
2:D:780:GLU:N	2:D:780:GLU:OE1	2.36	0.58
1:C:337:ASP:OD2	2:D:834:ARG:NE	2.37	0.58
1:A:169:ASN:HB2	1:A:170:PRO:HD2	1.86	0.58
1:A:252:GLU:OE1	1:A:252:GLU:N	2.25	0.58
2:B:1152:GLN:NE2	2:B:1198:GLN:HE22	2.02	0.58
2:B:1202:LEU:CA	2:B:1206:LEU:HD11	2.33	0.58
1:C:47:HIS:ND1	1:C:489:TYR:OH	2.34	0.58
1:C:72:GLU:HB2	1:C:86:VAL:HG21	1.85	0.58
2:D:1600:LYS:HE3	2:D:1630:HIS:NE2	2.19	0.58
2:D:1631:TRP:CD1	2:D:1649:LEU:CD2	2.86	0.58
1:A:332:LEU:HD12	1:A:337:ASP:HB2	1.84	0.58
1:A:359:LYS:HD2	1:A:552:TRP:CZ3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLU:OE1	1:A:534:TYR:OH	2.22	0.58
1:A:122:LEU:HD21	1:A:657:ARG:HG2	1.85	0.58
2:B:1049:ILE:HG22	2:B:1093:ILE:HD13	1.84	0.58
2:B:1592:GLU:O	2:B:1595:LYS:NZ	2.28	0.58
1:C:324:LEU:HB2	1:C:346:ILE:CG1	2.34	0.58
1:C:39:GLU:OE1	1:C:39:GLU:N	2.24	0.58
3:F:186:ILE:HD11	3:F:202:SER:HB2	1.84	0.58
2:B:958:GLN:OE1	2:B:958:GLN:N	2.37	0.58
2:D:1067:ALA:HA	2:D:1078:LEU:HD21	1.86	0.58
2:D:1096:ASP:OD2	2:D:1098:GLN:NE2	2.37	0.58
2:D:1255:TRP:HE3	2:D:1256:LEU:HD12	1.67	0.58
2:D:1550:VAL:CG2	2:D:1581:GLN:NE2	2.67	0.58
3:E:197:PHE:HE2	3:E:221:ARG:HD2	1.67	0.58
1:A:104:LYS:CG	1:A:105:PHE:N	2.66	0.58
1:A:563:LEU:HD22	2:B:808:SER:HB3	1.85	0.58
1:C:552:TRP:CH2	1:C:554:ASP:HB2	2.38	0.58
2:D:1105:LYS:CE	2:D:1106:TRP:HE1	2.12	0.58
2:D:1416:ASP:OD1	2:D:1417:ASP:N	2.37	0.58
1:C:119:LYS:NZ	1:C:654:THR:O	2.36	0.57
2:D:1494:HIS:CD2	2:D:1497:LYS:HD2	2.39	0.57
3:E:224:TYR:HD2	3:E:242:HIS:HB3	1.67	0.57
3:F:135:ARG:HE	3:F:141:PRO:HB3	1.68	0.57
1:A:338:MET:CE	2:B:1485:LEU:HB2	2.34	0.57
2:B:1554:LEU:HD12	2:B:1555:SER:H	1.69	0.57
1:C:125:LEU:HB2	1:C:215:GLN:NE2	2.19	0.57
2:D:1240:LEU:HD11	2:D:1248:PHE:HB3	1.85	0.57
2:D:1475:GLY:HA3	2:D:1493:TYR:CZ	2.39	0.57
2:D:1035:GLU:HA	2:D:1039:LEU:HD11	1.86	0.57
2:D:794:PHE:CE2	3:F:176:VAL:HB	2.39	0.57
1:A:135:ASP:OD1	1:A:139:TYR:OH	2.22	0.57
1:A:57:VAL:HG21	1:A:86:VAL:HG21	1.86	0.57
2:B:1043:GLN:O	2:B:1046:LEU:HG	2.04	0.57
2:B:1496:GLU:HG2	2:B:1497:LYS:N	2.20	0.57
2:D:835:LEU:HD23	2:D:929:LEU:HB3	1.86	0.57
1:A:272:ILE:HG22	1:A:327:SER:HB3	1.87	0.57
2:B:1084:LYS:HE2	2:B:1273:PHE:CE2	2.40	0.57
2:B:1549:LEU:HD13	2:B:1563:MET:CE	2.33	0.57
2:B:846:GLU:OE2	2:B:897:PRO:HB3	2.05	0.57
2:D:1597:GLU:HG3	2:D:1600:LYS:CG	2.34	0.57
2:D:763:SER:OG	2:D:911:GLU:OE2	2.14	0.57
2:B:939:ASN:C	2:B:940:LYS:HD3	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1027:TYR:CZ	2:D:1031:THR:HG21	2.40	0.57
2:D:1190:ALA:HB2	2:D:1220:TRP:HE3	1.70	0.57
2:D:1217:LYS:HG2	2:D:1217:LYS:O	2.05	0.57
2:D:1382:ASN:OD1	2:D:1383:THR:N	2.38	0.57
2:D:1644:LYS:HA	2:D:1647:GLN:OE1	2.04	0.57
1:C:560:VAL:HG13	2:D:813:LYS:HE3	1.85	0.57
2:D:951:ARG:O	2:D:952:LEU:HG	2.05	0.57
2:D:975:GLU:N	2:D:975:GLU:OE1	2.26	0.57
1:C:508:ARG:HH22	1:C:512:GLN:N	2.03	0.57
1:C:66:LYS:HE3	3:E:147:GLN:N	2.20	0.57
2:D:1547:THR:HB	2:D:1563:MET:HG3	1.87	0.57
2:D:1577:GLN:N	2:D:1580:GLN:HE21	1.86	0.57
2:B:1015:MET:CG	2:B:1056:GLN:HE22	2.18	0.57
2:B:801:THR:OG1	2:B:824:THR:HG22	2.05	0.57
1:C:422:ILE:HB	1:C:441:MET:HE3	1.87	0.57
2:D:1149:ILE:HD11	2:D:1153:GLU:OE2	2.04	0.57
1:C:146:LEU:HD13	2:D:773:TRP:CE3	2.39	0.57
1:A:209:TYR:CD2	1:A:214:PRO:HA	2.39	0.57
2:B:1292:LEU:O	2:B:1313:TRP:CE3	2.57	0.57
3:E:224:TYR:CE2	3:E:242:HIS:HB3	2.40	0.57
2:D:962:ILE:HD11	2:D:1330:PHE:CD2	2.40	0.56
3:E:282:GLU:OE2	3:E:284:ARG:HG2	2.04	0.56
3:F:188:PHE:CD2	3:F:218:PRO:HD2	2.39	0.56
1:A:125:LEU:H	1:A:125:LEU:HD12	1.69	0.56
1:C:26:TYR:O	1:C:649:SER:N	2.38	0.56
2:D:1065:ALA:HB3	2:D:1074:PRO:HB3	1.87	0.56
1:A:372:LEU:HD11	1:A:422:ILE:HG12	1.87	0.56
1:A:28:ILE:HD12	1:A:43:VAL:O	2.05	0.56
1:A:495:MET:HE1	1:A:625:ILE:HD11	1.87	0.56
2:B:1237:LEU:O	2:B:1241:LEU:HG	2.05	0.56
2:B:879:LYS:NZ	2:B:1521:GLN:HE22	2.03	0.56
2:B:904:LYS:HE3	2:B:908:GLN:HE22	1.69	0.56
2:D:1117:VAL:HA	2:D:1144:THR:HG21	1.86	0.56
2:D:1148:LEU:HD21	2:D:1195:ALA:HB1	1.85	0.56
2:D:1217:LYS:HG3	2:D:1248:PHE:CZ	2.39	0.56
2:D:1298:LEU:CD1	2:D:1307:ILE:HB	2.35	0.56
1:C:599:ASP:HB2	2:D:802:TRP:CZ3	2.40	0.56
3:F:239:GLU:OE1	3:F:240:ARG:O	2.23	0.56
1:A:30:THR:HG22	1:A:645:THR:OG1	2.06	0.56
2:B:949:PRO:HG3	2:B:958:GLN:HE22	1.70	0.56
2:D:1216:ASP:OD2	2:D:1219:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1551:LYS:HE3	2:D:1562:ILE:HD13	1.86	0.56
2:D:756:ILE:HB	3:F:134:ARG:NH2	2.19	0.56
1:C:263:LYS:HD2	2:D:854:TYR:CE1	2.40	0.56
1:A:366:PRO:HD2	1:A:455:TYR:CE1	2.41	0.56
1:A:390:ALA:HB3	1:A:427:LYS:HE3	1.86	0.56
1:C:196:PRO:HD2	1:C:199:VAL:CG2	2.36	0.56
2:D:1654:GLU:O	2:D:1658:VAL:HG13	2.05	0.56
3:E:203:PHE:HB3	3:E:214:SER:HB3	1.87	0.56
3:E:248:SER:OG	3:E:266:TYR:HB3	2.05	0.56
3:F:186:ILE:HG13	3:F:188:PHE:CE1	2.41	0.56
2:D:1433:GLU:CD	2:D:1445:ILE:H	2.08	0.56
2:D:826:MET:HG2	2:D:827:GLN:N	2.19	0.56
2:D:912:VAL:HG13	2:D:925:VAL:HG23	1.87	0.56
2:D:1241:LEU:HD11	2:D:1285:ASP:HB3	1.85	0.56
2:D:904:LYS:HG3	2:D:908:GLN:NE2	2.21	0.56
1:A:178:ASP:OD2	3:E:247:GLN:NE2	2.39	0.56
3:F:157:PHE:C	3:F:159:LYS:HZ2	2.05	0.56
3:F:186:ILE:HD13	3:F:213:TRP:CZ3	2.41	0.56
1:A:235:ILE:HD11	1:A:256:THR:HB	1.88	0.56
2:B:1367:ILE:HD11	2:B:1384:MET:HB2	1.88	0.56
1:C:523:THR:CB	1:C:560:VAL:HG23	2.31	0.56
2:D:856:GLN:OE1	2:D:856:GLN:N	2.35	0.56
2:D:945:ARG:HB2	2:D:1342:LEU:HD23	1.88	0.56
3:F:124:VAL:HA	3:F:143:LEU:O	2.05	0.56
2:B:1086:PHE:O	2:B:1095:ILE:HD12	2.06	0.56
2:D:1004:ILE:O	2:D:1004:ILE:HG13	2.05	0.56
2:D:1210:PHE:CD1	2:D:1220:TRP:HH2	2.23	0.56
3:F:190:CYS:SG	3:F:196:LEU:HD12	2.45	0.56
2:B:1303:ARG:NH1	2:B:1306:LYS:CA	2.69	0.56
2:D:1255:TRP:CE3	2:D:1256:LEU:HD12	2.40	0.56
3:E:116:GLN:HG2	3:E:119:PHE:CE1	2.40	0.56
2:B:1607:LEU:HD22	2:B:1609:SER:H	1.71	0.56
1:C:182:SER:O	1:C:185:GLN:HB2	2.06	0.56
1:C:397:VAL:HG13	1:C:409:LEU:HD22	1.87	0.56
1:C:650:SER:OG	1:C:652:GLN:OE1	2.10	0.56
1:A:140:THR:HG23	1:A:227:TYR:CZ	2.40	0.55
1:A:496:ASN:O	1:A:498:GLY:N	2.39	0.55
1:C:365:LYS:NZ	1:C:456:LEU:O	2.36	0.55
2:D:802:TRP:HB2	2:D:823:VAL:HG23	1.86	0.55
2:D:937:ARG:NH2	2:D:1349:HIS:CE1	2.73	0.55
2:D:945:ARG:HB2	2:D:1342:LEU:CD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:157:PHE:H	3:F:157:PHE:HD1	1.53	0.55
2:B:1507:ARG:NH1	2:B:1508:ASP:OD1	2.39	0.55
1:C:35:ARG:NH2	1:C:498:GLY:O	2.38	0.55
1:A:166:ASN:OD1	1:A:167:ILE:N	2.40	0.55
1:A:332:LEU:CD1	1:A:337:ASP:HB2	2.36	0.55
1:C:397:VAL:HG12	1:C:409:LEU:HD22	1.88	0.55
1:C:496:ASN:C	1:C:498:GLY:H	2.08	0.55
1:C:57:VAL:O	1:C:71:SER:HA	2.06	0.55
2:D:1218:ASN:HB2	2:D:1251:PRO:O	2.07	0.55
1:A:31:PRO:HA	1:A:644:LEU:HD23	1.89	0.55
2:B:1521:GLN:H	2:B:1521:GLN:CD	2.08	0.55
2:B:757:ALA:N	2:B:760:ASN:HD21	2.03	0.55
2:D:1016:ILE:HD12	2:D:1016:ILE:O	2.07	0.55
3:E:233:ASN:HB2	3:E:283:CYS:SG	2.46	0.55
2:B:1014:ASN:HD22	2:B:1055:GLN:HG3	1.72	0.55
2:B:1052:GLY:O	2:B:1056:GLN:HG2	2.07	0.55
2:B:761:ILE:HG21	2:B:913:LYS:CE	2.37	0.55
1:C:190:PRO:HD2	3:F:246:ARG:NH2	2.22	0.55
2:D:1636:GLU:N	2:D:1636:GLU:OE1	2.39	0.55
3:E:273:GLU:CG	3:E:275:GLU:OE2	2.54	0.55
1:A:263:LYS:HG3	2:B:854:TYR:CE1	2.42	0.55
2:B:1203:LYS:O	2:B:1206:LEU:HG	2.07	0.55
2:B:1507:ARG:HD2	2:B:1508:ASP:OD1	2.06	0.55
2:B:1544:VAL:HG13	2:B:1570:LYS:CB	2.37	0.55
2:B:1608:SER:O	2:B:1611:PHE:HD2	1.89	0.55
1:C:394:GLU:HB3	1:C:397:VAL:HG23	1.87	0.55
1:C:488:ARG:NH2	1:C:509:GLU:OE2	2.39	0.55
2:D:1118:PHE:N	2:D:1144:THR:HG23	2.21	0.55
2:D:1564:ALA:HB2	2:D:1581:GLN:HE22	1.71	0.55
3:E:197:PHE:CE2	3:E:221:ARG:HD2	2.41	0.55
2:B:1012:GLU:OE2	2:B:1068:ALA:HB2	2.06	0.55
2:B:1085:VAL:HG12	2:B:1086:PHE:CD1	2.41	0.55
2:D:1233:THR:CG2	2:D:1256:LEU:HD11	2.36	0.55
2:D:768:PRO:HD3	2:D:796:LYS:NZ	2.21	0.55
1:A:196:PRO:HD2	1:A:199:VAL:CG2	2.35	0.55
2:B:1263:GLY:CA	2:B:1272:THR:HG22	2.36	0.55
1:C:95:GLU:O	1:C:97:LYS:N	2.40	0.55
2:D:846:GLU:OE2	2:D:897:PRO:HB3	2.07	0.55
2:B:1300:LEU:CD1	2:B:1303:ARG:HE	2.20	0.55
1:C:157:LEU:HD11	2:D:811:ASP:C	2.27	0.55
1:A:628:THR:HG21	1:A:641:ASP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:962:ILE:HG12	2:B:1330:PHE:CE1	2.42	0.55
2:B:967:LEU:CD1	2:B:1327:ASN:HD22	2.19	0.55
2:D:1132:GLY:HA2	2:D:1228:TYR:CE1	2.42	0.55
2:D:1597:GLU:OE2	2:D:1600:LYS:HE2	2.07	0.55
2:B:1497:LYS:NZ	2:B:1501:LYS:O	2.35	0.54
1:C:540:ALA:HB3	1:C:543:GLN:HG2	1.89	0.54
2:D:1355:GLN:HA	2:D:1357:THR:HG23	1.89	0.54
2:D:761:ILE:CG2	2:D:762:VAL:N	2.70	0.54
3:E:276:TRP:H	3:E:276:TRP:HE3	1.54	0.54
3:F:106:SER:HA	3:F:133:TYR:CD2	2.42	0.54
1:A:566:LYS:HE3	1:A:584:LYS:CD	2.37	0.54
2:B:1136:ASN:HD22	2:B:1139:LYS:HZ3	1.55	0.54
2:B:1558:PHE:CD1	2:B:1587:PRO:HA	2.41	0.54
1:C:54:PRO:HG2	1:C:113:GLY:HA2	1.89	0.54
2:D:766:GLU:CB	2:D:796:LYS:NZ	2.66	0.54
2:D:905:THR:HA	2:D:931:VAL:CG2	2.36	0.54
3:E:109:LEU:O	3:E:114:ILE:HD11	2.08	0.54
3:E:130:ARG:HH11	3:E:130:ARG:HG3	1.72	0.54
1:A:471:LEU:HD21	1:A:519:LEU:HD23	1.89	0.54
1:C:508:ARG:HH12	1:C:512:GLN:C	2.06	0.54
2:D:1135:ASN:O	2:D:1136:ASN:HB2	2.07	0.54
2:D:1517:ASN:ND2	2:D:1521:GLN:HB2	2.20	0.54
3:F:180:ILE:HD12	3:F:180:ILE:C	2.28	0.54
1:A:60:HIS:ND1	1:A:67:LEU:O	2.34	0.54
2:D:1194:TYR:OH	2:D:1198:GLN:NE2	2.40	0.54
1:A:462:ARG:NH2	1:A:463:THR:O	2.30	0.54
