



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:27 PM UTC

PDB ID : 3NOG / pdb_00003nog
Title : Designed ankyrin repeat protein (DARPin) Binders to AcrB: Plasticity of the Interface
Authors : Monroe, N.; Briand, C.; Gruetter, M.G.
Deposited on : 2010-06-25
Resolution : 3.34 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

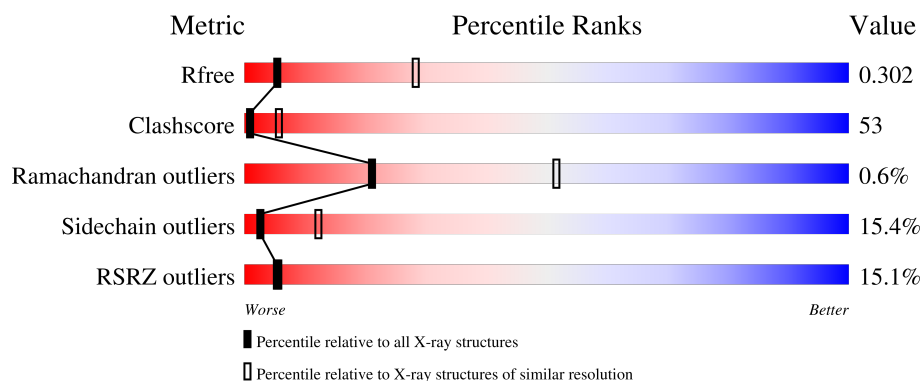
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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 of 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	1049	13% 45% 40% 10% ..
1	B	1049	14% 37% 46% 13% ..
1	C	1049	13% 41% 43% 12% ..
2	D	169	12% 40% 36% 13% 9%
2	E	169	39% 47% 37% .. 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	FME	B	1	-	-	X	-
1	FME	C	1	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24874 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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1012	Total	C	N	O	S	27	0	0
			7464	4806	1218	1399	41			
1	B	1028	Total	C	N	O	S	0	0	0
			7547	4853	1237	1414	43			
1	C	1040	Total	C	N	O	S	20	0	0
			7736	4979	1270	1444	43			

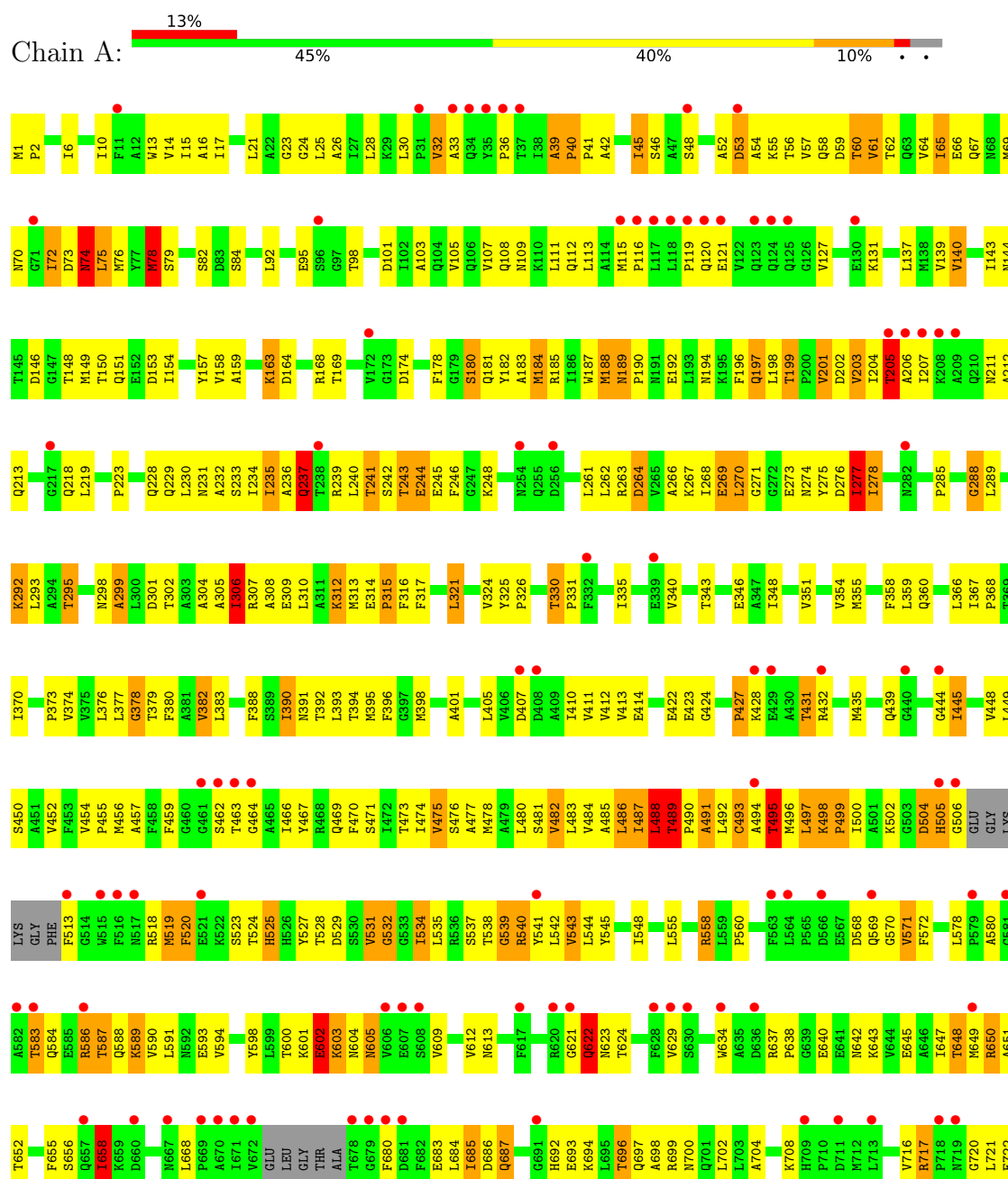
- Molecule 2 is a protein called Designed ankyrin repeat protein.

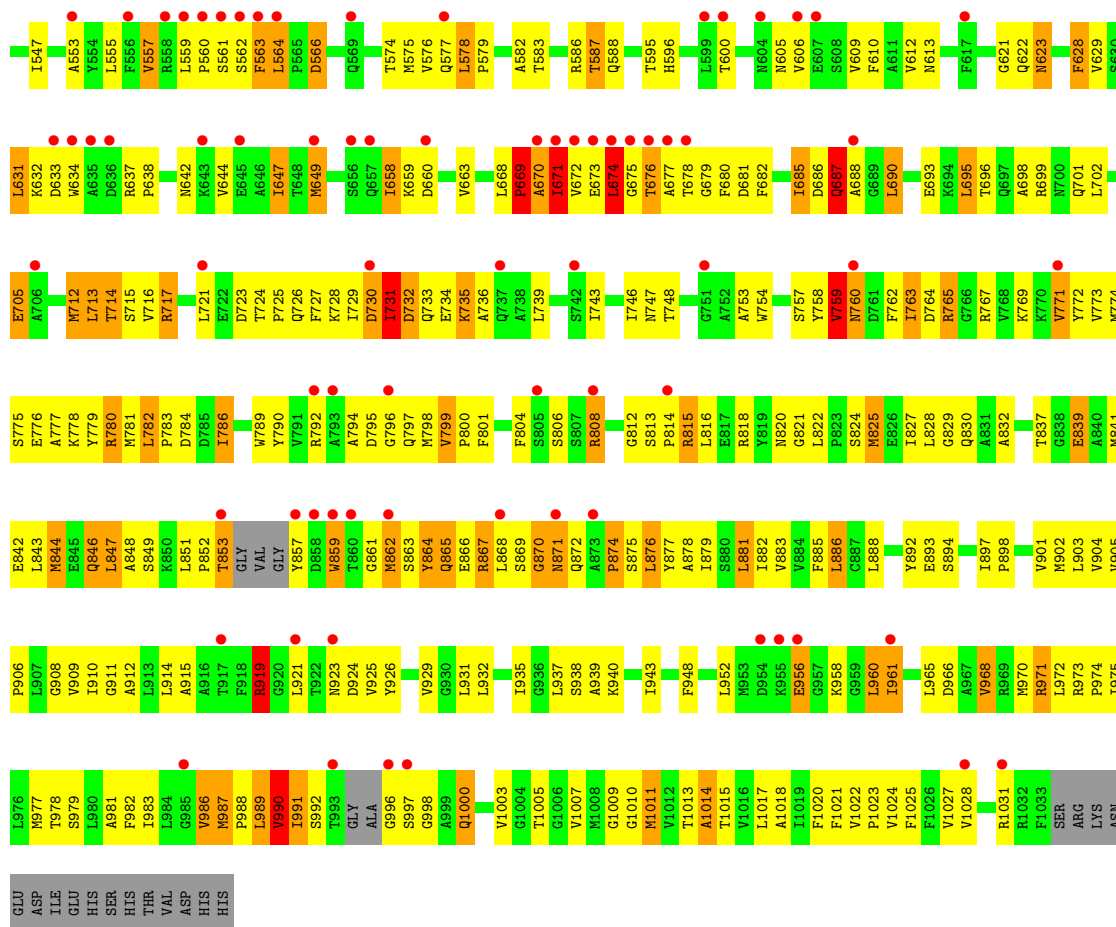
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	154	Total	C	N	O	S	4	0	0
			1097	686	194	216	1			
2	E	151	Total	C	N	O	S	21	0	0
			1030	641	185	203	1			

3 Residue-property plots

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

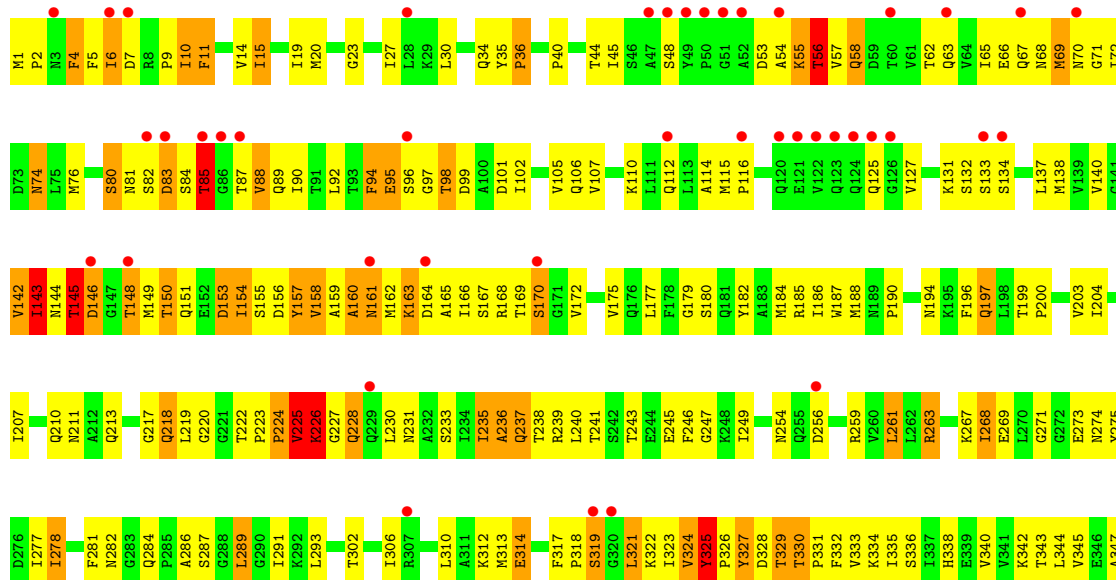
• Molecule 1: Acriflavine resistance protein B

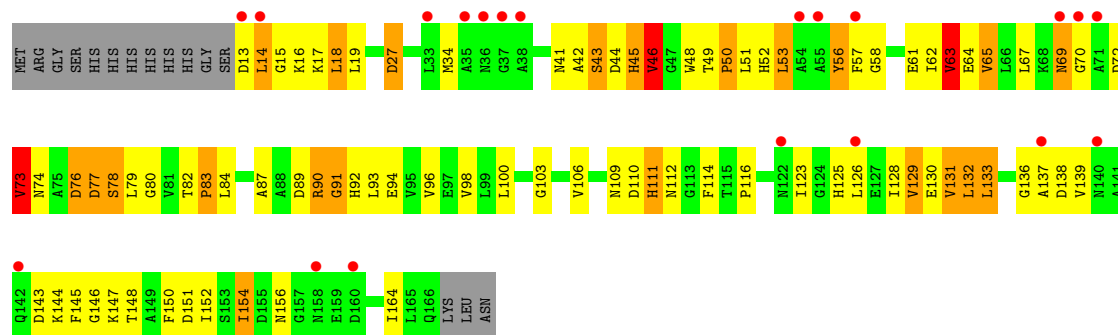




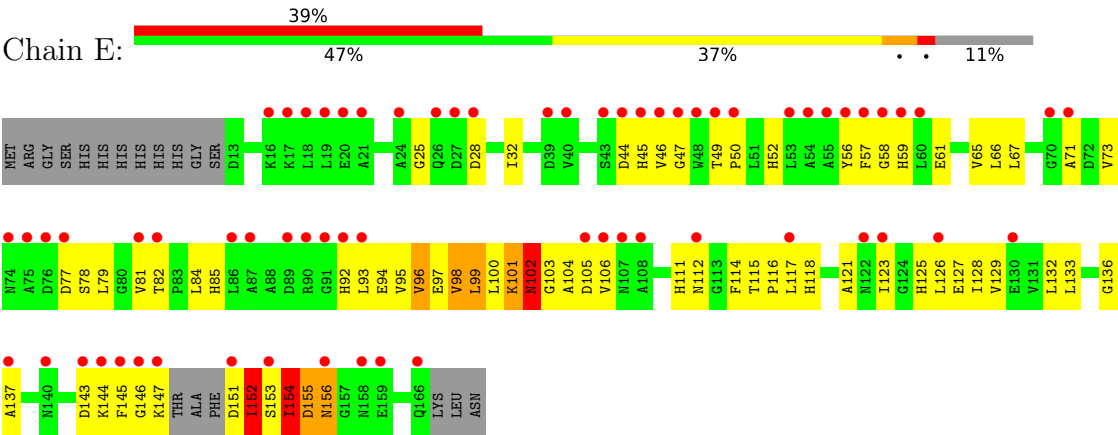
● Molecule 1: Acriflavine resistance protein B

Chain C: 13% 41% 43% 12% ..





● Molecule 2: Designed ankyrin repeat protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.40Å 158.00Å 258.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.78 – 3.34 48.78 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.78-3.34) 99.8 (48.78-3.34)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.6.2_432	Depositor
R, R_{free}	0.257 , 0.307 0.255 , 0.302	Depositor DCC
R_{free} test set	1043 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å ²)	70.8	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	24874	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.08	24/7591 (0.3%)	1.22	77/10342 (0.7%)
1	B	1.08	20/7675 (0.3%)	1.28	106/10467 (1.0%)
1	C	1.14	15/7874 (0.2%)	1.29	106/10720 (1.0%)
2	D	1.27	6/1115 (0.5%)	1.43	22/1525 (1.4%)
2	E	0.60	1/1046 (0.1%)	1.12	10/1434 (0.7%)
All	All	1.09	66/25301 (0.3%)	1.27	321/34488 (0.9%)

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	799	VAL	CA-CB	-9.14	1.47	1.54
1	C	225	VAL	CA-CB	-8.96	1.43	1.54
1	A	475	VAL	CA-CB	-8.16	1.43	1.54
1	C	324	VAL	CA-CB	-7.46	1.47	1.55
1	C	626	ILE	CA-CB	-7.14	1.44	1.55
1	A	57	VAL	CA-CB	-7.13	1.46	1.54
1	B	102	ILE	CA-CB	-6.97	1.46	1.54
1	C	925	VAL	CA-CB	-6.96	1.46	1.54
1	A	724	THR	CA-CB	-6.83	1.45	1.53
1	B	61	VAL	CA-CB	-6.76	1.46	1.54
1	C	166	ILE	CA-CB	-6.73	1.46	1.54
1	C	10	ILE	CA-CB	-6.72	1.46	1.54
1	C	724	THR	CA-CB	-6.65	1.45	1.54
2	D	73	VAL	CA-CB	-6.39	1.45	1.54
1	B	207	ILE	CA-CB	-6.29	1.46	1.54
1	B	57	VAL	CA-CB	-6.17	1.46	1.54
1	A	306	ILE	CA-CB	-6.13	1.47	1.54
1	A	42	ALA	CA-CB	-6.12	1.43	1.53
1	A	199	THR	CA-CB	-6.07	1.45	1.54
1	A	72	ILE	CA-CB	-6.02	1.47	1.54
1	B	731	ILE	CA-CB	-6.01	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	LYS	CA-C	-5.87	1.45	1.52
1	A	64	VAL	CA-CB	-5.86	1.47	1.54
1	A	270	LEU	CA-C	-5.86	1.45	1.52
1	B	629	VAL	CA-CB	-5.76	1.47	1.54
1	B	760	ASN	C-O	-5.75	1.19	1.24
1	B	61	VAL	N-CA	-5.73	1.39	1.46
1	C	145	THR	CA-CB	-5.61	1.44	1.53
1	B	799	VAL	CA-CB	-5.59	1.47	1.54
2	D	46	VAL	CA-CB	-5.57	1.47	1.54
1	A	305	ALA	CA-CB	-5.56	1.44	1.53
1	A	54	ALA	CA-CB	-5.54	1.44	1.53
2	D	65	VAL	CA-CB	-5.50	1.47	1.54
1	C	436	GLY	C-O	5.50	1.31	1.23
1	B	61	VAL	CA-C	-5.44	1.46	1.52
1	B	961	ILE	CA-CB	-5.42	1.47	1.54
2	D	63	VAL	CA-CB	-5.42	1.48	1.54
1	A	204	ILE	CA-CB	-5.42	1.47	1.54
1	C	95	GLU	CA-C	-5.41	1.46	1.52
1	A	65	ILE	CA-CB	-5.36	1.47	1.54
2	D	43	SER	CA-C	-5.32	1.46	1.52
2	D	42	ALA	CA-C	-5.31	1.46	1.52
1	A	203	VAL	CA-CB	-5.26	1.47	1.54
1	B	688	ALA	CA-CB	-5.24	1.45	1.54
1	B	183	ALA	CA-CB	-5.22	1.44	1.54
1	A	268	ILE	C-O	-5.19	1.18	1.24
1	A	382	VAL	C-O	-5.19	1.18	1.24
1	B	100	ALA	CA-CB	-5.18	1.45	1.53
1	A	201	VAL	CA-CB	-5.18	1.47	1.54
1	B	214	VAL	CA-CB	-5.17	1.48	1.54
2	E	98	VAL	CA-CB	-5.17	1.48	1.54
1	A	40	PRO	C-O	-5.17	1.20	1.24
1	C	571	VAL	CA-CB	-5.16	1.47	1.54
1	A	268	ILE	CA-C	-5.15	1.46	1.52
1	B	986	VAL	CA-CB	-5.15	1.48	1.54
1	A	489	THR	CA-CB	-5.14	1.46	1.53
1	C	57	VAL	CA-CB	-5.13	1.48	1.54
1	A	268	ILE	CA-CB	-5.12	1.48	1.54
1	B	671	ILE	CA-CB	-5.12	1.47	1.54
1	A	299	ALA	CA-CB	-5.11	1.45	1.53
1	C	442	LEU	CA-C	-5.11	1.45	1.52
1	B	990	VAL	CA-CB	-5.06	1.47	1.54
1	A	61	VAL	CA-CB	-5.04	1.47	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	513	PHE	CA-C	-5.02	1.48	1.53
1	B	382	VAL	CA-CB	-5.02	1.47	1.54
1	C	750	LEU	CA-C	-5.01	1.46	1.52