2:B:1303:ARG:HH12	2:B:1306:LYS:C	2.11	0.54
2:B:1475:GLY:HA3	2:B:1493:TYR:CZ	2.43	0.54
2:B:1521:GLN:N	2:B:1521:GLN:OE1	2.25	0.54
2:B:830:PHE:CE1	2:B:852:TYR:HD2	2.25	0.54
1:C:50:GLN:NE2	1:C:51:GLY:H	1.98	0.54
3:E:175:ASP:HB3	3:E:187:SER:OG	2.07	0.54
2:B:1152:GLN:HE21	2:B:1198:GLN:HE22	1.54	0.54
2:B:980:ILE:HG22	2:B:1344:VAL:HG22	1.89	0.54
1:C:368:MET:O	1:C:413:THR:HG22	2.07	0.54
2:B:897:PRO:O	2:B:1473:GLN:NE2	2.41	0.54
2:D:1436:LYS:O	2:D:1441:ARG:NH2	2.36	0.54
3:E:143:LEU:HD11	3:E:151:TRP:CE3	2.43	0.54
1:A:221:GLU:HB2	1:A:609:ASN:ND2	2.23	0.54
2:B:1202:LEU:HD11	2:B:1243:LEU:CD2	2.30	0.54
1:C:32:ASN:HD22	1:C:33:ILE:HG12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:156:GLU:OE2	3:E:158:CYS:O	2.26	0.54
3:F:113:TYR:HA	3:F:116:GLN:CG	2.37	0.54
2:B:1082:VAL:HG13	2:B:1086:PHE:CE1	2.43	0.54
2:B:1238:LEU:CD1	2:B:1277:GLN:HE21	2.17	0.54
2:B:1429:ILE:HD11	2:B:1433:GLU:HB2	1.89	0.54
1:A:338:MET:HE1	2:B:1485:LEU:HB2	1.90	0.54
1:C:66:LYS:O	1:C:66:LYS:NZ	2.34	0.54
2:D:1417:ASP:OD1	2:D:1418:LEU:N	2.41	0.54
3:E:170:ARG:HG3	3:E:170:ARG:NH1	2.16	0.54
1:A:28:ILE:HD11	1:A:42:MET:CG	2.38	0.54
1:A:412:ASN:ND2	3:F:101:PRO:O	2.40	0.54
1:A:44:LEU:N	1:A:44:LEU:HD12	2.23	0.54
2:D:1562:ILE:HG13	2:D:1581:GLN:HE21	1.71	0.54
1:A:25:MET:HG3	1:A:650:SER:HG	1.72	0.53
2:B:1358:CYS:HB3	2:B:1361:PHE:O	2.07	0.53
2:B:974:THR:HG21	2:B:1349:HIS:CD2	2.43	0.53
1:C:657:ARG:NE	1:C:659:GLU:O	2.38	0.53
1:A:26:TYR:HD2	1:A:112:PHE:CD2	2.26	0.53
1:A:412:ASN:OD1	3:F:103:ARG:HB2	2.09	0.53
1:C:169:ASN:HB2	1:C:170:PRO:HD2	1.90	0.53
1:C:273:PHE:CE2	1:C:326:VAL:HG22	2.43	0.53
2:D:1192:ALA:HA	2:D:1195:ALA:HB3	1.89	0.53
3:F:282:GLU:OE2	3:F:284:ARG:NH2	2.41	0.53
2:B:1357:THR:HA	2:B:1358:CYS:C	2.29	0.53
2:D:1180:TYR:CD2	2:D:1206:LEU:HG	2.43	0.53
2:D:1352:ALA:HB3	2:D:1353:LYS:HA	1.90	0.53
2:D:810:SER:CB	2:D:813:LYS:HB3	2.30	0.53
2:D:758:GLU:HG2	2:D:867:LEU:HG	1.90	0.53
3:F:187:SER:C	3:F:188:PHE:HD1	2.11	0.53
1:A:496:ASN:C	1:A:498:GLY:H	2.12	0.53
1:C:132:ILE:HD13	1:C:206:ILE:HG22	1.91	0.53
2:B:1554:LEU:CD1	2:B:1591:ARG:HH22	2.21	0.53
2:B:929:LEU:HD12	2:B:930:LYS:N	2.23	0.53
2:B:977:GLU:OE2	2:B:979:ARG:NE	2.42	0.53
1:C:37:GLU:OE2	1:C:212:ASN:ND2	2.41	0.53
2:D:1280:ALA:O	2:D:1283:GLN:NE2	2.41	0.53
3:F:126:GLU:HG3	3:F:142:LYS:HG2	1.90	0.53
3:F:233:ASN:HD21	3:F:283:CYS:HB3	1.71	0.53
1:A:647:THR:CB	1:A:653:GLN:HE22	2.21	0.53
2:B:764:ARG:N	2:B:924:GLY:O	2.31	0.53
2:D:1417:ASP:OD2	2:D:1461:PHE:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1517:ASN:ND2	2:D:1519:PHE:O	2.42	0.53
3:E:104:LEU:O	3:E:130:ARG:CZ	2.56	0.53
1:A:61:ASP:OD1	1:A:65:LYS:N	2.42	0.53
2:B:1497:LYS:HZ1	2:B:1501:LYS:C	2.11	0.53
2:B:1576:VAL:HA	2:B:1580:GLN:HE22	1.74	0.53
2:D:1089:ALA:HA	2:D:1092:LEU:CD1	2.38	0.53
2:D:1554:LEU:HD11	2:D:1591:ARG:CZ	2.39	0.53
2:D:841:ARG:HH22	2:D:903:LEU:HA	1.73	0.53
1:A:126:GLN:HE21	1:A:154:HIS:CD2	2.26	0.53
2:B:1105:LYS:HG2	2:B:1162:VAL:CG2	2.37	0.53
2:B:874:SER:HB3	2:B:900:ILE:HG22	1.89	0.53
2:D:1061:GLN:C	2:D:1063:SER:N	2.61	0.53
2:D:1252:VAL:O	2:D:1256:LEU:HD13	2.09	0.53
1:C:565:VAL:HG13	2:D:821:PHE:HB2	1.90	0.53
1:A:181:SER:CB	3:E:246:ARG:HE	2.15	0.53
1:A:125:LEU:CD2	1:A:215:GLN:HE22	2.22	0.53
1:A:242:PHE:CD2	1:A:379:PRO:HG2	2.44	0.53
1:A:235:ILE:CD1	1:A:256:THR:HB	2.38	0.53
2:B:1255:TRP:O	2:B:1259:GLN:HG2	2.09	0.53
2:D:1047:GLU:HG3	2:D:1051:LYS:NZ	2.23	0.53
2:D:1298:LEU:HD12	2:D:1307:ILE:HB	1.90	0.53
2:D:1414:ASP:O	2:D:1417:ASP:OD1	2.27	0.53
2:D:1533:LEU:HA	2:D:1652:PHE:HE1	1.73	0.53
2:D:841:ARG:HH12	2:D:903:LEU:C	2.12	0.53
2:D:1001:LYS:O	2:D:1004:ILE:HG12	2.09	0.53
3:F:133:TYR:O	3:F:134:ARG:HD2	2.09	0.53
1:A:130:LEU:HD21	1:A:163:VAL:CG1	2.38	0.52
2:B:1045:ALA:O	2:B:1049:ILE:HD12	2.09	0.52
2:B:886:VAL:HG11	2:B:894:LEU:HD22	1.90	0.52
2:B:957:VAL:HG21	2:B:1335:GLU:HG3	1.91	0.52
1:C:573:ARG:HE	1:C:579:GLN:HE21	1.58	0.52
2:D:1172:ALA:O	2:D:1176:LEU:HD13	2.08	0.52
2:D:831:ILE:HG13	2:D:923:ASP:OD2	2.09	0.52
3:F:233:ASN:HD21	3:F:283:CYS:C	2.08	0.52
1:A:35:ARG:HG2	1:A:124:SER:HB3	1.91	0.52
2:B:1112:GLN:HE22	2:B:1117:VAL:N	2.08	0.52
2:B:907:LEU:O	2:B:907:LEU:HD12	2.09	0.52
1:C:43:VAL:HG11	1:C:493:LEU:HD21	1.91	0.52
2:D:1313:TRP:HA	2:D:1313:TRP:CE3	2.44	0.52
2:D:1494:HIS:CE1	2:D:1496:GLU:OE1	2.62	0.52
3:F:246:ARG:HB3	3:F:246:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1508:ASP:N	2:B:1508:ASP:OD1	2.40	0.52
2:B:1561:TYR:HB3	2:B:1563:MET:HE3	1.91	0.52
2:B:978:THR:OG1	2:B:1346:THR:HG22	2.10	0.52
2:D:1077:TRP:CD2	2:D:1130:ILE:HG22	2.44	0.52
1:A:326:VAL:CG2	1:A:343:ARG:HB3	2.39	0.52
2:B:1174:ASP:HA	2:B:1201:ARG:NH2	2.21	0.52
2:B:1291:GLU:OE1	2:B:1291:GLU:N	2.43	0.52
1:A:261:TYR:CD2	2:B:826:MET:SD	3.03	0.52
1:C:230:PRO:HB2	1:C:339:VAL:CG2	2.40	0.52
2:D:1495:PRO:HG2	2:D:1496:GLU:OE1	2.10	0.52
2:D:872:PHE:CD1	2:D:902:PRO:HA	2.44	0.52
3:E:116:GLN:O	3:E:117:ASN:ND2	2.42	0.52
3:E:156:GLU:OE2	3:E:158:CYS:N	2.43	0.52
2:B:1576:VAL:CG1	2:B:1582:ARG:HE	2.22	0.52
2:D:1132:GLY:HA2	2:D:1228:TYR:CD1	2.45	0.52
2:D:764:ARG:HB3	2:D:767:PHE:CZ	2.44	0.52
2:D:957:VAL:CG2	2:D:1335:GLU:HA	2.39	0.52
2:D:980:ILE:HD11	2:D:1322:GLU:HB2	1.90	0.52
2:B:761:ILE:CG2	2:B:913:LYS:HE3	2.39	0.52
1:C:183:GLN:HG3	3:F:266:TYR:CZ	2.45	0.52
1:C:496:ASN:O	1:C:498:GLY:N	2.42	0.52
3:F:188:PHE:CD1	3:F:188:PHE:N	2.78	0.52
2:D:1310:ARG:NH2	3:F:235:ILE:HG12	2.24	0.52
1:A:376:VAL:HG11	1:A:401:THR:HG21	1.90	0.52
2:B:1149:ILE:CA	2:B:1152:GLN:HE22	2.23	0.52
1:C:36:LEU:HD12	1:C:90:ILE:O	2.10	0.52
2:D:1190:ALA:HB2	2:D:1220:TRP:CE3	2.45	0.52
2:B:1577:GLN:N	2:B:1580:GLN:HE22	2.08	0.52
2:B:865:GLU:CD	2:B:883:GLN:HE21	2.13	0.52
1:C:96:PHE:HD1	1:C:104:LYS:HG2	1.74	0.52
1:C:175:VAL:HB	2:D:979:ARG:CZ	2.40	0.52
2:D:1102:GLY:HA2	2:D:1105:LYS:HE2	1.92	0.52
2:D:1197:ALA:HB2	2:D:1202:LEU:CD2	2.38	0.52
1:C:148:ARG:NH2	2:D:773:TRP:CZ3	2.78	0.52
3:E:194:TYR:CD1	3:E:222:GLU:HA	2.45	0.52
1:A:129:TYR:HA	1:A:218:PHE:CE2	2.44	0.52
1:A:181:SER:HB3	3:E:246:ARG:CZ	2.40	0.52
2:B:1202:LEU:HB2	2:B:1206:LEU:HD11	1.91	0.52
2:B:1240:LEU:HD12	2:B:1240:LEU:C	2.30	0.52
2:D:1174:ASP:HA	2:D:1177:GLU:HG2	1.90	0.52
2:D:1254:ARG:O	2:D:1258:GLU:OE1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:596:VAL:O	2:D:804:ILE:HA	2.10	0.52
2:B:1112:GLN:NE2	2:B:1116:GLY:C	2.63	0.52
2:B:1549:LEU:HD12	2:B:1550:VAL:N	2.25	0.52
2:B:760:ASN:OD1	2:B:761:ILE:HG23	2.10	0.52
2:B:811:ASP:OD1	2:B:811:ASP:N	2.42	0.52
1:C:491:THR:HG22	1:C:505:ARG:NE	2.25	0.52
2:D:979:ARG:HG3	2:D:1323:GLU:HG3	1.91	0.52
2:D:1544:VAL:HG23	2:D:1570:LYS:HG2	1.91	0.52
3:F:139:LEU:HD11	3:F:155:VAL:HG21	1.92	0.52
1:A:474:ASN:OD1	1:A:516:VAL:HG12	2.10	0.51
2:B:1312:HIS:HA	2:B:1313:TRP:CE3	2.46	0.51
2:B:1577:GLN:N	2:B:1580:GLN:NE2	2.59	0.51
2:B:935:GLY:HA3	2:B:1349:HIS:CE1	2.45	0.51
3:F:116:GLN:HG3	3:F:119:PHE:CE1	2.45	0.51
3:F:135:ARG:HH12	3:F:137:PRO:HA	1.75	0.51
1:A:103:ASN:OD1	1:A:103:ASN:N	2.40	0.51
1:A:448:THR:HG23	1:A:451:ASN:HA	1.92	0.51
2:B:1516:GLU:CD	2:B:1624:LYS:HG2	2.31	0.51
1:C:391:VAL:CG2	1:C:394:GLU:HB2	2.40	0.51
2:D:1063:SER:O	2:D:1065:ALA:N	2.43	0.51
2:D:1145:ALA:O	2:D:1149:ILE:HG22	2.10	0.51
3:E:235:ILE:HG22	3:E:236:ILE:H	1.74	0.51
2:B:1084:LYS:HE3	2:B:1149:ILE:HD13	1.91	0.51
2:B:1248:PHE:O	2:B:1251:PRO:HD2	2.10	0.51
2:B:1317:SER:O	2:B:1319:LEU:HG	2.10	0.51
2:B:764:ARG:HD2	2:B:797:ASP:O	2.09	0.51
2:D:1149:ILE:HA	2:D:1152:GLN:HE21	1.75	0.51
2:D:1159:GLU:OE2	2:D:1165:LEU:HD23	2.11	0.51
3:E:107:ALA:N	3:E:130:ARG:NH1	2.58	0.51
3:E:235:ILE:HG22	3:E:236:ILE:N	2.26	0.51
2:D:756:ILE:CD1	3:F:134:ARG:HH22	2.23	0.51
1:A:540:ALA:HB3	1:A:543:GLN:HG2	1.91	0.51
2:B:1226:GLN:O	2:B:1230:VAL:HG23	2.11	0.51
2:D:1065:ALA:CB	2:D:1074:PRO:HB3	2.41	0.51
2:D:1313:TRP:HZ3	2:D:1318:LEU:HD11	1.73	0.51
2:D:1423:ASN:O	2:D:1425:VAL:HG12	2.10	0.51
2:D:1547:THR:HG22	2:D:1565:ILE:HD13	1.93	0.51
2:B:1192:ALA:O	2:B:1196:LEU:HG	2.10	0.51
2:B:1261:TYR:OH	2:B:1268:SER:HB2	2.11	0.51
1:C:489:TYR:CD2	1:C:505:ARG:HD2	2.46	0.51
1:C:148:ARG:CZ	1:C:594:VAL:CG2	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1255:TRP:HA	2:D:1258:GLU:CD	2.30	0.51
3:E:232:ASP:O	3:E:283:CYS:SG	2.69	0.51
2:D:756:ILE:CB	3:F:134:ARG:HH22	2.24	0.51
3:F:203:PHE:O	3:F:214:SER:N	2.36	0.51
1:C:508:ARG:HH12	1:C:512:GLN:HB2	1.76	0.51
2:D:1216:ASP:OD1	2:D:1218:ASN:OD1	2.29	0.51
2:D:1639:ASP:OD2	2:D:1642:ASN:HB2	2.11	0.51
2:D:841:ARG:HH12	2:D:903:LEU:CA	2.23	0.51
3:E:107:ALA:HB1	3:E:127:TYR:HB3	1.91	0.51
1:A:368:MET:O	1:A:413:THR:HG22	2.09	0.51
2:B:1313:TRP:O	2:B:1314:GLU:HB2	2.11	0.51
2:B:1541:VAL:HG13	2:B:1570:LYS:HZ1	1.76	0.51
2:B:1549:LEU:HD13	2:B:1563:MET:HE1	1.92	0.51
2:B:1634:GLU:OE2	2:B:1638:GLN:NE2	2.44	0.51
1:A:610:LYS:O	1:A:615:LYS:NZ	2.43	0.51
1:A:646:PHE:H	1:A:654:THR:HG21	1.76	0.51
2:B:1149:ILE:HA	2:B:1152:GLN:NE2	2.24	0.51
1:C:201:MET:HE3	1:C:225:LYS:HA	1.92	0.51
1:C:41:THR:HG22	1:C:500:LEU:HB2	1.92	0.51
1:C:42:MET:HB3	1:C:86:VAL:HG12	1.91	0.51
2:D:1400:MET:CE	2:D:1447:TYR:HB3	2.40	0.51
1:A:236:VAL:HG22	1:A:255:ILE:HD13	1.93	0.51
2:B:1118:PHE:HZ	2:B:1151:LEU:HD11	1.76	0.51
2:B:1435:ASP:OD1	2:B:1435:ASP:N	2.43	0.51
1:C:355:ILE:HG12	1:C:376:VAL:HG22	1.91	0.51
1:C:365:LYS:HZ1	1:C:549:ASP:CG	2.13	0.51
2:D:1588:ILE:HG22	2:D:1591:ARG:HH21	1.75	0.51
3:E:276:TRP:N	3:E:276:TRP:CD2	2.77	0.51
3:F:107:ALA:HB1	3:F:127:TYR:HB3	1.93	0.51
3:F:258:THR:O	3:F:283:CYS:HA	2.11	0.51
1:A:37:GLU:CD	1:A:161:ARG:NH1	2.63	0.51
2:B:1060:ARG:NH2	2:B:1099:VAL:HA	2.26	0.51
2:B:1407:MET:SD	2:B:1413:PRO:HD3	2.51	0.51
2:B:1559:ASP:OD1	2:B:1586:SER:O	2.29	0.51
2:B:967:LEU:HD22	2:B:1348:TYR:HD2	1.71	0.51
2:D:1547:THR:HB	2:D:1563:MET:CG	2.41	0.51
2:D:1505:LEU:CD1	2:D:1585:ILE:HD11	2.39	0.51
2:D:1631:TRP:HZ3	2:D:1633:GLU:HA	1.75	0.51
2:D:996:ASP:O	2:D:999:ARG:HB2	2.11	0.51
3:F:195:LYS:HD2	3:F:196:LEU:N	2.24	0.51
2:D:1156:ASP:OD1	2:D:1157:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:129:CYS:HB3	3:F:133:TYR:HB2	1.91	0.50
1:A:376:VAL:HG12	1:A:401:THR:HG21	1.93	0.50
1:A:462:ARG:HH21	1:A:463:THR:C	2.13	0.50
1:A:39:GLU:HG3	1:A:87:THR:HG22	1.93	0.50
2:B:1191:ILE:HG22	2:B:1235:TYR:CD1	2.47	0.50
1:C:465:LEU:HD11	1:C:555:VAL:HG22	1.93	0.50
2:D:1252:VAL:O	2:D:1255:TRP:HB3	2.11	0.50
2:D:1533:LEU:HD21	2:D:1655:SER:OG	2.11	0.50
1:A:397:VAL:HG12	1:A:409:LEU:HD23	1.93	0.50
1:A:362:LYS:NZ	1:A:442:GLN:O	2.30	0.50
2:B:1116:GLY:HA2	2:B:1171:LYS:HG2	1.94	0.50
2:B:841:ARG:NH2	2:B:903:LEU:HA	2.26	0.50
1:C:104:LYS:O	1:C:122:LEU:HD12	2.10	0.50
1:C:167:ILE:O	1:C:175:VAL:HG22	2.11	0.50
1:C:198:LEU:HD11	2:D:1349:HIS:NE2	2.27	0.50
1:C:460:VAL:HG13	1:C:462:ARG:HD3	1.92	0.50
2:D:979:ARG:HG3	2:D:1323:GLU:CG	2.42	0.50
2:D:1392:TYR:CE1	2:D:1398:ALA:HB2	2.47	0.50
2:D:798:SER:HB2	2:D:802:TRP:CZ2	2.47	0.50
2:D:758:GLU:CA	2:D:913:LYS:HZ3	2.09	0.50
3:E:107:ALA:C	3:E:130:ARG:HH12	2.15	0.50
3:E:245:TYR:C	3:E:245:TYR:CD1	2.84	0.50
1:A:647:THR:CG2	1:A:653:GLN:HE22	2.24	0.50
2:B:870:PRO:O	2:B:903:LEU:HD12	2.12	0.50
2:D:1133:LEU:O	2:D:1139:LYS:HE3	2.11	0.50
2:D:1210:PHE:O	2:D:1213:THR:HG22	2.11	0.50
2:D:1128:GLU:OE1	2:D:1267:GLY:CA	2.59	0.50
3:F:241:ASP:N	3:F:241:ASP:OD1	2.43	0.50
1:A:36:LEU:O	1:A:37:GLU:HG2	2.12	0.50
1:A:39:GLU:OE1	1:A:89:THR:HG23	2.12	0.50
2:B:1281:GLN:OE1	2:B:1284:LYS:HE2	2.11	0.50
2:B:831:ILE:HD12	2:B:925:VAL:HG23	1.92	0.50
1:C:456:LEU:HB2	1:C:535:TYR:HE2	1.77	0.50
1:A:59:VAL:HG13	1:A:106:VAL:HG21	1.94	0.50
1:A:612:THR:HG23	1:A:615:LYS:HZ3	1.76	0.50
2:B:967:LEU:HD22	2:B:1348:TYR:CE2	2.47	0.50
2:B:1608:SER:HA	2:B:1611:PHE:CE2	2.46	0.50
1:C:508:ARG:CG	1:C:508:ARG:NH1	2.68	0.50
2:D:1060:ARG:NH2	2:D:1099:VAL:HA	2.27	0.50
3:F:204:CYS:SG	3:F:211:VAL:HG21	2.51	0.50
1:A:166:ASN:HD21	1:A:174:PRO:CG	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PHE:HE2	1:A:330:VAL:CG2	2.25	0.50
2:B:1643:GLN:HG3	2:B:1644:LYS:H	1.75	0.50
2:B:826:MET:HG3	2:B:827:GLN:H	1.77	0.50
2:D:757:ALA:O	2:D:761:ILE:CD1	2.59	0.50
1:C:313:ASN:ND2	1:C:318:ASP:HB2	2.27	0.50
1:C:365:LYS:HZ3	1:C:457:HIS:HA	1.75	0.50
1:C:460:VAL:CG2	1:C:471:LEU:HD21	2.41	0.50
1:C:97:LYS:CG	2:D:1314:GLU:HB3	2.42	0.50
2:D:1348:TYR:HE1	2:D:1350:ALA:HB2	1.76	0.50
2:D:761:ILE:HD13	2:D:913:LYS:NZ	2.27	0.50
3:E:171:ASN:ND2	3:E:194:TYR:CE1	2.80	0.50
3:F:116:GLN:HG3	3:F:119:PHE:CZ	2.46	0.50
1:A:380:ASP:OD1	1:A:381:GLY:N	2.45	0.50
1:A:35:ARG:HH22	1:A:498:GLY:HA3	1.76	0.50
1:A:63:PRO:HD3	2:B:1034:TRP:CZ3	2.46	0.50
2:B:1141:MET:HA	2:B:1141:MET:HE2	1.94	0.50
2:B:1497:LYS:NZ	2:B:1502:LEU:HA	2.26	0.50
2:B:1551:LYS:HD2	2:B:1552:VAL:H	1.76	0.50
2:B:752:ASP:HB3	2:B:753:GLU:OE1	2.12	0.50
1:C:475:PHE:HB2	1:C:515:VAL:HG13	1.94	0.50
2:D:1210:PHE:CE1	2:D:1220:TRP:CH2	3.00	0.50
2:D:1313:TRP:CE3	2:D:1318:LEU:HD21	2.47	0.50
2:D:1492:PHE:HE2	2:D:1500:GLY:C	2.16	0.50
2:D:811:ASP:OD1	2:D:811:ASP:N	2.44	0.50
3:E:101:PRO:HB3	3:E:143:LEU:HD21	1.94	0.50
1:A:329:THR:HA	1:A:340:GLN:OE1	2.12	0.49
2:B:1032:GLU:HA	2:B:1034:TRP:CE3	2.47	0.49
2:D:1472:ILE:HD11	2:D:1494:HIS:NE2	2.27	0.49
3:E:133:TYR:O	3:E:161:LYS:HE3	2.12	0.49
3:F:246:ARG:CB	3:F:246:ARG:NH1	2.74	0.49
1:A:484:GLU:O	1:A:487:ILE:HG22	2.12	0.49
1:A:489:TYR:CD2	1:A:505:ARG:NH2	2.80	0.49
2:B:1300:LEU:HD11	2:B:1303:ARG:CG	2.23	0.49
2:B:755:ILE:HD12	2:B:756:ILE:O	2.12	0.49
2:D:1037:PHE:O	2:D:1041:LYS:HD2	2.13	0.49
3:E:222:GLU:HG2	3:E:224:TYR:CE1	2.47	0.49
1:A:122:LEU:H	1:A:122:LEU:HD12	1.77	0.49
2:B:795:LEU:HD11	2:B:825:VAL:HB	1.93	0.49
2:B:764:ARG:HB3	2:B:797:ASP:HB3	1.95	0.49
1:C:72:GLU:HB2	1:C:86:VAL:CG2	2.42	0.49
2:D:1294:LEU:HB3	2:D:1311:ILE:CG2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:971:VAL:HA	2:D:1351:LYS:HE3	1.94	0.49
2:D:763:SER:CB	2:D:926:ARG:HB2	2.43	0.49
2:D:972:PRO:HD3	2:D:1351:LYS:HE3	1.93	0.49
2:D:996:ASP:OD1	2:D:1036:LYS:CE	2.60	0.49
3:E:132:GLY:HA2	3:E:161:LYS:NZ	2.27	0.49
2:B:1299:GLN:HA	2:B:1303:ARG:HH21	1.76	0.49
1:C:453:ASN:OD1	1:C:455:TYR:HE2	1.95	0.49
2:D:1029:ASP:OD1	2:D:1034:TRP:NE1	2.32	0.49
2:D:1060:ARG:HD2	2:D:1064:SER:HA	1.94	0.49
2:D:898:TYR:HA	2:D:1473:GLN:HE22	1.78	0.49
3:F:157:PHE:CD1	3:F:157:PHE:N	2.81	0.49
3:F:224:TYR:CD1	3:F:242:HIS:HB3	2.47	0.49
1:A:326:VAL:O	1:A:342:GLU:HA	2.12	0.49
2:B:1159:GLU:OE2	2:B:1166:PRO:HG3	2.12	0.49
2:B:1249:VAL:HB	2:B:1250:PRO:CD	2.42	0.49
2:B:1512:ARG:NH1	2:B:1621:ILE:HD11	2.28	0.49
1:C:355:ILE:HG23	1:C:374:VAL:HG13	1.94	0.49
1:C:625:ILE:CD1	1:C:643:GLY:HA3	2.42	0.49
2:D:1047:GLU:O	2:D:1050:LYS:HG2	2.12	0.49
2:D:1249:VAL:HG23	2:D:1250:PRO:HD3	1.92	0.49
2:D:1249:VAL:O	2:D:1252:VAL:HG12	2.13	0.49
2:D:1295:ASP:HB2	2:D:1335:GLU:HB3	1.94	0.49
2:D:1506:CYS:HG	2:D:1511:CYS:CB	2.25	0.49
2:D:1601:HIS:HB2	2:D:1631:TRP:HB3	1.94	0.49
2:B:1027:TYR:CZ	2:B:1031:THR:HG21	2.46	0.49
2:B:1082:VAL:O	2:B:1086:PHE:CD1	2.65	0.49
2:B:1420:GLN:O	2:B:1423:ASN:OD1	2.31	0.49
1:C:59:VAL:CG1	1:C:70:SER:H	2.25	0.49
1:C:67:LEU:CD2	1:C:67:LEU:CB	2.82	0.49
1:C:36:LEU:HD11	1:C:91:PRO:C	2.33	0.49
2:D:1063:SER:HA	2:D:1106:TRP:HZ3	1.78	0.49
1:A:105:PHE:CE2	1:A:122:LEU:HG	2.46	0.49
2:B:1022:VAL:HG22	2:B:1049:ILE:HG12	1.94	0.49
2:B:1259:GLN:C	2:B:1260:ARG:HG3	2.33	0.49
2:B:1601:HIS:HB2	2:B:1631:TRP:HB3	1.95	0.49
1:C:367:GLY:H	1:C:413:THR:HG23	1.77	0.49
2:D:1303:ARG:NH2	3:F:241:ASP:HA	2.27	0.49
2:B:1554:LEU:HD13	2:B:1591:ARG:HH22	1.78	0.49
2:B:1638:GLN:OE1	2:B:1638:GLN:N	2.38	0.49
1:A:586:GLU:HG2	2:B:788:THR:HG23	1.95	0.49
1:C:95:GLU:C	1:C:97:LYS:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:778:LEU:CG	2:D:787:SER:HB3	2.42	0.49
2:D:802:TRP:HB2	2:D:823:VAL:CG2	2.43	0.49
3:F:180:ILE:HD12	3:F:180:ILE:O	2.13	0.49
1:A:130:LEU:HD13	1:A:210:TYR:CZ	2.48	0.49
1:A:126:GLN:HG2	1:A:154:HIS:NE2	2.27	0.49
1:A:431:LEU:HD11	1:A:436:GLN:NE2	2.27	0.49
2:B:1012:GLU:CD	2:B:1124:VAL:HG22	2.33	0.49
2:B:1053:TYR:HD2	2:B:1086:PHE:CE2	2.30	0.49
2:B:1130:ILE:HG23	2:B:1133:LEU:HB2	1.95	0.49
2:B:753:GLU:O	2:B:754:ASP:OD1	2.30	0.49
2:B:846:GLU:OE1	2:B:1476:ALA:HB3	2.13	0.49
1:C:236:VAL:HG22	1:C:255:ILE:HD13	1.93	0.49
2:D:1063:SER:O	2:D:1063:SER:OG	2.18	0.49
2:D:936:ILE:HG13	2:D:937:ARG:N	2.27	0.49
3:E:105:ASN:OD1	3:E:105:ASN:N	2.41	0.49
2:B:1238:LEU:HD21	2:B:1278:ALA:HA	1.94	0.49
1:C:230:PRO:HB2	1:C:339:VAL:HG22	1.95	0.49
1:C:272:ILE:HG22	1:C:327:SER:HB3	1.94	0.49
1:C:385:TYR:CD1	1:C:386:ARG:HG3	2.47	0.49
1:C:45:GLU:OE1	1:C:534:TYR:OH	2.27	0.49
1:C:78:PRO:HA	1:C:82:HIS:CE1	2.48	0.49
1:A:181:SER:N	3:E:246:ARG:CZ	2.75	0.49
1:A:59:VAL:HG13	1:A:106:VAL:CG2	2.42	0.48
1:A:37:GLU:OE1	1:A:161:ARG:NH1	2.45	0.48
2:B:800:THR:H	2:B:825:VAL:HG13	1.77	0.48
1:C:183:GLN:H	1:C:183:GLN:CD	2.14	0.48
1:C:489:TYR:HD2	1:C:505:ARG:HD2	1.78	0.48
2:D:1158:CYS:HA	2:D:1161:GLN:HE22	1.75	0.48
2:D:758:GLU:H	2:D:881:ARG:HH12	1.61	0.48
1:A:130:LEU:HD21	1:A:163:VAL:HG12	1.94	0.48
1:A:119:LYS:HB2	1:A:647:THR:HG21	1.95	0.48
2:B:1084:LYS:HE2	2:B:1273:PHE:HE2	1.77	0.48
2:B:1115:ASP:O	2:B:1175:PHE:CD2	2.66	0.48
2:B:1136:ASN:HD22	2:B:1139:LYS:HZ1	1.57	0.48
2:B:1149:ILE:O	2:B:1152:GLN:NE2	2.46	0.48
1:A:335:GLY:HA3	2:B:1404:ASP:OD2	2.14	0.48
2:B:877:THR:HG23	2:B:879:LYS:N	2.28	0.48
1:C:355:ILE:HD11	1:C:426:THR:HG23	1.95	0.48
3:F:188:PHE:HD1	3:F:188:PHE:N	2.11	0.48
3:F:194:TYR:CE1	3:F:222:GLU:HB3	2.48	0.48
1:A:365:LYS:N	1:A:365:LYS:HD3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:GLU:OE1	1:A:484:GLU:N	2.41	0.48
2:B:1554:LEU:HD12	2:B:1555:SER:O	2.13	0.48
2:B:1607:LEU:HD13	2:B:1609:SER:OG	2.14	0.48
1:C:183:GLN:O	1:C:185:GLN:HG2	2.13	0.48
1:C:29:ILE:HB	1:C:43:VAL:HG13	1.94	0.48
1:C:50:GLN:HE21	1:C:51:GLY:N	1.95	0.48
1:C:634:ASP:O	1:C:638:VAL:HG23	2.13	0.48
2:D:1157:ILE:O	2:D:1161:GLN:NE2	2.35	0.48
2:D:1543:TYR:HB2	2:D:1545:TYR:CZ	2.48	0.48
2:D:1512:ARG:NH1	2:D:1621:ILE:HD13	2.29	0.48
2:D:761:ILE:HD13	2:D:913:LYS:HZ1	1.78	0.48
3:E:170:ARG:NH1	3:E:170:ARG:CG	2.71	0.48
1:A:85:ASN:N	1:A:85:ASN:OD1	2.46	0.48
2:B:826:MET:CG	2:B:827:GLN:H	2.27	0.48
2:B:868:HIS:CD2	2:B:877:THR:HA	2.48	0.48
2:B:913:LYS:HD2	2:B:914:ALA:H	1.79	0.48
1:C:175:VAL:HB	2:D:979:ARG:NH1	2.27	0.48
1:C:385:TYR:HD2	1:C:403:GLY:HA2	1.77	0.48
2:B:1061:GLN:OE1	2:B:1074:PRO:HG3	2.13	0.48