All (321) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	VAL	N-CA-C	17.50	125.44	111.62
2	E	156	ASN	N-CA-C	16.82	129.30	110.97
1	A	759	VAL	N-CA-C	16.67	126.20	110.53
1	C	83	ASP	N-CA-C	16.45	129.21	111.28
1	C	85	THR	N-CA-C	-16.28	92.65	113.17
1	B	685	ILE	N-CA-C	16.08	127.58	110.05
1	A	540	ARG	N-CA-C	-14.90	95.04	111.28
1	A	61	VAL	CB-CA-C	-14.04	98.55	111.05
1	C	235	ILE	N-CA-C	12.75	122.51	110.53
1	B	514	GLY	N-CA-C	-12.58	98.79	115.40
2	D	138	ASP	N-CA-C	-12.34	88.30	108.41
1	B	759	VAL	N-CA-C	11.91	122.75	110.72
1	A	900	SER	N-CA-C	-11.69	96.79	111.75
1	A	945	ILE	CB-CA-C	-11.64	97.07	111.97
1	C	327	TYR	N-CA-C	11.63	127.29	111.24
1	B	509	LYS	N-CA-C	-11.55	97.45	112.24
2	D	42	ALA	N-CA-C	-11.39	93.43	110.28
1	C	56	THR	N-CA-C	-11.20	99.07	111.28
1	B	515	TRP	N-CA-C	-11.17	99.08	111.14
1	C	672	VAL	N-CA-C	11.14	124.97	111.05
1	A	270	LEU	N-CA-C	-11.04	94.22	110.23
1	B	513	PHE	CB-CA-C	-10.86	104.04	116.63
1	B	685	ILE	CB-CA-C	-10.68	99.84	111.59
1	A	505	HIS	N-CA-C	-10.41	100.05	113.17
1	C	1032	ARG	N-CA-C	-10.35	93.16	109.72
1	B	255	GLN	N-CA-C	-10.33	100.02	111.28
2	D	111	HIS	N-CA-C	-10.32	100.62	113.01
1	B	687	GLN	N-CA-C	10.23	125.15	112.87
1	B	674	LEU	N-CA-C	-10.03	100.98	113.01
1	C	131	LYS	N-CA-C	-9.99	97.06	110.55
1	B	679	GLY	N-CA-C	-9.71	96.96	111.14
1	B	919	ARG	N-CA-C	9.62	121.53	111.14
1	C	925	VAL	CB-CA-C	-9.41	99.92	111.97
1	C	430	ALA	N-CA-C	-9.35	101.09	111.28
1	A	53	ASP	N-CA-C	-9.31	98.96	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	ASP	N-CA-C	-9.13	101.24	112.38
1	C	70	ASN	N-CA-C	9.08	121.18	111.28
1	B	690	LEU	N-CA-C	9.06	121.23	111.36
1	C	95	GLU	N-CA-C	-9.00	98.54	110.24
1	A	532	GLY	N-CA-C	-8.98	101.95	112.73
1	B	503	GLY	N-CA-C	-8.91	102.92	115.30
2	D	14	LEU	N-CA-C	-8.81	101.57	111.71
1	C	166	ILE	N-CA-C	8.69	119.48	110.62
2	D	69	ASN	N-CA-C	8.66	120.80	111.36
2	E	102	ASN	N-CA-C	-8.63	101.88	111.28
1	A	760	ASN	N-CA-C	8.62	119.31	108.19
1	C	759	VAL	N-CA-C	8.54	118.90	111.56
1	B	875	SER	N-CA-C	-8.47	102.94	113.28
2	D	56	TYR	N-CA-C	8.44	123.23	113.19
1	B	207	ILE	CB-CA-C	-8.41	100.61	112.22
1	B	505	HIS	N-CA-C	-8.39	96.71	109.79
1	A	759	VAL	CB-CA-C	-8.36	101.06	112.02
1	C	170	SER	N-CA-C	8.34	122.47	109.96
2	D	76	ASP	N-CA-C	8.29	120.31	111.28
1	C	57	VAL	CB-CA-C	-8.29	100.95	112.14
1	C	601	LYS	N-CA-C	8.28	120.09	111.14
1	C	872	GLN	N-CA-C	8.13	120.14	111.28
1	C	746	ILE	CB-CA-C	-8.11	101.58	111.97
1	C	750	LEU	N-CA-C	8.10	120.18	111.36
1	C	158	VAL	CB-CA-C	-8.06	101.65	111.97
1	B	366	LEU	N-CA-C	8.06	120.06	111.28
2	D	72	ASP	N-CA-C	-8.04	97.78	109.59
1	A	60	THR	N-CA-C	8.04	120.12	111.36
2	D	46	VAL	N-CA-C	-7.93	103.68	112.80
1	B	563	PHE	N-CA-C	7.91	119.53	111.07
1	C	444	GLY	CA-C-N	7.82	130.47	120.70
1	C	444	GLY	C-N-CA	7.82	130.47	120.70
1	B	259	ARG	N-CA-CB	-7.81	97.90	110.63
1	C	992	SER	N-CA-C	7.81	121.72	110.24
1	A	378	GLY	N-CA-C	-7.78	103.05	113.24
1	C	6	ILE	N-CA-C	-7.77	101.34	111.05
1	B	760	ASN	CB-CA-C	-7.75	97.92	113.80
1	A	954	ASP	N-CA-C	7.71	119.32	111.07
1	A	603	LYS	N-CA-C	7.67	121.90	112.54
1	B	82	SER	N-CA-C	7.65	121.87	108.56
1	C	166	ILE	CB-CA-C	-7.61	101.87	112.14
1	A	488	LEU	N-CA-C	7.61	119.65	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	VAL	CB-CA-C	-7.61	102.24	111.97
1	A	491	ALA	N-CA-C	-7.60	103.00	111.28
1	A	754	TRP	N-CA-C	-7.59	97.85	109.85
1	C	314	GLU	N-CA-C	7.59	122.52	112.35
1	C	225	VAL	N-CA-C	-7.55	99.17	109.37
1	C	673	GLU	N-CA-C	7.52	119.48	111.28
1	B	61	VAL	CB-CA-C	-7.46	102.43	111.97
1	C	57	VAL	N-CA-C	7.41	118.17	110.62
1	B	259	ARG	N-CA-C	7.37	122.04	110.17
1	B	497	LEU	N-CA-C	7.35	122.31	109.96
1	C	163	LYS	CA-C-N	-7.33	110.91	120.44
1	C	163	LYS	C-N-CA	-7.33	110.91	120.44
1	A	243	THR	N-CA-C	-7.27	103.35	111.28
1	B	676	THR	N-CA-C	-7.27	100.46	110.35
1	A	57	VAL	N-CA-C	7.26	117.39	110.42
1	A	189	ASN	CA-C-N	7.24	126.77	119.24
1	A	189	ASN	C-N-CA	7.24	126.77	119.24
1	C	640	GLU	N-CA-C	-7.18	104.25	113.16
1	C	284	GLN	CA-C-N	7.17	128.80	119.84
1	C	284	GLN	C-N-CA	7.17	128.80	119.84
1	A	205	THR	N-CA-C	7.16	119.08	111.28
1	C	514	GLY	N-CA-C	-7.12	103.91	113.24
1	A	919	ARG	N-CA-C	-7.08	104.63	113.20
1	C	887	CYS	N-CA-C	-7.05	103.59	111.28
1	C	20	MET	N-CA-C	7.02	118.72	111.14
1	A	163	LYS	N-CA-C	7.01	118.57	111.07
1	C	325	TYR	N-CA-C	6.94	122.97	108.39
1	A	539	GLY	N-CA-C	-6.94	104.28	114.61
1	B	566	ASP	N-CA-C	-6.93	101.38	110.53
1	C	466	ILE	CB-CA-C	-6.92	102.95	112.02
1	A	818	ARG	N-CA-C	-6.91	98.81	109.52
1	C	786	ILE	CB-CA-C	-6.91	102.81	112.14
2	D	131	VAL	CB-CA-C	-6.90	102.83	112.14
2	D	109	ASN	N-CA-C	6.89	120.17	109.07
1	C	623	ASN	N-CA-C	6.88	121.28	113.02
1	C	495	THR	N-CA-C	6.87	118.56	111.14
1	B	225	VAL	N-CA-C	-6.86	98.45	108.87
1	C	443	VAL	CA-C-N	-6.86	112.37	119.98
1	C	443	VAL	C-N-CA	-6.86	112.37	119.98
2	D	139	VAL	N-CA-C	-6.84	106.06	112.83
1	C	492	LEU	N-CA-C	-6.83	103.83	111.28
1	B	870	GLY	N-CA-C	-6.83	104.19	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1000	GLN	N-CA-C	6.82	118.37	111.07
1	A	622	GLN	N-CA-C	-6.81	104.97	113.55
1	C	669	PRO	N-CA-C	-6.80	100.40	111.21
1	B	181	GLN	N-CA-C	-6.79	100.15	110.14
1	C	97	GLY	N-CA-C	-6.79	97.10	113.18
1	A	656	SER	N-CA-C	-6.76	103.98	111.82
1	A	726	GLN	N-CA-C	-6.67	99.19	109.52
1	B	867	ARG	N-CA-C	6.66	118.20	111.07
2	D	73	VAL	CB-CA-C	-6.64	103.35	112.24
2	E	156	ASN	CA-C-N	6.63	134.40	121.41
2	E	156	ASN	C-N-CA	6.63	134.40	121.41
2	D	146	GLY	N-CA-C	-6.62	106.67	115.40
2	D	17	LYS	N-CA-C	-6.60	104.08	111.28
1	A	796	GLY	N-CA-C	6.60	124.47	115.30
1	A	431	THR	CA-C-N	-6.57	111.90	120.44
1	A	431	THR	C-N-CA	-6.57	111.90	120.44
1	C	751	GLY	N-CA-C	-6.56	104.55	112.49
2	E	152	ILE	CB-CA-C	-6.56	103.58	111.97
1	C	326	PRO	N-CA-C	-6.55	101.62	111.57
1	A	237	GLN	N-CA-C	6.54	119.20	111.02
1	A	64	VAL	CB-CA-C	-6.53	103.61	111.97
1	C	786	ILE	N-CA-C	6.51	117.26	110.62
2	D	90	ARG	N-CA-C	-6.49	104.46	112.38
1	C	434	SER	N-CA-C	-6.49	104.21	111.28
1	B	506	GLY	N-CA-C	6.49	120.51	112.73
1	C	94	PHE	N-CA-C	6.48	120.47	110.42
1	C	441	ALA	N-CA-C	6.47	118.33	111.28
1	A	760	ASN	CB-CA-C	-6.45	100.49	114.10
1	B	669	PRO	CB-CA-C	-6.45	103.14	111.46
1	B	512	PHE	CA-C-N	-6.43	111.53	122.66
1	B	512	PHE	C-N-CA	-6.43	111.53	122.66
1	A	306	ILE	CB-CA-C	-6.43	103.78	111.81
1	C	910	ILE	N-CA-C	-6.42	104.08	110.62
1	B	677	ALA	N-CA-C	6.41	118.29	110.41
1	C	237	GLN	N-CA-C	6.40	118.28	110.41
2	D	144	LYS	N-CA-C	-6.40	104.35	111.71
1	B	209	ALA	N-CA-C	6.35	117.99	111.14
1	B	513	PHE	N-CA-C	-6.34	97.36	108.08
1	C	326	PRO	CA-C-O	-6.33	114.27	122.12
1	C	802	SER	N-CA-C	-6.31	104.45	111.71
1	C	163	LYS	N-CA-C	-6.31	104.40	111.28
1	C	896	SER	CB-CA-C	-6.28	100.98	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ILE	CB-CA-C	-6.28	101.47	110.83
1	B	331	PRO	N-CA-C	-6.27	104.81	113.53
1	B	60	THR	CA-C-N	-6.22	112.72	120.56
1	B	60	THR	C-N-CA	-6.22	112.72	120.56
1	C	74	ASN	N-CA-C	6.21	119.99	111.54
1	C	319	SER	CB-CA-C	-6.21	109.40	116.54
1	A	74	ASN	N-CA-C	6.21	120.18	112.24
1	B	62	THR	N-CA-C	6.21	118.12	111.36
1	B	222	THR	N-CA-C	-6.20	101.76	109.64
1	A	325	TYR	CA-C-N	6.17	126.07	119.28
1	A	325	TYR	C-N-CA	6.17	126.07	119.28
2	E	98	VAL	CB-CA-C	-6.15	104.09	111.97
1	A	813	SER	CA-C-N	6.15	125.55	118.85
1	A	813	SER	C-N-CA	6.15	125.55	118.85
2	E	152	ILE	N-CA-C	6.15	116.33	110.42
1	B	861	GLY	N-CA-C	-6.13	98.65	113.18
1	B	839	GLU	N-CA-C	6.12	117.74	111.14
1	B	425	LEU	CA-C-N	6.11	124.06	119.66
1	B	425	LEU	C-N-CA	6.11	124.06	119.66
1	C	743	ILE	N-CA-C	-6.11	103.42	111.05
1	B	671	ILE	CB-CA-C	-6.09	101.31	111.29
1	B	504	ASP	CA-C-N	-6.08	111.82	121.86
1	B	504	ASP	C-N-CA	-6.08	111.82	121.86
1	A	277	ILE	N-CA-C	6.05	116.64	108.17
1	B	98	THR	N-CA-C	-6.04	102.56	110.53
1	C	228	GLN	N-CA-C	-6.03	102.14	110.35
1	B	94	PHE	N-CA-C	6.03	119.77	110.42
1	B	195	LYS	N-CA-C	-6.00	104.74	111.28
1	C	143	ILE	N-CA-C	5.98	118.83	108.90
2	D	73	VAL	N-CA-C	-5.95	104.51	111.00
1	B	62	THR	CA-C-N	-5.95	111.84	120.29
1	B	62	THR	C-N-CA	-5.95	111.84	120.29
1	A	804	PHE	CB-CA-C	-5.94	101.44	110.83
1	B	500	ILE	N-CA-C	5.94	118.43	108.81
1	A	534	ILE	CB-CA-C	-5.94	104.03	112.22
1	B	83	ASP	N-CA-C	5.93	117.70	110.41
1	A	78	MET	N-CA-C	5.91	118.02	107.80
1	A	61	VAL	N-CA-CB	-5.86	106.84	111.64
2	D	50	PRO	CA-C-N	-5.84	111.99	120.29
2	D	50	PRO	C-N-CA	-5.84	111.99	120.29
1	B	508	GLY	N-CA-C	-5.84	105.75	112.29
1	C	787	GLY	N-CA-C	-5.84	108.25	114.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	ALA	N-CA-C	-5.83	104.92	111.28
1	B	495	THR	CB-CA-C	-5.83	100.80	110.37
1	B	383	LEU	N-CA-C	-5.83	104.93	111.28
1	B	52	ALA	N-CA-C	5.82	118.22	110.53
1	A	39	ALA	CA-C-N	5.82	123.85	119.66
1	A	39	ALA	C-N-CA	5.82	123.85	119.66
1	C	80	SER	N-CA-C	5.81	117.60	107.49
1	C	153	ASP	CA-C-N	-5.81	113.12	120.56
1	C	153	ASP	C-N-CA	-5.81	113.12	120.56
1	C	96	SER	N-CA-C	5.75	117.55	111.28
1	B	735	LYS	N-CA-C	-5.75	105.02	111.28
1	B	365	THR	CB-CA-C	-5.74	101.26	110.79
1	C	227	GLY	N-CA-C	5.74	123.24	115.32
1	C	508	GLY	N-CA-C	-5.73	107.28	115.64
1	A	698	ALA	N-CA-C	-5.71	105.06	111.28
1	C	997	SER	N-CA-C	-5.71	104.52	113.02
1	B	197	GLN	N-CA-C	-5.70	103.52	111.39
1	C	134	SER	N-CA-C	5.70	122.15	113.61
1	A	40	PRO	CB-CA-C	-5.69	105.82	111.17
2	E	96	VAL	CB-CA-C	-5.68	104.70	111.97
1	C	55	LYS	N-CA-C	5.65	117.52	111.36
1	B	631	LEU	N-CA-C	5.63	119.15	110.42
1	C	924	ASP	N-CA-C	-5.62	103.28	110.53
1	B	427	PRO	CA-C-N	-5.59	113.17	120.44
1	B	427	PRO	C-N-CA	-5.59	113.17	120.44
1	C	334	LYS	N-CA-C	5.59	117.46	111.36
1	A	806	SER	N-CA-C	-5.59	100.80	109.24
1	C	995	ALA	N-CA-C	-5.58	102.02	110.28
1	B	956	GLU	N-CA-C	5.58	119.78	112.92
1	A	493	CYS	N-CA-C	-5.58	105.20	111.28
1	B	862	MET	N-CA-C	-5.58	100.09	109.07
1	C	1032	ARG	CA-C-N	-5.57	115.35	123.93
1	C	1032	ARG	C-N-CA	-5.57	115.35	123.93
1	A	602	GLU	N-CA-C	5.57	119.06	112.72
1	C	170	SER	CB-CA-C	-5.57	100.98	109.89
1	C	506	GLY	N-CA-C	-5.57	108.35	115.42
1	B	57	VAL	CB-CA-C	-5.55	104.65	112.14
1	A	499	PRO	N-CA-C	-5.54	102.49	111.14
1	A	475	VAL	CB-CA-C	-5.54	104.58	112.22
1	C	693	GLU	N-CA-C	-5.54	105.24	111.28
1	C	669	PRO	CA-C-O	-5.53	115.14	121.56
1	B	996	GLY	CA-C-N	5.53	131.28	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	996	GLY	C-N-CA	5.53	131.28	120.99
1	C	352	PHE	N-CA-C	-5.53	105.25	111.28
1	A	495	THR	N-CA-C	5.52	120.17	113.38
1	A	475	VAL	N-CA-C	5.50	116.28	110.72
2	E	154	ILE	N-CA-C	-5.50	105.01	110.62
1	A	799	VAL	CB-CA-C	-5.50	104.61	110.16
1	B	225	VAL	CB-CA-C	-5.50	103.68	111.21
1	B	159	ALA	N-CA-C	5.48	117.25	111.28
1	A	792	ARG	N-CA-C	5.48	118.39	110.28
1	A	525	HIS	N-CA-C	-5.47	105.39	111.36
2	E	101	LYS	N-CA-C	-5.46	105.33	111.28
1	C	552	MET	N-CA-C	-5.45	105.45	111.71
1	B	846	GLN	N-CA-C	5.43	117.00	111.14
1	B	385	ALA	N-CA-C	5.43	117.95	111.71
1	B	670	ALA	N-CA-C	-5.43	102.25	110.28
1	B	782	LEU	CA-C-N	5.42	125.24	119.28
1	B	782	LEU	C-N-CA	5.42	125.24	119.28
1	B	847	LEU	N-CA-C	-5.42	104.77	111.33
1	A	918	PHE	N-CA-C	5.41	117.25	111.36
1	B	986	VAL	N-CA-C	5.40	120.41	113.07
2	D	91	GLY	N-CA-C	5.39	125.96	113.18
1	C	1001	ASN	N-CA-C	-5.39	105.41	111.28
1	C	801	PHE	N-CA-C	-5.39	106.54	113.01
1	C	629	VAL	CB-CA-C	-5.38	102.60	110.62
1	B	865	GLN	N-CA-C	-5.37	104.66	111.11
1	B	427	PRO	N-CA-C	5.37	121.75	113.75
1	C	226	LYS	N-CA-C	-5.36	102.45	110.23
1	A	658	ILE	N-CA-C	5.36	116.32	109.30
1	B	63	GLN	N-CA-C	5.36	117.20	111.36
1	B	39	ALA	CA-C-N	5.33	123.50	119.66
1	B	39	ALA	C-N-CA	5.33	123.50	119.66
1	B	510	LYS	N-CA-C	5.31	117.73	110.24
1	A	203	VAL	CB-CA-C	-5.30	104.98	112.14
1	C	236	ALA	CB-CA-C	-5.30	110.45	116.54
1	B	158	VAL	CB-CA-C	-5.29	104.99	112.14
1	C	873	ALA	N-CA-C	5.28	120.66	113.16
1	C	165	ALA	N-CA-C	5.26	117.01	111.28
1	B	56	THR	N-CA-C	-5.26	105.45	111.07
1	B	81	ASN	N-CA-C	5.21	116.91	108.26
1	B	680	PHE	N-CA-C	-5.21	101.84	109.81
1	C	890	ALA	N-CA-C	5.19	116.74	111.14
1	C	10	ILE	CB-CA-C	-5.18	105.14	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	PRO	CA-C-N	-5.18	113.39	120.44
1	A	427	PRO	C-N-CA	-5.18	113.39	120.44
1	B	277	ILE	CB-CA-C	-5.18	102.97	110.63
1	C	724	THR	CA-C-N	5.17	125.07	119.85
1	C	724	THR	C-N-CA	5.17	125.07	119.85
1	B	49	TYR	CA-C-N	5.16	125.96	119.98
1	B	49	TYR	C-N-CA	5.16	125.96	119.98
1	C	146	ASP	N-CA-C	5.15	118.67	112.38
1	C	739	LEU	N-CA-C	-5.15	103.59	110.55
1	A	276	ASP	N-CA-C	5.13	116.95	111.36
1	C	994	GLY	CA-C-N	-5.13	113.59	120.87
1	C	994	GLY	C-N-CA	-5.13	113.59	120.87
1	B	276	ASP	N-CA-C	5.13	116.87	111.28
1	A	722	GLU	N-CA-C	5.11	117.27	110.53
2	D	63	VAL	CB-CA-C	-5.10	105.44	111.97
1	A	40	PRO	O-C-N	5.10	123.55	121.15
1	A	288	GLY	N-CA-C	5.10	117.50	110.56
1	B	612	VAL	N-CA-C	5.09	114.95	107.15
1	C	160	ALA	CA-C-N	-5.09	113.98	122.08
1	C	160	ALA	C-N-CA	-5.09	113.98	122.08
1	A	304	ALA	N-CA-C	-5.09	105.73	111.28
1	A	717	ARG	N-CA-C	5.08	114.15	108.25
1	A	268	ILE	N-CA-C	5.08	116.05	108.54
1	C	1034	SER	N-CA-C	5.08	116.56	108.79
1	C	142	VAL	N-CA-C	5.06	117.11	108.86
1	B	990	VAL	CB-CA-C	-5.05	105.25	112.22
1	B	58	GLN	CA-C-N	-5.05	113.88	120.44
1	B	58	GLN	C-N-CA	-5.05	113.88	120.44
1	A	720	GLY	N-CA-C	-5.04	103.68	112.55
1	B	186	ILE	CB-CA-C	-5.02	104.21	111.19
1	B	644	VAL	CA-C-N	-5.02	113.56	120.28
1	B	644	VAL	C-N-CA	-5.02	113.56	120.28
1	C	429	GLU	N-CA-C	5.02	120.24	113.72
1	B	1011	MET	N-CA-C	5.01	116.55	111.14

There are no chirality outliers.

There are no planarity outliers.

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	7464	0	7440	697	0
1	B	7547	0	7469	895	0
1	C	7736	0	7730	872	0
2	D	1097	0	1008	146	0
2	E	1030	0	896	95	0
All	All	24874	0	24543	2636	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 53.