2:B:1436:LYS:HB3	2:B:1441:ARG:HE	1.79	0.48
2:B:1411:PHE:C	2:B:1466:TYR:HE1	2.17	0.48
2:B:1496:GLU:O	2:B:1497:LYS:C	2.52	0.48
2:B:1505:LEU:HG	2:B:1612:TRP:CH2	2.49	0.48
2:B:1557:ASP:O	2:B:1588:ILE:HG23	2.12	0.48
1:C:77:THR:O	1:C:80:THR:HG22	2.14	0.48
2:D:1246:PHE:CE1	2:D:1286:ALA:HB3	2.48	0.48
2:D:934:GLU:HG2	2:D:1352:ALA:O	2.14	0.48
2:D:756:ILE:CD1	2:D:761:ILE:HG13	2.39	0.48
3:E:146:LEU:N	3:E:150:LYS:O	2.41	0.48
1:A:487:ILE:CD1	1:A:535:TYR:HB2	2.42	0.48
2:B:996:ASP:OD1	2:B:999:ARG:HB2	2.13	0.48
1:C:209:TYR:CD2	1:C:214:PRO:HA	2.48	0.48
1:C:479:MET:HG3	1:C:480:ASP:N	2.29	0.48
2:D:1643:GLN:HE21	2:D:1644:LYS:NZ	2.12	0.48
1:A:471:LEU:O	1:A:471:LEU:HD12	2.14	0.48
1:A:628:THR:HG23	1:A:630:GLY:H	1.79	0.48
2:B:1507:ARG:CZ	2:B:1508:ASP:OD1	2.62	0.48
2:B:1544:VAL:CG1	2:B:1570:LYS:HB3	2.42	0.48
2:B:1574:ASP:O	2:B:1576:VAL:HG22	2.14	0.48
2:D:1202:LEU:O	2:D:1207:LEU:HB2	2.14	0.48
2:D:978:THR:HG1	2:D:1324:THR:HG23	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:796:LYS:HG3	2:D:797:ASP:H	1.78	0.48
2:B:1032:GLU:HA	2:B:1034:TRP:CZ3	2.49	0.48
2:B:1576:VAL:HG11	2:B:1582:ARG:HE	1.78	0.48
2:B:971:VAL:HG21	2:B:1349:HIS:CE1	2.48	0.48
1:C:115:GLN:HG2	1:C:649:SER:HB2	1.94	0.48
1:C:527:PRO:O	1:C:555:VAL:N	2.34	0.48
2:D:1470:GLU:HG3	2:D:1471:LEU:HD22	1.94	0.48
2:D:796:LYS:HA	2:D:796:LYS:HD2	1.57	0.48
2:D:888:ILE:HD12	2:D:889:PRO:HD2	1.96	0.48
3:E:222:GLU:HB3	3:E:224:TYR:HE1	1.78	0.48
1:C:189:LEU:CD1	3:F:246:ARG:HH12	2.26	0.48
1:A:130:LEU:CB	1:A:218:PHE:HD2	2.26	0.48
1:A:119:LYS:CB	1:A:647:THR:HG21	2.43	0.48
2:B:965:ALA:H	2:B:1327:ASN:HD21	1.60	0.48
1:C:28:ILE:HD13	1:C:44:LEU:HD23	1.94	0.48
1:C:508:ARG:NH1	1:C:512:GLN:HB2	2.28	0.48
1:C:561:GLY:HA3	2:D:813:LYS:CE	2.42	0.48
1:C:617:TRP:CE3	1:C:617:TRP:HA	2.49	0.48
1:C:532:VAL:HG11	1:C:644:LEU:HD12	1.96	0.48
2:D:1250:PRO:O	2:D:1254:ARG:HG2	2.14	0.48
2:D:1508:ASP:OD1	2:D:1509:GLU:N	2.40	0.48
2:D:856:GLN:HG2	2:D:857:ASN:N	2.28	0.48
3:E:203:PHE:O	3:E:214:SER:N	2.40	0.48
1:A:144:THR:HG23	1:A:194:ASP:OD1	2.13	0.48
1:A:476:LEU:HD13	1:A:514:LEU:CD1	2.44	0.48
1:A:487:ILE:HD11	1:A:535:TYR:HB2	1.95	0.48
1:A:502:LYS:HD2	1:A:503:ALA:N	2.29	0.48
2:B:1136:ASN:HA	2:B:1139:LYS:CE	2.43	0.48
2:B:1635:ASP:CA	2:B:1638:GLN:HE22	2.16	0.48
1:C:275:ILE:HG13	1:C:282:ILE:HB	1.95	0.48
1:C:488:ARG:HH12	1:C:507:VAL:CG1	2.27	0.48
2:D:1060:ARG:NH1	2:D:1060:ARG:HG3	2.28	0.48
3:F:187:SER:C	3:F:188:PHE:CD1	2.87	0.48
3:F:222:GLU:OE2	3:F:224:TYR:CZ	2.67	0.48
1:A:166:ASN:HD21	1:A:174:PRO:HB3	1.79	0.47
1:A:132:ILE:HD13	1:A:206:ILE:HG22	1.95	0.47
2:B:1152:GLN:HE21	2:B:1153:GLU:HG2	1.79	0.47
2:B:1166:PRO:O	2:B:1170:THR:OG1	2.30	0.47
2:B:1191:ILE:HG22	2:B:1235:TYR:CE1	2.48	0.47
2:B:980:ILE:HG13	2:B:1322:GLU:O	2.14	0.47
2:B:974:THR:HG21	2:B:1349:HIS:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:588:ASP:O	2:D:778:LEU:HD23	2.14	0.47
3:E:222:GLU:HB3	3:E:224:TYR:CE1	2.49	0.47
3:F:188:PHE:CE2	3:F:218:PRO:HD2	2.48	0.47
1:A:191:LEU:HD12	1:A:192:SER:H	1.79	0.47
1:A:481:ARG:HA	1:A:484:GLU:CD	2.34	0.47
2:B:1031:THR:HB	2:B:1033:GLN:HE21	1.79	0.47
2:B:1044:GLY:O	2:B:1048:LEU:HD13	2.14	0.47
1:C:23:SER:O	1:C:544:ARG:NH2	2.42	0.47
1:C:346:ILE:HG13	1:C:346:ILE:O	2.14	0.47
1:C:36:LEU:HD21	1:C:92:ALA:HA	1.97	0.47
2:D:911:GLU:HB2	2:D:926:ARG:HG3	1.96	0.47
3:E:124:VAL:HA	3:E:143:LEU:O	2.14	0.47
3:E:260:ILE:CD1	3:E:284:ARG:HD3	2.35	0.47
3:F:231:ILE:HD11	3:F:234:GLY:HA3	1.96	0.47
1:A:36:LEU:O	1:A:37:GLU:CG	2.62	0.47
1:A:496:ASN:ND2	1:A:501:LEU:HD22	2.22	0.47
2:B:1152:GLN:NE2	2:B:1153:GLU:HG2	2.28	0.47
2:B:1233:THR:CG2	2:B:1256:LEU:HD11	2.38	0.47
2:B:1494:HIS:CD2	2:B:1495:PRO:HD2	2.39	0.47
2:D:1215:LYS:HD2	2:D:1215:LYS:C	2.34	0.47
2:D:1538:GLU:HB3	2:D:1539:PRO:HD2	1.96	0.47
2:D:794:PHE:CZ	3:F:176:VAL:HB	2.49	0.47
3:F:255:LYS:HB2	3:F:255:LYS:HE2	1.58	0.47
2:B:1051:LYS:O	2:B:1055:GLN:HG2	2.15	0.47
2:B:1130:ILE:HA	2:B:1130:ILE:HD12	1.54	0.47
2:B:1431:LYS:O	2:B:1434:LEU:HB2	2.13	0.47
1:C:275:ILE:HG22	1:C:324:LEU:CD2	2.44	0.47
2:D:1056:GLN:HE22	2:D:1082:VAL:HG22	1.79	0.47
2:D:1186:SER:HA	2:D:1189:VAL:CG2	2.43	0.47
2:D:1002:HIS:NE2	2:D:1262:TYR:O	2.40	0.47
2:D:1328:GLU:OE1	2:D:1330:PHE:HB3	2.14	0.47
2:D:1485:LEU:HD12	2:D:1486:GLU:N	2.27	0.47
2:D:1636:GLU:O	2:D:1639:ASP:HB3	2.14	0.47
1:A:29:ILE:HG12	1:A:646:PHE:HD2	1.79	0.47
2:B:1077:TRP:CD1	2:B:1130:ILE:HD11	2.50	0.47
2:B:949:PRO:O	2:B:950:GLU:HG2	2.15	0.47
2:D:753:GLU:O	2:D:753:GLU:HG2	2.13	0.47
2:D:755:ILE:CG2	2:D:756:ILE:N	2.77	0.47
2:D:764:ARG:HB3	2:D:767:PHE:HZ	1.79	0.47
3:F:245:TYR:CG	3:F:245:TYR:O	2.68	0.47
2:B:1157:ILE:HD12	2:B:1158:CYS:SG	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1237:LEU:HD23	2:B:1278:ALA:HB1	1.96	0.47
2:B:1356:LEU:HD13	2:B:1357:THR:N	2.27	0.47
2:B:833:LEU:HG	2:B:835:LEU:HD13	1.97	0.47
2:D:1056:GLN:NE2	2:D:1082:VAL:HG22	2.29	0.47
2:D:1186:SER:O	2:D:1189:VAL:HG23	2.13	0.47
2:D:1193:GLY:O	2:D:1202:LEU:HD23	2.14	0.47
3:E:182:PHE:CE1	3:E:206:ILE:HG22	2.50	0.47
2:B:1312:HIS:HE1	3:E:237:GLN:HE22	1.62	0.47
1:A:431:LEU:HD12	1:A:431:LEU:C	2.35	0.47
1:A:83:MET:HE2	1:A:505:ARG:NH1	2.28	0.47
2:B:949:PRO:HG3	2:B:958:GLN:OE1	2.15	0.47
2:B:960:GLU:HB3	2:B:1332:VAL:O	2.15	0.47
1:C:508:ARG:HH12	1:C:512:GLN:CB	2.27	0.47
1:C:105:PHE:CZ	1:C:658:ALA:HA	2.50	0.47
2:D:831:ILE:N	2:D:923:ASP:OD2	2.47	0.47
1:A:42:MET:HE1	1:A:57:VAL:HG13	1.95	0.47
1:A:496:ASN:OD1	1:A:496:ASN:C	2.52	0.47
2:B:1549:LEU:HD13	2:B:1563:MET:HE2	1.96	0.47
2:B:913:LYS:HZ2	2:B:913:LYS:HG2	1.31	0.47
1:C:203:GLN:NE2	1:C:223:GLU:OE1	2.47	0.47
1:C:386:ARG:HG2	1:C:400:LEU:HD21	1.96	0.47
1:C:465:LEU:HD12	1:C:555:VAL:HG22	1.96	0.47
2:D:1310:ARG:HH21	3:F:235:ILE:HG12	1.80	0.47
1:A:169:ASN:HD21	1:A:173:ILE:HB	1.79	0.47
1:A:491:THR:O	1:A:533:ALA:HA	2.14	0.47
2:B:1434:LEU:HD23	2:B:1434:LEU:HA	1.81	0.47
1:C:135:ASP:HB3	1:C:146:LEU:CD1	2.42	0.47
1:C:229:LEU:CD2	1:C:601:GLY:HA3	2.45	0.47
2:D:995:VAL:HG13	2:D:1027:TYR:CE2	2.50	0.47
2:D:1261:TYR:OH	2:D:1268:SER:HB3	2.14	0.47
2:D:932:VAL:HG13	2:D:933:PRO:HD2	1.96	0.47
3:E:107:ALA:N	3:E:130:ARG:HH12	2.13	0.47
3:F:105:ASN:OD1	3:F:106:SER:N	2.48	0.47
1:A:151:THR:HG21	1:A:182:SER:HB3	1.95	0.47
1:C:463:THR:O	1:C:465:LEU:N	2.48	0.47
2:D:1061:GLN:CG	2:D:1062:PRO:HD2	2.45	0.47
2:D:1102:GLY:HA2	2:D:1105:LYS:CE	2.45	0.47
2:D:985:THR:HA	2:D:986:PRO:HD3	1.83	0.47
2:D:987:VAL:CG2	2:D:988:ALA:N	2.77	0.47
1:A:35:ARG:HD3	1:A:154:HIS:CD2	2.49	0.47
1:A:492:TYR:HB2	1:A:531:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:LEU:HD11	1:A:533:ALA:HB3	1.97	0.47
2:D:1136:ASN:CA	2:D:1139:LYS:HE2	2.45	0.47
2:D:1160:GLU:OE2	3:E:117:ASN:HB2	2.15	0.47
2:D:772:LEU:O	2:D:774:ASN:N	2.47	0.47
3:E:104:LEU:O	3:E:130:ARG:NH2	2.48	0.47
2:B:1039:LEU:HD12	2:B:1039:LEU:HA	1.57	0.46
2:B:980:ILE:HG22	2:B:1344:VAL:HG13	1.97	0.46
2:B:913:LYS:HG3	2:B:914:ALA:N	2.30	0.46
2:B:970:GLN:NE2	2:B:974:THR:O	2.48	0.46
1:C:150:PHE:CZ	2:D:807:VAL:HG21	2.51	0.46
1:C:32:ASN:HD21	1:C:657:ARG:CD	2.01	0.46
1:C:575:PRO:HG2	2:D:824:THR:O	2.16	0.46
1:C:636:ALA:HB1	1:C:654:THR:HA	1.96	0.46
1:C:647:THR:HG23	1:C:653:GLN:HB3	1.97	0.46
2:D:1366:THR:OG1	2:D:1387:GLU:HB3	2.15	0.46
2:D:904:LYS:HG3	2:D:908:GLN:HE22	1.79	0.46
1:A:130:LEU:HB2	1:A:218:PHE:HD2	1.80	0.46
1:A:299:GLU:OE1	1:A:299:GLU:N	2.48	0.46
2:B:833:LEU:HD21	2:B:910:VAL:HG12	1.96	0.46
2:B:861:LYS:HD3	2:B:887:THR:HG23	1.96	0.46
1:C:463:THR:O	1:C:465:LEU:HD23	2.15	0.46
2:D:1217:LYS:NZ	2:D:1251:PRO:HG2	2.30	0.46
2:D:1450:LYS:HG3	2:D:1451:VAL:N	2.25	0.46
1:C:157:LEU:HD21	2:D:811:ASP:O	2.15	0.46
2:D:877:THR:HG23	2:D:879:LYS:N	2.30	0.46
2:D:894:LEU:HA	2:D:894:LEU:HD12	1.72	0.46
3:F:226:PRO:O	3:F:276:TRP:NE1	2.44	0.46
1:A:104:LYS:HG2	1:A:105:PHE:N	2.30	0.46
1:A:215:GLN:HG2	1:A:216:GLN:H	1.79	0.46
2:B:1191:ILE:HG13	2:B:1191:ILE:H	1.43	0.46
2:B:1413:PRO:HD2	2:B:1441:ARG:HD2	1.96	0.46
1:C:36:LEU:HD11	1:C:92:ALA:N	2.30	0.46
1:A:195:ILE:O	1:A:195:ILE:HG13	2.15	0.46
1:A:456:LEU:HB2	1:A:535:TYR:CE2	2.47	0.46
2:B:1060:ARG:CZ	2:B:1099:VAL:HG13	2.45	0.46
1:C:353:TYR:CE1	1:C:387:VAL:HG21	2.49	0.46
1:C:569:GLN:HB2	1:C:570:SER:H	1.49	0.46
2:D:1294:LEU:HB3	2:D:1311:ILE:HG23	1.97	0.46
2:D:1554:LEU:HD12	2:D:1555:SER:N	2.30	0.46
2:D:1640:GLU:O	2:D:1643:GLN:HG2	2.15	0.46
3:F:113:TYR:HA	3:F:116:GLN:CD	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1174:ASP:OD1	2:B:1175:PHE:HD2	1.98	0.46
2:B:1265:GLY:N	2:B:1268:SER:OG	2.48	0.46
2:B:1512:ARG:HH12	2:B:1610:ASP:HA	1.80	0.46
2:D:1066:PHE:CE1	2:D:1082:VAL:HG11	2.51	0.46
2:D:1152:GLN:O	2:D:1155:LYS:HB2	2.16	0.46
2:D:1275:VAL:HG13	2:D:1276:PHE:CD1	2.51	0.46
2:D:1492:PHE:N	2:D:1492:PHE:CD1	2.63	0.46
2:D:974:THR:HB	2:D:1349:HIS:HD2	1.80	0.46
3:E:107:ALA:O	3:E:130:ARG:NH1	2.49	0.46
2:B:1384:MET:HE3	2:B:1411:PHE:CZ	2.50	0.46
2:B:1541:VAL:HG13	2:B:1570:LYS:NZ	2.30	0.46
2:B:878:THR:HG21	2:B:1624:LYS:NZ	2.30	0.46
1:C:484:GLU:HA	1:C:487:ILE:CD1	2.46	0.46
3:F:136:GLU:CB	3:F:159:LYS:HE2	2.39	0.46
1:A:303:SER:OG	1:A:306:VAL:HG12	2.16	0.46
2:B:1243:LEU:HA	2:B:1243:LEU:HD23	1.50	0.46