All (2636) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:C	1:A:235:ILE:HD13	1.18	1.55
1:B:563:PHE:C	1:B:564:LEU:HD12	1.33	1.53
1:C:314:GLU:HA	1:C:317:PHE:CE1	1.48	1.48
1:B:705:GLU:HG2	1:B:847:LEU:CD2	1.40	1.47
1:C:689:GLY:C	1:C:690:LEU:HD23	1.36	1.44
1:A:496:MET:C	1:A:497:LEU:HD23	1.44	1.41
1:B:919:ARG:NH1	1:B:919:ARG:HB3	1.39	1.38
1:B:222:THR:CG2	1:C:275:TYR:HB2	1.55	1.35
1:A:75:LEU:HD12	1:A:76:MET:N	1.39	1.34
1:A:808:ARG:NH1	1:A:808:ARG:HB2	1.42	1.34
1:C:671:ILE:CD1	1:C:674:LEU:HD11	1.59	1.33
1:B:250:LEU:HD23	1:B:251:LEU:N	1.43	1.32
2:D:56:TYR:CE1	2:D:90:ARG:HD3	1.64	1.31
1:B:197:GLN:CA	1:B:798:MET:HE3	1.61	1.30
1:B:270:LEU:HD23	1:B:271:GLY:N	1.46	1.30
1:B:799:VAL:HG13	1:B:800:PRO:CD	1.59	1.30
1:A:482:VAL:O	1:A:486:LEU:HD21	1.28	1.30
1:B:197:GLN:HA	1:B:798:MET:CE	1.61	1.29
1:A:234:ILE:C	1:A:235:ILE:CD1	2.05	1.29
1:A:721:LEU:CD1	1:A:814:PRO:HG3	1.62	1.29
1:C:154:ILE:HD12	1:C:154:ILE:C	1.56	1.27
1:B:960:LEU:HD23	1:B:960:LEU:O	1.33	1.27
1:C:185:ARG:HH12	1:C:774:MET:CE	1.48	1.27
1:B:270:LEU:HD23	1:B:270:LEU:C	1.49	1.26
1:C:879:ILE:O	1:C:879:ILE:HD12	1.35	1.26
1:C:741:VAL:CG1	1:C:746:ILE:HD11	1.64	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:750:LEU:HD23	1:C:750:LEU:C	1.59	1.25
2:E:152:ILE:C	2:E:152:ILE:HD12	1.62	1.24
1:B:960:LEU:HD23	1:B:960:LEU:C	1.59	1.24
2:D:56:TYR:CE1	2:D:90:ARG:CD	2.21	1.23
1:B:919:ARG:HH11	1:B:919:ARG:CB	1.51	1.23
2:D:51:LEU:HD23	2:D:51:LEU:O	1.34	1.23
2:D:56:TYR:HE1	2:D:90:ARG:CD	1.51	1.22
1:B:230:LEU:O	1:B:230:LEU:HD23	1.33	1.22
1:C:671:ILE:CG1	1:C:674:LEU:HD21	1.71	1.21
1:B:188:MET:HE2	1:B:773:VAL:CG2	1.69	1.20
1:B:799:VAL:CG1	1:B:800:PRO:HD2	1.70	1.20
1:B:562:SER:O	1:B:924:ASP:HA	1.39	1.19
1:B:668:LEU:C	1:B:668:LEU:HD12	1.67	1.19
1:B:668:LEU:HD12	1:B:668:LEU:O	1.39	1.19
1:C:750:LEU:HD23	1:C:750:LEU:O	1.34	1.19
2:D:18:LEU:HD23	2:D:18:LEU:O	1.42	1.19
2:D:129:VAL:O	2:D:133:LEU:HD12	1.38	1.19
1:A:488:LEU:HD12	1:A:488:LEU:O	1.40	1.19
1:A:428:LYS:O	1:A:431:THR:HG22	1.39	1.19
1:C:607:GLU:OE2	1:C:632:LYS:HG2	1.38	1.18
1:C:671:ILE:HD11	1:C:674:LEU:CD1	1.71	1.18
1:C:154:ILE:HD12	1:C:154:ILE:O	1.37	1.18
1:C:879:ILE:HD12	1:C:879:ILE:C	1.62	1.18
1:B:230:LEU:HD23	1:B:230:LEU:C	1.60	1.18
2:E:46:VAL:HG13	2:E:47:GLY:H	1.02	1.18
1:C:674:LEU:H	1:C:674:LEU:CD2	1.52	1.17
1:C:314:GLU:HA	1:C:317:PHE:CD1	1.79	1.16
1:B:188:MET:CE	1:B:773:VAL:HG22	1.74	1.16
1:C:688:ALA:HB3	1:C:690:LEU:HD21	1.20	1.16
1:A:423:GLU:CA	1:A:502:LYS:HE3	1.76	1.16
1:A:486:LEU:H	1:A:486:LEU:CD2	1.52	1.16
1:A:721:LEU:CD1	1:A:814:PRO:CG	2.24	1.16
1:B:254:ASN:HD22	1:B:258:SER:HB3	1.11	1.16
1:C:960:LEU:O	1:C:960:LEU:HD13	1.43	1.16
1:A:498:LYS:HE3	1:A:498:LYS:O	1.45	1.15
1:A:519:MET:SD	1:A:519:MET:C	2.30	1.15
1:B:989:LEU:HD23	1:B:1000:GLN:HG2	1.26	1.15
1:A:808:ARG:CB	1:A:808:ARG:HH11	1.61	1.14
1:B:705:GLU:HG2	1:B:847:LEU:HD22	1.26	1.14
2:D:53:LEU:H	2:D:53:LEU:CD2	1.58	1.14
1:A:478:MET:O	1:A:482:VAL:HG23	1.45	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:MET:HG3	1:C:575:MET:O	1.43	1.14
1:B:197:GLN:CA	1:B:798:MET:CE	2.22	1.13
1:C:144:ASN:HD22	1:C:149:MET:CB	1.60	1.13
1:A:486:LEU:HD22	1:A:486:LEU:N	1.60	1.13
1:B:193:LEU:HD23	1:B:193:LEU:N	1.52	1.13
1:B:563:PHE:C	1:B:564:LEU:CD1	2.19	1.13
1:C:674:LEU:HD22	1:C:674:LEU:N	1.59	1.13
1:B:991:ILE:HD12	1:B:991:ILE:O	1.49	1.12
1:C:435:MET:HA	1:C:435:MET:HE3	1.24	1.12
1:B:222:THR:HG21	1:C:275:TYR:HB2	1.26	1.12
2:D:61:GLU:O	2:D:65:VAL:HG23	1.49	1.12
1:A:931:LEU:O	1:A:935:ILE:HG22	1.50	1.11
1:C:739:LEU:HD13	1:C:739:LEU:N	1.50	1.11
1:B:705:GLU:CG	1:B:847:LEU:CD2	2.28	1.11
1:B:848:ALA:HA	1:B:851:LEU:CD1	1.79	1.11
1:A:360:GLN:HG2	1:A:513:PHE:CZ	1.84	1.11
1:A:486:LEU:N	1:A:486:LEU:HD13	1.59	1.11
1:B:649:MET:HA	1:B:649:MET:HE3	1.21	1.11
2:E:112:ASN:O	2:E:144:LYS:HG2	1.51	1.11
1:C:83:ASP:HB3	1:C:85:THR:HG23	1.24	1.10
1:B:222:THR:CG2	1:C:275:TYR:CB	2.28	1.10
1:C:879:ILE:HD11	1:C:883:VAL:HG23	1.30	1.10
1:B:188:MET:HE2	1:B:773:VAL:HG22	1.16	1.10
1:C:671:ILE:HG13	1:C:671:ILE:O	1.41	1.10
1:C:200:PRO:CD	1:C:749:THR:HG23	1.79	1.10
1:C:447:MET:SD	1:C:891:LEU:HD21	1.91	1.09
1:A:971:ARG:O	1:A:974:PRO:HD2	1.52	1.09
1:B:534:ILE:HG13	1:B:541:TYR:CE2	1.87	1.09
1:C:741:VAL:HG13	1:C:746:ILE:CD1	1.81	1.09
2:D:51:LEU:HD23	2:D:51:LEU:C	1.71	1.09
1:A:234:ILE:O	1:A:235:ILE:CD1	2.00	1.09
1:A:971:ARG:HH11	1:A:971:ARG:HG3	1.06	1.08
1:C:497:LEU:HD23	1:C:498:LYS:H	1.03	1.08
1:C:671:ILE:HD11	1:C:674:LEU:HD11	1.10	1.08
1:A:721:LEU:HD12	1:A:814:PRO:HG3	1.31	1.08
1:B:182:TYR:HB3	1:B:270:LEU:HD11	1.31	1.08
1:C:144:ASN:ND2	1:C:149:MET:HB2	1.68	1.08
1:C:435:MET:HA	1:C:435:MET:CE	1.84	1.08
2:E:152:ILE:HD12	2:E:152:ILE:O	1.53	1.08
1:A:971:ARG:HH11	1:A:971:ARG:CG	1.67	1.08
1:B:871:ASN:HB3	1:B:872:GLN:HG2	1.35	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:HD13	1:A:235:ILE:N	1.57	1.07
1:A:379:THR:O	1:A:383:LEU:HD23	1.50	1.07
1:C:919:ARG:HH12	1:C:990:VAL:HG12	1.20	1.07
1:B:671:ILE:HD13	1:B:671:ILE:O	1.52	1.07
1:A:498:LYS:HD3	1:A:498:LYS:H	1.14	1.07
1:A:808:ARG:HB2	1:A:808:ARG:HH11	0.91	1.07
1:B:534:ILE:HG13	1:B:541:TYR:CZ	1.89	1.07
1:B:649:MET:HA	1:B:649:MET:CE	1.82	1.07
1:A:721:LEU:HD12	1:A:814:PRO:CG	1.84	1.06
1:B:717:ARG:HG2	1:B:717:ARG:HH11	0.95	1.06
1:B:194:ASN:ND2	1:B:790:TYR:CG	2.22	1.06
1:B:250:LEU:HD23	1:B:250:LEU:C	1.76	1.06
1:B:658:ILE:CD1	1:B:658:ILE:H	1.67	1.06
1:A:519:MET:SD	1:A:520:PHE:N	2.29	1.06
1:B:182:TYR:CB	1:B:270:LEU:HD11	1.84	1.06
1:C:11:PHE:O	1:C:11:PHE:HD1	1.38	1.05
1:C:689:GLY:C	1:C:690:LEU:CD2	2.29	1.05
1:C:54:ALA:HB2	1:C:814:PRO:O	1.55	1.05
1:A:411:VAL:HG21	1:A:971:ARG:HH21	1.09	1.05
1:B:270:LEU:C	1:B:270:LEU:CD2	2.29	1.05
1:B:712:MET:C	1:B:713:LEU:CD1	2.30	1.05
1:B:712:MET:O	1:B:713:LEU:HD12	1.56	1.05
2:E:92:HIS:O	2:E:96:VAL:HG23	1.55	1.05
1:B:960:LEU:C	1:B:960:LEU:CD2	2.30	1.04
1:C:200:PRO:HD2	1:C:749:THR:HG23	1.08	1.04
1:C:623:ASN:C	1:C:623:ASN:HD22	1.65	1.04
1:B:207:ILE:HG22	1:B:760:ASN:ND2	1.72	1.04
2:E:112:ASN:HA	2:E:144:LYS:HE2	1.40	1.04
1:C:570:GLY:O	1:C:571:VAL:HG12	1.55	1.04
1:A:527:TYR:CE1	1:A:972:LEU:HD23	1.92	1.03
1:C:44:THR:HB	1:C:132:SER:OG	1.57	1.03
1:B:874:PRO:HB2	1:B:877:TYR:HD2	1.22	1.03
1:B:874:PRO:CB	1:B:877:TYR:HD2	1.70	1.03
1:C:497:LEU:CD2	1:C:498:LYS:H	1.69	1.03
1:C:567:GLU:OE1	1:C:998:GLY:HA3	1.59	1.03
1:A:498:LYS:H	1:A:498:LYS:CD	1.64	1.03
1:B:222:THR:HG22	1:C:275:TYR:HB2	1.39	1.03
2:D:18:LEU:HD23	2:D:18:LEU:C	1.81	1.02
1:C:314:GLU:CA	1:C:317:PHE:CE1	2.43	1.02
1:A:935:ILE:HD12	1:A:935:ILE:O	1.59	1.02
1:B:119:PRO:O	1:B:123:GLN:HG3	1.59	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:HD12	1:A:240:LEU:N	1.68	1.02
1:C:447:MET:HE1	1:C:891:LEU:HD23	1.40	1.02
1:C:671:ILE:HG13	1:C:674:LEU:HD21	1.05	1.02
1:A:360:GLN:HG2	1:A:513:PHE:HZ	1.15	1.02
1:B:156:ASP:CB	1:B:182:TYR:CE2	2.43	1.02
1:B:158:VAL:HA	1:B:162:MET:HG3	1.40	1.02
1:B:194:ASN:ND2	1:B:790:TYR:CD2	2.25	1.02
2:D:56:TYR:HE1	2:D:90:ARG:HD3	0.97	1.02
1:B:705:GLU:CG	1:B:847:LEU:HD22	1.88	1.01
1:C:989:LEU:HD22	1:C:1000:GLN:HB3	1.42	1.01
2:D:56:TYR:CE1	2:D:90:ARG:NE	2.26	1.01
1:B:204:ILE:O	1:B:208:LYS:HG3	1.58	1.01
1:B:250:LEU:C	1:B:250:LEU:CD2	2.30	1.01
2:D:53:LEU:H	2:D:53:LEU:HD23	1.18	1.01
2:E:152:ILE:HG13	2:E:153:SER:N	1.73	1.01
1:B:197:GLN:C	1:B:798:MET:CE	2.32	1.01
1:B:471:SER:O	1:B:475:VAL:HG12	1.61	1.01
1:B:672:VAL:O	1:B:672:VAL:HG22	1.53	1.01
1:C:673:GLU:H	1:C:673:GLU:CD	1.69	1.01
1:C:83:ASP:HB3	1:C:85:THR:CG2	1.91	1.01
1:C:879:ILE:CD1	1:C:883:VAL:HG23	1.90	1.01
1:A:73:ASP:HB3	1:A:74:ASN:OD1	1.60	1.00
1:C:497:LEU:HD23	1:C:498:LYS:N	1.74	1.00
1:C:896:SER:OG	1:C:897:ILE:HD12	1.61	1.00
1:C:671:ILE:HG13	1:C:674:LEU:CD2	1.91	1.00
2:E:93:LEU:CD2	2:E:128:ILE:HG12	1.92	1.00
1:B:799:VAL:CG1	1:B:800:PRO:CD	2.33	1.00
1:C:434:SER:O	1:C:438:ILE:HG12	1.60	1.00
1:B:164:ASP:O	1:B:168:ARG:HG3	1.62	1.00
1:A:423:GLU:HA	1:A:502:LYS:HE3	1.01	0.99
1:A:497:LEU:HD23	1:A:497:LEU:N	1.58	0.99
1:B:758:TYR:HB2	1:B:772:TYR:CE1	1.97	0.99
1:C:568:ASP:OD2	1:C:644:VAL:HG13	1.61	0.99
1:C:741:VAL:HG13	1:C:746:ILE:HD11	1.00	0.99
1:C:314:GLU:O	1:C:317:PHE:HD1	1.42	0.99
2:D:44:ASP:OD1	2:D:45:HIS:CB	2.10	0.99
1:C:185:ARG:HH12	1:C:774:MET:HE3	1.26	0.99
1:C:196:PHE:C	1:C:197:GLN:HG2	1.87	0.99
1:B:726:GLN:HE22	1:B:812:GLY:HA3	1.25	0.99
1:C:158:VAL:HA	1:C:162:MET:HE3	1.45	0.99
1:C:750:LEU:C	1:C:750:LEU:CD2	2.30	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:THR:HG21	1:C:275:TYR:CB	1.90	0.98
1:C:146:ASP:CB	1:C:148:THR:CG2	2.40	0.98
1:C:325:TYR:N	1:C:325:TYR:CD1	2.30	0.98
1:C:721:LEU:HD23	1:C:721:LEU:N	1.77	0.98
1:A:496:MET:C	1:A:497:LEU:CD2	2.36	0.98
1:C:144:ASN:HD22	1:C:149:MET:HB2	0.84	0.98
1:C:688:ALA:CB	1:C:690:LEU:HD21	1.94	0.98
1:C:200:PRO:HD2	1:C:749:THR:CG2	1.93	0.98
1:B:658:ILE:HD12	1:B:658:ILE:N	1.78	0.98
1:B:229:GLN:H	1:B:229:GLN:CD	1.64	0.98
1:C:736:ALA:O	1:C:741:VAL:HB	1.63	0.98
1:B:190:PRO:HG3	1:B:789:TRP:CH2	1.99	0.97
2:E:100:LEU:HD21	2:E:106:VAL:HG12	1.47	0.97
1:A:355:MET:HE2	1:A:368:PRO:HG2	1.47	0.97
1:B:193:LEU:HD23	1:B:193:LEU:H	1.29	0.97
2:E:152:ILE:C	2:E:152:ILE:CD1	2.30	0.97
1:B:511:GLY:HA2	1:B:513:PHE:O	1.64	0.96
1:C:960:LEU:HD13	1:C:960:LEU:C	1.90	0.96
1:A:527:TYR:CE1	1:A:972:LEU:CD2	2.48	0.96
1:C:154:ILE:C	1:C:154:ILE:CD1	2.32	0.96
1:C:879:ILE:HD11	1:C:883:VAL:CG2	1.95	0.96
1:B:207:ILE:CG2	1:B:760:ASN:ND2	2.27	0.96
1:A:32:VAL:HG12	1:A:390:ILE:HB	1.47	0.96
1:B:948:PHE:HE2	1:B:971:ARG:HE	1.02	0.96
1:B:61:VAL:O	1:B:65:ILE:HG13	1.66	0.96
1:B:69:MET:CE	1:B:72:ILE:HD11	1.96	0.96
1:B:422:GLU:C	1:B:423:GLU:HG2	1.87	0.96
1:B:712:MET:C	1:B:713:LEU:HD13	1.91	0.96
1:C:741:VAL:CG1	1:C:746:ILE:CD1	2.38	0.96
1:A:411:VAL:CG2	1:A:971:ARG:HH21	1.79	0.95
1:B:685:ILE:HG22	1:B:686:ASP:N	1.80	0.95
1:C:671:ILE:HD11	1:C:674:LEU:CG	1.95	0.95
1:A:498:LYS:N	1:A:498:LYS:CE	2.30	0.95
1:C:506:GLY:C	1:C:507:GLU:HG2	1.88	0.95
2:D:44:ASP:OD1	2:D:45:HIS:HB3	1.65	0.95
1:B:459:PHE:HB2	1:B:464:GLY:HA2	1.48	0.95
1:C:314:GLU:CA	1:C:317:PHE:HE1	1.77	0.95
1:A:527:TYR:O	1:A:531:VAL:HG23	1.64	0.95
1:B:207:ILE:CG2	1:B:760:ASN:HD22	1.79	0.95
1:B:361:ASN:H	1:B:361:ASN:HD22	1.01	0.95
1:A:423:GLU:HA	1:A:502:LYS:CE	1.95	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:671:ILE:CD1	1:C:674:LEU:HD21	1.96	0.95
2:E:46:VAL:HG13	2:E:47:GLY:N	1.82	0.94
2:D:14:LEU:H	2:D:14:LEU:HD12	1.31	0.94
1:C:919:ARG:HG3	1:C:919:ARG:O	1.67	0.94
1:B:717:ARG:HH11	1:B:717:ARG:CG	1.77	0.94
1:B:361:ASN:HD22	1:B:361:ASN:N	1.60	0.94
1:B:799:VAL:HG13	1:B:800:PRO:HD2	0.96	0.94
1:C:1:FME:N	1:C:2:PRO:CD	2.30	0.94
1:C:875:SER:O	1:C:879:ILE:HG22	1.68	0.94
1:C:976:LEU:O	1:C:980:LEU:HD23	1.66	0.94
1:B:685:ILE:CG2	1:B:686:ASP:N	2.29	0.94
1:A:973:ARG:O	1:A:977:MET:HG3	1.68	0.93
1:C:447:MET:SD	1:C:891:LEU:CD2	2.55	0.93
1:C:960:LEU:HD11	1:C:1027:VAL:HG22	1.47	0.93
1:A:480:LEU:O	1:A:484:VAL:HG23	1.67	0.93
1:B:196:PHE:HA	1:B:197:GLN:HE22	1.34	0.93
1:C:739:LEU:N	1:C:739:LEU:CD1	2.30	0.93
1:B:102:ILE:CG2	1:B:103:ALA:N	2.32	0.93
1:B:717:ARG:HG2	1:B:717:ARG:NH1	1.76	0.93
1:C:439:GLN:HA	1:C:442:LEU:HD12	1.49	0.93
1:C:4:PHE:O	1:C:4:PHE:HD2	1.49	0.93
1:B:678:THR:HG22	1:B:678:THR:O	1.65	0.93
1:C:690:LEU:HD23	1:C:690:LEU:N	1.84	0.93
1:C:733:GLN:HE22	1:C:743:ILE:HG21	1.34	0.93
1:B:230:LEU:C	1:B:230:LEU:CD2	2.37	0.93
1:B:712:MET:C	1:B:713:LEU:HD12	1.91	0.92
1:C:185:ARG:NH1	1:C:774:MET:CE	2.32	0.92
1:B:1:FME:CE	1:B:487:ILE:HD11	1.98	0.92
1:B:705:GLU:HG2	1:B:847:LEU:HD23	1.47	0.92
1:C:144:ASN:ND2	1:C:149:MET:CB	2.28	0.92
1:B:117:LEU:CD1	1:B:117:LEU:N	2.30	0.92
1:C:896:SER:OG	1:C:897:ILE:N	1.98	0.92
1:A:486:LEU:H	1:A:486:LEU:HD22	0.76	0.92
1:B:726:GLN:NE2	1:B:812:GLY:HA3	1.84	0.92
1:B:352:PHE:HD1	1:B:365:THR:HG1	0.97	0.92
1:C:68:ASN:HD22	1:C:114:ALA:HB2	1.35	0.92
1:B:563:PHE:O	1:B:564:LEU:HG	1.69	0.92
1:C:327:TYR:HD2	1:C:327:TYR:O	1.53	0.92
1:A:758:TYR:CD1	1:A:758:TYR:C	2.46	0.92
1:B:234:ILE:O	1:B:235:ILE:CD1	2.18	0.92
1:C:200:PRO:CD	1:C:749:THR:CG2	2.46	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:VAL:O	1:A:901:VAL:HG12	1.68	0.92
1:B:117:LEU:N	1:B:117:LEU:HD13	1.84	0.91
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.32	0.91
1:B:240:LEU:HD23	1:B:245:GLU:HB3	1.48	0.91
1:B:739:LEU:HD13	1:B:799:VAL:HG21	1.52	0.91
1:C:738:ALA:C	1:C:739:LEU:HD13	1.95	0.91
2:D:18:LEU:C	2:D:18:LEU:CD2	2.40	0.91
1:A:971:ARG:HG3	1:A:971:ARG:NH1	1.76	0.91
1:B:765:ARG:HB3	1:B:765:ARG:HH11	1.34	0.91
1:A:488:LEU:HD12	1:A:488:LEU:C	1.93	0.91
1:B:190:PRO:HG3	1:B:789:TRP:CZ2	2.06	0.91
1:B:197:GLN:HA	1:B:798:MET:HE3	0.91	0.91
1:B:234:ILE:C	1:B:235:ILE:HD13	1.96	0.91
1:C:146:ASP:CB	1:C:148:THR:HG23	2.01	0.91
1:C:447:MET:CE	1:C:891:LEU:CD2	2.48	0.91
1:A:904:VAL:O	1:A:904:VAL:HG22	1.67	0.91
1:B:563:PHE:O	1:B:564:LEU:CD1	2.17	0.91
1:A:240:LEU:N	1:A:240:LEU:CD1	2.33	0.91
1:B:874:PRO:HG2	1:B:874:PRO:O	1.68	0.90
2:D:53:LEU:CD2	2:D:53:LEU:N	2.30	0.90
1:A:358:PHE:CD1	1:A:977:MET:HE3	2.06	0.90
2:E:152:ILE:CG1	2:E:153:SER:N	2.33	0.90
1:B:705:GLU:HG2	1:B:847:LEU:HD21	1.50	0.90
1:C:83:ASP:CB	1:C:85:THR:HG23	2.01	0.90
1:C:960:LEU:C	1:C:960:LEU:CD1	2.43	0.90
1:C:497:LEU:CD2	1:C:498:LYS:N	2.30	0.90
1:C:674:LEU:H	1:C:674:LEU:HD22	0.73	0.90
1:B:361:ASN:H	1:B:361:ASN:ND2	1.66	0.90
1:B:563:PHE:O	1:B:564:LEU:CG	2.19	0.90
1:B:196:PHE:C	1:B:197:GLN:NE2	2.30	0.90
1:B:362:PHE:O	1:B:365:THR:HG22	1.72	0.90
1:A:298:ASN:ND2	1:A:301:ASP:H	1.70	0.89
1:C:268:ILE:HD13	1:C:268:ILE:N	1.85	0.89
1:C:84:SER:HB3	1:C:814:PRO:O	1.72	0.89
1:A:721:LEU:HD11	1:A:814:PRO:CG	2.02	0.89
1:B:193:LEU:N	1:B:193:LEU:CD2	2.30	0.89
1:A:248:LYS:O	1:A:261:LEU:HD23	1.73	0.89
1:B:874:PRO:HB2	1:B:877:TYR:CD2	2.07	0.89
2:D:125:HIS:ND1	2:D:128:ILE:HG13	1.88	0.89
1:B:815:ARG:HG2	1:B:815:ARG:HH11	1.38	0.89
1:A:431:THR:HG23	1:A:432:ARG:N	1.87	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:THR:CG2	1:A:432:ARG:N	2.36	0.88
1:C:54:ALA:CB	1:C:814:PRO:O	2.21	0.88
1:A:758:TYR:C	1:A:758:TYR:HD1	1.80	0.88
1:B:197:GLN:CD	1:B:197:GLN:N	2.30	0.88
1:C:896:SER:OG	1:C:897:ILE:CD1	2.20	0.88
2:D:49:THR:O	2:D:53:LEU:CD2	2.20	0.88
1:C:993:THR:HG23	1:C:993:THR:O	1.73	0.88
1:A:519:MET:C	1:A:519:MET:HE2	1.98	0.88
1:B:150:THR:HG23	1:B:153:ASP:OD2	1.72	0.88
2:E:94:GLU:O	2:E:98:VAL:HG23	1.73	0.88
1:A:218:GLN:HB2	1:A:233:SER:HA	1.56	0.88
1:C:185:ARG:HH12	1:C:774:MET:HE2	1.37	0.88
2:E:97:GLU:OE1	2:E:97:GLU:HA	1.71	0.88
1:A:534:ILE:HA	1:A:541:TYR:HE1	1.39	0.88
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.52	0.88
1:C:689:GLY:O	1:C:690:LEU:HD23	1.73	0.88
1:C:810:GLU:C	1:C:811:TYR:HD2	1.81	0.88
1:A:75:LEU:HD12	1:A:76:MET:H	0.98	0.88
1:A:234:ILE:O	1:A:235:ILE:HD12	1.74	0.88
1:B:196:PHE:C	1:B:197:GLN:CD	2.42	0.88
1:B:169:THR:HG22	1:B:172:VAL:HG13	1.56	0.87
1:A:67:GLN:HE21	1:C:767:ARG:NH1	1.72	0.87
1:A:519:MET:SD	1:A:520:PHE:CA	2.61	0.87
1:B:564:LEU:HD12	1:B:564:LEU:N	1.89	0.87
1:A:32:VAL:CG1	1:A:390:ILE:HB	2.04	0.87
1:A:482:VAL:O	1:A:486:LEU:CD2	2.21	0.87
1:A:491:ALA:O	1:A:495:THR:HG23	1.75	0.87
2:D:73:VAL:CG1	2:D:74:ASN:N	2.37	0.87
1:B:705:GLU:CB	1:B:847:LEU:HD22	2.04	0.87
1:A:524:THR:O	1:A:528:THR:HG23	1.75	0.87
1:A:971:ARG:C	1:A:974:PRO:HD2	1.99	0.87
1:B:853:THR:C	1:B:857:TYR:N	2.33	0.87
1:B:166:ILE:HG22	1:B:175:VAL:HG21	1.57	0.86
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.57	0.86
2:D:126:LEU:HA	2:D:129:VAL:HG21	1.56	0.86
1:A:519:MET:C	1:A:519:MET:CE	2.48	0.86
1:B:658:ILE:CD1	1:B:658:ILE:N	2.30	0.86
1:C:144:ASN:ND2	1:C:149:MET:HG3	1.90	0.86
1:A:519:MET:SD	1:A:520:PHE:HA	2.16	0.86
1:C:325:TYR:N	1:C:325:TYR:HD1	1.73	0.86
1:A:496:MET:O	1:A:497:LEU:HD23	1.73	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ILE:HG21	1:B:940:LYS:HG3	1.55	0.86
1:A:780:ARG:O	1:A:780:ARG:HG3	1.74	0.86
1:B:137:LEU:HD22	1:B:293:LEU:HD12	1.58	0.86
1:C:200:PRO:HG2	1:C:749:THR:HG22	1.56	0.86
1:C:989:LEU:CD2	1:C:1000:GLN:HB3	2.06	0.86
2:D:51:LEU:C	2:D:51:LEU:CD2	2.47	0.86
1:B:160:ALA:C	1:B:161:ASN:HD22	1.83	0.86
1:A:498:LYS:CD	1:A:498:LYS:N	2.35	0.85
1:B:563:PHE:CA	1:B:564:LEU:HD12	2.06	0.85
1:B:69:MET:HE3	1:B:72:ILE:HD11	1.58	0.85
1:C:735:LYS:O	1:C:739:LEU:HD22	1.76	0.85
1:A:75:LEU:CD1	1:A:76:MET:N	2.33	0.85
1:C:15:ILE:O	1:C:19:ILE:HG12	1.76	0.85
2:D:49:THR:O	2:D:53:LEU:HD21	1.77	0.85
2:D:56:TYR:O	2:D:56:TYR:CD1	2.29	0.85
1:A:758:TYR:CD1	1:A:758:TYR:O	2.29	0.85
1:B:348:ILE:HG21	1:B:369:THR:HG23	1.58	0.85
1:B:762:PHE:HE1	1:B:764:ASP:HB2	1.40	0.85
1:C:211:ASN:HD22	1:C:760:ASN:ND2	1.74	0.85
1:B:154:ILE:O	1:B:158:VAL:HG23	1.77	0.85
1:C:671:ILE:O	1:C:674:LEU:CD2	2.25	0.85
1:C:4:PHE:C	1:C:4:PHE:CD2	2.51	0.85
1:C:573:MET:HE3	1:C:626:ILE:HD11	1.59	0.85
1:B:420:MET:HE1	1:B:499:PRO:HA	1.59	0.85
1:C:4:PHE:O	1:C:4:PHE:CD2	2.30	0.85
1:C:154:ILE:HD11	1:C:287:SER:HB3	1.56	0.85
1:C:237:GLN:O	1:C:238:THR:HG23	1.77	0.85
1:A:749:THR:HG21	1:A:791:VAL:HG11	1.57	0.84
1:B:495:THR:HG22	1:B:496:MET:N	1.92	0.84
1:B:948:PHE:HE2	1:B:971:ARG:NE	1.73	0.84
1:C:671:ILE:HD12	1:C:674:LEU:HD11	1.59	0.84
2:E:73:VAL:HG12	2:E:104:ALA:HB2	1.58	0.84
1:C:447:MET:HE1	1:C:891:LEU:CD2	2.06	0.84
1:C:447:MET:CE	1:C:891:LEU:HD23	2.07	0.84
2:E:56:TYR:CD1	2:E:56:TYR:O	2.30	0.84
1:A:790:TYR:HB3	1:A:798:MET:HB3	1.59	0.84
2:E:144:LYS:O	2:E:145:PHE:CG	2.31	0.84
1:A:75:LEU:CD1	1:A:76:MET:H	1.87	0.84
1:B:207:ILE:HG22	1:B:760:ASN:HD21	1.42	0.84
1:B:561:SER:HB2	1:B:923:ASN:HB3	1.58	0.84
1:C:327:TYR:O	1:C:327:TYR:CD2	2.30	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:ILE:H	1:B:658:ILE:HD13	1.42	0.84
1:C:11:PHE:HD1	1:C:11:PHE:C	1.85	0.84
2:E:46:VAL:CG1	2:E:47:GLY:H	1.87	0.84
1:A:558:ARG:C	1:A:558:ARG:CD	2.50	0.84
1:B:563:PHE:O	1:B:564:LEU:HD12	1.75	0.84
1:C:876:LEU:C	1:C:876:LEU:CD2	2.50	0.84
1:C:879:ILE:C	1:C:879:ILE:CD1	2.38	0.83
2:E:144:LYS:O	2:E:145:PHE:CD2	2.30	0.83
1:B:281:PHE:HD1	1:B:610:PHE:HD1	1.26	0.83
1:C:185:ARG:NH1	1:C:774:MET:HE3	1.92	0.83
2:D:56:TYR:CD1	2:D:90:ARG:NE	2.45	0.83
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.60	0.83
1:A:486:LEU:N	1:A:486:LEU:CD1	2.30	0.83
1:B:885:PHE:HD1	1:B:902:MET:HE1	1.42	0.83
1:A:190:PRO:HG2	1:A:779:TYR:HB3	1.59	0.83
1:A:974:PRO:O	1:A:978:THR:HG23	1.77	0.83
1:B:229:GLN:OE1	1:B:230:LEU:N	2.11	0.83
1:B:837:THR:O	1:B:841:MET:HG3	1.78	0.83
1:B:1027:VAL:O	1:B:1031:ARG:HG2	1.78	0.83
2:D:125:HIS:O	2:D:129:VAL:HG22	1.78	0.83
1:B:53:ASP:O	1:B:57:VAL:HG23	1.78	0.83
1:B:250:LEU:CD2	1:B:251:LEU:N	2.34	0.83
1:C:11:PHE:O	1:C:11:PHE:CD1	2.30	0.83
1:A:411:VAL:HG21	1:A:971:ARG:NH2	1.94	0.83
1:B:1:FME:HE2	1:B:487:ILE:HD11	1.58	0.83
1:B:102:ILE:HG22	1:B:103:ALA:H	1.44	0.83
1:A:488:LEU:CD1	1:A:492:LEU:HD13	2.09	0.83
1:B:182:TYR:CG	1:B:270:LEU:HD11	2.13	0.82
1:B:254:ASN:ND2	1:B:258:SER:HB3	1.93	0.82
1:C:435:MET:CE	1:C:435:MET:CA	2.55	0.82
2:D:56:TYR:CD1	2:D:90:ARG:HG3	2.13	0.82
1:B:671:ILE:O	1:B:671:ILE:HG23	1.77	0.82
1:A:485:ALA:C	1:A:486:LEU:HD13	2.03	0.82
1:C:623:ASN:C	1:C:623:ASN:ND2	2.34	0.82
1:C:758:TYR:CE2	1:C:770:LYS:HB3	2.14	0.82
1:B:562:SER:O	1:B:924:ASP:CA	2.25	0.82
1:A:488:LEU:HD12	1:A:492:LEU:HD13	1.59	0.82
1:A:498:LYS:HE3	1:A:498:LYS:N	1.94	0.82
1:B:234:ILE:O	1:B:235:ILE:HD12	1.79	0.82
1:C:200:PRO:HG2	1:C:749:THR:CG2	2.09	0.82
2:D:44:ASP:OD1	2:D:45:HIS:CA	2.28	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:989:LEU:CD2	1:B:1000:GLN:HG2	2.09	0.82
1:A:558:ARG:O	1:A:558:ARG:HD2	1.79	0.82
1:C:733:GLN:NE2	1:C:743:ILE:HG21	1.94	0.82
1:C:157:TYR:C	1:C:157:TYR:CD2	2.58	0.82
1:A:445:ILE:HG21	1:A:940:LYS:HE2	1.62	0.81
1:A:519:MET:HE2	1:A:519:MET:O	1.80	0.81
1:B:563:PHE:CB	1:B:564:LEU:HD12	2.10	0.81
1:C:671:ILE:CD1	1:C:674:LEU:CD1	2.42	0.81
1:A:680:PHE:CZ	1:A:829:GLY:HA3	2.15	0.81
1:B:605:ASN:O	1:B:631:LEU:HD22	1.79	0.81
1:B:731:ILE:O	1:B:731:ILE:HG12	1.79	0.81
1:C:138:MET:HE2	1:C:140:VAL:HG23	1.61	0.81
2:D:56:TYR:CD1	2:D:90:ARG:CD	2.63	0.81
1:A:75:LEU:HD12	1:A:75:LEU:C	1.86	0.81
1:B:354:VAL:HG21	1:B:981:ALA:HB2	1.63	0.81
1:C:11:PHE:C	1:C:11:PHE:CD1	2.57	0.81
1:B:447:MET:HA	1:B:447:MET:HE2	1.62	0.81
1:B:587:THR:HG21	1:B:622:GLN:O	1.81	0.81
1:B:674:LEU:O	1:B:674:LEU:HD13	1.80	0.81
1:C:71:GLY:O	1:C:72:ILE:HG12	1.81	0.81
1:C:733:GLN:OE1	1:C:743:ILE:HD13	1.81	0.81
1:A:1:FME:N	1:A:2:PRO:CD	2.43	0.81
1:C:980:LEU:N	1:C:980:LEU:HD22	1.95	0.81
1:A:685:ILE:HD13	1:A:685:ILE:H	1.45	0.81
1:C:512:PHE:CD1	1:C:512:PHE:O	2.34	0.81
1:B:527:TYR:HE2	1:B:968:VAL:HG13	1.45	0.81
1:A:182:TYR:CD2	1:A:270:LEU:HD23	2.14	0.80
1:A:485:ALA:O	1:A:490:PRO:CD	2.29	0.80
1:B:775:SER:OG	1:B:780:ARG:HG2	1.80	0.80
1:A:519:MET:CE	1:A:519:MET:O	2.30	0.80
1:B:224:PRO:HA	1:C:781:MET:HE1	1.64	0.80
1:B:671:ILE:O	1:B:672:VAL:CG1	2.30	0.80
1:B:362:PHE:O	1:B:365:THR:CG2	2.30	0.80
1:B:561:SER:CB	1:B:923:ASN:HB3	2.10	0.80
1:B:668:LEU:C	1:B:668:LEU:CD1	2.46	0.80
1:C:85:THR:OG1	1:C:87:THR:HG23	1.80	0.80
2:D:73:VAL:CG1	2:D:74:ASN:OD1	2.28	0.80
1:A:379:THR:O	1:A:383:LEU:CD2	2.30	0.80
1:A:483:LEU:O	1:A:486:LEU:CD2	2.30	0.80
1:A:534:ILE:HA	1:A:541:TYR:CE1	2.16	0.80
2:D:46:VAL:CG2	2:D:46:VAL:O	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:MET:HG2	1:A:774:MET:O	1.82	0.80
1:C:83:ASP:O	1:C:84:SER:CB	2.29	0.80
1:C:570:GLY:O	1:C:571:VAL:CG1	2.30	0.80
1:B:278:ILE:HG12	1:B:278:ILE:O	1.82	0.80
1:C:496:MET:CG	1:C:496:MET:O	2.30	0.80
1:C:568:ASP:OD2	1:C:644:VAL:HG22	1.82	0.80
1:C:672:VAL:CG2	1:C:673:GLU:OE1	2.30	0.80
1:A:498:LYS:H	1:A:498:LYS:CE	1.93	0.80
1:B:848:ALA:O	1:B:851:LEU:CD1	2.29	0.80
1:C:88:VAL:HG23	1:C:89:GLN:N	1.95	0.80
1:C:570:GLY:C	1:C:571:VAL:CG1	2.53	0.80
1:C:927:PHE:CE2	1:C:931:LEU:HD11	2.16	0.80
1:C:976:LEU:O	1:C:980:LEU:CD2	2.30	0.80
1:A:647:ILE:O	1:A:650:ARG:HG2	1.81	0.80
1:B:671:ILE:O	1:B:671:ILE:CD1	2.30	0.80
1:B:774:MET:HE2	1:B:780:ARG:HH11	1.45	0.80
1:B:848:ALA:HA	1:B:851:LEU:HD13	1.62	0.79
1:C:160:ALA:C	1:C:161:ASN:OD1	2.25	0.79
1:A:73:ASP:CB	1:A:74:ASN:OD1	2.30	0.79
1:B:848:ALA:HA	1:B:851:LEU:HD11	1.63	0.79
1:C:71:GLY:O	1:C:72:ILE:CG1	2.30	0.79
1:C:196:PHE:C	1:C:197:GLN:CG	2.54	0.79
2:D:53:LEU:N	2:D:53:LEU:HD22	1.95	0.79
1:B:441:ALA:O	1:B:445:ILE:HG13	1.81	0.79
1:B:501:ALA:O	1:B:504:ASP:HB3	1.82	0.79
1:A:558:ARG:CD	1:A:558:ARG:O	2.30	0.79
1:B:182:TYR:HB3	1:B:270:LEU:CD1	2.10	0.79
1:C:566:ASP:OD2	1:C:678:THR:HG21	1.82	0.79
2:D:73:VAL:HG12	2:D:74:ASN:N	1.96	0.79
1:C:923:ASN:OD1	1:C:927:PHE:CD2	2.35	0.79
1:B:966:ASP:O	1:B:970:MET:HG3	1.80	0.79
1:C:144:ASN:ND2	1:C:149:MET:CG	2.45	0.79
1:C:314:GLU:CA	1:C:317:PHE:CD1	2.65	0.79
2:E:93:LEU:HD21	2:E:128:ILE:CG1	2.13	0.79
1:C:267:LYS:C	1:C:268:ILE:HD13	2.08	0.79
1:A:931:LEU:O	1:A:935:ILE:CG2	2.30	0.79
1:B:991:ILE:O	1:B:991:ILE:CD1	2.30	0.79
1:C:88:VAL:CG2	1:C:89:GLN:N	2.45	0.79
1:A:376:LEU:O	1:A:380:PHE:HD1	1.64	0.78
1:B:218:GLN:HB3	1:B:232:ALA:O	1.82	0.78
1:B:874:PRO:CB	1:B:877:TYR:CD2	2.61	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:ILE:O	1:A:935:ILE:CD1	2.30	0.78
1:B:24:GLY:O	1:B:27:ILE:HG22	1.83	0.78
1:A:263:ARG:HG3	1:A:264:ASP:OD2	1.83	0.78
1:C:149:MET:SD	1:C:321:LEU:CD1	2.72	0.78
1:C:512:PHE:CD1	1:C:512:PHE:C	2.57	0.78
1:C:758:TYR:HE2	1:C:770:LYS:HB3	1.48	0.78
2:D:56:TYR:HE1	2:D:90:ARG:NE	1.72	0.78
1:B:182:TYR:CD1	1:B:270:LEU:CD1	2.66	0.78
1:A:956:GLU:OE2	1:A:956:GLU:CA	2.30	0.78
1:B:302:THR:O	1:B:306:ILE:HG22	1.83	0.78
1:B:449:LEU:O	1:B:453:PHE:HD1	1.66	0.78
1:B:848:ALA:CA	1:B:851:LEU:CD1	2.60	0.78
1:C:673:GLU:CD	1:C:673:GLU:N	2.38	0.78
2:E:93:LEU:HD21	2:E:128:ILE:HG12	1.64	0.78
2:D:56:TYR:HD1	2:D:90:ARG:HG3	1.49	0.78
1:A:10:ILE:O	1:A:14:VAL:HG23	1.83	0.78
1:B:919:ARG:HB3	1:B:919:ARG:HH11	0.67	0.78
1:C:156:ASP:OD1	1:C:182:TYR:HB2	1.84	0.78
1:B:156:ASP:CB	1:B:182:TYR:HE2	1.96	0.78
1:C:68:ASN:ND2	1:C:114:ALA:HB2	1.98	0.78
1:C:724:THR:CB	1:C:725:PRO:CD	2.63	0.78
1:B:575:MET:HG3	1:B:576:VAL:N	1.99	0.77
1:B:534:ILE:HA	1:B:541:TYR:CZ	2.19	0.77
1:C:156:ASP:CG	1:C:182:TYR:CD2	2.62	0.77
1:A:67:GLN:NE2	1:C:767:ARG:NH1	2.32	0.77
1:C:927:PHE:CE2	1:C:931:LEU:CD1	2.67	0.77
1:A:181:GLN:HE21	1:A:769:LYS:HE3	1.49	0.77
1:A:348:ILE:O	1:A:351:VAL:HG12	1.84	0.77
1:A:496:MET:O	1:A:497:LEU:CD2	2.30	0.77
1:C:259:ARG:HH12	2:E:155:ASP:CG	1.93	0.77
1:C:568:ASP:OD2	1:C:644:VAL:CG1	2.32	0.77
1:C:1:FME:CN	1:C:2:PRO:HD2	2.15	0.77
2:E:146:GLY:HA2	2:E:147:LYS:CB	2.15	0.77
1:A:150:THR:O	1:A:154:ILE:HG13	1.85	0.77
1:B:218:GLN:NE2	1:B:231:ASN:HD21	1.82	0.77
1:B:762:PHE:HD2	1:B:771:VAL:HG23	1.48	0.77
1:B:103:ALA:O	1:B:107:VAL:HG23	1.84	0.77
1:A:498:LYS:HE3	1:A:498:LYS:C	2.08	0.77
1:C:669:PRO:HA	1:C:678:THR:HG22	1.66	0.77
2:D:126:LEU:O	2:D:129:VAL:HG23	1.85	0.77
1:A:498:LYS:O	1:A:498:LYS:CE	2.30	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLN:CA	1:B:798:MET:HE2	2.12	0.76
1:B:559:LEU:HD12	1:B:560:PRO:HD2	1.66	0.76
1:B:713:LEU:HD13	1:B:713:LEU:N	1.99	0.76
1:C:155:SER:HB3	1:C:287:SER:HB2	1.64	0.76
1:B:5:PHE:O	1:B:491:ALA:HB2	1.85	0.76
1:C:671:ILE:O	1:C:674:LEU:HD21	1.85	0.76
1:C:793:ALA:O	1:C:794:ALA:C	2.28	0.76
1:C:810:GLU:C	1:C:811:TYR:CD2	2.63	0.76
1:B:204:ILE:HG23	1:B:759:VAL:CG1	2.16	0.76
1:B:270:LEU:CD2	1:B:271:GLY:N	2.39	0.76
1:B:974:PRO:O	1:B:978:THR:HG23	1.85	0.76
1:B:188:MET:HE2	1:B:773:VAL:HG21	1.65	0.76
1:B:254:ASN:C	1:B:257:GLY:H	1.93	0.76
1:B:674:LEU:O	1:B:674:LEU:CD1	2.34	0.76
1:C:502:LYS:HG2	1:C:503:GLY:N	2.00	0.76
1:B:874:PRO:O	1:B:874:PRO:CG	2.30	0.76
2:D:126:LEU:HA	2:D:129:VAL:CG2	2.15	0.76
1:A:520:PHE:CD2	1:A:520:PHE:C	2.60	0.76
1:B:234:ILE:O	1:B:235:ILE:HD13	1.85	0.76
1:A:423:GLU:C	1:A:502:LYS:HG3	2.11	0.76
1:B:72:ILE:HG22	1:B:73:ASP:N	2.00	0.76
1:B:102:ILE:HG22	1:B:103:ALA:N	1.97	0.76
1:B:196:PHE:HA	1:B:197:GLN:NE2	2.00	0.76
1:C:607:GLU:OE2	1:C:632:LYS:CG	2.29	0.76
1:A:904:VAL:O	1:A:904:VAL:CG2	2.34	0.76
1:C:669:PRO:CA	1:C:678:THR:HG22	2.15	0.76
1:B:501:ALA:HB3	1:B:504:ASP:CB	2.17	0.75
1:B:712:MET:O	1:B:713:LEU:CD1	2.30	0.75
2:D:19:LEU:HD23	2:D:50:PRO:HG3	1.67	0.75
1:A:235:ILE:O	1:B:728:LYS:HA	1.87	0.75
1:C:369:THR:O	1:C:372:VAL:HG13	1.86	0.75
1:A:73:ASP:C	1:A:74:ASN:OD1	2.30	0.75
1:A:504:ASP:C	1:A:504:ASP:OD1	2.30	0.75
1:B:1:FME:N	1:B:2:PRO:CD	2.49	0.75
1:C:144:ASN:HD21	1:C:149:MET:HG3	1.52	0.75
1:A:829:GLY:C	1:A:830:GLN:OE1	2.29	0.75
1:B:513:PHE:C	1:B:515:TRP:H	1.94	0.75
1:C:34:GLN:HB2	1:C:333:VAL:HG13	1.67	0.75
1:C:429:GLU:C	1:C:429:GLU:OE1	2.29	0.75
1:C:795:ASP:C	1:C:795:ASP:OD1	2.30	0.75
1:C:876:LEU:CD2	1:C:876:LEU:O	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PHE:HB2	1:B:287:SER:O	1.86	0.75
1:B:229:GLN:OE1	1:B:229:GLN:C	2.30	0.75
1:C:724:THR:HB	1:C:725:PRO:CD	2.16	0.75
1:B:415:ASN:O	1:B:419:VAL:HG23	1.87	0.75
1:B:848:ALA:O	1:B:851:LEU:HD12	1.86	0.75
1:A:504:ASP:CG	1:A:504:ASP:O	2.30	0.75
1:A:101:ASP:O	1:A:105:VAL:HG23	1.87	0.75
1:B:204:ILE:HG23	1:B:759:VAL:HG12	1.69	0.75
1:B:213:GLN:C	1:B:213:GLN:OE1	2.30	0.75
1:B:229:GLN:CD	1:B:229:GLN:N	2.32	0.75
1:B:988:PRO:O	1:B:991:ILE:CG2	2.35	0.75
1:C:327:TYR:HD1	1:C:628:PHE:HB3	1.50	0.75
1:C:689:GLY:CA	1:C:690:LEU:HD23	2.17	0.75
1:C:157:TYR:CE2	1:C:162:MET:HE2	2.22	0.75
1:C:200:PRO:CG	1:C:749:THR:CG2	2.65	0.75
1:C:314:GLU:HA	1:C:317:PHE:HE1	1.01	0.75
1:B:10:ILE:HB	1:C:893:GLU:OE2	1.87	0.74
1:B:799:VAL:HG13	1:B:800:PRO:HD3	1.68	0.74
1:B:853:THR:CG2	1:B:853:THR:O	2.34	0.74
1:A:542:LEU:O	1:A:545:TYR:HB3	1.87	0.74
1:B:161:ASN:N	1:B:161:ASN:ND2	2.29	0.74
1:A:62:THR:O	1:A:66:GLU:HG3	1.86	0.74
2:D:18:LEU:O	2:D:18:LEU:CD2	2.30	0.74
1:C:102:ILE:O	1:C:106:GLN:HG3	1.87	0.74
2:E:152:ILE:HG13	2:E:153:SER:H	1.51	0.74
1:B:668:LEU:O	1:B:668:LEU:CD1	2.30	0.74
1:C:587:THR:HG21	1:C:622:GLN:O	1.87	0.74
1:C:742:SER:HB3	1:C:745:ASP:H	1.53	0.74
1:C:891:LEU:HD12	1:C:892:TYR:CD1	2.23	0.74
2:E:112:ASN:CA	2:E:144:LYS:HE2	2.17	0.74
1:B:229:GLN:OE1	1:B:229:GLN:CA	2.34	0.74
2:D:13:ASP:C	2:D:13:ASP:OD1	2.30	0.74
1:A:32:VAL:HG12	1:A:390:ILE:O	1.86	0.74
1:A:242:SER:HB2	1:A:244:GLU:HG2	1.70	0.74
1:A:428:LYS:O	1:A:431:THR:CG2	2.30	0.74
1:A:519:MET:HE2	1:A:519:MET:CA	2.16	0.74
1:B:670:ALA:O	1:B:671:ILE:HG22	1.87	0.74
2:E:93:LEU:HD23	2:E:128:ILE:HG12	1.68	0.74
1:A:942:ALA:O	1:A:946:VAL:HG12	1.87	0.74
1:B:990:VAL:HG12	1:B:991:ILE:N	2.00	0.74
1:A:721:LEU:HD12	1:A:814:PRO:HG2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:671:ILE:CG1	1:C:671:ILE:O	2.29	0.74
1:C:157:TYR:HE2	1:C:162:MET:HE2	1.51	0.74
1:C:247:GLY:O	1:C:263:ARG:CG	2.36	0.74
1:C:910:ILE:CG2	1:C:1013:THR:HG21	2.17	0.74
1:A:897:ILE:N	1:A:898:PRO:CD	2.51	0.73
1:B:713:LEU:CD1	1:B:713:LEU:N	2.41	0.73
1:C:327:TYR:CD1	1:C:628:PHE:HB3	2.23	0.73
1:C:732:ASP:C	1:C:732:ASP:OD1	2.30	0.73
2:E:100:LEU:HD21	2:E:106:VAL:CG1	2.17	0.73
1:A:580:ALA:HA	1:A:623:ASN:ND2	2.03	0.73
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.70	0.73
1:B:365:THR:HG23	1:B:366:LEU:HD23	1.70	0.73
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.14	0.73
1:A:721:LEU:CD1	1:A:814:PRO:HG2	2.13	0.73
1:B:169:THR:HG22	1:B:172:VAL:CG1	2.17	0.73
1:C:4:PHE:HD2	1:C:4:PHE:C	1.95	0.73
1:C:203:VAL:O	1:C:207:ILE:HG13	1.88	0.73
1:B:59:ASP:O	1:B:63:GLN:HB2	1.89	0.73
1:B:224:PRO:HA	1:C:781:MET:CE	2.18	0.73
1:C:247:GLY:O	1:C:263:ARG:HG3	1.88	0.73
2:D:77:ASP:C	2:D:77:ASP:OD1	2.30	0.73
1:A:478:MET:O	1:A:482:VAL:CG2	2.30	0.73
1:A:488:LEU:O	1:A:488:LEU:CD1	2.30	0.73
1:B:99:ASP:C	1:B:99:ASP:OD1	2.30	0.73
1:B:254:ASN:HB2	1:B:258:SER:O	1.88	0.73
1:B:274:ASN:C	1:B:274:ASN:OD1	2.30	0.73
1:B:671:ILE:C	1:B:672:VAL:HG12	2.13	0.73
1:C:94:PHE:O	1:C:95:GLU:C	2.30	0.73
1:C:876:LEU:O	1:C:876:LEU:HD23	1.88	0.73
1:A:423:GLU:C	1:A:502:LYS:HE3	2.12	0.73
1:A:860:THR:O	1:A:861:GLY:C	2.29	0.73
1:A:621:GLY:HA3	1:A:624:THR:HG22	1.71	0.73
1:A:808:ARG:NH1	1:A:808:ARG:CB	2.30	0.73
1:B:781:MET:HA	1:B:781:MET:HE2	1.71	0.73
1:C:671:ILE:CD1	1:C:674:LEU:CD2	2.67	0.73
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.22	0.73
1:A:956:GLU:OE2	1:A:956:GLU:HA	1.87	0.73
1:C:149:MET:SD	1:C:321:LEU:HD13	2.29	0.73
1:C:669:PRO:HD3	1:C:676:THR:O	1.89	0.73
1:C:754:TRP:CZ2	1:C:786:ILE:HG12	2.24	0.72
1:B:254:ASN:HD22	1:B:258:SER:CB	1.97	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:MET:HE3	1:C:500:ILE:HG13	1.69	0.72
2:D:34:MET:HE3	2:D:34:MET:HA	1.71	0.72
1:A:376:LEU:O	1:A:380:PHE:CD1	2.42	0.72
1:B:986:VAL:O	1:B:986:VAL:HG12	1.89	0.72
1:B:991:ILE:HD12	1:B:991:ILE:C	2.11	0.72
1:B:948:PHE:CE2	1:B:971:ARG:NE	2.53	0.72
1:A:488:LEU:C	1:A:488:LEU:CD1	2.62	0.72
1:B:183:ALA:N	1:B:271:GLY:O	2.22	0.72
1:B:771:VAL:O	1:B:771:VAL:HG12	1.88	0.72
1:A:407:ASP:OD1	1:A:978:THR:HG21	1.90	0.72
1:A:427:PRO:HD3	1:A:499:PRO:HB3	1.72	0.72
1:A:463:THR:O	1:A:467:TYR:HD2	1.73	0.72
1:A:535:LEU:HD22	1:A:1027:VAL:HG21	1.71	0.72
1:B:874:PRO:HB3	1:B:877:TYR:HD2	1.51	0.72
1:C:534:ILE:HG13	1:C:541:TYR:CE2	2.25	0.72
1:A:151:GLN:HB3	1:A:285:PRO:HB3	1.71	0.72
1:B:774:MET:HE2	1:B:780:ARG:NH1	2.05	0.72
1:C:757:SER:O	1:C:772:TYR:HD1	1.70	0.72
1:C:926:TYR:HD2	1:C:1003:VAL:HG22	1.55	0.72
1:A:383:LEU:HD11	1:A:473:THR:HG22	1.70	0.72
1:B:36:PRO:HG3	1:B:391:ASN:ND2	2.05	0.72
1:B:394:THR:HG22	1:B:473:THR:OG1	1.90	0.72
1:B:732:ASP:C	1:B:732:ASP:OD1	2.30	0.72
1:C:733:GLN:CD	1:C:743:ILE:HD13	2.15	0.72
1:B:69:MET:CE	1:B:72:ILE:CD1	2.67	0.72
1:B:671:ILE:O	1:B:672:VAL:HG12	1.89	0.72
1:C:314:GLU:O	1:C:317:PHE:CD1	2.35	0.72
1:A:519:MET:CG	1:A:520:PHE:N	2.52	0.72
1:B:102:ILE:HG23	1:B:103:ALA:N	2.02	0.72
1:B:254:ASN:HB2	1:B:258:SER:N	2.05	0.72
1:C:53:ASP:C	1:C:53:ASP:OD1	2.30	0.72
1:C:457:ALA:HB1	1:C:468:ARG:HG2	1.72	0.72
1:C:513:PHE:O	1:C:516:PHE:N	2.23	0.72
1:B:557:VAL:CG2	1:B:557:VAL:O	2.38	0.71
1:B:670:ALA:O	1:B:671:ILE:CB	2.33	0.71
1:B:188:MET:CE	1:B:773:VAL:CG2	2.48	0.71
1:C:204:ILE:HG23	1:C:759:VAL:CG2	2.20	0.71
2:E:125:HIS:ND1	2:E:128:ILE:HG13	2.06	0.71
1:C:582:ALA:HB3	1:C:623:ASN:HB2	1.72	0.71
1:C:891:LEU:HD12	1:C:892:TYR:CE1	2.25	0.71
1:C:230:LEU:O	1:C:230:LEU:HG	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:PHE:C	1:A:520:PHE:HD2	1.99	0.71
1:A:1016:VAL:HG23	1:A:1017:LEU:HD12	1.71	0.71
1:B:182:TYR:CD1	1:B:270:LEU:HD13	2.26	0.71
1:B:512:PHE:O	1:B:513:PHE:C	2.32	0.71
1:B:605:ASN:HD21	1:B:642:ASN:HB3	1.54	0.71
1:C:405:LEU:HD12	1:C:405:LEU:O	1.91	0.71
1:A:489:THR:CB	1:A:490:PRO:CD	2.69	0.71
1:A:527:TYR:CD1	1:A:972:LEU:HD23	2.25	0.71
1:B:702:LEU:HB2	1:B:851:LEU:HD21	1.73	0.71
1:A:6:ILE:HD13	1:A:431:THR:HG21	1.72	0.71
1:B:150:THR:OG1	1:B:152:GLU:HB2	1.91	0.71
1:C:739:LEU:HD22	1:C:739:LEU:H	1.55	0.71
1:A:234:ILE:CA	1:A:235:ILE:HD13	2.18	0.70
1:A:901:VAL:O	1:A:901:VAL:CG1	2.39	0.70
1:C:937:LEU:O	1:C:940:LYS:CG	2.39	0.70
1:B:512:PHE:O	1:B:513:PHE:CB	2.36	0.70
1:A:527:TYR:CD1	1:A:972:LEU:CD2	2.75	0.70
1:B:116:PRO:C	1:B:117:LEU:CD1	2.64	0.70
1:C:1032:ARG:O	1:C:1033:PHE:CB	2.37	0.70
1:A:317:PHE:HB3	1:A:321:LEU:HB3	1.71	0.70
1:A:489:THR:HB	1:A:490:PRO:CD	2.22	0.70
1:C:910:ILE:HG23	1:C:1013:THR:HG21	1.74	0.70
2:D:129:VAL:O	2:D:133:LEU:CD1	2.30	0.70
1:C:876:LEU:C	1:C:876:LEU:HD22	2.13	0.70
2:D:61:GLU:O	2:D:65:VAL:CG2	2.34	0.70
1:A:182:TYR:CD2	1:A:270:LEU:CD2	2.74	0.70
1:A:483:LEU:C	1:A:486:LEU:CD2	2.64	0.70
1:B:336:SER:OG	1:B:395:MET:HE1	1.91	0.70
1:C:724:THR:HB	1:C:725:PRO:HD2	1.73	0.70
1:A:58:GLN:NE2	1:A:818:ARG:HH11	1.88	0.70
1:B:534:ILE:HA	1:B:541:TYR:OH	1.90	0.70
1:B:818:ARG:NH1	1:B:821:GLY:O	2.25	0.70
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.74	0.70
1:C:325:TYR:HD1	1:C:325:TYR:H	1.39	0.70
2:D:73:VAL:HG13	2:D:74:ASN:OD1	1.92	0.70
1:A:989:LEU:HD22	1:A:1000:GLN:HB3	1.72	0.70
1:B:672:VAL:O	1:B:672:VAL:CG2	2.30	0.70
1:C:891:LEU:CD1	1:C:892:TYR:CE1	2.74	0.70
1:C:896:SER:HG	1:C:897:ILE:CD1	2.05	0.70
1:B:62:THR:OG1	1:B:88:VAL:HG21	1.92	0.70
2:D:152:ILE:O	2:D:156:ASN:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:VAL:HA	1:C:534:ILE:HG22	1.74	0.70
1:B:161:ASN:HD22	1:B:161:ASN:N	1.87	0.69
1:B:758:TYR:HB2	1:B:772:TYR:CD1	2.26	0.69
1:B:901:VAL:O	1:B:904:VAL:HG22	1.92	0.69
1:C:82:SER:O	1:C:815:ARG:HA	1.90	0.69
1:C:504:ASP:OD1	1:C:507:GLU:HA	1.92	0.69
1:B:459:PHE:O	1:B:464:GLY:HA3	1.92	0.69
1:C:1:FME:N	1:C:2:PRO:HD2	2.06	0.69
1:C:55:LYS:O	1:C:56:THR:C	2.32	0.69
1:B:713:LEU:HD22	1:B:843:LEU:HD23	1.73	0.69
1:B:780:ARG:HD2	1:B:780:ARG:O	1.92	0.69
1:C:672:VAL:HG23	1:C:673:GLU:OE1	1.90	0.69
2:D:56:TYR:CD1	2:D:90:ARG:CG	2.75	0.69
2:E:145:PHE:O	2:E:145:PHE:HD1	1.74	0.69
1:B:765:ARG:HB3	1:B:765:ARG:NH1	2.07	0.69
1:C:327:TYR:CD1	1:C:628:PHE:HD1	2.11	0.69
1:A:519:MET:HE1	1:A:523:SER:OG	1.92	0.69
1:B:5:PHE:CE1	1:B:487:ILE:HG12	2.27	0.69
1:B:182:TYR:CD1	1:B:270:LEU:HD11	2.27	0.69
1:B:450:SER:O	1:B:454:VAL:HG12	1.92	0.69
1:C:65:ILE:O	1:C:69:MET:HG2	1.92	0.69
1:C:816:LEU:HD12	1:C:816:LEU:N	2.07	0.69
1:B:183:ALA:HB3	1:B:271:GLY:O	1.92	0.69
1:B:274:ASN:OD1	1:B:276:ASP:N	2.22	0.69
1:C:190:PRO:HG3	1:C:789:TRP:CH2	2.27	0.69
1:A:360:GLN:CG	1:A:513:PHE:CZ	2.69	0.69
1:A:537:SER:OG	1:A:540:ARG:CB	2.41	0.69
1:A:580:ALA:HA	1:A:623:ASN:HD22	1.56	0.69
1:A:781:MET:SD	1:C:220:GLY:HA2	2.33	0.69
1:B:69:MET:HE1	1:B:72:ILE:HD11	1.74	0.69
1:B:184:MET:HB3	1:B:771:VAL:HG22	1.73	0.69
1:C:412:VAL:O	1:C:416:VAL:HG23	1.92	0.69
1:C:429:GLU:HA	1:C:432:ARG:HG3	1.75	0.69
2:E:156:ASN:HD22	2:E:156:ASN:C	2.01	0.69
1:A:463:THR:CG2	1:A:467:TYR:CE2	2.76	0.69
1:A:728:LYS:NZ	1:C:236:ALA:O	2.21	0.69
1:B:143:ILE:HG22	1:B:286:ALA:HB2	1.74	0.69
1:C:940:LYS:HG3	1:C:941:ASN:N	2.08	0.69
1:A:780:ARG:O	1:A:780:ARG:CG	2.41	0.68
1:C:449:LEU:HB2	1:C:478:MET:HE2	1.75	0.68
1:C:924:ASP:O	1:C:927:PHE:HB3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:LEU:C	2:D:129:VAL:HG23	2.17	0.68
1:A:483:LEU:O	1:A:486:LEU:HD23	1.93	0.68
1:A:966:ASP:HA	1:A:969:ARG:HD3	1.74	0.68
1:C:211:ASN:HD22	1:C:760:ASN:HD21	1.41	0.68
1:B:197:GLN:C	1:B:798:MET:HE2	2.18	0.68
1:B:234:ILE:C	1:B:235:ILE:CD1	2.62	0.68
1:B:764:ASP:OD1	1:B:765:ARG:CG	2.40	0.68
1:A:544:LEU:O	1:A:548:ILE:HG13	1.93	0.68
1:C:237:GLN:O	1:C:238:THR:CG2	2.41	0.68
1:A:423:GLU:O	1:A:502:LYS:CE	2.42	0.68
1:A:491:ALA:O	1:A:495:THR:CG2	2.41	0.68
1:B:188:MET:HE3	1:B:773:VAL:HG22	1.73	0.68
1:C:689:GLY:O	1:C:690:LEU:CD2	2.37	0.68
1:C:960:LEU:O	1:C:960:LEU:CD1	2.30	0.68
1:A:194:ASN:ND2	1:A:798:MET:HG3	2.08	0.68
1:B:795:ASP:OD2	1:B:797:GLN:HB2	1.94	0.68