2:B:1311:ILE:HD11	2:B:1320:ARG:HD2	1.98	0.46
1:C:599:ASP:O	1:C:601:GLY:N	2.48	0.46
2:D:1207:LEU:HA	2:D:1207:LEU:HD12	1.52	0.46
2:D:1469:VAL:HG13	2:D:1472:ILE:HG22	1.97	0.46
2:D:764:ARG:HH12	2:D:923:ASP:CG	2.12	0.46
1:A:167:ILE:HD12	1:A:193:TRP:CE2	2.51	0.46
1:A:273:PHE:CE1	1:A:326:VAL:HG12	2.51	0.46
2:B:1136:ASN:CA	2:B:1139:LYS:HZ1	2.20	0.46
2:B:1189:VAL:CG1	2:B:1213:THR:HG21	2.43	0.46
2:B:1268:SER:O	2:B:1272:THR:HG23	2.16	0.46
1:C:429:GLN:C	1:C:431:LEU:H	2.20	0.46
1:C:631:SER:O	1:C:641:ASP:OD2	2.33	0.46
2:D:1413:PRO:HD2	2:D:1441:ARG:HD2	1.97	0.46
2:D:841:ARG:NH1	2:D:902:PRO:O	2.49	0.46
1:C:175:VAL:O	2:D:979:ARG:NH1	2.48	0.46
3:F:175:ASP:HB3	3:F:187:SER:OG	2.16	0.46
1:A:104:LYS:HG3	1:A:105:PHE:H	1.81	0.46
1:A:492:TYR:CZ	1:A:504:GLY:HA3	2.51	0.46
2:B:999:ARG:NH1	2:B:1262:TYR:CZ	2.84	0.46
2:D:1025:VAL:HG23	2:D:1026:HIS:N	2.30	0.46
2:D:1472:ILE:HD11	2:D:1494:HIS:CD2	2.51	0.46
3:F:245:TYR:CD1	3:F:245:TYR:N	2.84	0.46
2:B:1312:HIS:CE1	3:E:237:GLN:HE22	2.34	0.46
2:B:977:GLU:HG2	2:B:1347:MET:HG2	1.98	0.46
2:D:1400:MET:HE1	2:D:1448:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1492:PHE:CE2	2:D:1500:GLY:HA3	2.51	0.46
2:D:979:ARG:NH1	2:D:979:ARG:HG3	2.31	0.46
3:E:131:PRO:HA	3:E:132:GLY:HA2	1.45	0.46
3:F:149:LEU:HD12	3:F:149:LEU:HA	1.48	0.46
1:A:478:ARG:NH1	1:A:479:MET:O	2.49	0.45
1:A:467:PRO:HA	1:A:521:ILE:HG22	1.97	0.45
1:A:67:LEU:CD2	1:A:68:VAL:H	2.29	0.45
2:B:1264:GLY:H	2:B:1272:THR:HG21	1.81	0.45
2:B:1478:LYS:HA	2:B:1489:CYS:O	2.16	0.45
2:B:1594:LEU:HB3	2:B:1596:LEU:HG	1.98	0.45
2:B:949:PRO:HG3	2:B:958:GLN:NE2	2.30	0.45
2:D:1190:ALA:HA	2:D:1220:TRP:CZ3	2.34	0.45
3:E:207:SER:OG	3:E:208:GLY:N	2.47	0.45
2:B:1524:ASP:HA	2:B:1527:VAL:CG2	2.46	0.45
1:C:135:ASP:OD1	1:C:135:ASP:N	2.47	0.45
2:D:1215:LYS:HD2	2:D:1216:ASP:N	2.31	0.45
3:E:156:GLU:C	3:E:156:GLU:OE2	2.55	0.45
2:B:1206:LEU:C	2:B:1206:LEU:HD12	2.36	0.45
1:C:148:ARG:NH2	2:D:773:TRP:CE3	2.84	0.45
3:F:163:CYS:HB2	3:F:180:ILE:O	2.16	0.45
2:B:1014:ASN:ND2	2:B:1055:GLN:HG3	2.31	0.45
2:B:1326:GLU:OE1	2:B:1326:GLU:N	2.49	0.45
2:B:1532:ARG:HH21	2:B:1629:GLU:CD	2.20	0.45
2:B:982:LEU:HG	2:B:1311:ILE:HD13	1.98	0.45
1:C:466:ARG:H	1:C:469:GLU:CD	2.19	0.45
2:D:1317:SER:OG	2:D:1320:ARG:NH2	2.50	0.45
2:D:1397:ASP:OD1	2:D:1453:HIS:N	2.49	0.45
3:E:245:TYR:CD1	3:E:246:ARG:HB2	2.51	0.45
3:F:197:PHE:CB	3:F:221:ARG:NH1	2.79	0.45
1:A:169:ASN:HB2	1:A:170:PRO:CD	2.46	0.45
1:A:240:GLU:HB3	1:A:242:PHE:CE1	2.52	0.45
1:A:25:MET:HE2	1:A:47:HIS:HD2	1.82	0.45
1:A:35:ARG:NH2	1:A:498:GLY:HA3	2.32	0.45
1:A:575:PRO:HA	1:A:579:GLN:OE1	2.17	0.45
2:B:1209:LYS:O	2:B:1213:THR:OG1	2.18	0.45
2:B:1367:ILE:HD12	2:B:1385:ILE:O	2.17	0.45
2:B:1429:ILE:HD13	2:B:1445:ILE:O	2.17	0.45
2:B:772:LEU:O	2:B:774:ASN:N	2.49	0.45
1:C:427:LYS:HE3	1:C:427:LYS:HB3	1.74	0.45
1:C:573:ARG:NE	1:C:579:GLN:HE21	2.15	0.45
2:D:1554:LEU:CD1	2:D:1591:ARG:CZ	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:SER:H	1:A:195:ILE:HD11	1.81	0.45
2:B:1407:MET:HE1	2:B:1463:VAL:CG1	2.47	0.45
2:D:1105:LYS:HB2	2:D:1162:VAL:HG21	1.97	0.45
2:D:1108:ILE:HD12	2:D:1168:SER:CB	2.46	0.45
3:E:203:PHE:CD2	3:E:205:LEU:HB3	2.52	0.45
2:B:1308:THR:O	3:E:238:GLY:HA2	2.17	0.45
3:F:198:GLY:HA3	3:F:218:PRO:HB3	1.99	0.45
1:A:93:ASN:ND2	1:A:95:GLU:HG2	2.31	0.45
2:B:1534:ASP:OD1	2:B:1535:LYS:N	2.50	0.45
2:D:1554:LEU:HD12	2:D:1555:SER:H	1.81	0.45
2:D:1577:GLN:N	2:D:1577:GLN:OE1	2.49	0.45
3:E:132:GLY:O	3:E:161:LYS:HB2	2.16	0.45
1:A:76:LEU:HG	1:A:82:HIS:CA	2.46	0.45
2:B:1300:LEU:HD23	2:B:1324:THR:CG2	2.39	0.45
2:B:1544:VAL:HB	2:B:1605:TRP:HB3	1.97	0.45
2:B:949:PRO:HD3	2:B:958:GLN:HE22	1.81	0.45
2:D:1542:ASP:O	2:D:1570:LYS:HE2	2.17	0.45
2:D:1544:VAL:HG22	2:D:1605:TRP:CB	2.46	0.45
2:D:781:PRO:HA	2:D:782:PRO:HD3	1.78	0.45
1:A:293:ILE:HG13	1:A:293:ILE:O	2.17	0.45
1:A:595:LEU:HD11	2:B:791:MET:HE1	1.98	0.45
2:B:1117:VAL:CA	2:B:1144:THR:HG21	2.45	0.45
2:B:1180:TYR:CZ	2:B:1189:VAL:HG22	2.52	0.45
2:B:1245:ASP:O	2:B:1249:VAL:HG23	2.17	0.45
2:B:1403:LEU:HB2	2:B:1446:ILE:O	2.17	0.45
2:B:1489:CYS:SG	2:B:1491:ARG:NH1	2.90	0.45
1:C:225:LYS:HG2	1:C:226:GLU:N	2.31	0.45
1:C:569:GLN:N	1:C:582:THR:OG1	2.50	0.45
2:D:1138:GLU:OE2	2:D:1185:ARG:HD2	2.17	0.45
1:C:579:GLN:H	2:D:795:LEU:HD11	1.82	0.45
2:D:841:ARG:NH1	2:D:903:LEU:C	2.70	0.45
2:D:983:GLN:HB3	2:D:1341:THR:HG1	1.81	0.45
3:E:226:PRO:CD	3:E:276:TRP:HH2	2.29	0.45
1:A:462:ARG:NH2	1:A:463:THR:C	2.69	0.45
1:A:569:GLN:N	1:A:582:THR:OG1	2.49	0.45
1:A:70:SER:OG	1:A:88:PHE:HB2	2.17	0.45
2:B:1053:TYR:CD2	2:B:1086:PHE:HE2	2.35	0.45
2:B:1202:LEU:CB	2:B:1206:LEU:HD11	2.46	0.45
2:B:1207:LEU:HD12	2:B:1207:LEU:HA	1.42	0.45
2:B:1415:THR:HG23	2:B:1416:ASP:N	2.32	0.45
2:B:1549:LEU:O	2:B:1599:LYS:N	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:ASP:OD1	1:C:480:ASP:N	2.50	0.45
2:D:1497:LYS:O	2:D:1500:GLY:N	2.50	0.45
2:D:1558:PHE:N	2:D:1558:PHE:CD1	2.85	0.45
2:D:1550:VAL:CG2	2:D:1581:GLN:HE22	2.29	0.45
2:D:1564:ALA:HB2	2:D:1581:GLN:NE2	2.31	0.45
2:D:810:SER:O	2:D:814:GLY:N	2.46	0.45
3:E:195:LYS:CE	3:E:197:PHE:HE1	2.27	0.45
3:F:156:GLU:OE2	3:F:158:CYS:O	2.35	0.45
1:A:125:LEU:HD12	1:A:125:LEU:N	2.31	0.44
2:B:1577:GLN:O	2:B:1580:GLN:NE2	2.50	0.44
2:B:1662:PRO:O	2:B:1663:ASN:HB2	2.16	0.44
2:B:945:ARG:HD2	2:B:960:GLU:OE2	2.16	0.44
1:C:76:LEU:HD13	1:C:82:HIS:O	2.17	0.44
2:D:1536:ALA:HB2	2:D:1605:TRP:CZ3	2.52	0.44
3:E:226:PRO:N	3:E:276:TRP:CH2	2.78	0.44
3:F:246:ARG:NH1	3:F:246:ARG:HG2	2.29	0.44
1:A:167:ILE:CG1	1:A:176:LYS:HB3	2.47	0.44
1:A:185:GLN:NE2	3:E:245:TYR:CE1	2.86	0.44
2:B:1418:LEU:HA	2:B:1421:LEU:HD22	2.00	0.44
2:B:1494:HIS:ND1	2:B:1497:LYS:CB	2.79	0.44
1:C:106:VAL:HG12	1:C:123:VAL:HG23	1.99	0.44
2:D:999:ARG:NH1	2:D:999:ARG:HG3	2.31	0.44
1:A:646:PHE:H	1:A:654:THR:CG2	2.30	0.44
2:B:1060:ARG:HG3	2:B:1060:ARG:NH1	2.30	0.44
2:B:1086:PHE:O	2:B:1090:VAL:HG13	2.16	0.44
2:B:1561:TYR:HB3	2:B:1563:MET:CE	2.47	0.44
2:B:1576:VAL:HB	2:B:1580:GLN:NE2	2.33	0.44
2:B:1607:LEU:C	2:B:1610:ASP:OD1	2.56	0.44
1:C:324:LEU:HB2	1:C:346:ILE:HG13	1.99	0.44
1:C:389:VAL:HG12	1:C:426:THR:HG22	1.98	0.44
2:D:1328:GLU:OE1	2:D:1330:PHE:HD2	1.99	0.44
2:D:1365:VAL:HG13	2:D:1386:LEU:HD11	1.99	0.44
2:D:812:LYS:HD2	2:D:812:LYS:HA	1.69	0.44
3:E:231:ILE:HD11	3:E:234:GLY:HA3	1.98	0.44
3:E:236:ILE:HB	3:E:239:GLU:HG2	1.99	0.44
1:A:386:ARG:HH11	1:A:386:ARG:HG3	1.82	0.44
2:B:1076:THR:H	2:B:1076:THR:HG23	1.39	0.44
1:C:186:LEU:HA	1:C:186:LEU:HD13	1.69	0.44
2:D:994:ALA:HB1	2:D:1027:TYR:OH	2.18	0.44
2:D:1492:PHE:CZ	2:D:1499:ASP:O	2.71	0.44
2:D:911:GLU:HA	2:D:925:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1015:MET:CG	2:B:1056:GLN:NE2	2.80	0.44
2:B:948:ASP:OD2	2:B:951:ARG:NE	2.51	0.44
1:C:496:ASN:C	1:C:498:GLY:N	2.70	0.44
2:D:1153:GLU:N	2:D:1153:GLU:OE1	2.50	0.44
2:D:1651:ALA:O	2:D:1655:SER:HB3	2.18	0.44
2:B:1312:HIS:CA	2:B:1313:TRP:CE3	3.00	0.44
2:B:1407:MET:CE	2:B:1463:VAL:HB	2.48	0.44
1:A:268:THR:HB	2:B:1447:TYR:OH	2.18	0.44
2:B:951:ARG:HH21	2:B:1339:GLN:CG	2.17	0.44
1:C:398:GLN:CD	1:C:427:LYS:HE2	2.38	0.44
1:C:561:GLY:N	2:D:813:LYS:CE	2.80	0.44
2:D:1067:ALA:CA	2:D:1078:LEU:HD21	2.47	0.44
2:D:1190:ALA:CA	2:D:1220:TRP:HZ3	2.22	0.44
1:A:169:ASN:ND2	1:A:173:ILE:HB	2.33	0.44
2:B:992:GLU:HA	2:B:992:GLU:OE1	2.18	0.44
1:C:479:MET:HB3	1:C:479:MET:HE2	1.67	0.44
2:D:997:ALA:O	2:D:1037:PHE:HE2	2.00	0.44
2:D:833:LEU:HG	2:D:835:LEU:HD13	1.98	0.44
3:E:165:ASN:OD1	3:E:166:PRO:HD2	2.18	0.44
1:A:161:ARG:HH22	1:A:212:ASN:ND2	2.16	0.44
1:A:479:MET:CG	1:A:484:GLU:HG3	2.48	0.44
1:A:465:LEU:HD11	1:A:521:ILE:HD13	1.99	0.44
2:B:1136:ASN:HA	2:B:1139:LYS:HE3	1.99	0.44
2:B:1230:VAL:HG12	2:B:1275:VAL:CG2	2.47	0.44
2:B:1312:HIS:HA	2:B:1313:TRP:HE3	1.81	0.44
2:B:1363:LEU:HD21	2:B:1477:VAL:HG12	1.98	0.44
2:B:879:LYS:HZ1	2:B:1521:GLN:HE22	1.65	0.44
2:B:1652:PHE:HE1	2:B:1656:MET:HE3	1.82	0.44
1:C:55:VAL:HA	1:C:111:THR:O	2.18	0.44
1:C:291:ILE:HA	1:C:292:PRO:HD3	1.70	0.44
1:C:385:TYR:CD2	1:C:403:GLY:HA2	2.52	0.44
1:C:496:ASN:CB	1:C:501:LEU:HG	2.34	0.44
1:C:67:LEU:HD12	1:C:68:VAL:N	2.27	0.44
2:D:793:ILE:HD12	2:D:794:PHE:H	1.83	0.44
2:D:947:LEU:HD12	2:D:947:LEU:H	1.80	0.44
3:E:146:LEU:HD12	3:E:150:LYS:H	1.83	0.44
3:E:282:GLU:OE2	3:E:284:ARG:CG	2.66	0.44
1:A:351:SER:OG	1:A:353:TYR:O	2.36	0.44
1:A:242:PHE:HD2	1:A:379:PRO:HG2	1.81	0.44
2:B:1077:TRP:CE2	2:B:1130:ILE:CD1	3.00	0.44
2:B:1444:LEU:HG	2:B:1445:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1554:LEU:HD13	2:B:1591:ARG:CZ	2.48	0.44
1:C:106:VAL:HG12	1:C:123:VAL:CG2	2.48	0.44
1:C:26:TYR:HB2	1:C:649:SER:HB3	1.99	0.44
2:D:1061:GLN:O	2:D:1062:PRO:C	2.55	0.44
2:D:1300:LEU:O	2:D:1300:LEU:HD12	2.18	0.44
2:D:771:TRP:CE3	2:D:772:LEU:HB2	2.53	0.44
1:C:198:LEU:HD13	2:D:975:GLU:OE2	2.18	0.44
3:F:110:LYS:O	3:F:114:ILE:HG13	2.18	0.44
2:B:1479:VAL:HG12	2:B:1480:TYR:N	2.33	0.43
2:B:838:SER:HB2	2:B:932:VAL:CG2	2.47	0.43
1:C:169:ASN:HB2	1:C:170:PRO:CD	2.48	0.43
1:C:420:LEU:HD11	1:C:422:ILE:HD11	2.00	0.43
2:D:1063:SER:HA	2:D:1106:TRP:CZ3	2.53	0.43
2:D:1641:GLU:OE1	2:D:1641:GLU:N	2.50	0.43
3:E:212:GLN:HG3	3:E:213:TRP:N	2.33	0.43
1:A:270:PHE:CE1	1:A:290:ARG:HD3	2.53	0.43
2:B:1264:GLY:H	2:B:1272:THR:CG2	2.31	0.43
2:B:1634:GLU:CD	2:B:1634:GLU:C	2.77	0.43
2:B:943:ALA:O	2:B:1343:SER:HA	2.19	0.43
2:D:1078:LEU:HD12	2:D:1078:LEU:C	2.38	0.43
2:D:1554:LEU:HD12	2:D:1554:LEU:HA	1.48	0.43
2:D:813:LYS:HA	2:D:813:LYS:HD2	1.80	0.43
1:C:563:LEU:HB3	2:D:818:ALA:HB2	1.98	0.43
1:A:77:THR:OG1	1:A:80:THR:HG23	2.17	0.43
2:B:1077:TRP:NE1	2:B:1146:PHE:CZ	2.86	0.43
2:B:1358:CYS:CB	2:B:1361:PHE:O	2.66	0.43
2:B:1368:LYS:O	2:B:1385:ILE:HG22	2.18	0.43
2:B:1429:ILE:HD11	2:B:1433:GLU:CB	2.48	0.43
2:B:1558:PHE:HD1	2:B:1587:PRO:HA	1.81	0.43
1:C:60:HIS:NE2	1:C:109:GLN:HB2	2.33	0.43
1:C:332:LEU:C	1:C:334:SER:H	2.21	0.43
1:C:77:THR:H	1:C:80:THR:HG22	1.83	0.43
2:D:942:VAL:HG21	2:D:1346:THR:HG23	2.00	0.43
2:D:1498:GLU:C	2:D:1500:GLY:N	2.64	0.43
2:D:997:ALA:H	2:D:1036:LYS:CE	2.30	0.43
1:A:552:TRP:CH2	1:A:554:ASP:HB2	2.54	0.43
2:B:1238:LEU:HD11	2:B:1277:GLN:NE2	2.25	0.43
2:B:1465:GLN:HG2	2:B:1465:GLN:O	2.18	0.43
2:B:1503:ASN:OD1	2:B:1515:GLU:HG2	2.18	0.43
2:B:1506:CYS:HA	2:B:1511:CYS:HA	2.00	0.43
1:C:90:ILE:HG13	1:C:90:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1303:ARG:NH1	3:F:241:ASP:OD1	2.52	0.43
1:A:130:LEU:HD13	1:A:210:TYR:OH	2.18	0.43
2:B:792:ASN:ND2	2:B:792:ASN:O	2.26	0.43
2:B:884:GLN:HG3	2:B:885:THR:N	2.33	0.43
1:C:263:LYS:HE3	1:C:263:LYS:HB2	1.63	0.43
2:D:1317:SER:OG	2:D:1318:LEU:N	2.51	0.43
2:D:1515:GLU:HA	2:D:1589:LYS:HZ3	1.84	0.43
3:E:170:ARG:C	3:E:171:ASN:OD1	2.56	0.43
3:F:106:SER:HB3	3:F:158:CYS:HB2	1.99	0.43
2:B:1300:LEU:CD1	2:B:1300:LEU:O	2.63	0.43
2:B:1348:TYR:HD1	2:B:1349:HIS:C	2.22	0.43
2:B:1360:LYS:HG3	2:B:1487:GLU:HB3	2.01	0.43
2:B:1502:LEU:HA	2:B:1502:LEU:HD12	1.79	0.43
2:B:1559:ASP:OD1	2:B:1586:SER:N	2.51	0.43
2:B:932:VAL:HG12	2:B:933:PRO:HD2	2.00	0.43
1:C:599:ASP:C	1:C:601:GLY:N	2.70	0.43
2:D:1214:ALA:HB2	2:D:1220:TRP:NE1	2.31	0.43
2:D:756:ILE:HG12	2:D:761:ILE:HD11	2.00	0.43
2:D:856:GLN:HG2	2:D:857:ASN:H	1.83	0.43
2:D:899:VAL:HG23	2:D:1473:GLN:NE2	2.32	0.43
2:D:971:VAL:HG12	2:D:1349:HIS:CB	2.48	0.43
3:E:223:ILE:HD11	3:E:269:VAL:CG2	2.42	0.43
3:E:226:PRO:O	3:E:276:TRP:CH2	2.71	0.43
3:F:116:GLN:NE2	3:F:119:PHE:HE1	2.15	0.43
2:B:1083:VAL:HG13	2:B:1100:LEU:HD11	2.00	0.43
2:B:1214:ALA:HB2	2:B:1220:TRP:CD2	2.54	0.43
2:B:1360:LYS:HA	2:B:1360:LYS:HE2	2.01	0.43
2:B:831:ILE:CD1	2:B:925:VAL:HG23	2.48	0.43
1:C:58:THR:OG1	1:C:60:HIS:HE1	2.02	0.43
2:D:1015:MET:HA	2:D:1015:MET:CE	2.49	0.43
2:D:1536:ALA:HB3	2:D:1652:PHE:HZ	1.83	0.43
3:E:197:PHE:HB2	3:E:219:GLU:HG2	2.01	0.43
1:A:166:ASN:HD21	1:A:174:PRO:CB	2.31	0.43
1:A:27:SER:OG	1:A:45:GLU:HB2	2.19	0.43
1:A:471:LEU:CB	1:A:521:ILE:HD11	2.43	0.43
1:A:634:ASP:OD1	1:A:637:GLY:N	2.51	0.43
1:A:99:GLU:HA	1:A:100:LYS:HA	1.72	0.43
1:A:338:MET:HE2	2:B:1485:LEU:HB2	2.00	0.43
2:B:753:GLU:O	2:B:755:ILE:HG23	2.18	0.43
1:C:120:VAL:HB	1:C:656:GLN:NE2	2.34	0.43
2:D:1207:LEU:O	2:D:1210:PHE:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1464:HIS:HB2	2:D:1466:TYR:CZ	2.53	0.43
2:D:1652:PHE:CE1	2:D:1656:MET:HE2	2.53	0.43
3:E:146:LEU:HG	3:E:150:LYS:CB	2.40	0.43
3:E:193:GLY:O	3:E:223:ILE:HG23	2.19	0.43
3:E:236:ILE:CG2	3:E:239:GLU:HG2	2.49	0.43
1:A:181:SER:H	3:E:246:ARG:NE	2.17	0.43
1:A:30:THR:HG22	1:A:645:THR:HG1	1.84	0.43
2:B:1060:ARG:NH1	2:B:1099:VAL:HG13	2.34	0.43
2:B:1154:ALA:O	2:B:1157:ILE:HG13	2.19	0.43
2:B:1206:LEU:HD12	2:B:1207:LEU:N	2.34	0.43
2:B:1425:VAL:O	2:B:1426:ASP:HB2	2.18	0.43
2:B:807:VAL:HG22	2:B:817:VAL:HG22	2.01	0.43
2:B:949:PRO:CG	2:B:958:GLN:HE22	2.31	0.43
1:C:205:LYS:HD2	1:C:221:GLU:HG2	2.01	0.43
2:D:1507:ARG:HG3	2:D:1507:ARG:O	2.19	0.43
2:D:759:GLU:O	2:D:760:ASN:ND2	2.52	0.43
2:D:813:LYS:O	2:D:813:LYS:HG3	2.18	0.43
1:C:175:VAL:HB	2:D:979:ARG:NH2	2.34	0.43
3:E:224:TYR:CD1	3:E:224:TYR:N	2.87	0.43
3:F:245:TYR:H	3:F:245:TYR:HD1	1.65	0.43
1:A:26:TYR:CD1	1:A:26:TYR:N	2.87	0.43
1:A:550:SER:OG	1:A:631:SER:N	2.52	0.43
2:B:1576:VAL:HG12	2:B:1582:ARG:HH21	1.82	0.43
1:C:312:GLN:H	1:C:312:GLN:CD	2.16	0.43
2:D:1237:LEU:HD22	2:D:1256:LEU:CD2	2.48	0.43
2:D:962:ILE:HG12	2:D:1330:PHE:CE1	2.53	0.43
2:D:1496:GLU:HG2	2:D:1497:LYS:N	2.34	0.43
2:D:872:PHE:HE1	2:D:902:PRO:HB3	1.84	0.43
3:E:120:PRO:HG2	3:E:123:THR:CG2	2.49	0.43
1:A:161:ARG:O	1:A:181:SER:HA	2.19	0.42
1:A:490:TYR:OH	1:A:508:ARG:HD2	2.19	0.42
2:B:781:PRO:HA	2:B:782:PRO:HD3	1.87	0.42
1:C:66:LYS:HD3	3:E:147:GLN:HG2	2.00	0.42
1:C:70:SER:OG	1:C:88:PHE:HB2	2.19	0.42
2:D:1023:ILE:HD12	2:D:1023:ILE:HA	1.91	0.42
2:D:1310:ARG:CD	2:D:1312:HIS:NE2	2.82	0.42
2:D:1400:MET:HE1	2:D:1447:TYR:HB3	2.01	0.42
2:D:1400:MET:HE2	2:D:1447:TYR:HB3	2.00	0.42
2:D:851:LEU:HD23	2:D:862:VAL:HG21	2.01	0.42
3:E:125:VAL:HG23	3:E:143:LEU:HG	2.01	0.42
3:E:132:GLY:HA2	3:E:161:LYS:HZ3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:THR:CG2	1:A:116:VAL:HG23	2.42	0.42
1:A:277:ASP:O	1:A:280:GLN:HG2	2.18	0.42
1:A:420:LEU:O	1:A:443:ALA:N	2.48	0.42
1:A:637:GLY:O	1:A:641:ASP:HB2	2.19	0.42
2:B:1115:ASP:O	2:B:1175:PHE:CG	2.71	0.42
2:B:1118:PHE:N	2:B:1144:THR:CG2	2.79	0.42
2:B:1429:ILE:HD11	2:B:1433:GLU:CG	2.48	0.42
2:B:1559:ASP:OD2	2:B:1561:TYR:CZ	2.71	0.42
2:B:783:LYS:HE3	3:F:197:PHE:CD1	2.55	0.42
1:C:449:VAL:HG23	1:C:449:VAL:O	2.19	0.42
2:D:1208:ASN:O	2:D:1211:LEU:HG	2.18	0.42
2:D:1225:LYS:HE3	2:D:1227:LEU:CD1	2.48	0.42
2:D:1659:PHE:CE2	2:D:1662:PRO:HD3	2.49	0.42
2:D:874:SER:HB3	2:D:900:ILE:HG22	2.01	0.42
2:D:916:VAL:HG22	2:D:921:ILE:O	2.19	0.42
3:F:97:SER:OG	3:F:98:CYS:O	2.36	0.42
1:A:366:PRO:HD2	1:A:455:TYR:CZ	2.54	0.42
1:A:46:ALA:HB3	1:A:76:LEU:HD11	2.01	0.42
1:A:532:VAL:HG11	1:A:644:LEU:HD12	2.01	0.42
2:B:1128:GLU:HG3	2:B:1267:GLY:HA2	2.00	0.42
2:B:982:LEU:HD22	2:B:1296:VAL:HG11	2.00	0.42
2:B:1303:ARG:CZ	2:B:1307:ILE:HG12	2.49	0.42
2:B:1347:MET:HE3	2:B:1347:MET:HB2	1.81	0.42
1:C:641:ASP:OD1	1:C:642:ALA:N	2.53	0.42
2:D:1047:GLU:HG3	2:D:1051:LYS:HZ2	1.84	0.42
2:D:1061:GLN:OE1	2:D:1061:GLN:HA	2.20	0.42
2:D:1494:HIS:ND1	2:D:1496:GLU:OE1	2.52	0.42
2:D:1507:ARG:NH1	2:D:1613:GLY:HA2	2.34	0.42
2:D:752:ASP:CG	2:D:753:GLU:H	2.23	0.42
2:D:756:ILE:HD11	3:F:134:ARG:HH12	1.82	0.42
2:D:759:GLU:O	2:D:760:ASN:CG	2.57	0.42
2:D:839:VAL:HG22	2:D:929:LEU:CD1	2.49	0.42
1:A:444:LEU:HG	1:A:445:PRO:HD2	2.00	0.42
2:B:1010:CYS:O	2:B:1012:GLU:N	2.53	0.42
2:B:1408:MET:HG3	2:B:1411:PHE:HB2	2.01	0.42
2:B:896:VAL:HA	2:B:897:PRO:HD3	1.76	0.42
1:C:488:ARG:O	1:C:508:ARG:N	2.48	0.42
1:C:495:MET:CE	1:C:625:ILE:HD11	2.49	0.42
2:D:1258:GLU:OE1	2:D:1258:GLU:N	2.49	0.42
3:F:131:PRO:HA	3:F:132:GLY:HA2	1.35	0.42
1:A:120:VAL:HG11	2:B:1039:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:TYR:CZ	1:A:191:LEU:HG	2.54	0.42
1:A:385:TYR:C	1:A:386:ARG:HG2	2.40	0.42
2:B:1117:VAL:HA	2:B:1144:THR:CG2	2.47	0.42
1:C:508:ARG:HG2	1:C:509:GLU:N	2.34	0.42
2:D:1368:LYS:O	2:D:1385:ILE:HG13	2.19	0.42
2:D:1501:LYS:HD2	2:D:1557:ASP:OD2	2.19	0.42
2:D:1603:LEU:HD22	2:D:1649:LEU:CD1	2.49	0.42
2:D:948:ASP:OD2	2:D:951:ARG:CZ	2.67	0.42
2:D:959:LYS:HE3	2:D:961:ASP:OD1	2.20	0.42
3:E:157:PHE:N	3:E:157:PHE:CD1	2.84	0.42
3:E:258:THR:O	3:E:283:CYS:HA	2.19	0.42
1:A:354:GLN:O	1:A:376:VAL:HA	2.18	0.42
1:A:428:LYS:O	1:A:431:LEU:HG	2.20	0.42
1:C:65:LYS:HB3	1:C:65:LYS:HE3	1.48	0.42
2:D:1118:PHE:HD2	2:D:1144:THR:CG2	2.32	0.42
2:D:985:THR:HB	2:D:1339:GLN:O	2.19	0.42
2:D:1544:VAL:CG2	2:D:1570:LYS:HD3	2.46	0.42
3:E:143:LEU:CD1	3:E:151:TRP:CE3	3.03	0.42
1:A:43:VAL:HG21	1:A:493:LEU:HD23	2.00	0.42
2:B:1167:GLY:O	2:B:1171:LYS:HB2	2.20	0.42
1:C:422:ILE:HD12	1:C:422:ILE:HG23	1.67	0.42
1:C:529:PHE:CZ	1:C:553:VAL:HG11	2.55	0.42
2:D:1237:LEU:HD22	2:D:1256:LEU:HD21	2.02	0.42
2:D:1470:GLU:C	2:D:1471:LEU:HD22	2.40	0.42
2:D:1562:ILE:CG1	2:D:1562:ILE:O	2.67	0.42
1:A:28:ILE:HA	1:A:28:ILE:HD12	1.75	0.42
1:A:253:VAL:CG1	1:A:300:VAL:HG13	2.50	0.42
1:A:232:PHE:CE1	1:A:339:VAL:HG23	2.55	0.42
1:A:46:ALA:O	1:A:82:HIS:CG	2.72	0.42
2:B:1141:MET:HG3	2:B:1183:LEU:HD11	2.02	0.42
2:B:1084:LYS:HE3	2:B:1149:ILE:CD1	2.49	0.42
1:C:391:VAL:HG13	1:C:397:VAL:HG11	2.02	0.42
1:C:35:ARG:NH1	1:C:40:GLU:OE2	2.37	0.42
2:D:1300:LEU:HD11	2:D:1303:ARG:HB2	2.00	0.42
2:D:1403:LEU:HB2	2:D:1446:ILE:O	2.19	0.42
3:E:157:PHE:H	3:E:157:PHE:HD1	1.65	0.42
3:F:245:TYR:O	3:F:246:ARG:HB2	2.19	0.42
1:A:37:GLU:OE2	1:A:127:SER:HB3	2.19	0.42
1:A:88:PHE:HE2	1:A:90:ILE:HD11	1.85	0.42
2:B:1149:ILE:HA	2:B:1152:GLN:OE1	2.19	0.42
2:B:1144:THR:HB	2:B:1176:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1554:LEU:HD13	2:B:1591:ARG:NH2	2.34	0.42
1:C:473:VAL:HG11	1:C:517:LEU:HD23	2.01	0.42
1:C:102:ARG:NH2	2:D:1035:GLU:HB3	2.35	0.42
2:D:1225:LYS:HE2	2:D:1228:TYR:CZ	2.55	0.42
2:D:1508:ASP:CG	2:D:1509:GLU:N	2.70	0.42
2:D:877:THR:HG23	2:D:880:ARG:H	1.85	0.42
3:E:135:ARG:CZ	3:E:137:PRO:HA	2.49	0.42
3:E:237:GLN:HB3	3:E:250:THR:CG2	2.42	0.42
3:F:156:GLU:O	3:F:159:LYS:HE3	2.19	0.42
1:A:28:ILE:HD11	1:A:42:MET:HG3	2.01	0.42
1:A:449:VAL:O	1:A:449:VAL:HG23	2.20	0.42
2:B:981:LEU:HD11	2:B:1343:SER:OG	2.19	0.42