1:B:222:THR:CG2	1:C:275:TYR:HB3	2.24	0.68
1:B:231:ASN:HD22	1:B:232:ALA:N	1.92	0.68
1:B:355:MET:HE3	1:B:368:PRO:HG2	1.75	0.68
1:B:670:ALA:O	1:B:671:ILE:CG2	2.42	0.68
2:D:14:LEU:HD12	2:D:14:LEU:N	2.08	0.68
1:B:166:ILE:O	1:B:172:VAL:HG21	1.93	0.68
1:B:169:THR:CG2	1:B:172:VAL:CG1	2.72	0.68
1:B:871:ASN:CB	1:B:872:GLN:HG2	2.19	0.68
1:C:707:ALA:O	1:C:710:PRO:HD3	1.94	0.68
2:D:76:ASP:O	2:D:77:ASP:HB3	1.94	0.68
1:B:403:GLY:HA3	1:B:982:PHE:CE1	2.28	0.68
1:B:712:MET:HE1	1:B:839:GLU:OE2	1.93	0.68
1:C:980:LEU:HD22	1:C:980:LEU:H	1.56	0.68
2:D:92:HIS:O	2:D:96:VAL:HG23	1.93	0.68
1:A:218:GLN:HA	1:A:234:ILE:HG13	1.76	0.67
1:A:899:PHE:O	1:A:900:SER:C	2.36	0.67
1:B:140:VAL:O	1:B:288:GLY:HA2	1.94	0.67
1:B:815:ARG:HG2	1:B:815:ARG:NH1	2.09	0.67
1:B:13:TRP:O	1:B:17:ILE:HG13	1.95	0.67
1:B:764:ASP:OD1	1:B:765:ARG:HG3	1.93	0.67
1:C:336:SER:O	1:C:340:VAL:HG23	1.95	0.67
2:D:77:ASP:OD1	2:D:79:LEU:N	2.26	0.67
1:A:586:ARG:O	1:A:590:VAL:HG23	1.95	0.67
1:B:670:ALA:O	1:B:671:ILE:HB	1.94	0.67
1:B:800:PRO:HD2	1:B:800:PRO:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:760:ASN:O	1:C:771:VAL:HB	1.95	0.67
1:C:879:ILE:O	1:C:879:ILE:CD1	2.30	0.67
1:C:237:GLN:C	1:C:238:THR:HG23	2.19	0.67
1:C:742:SER:O	1:C:746:ILE:HD13	1.93	0.67
1:A:298:ASN:HD22	1:A:301:ASP:CB	2.07	0.67
1:B:939:ALA:O	1:B:943:ILE:HG13	1.95	0.67
1:A:39:ALA:HB1	1:A:40:PRO:HD2	1.76	0.67
1:C:200:PRO:CG	1:C:749:THR:HG23	2.23	0.67
1:C:925:VAL:O	1:C:926:TYR:C	2.35	0.67
1:A:137:LEU:HD13	1:A:293:LEU:HD12	1.77	0.67
1:B:10:ILE:CB	1:C:893:GLU:OE2	2.43	0.67
1:B:281:PHE:HD1	1:B:610:PHE:CD1	2.11	0.67
1:A:721:LEU:HD13	1:A:814:PRO:HG3	1.71	0.67
1:C:937:LEU:HB3	1:C:1011:MET:HE3	1.76	0.67
2:E:152:ILE:CD1	2:E:153:SER:N	2.58	0.67
1:B:1:FME:HE2	1:B:487:ILE:CD1	2.23	0.67
1:B:61:VAL:O	1:B:65:ILE:CG1	2.42	0.67
1:B:1022:VAL:HA	1:B:1025:PHE:HD1	1.60	0.67
1:C:815:ARG:C	1:C:816:LEU:HD12	2.20	0.67
1:A:423:GLU:O	1:A:502:LYS:CD	2.43	0.66
1:B:512:PHE:O	1:B:513:PHE:HB2	1.94	0.66
1:B:874:PRO:HB3	1:B:877:TYR:CD2	2.28	0.66
2:D:79:LEU:HD22	2:D:111:HIS:CE1	2.29	0.66
1:C:896:SER:HG	1:C:897:ILE:HD13	1.61	0.66
1:A:445:ILE:HD11	1:A:943:ILE:HG21	1.77	0.66
1:A:534:ILE:HG13	1:A:535:LEU:N	2.10	0.66
1:C:314:GLU:C	1:C:317:PHE:HD1	2.02	0.66
1:C:563:PHE:CE2	1:C:564:LEU:HD12	2.30	0.66
1:C:689:GLY:N	1:C:690:LEU:HD23	2.09	0.66
1:C:757:SER:O	1:C:772:TYR:CD1	2.47	0.66
1:A:74:ASN:OD1	1:A:74:ASN:N	2.28	0.66
1:A:652:THR:HA	1:A:655:PHE:HD2	1.59	0.66
1:B:10:ILE:HG12	1:C:893:GLU:OE2	1.94	0.66
1:B:561:SER:HA	1:B:923:ASN:HB3	1.78	0.66
1:B:853:THR:O	1:B:853:THR:HG22	1.95	0.66
1:C:53:ASP:CG	1:C:56:THR:OG1	2.38	0.66
1:C:463:THR:HG22	1:C:467:TYR:CE1	2.30	0.66
1:C:972:LEU:HD13	1:C:976:LEU:HD23	1.78	0.66
1:A:373:PRO:O	1:A:377:LEU:HG	1.95	0.66
1:B:38:ILE:HD11	1:B:671:ILE:HD11	1.78	0.66
1:C:575:MET:O	1:C:575:MET:CG	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:THR:O	1:B:587:THR:HG22	1.96	0.66
1:B:762:PHE:CD2	1:B:771:VAL:HG23	2.31	0.66
1:A:360:GLN:CG	1:A:513:PHE:HZ	2.00	0.66
1:B:563:PHE:CB	1:B:564:LEU:CD1	2.73	0.66
2:D:57:PHE:H	2:D:58:GLY:HA2	1.60	0.66
1:B:727:PHE:CE1	1:B:783:PRO:HB3	2.30	0.66
1:C:559:LEU:HD12	1:C:560:PRO:HD2	1.77	0.66
1:C:671:ILE:CG1	1:C:674:LEU:CD2	2.62	0.66
2:D:46:VAL:O	2:D:46:VAL:HG23	1.94	0.66
1:B:1:FME:CE	1:B:487:ILE:CD1	2.73	0.66
1:B:63:GLN:O	1:B:67:GLN:HG3	1.96	0.66
1:C:345:VAL:O	1:C:349:ILE:HG13	1.95	0.66
1:C:497:LEU:HD22	1:C:498:LYS:N	2.09	0.66
1:A:242:SER:OG	1:A:245:GLU:HG3	1.94	0.66
1:A:955:LYS:C	1:A:956:GLU:OE2	2.38	0.66
1:B:196:PHE:CA	1:B:197:GLN:NE2	2.59	0.66
1:C:187:TRP:NE1	1:C:269:GLU:OE2	2.28	0.66
1:C:429:GLU:OE1	1:C:430:ALA:N	2.29	0.66
1:C:876:LEU:C	1:C:876:LEU:HD23	2.20	0.66
1:A:463:THR:HG22	1:A:467:TYR:CD2	2.30	0.65
1:A:568:ASP:OD2	1:A:643:LYS:HG3	1.96	0.65
1:B:541:TYR:O	1:B:544:LEU:HB2	1.96	0.65
1:C:919:ARG:NH1	1:C:990:VAL:HG12	2.03	0.65
1:A:463:THR:HG22	1:A:467:TYR:CE2	2.31	0.65
1:A:483:LEU:O	1:A:486:LEU:HD22	1.96	0.65
1:C:546:LEU:O	1:C:550:VAL:HG23	1.95	0.65
1:C:937:LEU:O	1:C:940:LYS:HG3	1.96	0.65
1:A:754:TRP:CD1	1:A:754:TRP:N	2.62	0.65
1:B:254:ASN:O	1:B:257:GLY:N	2.30	0.65
1:C:563:PHE:HE2	1:C:862:MET:HE1	1.61	0.65
1:B:229:GLN:OE1	1:B:229:GLN:N	2.29	0.65
1:B:365:THR:O	1:B:368:PRO:HD2	1.96	0.65
1:B:848:ALA:CA	1:B:851:LEU:HD13	2.26	0.65
1:C:332:PHE:CE2	1:C:569:GLN:NE2	2.64	0.65
1:C:640:GLU:OE1	1:C:640:GLU:N	2.29	0.65
1:B:274:ASN:OD1	1:B:275:TYR:N	2.30	0.65
1:C:1:FME:N	1:C:2:PRO:HD3	2.09	0.65
1:C:361:ASN:OD1	1:C:362:PHE:N	2.30	0.65
1:C:982:PHE:CD2	1:C:1011:MET:HG3	2.30	0.65
2:E:143:ASP:N	2:E:146:GLY:O	2.30	0.65
1:A:726:GLN:CG	1:A:812:GLY:HA3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:TYR:CE2	1:B:968:VAL:HG13	2.31	0.65
1:C:145:THR:OG1	1:C:146:ASP:N	2.29	0.65
1:C:724:THR:CB	1:C:725:PRO:HD2	2.26	0.65
1:A:489:THR:CB	1:A:490:PRO:HD3	2.27	0.65
1:B:213:GLN:OE1	1:B:214:VAL:N	2.30	0.65
1:C:616:GLY:O	1:C:619:GLY:N	2.30	0.65
1:B:1018:ALA:O	1:B:1022:VAL:HG22	1.96	0.65
1:B:160:ALA:C	1:B:161:ASN:ND2	2.52	0.65
1:B:407:ASP:OD2	1:B:978:THR:HB	1.97	0.65
1:B:513:PHE:C	1:B:515:TRP:N	2.53	0.65
1:B:712:MET:HB3	1:B:713:LEU:HD13	1.79	0.65
1:C:225:VAL:HG12	1:C:226:LYS:O	1.97	0.65
1:A:55:LYS:NZ	1:A:59:ASP:OD1	2.30	0.65
1:A:70:ASN:C	1:A:70:ASN:OD1	2.40	0.65
1:A:489:THR:HB	1:A:490:PRO:HD3	1.78	0.65
1:B:628:PHE:N	1:B:628:PHE:CD2	2.64	0.65
1:C:83:ASP:O	1:C:84:SER:HB3	1.95	0.65
1:C:435:MET:CA	1:C:435:MET:HE2	2.27	0.65
1:C:671:ILE:O	1:C:674:LEU:HD23	1.96	0.65
1:B:99:ASP:OD1	1:B:101:ASP:N	2.29	0.64
1:B:633:ASP:OD1	1:B:634:TRP:N	2.29	0.64
1:C:161:ASN:OD1	1:C:161:ASN:N	2.29	0.64
2:E:95:VAL:O	2:E:99:LEU:HG	1.98	0.64
1:A:956:GLU:OE2	1:A:956:GLU:N	2.29	0.64
1:B:174:ASP:OD2	1:B:175:VAL:N	2.30	0.64
1:C:71:GLY:C	1:C:72:ILE:HG13	2.22	0.64
1:C:743:ILE:O	1:C:747:ASN:ND2	2.30	0.64
1:A:445:ILE:HD11	1:A:943:ILE:CG2	2.27	0.64
1:B:715:SER:O	1:B:717:ARG:NH1	2.30	0.64
1:C:640:GLU:H	1:C:640:GLU:CD	2.04	0.64
1:C:893:GLU:O	1:C:894:SER:HB2	1.96	0.64
1:A:463:THR:CG2	1:A:467:TYR:HE2	2.10	0.64
1:C:761:ASP:HB3	1:C:768:VAL:CG1	2.28	0.64
1:A:240:LEU:CD1	1:A:240:LEU:H	2.10	0.64
1:A:370:ILE:O	1:A:374:VAL:HG23	1.97	0.64
1:B:210:GLN:OE1	1:B:249:ILE:HG23	1.97	0.64
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.80	0.64
1:B:705:GLU:CG	1:B:847:LEU:HD21	2.18	0.64
1:C:138:MET:HE2	1:C:140:VAL:CG2	2.28	0.64
1:C:230:LEU:HD23	1:C:230:LEU:H	1.62	0.64
1:C:736:ALA:HB1	1:C:741:VAL:HG11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:ASP:C	2:D:112:ASN:N	2.53	0.64
1:A:894:SER:HB2	1:A:897:ILE:HD12	1.79	0.64
1:B:197:GLN:N	1:B:197:GLN:OE1	2.30	0.64
1:B:435:MET:O	1:B:437:GLN:N	2.31	0.64
1:B:988:PRO:O	1:B:991:ILE:HG23	1.98	0.64
2:D:77:ASP:OD1	2:D:78:SER:N	2.30	0.64
2:E:145:PHE:CD1	2:E:145:PHE:C	2.75	0.64
1:A:236:ALA:HB2	1:B:729:ILE:CG2	2.28	0.64
1:A:298:ASN:HD22	1:A:301:ASP:H	1.44	0.64
1:A:379:THR:HG22	1:A:383:LEU:HD21	1.80	0.64
1:A:488:LEU:HD11	1:A:492:LEU:CD1	2.28	0.64
1:A:696:THR:O	1:A:700:ASN:ND2	2.31	0.64
1:A:754:TRP:HZ3	1:C:219:LEU:CD2	2.09	0.64
1:B:717:ARG:CG	1:B:717:ARG:NH1	2.43	0.64
1:B:746:ILE:HD13	1:B:804:PHE:CE2	2.32	0.64
2:E:61:GLU:O	2:E:65:VAL:HG23	1.98	0.64
1:A:527:TYR:O	1:A:531:VAL:CG2	2.43	0.64
1:B:254:ASN:O	1:B:257:GLY:HA2	1.98	0.64
1:B:848:ALA:C	1:B:851:LEU:CD1	2.71	0.64
1:A:463:THR:HG23	1:A:467:TYR:HE2	1.61	0.64
1:B:54:ALA:HB1	1:B:82:SER:O	1.98	0.64
1:B:144:ASN:OD1	1:B:149:MET:HG2	1.98	0.64
1:B:225:VAL:O	1:B:225:VAL:CG2	2.46	0.64
1:B:225:VAL:O	1:B:225:VAL:HG23	1.96	0.64
1:B:355:MET:HG2	1:B:365:THR:HA	1.80	0.64
1:B:459:PHE:HB2	1:B:464:GLY:CA	2.26	0.64
1:B:800:PRO:CD	1:B:800:PRO:O	2.44	0.64
1:B:848:ALA:O	1:B:851:LEU:HD13	1.97	0.64
1:B:871:ASN:HB3	1:B:872:GLN:CG	2.22	0.64
1:C:583:THR:O	1:C:587:THR:HG22	1.98	0.64
1:C:696:THR:HB	1:C:825:MET:HE1	1.80	0.64
2:E:112:ASN:HA	2:E:144:LYS:CE	2.22	0.64
1:A:109:ASN:O	1:A:112:GLN:HG3	1.99	0.63
1:A:181:GLN:HE21	1:A:769:LYS:CE	2.10	0.63
1:A:190:PRO:HG3	1:A:789:TRP:CZ2	2.33	0.63
1:C:163:LYS:HD2	1:C:177:LEU:HB2	1.79	0.63
1:C:733:GLN:OE1	1:C:743:ILE:CD1	2.46	0.63
2:D:93:LEU:HD23	2:D:128:ILE:HG12	1.80	0.63
1:A:218:GLN:HB2	1:A:232:ALA:O	1.98	0.63
1:B:1:FME:HE1	1:B:487:ILE:HD11	1.80	0.63
1:B:60:THR:OG1	1:B:61:VAL:N	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASP:OD2	1:B:153:ASP:N	2.30	0.63
1:C:568:ASP:OD2	1:C:644:VAL:CG2	2.46	0.63
1:C:570:GLY:C	1:C:571:VAL:HG13	2.22	0.63
1:A:358:PHE:CG	1:A:977:MET:HE3	2.33	0.63
1:B:116:PRO:C	1:B:117:LEU:HD12	2.23	0.63
1:B:848:ALA:C	1:B:851:LEU:HD12	2.24	0.63
1:C:98:THR:CG2	1:C:99:ASP:N	2.61	0.63
1:C:989:LEU:HD22	1:C:1000:GLN:CB	2.23	0.63
1:B:150:THR:OG1	1:B:152:GLU:N	2.30	0.63
1:B:501:ALA:HB3	1:B:504:ASP:OD2	1.98	0.63
1:B:649:MET:HE3	1:B:649:MET:CA	2.13	0.63
1:B:669:PRO:O	1:B:669:PRO:HG2	1.97	0.63
1:B:919:ARG:NH1	1:B:919:ARG:CB	2.30	0.63
1:C:88:VAL:HG23	1:C:89:GLN:H	1.63	0.63
1:C:506:GLY:C	1:C:507:GLU:CG	2.65	0.63
1:B:116:PRO:C	1:B:117:LEU:HD13	2.22	0.63
1:B:871:ASN:OD1	1:B:871:ASN:N	2.30	0.63
1:C:259:ARG:NH1	2:E:155:ASP:CG	2.55	0.63
1:C:435:MET:O	1:C:439:GLN:HB2	1.98	0.63
1:A:531:VAL:O	1:A:534:ILE:HG12	1.99	0.63
1:B:669:PRO:O	1:B:669:PRO:CG	2.45	0.63
1:A:897:ILE:O	1:A:897:ILE:HG22	1.97	0.63
1:C:531:VAL:HA	1:C:534:ILE:CG2	2.29	0.63
1:C:681:ASP:HB3	1:C:860:THR:HG23	1.81	0.63
1:C:730:ASP:N	1:C:730:ASP:OD1	2.30	0.63
1:C:919:ARG:HH12	1:C:990:VAL:CG1	2.04	0.63
1:A:527:TYR:CE1	1:A:972:LEU:HD21	2.31	0.63
1:B:150:THR:CG2	1:B:153:ASP:OD2	2.46	0.63
1:B:501:ALA:HB3	1:B:504:ASP:HB2	1.80	0.63
1:A:498:LYS:NZ	1:A:500:ILE:HD11	2.14	0.63
1:B:561:SER:CA	1:B:923:ASN:HB3	2.29	0.63
1:C:739:LEU:HB2	1:C:741:VAL:HG23	1.81	0.63
2:D:76:ASP:O	2:D:77:ASP:CB	2.44	0.63
1:A:379:THR:HG22	1:A:383:LEU:CD2	2.29	0.62
1:A:489:THR:CG2	1:A:490:PRO:HD3	2.29	0.62
1:A:758:TYR:HE1	1:A:760:ASN:O	1.82	0.62
1:A:997:SER:C	1:A:999:ALA:N	2.54	0.62
1:B:851:LEU:HB3	1:B:852:PRO:HD2	1.79	0.62
1:C:71:GLY:C	1:C:72:ILE:CG1	2.71	0.62
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.80	0.62
1:C:259:ARG:NH1	2:E:155:ASP:OD2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:721:LEU:N	1:C:721:LEU:CD2	2.52	0.62
1:C:884:VAL:O	1:C:888:LEU:HG	1.98	0.62
1:A:163:LYS:HG3	1:A:164:ASP:N	2.14	0.62
1:A:971:ARG:O	1:A:974:PRO:CD	2.37	0.62
1:B:83:ASP:HA	1:B:815:ARG:H	1.64	0.62
1:C:1030:ARG:O	1:C:1034:SER:HB2	1.99	0.62
1:B:765:ARG:HH11	1:B:765:ARG:CB	2.09	0.62
1:C:36:PRO:HG3	1:C:391:ASN:HD21	1.64	0.62
1:C:324:VAL:C	1:C:325:TYR:CD1	2.76	0.62
1:C:926:TYR:CD2	1:C:1003:VAL:HG22	2.33	0.62
1:A:455:PRO:HG2	1:A:880:SER:OG	2.00	0.62
1:B:270:LEU:HD23	1:B:271:GLY:CA	2.27	0.62
1:B:678:THR:O	1:B:678:THR:CG2	2.39	0.62
1:C:724:THR:CG2	1:C:814:PRO:HG3	2.29	0.62
1:C:937:LEU:HD13	1:C:1011:MET:HG2	1.81	0.62
2:D:14:LEU:H	2:D:14:LEU:CD1	2.09	0.62
1:B:1:FME:HE2	1:B:487:ILE:CG1	2.28	0.62
1:B:1:FME:H	1:B:2:PRO:HD3	1.64	0.62
1:B:412:VAL:HG13	1:B:435:MET:SD	2.40	0.62
1:B:668:LEU:HB2	1:B:669:PRO:HD2	1.81	0.62
1:C:382:VAL:HG11	1:C:476:SER:OG	2.00	0.62
1:C:638:PRO:O	1:C:642:ASN:ND2	2.30	0.62
1:A:392:THR:O	1:A:396:PHE:HD1	1.82	0.62
1:A:782:LEU:HB2	1:A:785:ASP:OD1	1.99	0.62
1:B:1:FME:N	1:B:2:PRO:HD3	2.15	0.62
1:B:534:ILE:HA	1:B:541:TYR:CE1	2.35	0.62
1:B:575:MET:HG3	1:B:576:VAL:H	1.65	0.62
1:B:990:VAL:HG22	1:B:1005:THR:HG22	1.82	0.62
1:C:1008:MET:O	1:C:1012:VAL:HG23	2.00	0.62
2:E:121:ALA:HB1	2:E:152:ILE:HG12	1.82	0.62
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.81	0.62
1:B:732:ASP:OD1	1:B:734:GLU:N	2.33	0.62
1:C:268:ILE:N	1:C:268:ILE:CD1	2.58	0.62
1:C:379:THR:O	1:C:383:LEU:HB2	2.00	0.62
2:E:84:LEU:HD22	2:E:116:PRO:HB3	1.82	0.62
1:A:394:THR:HG23	1:A:473:THR:HG21	1.81	0.62
1:B:176:GLN:O	1:B:289:LEU:HD23	1.99	0.62
1:B:903:LEU:O	1:B:906:PRO:HD2	1.99	0.62
1:C:566:ASP:OD2	1:C:678:THR:CG2	2.48	0.62
1:C:983:ILE:HG23	1:C:1008:MET:HG3	1.81	0.62
2:E:67:LEU:CD2	2:E:73:VAL:HG22	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLY:O	1:A:382:VAL:HG23	1.99	0.61
2:D:110:ASP:C	2:D:112:ASN:H	2.03	0.61
1:A:115:MET:HB2	1:A:116:PRO:HD3	1.81	0.61
1:A:410:ILE:HD12	1:A:978:THR:HG22	1.80	0.61
1:A:1024:VAL:O	1:A:1028:VAL:HG23	1.99	0.61
1:B:61:VAL:CG2	1:B:122:VAL:HG21	2.29	0.61
1:B:324:VAL:HG22	1:B:325:TYR:N	2.15	0.61
1:C:911:GLY:HA3	1:C:1013:THR:OG1	1.99	0.61
1:A:498:LYS:HD3	1:A:498:LYS:N	1.98	0.61
1:C:324:VAL:HG22	1:C:325:TYR:N	2.14	0.61
1:C:671:ILE:CD1	1:C:674:LEU:CG	2.74	0.61
1:C:952:LEU:N	1:C:952:LEU:CD1	2.61	0.61
1:A:459:PHE:HB2	1:A:464:GLY:HA2	1.83	0.61
1:B:333:VAL:O	1:B:337:ILE:HG13	1.99	0.61
1:B:402:ILE:O	1:B:406:VAL:HG23	2.00	0.61
1:B:534:ILE:CG1	1:B:541:TYR:CZ	2.78	0.61
1:C:527:TYR:CZ	1:C:968:VAL:HG13	2.35	0.61
1:C:910:ILE:HG23	1:C:911:GLY:N	2.15	0.61
1:B:461:GLY:HA3	1:B:868:LEU:HD22	1.82	0.61
1:C:200:PRO:CG	1:C:749:THR:HG22	2.24	0.61
1:C:318:PRO:O	1:C:319:SER:OG	2.16	0.61
1:A:187:TRP:HH2	1:A:275:TYR:HE1	1.49	0.61
2:E:145:PHE:O	2:E:145:PHE:CD1	2.53	0.61
1:C:44:THR:HB	1:C:132:SER:HG	1.60	0.61
1:C:225:VAL:HG12	1:C:225:VAL:O	1.93	0.61
1:C:496:MET:O	1:C:496:MET:HG2	1.99	0.61
2:D:53:LEU:H	2:D:53:LEU:HD22	1.50	0.61
1:C:36:PRO:HG3	1:C:391:ASN:ND2	2.14	0.61
1:C:567:GLU:OE2	1:C:998:GLY:N	2.20	0.61
1:C:682:PHE:HE2	1:C:684:LEU:HD23	1.65	0.61
1:A:558:ARG:C	1:A:558:ARG:HD2	2.23	0.61
1:B:988:PRO:O	1:B:991:ILE:HG22	1.98	0.61
1:C:502:LYS:HG2	1:C:503:GLY:H	1.65	0.61
1:A:236:ALA:CB	1:B:729:ILE:O	2.49	0.60
1:B:492:LEU:HB3	1:B:496:MET:CE	2.31	0.60
1:B:495:THR:HG22	1:B:496:MET:HG3	1.82	0.60
1:B:966:ASP:O	1:B:970:MET:CG	2.48	0.60
1:C:937:LEU:O	1:C:940:LYS:HG2	2.01	0.60
1:C:937:LEU:HA	1:C:940:LYS:HG2	1.83	0.60
1:C:983:ILE:O	1:C:1008:MET:HE2	2.00	0.60
1:B:553:ALA:O	1:B:557:VAL:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:ASP:OD2	1:B:730:ASP:N	2.30	0.60
1:C:372:VAL:O	1:C:376:LEU:HB2	2.02	0.60
1:C:567:GLU:CD	1:C:998:GLY:HA3	2.26	0.60
1:C:689:GLY:N	1:C:690:LEU:CD2	2.64	0.60
1:C:736:ALA:HB1	1:C:741:VAL:CG1	2.31	0.60
1:A:684:LEU:O	1:A:824:SER:HA	2.00	0.60
1:B:632:LYS:O	1:B:637:ARG:NH2	2.33	0.60
1:C:482:VAL:O	1:C:486:LEU:HD12	2.02	0.60
1:A:202:ASP:OD2	1:A:792:ARG:NH2	2.34	0.60
1:A:997:SER:O	1:A:999:ALA:N	2.34	0.60
1:B:859:TRP:HA	1:B:859:TRP:CE3	2.36	0.60
1:C:158:VAL:HG22	1:C:162:MET:HE3	1.82	0.60
1:C:960:LEU:CD1	1:C:1027:VAL:HG22	2.26	0.60
2:E:151:ASP:O	2:E:154:ILE:HG12	2.00	0.60
1:A:277:ILE:C	1:A:278:ILE:HG12	2.27	0.60
1:A:527:TYR:HE1	1:A:972:LEU:HD23	1.62	0.60
1:A:694:LYS:C	1:A:697:GLN:OE1	2.44	0.60
1:C:150:THR:OG1	1:C:151:GLN:N	2.30	0.60
1:C:902:MET:HE2	1:C:902:MET:HA	1.84	0.60
1:B:348:ILE:CG2	1:B:369:THR:HG23	2.30	0.60
1:C:629:VAL:CG2	1:C:629:VAL:O	2.43	0.60
2:D:49:THR:HB	2:D:50:PRO:CD	2.31	0.60
2:E:156:ASN:C	2:E:156:ASN:ND2	2.59	0.60
1:A:489:THR:HG22	1:A:490:PRO:HD3	1.82	0.60
1:B:72:ILE:CG2	1:B:73:ASP:N	2.65	0.60
1:B:150:THR:HG1	1:B:152:GLU:HB2	1.64	0.60
1:C:155:SER:HB3	1:C:287:SER:CB	2.32	0.60
1:C:596:HIS:NE2	1:C:600:THR:HG21	2.17	0.60
1:C:723:ASP:OD1	1:C:723:ASP:N	2.31	0.60
1:B:715:SER:HB2	1:B:830:GLN:HG2	1.83	0.60
1:C:464:GLY:HA2	1:C:467:TYR:HD1	1.66	0.60
2:D:49:THR:HB	2:D:50:PRO:HD2	1.82	0.60
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.83	0.60
1:B:347:ALA:O	1:B:351:VAL:HG23	2.00	0.60
1:B:421:ALA:HA	1:B:500:ILE:HG21	1.83	0.60
1:B:534:ILE:HG13	1:B:541:TYR:CD2	2.33	0.60
2:D:44:ASP:OD1	2:D:45:HIS:N	2.35	0.60
2:E:84:LEU:O	2:E:84:LEU:HD23	2.01	0.60
1:A:964:THR:O	1:A:968:VAL:HG23	2.02	0.60
1:C:211:ASN:ND2	1:C:760:ASN:ND2	2.49	0.60
1:C:327:TYR:CD2	1:C:327:TYR:C	2.80	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:92:HIS:O	2:E:96:VAL:CG2	2.41	0.60
1:A:945:ILE:HG22	1:A:946:VAL:N	2.10	0.59
1:A:457:ALA:HB2	1:A:471:SER:CB	2.32	0.59
1:A:685:ILE:HD13	1:A:685:ILE:N	2.16	0.59
1:A:694:LYS:HA	1:A:697:GLN:OE1	2.01	0.59
1:A:777:ALA:O	1:A:781:MET:HG2	2.03	0.59
1:A:899:PHE:C	1:A:901:VAL:N	2.52	0.59
1:B:254:ASN:CB	1:B:258:SER:O	2.49	0.59
1:B:842:GLU:O	1:B:846:GLN:HG3	2.02	0.59
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.83	0.59
1:A:423:GLU:C	1:A:502:LYS:CG	2.75	0.59
1:C:259:ARG:NH2	2:E:155:ASP:OD2	2.35	0.59
1:A:69:MET:O	1:C:168:ARG:HD3	2.02	0.59
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.85	0.59
1:B:382:VAL:O	1:B:382:VAL:CG2	2.48	0.59
1:B:726:GLN:NE2	1:B:812:GLY:CA	2.63	0.59
1:C:69:MET:HE2	1:C:92:LEU:HD21	1.83	0.59
1:B:739:LEU:HD13	1:B:799:VAL:CG2	2.31	0.59
1:C:490:PRO:O	1:C:493:CYS:HB2	2.02	0.59
2:E:93:LEU:HD21	2:E:128:ILE:HG13	1.83	0.59
1:A:444:GLY:O	1:A:448:VAL:HG12	2.03	0.59
1:B:671:ILE:C	1:B:672:VAL:CG1	2.74	0.59
1:C:496:MET:O	1:C:496:MET:HG3	2.03	0.59
1:C:541:TYR:HA	1:C:544:LEU:HD23	1.85	0.59
1:C:563:PHE:CE2	1:C:862:MET:HE1	2.38	0.59
1:A:308:ALA:O	1:A:312:LYS:HG3	2.02	0.59
1:A:795:ASP:OD1	1:A:795:ASP:N	2.30	0.59
1:B:117:LEU:N	1:B:117:LEU:HD12	2.16	0.59
1:B:685:ILE:HG23	1:B:686:ASP:N	2.16	0.59
1:B:714:THR:CG2	1:B:832:ALA:HA	2.31	0.59
1:C:204:ILE:HG23	1:C:759:VAL:HG22	1.83	0.59
2:D:133:LEU:HA	2:D:137:ALA:HB2	1.84	0.59
1:A:78:MET:O	1:A:78:MET:CG	2.50	0.59
1:A:983:ILE:HG23	1:A:1008:MET:HG3	1.85	0.59
1:B:241:THR:HA	1:B:763:ILE:O	2.03	0.59
1:B:254:ASN:O	1:B:257:GLY:CA	2.50	0.59
1:B:988:PRO:C	1:B:991:ILE:HG22	2.27	0.59
1:C:651:ALA:O	1:C:655:PHE:CD2	2.56	0.59
1:A:412:VAL:HG11	1:A:489:THR:HG21	1.85	0.59
1:A:485:ALA:O	1:A:490:PRO:HD2	2.00	0.59
1:B:60:THR:O	1:B:64:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.35	0.59
1:B:776:GLU:O	1:B:777:ALA:C	2.45	0.59
1:C:225:VAL:CG1	1:C:226:LYS:O	2.51	0.59
1:C:667:ASN:OD1	1:C:668:LEU:N	2.30	0.59
1:C:793:ALA:O	1:C:795:ASP:N	2.35	0.59
1:A:485:ALA:O	1:A:490:PRO:CG	2.51	0.59
1:B:250:LEU:HD23	1:B:251:LEU:H	1.55	0.59
1:B:293:LEU:HD11	1:B:299:ALA:HB2	1.84	0.59
1:B:352:PHE:HD2	1:B:353:LEU:HD12	1.68	0.59
1:B:435:MET:C	1:B:437:GLN:N	2.58	0.59
1:B:715:SER:O	1:B:829:GLY:HA2	2.03	0.59
1:B:759:VAL:HG23	1:B:771:VAL:HG12	1.84	0.59
1:B:765:ARG:NH1	1:B:765:ARG:CB	2.65	0.59
1:A:971:ARG:CG	1:A:971:ARG:NH1	2.38	0.58
1:B:83:ASP:OD2	1:B:83:ASP:N	2.34	0.58
1:C:927:PHE:CE2	1:C:931:LEU:HD12	2.38	0.58
1:B:422:GLU:O	1:B:423:GLU:HG2	2.03	0.58
1:B:712:MET:CE	1:B:839:GLU:OE2	2.51	0.58
1:C:1:FME:CN	1:C:2:PRO:CD	2.79	0.58