2:B:1502:LEU:HD11	2:B:1515:GLU:HG3	2.02	0.42
2:B:960:GLU:O	2:B:960:GLU:HG3	2.20	0.42
1:C:324:LEU:HB2	1:C:346:ILE:HD11	2.02	0.42
1:C:659:GLU:N	1:C:659:GLU:CD	2.72	0.42
2:D:1313:TRP:HE3	2:D:1318:LEU:HD21	1.83	0.42
2:D:962:ILE:HD11	2:D:1330:PHE:CE2	2.54	0.42
2:D:1408:MET:HB2	2:D:1411:PHE:CD1	2.55	0.42
2:D:1544:VAL:HG23	2:D:1570:LYS:CD	2.45	0.42
3:E:246:ARG:CZ	3:E:266:TYR:HB2	2.50	0.42
3:F:109:LEU:HD22	3:F:125:VAL:CG1	2.50	0.42
3:F:113:TYR:CA	3:F:116:GLN:HG2	2.47	0.42
1:A:471:LEU:C	1:A:471:LEU:HD12	2.41	0.41
2:B:911:GLU:HA	2:B:925:VAL:O	2.19	0.41
1:C:293:ILE:HG13	1:C:293:ILE:O	2.20	0.41
1:C:55:VAL:HG23	1:C:74:THR:HG22	2.02	0.41
2:D:1027:TYR:CE2	2:D:1031:THR:HG21	2.54	0.41
2:D:1471:LEU:HD13	2:D:1471:LEU:HA	1.58	0.41
2:D:1479:VAL:O	2:D:1480:TYR:HB3	2.19	0.41
2:D:948:ASP:OD2	2:D:951:ARG:NH2	2.53	0.41
3:E:243:TYR:CZ	3:E:249:VAL:HG12	2.55	0.41
2:D:1310:ARG:HH21	3:F:235:ILE:CG1	2.33	0.41
2:B:1111:LYS:HA	2:B:1111:LYS:HD2	1.64	0.41
2:B:1549:LEU:HD11	2:B:1551:LYS:O	2.20	0.41
2:B:752:ASP:HB3	2:B:753:GLU:H	1.54	0.41
1:C:244:TYR:CE2	1:C:246:TYR:HB2	2.56	0.41
2:D:1077:TRP:CE2	2:D:1130:ILE:HG22	2.55	0.41
2:D:1216:ASP:OD1	2:D:1216:ASP:C	2.57	0.41
2:D:1131:GLY:C	2:D:1228:TYR:HE1	2.22	0.41
2:D:1220:TRP:CE3	2:D:1236:ALA:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:951:ARG:HH22	2:D:1339:GLN:HB3	1.84	0.41
3:F:103:ARG:O	3:F:104:LEU:HD23	2.20	0.41
3:F:206:ILE:O	3:F:206:ILE:HG13	2.20	0.41
3:F:207:SER:OG	3:F:208:GLY:N	2.51	0.41
1:A:65:LYS:HB2	1:A:65:LYS:HE3	1.69	0.41
1:A:67:LEU:HD23	1:A:68:VAL:H	1.85	0.41
2:B:1023:ILE:HG13	2:B:1276:PHE:HB2	2.03	0.41
2:B:1348:TYR:HE1	2:B:1350:ALA:HB2	1.85	0.41
2:B:1505:LEU:HD23	2:B:1621:ILE:HG21	2.03	0.41
2:B:1592:GLU:O	2:B:1595:LYS:HD2	2.20	0.41
3:E:224:TYR:CD2	3:E:242:HIS:CD2	3.08	0.41
1:A:185:GLN:NE2	3:E:245:TYR:HE1	2.18	0.41
1:A:475:PHE:HB2	1:A:515:VAL:HG23	2.02	0.41
1:A:535:TYR:CZ	1:A:547:VAL:HB	2.56	0.41
2:B:875:LEU:HD23	2:B:875:LEU:HA	1.74	0.41
1:C:230:PRO:CB	1:C:339:VAL:HG22	2.50	0.41
2:D:1136:ASN:O	2:D:1137:ASN:HB2	2.20	0.41
2:D:798:SER:HB2	2:D:802:TRP:HZ2	1.85	0.41
3:F:194:TYR:HE1	3:F:222:GLU:HB3	1.85	0.41
1:A:332:LEU:C	1:A:334:SER:H	2.24	0.41
1:A:414:HIS:HA	1:A:415:PRO:HD3	1.93	0.41
1:A:487:ILE:HA	1:A:487:ILE:HD12	1.83	0.41
1:A:608:LYS:HB3	1:A:608:LYS:HE2	1.84	0.41
2:B:1187:TYR:CD1	2:B:1232:ALA:HB2	2.50	0.41
2:B:1403:LEU:HD12	2:B:1448:LEU:HD11	2.02	0.41
2:B:783:LYS:NZ	3:F:197:PHE:HD1	2.18	0.41
1:C:457:HIS:ND1	1:C:457:HIS:C	2.73	0.41
1:C:599:ASP:HB2	2:D:802:TRP:HZ3	1.83	0.41
2:D:1117:VAL:HG12	2:D:1175:PHE:CD2	2.55	0.41
2:D:983:GLN:OE1	2:D:1319:LEU:HD21	2.20	0.41
3:E:139:LEU:HA	3:E:139:LEU:HD12	1.81	0.41
3:E:206:ILE:O	3:E:206:ILE:HG13	2.16	0.41
3:F:268:THR:HG22	3:F:275:GLU:O	2.20	0.41
3:F:98:CYS:HA	3:F:149:LEU:HD11	2.02	0.41
1:A:125:LEU:HD12	1:A:126:GLN:H	1.86	0.41
1:A:159:VAL:O	1:A:182:SER:OG	2.38	0.41
1:A:273:PHE:CD1	1:A:326:VAL:HG12	2.55	0.41
2:B:1128:GLU:HA	2:B:1134:ARG:CZ	2.50	0.41
1:C:144:THR:HG22	1:C:194:ASP:OD1	2.20	0.41
1:C:368:MET:O	1:C:413:THR:CG2	2.68	0.41
1:C:100:LYS:HD3	2:D:1313:TRP:CH2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1425:VAL:O	2:D:1426:ASP:HB2	2.20	0.41
2:D:1545:TYR:CG	2:D:1565:ILE:HD12	2.55	0.41
2:D:1643:GLN:HE21	2:D:1644:LYS:HZ3	1.69	0.41
2:D:833:LEU:HD13	2:D:912:VAL:HG11	2.03	0.41
2:D:888:ILE:HA	2:D:889:PRO:HD3	1.89	0.41
2:D:863:ARG:HG2	2:D:915:ALA:O	2.21	0.41
2:D:909:GLU:OE2	2:D:926:ARG:HD2	2.20	0.41
2:B:981:LEU:O	2:B:1342:LEU:HD12	2.20	0.41
2:B:841:ARG:O	2:B:842:ASN:OD1	2.39	0.41
1:C:275:ILE:CG1	1:C:282:ILE:HB	2.51	0.41
2:D:880:ARG:HD3	2:D:880:ARG:HH11	1.72	0.41
2:D:860:LEU:O	2:D:888:ILE:HG22	2.20	0.41
2:D:913:LYS:HE3	2:D:913:LYS:HB2	1.60	0.41
3:E:120:PRO:HD2	3:E:123:THR:HG21	2.03	0.41
3:E:250:THR:HA	3:E:264:SER:HB2	2.01	0.41
1:A:178:ASP:OD1	1:A:179:SER:N	2.53	0.41
1:A:161:ARG:NH2	1:A:212:ASN:ND2	2.69	0.41
1:A:273:PHE:CG	1:A:302:LEU:HD22	2.55	0.41
1:A:232:PHE:CZ	1:A:339:VAL:HG23	2.55	0.41
1:C:134:THR:HG22	1:C:147:TYR:HB3	2.02	0.41
1:C:156:LEU:HA	1:C:156:LEU:HD23	1.77	0.41
1:C:491:THR:HG22	1:C:505:ARG:CD	2.50	0.41
2:D:1476:ALA:HA	2:D:1492:PHE:HA	2.02	0.41
3:E:109:LEU:CB	3:E:114:ILE:HG12	2.43	0.41
3:F:120:PRO:HG2	3:F:123:THR:OG1	2.21	0.41
3:F:110:LYS:HG3	3:F:126:GLU:O	2.20	0.41
1:A:104:LYS:CG	1:A:105:PHE:H	2.33	0.41
1:A:473:VAL:HG21	1:A:531:LEU:CD2	2.51	0.41
1:A:59:VAL:HG12	1:A:69:LEU:HB2	2.03	0.41
2:D:1062:PRO:O	2:D:1106:TRP:CZ3	2.74	0.41
2:D:1311:ILE:CD1	2:D:1318:LEU:HA	2.50	0.41
2:D:1631:TRP:CZ3	2:D:1633:GLU:HA	2.54	0.41
3:E:146:LEU:HD12	3:E:150:LYS:N	2.35	0.41
1:A:104:LYS:HE3	1:A:104:LYS:HB2	1.70	0.41
1:A:253:VAL:HG12	1:A:300:VAL:HG13	2.03	0.41
1:A:617:TRP:CE3	1:A:617:TRP:HA	2.56	0.41
2:B:1076:THR:OG1	2:B:1120:GLU:OE1	2.27	0.41
2:B:1256:LEU:N	2:B:1256:LEU:HD13	2.36	0.41
2:B:1453:HIS:ND1	2:B:1453:HIS:C	2.74	0.41
2:B:1559:ASP:OD2	2:B:1561:TYR:CE2	2.74	0.41
1:C:170:PRO:HD3	1:C:204:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1197:ALA:HA	2:D:1202:LEU:HG	2.02	0.41
2:D:1313:TRP:CG	2:D:1314:GLU:N	2.88	0.41
2:D:1550:VAL:HG23	2:D:1562:ILE:HG13	2.02	0.41
3:F:181:LEU:HA	3:F:181:LEU:HD23	1.60	0.41
1:A:291:ILE:HA	1:A:292:PRO:HD3	1.71	0.41
1:A:360:THR:HG21	1:A:372:LEU:HD23	2.02	0.41
2:B:1325:LYS:HE2	2:B:1325:LYS:HB3	1.81	0.41
2:B:1417:ASP:O	2:B:1421:LEU:HD22	2.21	0.41
2:B:1418:LEU:HA	2:B:1418:LEU:HD23	2.00	0.41
2:B:1471:LEU:HA	2:B:1471:LEU:HD13	1.95	0.41
2:B:1636:GLU:O	2:B:1639:ASP:HB2	2.21	0.41
1:C:351:SER:C	1:C:353:TYR:H	2.23	0.41
1:C:569:GLN:OE1	1:C:581:MET:SD	2.79	0.41
1:C:592:ARG:HB2	2:D:777:ASP:OD1	2.21	0.41
2:D:1124:VAL:O	2:D:1127:GLN:HG2	2.21	0.41
2:D:1505:LEU:HA	2:D:1505:LEU:HD23	1.67	0.41
3:E:249:VAL:CG2	3:E:265:ILE:HG22	2.50	0.41
3:F:116:GLN:NE2	3:F:119:PHE:CE1	2.89	0.41
3:F:143:LEU:HD23	3:F:143:LEU:HA	1.76	0.41
1:A:449:VAL:HG21	1:A:545:GLU:CG	2.45	0.40
1:A:576:VAL:HG13	1:A:577:PRO:HD2	2.03	0.40
2:B:1403:LEU:HD23	2:B:1479:VAL:HG22	2.03	0.40
2:B:753:GLU:N	2:B:753:GLU:OE1	2.45	0.40
1:A:261:TYR:HD2	2:B:826:MET:SD	2.45	0.40
2:B:996:ASP:OD1	2:B:999:ARG:N	2.54	0.40
1:C:646:PHE:H	1:C:654:THR:HG23	1.80	0.40
1:C:55:VAL:CG2	1:C:74:THR:HG22	2.50	0.40
2:D:1171:LYS:O	2:D:1174:ASP:HB2	2.21	0.40
2:D:1240:LEU:CD1	2:D:1248:PHE:HB3	2.51	0.40
2:D:1496:GLU:HG2	2:D:1497:LYS:H	1.86	0.40
2:D:762:VAL:O	2:D:924:GLY:HA3	2.21	0.40
2:D:934:GLU:HB2	2:D:1354:ASP:O	2.22	0.40
2:D:967:LEU:HD22	2:D:1348:TYR:CD2	2.56	0.40
3:E:229:PRO:HG2	3:E:280:PRO:CG	2.46	0.40
2:B:1382:ASN:OD1	2:B:1383:THR:HG22	2.21	0.40
1:C:180:LEU:HD22	1:C:191:LEU:HD11	2.04	0.40
1:C:449:VAL:HG21	1:C:545:GLU:CG	2.50	0.40
1:C:607:LYS:O	1:C:607:LYS:HG3	2.21	0.40
2:D:1149:ILE:CD1	2:D:1153:GLU:OE2	2.69	0.40
2:D:1494:HIS:CE1	2:D:1497:LYS:HG3	2.56	0.40
2:D:796:LYS:HE2	3:F:168:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:945:ARG:NH1	2:B:962:ILE:HG22	2.37	0.40
1:C:135:ASP:OD2	1:C:136:LYS:HG3	2.21	0.40
1:C:274:GLY:HA3	1:C:325:TYR:CZ	2.56	0.40
1:C:229:LEU:HD21	1:C:601:GLY:HA3	2.04	0.40
2:D:1066:PHE:HB2	2:D:1078:LEU:CD1	2.47	0.40
2:D:1175:PHE:CE1	2:D:1179:ASN:ND2	2.90	0.40
2:D:1258:GLU:HA	2:D:1260:ARG:HH11	1.76	0.40
2:D:1310:ARG:HD2	2:D:1312:HIS:CD2	2.56	0.40
2:D:935:GLY:CA	2:D:1353:LYS:H	2.30	0.40
2:D:1367:ILE:HD12	2:D:1367:ILE:HG23	1.83	0.40
2:D:1494:HIS:CE1	2:D:1496:GLU:CD	2.94	0.40
2:D:756:ILE:HD12	3:F:134:ARG:NH2	2.34	0.40
3:F:127:TYR:HE2	3:F:143:LEU:HD12	1.87	0.40
1:A:183:GLN:O	1:A:184:ASN:OD1	2.40	0.40
1:A:477:LEU:HD11	1:A:487:ILE:HG21	2.04	0.40
2:B:1130:ILE:CG2	2:B:1134:ARG:H	2.35	0.40
2:B:1135:ASN:HB2	2:B:1185:ARG:NH2	2.37	0.40
2:B:1253:VAL:HG23	2:B:1253:VAL:H	1.57	0.40
1:C:104:LYS:HD2	1:C:104:LYS:HA	1.81	0.40
1:C:229:LEU:HD22	1:C:231:SER:H	1.86	0.40
1:C:269:ALA:HB2	1:C:330:VAL:HG22	2.03	0.40
1:C:456:LEU:HB2	1:C:535:TYR:CE2	2.57	0.40
1:C:589:HIS:HB2	2:D:782:PRO:HB3	2.02	0.40
2:D:1132:GLY:HA3	2:D:1187:TYR:CZ	2.57	0.40
2:D:1352:ALA:N	2:D:1353:LYS:HA	2.36	0.40
2:D:898:TYR:CA	2:D:1473:GLN:HE22	2.34	0.40
2:D:1484:ASN:HB3	2:D:1487:GLU:CD	2.42	0.40
2:D:1544:VAL:HG22	2:D:1605:TRP:HB2	2.04	0.40
2:D:778:LEU:HA	2:D:778:LEU:HD12	1.83	0.40
3:E:133:TYR:CB	3:E:158:CYS:HB3	2.47	0.40
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.88	0.40
1:A:480:ASP:O	1:A:484:GLU:OE1	2.38	0.40
1:A:464:GLU:CB	1:A:556:LYS:HE3	2.49	0.40
1:A:615:LYS:HE2	1:A:615:LYS:HB2	1.69	0.40
2:B:1249:VAL:O	2:B:1253:VAL:HG23	2.21	0.40
2:B:1422:ALA:CB	2:B:1429:ILE:HG22	2.52	0.40
2:B:1653:THR:HG23	2:B:1654:GLU:HG2	2.03	0.40
1:C:27:SER:OG	1:C:45:GLU:HB2	2.21	0.40
1:C:67:LEU:HD21	1:C:69:LEU:HD12	2.03	0.40
2:D:1066:PHE:HB3	2:D:1078:LEU:HD11	2.02	0.40
2:D:1137:ASN:HB2	2:D:1185:ARG:HE	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1241:LEU:HA	2:D:1241:LEU:HD12	1.64	0.40
2:D:1217:LYS:O	2:D:1251:PRO:HB2	2.21	0.40
3:F:143:LEU:HD22	3:F:152:SER:O	2.22	0.40
3:F:106:SER:CB	3:F:158:CYS:HB2	2.52	0.40

All (4) 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:A:77:THR:OG1	2:B:954:ARG:NH2[3_455]	2.06	0.14
1:C:413:THR:O	1:C:512:GLN:NE2[2_755]	2.15	0.05