1:C:361:ASN:OD1	1:C:361:ASN:C	2.46	0.58
1:C:435:MET:O	1:C:439:GLN:CB	2.51	0.58
1:A:14:VAL:HG11	1:B:886:LEU:O	2.03	0.58
1:A:894:SER:CB	1:A:897:ILE:HD12	2.34	0.58
1:B:435:MET:O	1:B:438:ILE:N	2.27	0.58
1:C:154:ILE:O	1:C:154:ILE:CD1	2.31	0.58
1:C:731:ILE:CD1	1:C:746:ILE:HG21	2.33	0.58
1:C:773:VAL:O	1:C:773:VAL:HG13	2.04	0.58
1:C:876:LEU:O	1:C:876:LEU:HD22	2.02	0.58
2:D:49:THR:C	2:D:53:LEU:HD21	2.28	0.58
1:A:183:ALA:O	1:A:271:GLY:O	2.22	0.58
1:A:758:TYR:CE1	1:A:760:ASN:O	2.57	0.58
1:B:278:ILE:O	1:B:278:ILE:CG1	2.47	0.58
1:B:452:VAL:CG1	1:B:932:LEU:HD22	2.33	0.58
1:C:115:MET:N	1:C:116:PRO:HD2	2.18	0.58
1:A:146:ASP:HB3	1:A:148:THR:HG23	1.85	0.58
1:A:366:LEU:O	1:A:370:ILE:HG13	2.03	0.58
1:A:411:VAL:CG2	1:A:971:ARG:NH2	2.58	0.58
1:B:685:ILE:CG2	1:B:686:ASP:H	2.16	0.58
2:D:49:THR:CB	2:D:50:PRO:CD	2.82	0.58
1:B:724:THR:HB	1:B:725:PRO:CD	2.33	0.58
1:C:629:VAL:O	1:C:629:VAL:HG23	1.96	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1016:VAL:HG23	1:C:1017:LEU:HD12	1.86	0.58
2:D:44:ASP:OD1	2:D:45:HIS:CG	2.56	0.58
2:D:63:VAL:O	2:D:67:LEU:HG	2.03	0.58
1:A:972:LEU:O	1:A:975:ILE:HG22	2.04	0.58
1:B:197:GLN:C	1:B:798:MET:HE3	2.11	0.58
1:B:878:ALA:O	1:B:882:ILE:HG13	2.04	0.58
2:D:13:ASP:O	2:D:14:LEU:C	2.44	0.58
1:B:414:GLU:OE2	1:B:974:PRO:HG3	2.04	0.58
1:B:671:ILE:O	1:B:672:VAL:HG13	2.03	0.58
1:C:72:ILE:CG2	1:C:94:PHE:HE2	2.16	0.58
1:C:98:THR:HG23	1:C:99:ASP:N	2.19	0.58
1:C:447:MET:SD	1:C:891:LEU:HD23	2.44	0.58
1:C:688:ALA:HB2	1:C:854:GLY:CA	2.33	0.58
1:C:720:GLY:C	1:C:721:LEU:HD23	2.27	0.58
1:A:359:LEU:HD11	1:A:413:VAL:HG11	1.86	0.58
1:B:668:LEU:HD13	1:B:669:PRO:HD2	1.86	0.58
1:B:713:LEU:CD2	1:B:843:LEU:HD23	2.33	0.58
1:C:733:GLN:NE2	1:C:743:ILE:HD13	2.18	0.58
1:C:980:LEU:CD2	1:C:980:LEU:H	2.16	0.58
1:A:704:ALA:O	1:A:708:LYS:HG3	2.03	0.58
1:B:10:ILE:HG23	1:C:895:TRP:CZ2	2.39	0.58
1:C:735:LYS:O	1:C:739:LEU:CD2	2.49	0.58
1:A:423:GLU:O	1:A:502:LYS:HD2	2.03	0.57
1:B:250:LEU:C	1:B:250:LEU:HD22	2.24	0.57
1:B:365:THR:HG23	1:B:366:LEU:N	2.19	0.57
1:B:531:VAL:O	1:B:534:ILE:HG22	2.04	0.57
1:C:453:PHE:CE1	1:C:474:ILE:HG21	2.38	0.57
1:C:527:TYR:CE2	1:C:968:VAL:HG13	2.38	0.57
1:C:531:VAL:HG21	1:C:968:VAL:HG11	1.84	0.57
1:A:230:LEU:HD12	1:A:231:ASN:H	1.69	0.57
1:B:449:LEU:O	1:B:453:PHE:CD1	2.53	0.57
1:C:30:LEU:HD13	1:C:390:ILE:HG13	1.86	0.57
1:C:837:THR:O	1:C:841:MET:HG3	2.04	0.57
1:A:815:ARG:O	1:A:815:ARG:HG3	2.05	0.57
1:B:534:ILE:HG13	1:B:541:TYR:CE1	2.36	0.57
1:B:578:LEU:HD12	1:B:579:PRO:HD3	1.87	0.57
1:B:685:ILE:HG23	1:B:686:ASP:H	1.68	0.57
1:C:879:ILE:HG23	1:C:880:SER:H	1.69	0.57
1:A:774:MET:HG2	1:A:775:SER:H	1.69	0.57
1:B:764:ASP:CG	1:B:765:ARG:HG3	2.30	0.57
1:C:58:GLN:OE1	1:C:818:ARG:HD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:O	1:A:14:VAL:HG12	2.04	0.57
1:A:189:ASN:HD22	1:A:192:GLU:CD	2.12	0.57
1:A:949:ALA:O	1:A:953:MET:HG2	2.04	0.57
1:C:230:LEU:HD23	1:C:230:LEU:N	2.19	0.57
1:B:853:THR:CA	1:B:857:TYR:N	2.67	0.57
1:C:567:GLU:CD	1:C:998:GLY:H	2.10	0.57
1:A:223:PRO:HD2	1:B:780:ARG:NH2	2.19	0.57
1:A:315:PRO:HB2	1:A:316:PHE:CE1	2.39	0.57
1:A:534:ILE:HG22	1:A:541:TYR:CE1	2.40	0.57
1:C:793:ALA:C	1:C:795:ASP:N	2.59	0.57
2:D:46:VAL:O	2:D:46:VAL:HG22	2.03	0.57
1:A:36:PRO:HD3	1:A:391:ASN:ND2	2.19	0.57
1:A:423:GLU:CA	1:A:502:LYS:HG3	2.35	0.57
1:A:449:LEU:O	1:A:452:VAL:HG22	2.05	0.57
1:A:591:LEU:HD12	1:A:613:ASN:ND2	2.20	0.57
1:A:878:ALA:O	1:A:882:ILE:HG12	2.04	0.57
1:B:47:ALA:HB2	1:B:127:VAL:HG13	1.85	0.57
1:B:452:VAL:HG12	1:B:932:LEU:HD22	1.87	0.57
1:B:501:ALA:CB	1:B:504:ASP:HB2	2.33	0.57
1:C:572:PHE:CZ	1:C:629:VAL:HG21	2.39	0.57
1:C:714:THR:HG22	1:C:715:SER:N	2.19	0.57
1:C:927:PHE:CZ	1:C:931:LEU:HD11	2.40	0.57
1:A:188:MET:HE1	1:A:203:VAL:HG11	1.86	0.57
1:B:403:GLY:HA3	1:B:982:PHE:HE1	1.69	0.57
1:B:493:CYS:O	1:B:497:LEU:HB2	2.04	0.57
1:B:1022:VAL:HA	1:B:1025:PHE:CD1	2.39	0.57
1:C:332:PHE:CD2	1:C:569:GLN:NE2	2.73	0.57
1:C:667:ASN:CG	1:C:668:LEU:H	2.11	0.57
1:B:11:PHE:HE1	1:B:15:ILE:HD11	1.70	0.57
1:B:726:GLN:HE22	1:B:812:GLY:CA	2.11	0.57
1:C:156:ASP:OD1	1:C:182:TYR:CB	2.52	0.57
1:C:190:PRO:HG3	1:C:789:TRP:CZ3	2.39	0.57
1:B:686:ASP:HB2	1:B:695:LEU:HD12	1.87	0.56
1:B:775:SER:OG	1:B:780:ARG:CG	2.50	0.56
1:C:153:ASP:OD1	1:C:182:TYR:OH	2.23	0.56
1:C:448:VAL:HG11	1:C:939:ALA:HB3	1.85	0.56
1:A:194:ASN:HD22	1:A:798:MET:HG3	1.68	0.56
1:A:621:GLY:HA3	1:A:624:THR:CG2	2.34	0.56
1:A:668:LEU:HD23	1:A:668:LEU:N	2.18	0.56
1:A:892:TYR:OH	1:A:946:VAL:HG13	2.04	0.56
1:B:56:THR:O	1:B:60:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:MET:HE1	1:B:107:VAL:HG13	1.87	0.56
1:C:34:GLN:HG2	1:C:35:TYR:CD1	2.40	0.56
1:C:482:VAL:HG12	1:C:486:LEU:CD1	2.35	0.56
2:D:87:ALA:O	2:D:91:GLY:N	2.37	0.56
1:A:269:GLU:O	1:A:270:LEU:C	2.41	0.56
1:A:686:ASP:HB3	1:A:823:PRO:HB2	1.87	0.56
1:A:742:SER:OG	1:A:744:ASN:HB2	2.05	0.56
1:A:892:TYR:HE2	1:A:947:GLU:HA	1.70	0.56
1:A:943:ILE:O	1:A:946:VAL:HG13	2.06	0.56
1:B:62:THR:O	1:B:62:THR:HG22	2.05	0.56
1:B:596:HIS:CD2	1:B:600:THR:OG1	2.57	0.56
1:B:958:LYS:NZ	1:B:966:ASP:OD2	2.38	0.56
1:C:247:GLY:O	1:C:263:ARG:HG2	2.04	0.56
1:C:448:VAL:HG21	1:C:943:ILE:HD11	1.86	0.56
1:C:671:ILE:HD11	1:C:674:LEU:HG	1.84	0.56
2:D:34:MET:HA	2:D:34:MET:CE	2.35	0.56
1:B:189:ASN:OD1	1:B:189:ASN:N	2.38	0.56
1:C:164:ASP:OD2	1:C:767:ARG:NH2	2.31	0.56
2:D:27:ASP:OD2	2:D:27:ASP:N	2.39	0.56
2:E:105:ASP:OD1	2:E:106:VAL:N	2.38	0.56
1:A:236:ALA:HB2	1:B:729:ILE:HG23	1.87	0.56
1:A:488:LEU:HD11	1:A:492:LEU:HD13	1.88	0.56
1:B:987:MET:HG2	1:B:988:PRO:CD	2.35	0.56
1:C:240:LEU:HD22	1:C:245:GLU:HB3	1.87	0.56
1:C:879:ILE:HG23	1:C:880:SER:N	2.20	0.56
1:A:469:GLN:OE1	1:A:469:GLN:HA	2.05	0.56
1:A:897:ILE:N	1:A:898:PRO:HD2	2.21	0.56
1:B:712:MET:CB	1:B:713:LEU:HD13	2.36	0.56
1:B:893:GLU:HG3	1:B:893:GLU:O	2.05	0.56
1:B:987:MET:HG2	1:B:988:PRO:N	2.21	0.56
1:C:672:VAL:HG22	1:C:673:GLU:OE1	2.04	0.56
1:B:10:ILE:CG1	1:C:893:GLU:OE2	2.54	0.56
1:B:540:ARG:O	1:B:544:LEU:HD13	2.05	0.56
1:B:673:GLU:C	1:B:675:GLY:N	2.59	0.56
1:B:516:PHE:C	1:B:516:PHE:CD1	2.83	0.56
1:A:248:LYS:O	1:A:261:LEU:CD2	2.49	0.56
1:B:987:MET:HG2	1:B:988:PRO:HD3	1.88	0.56
1:C:34:GLN:NE2	1:C:333:VAL:HG22	2.20	0.56
1:C:903:LEU:O	1:C:906:PRO:HD2	2.06	0.56
2:E:56:TYR:O	2:E:56:TYR:CG	2.58	0.56
1:A:205:THR:HG22	1:A:206:ALA:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ARG:C	1:A:240:LEU:HD12	2.31	0.56
1:B:188:MET:C	1:B:189:ASN:OD1	2.49	0.56
1:B:979:SER:O	1:B:983:ILE:HG13	2.07	0.56
1:C:146:ASP:CB	1:C:148:THR:HG21	2.35	0.56
1:C:318:PRO:C	1:C:319:SER:HG	2.10	0.56
1:C:324:VAL:CG2	1:C:325:TYR:N	2.69	0.56
1:C:572:PHE:CE2	1:C:629:VAL:HG21	2.40	0.55
1:C:729:ILE:C	1:C:730:ASP:OD1	2.49	0.55
2:D:44:ASP:OD1	2:D:45:HIS:CD2	2.60	0.55
2:D:73:VAL:HG12	2:D:74:ASN:H	1.68	0.55
2:E:100:LEU:O	2:E:103:GLY:HA2	2.06	0.55
1:A:23:GLY:O	1:A:26:ALA:HB3	2.05	0.55
1:A:456:MET:HG3	1:A:467:TYR:HB3	1.88	0.55
1:A:588:GLN:O	1:A:589:LYS:C	2.49	0.55
1:B:231:ASN:HD22	1:B:231:ASN:C	2.14	0.55
1:B:764:ASP:OD1	1:B:765:ARG:HG2	2.05	0.55
1:C:993:THR:O	1:C:993:THR:CG2	2.35	0.55
2:E:57:PHE:H	2:E:58:GLY:HA2	1.70	0.55
1:A:997:SER:O	1:A:998:GLY:C	2.48	0.55
1:A:583:THR:H	1:A:586:ARG:HG3	1.72	0.55
1:A:655:PHE:O	1:A:658:ILE:HG13	2.07	0.55
1:A:949:ALA:O	1:A:953:MET:CG	2.54	0.55
1:B:328:ASP:OD1	1:B:329:THR:N	2.40	0.55
1:C:94:PHE:C	1:C:95:GLU:O	2.44	0.55
1:C:637:ARG:N	1:C:638:PRO:HD3	2.21	0.55
1:A:435:MET:HE2	1:A:490:PRO:HG3	1.87	0.55
1:A:542:LEU:O	1:A:545:TYR:CB	2.55	0.55
1:B:72:ILE:HG22	1:B:73:ASP:H	1.70	0.55
1:B:169:THR:CG2	1:B:172:VAL:HG11	2.36	0.55
1:C:816:LEU:N	1:C:816:LEU:CD1	2.70	0.55
1:C:933:THR:O	1:C:937:LEU:HG	2.07	0.55
1:A:391:ASN:O	1:A:395:MET:HG2	2.07	0.55
1:A:555:LEU:CD1	1:A:914:LEU:HD23	2.37	0.55
1:A:1026:PHE:CD2	1:A:1026:PHE:O	2.59	0.55
1:B:162:MET:O	1:B:166:ILE:HG12	2.07	0.55
1:B:336:SER:OG	1:B:395:MET:CE	2.55	0.55
1:C:327:TYR:CD1	1:C:628:PHE:CD1	2.94	0.55
1:C:482:VAL:HG12	1:C:486:LEU:HD11	1.88	0.55
1:C:894:SER:O	1:C:898:PRO:CD	2.54	0.55
1:A:139:VAL:O	1:A:326:PRO:HD2	2.07	0.55
1:A:184:MET:HG2	1:A:246:PHE:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:C	1:A:261:LEU:HD23	2.31	0.55
1:B:623:ASN:HD22	1:B:623:ASN:C	2.14	0.55
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.87	0.55
1:C:674:LEU:CD2	1:C:674:LEU:N	2.30	0.55
2:D:132:LEU:O	2:D:136:GLY:O	2.25	0.55
2:E:77:ASP:HB3	2:E:81:VAL:H	1.71	0.55
1:A:16:ALA:HB2	1:A:488:LEU:HD23	1.89	0.55
1:A:749:THR:HG21	1:A:791:VAL:CG1	2.33	0.55
1:A:792:ARG:HG3	1:A:793:ALA:N	2.21	0.55
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.87	0.55
1:B:184:MET:CE	1:B:268:ILE:CG2	2.85	0.55
1:B:952:LEU:O	1:B:956:GLU:HB2	2.07	0.55
2:D:100:LEU:HD21	2:D:106:VAL:HG13	1.88	0.55
1:A:471:SER:O	1:A:475:VAL:HG23	2.06	0.55
1:B:668:LEU:HB2	1:B:669:PRO:CD	2.36	0.55
1:C:688:ALA:HB2	1:C:854:GLY:HA3	1.87	0.55
1:C:876:LEU:O	1:C:880:SER:HB2	2.06	0.55
1:C:940:LYS:HG3	1:C:941:ASN:H	1.72	0.55
2:E:46:VAL:HG22	2:E:78:SER:HB3	1.89	0.55
1:A:899:PHE:C	1:A:902:MET:H	2.13	0.55
1:C:184:MET:HB3	1:C:771:VAL:HG22	1.89	0.55
1:C:948:PHE:HD1	1:C:967:ALA:HA	1.71	0.55
2:D:44:ASP:CG	2:D:45:HIS:CA	2.80	0.55
2:E:154:ILE:CG1	2:E:155:ASP:N	2.70	0.55
1:A:219:LEU:CD1	1:B:783:PRO:HG3	2.37	0.54
1:A:572:PHE:CZ	1:A:629:VAL:HG11	2.43	0.54
1:A:972:LEU:CD1	1:A:972:LEU:C	2.80	0.54
1:B:634:TRP:O	1:B:637:ARG:O	2.25	0.54
1:B:705:GLU:HB3	1:B:847:LEU:CD2	2.37	0.54
1:B:987:MET:O	1:B:991:ILE:HG22	2.08	0.54
1:C:480:LEU:O	1:C:484:VAL:HG23	2.06	0.54
2:E:49:THR:O	2:E:52:HIS:HB2	2.08	0.54
1:A:380:PHE:CD1	1:A:380:PHE:N	2.75	0.54
1:A:899:PHE:O	1:A:902:MET:N	2.30	0.54
1:B:194:ASN:ND2	1:B:790:TYR:CB	2.70	0.54
1:A:598:TYR:HA	1:A:602:GLU:CB	2.37	0.54
1:A:898:PRO:O	1:A:901:VAL:HB	2.08	0.54
1:B:414:GLU:CD	1:B:974:PRO:HG3	2.32	0.54
1:B:729:ILE:C	1:B:730:ASP:OD2	2.50	0.54
1:C:343:THR:HG21	1:C:989:LEU:HD23	1.90	0.54
1:C:626:ILE:O	1:C:626:ILE:CG2	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:789:TRP:O	1:C:801:PHE:HB2	2.06	0.54
2:E:66:LEU:O	2:E:71:ALA:HB2	2.07	0.54
1:A:685:ILE:HG12	1:A:687:GLN:HE22	1.73	0.54
1:B:557:VAL:O	1:B:557:VAL:HG23	2.06	0.54
1:B:330:THR:N	1:B:331:PRO:CD	2.71	0.54
1:B:352:PHE:CD2	1:B:353:LEU:HD12	2.43	0.54
1:B:859:TRP:HA	1:B:859:TRP:HE3	1.69	0.54
1:C:169:THR:HG22	1:C:170:SER:N	2.21	0.54
1:A:236:ALA:HB1	1:B:729:ILE:O	2.07	0.54
1:A:528:THR:OG1	1:A:529:ASP:N	2.39	0.54
1:B:138:MET:HE2	1:B:140:VAL:HG22	1.89	0.54
1:C:72:ILE:HG22	1:C:94:PHE:HE2	1.73	0.54
1:C:327:TYR:HB2	1:C:628:PHE:HB3	1.89	0.54
1:C:607:GLU:HG3	1:C:607:GLU:O	2.08	0.54
1:C:793:ALA:N	1:C:797:GLN:O	2.41	0.54
2:E:115:THR:OG1	2:E:118:HIS:CD2	2.60	0.54
1:A:489:THR:O	1:A:493:CYS:N	2.37	0.54
1:A:527:TYR:CD1	1:A:972:LEU:HD21	2.42	0.54
1:A:598:TYR:HA	1:A:602:GLU:HB3	1.89	0.54
1:B:367:ILE:N	1:B:368:PRO:CD	2.71	0.54
1:C:894:SER:O	1:C:898:PRO:HG2	2.08	0.54
2:D:50:PRO:HA	2:D:53:LEU:CD2	2.37	0.54
1:A:527:TYR:HE1	1:A:968:VAL:HG12	1.72	0.54
1:B:143:ILE:HG22	1:B:286:ALA:CB	2.37	0.54
1:B:414:GLU:HG3	1:B:977:MET:HE1	1.90	0.54
1:C:687:GLN:HA	1:C:822:LEU:HD23	1.89	0.54
1:C:810:GLU:O	1:C:811:TYR:CD2	2.59	0.54
1:B:53:ASP:CG	1:B:56:THR:OG1	2.50	0.54
1:C:36:PRO:HD2	1:C:393:LEU:HD12	1.90	0.54
1:C:754:TRP:CZ2	1:C:786:ILE:CG1	2.91	0.54
1:C:910:ILE:CG2	1:C:911:GLY:N	2.70	0.54
1:A:594:VAL:HG22	1:A:655:PHE:CE1	2.43	0.54
1:B:668:LEU:CD1	1:B:669:PRO:HD2	2.38	0.54
1:C:157:TYR:C	1:C:157:TYR:HD2	2.13	0.54
1:A:6:ILE:HG23	1:A:494:ALA:CB	2.38	0.53
1:A:24:GLY:O	1:A:28:LEU:HG	2.08	0.53
1:B:242:SER:HB3	1:B:245:GLU:HG3	1.89	0.53
1:B:853:THR:HA	1:B:857:TYR:N	2.23	0.53
1:C:261:LEU:HD12	1:C:263:ARG:HD2	1.89	0.53
1:C:640:GLU:N	1:C:640:GLU:CD	2.66	0.53
1:C:681:ASP:HB3	1:C:860:THR:CG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:815:ARG:O	1:C:815:ARG:HG2	2.09	0.53
2:D:110:ASP:HB3	2:D:112:ASN:H	1.73	0.53
1:A:1:FME:CN	1:A:2:PRO:HD2	2.38	0.53
1:A:466:ILE:HD13	1:A:466:ILE:N	2.22	0.53
1:B:794:ALA:C	1:B:796:GLY:H	2.14	0.53
1:B:885:PHE:CD1	1:B:902:MET:HE1	2.32	0.53
1:C:302:THR:O	1:C:306:ILE:HG13	2.08	0.53
1:C:375:VAL:HB	1:C:405:LEU:HD13	1.88	0.53
1:C:753:ALA:O	1:C:775:SER:HB3	2.08	0.53
1:C:926:TYR:HD2	1:C:1003:VAL:CG2	2.20	0.53
1:A:243:THR:OG1	1:A:244:GLU:N	2.38	0.53
1:B:197:GLN:C	1:B:798:MET:HE1	2.31	0.53
1:B:419:VAL:O	1:B:423:GLU:HG3	2.08	0.53
1:C:71:GLY:O	1:C:72:ILE:HG13	2.07	0.53
1:C:158:VAL:CA	1:C:162:MET:HE3	2.28	0.53
1:C:754:TRP:HZ2	1:C:786:ILE:HG12	1.73	0.53
2:D:13:ASP:OD1	2:D:14:LEU:N	2.42	0.53
2:D:57:PHE:N	2:D:58:GLY:HA2	2.20	0.53
1:A:445:ILE:CG2	1:A:940:LYS:HE2	2.35	0.53
1:B:988:PRO:HA	1:B:991:ILE:CG2	2.38	0.53
1:C:1:FME:HB2	1:C:2:PRO:HD3	1.90	0.53
1:C:449:LEU:CB	1:C:478:MET:HE2	2.38	0.53
1:C:712:MET:SD	1:C:835:LYS:HG3	2.49	0.53
2:D:129:VAL:C	2:D:133:LEU:HD12	2.27	0.53
1:A:694:LYS:CA	1:A:697:GLN:OE1	2.56	0.53
1:A:815:ARG:O	1:A:815:ARG:CG	2.56	0.53
1:C:361:ASN:O	1:C:365:THR:HG22	2.08	0.53
1:C:750:LEU:O	1:C:750:LEU:CD2	2.30	0.53
1:A:539:GLY:O	1:A:543:VAL:CG2	2.57	0.53
1:B:196:PHE:CA	1:B:197:GLN:HE22	2.13	0.53
1:B:435:MET:O	1:B:436:GLY:C	2.47	0.53
1:B:777:ALA:HA	1:B:780:ARG:NH2	2.23	0.53
1:C:741:VAL:CG1	1:C:746:ILE:HD13	2.36	0.53
1:C:923:ASN:OD1	1:C:927:PHE:HD2	1.90	0.53
1:A:298:ASN:ND2	1:A:301:ASP:N	2.50	0.53
1:A:314:GLU:N	1:A:315:PRO:CD	2.72	0.53
1:A:424:GLY:CA	1:A:502:LYS:HB2	2.39	0.53
1:B:504:ASP:C	1:B:505:HIS:O	2.41	0.53
1:C:880:SER:O	1:C:884:VAL:HG23	2.07	0.53
1:C:926:TYR:CD2	1:C:1003:VAL:CG2	2.92	0.53
2:E:133:LEU:HA	2:E:136:GLY:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ASP:O	1:C:105:VAL:HG23	2.08	0.53
1:C:204:ILE:HG23	1:C:759:VAL:HG21	1.88	0.53
1:C:323:ILE:HG22	1:C:324:VAL:N	2.24	0.53
1:C:429:GLU:OE1	1:C:429:GLU:CA	2.55	0.53
1:C:673:GLU:N	1:C:673:GLU:OE2	2.30	0.53
1:C:901:VAL:HG12	1:C:946:VAL:HG21	1.91	0.53
1:C:978:THR:OG1	1:C:979:SER:N	2.39	0.53
1:B:1:FME:CE	1:B:487:ILE:CG1	2.87	0.53
1:B:596:HIS:CD2	1:B:600:THR:HG1	2.27	0.53
1:C:623:ASN:ND2	1:C:623:ASN:O	2.29	0.53
1:C:687:GLN:HA	1:C:822:LEU:CD2	2.39	0.53
1:C:811:TYR:HD2	1:C:811:TYR:N	2.07	0.53
2:D:126:LEU:CA	2:D:129:VAL:CG2	2.86	0.53
1:A:743:ILE:HD12	1:A:743:ILE:N	2.23	0.53
1:B:217:GLY:O	1:B:234:ILE:HG13	2.09	0.53
1:B:714:THR:HG21	1:B:832:ALA:HA	1.90	0.53
1:C:207:ILE:HG22	1:C:760:ASN:HD21	1.72	0.53
2:D:100:LEU:HD21	2:D:106:VAL:CG1	2.39	0.53
1:B:207:ILE:CG2	1:B:207:ILE:O	2.50	0.52
1:B:443:VAL:O	1:B:446:ALA:HB3	2.09	0.52
1:B:879:ILE:O	1:B:883:VAL:HG23	2.07	0.52
1:C:74:ASN:OD1	1:C:74:ASN:N	2.41	0.52
1:C:686:ASP:OD1	1:C:686:ASP:C	2.48	0.52
1:C:695:LEU:O	1:C:695:LEU:HD23	2.09	0.52
1:C:724:THR:HG21	1:C:814:PRO:HG3	1.91	0.52
1:C:1036:LYS:O	1:C:1037:ASN:C	2.48	0.52
2:D:13:ASP:C	2:D:15:GLY:N	2.62	0.52
2:D:77:ASP:CG	2:D:78:SER:N	2.67	0.52
2:E:93:LEU:CD2	2:E:128:ILE:CG1	2.70	0.52
1:B:62:THR:O	1:B:66:GLU:HG3	2.09	0.52
1:B:501:ALA:O	1:B:504:ASP:CB	2.56	0.52
1:B:844:MET:HA	1:B:844:MET:HE3	1.90	0.52
1:C:157:TYR:CD2	1:C:157:TYR:O	2.62	0.52
1:C:506:GLY:O	1:C:507:GLU:CG	2.58	0.52
2:D:94:GLU:H	2:D:94:GLU:CD	2.18	0.52
1:A:1:FME:N	1:A:2:PRO:HD3	2.21	0.52
1:A:207:ILE:HG22	1:A:760:ASN:HD22	1.75	0.52
1:B:173:GLY:CA	1:B:294:ALA:HB2	2.40	0.52
1:C:724:THR:HB	1:C:725:PRO:HD3	1.91	0.52
2:D:51:LEU:HD22	2:D:83:PRO:CG	2.39	0.52
2:E:143:ASP:H	2:E:146:GLY:C	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ILE:O	1:A:449:LEU:HB2	2.09	0.52
1:B:166:ILE:O	1:B:169:THR:HB	2.09	0.52
1:B:328:ASP:OD1	1:B:328:ASP:C	2.51	0.52
1:C:924:ASP:OD2	1:C:924:ASP:N	2.35	0.52
2:D:44:ASP:CG	2:D:45:HIS:HA	2.33	0.52
1:A:558:ARG:O	1:A:558:ARG:HD3	2.08	0.52
1:A:935:ILE:O	1:A:935:ILE:CG1	2.56	0.52
1:B:196:PHE:O	1:B:197:GLN:C	2.47	0.52
1:B:926:TYR:HB3	1:B:1003:VAL:HG13	1.90	0.52
1:C:347:ALA:O	1:C:351:VAL:HG23	2.09	0.52
1:C:736:ALA:O	1:C:741:VAL:CB	2.49	0.52
1:B:687:GLN:NE2	1:B:859:TRP:HB2	2.24	0.52
1:C:512:PHE:O	1:C:512:PHE:HD1	1.88	0.52
1:C:681:ASP:O	1:C:859:TRP:HE3	1.93	0.52
2:D:145:PHE:C	2:D:147:LYS:H	2.16	0.52
2:E:100:LEU:O	2:E:103:GLY:N	2.42	0.52
1:A:481:SER:OG	1:A:482:VAL:N	2.39	0.52
1:B:61:VAL:HG13	1:B:65:ILE:HD11	1.91	0.52
1:C:378:GLY:O	1:C:382:VAL:HG23	2.10	0.52
1:A:423:GLU:C	1:A:502:LYS:CE	2.81	0.52
1:A:531:VAL:HA	1:A:534:ILE:HG12	1.92	0.52
1:A:782:LEU:HB2	1:A:785:ASP:CG	2.35	0.52
1:B:659:LYS:O	1:B:660:ASP:HB2	2.09	0.52
1:C:631:LEU:HD11	1:C:644:VAL:HG12	1.91	0.52
1:C:952:LEU:O	1:C:956:GLU:HB3	2.09	0.52
2:D:73:VAL:HG13	2:D:74:ASN:N	2.16	0.52
2:E:117:LEU:HD12	2:E:132:LEU:HD12	1.92	0.52
1:A:236:ALA:HB2	1:B:729:ILE:HG22	1.92	0.52
1:A:519:MET:HG3	1:A:520:PHE:N	2.25	0.52
1:B:126:GLY:HA2	1:C:116:PRO:HB3	1.91	0.52
1:B:729:ILE:HG13	1:B:806:SER:O	2.10	0.52
1:C:44:THR:HB	1:C:132:SER:CB	2.39	0.52
1:C:158:VAL:HG22	1:C:162:MET:CE	2.39	0.52
1:C:278:ILE:HD13	1:C:278:ILE:H	1.75	0.52
1:C:330:THR:N	1:C:331:PRO:CD	2.73	0.52
1:C:505:HIS:O	1:C:505:HIS:ND1	2.39	0.52
1:C:669:PRO:O	1:C:669:PRO:CD	2.53	0.52
1:C:969:ARG:NH2	1:C:970:MET:HE3	2.24	0.52
1:A:139:VAL:HG13	1:A:178:PHE:HE2	1.75	0.52
1:A:288:GLY:O	1:A:289:LEU:HD23	2.10	0.52
1:A:498:LYS:HZ2	1:A:500:ILE:HD11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:PHE:HB3	1:A:1025:PHE:CZ	2.45	0.52
1:B:108:GLN:HG3	1:C:112:GLN:CG	2.40	0.52
1:B:184:MET:CB	1:B:771:VAL:HG22	2.38	0.52
1:B:255:GLN:C	1:B:257:GLY:N	2.64	0.52
1:C:156:ASP:OD1	1:C:182:TYR:CD2	2.62	0.52
1:C:169:THR:CG2	1:C:170:SER:N	2.72	0.52
1:A:92:LEU:N	1:A:92:LEU:HD12	2.25	0.51
1:B:489:THR:N	1:B:490:PRO:CD	2.74	0.51
1:C:960:LEU:C	1:C:960:LEU:HD12	2.31	0.51
1:A:488:LEU:HD11	1:A:492:LEU:HD11	1.91	0.51
1:B:905:VAL:O	1:B:909:VAL:HG23	2.10	0.51
1:C:957:GLY:O	1:C:958:LYS:HG2	2.11	0.51
2:E:57:PHE:HB2	2:E:58:GLY:HA2	1.92	0.51
1:A:489:THR:HG22	1:A:490:PRO:CD	2.40	0.51
1:A:504:ASP:OD1	1:A:506:GLY:N	2.44	0.51
1:B:846:GLN:O	1:B:849:SER:OG	2.23	0.51
1:C:74:ASN:HB3	1:C:95:GLU:CB	2.34	0.51
1:C:87:THR:C	1:C:88:VAL:HG12	2.35	0.51
1:C:785:ASP:O	1:C:788:ASP:HB2	2.09	0.51
1:A:213:GLN:HA	1:A:237:GLN:O	2.10	0.51
1:A:609:VAL:HG22	1:A:629:VAL:HG22	1.92	0.51
1:B:26:ALA:O	1:B:30:LEU:HD22	2.10	0.51
1:C:71:GLY:H	1:C:110:LYS:NZ	2.09	0.51
1:C:160:ALA:CB	1:C:161:ASN:OD1	2.59	0.51
1:C:247:GLY:C	1:C:263:ARG:HG2	2.36	0.51
2:D:93:LEU:CD2	2:D:128:ILE:HG12	2.39	0.51
1:A:450:SER:O	1:A:454:VAL:HG23	2.10	0.51
1:A:685:ILE:HG12	1:A:687:GLN:NE2	2.26	0.51
1:B:482:VAL:HG12	1:B:486:LEU:HD13	1.91	0.51
1:B:1007:VAL:O	1:B:1011:MET:HB2	2.11	0.51
1:C:889:ALA:O	1:C:892:TYR:O	2.29	0.51
1:C:974:PRO:O	1:C:978:THR:HG23	2.11	0.51
1:A:683:GLU:OE2	1:A:860:THR:HG21	2.11	0.51
1:A:767:ARG:HG3	1:A:768:VAL:N	2.26	0.51
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.32	0.51
1:B:776:GLU:HB3	1:B:779:TYR:HD1	1.76	0.51
1:C:724:THR:HG23	1:C:814:PRO:HG3	1.92	0.51
1:C:958:LYS:HD3	1:C:962:GLU:CD	2.36	0.51
1:A:975:ILE:HD13	1:A:1019:ILE:CD1	2.41	0.51
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.46	0.51
1:B:435:MET:C	1:B:437:GLN:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:ASP:OD1	1:C:686:ASP:O	2.29	0.51
1:A:180:SER:HB3	1:A:274:ASN:ND2	2.26	0.51
1:B:310:LEU:HD13	1:B:323:ILE:CD1	2.41	0.51
1:B:960:LEU:HD21	1:B:1027:VAL:HG22	1.92	0.51
1:C:616:GLY:O	1:C:619:GLY:O	2.29	0.51
1:C:692:HIS:O	1:C:696:THR:HG22	2.11	0.51
1:A:807:SER:O	1:A:808:ARG:HG3	2.11	0.51
1:B:60:THR:O	1:B:61:VAL:C	2.49	0.51
1:B:508:GLY:C	1:B:510:LYS:N	2.63	0.51
1:B:790:TYR:CD1	1:B:800:PRO:HA	2.46	0.51
1:C:925:VAL:C	1:C:927:PHE:N	2.65	0.51
1:A:183:ALA:N	1:A:271:GLY:O	2.39	0.50
1:B:102:ILE:O	1:B:103:ALA:C	2.54	0.50
1:B:146:ASP:HB2	1:B:320:GLY:HA3	1.93	0.50
1:C:53:ASP:OD2	1:C:56:THR:OG1	2.29	0.50
1:C:196:PHE:O	1:C:197:GLN:CG	2.59	0.50
1:C:278:ILE:HD11	1:C:613:ASN:HB3	1.91	0.50
1:C:328:ASP:OD1	1:C:329:THR:N	2.43	0.50
1:A:33:ALA:O	1:A:391:ASN:HA	2.11	0.50
1:A:70:ASN:OD1	1:A:70:ASN:O	2.29	0.50
1:A:830:GLN:OE1	1:A:830:GLN:N	2.44	0.50
1:B:61:VAL:CG1	1:B:65:ILE:HD11	2.42	0.50
1:C:451:ALA:O	1:C:455:PRO:HD2	2.10	0.50
1:C:504:ASP:OD1	1:C:504:ASP:O	2.29	0.50
1:C:741:VAL:HG12	1:C:746:ILE:CD1	2.38	0.50
1:A:84:SER:OG	1:A:814:PRO:HA	2.12	0.50
1:A:150:THR:HG23	1:A:153:ASP:H	1.76	0.50
1:A:693:GLU:H	1:A:693:GLU:CD	2.16	0.50
1:B:69:MET:HE3	1:B:72:ILE:CD1	2.34	0.50
1:B:175:VAL:CG1	1:B:289:LEU:CD2	2.89	0.50
1:B:199:THR:HG21	1:B:792:ARG:H	1.77	0.50
1:B:595:THR:HG23	1:B:609:VAL:HB	1.93	0.50
1:A:58:GLN:NE2	1:A:818:ARG:NH1	2.57	0.50
1:A:394:THR:HG23	1:A:473:THR:CG2	2.41	0.50
1:A:448:VAL:HG21	1:A:888:LEU:HD21	1.94	0.50
1:B:158:VAL:CA	1:B:162:MET:HG3	2.27	0.50
1:B:746:ILE:C	1:B:748:THR:H	2.20	0.50
1:B:778:LYS:HG3	1:B:778:LYS:O	2.12	0.50
1:B:799:VAL:HG12	1:B:800:PRO:O	2.11	0.50
1:B:982:PHE:O	1:B:986:VAL:HG23	2.12	0.50
1:C:23:GLY:O	1:C:27:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:O	1:A:358:PHE:HD1	1.93	0.50
1:B:324:VAL:HG22	1:B:325:TYR:H	1.75	0.50
1:B:605:ASN:ND2	1:B:642:ASN:HB3	2.23	0.50
1:B:673:GLU:C	1:B:675:GLY:H	2.18	0.50
1:B:682:PHE:N	1:B:827:ILE:O	2.38	0.50
1:B:925:VAL:O	1:B:929:VAL:HG23	2.12	0.50
1:B:988:PRO:HA	1:B:991:ILE:HG21	1.93	0.50
1:C:395:MET:HA	1:C:395:MET:HE2	1.94	0.50
1:C:801:PHE:O	1:C:805:SER:OG	2.30	0.50
2:E:49:THR:HG22	2:E:52:HIS:CE1	2.47	0.50
1:A:431:THR:HG22	1:A:432:ARG:N	2.23	0.50
1:A:528:THR:OG1	1:A:529:ASP:OD2	2.30	0.50
1:B:194:ASN:O	1:B:194:ASN:OD1	2.30	0.50
1:C:592:ASN:O	1:C:596:HIS:HB2	2.11	0.50
1:C:761:ASP:HB3	1:C:768:VAL:HG13	1.92	0.50
1:A:589:LYS:NZ	1:A:593:GLU:OE2	2.45	0.50
1:B:397:GLY:O	1:B:474:ILE:HG12	2.12	0.50
1:C:504:ASP:O	1:C:504:ASP:CG	2.52	0.50
1:C:559:LEU:HD12	1:C:560:PRO:CD	2.41	0.50
1:C:780:ARG:HH11	1:C:780:ARG:HG3	1.77	0.50
2:D:143:ASP:HB2	2:D:147:LYS:O	2.10	0.50
1:A:1:FME:CN	1:A:2:PRO:CD	2.90	0.50
1:A:13:TRP:O	1:A:17:ILE:HG12	2.12	0.50
1:A:36:PRO:HD3	1:A:391:ASN:HD22	1.77	0.50
1:A:525:HIS:O	1:A:528:THR:OG1	2.30	0.50
1:A:721:LEU:HD11	1:A:814:PRO:CB	2.42	0.50
1:B:58:GLN:HA	1:B:62:THR:HB	1.94	0.50
1:B:324:VAL:O	1:B:326:PRO:HD3	2.11	0.50
1:C:53:ASP:OD1	1:C:56:THR:OG1	2.30	0.50
1:C:927:PHE:O	1:C:930:GLY:N	2.41	0.50
1:B:53:ASP:OD2	1:B:56:THR:OG1	2.30	0.50
1:B:218:GLN:HE22	1:B:231:ASN:HD21	1.58	0.50
1:B:291:ILE:HD12	1:B:306:ILE:HD12	1.94	0.50
1:C:497:LEU:O	1:C:499:PRO:HD3	2.12	0.50
1:C:531:VAL:CA	1:C:534:ILE:HG22	2.41	0.50
1:C:695:LEU:C	1:C:695:LEU:CD2	2.85	0.50
1:A:146:ASP:CB	1:A:148:THR:HG23	2.41	0.49
1:A:488:LEU:CD1	1:A:492:LEU:CD1	2.81	0.49
1:A:647:ILE:HA	1:A:650:ARG:HD2	1.93	0.49
1:B:6:ILE:HG12	1:B:490:PRO:O	2.11	0.49
1:B:705:GLU:CB	1:B:847:LEU:CD2	2.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:PRO:HG3	1:C:76:MET:HE1	1.93	0.49
1:C:186:ILE:HB	1:C:773:VAL:HG23	1.94	0.49
1:C:719:ASN:OD1	1:C:719:ASN:O	2.29	0.49
1:C:732:ASP:OD1	1:C:734:GLU:N	2.45	0.49
2:D:150:PHE:O	2:D:154:ILE:HG13	2.11	0.49
1:A:55:LYS:O	1:A:56:THR:C	2.50	0.49
1:A:187:TRP:HD1	1:A:267:LYS:O	1.94	0.49
1:A:412:VAL:CG1	1:A:489:THR:HG21	2.42	0.49
1:A:424:GLY:HA3	1:A:502:LYS:HB2	1.94	0.49
1:A:944:LEU:CD1	1:A:971:ARG:NH2	2.76	0.49
1:A:997:SER:C	1:A:999:ALA:H	2.20	0.49
1:B:195:LYS:O	1:B:197:GLN:OE1	2.30	0.49
1:B:211:ASN:OD1	1:B:211:ASN:O	2.29	0.49
1:B:250:LEU:HD23	1:B:251:LEU:CA	2.37	0.49
1:B:775:SER:HG	1:B:780:ARG:HG2	1.76	0.49
1:B:897:ILE:N	1:B:898:PRO:HD2	2.26	0.49
1:C:137:LEU:HD22	1:C:293:LEU:HD13	1.92	0.49
1:C:420:MET:HE3	1:C:500:ILE:CG1	2.41	0.49
2:D:61:GLU:HG2	2:D:62:ILE:N	2.28	0.49
2:E:143:ASP:O	2:E:146:GLY:O	2.29	0.49
1:A:498:LYS:HE3	1:A:498:LYS:CA	2.43	0.49
1:B:81:ASN:OD1	1:B:81:ASN:O	2.30	0.49
1:B:606:VAL:HA	1:B:631:LEU:HD23	1.93	0.49
1:B:973:ARG:HB3	1:B:974:PRO:HD3	1.94	0.49
1:C:373:PRO:O	1:C:377:LEU:HB2	2.12	0.49
1:C:607:GLU:OE2	1:C:632:LYS:HE3	2.12	0.49
2:D:14:LEU:O	2:D:15:GLY:C	2.52	0.49
1:B:8:ARG:N	1:B:9:PRO:HD3	2.27	0.49
1:B:182:TYR:HD1	1:B:270:LEU:CD1	2.24	0.49
1:B:501:ALA:HB3	1:B:504:ASP:CG	2.38	0.49
1:C:312:LYS:HG2	1:C:313:MET:N	2.28	0.49
2:D:19:LEU:CD2	2:D:50:PRO:HG3	2.41	0.49
2:D:43:SER:O	2:D:43:SER:OG	2.30	0.49
1:A:174:ASP:HB3	1:A:292:LYS:HB2	1.95	0.49
1:A:829:GLY:O	1:A:830:GLN:OE1	2.30	0.49
1:B:173:GLY:N	1:B:294:ALA:HB2	2.27	0.49
1:B:340:VAL:HG21	1:B:395:MET:HB3	1.95	0.49
1:C:92:LEU:N	1:C:92:LEU:HD12	2.26	0.49
1:C:261:LEU:CD1	1:C:263:ARG:HD2	2.42	0.49
1:C:780:ARG:HG3	1:C:780:ARG:O	2.12	0.49
1:C:782:LEU:O	1:C:785:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:LEU:HD12	1:A:613:ASN:HD22	1.77	0.49
1:B:733:GLN:NE2	1:B:743:ILE:HD11	2.27	0.49
1:C:391:ASN:H	1:C:394:THR:HG22	1.77	0.49
1:A:423:GLU:O	1:A:502:LYS:HE3	2.09	0.49
1:B:160:ALA:HB3	1:B:161:ASN:ND2	2.28	0.49
1:B:281:PHE:CD1	1:B:610:PHE:HD1	2.17	0.49
1:B:353:LEU:C	1:B:355:MET:H	2.20	0.49
1:B:808:ARG:HA	2:D:79:LEU:HD13	1.95	0.49
1:C:561:SER:HA	1:C:923:ASN:HB3	1.94	0.49
1:C:567:GLU:OE1	1:C:998:GLY:CA	2.47	0.49
1:C:979:SER:O	1:C:983:ILE:HG13	2.12	0.49
2:D:51:LEU:HD22	2:D:83:PRO:HG3	1.95	0.49
1:B:180:SER:HB2	1:B:273:GLU:HG3	1.95	0.49
1:B:911:GLY:C	1:B:1010:GLY:HA2	2.37	0.49
1:C:886:LEU:O	1:C:887:CYS:C	2.55	0.49
1:C:887:CYS:O	1:C:891:LEU:HG	2.13	0.49
2:D:63:VAL:HG12	2:D:64:GLU:N	2.23	0.49
1:A:987:MET:C	1:A:989:LEU:H	2.20	0.49
1:B:302:THR:O	1:B:306:ILE:CG2	2.58	0.49
1:B:365:THR:C	1:B:368:PRO:HD2	2.37	0.49
1:B:447:MET:HE2	1:B:447:MET:CA	2.40	0.49
1:B:682:PHE:HB3	1:B:827:ILE:HB	1.94	0.49
1:B:866:GLU:O	1:B:869:SER:OG	2.25	0.49
1:A:358:PHE:HB2	1:A:977:MET:CE	2.42	0.49
1:A:539:GLY:HA2	1:A:542:LEU:H	1.78	0.49
1:A:693:GLU:OE1	1:A:693:GLU:N	2.30	0.49
1:A:743:ILE:HD12	1:A:743:ILE:H	1.78	0.49
1:B:53:ASP:OD1	1:B:56:THR:OG1	2.29	0.49
1:B:382:VAL:O	1:B:382:VAL:HG23	2.13	0.49
1:C:53:ASP:OD1	1:C:56:THR:N	2.30	0.49
1:C:342:LYS:O	1:C:343:THR:C	2.53	0.49
1:C:431:THR:O	1:C:435:MET:HG2	2.13	0.49
1:C:521:GLU:O	1:C:525:HIS:HD2	1.95	0.49
1:C:616:GLY:N	1:C:619:GLY:O	2.37	0.49
1:A:223:PRO:HD2	1:B:780:ARG:HH22	1.78	0.48
1:A:488:LEU:O	1:A:492:LEU:HD13	2.13	0.48
1:B:388:PHE:CE2	1:B:472:ILE:HG21	2.48	0.48
1:C:754:TRP:CE3	1:C:780:ARG:HB2	2.48	0.48
1:A:754:TRP:HE3	1:C:218:GLN:O	1.96	0.48
1:B:218:GLN:CB	1:B:232:ALA:O	2.57	0.48
1:B:668:LEU:CB	1:B:669:PRO:CD	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:VAL:O	1:C:14:VAL:HG12	2.13	0.48
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.48	0.48
1:C:278:ILE:CD1	1:C:613:ASN:HB3	2.44	0.48
2:D:79:LEU:HD22	2:D:111:HIS:NE2	2.28	0.48
2:E:101:LYS:O	2:E:102:ASN:C	2.50	0.48
1:A:380:PHE:CZ	1:A:398:MET:HE3	2.48	0.48
1:A:382:VAL:HG11	1:A:476:SER:HB3	1.94	0.48
1:A:504:ASP:OD1	1:A:504:ASP:O	2.30	0.48
1:A:1013:THR:C	1:A:1015:THR:H	2.21	0.48
1:B:222:THR:HG23	1:C:275:TYR:CB	2.36	0.48
1:C:23:GLY:HA3	1:C:377:LEU:O	2.13	0.48
1:C:314:GLU:N	1:C:317:PHE:HE1	2.11	0.48
1:C:448:VAL:HG11	1:C:939:ALA:CB	2.42	0.48
1:C:616:GLY:HA3	1:C:624:THR:HG22	1.95	0.48
1:C:672:VAL:HG23	1:C:673:GLU:CD	2.37	0.48
1:C:737:GLN:O	1:C:738:ALA:C	2.53	0.48
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.95	0.48
1:A:240:LEU:H	1:A:240:LEU:HD13	1.78	0.48
1:A:457:ALA:HB2	1:A:471:SER:HB3	1.95	0.48
1:B:115:MET:N	1:B:116:PRO:CD	2.76	0.48
1:B:137:LEU:HD22	1:B:293:LEU:CD1	2.39	0.48
1:B:534:ILE:HG23	1:B:535:LEU:HG	1.95	0.48
1:B:808:ARG:HA	2:D:79:LEU:CD1	2.44	0.48
1:B:903:LEU:HD13	1:B:1025:PHE:CD2	2.48	0.48
1:C:69:MET:HA	1:C:69:MET:HE3	1.94	0.48
1:C:313:MET:O	1:C:317:PHE:CE1	2.67	0.48
1:A:139:VAL:CG1	1:A:178:PHE:HE2	2.26	0.48
1:A:164:ASP:OD2	1:A:767:ARG:NH2	2.44	0.48
1:A:445:ILE:HA	1:A:448:VAL:CG1	2.43	0.48
1:B:166:ILE:HD13	1:B:166:ILE:N	2.28	0.48
1:B:531:VAL:C	1:B:534:ILE:HG22	2.38	0.48
1:B:910:ILE:HG23	1:B:1013:THR:HG21	1.95	0.48
1:C:259:ARG:CZ	2:E:155:ASP:OD2	2.62	0.48
1:C:406:VAL:O	1:C:410:ILE:HG13	2.14	0.48
1:C:447:MET:SD	1:C:887:CYS:HB3	2.53	0.48
1:C:795:ASP:OD1	1:C:795:ASP:O	2.30	0.48
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.13	0.48
1:B:157:TYR:C	1:B:157:TYR:CD2	2.91	0.48
1:B:183:ALA:CB	1:B:271:GLY:O	2.60	0.48
1:B:324:VAL:CG2	1:B:325:TYR:N	2.76	0.48
1:B:406:VAL:C	1:B:408:ASP:H	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ARG:O	1:B:422:GLU:HG3	2.14	0.48
1:B:727:PHE:HE1	1:B:783:PRO:HB3	1.76	0.48
1:C:598:TYR:HB3	1:C:606:VAL:HG21	1.95	0.48
1:C:714:THR:CG2	1:C:715:SER:N	2.76	0.48
1:A:236:ALA:HB2	1:B:729:ILE:O	2.13	0.48
1:A:410:ILE:CD1	1:A:978:THR:HG22	2.44	0.48
1:A:459:PHE:CB	1:A:464:GLY:HA2	2.43	0.48
1:B:184:MET:CE	1:B:268:ILE:HG22	2.43	0.48
1:B:222:THR:HG22	1:C:275:TYR:CB	2.24	0.48
2:D:50:PRO:C	2:D:53:LEU:HD23	2.39	0.48
2:E:84:LEU:CD2	2:E:116:PRO:HB3	2.44	0.48
1:A:242:SER:HB2	1:A:244:GLU:CG	2.41	0.48
1:A:380:PHE:HD1	1:A:380:PHE:H	1.61	0.48
1:A:527:TYR:CE1	1:A:968:VAL:HG12	2.48	0.48
1:A:534:ILE:CA	1:A:541:TYR:CE1	2.94	0.48
1:A:987:MET:N	1:A:988:PRO:CD	2.77	0.48
1:B:182:TYR:HB3	1:B:270:LEU:CG	2.44	0.48
1:B:198:LEU:N	1:B:798:MET:CE	2.76	0.48
1:C:199:THR:HB	1:C:200:PRO:HD2	1.96	0.48
1:A:190:PRO:HD2	1:A:779:TYR:CG	2.49	0.48
1:A:497:LEU:HB3	1:A:498:LYS:HE2	1.95	0.48
1:A:758:TYR:O	1:A:758:TYR:CG	2.61	0.48
1:B:351:VAL:O	1:B:355:MET:HB2	2.12	0.48
1:B:660:ASP:OD1	2:D:16:LYS:NZ	2.41	0.48
1:C:210:GLN:NE2	1:C:249:ILE:HG23	2.29	0.48
1:C:391:ASN:O	1:C:395:MET:HG2	2.14	0.48
1:C:429:GLU:CA	1:C:432:ARG:HG3	2.43	0.48
2:E:143:ASP:O	2:E:144:LYS:C	2.55	0.48
1:A:497:LEU:HD22	1:A:497:LEU:HA	1.58	0.48
1:A:751:GLY:O	1:A:754:TRP:O	2.32	0.48
1:B:561:SER:O	1:B:562:SER:OG	2.30	0.48
1:B:668:LEU:CB	1:B:669:PRO:HD2	2.44	0.48
1:B:729:ILE:O	1:B:729:ILE:HG23	2.14	0.48
2:D:56:TYR:O	2:D:56:TYR:CG	2.66	0.48
2:D:61:GLU:HG2	2:D:62:ILE:H	1.78	0.48
2:D:110:ASP:HB3	2:D:112:ASN:HB2	1.96	0.48
1:A:314:GLU:C	1:A:316:PHE:H	2.22	0.47
1:A:448:VAL:HG21	1:A:888:LEU:CD2	2.44	0.47
1:A:813:SER:HB2	1:A:814:PRO:HD2	1.95	0.47
1:A:910:ILE:CG2	1:A:911:GLY:N	2.77	0.47
1:B:324:VAL:CG2	1:B:325:TYR:H	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:TYR:CE1	1:B:800:PRO:HB3	2.49	0.47
1:C:318:PRO:C	1:C:319:SER:OG	2.55	0.47
2:D:126:LEU:C	2:D:129:VAL:CG2	2.86	0.47
2:E:93:LEU:HD11	2:E:127:GLU:CB	2.44	0.47
1:A:489:THR:N	1:A:490:PRO:HD2	2.30	0.47
1:A:972:LEU:O	1:A:972:LEU:CD1	2.62	0.47
1:B:231:ASN:OD1	1:C:622:GLN:CG	2.62	0.47
1:B:716:VAL:O	1:B:716:VAL:HG13	2.13	0.47
1:B:767:ARG:HH22	1:C:67:GLN:HE22	1.62	0.47
1:C:278:ILE:HD12	1:C:584:GLN:OE1	2.14	0.47
1:C:948:PHE:HE1	1:C:970:MET:SD	2.37	0.47
2:D:130:GLU:HG3	2:D:131:VAL:N	2.29	0.47
1:A:74:ASN:HB3	1:A:95:GLU:HG3	1.96	0.47
1:B:480:LEU:HA	1:B:483:LEU:HD23	1.95	0.47
1:B:674:LEU:O	1:B:674:LEU:HD12	2.12	0.47
1:A:431:THR:O	1:A:432:ARG:C	2.53	0.47
1:A:648:THR:O	1:A:652:THR:HG22	2.14	0.47
1:A:650:ARG:CG	1:A:651:ALA:N	2.77	0.47
1:B:235:ILE:HD13	1:B:235:ILE:N	2.26	0.47
1:B:686:ASP:HB2	1:B:695:LEU:CD1	2.44	0.47
1:B:687:GLN:NE2	1:B:859:TRP:CB	2.77	0.47
1:C:842:GLU:O	1:C:846:GLN:HG3	2.14	0.47
1:C:1037:ASN:OD1	1:C:1039:ASP:O	2.32	0.47
2:D:44:ASP:CG	2:D:45:HIS:HB3	2.37	0.47
1:A:697:GLN:HA	1:A:700:ASN:HD22	1.80	0.47
1:A:1012:VAL:O	1:A:1016:VAL:HG22	2.14	0.47
1:B:2:PRO:O	1:B:6:ILE:HG13	2.14	0.47
1:B:47:ALA:HB3	1:B:88:VAL:CG1	2.44	0.47
1:B:263:ARG:O	1:B:263:ARG:HG2	2.14	0.47
1:B:378:GLY:HA3	1:B:480:LEU:HD23	1.95	0.47
1:B:576:VAL:HG22	1:B:663:VAL:HG22	1.96	0.47
1:C:733:GLN:NE2	1:C:743:ILE:CG2	2.72	0.47
1:C:1033:PHE:O	1:C:1034:SER:OG	2.30	0.47
1:A:181:GLN:NE2	1:A:769:LYS:HE3	2.25	0.47
1:A:454:VAL:N	1:A:455:PRO:CD	2.77	0.47
1:A:971:ARG:HH11	1:A:971:ARG:HG2	1.69	0.47
1:B:193:LEU:CD2	1:B:265:VAL:HB	2.44	0.47
1:C:231:ASN:O	1:C:231:ASN:CG	2.56	0.47
1:A:78:MET:O	1:A:78:MET:HG3	2.14	0.47
1:A:306:ILE:H	1:A:306:ILE:HG12	1.34	0.47
1:A:492:LEU:CD1	1:A:492:LEU:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ILE:HG22	1:A:541:TYR:CZ	2.50	0.47
1:A:539:GLY:O	1:A:540:ARG:C	2.58	0.47
1:A:953:MET:HE3	1:A:953:MET:HB3	1.69	0.47
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.97	0.47
1:B:293:LEU:HD11	1:B:299:ALA:CB	2.45	0.47
1:B:504:ASP:OD1	1:B:505:HIS:O	2.33	0.47
1:B:537:SER:O	1:B:541:TYR:HD1	1.97	0.47
1:B:774:MET:CE	1:B:780:ARG:NH1	2.75	0.47
1:C:94:PHE:O	1:C:95:GLU:O	2.31	0.47
1:C:163:LYS:O	1:C:164:ASP:C	2.56	0.47
1:C:367:ILE:HG12	1:C:496:MET:HE2	1.96	0.47
1:C:488:LEU:O	1:C:492:LEU:HG	2.15	0.47
1:C:597:TYR:C	1:C:597:TYR:CD2	2.93	0.47
1:C:669:PRO:N	1:C:678:THR:HG22	2.29	0.47
1:C:727:PHE:CE1	1:C:807:SER:HB3	2.50	0.47
1:C:908:GLY:HA3	1:C:938:SER:OG	2.14	0.47
2:D:48:TRP:NE1	2:D:77:ASP:OD2	2.44	0.47
2:D:94:GLU:O	2:D:98:VAL:HG23	2.15	0.47
2:D:110:ASP:CB	2:D:112:ASN:HB2	2.45	0.47
1:A:182:TYR:HD2	1:A:270:LEU:CD2	2.26	0.47
1:A:423:GLU:N	1:A:502:LYS:HG3	2.29	0.47
1:B:365:THR:HG23	1:B:366:LEU:H	1.79	0.47
1:B:511:GLY:HA2	1:B:512:PHE:C	2.40	0.47
1:C:162:MET:O	1:C:163:LYS:C	2.55	0.47
1:C:332:PHE:HA	1:C:335:ILE:HG22	1.96	0.47
1:C:632:LYS:O	1:C:633:ASP:C	2.58	0.47
1:A:41:PRO:HD2	1:A:95:GLU:O	2.15	0.47
1:B:72:ILE:CG2	1:B:73:ASP:H	2.25	0.47
1:B:182:TYR:HD1	1:B:270:LEU:CD2	2.27	0.47
1:B:243:THR:HG23	1:B:244:GLU:N	2.30	0.47
1:C:254:ASN:C	1:C:256:ASP:H	2.23	0.47
1:C:631:LEU:HD12	1:C:637:ARG:CZ	2.45	0.47
1:C:885:PHE:HE1	1:C:898:PRO:HB2	1.80	0.47
2:D:49:THR:O	2:D:52:HIS:HB2	2.15	0.47
2:D:49:THR:O	2:D:53:LEU:HD23	2.10	0.47
2:D:125:HIS:O	2:D:129:VAL:CG2	2.57	0.47
1:A:211:ASN:HA	1:A:240:LEU:HD13	1.97	0.47
1:A:241:THR:HG23	1:A:763:ILE:O	2.15	0.47
1:A:314:GLU:N	1:A:315:PRO:HD2	2.30	0.47
1:A:343:THR:HA	1:A:346:GLU:HB2	1.96	0.47
1:A:539:GLY:O	1:A:543:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:GLY:N	1:A:634:TRP:HH2	2.13	0.47
1:A:621:GLY:CA	1:A:624:THR:HG22	2.44	0.47
1:C:598:TYR:HB3	1:C:606:VAL:HG11	1.97	0.47
2:E:57:PHE:N	2:E:58:GLY:HA2	2.30	0.47
1:A:692:HIS:O	1:A:696:THR:OG1	2.33	0.46
1:B:370:ILE:HG21	1:B:492:LEU:HD11	1.97	0.46
1:B:456:MET:HG2	1:B:456:MET:O	2.14	0.46
1:B:869:SER:C	1:B:871:ASN:N	2.66	0.46
1:C:746:ILE:HG22	1:C:747:ASN:N	2.20	0.46
1:A:360:GLN:CD	1:A:513:PHE:CE1	2.93	0.46
1:A:815:ARG:HE	1:A:815:ARG:HB2	1.22	0.46
1:A:944:LEU:HD12	1:A:971:ARG:NH2	2.29	0.46
1:A:977:MET:HE2	1:A:977:MET:HB3	1.85	0.46
1:A:1026:PHE:O	1:A:1026:PHE:CG	2.68	0.46
1:B:605:ASN:HD22	1:B:647:ILE:HD11	1.80	0.46
1:B:733:GLN:HE22	1:B:743:ILE:HD11	1.80	0.46
1:B:864:TYR:O	1:B:865:GLN:C	2.58	0.46
1:C:76:MET:HG2	1:C:95:GLU:OE2	2.15	0.46
1:C:412:VAL:HG23	1:C:442:LEU:HD21	1.96	0.46
1:C:885:PHE:CE1	1:C:898:PRO:HB2	2.50	0.46
1:C:987:MET:O	1:C:990:VAL:N	2.45	0.46
2:D:65:VAL:O	2:D:69:ASN:ND2	2.40	0.46
1:A:212:ALA:O	1:A:237:GLN:HG2	2.15	0.46
1:A:539:GLY:C	1:A:541:TYR:N	2.68	0.46
1:B:222:THR:HG23	1:C:275:TYR:HB3	1.95	0.46
1:B:393:LEU:HD12	1:B:469:GLN:HG3	1.97	0.46
1:B:669:PRO:O	1:B:669:PRO:CD	2.63	0.46
1:B:671:ILE:HG23	1:B:673:GLU:N	2.30	0.46
1:C:719:ASN:HB2	1:C:828:LEU:CD1	2.46	0.46
1:C:722:GLU:HG3	1:C:723:ASP:H	1.81	0.46
1:C:952:LEU:N	1:C:952:LEU:HD13	2.30	0.46
1:A:219:LEU:HD13	1:B:783:PRO:HD3	1.96	0.46
1:A:414:GLU:CD	1:A:414:GLU:C	2.83	0.46
1:A:427:PRO:HD3	1:A:499:PRO:CB	2.44	0.46
1:A:435:MET:O	1:A:439:GLN:HB2	2.14	0.46
1:A:584:GLN:N	1:A:622:GLN:OE1	2.49	0.46
1:A:754:TRP:N	1:A:754:TRP:HD1	2.12	0.46
1:C:63:GLN:O	1:C:67:GLN:HG2	2.15	0.46
1:C:436:GLY:O	1:C:439:GLN:HB3	2.15	0.46
2:E:67:LEU:HD22	2:E:73:VAL:HG22	1.97	0.46
1:A:248:LYS:HA	1:A:261:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:VAL:O	1:B:345:VAL:HG23	2.15	0.46
1:B:733:GLN:O	1:B:736:ALA:HB3	2.15	0.46
1:A:685:ILE:HA	1:A:823:PRO:O	2.16	0.46
1:A:789:TRP:C	1:A:790:TYR:HD2	2.23	0.46
1:B:420:MET:HE3	1:B:425:LEU:O	2.15	0.46
1:B:605:ASN:HD21	1:B:642:ASN:CB	2.26	0.46
1:B:870:GLY:C	1:B:871:ASN:OD1	2.59	0.46
1:B:881:LEU:O	1:B:881:LEU:HD22	2.16	0.46
1:C:184:MET:HE1	1:C:243:THR:HG22	1.97	0.46
1:C:569:GLN:C	1:C:634:TRP:HZ2	2.24	0.46
2:D:43:SER:HA	2:D:49:THR:HA	1.97	0.46
1:A:229:GLN:OE1	1:B:586:ARG:HD2	2.15	0.46
1:B:291:ILE:CD1	1:B:306:ILE:HD12	2.46	0.46
1:B:758:TYR:HB2	1:B:772:TYR:HE1	1.70	0.46
1:C:188:MET:HE1	1:C:200:PRO:HB3	1.98	0.46
1:C:466:ILE:H	1:C:466:ILE:HG12	1.40	0.46
1:C:713:LEU:HD21	1:C:843:LEU:HD23	1.96	0.46
1:A:449:LEU:HD23	1:A:478:MET:SD	2.56	0.46
1:A:480:LEU:HA	1:A:480:LEU:HD23	1.69	0.46
1:B:88:VAL:HG22	1:B:89:GLN:N	2.30	0.46
1:B:183:ALA:CA	1:B:271:GLY:O	2.64	0.46
1:C:454:VAL:O	1:C:455:PRO:C	2.58	0.46
1:C:667:ASN:CG	1:C:668:LEU:N	2.74	0.46
1:C:811:TYR:CD2	1:C:811:TYR:N	2.76	0.46
1:C:907:LEU:O	1:C:910:ILE:HG22	2.14	0.46
2:D:76:ASP:HB3	2:D:80:GLY:HA2	1.97	0.46
1:A:17:ILE:O	1:A:21:LEU:HB2	2.16	0.46
1:A:159:ALA:HB1	1:A:181:GLN:HB2	1.97	0.46
1:A:492:LEU:O	1:A:493:CYS:C	2.57	0.46