2:B:1577:GLN:NE2	3:E:133:TYR:OH[3_565]	2.15	0.05
1:A:435:GLU:OE2	2:D:1431:LYS:NZ[2_755]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	640/645 (99%)	598 (93%)	37 (6%)	5 (1%)	19	59
1	C	640/645 (99%)	599 (94%)	34 (5%)	7 (1%)	14	51
2	B	898/915 (98%)	822 (92%)	58 (6%)	18 (2%)	7	40
2	D	898/915 (98%)	818 (91%)	57 (6%)	23 (3%)	5	35
3	E	187/194 (96%)	165 (88%)	17 (9%)	5 (3%)	5	34
3	F	187/194 (96%)	165 (88%)	17 (9%)	5 (3%)	5	34
All	All	3450/3508 (98%)	3167 (92%)	220 (6%)	63 (2%)	8	42

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	950	GLU

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Mol	Chain	Res	Type
2	B	1137	ASN
2	B	1286	ALA
2	B	1287	PRO
2	B	1573	SER
1	C	397	VAL
1	C	497	LYS
2	D	950	GLU
2	D	988	ALA
2	D	1497	LYS
3	E	239	GLU
3	F	239	GLU
1	A	397	VAL
1	A	497	LYS
1	A	540	ALA
2	B	957	VAL
2	B	992	GLU
2	B	1011	GLY
2	B	1264	GLY
2	B	1301	PRO
1	C	96	PHE
1	C	540	ALA
2	D	757	ALA
2	D	957	VAL
2	D	989	GLN
2	D	1011	GLY
2	D	1264	GLY
2	D	1289	HIS
2	D	1301	PRO
2	D	1358	CYS
1	A	600	LYS
2	B	1135	ASN
1	C	333	HIS
2	D	1498	GLU
2	D	1633	GLU
3	E	131	PRO
3	F	131	PRO
2	B	1317	SER
2	B	1354	ASP
2	B	1480	TYR
1	C	569	GLN
1	C	600	LYS
2	D	760	ASN

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Mol	Chain	Res	Type
2	D	1064	SER
2	D	1480	TYR
2	D	1499	ASP
3	E	156	GLU
3	E	237	GLN
3	F	237	GLN
2	B	796	LYS
2	B	935	GLY
2	B	1508	ASP
2	D	1136	ASN
2	D	1286	ALA
2	D	1287	PRO
2	D	1317	SER
2	D	1508	ASP
1	A	333	HIS
2	D	1399	THR
3	F	137	PRO
3	F	155	VAL
3	E	137	PRO
2	B	1520	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	564/567 (100%)	522 (93%)	42 (7%)	13	40
1	C	564/567 (100%)	527 (93%)	37 (7%)	16	43
2	B	791/810 (98%)	719 (91%)	72 (9%)	9	32
2	D	787/810 (97%)	715 (91%)	72 (9%)	9	32
3	E	166/167 (99%)	138 (83%)	28 (17%)	2	13
3	F	166/167 (99%)	138 (83%)	28 (17%)	2	13
All	All	3038/3088 (98%)	2759 (91%)	279 (9%)	9	31

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	TYR
1	A	30	THR
1	A	59	VAL
1	A	67	LEU
1	A	68	VAL
1	A	71	SER
1	A	76	LEU
1	A	83	MET
1	A	85	ASN
1	A	87	THR
1	A	89	THR
1	A	116	VAL
1	A	117	VAL
1	A	122	LEU
1	A	125	LEU
1	A	130	LEU
1	A	133	GLN
1	A	134	THR
1	A	163	VAL
1	A	177	GLN
1	A	213	SER
1	A	228	VAL
1	A	235	ILE
1	A	239	THR
1	A	242	PHE
1	A	252	GLU
1	A	293	ILE
1	A	306	VAL
1	A	330	VAL
1	A	413	THR
1	A	421	SER
1	A	423	THR
1	A	448	THR
1	A	463	THR
1	A	465	LEU
1	A	471	LEU
1	A	491	THR
1	A	496	ASN
1	A	583	LEU
1	A	605	LEU
1	A	622	LYS
1	A	650	SER
2	B	755	ILE

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Mol	Chain	Res	Type
2	B	759	GLU
2	B	763	SER
2	B	774	ASN
2	B	792	ASN
2	B	826	MET
2	B	831	ILE
2	B	842	ASN
2	B	907	LEU
2	B	929	LEU
2	B	932	VAL
2	B	939	ASN
2	B	940	LYS
2	B	946	THR
2	B	952	LEU
2	B	957	VAL
2	B	962	ILE
2	B	981	LEU
2	B	982	LEU
2	B	983	GLN
2	B	991	THR
2	B	995	VAL
2	B	996	ASP
2	B	1048	LEU
2	B	1051	LYS
2	B	1070	VAL
2	B	1072	ARG
2	B	1085	VAL
2	B	1117	VAL
2	B	1130	ILE
2	B	1157	ILE
2	B	1170	THR
2	B	1189	VAL
2	B	1191	ILE
2	B	1206	LEU
2	B	1244	LYS
2	B	1250	PRO
2	B	1256	LEU
2	B	1260	ARG
2	B	1269	THR
2	B	1291	GLU
2	B	1292	LEU
2	B	1298	LEU

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Mol	Chain	Res	Type
2	B	1300	LEU
2	B	1311	ILE
2	B	1319	LEU
2	B	1320	ARG
2	B	1349	HIS
2	B	1356	LEU
2	B	1357	THR
2	B	1366	THR
2	B	1384	MET
2	B	1407	MET
2	B	1414	ASP
2	B	1421	LEU
2	B	1453	HIS
2	B	1499	ASP
2	B	1503	ASN
2	B	1504	LYS
2	B	1507	ARG
2	B	1508	ASP
2	B	1511	CYS
2	B	1522	LYS
2	B	1525	ASP
2	B	1544	VAL
2	B	1550	VAL
2	B	1610	ASP
2	B	1624	LYS
2	B	1628	VAL
2	B	1633	GLU
2	B	1634	GLU
2	B	1637	CYS
1	C	30	THR
1	C	35	ARG
1	C	41	THR
1	C	60	HIS
1	C	67	LEU
1	C	71	SER
1	C	77	THR
1	C	86	VAL
1	C	90	ILE
1	C	94	ARG
1	C	95	GLU
1	C	97	LYS
1	C	106	VAL

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Mol	Chain	Res	Type
1	C	127	SER
1	C	146	LEU
1	C	191	LEU
1	C	226	GLU
1	C	229	LEU
1	C	293	ILE
1	C	301	VAL
1	C	302	LEU
1	C	338	MET
1	C	343	ARG
1	C	346	ILE
1	C	359	LYS
1	C	365	LYS
1	C	398	GLN
1	C	413	THR
1	C	441	MET
1	C	457	HIS
1	C	465	LEU
1	C	470	THR
1	C	473	VAL
1	C	546	VAL
1	C	547	VAL
1	C	560	VAL
1	C	605	LEU
2	D	756	ILE
2	D	762	VAL
2	D	795	LEU
2	D	796	LYS
2	D	807	VAL
2	D	824	THR
2	D	862	VAL
2	D	883	GLN
2	D	885	THR
2	D	886	VAL
2	D	904	LYS
2	D	907	LEU
2	D	912	VAL
2	D	936	ILE
2	D	937	ARG
2	D	939	ASN
2	D	946	THR
2	D	995	VAL

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Mol	Chain	Res	Type
2	D	1016	ILE
2	D	1021	THR
2	D	1039	LEU
2	D	1050	LYS
2	D	1078	LEU
2	D	1107	LEU
2	D	1109	LEU
2	D	1117	VAL
2	D	1144	THR
2	D	1148	LEU
2	D	1149	ILE
2	D	1151	LEU
2	D	1152	GLN
2	D	1159	GLU
2	D	1161	GLN
2	D	1189	VAL
2	D	1191	ILE
2	D	1202	LEU
2	D	1215	LYS
2	D	1244	LYS
2	D	1256	LEU
2	D	1297	SER
2	D	1298	LEU
2	D	1302	SER
2	D	1315	SER
2	D	1320	ARG
2	D	1324	THR
2	D	1331	THR
2	D	1341	THR
2	D	1342	LEU
2	D	1356	LEU
2	D	1395	ASP
2	D	1423	ASN
2	D	1435	ASP
2	D	1440	ASP
2	D	1450	LYS
2	D	1485	LEU
2	D	1487	GLU
2	D	1491	ARG
2	D	1492	PHE
2	D	1506	CYS
2	D	1511	CYS

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Mol	Chain	Res	Type
2	D	1528	THR
2	D	1529	LEU
2	D	1548	ARG
2	D	1550	VAL
2	D	1551	LYS
2	D	1552	VAL
2	D	1558	PHE
2	D	1563	MET
2	D	1585	ILE
2	D	1624	LYS
2	D	1628	VAL
2	D	1658	VAL
3	E	102	THR
3	E	104	LEU
3	E	105	ASN
3	E	129	CYS
3	E	143	LEU
3	E	146	LEU
3	E	150	LYS
3	E	156	GLU
3	E	160	LYS
3	E	163	CYS
3	E	170	ARG
3	E	171	ASN
3	E	174	ILE
3	E	181	LEU
3	E	185	THR
3	E	192	THR
3	E	199	SER
3	E	205	LEU
3	E	206	ILE
3	E	223	ILE
3	E	225	CYS
3	E	241	ASP
3	E	245	TYR
3	E	246	ARG
3	E	248	SER
3	E	253	CYS
3	E	265	ILE
3	E	283	CYS
3	F	102	THR
3	F	106	SER

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Mol	Chain	Res	Type
3	F	113	TYR
3	F	135	ARG
3	F	145	CYS
3	F	146	LEU
3	F	155	VAL
3	F	156	GLU
3	F	157	PHE
3	F	159	LYS
3	F	163	CYS
3	F	174	ILE
3	F	180	ILE
3	F	185	THR
3	F	188	PHE
3	F	195	LYS
3	F	196	LEU
3	F	206	ILE
3	F	217	LEU
3	F	222	GLU
3	F	225	CYS
3	F	239	GLU
3	F	246	ARG
3	F	248	SER
3	F	253	CYS
3	F	255	LYS
3	F	272	ASP
3	F	283	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	126	GLN
1	A	184	ASN
1	A	212	ASN
1	A	216	GLN
1	A	453	ASN
1	A	609	ASN
2	B	774	ASN
2	B	842	ASN
2	B	1055	GLN
2	B	1056	GLN
2	B	1136	ASN

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Mol	Chain	Res	Type
2	B	1152	GLN
2	B	1277	GLN
2	B	1453	HIS
2	B	1580	GLN
2	B	1642	ASN
1	C	32	ASN
1	C	50	GLN
1	C	60	HIS
1	C	126	GLN
1	C	185	GLN
1	C	215	GLN
1	C	589	HIS
1	C	656	GLN
2	D	1112	GLN
2	D	1152	GLN
2	D	1198	GLN
2	D	1349	HIS
2	D	1473	GLN
2	D	1503	ASN
2	D	1517	ASN
2	D	1580	GLN
2	D	1581	GLN
2	D	1643	GLN
3	E	117	ASN
3	E	237	GLN
3	E	242	HIS
3	E	254	ASN
3	F	173	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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	642/645 (99%)	0.15	21 (3%)	46	37	19, 107, 194, 287	0
1	C	642/645 (99%)	0.14	10 (1%)	72	62	16, 91, 178, 269	0
2	B	902/915 (98%)	0.22	23 (2%)	57	47	21, 143, 235, 308	0
2	D	902/915 (98%)	0.20	17 (1%)	66	58	16, 124, 224, 358	0
3	E	189/194 (97%)	0.39	12 (6%)	20	16	45, 129, 218, 254	0
3	F	189/194 (97%)	0.45	20 (10%)	6	6	38, 139, 231, 279	0
All	All	3466/3508 (98%)	0.21	103 (2%)	50	39	16, 118, 221, 358	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	985	THR	6.6
3	F	154	ALA	6.3
1	A	99	GLU	5.7
1	A	396	THR	4.8
2	B	1438	PHE	4.7
1	C	66	LYS	4.6
2	D	760	ASN	4.6
2	D	1640	GLU	4.3
3	F	138	SER	4.2
2	B	984	GLY	4.1
1	A	397	VAL	4.1
1	C	99	GLU	4.0
2	B	1066	PHE	3.7
1	A	100	LYS	3.7
2	B	1441	ARG	3.6
2	D	752	ASP	3.5
2	B	1119	GLN	3.4
1	C	410	SER	3.4
2	D	759	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	1065	ALA	3.3
3	F	102	THR	3.3
2	B	1466	TYR	3.3
2	D	993	ASP	3.2
3	F	107	ALA	3.1
2	B	990	MET	3.1
2	D	1546	LYS	3.0
1	A	365	LYS	2.9
3	F	135	ARG	2.9
1	A	398	GLN	2.9
1	A	98	SER	2.9
2	B	986	PRO	2.9
2	B	1437	ALA	2.9
1	A	96	PHE	2.9
2	D	1638	GLN	2.8
1	A	366	PRO	2.8
1	C	411	ILE	2.8
1	C	514	LEU	2.8
3	F	155	VAL	2.8
3	E	269	VAL	2.7
2	D	1134	ARG	2.7
2	B	947	LEU	2.7
3	F	127	TYR	2.7
2	D	915	ALA	2.6
3	E	231	ILE	2.6
2	B	1266	TYR	2.6
3	F	103	ARG	2.6
2	B	1287	PRO	2.6
3	F	153	THR	2.5
3	F	118	TYR	2.5
2	B	1314	GLU	2.5
2	B	1337	LYS	2.5
3	E	147	GLN	2.4
1	C	541	SER	2.4
1	A	364	PHE	2.4
3	F	125	VAL	2.4
1	A	50	GLN	2.4
3	E	131	PRO	2.4
3	E	281	PRO	2.4
1	C	542	GLY	2.4
3	F	157	PHE	2.4
1	A	118	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	219	GLU	2.3
3	F	122	GLY	2.3
1	A	642	ALA	2.3
3	F	182	PHE	2.3
2	D	1354	ASP	2.3
2	D	1116	GLY	2.3
3	E	132	GLY	2.3
3	E	126	GLU	2.3
2	B	1223	PRO	2.3
2	D	1008	SER	2.3
1	C	625	ILE	2.3
1	A	541	SER	2.3
1	A	455	TYR	2.3
3	F	131	PRO	2.3
1	A	631	SER	2.2
3	E	261	GLY	2.2
2	D	1527	VAL	2.2
3	F	285	GLY	2.2
2	D	1119	GLN	2.2
3	F	126	GLU	2.2
2	B	975	GLU	2.2
2	B	1110	GLU	2.2
2	B	756	ILE	2.2
1	A	221	GLU	2.2
2	B	1305	SER	2.2
1	A	420	LEU	2.2
3	F	104	LEU	2.2
1	A	477	LEU	2.2
3	F	124	VAL	2.1
2	D	1133	LEU	2.1
1	C	512	GLN	2.1
3	E	128	GLU	2.1
2	D	1569	ILE	2.1
1	A	368	MET	2.1
1	A	487	ILE	2.1
2	D	1113	LYS	2.1
3	E	118	TYR	2.1
1	C	370	PHE	2.1
3	E	197	PHE	2.1
2	B	1296	VAL	2.1
2	B	1509	GLU	2.0
3	F	137	PRO	2.0

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.