1:A:558:ARG:C	1:A:558:ARG:HD3	2.38	0.46
1:B:445:ILE:HD13	1:B:940:LYS:HG3	1.98	0.46
1:B:717:ARG:HG3	1:B:828:LEU:HD12	1.98	0.46
1:B:1013:THR:C	1:B:1015:THR:H	2.24	0.46
1:C:925:VAL:O	1:C:928:GLN:N	2.49	0.46
1:A:182:TYR:CD2	1:A:270:LEU:HD21	2.51	0.46
1:B:235:ILE:HD12	1:B:235:ILE:HA	1.60	0.46
1:B:350:LEU:O	1:B:354:VAL:HG13	2.16	0.46
1:C:465:ALA:O	1:C:469:GLN:HG2	2.15	0.46
1:C:1015:THR:O	1:C:1019:ILE:HB	2.15	0.46
2:E:143:ASP:O	2:E:146:GLY:N	2.39	0.46
1:A:1:FME:N	1:A:2:PRO:HD2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:TYR:HD2	1:A:270:LEU:HD21	1.81	0.45
1:A:519:MET:SD	1:A:519:MET:O	2.67	0.45
1:A:813:SER:CB	1:A:814:PRO:HD2	2.45	0.45
1:B:733:GLN:HE22	1:B:743:ILE:CD1	2.28	0.45
1:B:846:GLN:O	1:B:847:LEU:C	2.58	0.45
1:C:672:VAL:HG23	1:C:673:GLU:N	2.30	0.45
2:D:13:ASP:O	2:D:16:LYS:N	2.50	0.45
1:A:470:PHE:O	1:A:474:ILE:HG13	2.16	0.45
1:B:903:LEU:HD13	1:B:1025:PHE:HD2	1.81	0.45
1:C:62:THR:O	1:C:66:GLU:HB2	2.15	0.45
1:C:513:PHE:O	1:C:514:GLY:C	2.58	0.45
1:C:999:ALA:O	1:C:1000:GLN:C	2.55	0.45
2:D:18:LEU:C	2:D:18:LEU:HD22	2.36	0.45
2:D:80:GLY:O	2:D:82:THR:HG23	2.15	0.45
2:E:97:GLU:OE1	2:E:97:GLU:CA	2.46	0.45
1:A:228:GLN:C	1:B:583:THR:HG21	2.41	0.45
1:A:351:VAL:HG23	1:A:981:ALA:HB1	1.98	0.45
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	1.98	0.45
1:B:44:THR:HG21	1:B:89:GLN:NE2	2.31	0.45
1:B:733:GLN:H	1:B:733:GLN:HG2	1.53	0.45
1:B:815:ARG:NH1	1:B:815:ARG:CG	2.73	0.45
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	1.99	0.45
1:C:351:VAL:O	1:C:352:PHE:C	2.57	0.45
1:C:446:ALA:CB	1:C:482:VAL:HG22	2.46	0.45
1:C:801:PHE:O	1:C:801:PHE:CD1	2.70	0.45
1:C:876:LEU:HD11	1:C:932:LEU:HD11	1.98	0.45
1:C:879:ILE:HD12	1:C:883:VAL:HG23	1.91	0.45
2:D:56:TYR:HD1	2:D:90:ARG:CG	2.19	0.45
2:E:106:VAL:HG21	2:E:136:GLY:HA3	1.98	0.45
1:A:650:ARG:HG2	1:A:651:ALA:N	2.32	0.45
1:B:214:VAL:CG1	1:B:215:ALA:N	2.79	0.45
1:C:269:GLU:O	1:C:269:GLU:HG3	2.15	0.45
1:C:514:GLY:O	1:C:518:ARG:HG3	2.17	0.45
1:C:555:LEU:HD23	1:C:555:LEU:HA	1.84	0.45
1:C:616:GLY:HA3	1:C:624:THR:CG2	2.47	0.45
1:C:894:SER:O	1:C:898:PRO:CG	2.64	0.45
1:C:986:VAL:O	1:C:986:VAL:HG13	2.16	0.45
2:D:57:PHE:N	2:D:58:GLY:CA	2.79	0.45
2:E:82:THR:O	2:E:85:HIS:HB2	2.16	0.45
1:A:219:LEU:HD11	1:B:783:PRO:HG3	1.98	0.45
1:A:943:ILE:O	1:A:946:VAL:CG1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:MET:HG2	1:B:95:GLU:OE2	2.17	0.45
1:B:178:PHE:HE2	1:B:290:GLY:N	2.15	0.45
1:C:83:ASP:O	1:C:84:SER:OG	2.30	0.45
1:C:154:ILE:HG13	1:C:155:SER:N	2.30	0.45
1:C:314:GLU:C	1:C:317:PHE:CD1	2.85	0.45
1:A:58:GLN:HE21	1:A:818:ARG:HH11	1.60	0.45
1:A:189:ASN:HD22	1:A:192:GLU:CG	2.29	0.45
1:A:196:PHE:C	1:A:197:GLN:CG	2.85	0.45
1:A:199:THR:O	1:A:199:THR:HG23	2.17	0.45
1:A:244:GLU:HG2	1:A:244:GLU:H	1.36	0.45
1:A:378:GLY:HA3	1:A:480:LEU:CD1	2.47	0.45
1:A:578:LEU:HD13	1:A:587:THR:HG23	1.99	0.45
1:A:888:LEU:HD13	1:A:901:VAL:HB	1.97	0.45
1:B:21:LEU:HD13	1:B:21:LEU:HA	1.81	0.45
1:B:522:LYS:O	1:B:525:HIS:HB2	2.15	0.45
1:B:588:GLN:HB2	1:B:613:ASN:HD22	1.80	0.45
1:B:713:LEU:HD12	1:B:713:LEU:HA	1.64	0.45
1:C:444:GLY:O	1:C:448:VAL:HG23	2.16	0.45
1:C:542:LEU:O	1:C:546:LEU:HD13	2.16	0.45
1:C:586:ARG:O	1:C:590:VAL:HG23	2.17	0.45
1:A:40:PRO:HA	1:A:41:PRO:HD3	1.82	0.45
1:A:264:ASP:OD2	1:A:264:ASP:N	2.48	0.45
1:A:306:ILE:O	1:A:307:ARG:C	2.60	0.45
1:A:427:PRO:CG	1:A:497:LEU:O	2.65	0.45
1:A:972:LEU:O	1:A:972:LEU:HD13	2.16	0.45
1:B:674:LEU:CD1	1:B:674:LEU:C	2.85	0.45
1:B:734:GLU:O	1:B:735:LYS:C	2.58	0.45
1:B:892:TYR:OH	1:B:943:ILE:HA	2.17	0.45
1:C:335:ILE:HD12	1:C:338:HIS:HB3	1.98	0.45
1:C:775:SER:HG	1:C:789:TRP:HZ2	1.64	0.45
1:C:937:LEU:CA	1:C:940:LYS:HG2	2.47	0.45
2:D:89:ASP:C	2:D:91:GLY:N	2.65	0.45
2:E:100:LEU:O	2:E:103:GLY:CA	2.65	0.45
2:E:112:ASN:HB2	2:E:114:PHE:HD2	1.82	0.45
1:A:144:ASN:OD1	1:A:149:MET:HG3	2.16	0.45
1:A:531:VAL:O	1:A:532:GLY:C	2.59	0.45
1:A:753:ALA:HB3	1:A:754:TRP:HD1	1.82	0.45
1:A:913:LEU:HD23	1:A:927:PHE:HZ	1.82	0.45
1:A:1008:MET:O	1:A:1012:VAL:HG23	2.17	0.45
1:B:169:THR:CG2	1:B:172:VAL:HG13	2.34	0.45
1:B:447:MET:HA	1:B:447:MET:CE	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:MET:O	1:B:467:TYR:HB3	2.17	0.45
1:B:1013:THR:CG2	1:B:1017:LEU:HD12	2.47	0.45
1:C:98:THR:HG23	1:C:99:ASP:H	1.80	0.45
1:C:472:ILE:HG23	1:C:473:THR:N	2.31	0.45
1:C:567:GLU:OE2	1:C:997:SER:N	2.50	0.45
1:C:750:LEU:CD2	1:C:751:GLY:N	2.77	0.45
1:A:230:LEU:HD23	1:B:782:LEU:HD22	1.99	0.45
1:A:807:SER:C	1:A:808:ARG:HG3	2.41	0.45
1:A:910:ILE:HG23	1:A:911:GLY:N	2.32	0.45
1:B:118:LEU:O	1:B:123:GLN:OE1	2.33	0.45
1:B:575:MET:O	1:B:576:VAL:HG23	2.16	0.45
2:D:50:PRO:HA	2:D:53:LEU:HD23	1.98	0.45
1:A:316:PHE:CD2	1:B:687:GLN:HB3	2.52	0.45
1:A:694:LYS:O	1:A:697:GLN:HB2	2.17	0.45
1:A:908:GLY:CA	1:A:1014:ALA:HB2	2.47	0.45
1:B:62:THR:O	1:B:62:THR:CG2	2.63	0.45
1:B:293:LEU:CD1	1:B:299:ALA:HB2	2.46	0.45
1:B:361:ASN:N	1:B:361:ASN:ND2	2.32	0.45
1:B:488:LEU:O	1:B:492:LEU:HG	2.17	0.45
1:B:698:ALA:O	1:B:851:LEU:HD23	2.16	0.45
1:C:719:ASN:HD22	1:C:828:LEU:HD11	1.82	0.45
1:B:10:ILE:HD12	1:C:895:TRP:NE1	2.32	0.44
1:B:254:ASN:CG	1:B:258:SER:O	2.60	0.44
1:B:702:LEU:HD21	1:B:844:MET:HE1	1.98	0.44
1:B:813:SER:HB3	1:B:816:LEU:CD2	2.48	0.44
1:C:5:PHE:CE2	1:C:487:ILE:HG12	2.51	0.44
1:C:5:PHE:CE2	1:C:487:ILE:HG23	2.53	0.44
1:C:53:ASP:OD1	1:C:53:ASP:O	2.35	0.44
1:C:53:ASP:CG	1:C:56:THR:HG1	2.17	0.44
2:D:73:VAL:HG11	2:D:103:GLY:O	2.17	0.44
2:E:77:ASP:HB2	2:E:81:VAL:O	2.17	0.44
1:A:273:GLU:CD	1:A:770:LYS:HD2	2.42	0.44
1:A:427:PRO:HG2	1:A:497:LEU:O	2.17	0.44
1:A:483:LEU:HA	1:A:486:LEU:HD23	1.99	0.44
1:A:980:LEU:HD23	1:A:980:LEU:C	2.42	0.44
1:B:340:VAL:O	1:B:344:LEU:HG	2.17	0.44
1:B:416:VAL:HG22	1:B:434:SER:CB	2.47	0.44
1:B:456:MET:HE2	1:B:456:MET:HB3	1.84	0.44
1:B:784:ASP:C	1:B:786:ILE:H	2.26	0.44
1:B:988:PRO:C	1:B:991:ILE:CG2	2.90	0.44
1:C:9:PRO:HD2	1:C:10:ILE:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:LEU:HA	1:C:560:PRO:HD3	1.87	0.44
1:A:899:PHE:O	1:A:903:LEU:HD12	2.17	0.44
1:B:95:GLU:O	1:B:98:THR:OG1	2.32	0.44
1:B:98:THR:HG22	1:B:99:ASP:N	2.32	0.44
1:B:746:ILE:C	1:B:748:THR:N	2.75	0.44
1:C:45:ILE:HD11	1:C:107:VAL:CG1	2.47	0.44
1:C:367:ILE:CB	1:C:368:PRO:HD3	2.47	0.44
1:C:568:ASP:HA	1:C:644:VAL:CG2	2.47	0.44
2:D:164:ILE:H	2:D:164:ILE:HG13	1.57	0.44
1:A:725:PRO:HA	1:A:810:GLU:O	2.17	0.44
1:A:726:GLN:HB3	1:C:235:ILE:HG12	1.99	0.44
1:B:184:MET:HE3	1:B:268:ILE:CG2	2.47	0.44
1:B:211:ASN:OD1	1:B:211:ASN:C	2.60	0.44
1:B:416:VAL:HG22	1:B:434:SER:HB3	1.99	0.44
1:B:869:SER:O	1:B:870:GLY:C	2.59	0.44
1:B:1020:PHE:O	1:B:1023:PRO:HD2	2.18	0.44
1:C:429:GLU:O	1:C:430:ALA:C	2.60	0.44
1:C:952:LEU:HA	1:C:952:LEU:HD12	1.40	0.44
1:B:33:ALA:O	1:B:391:ASN:HA	2.18	0.44
1:B:62:THR:OG1	1:B:88:VAL:CG2	2.65	0.44
1:B:754:TRP:CE3	1:B:780:ARG:HB2	2.52	0.44
1:B:853:THR:O	1:B:853:THR:HG23	2.14	0.44
1:C:5:PHE:O	1:C:6:ILE:C	2.59	0.44
1:C:158:VAL:CG2	1:C:162:MET:HE3	2.46	0.44
1:C:390:ILE:O	1:C:390:ILE:HG22	2.17	0.44
1:C:736:ALA:C	1:C:741:VAL:HB	2.37	0.44
2:E:44:ASP:HA	2:E:45:HIS:HA	1.50	0.44
2:E:57:PHE:H	2:E:58:GLY:CA	2.31	0.44
2:E:126:LEU:HA	2:E:129:VAL:HG22	2.00	0.44
1:A:388:PHE:CE1	1:A:469:GLN:OE1	2.71	0.44
1:A:401:ALA:O	1:A:405:LEU:HD13	2.18	0.44
1:B:814:PRO:O	1:B:815:ARG:C	2.57	0.44
1:B:1020:PHE:C	1:B:1023:PRO:HD2	2.41	0.44
1:C:48:SER:HB3	1:C:125:GLN:HG2	1.99	0.44
1:C:367:ILE:HG23	1:C:492:LEU:HD12	1.99	0.44
1:C:567:GLU:CD	1:C:998:GLY:CA	2.91	0.44
1:C:668:LEU:O	1:C:669:PRO:C	2.60	0.44
1:C:733:GLN:O	1:C:734:GLU:C	2.55	0.44
1:C:911:GLY:O	1:C:912:ALA:C	2.59	0.44
1:C:1013:THR:C	1:C:1015:THR:H	2.26	0.44
1:A:190:PRO:HG3	1:A:789:TRP:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:ALA:HB3	1:A:754:TRP:CD1	2.52	0.44
1:B:702:LEU:HD11	1:B:844:MET:CE	2.48	0.44
1:B:724:THR:HB	1:B:725:PRO:HD2	1.99	0.44
1:C:156:ASP:CG	1:C:182:TYR:HD2	2.22	0.44
1:C:172:VAL:HG13	1:C:291:ILE:HG23	2.00	0.44
1:C:527:TYR:CZ	1:C:1019:ILE:HG13	2.53	0.44
1:C:952:LEU:N	1:C:952:LEU:HD12	2.27	0.44
1:A:462:SER:OG	1:A:463:THR:N	2.49	0.44
1:A:518:ARG:O	1:A:519:MET:C	2.60	0.44
1:A:531:VAL:O	1:A:534:ILE:CG1	2.66	0.44
1:A:721:LEU:HD11	1:A:814:PRO:HG2	1.85	0.44
1:A:902:MET:HB3	1:A:902:MET:HE2	1.68	0.44
1:B:166:ILE:CG2	1:B:175:VAL:HG21	2.38	0.44
1:B:578:LEU:CD1	1:B:579:PRO:HD3	2.48	0.44
1:C:5:PHE:C	1:C:7:ASP:N	2.69	0.44
1:C:448:VAL:HG12	1:C:936:GLY:HA2	2.00	0.44
1:A:72:ILE:HD13	1:A:107:VAL:HG22	1.99	0.44
1:A:159:ALA:O	1:A:163:LYS:HE2	2.18	0.44
1:A:492:LEU:N	1:A:492:LEU:HD12	2.32	0.44
1:A:645:GLU:O	1:A:649:MET:HG3	2.18	0.44
1:A:896:SER:C	1:A:898:PRO:HD2	2.42	0.44
1:B:960:LEU:HD22	1:B:961:ILE:HD13	1.99	0.44
1:C:281:PHE:O	1:C:282:ASN:HB2	2.18	0.44
1:C:431:THR:HG22	1:C:435:MET:HG3	1.98	0.44
1:C:471:SER:O	1:C:475:VAL:HG23	2.17	0.44
1:C:144:ASN:ND2	1:C:149:MET:N	2.66	0.43
1:C:151:GLN:HA	1:C:154:ILE:HG23	2.00	0.43
2:E:152:ILE:HD12	2:E:153:SER:N	2.17	0.43
1:A:98:THR:CG2	1:A:103:ALA:HB2	2.47	0.43
1:A:157:TYR:O	1:A:158:VAL:C	2.61	0.43
1:A:190:PRO:HD2	1:A:779:TYR:CD2	2.53	0.43
1:A:538:THR:C	1:A:540:ARG:N	2.69	0.43
1:A:897:ILE:O	1:A:897:ILE:CG2	2.64	0.43
1:B:139:VAL:HG22	1:B:327:TYR:HB3	1.99	0.43
1:B:187:TRP:HD1	1:B:267:LYS:O	2.00	0.43
1:B:561:SER:HA	1:B:923:ASN:CB	2.48	0.43
1:B:671:ILE:O	1:B:672:VAL:C	2.59	0.43
1:C:318:PRO:O	1:C:319:SER:C	2.61	0.43
1:C:358:PHE:CG	1:C:977:MET:HG2	2.54	0.43
1:C:404:LEU:HD22	1:C:404:LEU:N	2.33	0.43
1:C:594:VAL:CG1	1:C:598:TYR:HE2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:648:THR:HA	1:C:651:ALA:HB3	2.00	0.43
1:C:724:THR:HG23	1:C:814:PRO:CG	2.48	0.43
1:C:725:PRO:CD	1:C:725:PRO:O	2.64	0.43
1:C:741:VAL:HG11	1:C:746:ILE:HD11	1.84	0.43
2:D:148:THR:H	2:D:151:ASP:HB2	1.83	0.43
2:E:25:GLY:CA	2:E:59:HIS:CE1	3.01	0.43
1:A:184:MET:HG2	1:A:246:PHE:CD1	2.53	0.43
1:A:189:ASN:ND2	1:A:192:GLU:HG3	2.34	0.43
1:A:534:ILE:HD12	1:A:1024:VAL:CG2	2.48	0.43
1:A:971:ARG:O	1:A:972:LEU:C	2.61	0.43
1:B:10:ILE:HB	1:C:893:GLU:CD	2.44	0.43
1:B:531:VAL:HA	1:B:534:ILE:HG22	2.00	0.43
1:B:699:ARG:HD3	1:B:825:MET:HG2	2.00	0.43
1:B:733:GLN:HA	1:B:736:ALA:HB3	2.00	0.43
1:C:226:LYS:HD3	1:C:226:LYS:HA	1.83	0.43
1:C:372:VAL:H	1:C:373:PRO:HD2	1.83	0.43
1:C:415:ASN:HD22	1:C:434:SER:HB3	1.84	0.43
1:C:521:GLU:O	1:C:525:HIS:CD2	2.71	0.43
1:C:563:PHE:CE2	1:C:862:MET:CE	3.01	0.43
1:C:993:THR:HA	1:C:997:SER:CB	2.49	0.43
1:A:485:ALA:HB3	1:A:486:LEU:CD1	2.49	0.43
1:A:739:LEU:HD13	1:A:799:VAL:HG11	2.00	0.43
1:B:310:LEU:HD13	1:B:323:ILE:HD12	2.00	0.43
1:C:194:ASN:O	1:C:194:ASN:ND2	2.52	0.43
1:C:217:GLY:C	1:C:218:GLN:HG2	2.42	0.43
1:C:391:ASN:H	1:C:394:THR:CG2	2.31	0.43
1:C:780:ARG:O	1:C:780:ARG:CG	2.66	0.43
1:A:185:ARG:HA	1:A:185:ARG:HD2	1.86	0.43
1:A:587:THR:HB	1:A:613:ASN:HD21	1.82	0.43
1:B:11:PHE:CD1	1:B:11:PHE:O	2.72	0.43
1:B:223:PRO:HA	1:B:224:PRO:HD3	1.78	0.43
1:B:746:ILE:HG23	1:B:801:PHE:CE1	2.53	0.43
1:C:177:LEU:HD13	1:C:179:GLY:N	2.34	0.43
1:C:207:ILE:HG22	1:C:760:ASN:ND2	2.33	0.43
1:C:972:LEU:HD13	1:C:972:LEU:C	2.43	0.43
1:A:263:ARG:HG3	1:A:264:ASP:N	2.32	0.43
1:A:379:THR:CG2	1:A:383:LEU:HD21	2.47	0.43
1:A:483:LEU:C	1:A:486:LEU:HD23	2.38	0.43
1:A:696:THR:O	1:A:699:ARG:HB3	2.18	0.43
1:B:83:ASP:HA	1:B:815:ARG:N	2.30	0.43
1:B:420:MET:CE	1:B:499:PRO:HA	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:THR:HG22	1:B:496:MET:CG	2.48	0.43
1:B:497:LEU:HD12	1:B:497:LEU:HA	1.73	0.43
1:B:502:LYS:C	1:B:504:ASP:H	2.26	0.43
1:B:754:TRP:CH2	1:B:780:ARG:HA	2.54	0.43
1:B:997:SER:O	1:B:1000:GLN:N	2.52	0.43
1:C:263:ARG:HG3	1:C:263:ARG:H	1.57	0.43
1:C:577:GLN:HE22	1:C:623:ASN:HD21	1.65	0.43
1:C:614:GLY:HA2	1:C:621:GLY:O	2.19	0.43
1:C:741:VAL:HG12	1:C:746:ILE:HD13	1.97	0.43
2:D:50:PRO:CA	2:D:53:LEU:HD23	2.49	0.43
2:E:28:ASP:O	2:E:32:ILE:HG13	2.19	0.43
1:A:431:THR:HG22	1:A:432:ARG:H	1.82	0.43
1:A:923:ASN:OD1	1:A:923:ASN:C	2.62	0.43
1:B:351:VAL:O	1:B:355:MET:CB	2.66	0.43
1:B:391:ASN:O	1:B:395:MET:HG3	2.19	0.43
1:B:410:ILE:CG2	1:B:977:MET:HE3	2.49	0.43
1:B:448:VAL:O	1:B:452:VAL:HG23	2.19	0.43
1:B:774:MET:SD	1:B:780:ARG:NH1	2.91	0.43
1:C:522:LYS:HG2	1:C:526:HIS:HE1	1.83	0.43
1:C:695:LEU:HD23	1:C:695:LEU:C	2.43	0.43
1:C:1019:ILE:HD12	1:C:1019:ILE:HA	1.84	0.43
2:E:100:LEU:HA	2:E:100:LEU:HD23	1.64	0.43
1:A:187:TRP:O	1:A:266:ALA:HA	2.18	0.43
1:A:961:ILE:O	1:A:961:ILE:HD13	2.19	0.43
1:B:351:VAL:HG13	1:B:410:ILE:HD11	2.00	0.43
1:B:557:VAL:O	1:B:557:VAL:HG22	2.08	0.43
1:B:566:ASP:OD1	1:B:566:ASP:N	2.52	0.43
1:C:822:LEU:N	1:C:822:LEU:HD12	2.33	0.43
1:C:925:VAL:O	1:C:927:PHE:N	2.51	0.43
2:E:61:GLU:H	2:E:61:GLU:CD	2.27	0.43
1:A:14:VAL:HG13	1:B:886:LEU:HD12	2.01	0.43
1:A:52:ALA:C	1:A:53:ASP:O	2.54	0.43
1:A:497:LEU:CA	1:A:498:LYS:HE2	2.49	0.43
1:A:973:ARG:O	1:A:977:MET:CG	2.53	0.43
1:B:753:ALA:HB1	1:B:789:TRP:CZ2	2.54	0.43
1:C:1:FME:HE3	1:C:1:FME:HB3	1.60	0.43
1:C:213:GLN:HG2	1:C:239:ARG:HD3	2.00	0.43
1:C:578:LEU:N	1:C:578:LEU:HD12	2.33	0.43
1:C:604:ASN:HD22	1:C:604:ASN:HA	1.60	0.43
1:C:669:PRO:HG3	1:C:675:GLY:O	2.19	0.43
1:C:945:ILE:HD11	1:C:1019:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:TYR:HD1	2:D:90:ARG:HE	1.61	0.43
1:A:886:LEU:HB3	1:C:14:VAL:HG13	2.00	0.43
1:A:996:GLY:O	1:A:999:ALA:HB3	2.19	0.43
1:B:102:ILE:O	1:B:105:VAL:HG12	2.18	0.43
1:B:909:VAL:O	1:B:912:ALA:HB3	2.18	0.43
1:C:185:ARG:HG3	1:C:271:GLY:HA3	2.00	0.43
1:C:911:GLY:CA	1:C:1013:THR:OG1	2.64	0.43
2:D:145:PHE:C	2:D:147:LYS:N	2.77	0.43
1:A:45:ILE:HG12	1:A:111:LEU:HD12	2.00	0.42
1:A:158:VAL:CG1	1:A:289:LEU:HD21	2.49	0.42
1:A:315:PRO:C	1:A:316:PHE:CD1	2.97	0.42
1:B:353:LEU:HD12	1:B:353:LEU:N	2.34	0.42
1:B:613:ASN:C	1:B:613:ASN:OD1	2.61	0.42
1:B:794:ALA:C	1:B:796:GLY:N	2.76	0.42
1:C:735:LYS:O	1:C:736:ALA:C	2.60	0.42
1:C:977:MET:HE2	1:C:977:MET:HB3	1.73	0.42
1:A:140:VAL:O	1:A:140:VAL:HG22	2.17	0.42
1:A:275:TYR:CD1	1:C:223:PRO:HD3	2.55	0.42
1:A:570:GLY:N	1:A:634:TRP:CH2	2.87	0.42
1:B:107:VAL:HG23	1:B:107:VAL:H	1.44	0.42
1:B:687:GLN:HE22	1:B:859:TRP:CB	2.32	0.42
1:B:871:ASN:HA	1:B:872:GLN:HA	1.35	0.42
1:B:1022:VAL:N	1:B:1023:PRO:CD	2.82	0.42
1:C:372:VAL:N	1:C:373:PRO:HD2	2.34	0.42
1:C:719:ASN:HB2	1:C:828:LEU:HD11	2.00	0.42
1:A:489:THR:CG2	1:A:490:PRO:CD	2.95	0.42
1:A:814:PRO:HG2	1:A:815:ARG:H	1.85	0.42
1:B:5:PHE:CD1	1:B:487:ILE:HG12	2.55	0.42
1:B:11:PHE:CE2	1:C:890:ALA:HB1	2.54	0.42
1:B:160:ALA:HB3	1:B:161:ASN:HD21	1.85	0.42
1:B:371:ALA:HB2	1:B:489:THR:CG2	2.48	0.42
1:B:534:ILE:HG23	1:B:535:LEU:N	2.32	0.42
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	2.00	0.42
1:C:742:SER:HB3	1:C:745:ASP:HB2	2.00	0.42
1:C:793:ALA:HB3	1:C:797:GLN:H	1.84	0.42
2:D:82:THR:O	2:D:83:PRO:C	2.61	0.42
1:A:60:THR:HG22	1:A:61:VAL:HG23	2.01	0.42
1:A:912:ALA:O	1:A:927:PHE:CE2	2.73	0.42
1:B:199:THR:CG2	1:B:792:ARG:H	2.33	0.42
1:B:799:VAL:HG12	1:B:800:PRO:HD2	1.84	0.42
1:B:991:ILE:HG23	1:B:992:SER:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:GLU:CD	1:C:998:GLY:N	2.75	0.42
2:D:27:ASP:HB3	2:D:62:ILE:CG1	2.49	0.42
1:A:302:THR:O	1:A:306:ILE:HG12	2.20	0.42
1:A:912:ALA:O	1:A:927:PHE:HE2	2.03	0.42
1:A:975:ILE:O	1:A:979:SER:HB2	2.18	0.42
1:B:212:ALA:O	1:B:237:GLN:HG3	2.20	0.42
1:B:383:LEU:O	1:B:384:ALA:C	2.60	0.42
1:B:931:LEU:O	1:B:935:ILE:HG13	2.19	0.42
1:C:185:ARG:NH1	1:C:774:MET:HE2	2.18	0.42
1:C:412:VAL:HA	1:C:438:ILE:CD1	2.50	0.42
1:C:431:THR:O	1:C:435:MET:CG	2.67	0.42
1:C:943:ILE:O	1:C:947:GLU:HB3	2.19	0.42
1:C:987:MET:C	1:C:989:LEU:N	2.78	0.42
2:E:25:GLY:HA3	2:E:59:HIS:CE1	2.55	0.42
1:A:66:GLU:O	1:C:168:ARG:NH1	2.53	0.42
1:A:423:GLU:C	1:A:502:LYS:CD	2.93	0.42
1:A:537:SER:HB3	1:A:541:TYR:CD1	2.55	0.42
1:B:377:LEU:HD12	1:B:377:LEU:HA	1.63	0.42
1:B:431:THR:O	1:B:432:ARG:C	2.59	0.42
1:B:690:LEU:HD11	1:B:857:TYR:CB	2.50	0.42
1:B:848:ALA:C	1:B:851:LEU:HD13	2.40	0.42
1:B:961:ILE:HG22	1:B:965:LEU:HD13	2.02	0.42
1:C:65:ILE:O	1:C:69:MET:CG	2.65	0.42
1:C:453:PHE:O	1:C:456:MET:HG2	2.20	0.42
1:A:74:ASN:O	1:A:95:GLU:HG2	2.20	0.42
1:A:570:GLY:HA3	1:A:634:TRP:CH2	2.54	0.42
1:A:800:PRO:C	1:A:802:SER:N	2.77	0.42
1:B:182:TYR:HB3	1:B:270:LEU:HD21	2.02	0.42
1:B:764:ASP:HB3	1:B:769:LYS:HD2	2.02	0.42
1:B:828:LEU:HD12	1:B:828:LEU:O	2.20	0.42
1:B:997:SER:O	1:B:998:GLY:C	2.60	0.42
1:C:980:LEU:HA	1:C:980:LEU:HD13	1.73	0.42
2:D:53:LEU:HD23	2:D:53:LEU:N	2.03	0.42
1:A:600:THR:O	1:A:603:LYS:HG2	2.20	0.42
1:A:781:MET:HB3	1:A:781:MET:HE3	1.83	0.42
1:A:841:MET:O	1:A:844:MET:HB2	2.20	0.42
1:B:156:ASP:CB	1:B:182:TYR:CD2	2.98	0.42
1:B:519:MET:CG	1:B:520:PHE:N	2.78	0.42
1:B:671:ILE:CG2	1:B:673:GLU:N	2.82	0.42
1:B:777:ALA:HA	1:B:780:ARG:HH21	1.85	0.42
1:C:142:VAL:HG13	1:C:322:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ILE:N	1:C:277:ILE:HD12	2.34	0.42
1:C:404:LEU:C	1:C:406:VAL:H	2.28	0.42
1:C:507:GLU:HB2	1:C:508:GLY:H	1.58	0.42
1:C:571:VAL:HB	1:C:629:VAL:O	2.19	0.42
1:C:222:THR:HA	1:C:224:PRO:HD3	2.02	0.42
1:C:567:GLU:OE2	1:C:996:GLY:CA	2.68	0.42
1:C:898:PRO:O	1:C:902:MET:HB2	2.20	0.42
1:A:470:PHE:CD1	1:A:929:VAL:HG11	2.55	0.42
1:A:580:ALA:CA	1:A:623:ASN:ND2	2.81	0.42
1:A:794:ALA:C	1:A:796:GLY:H	2.27	0.42
1:A:973:ARG:HB3	1:A:974:PRO:HD3	2.01	0.42
1:B:502:LYS:C	1:B:504:ASP:N	2.77	0.42
1:B:575:MET:CG	1:B:576:VAL:N	2.76	0.42
1:B:623:ASN:O	1:B:623:ASN:ND2	2.50	0.42
1:C:342:LYS:O	1:C:344:LEU:N	2.53	0.42
1:C:454:VAL:HB	1:C:455:PRO:CD	2.48	0.42
1:C:528:THR:HG22	1:C:529:ASP:N	2.34	0.42
1:C:761:ASP:HB3	1:C:768:VAL:HG12	1.99	0.42
1:C:988:PRO:O	1:C:992:SER:HB3	2.20	0.42
1:A:376:LEU:O	1:A:379:THR:HB	2.20	0.41
1:B:672:VAL:O	1:B:672:VAL:HG13	2.19	0.41
1:B:715:SER:CB	1:B:830:GLN:HE21	2.33	0.41
1:C:54:ALA:N	1:C:84:SER:HA	2.35	0.41
1:C:153:ASP:OD1	1:C:153:ASP:N	2.52	0.41
1:C:154:ILE:HD12	1:C:155:SER:N	2.24	0.41
1:C:225:VAL:O	1:C:226:LYS:C	2.61	0.41
1:C:896:SER:OG	1:C:897:ILE:HD13	2.04	0.41
1:C:934:THR:HA	1:C:937:LEU:HD12	2.02	0.41
1:A:111:LEU:HD23	1:A:111:LEU:O	2.20	0.41
1:A:900:SER:HA	1:A:1025:PHE:HB3	2.02	0.41
1:A:971:ARG:HA	1:A:971:ARG:HD2	1.49	0.41
1:A:975:ILE:O	1:A:979:SER:CB	2.68	0.41
1:A:1016:VAL:HG23	1:A:1017:LEU:CD1	2.45	0.41
1:B:74:ASN:OD1	1:B:74:ASN:N	2.52	0.41
1:B:631:LEU:HD23	1:B:631:LEU:HA	1.77	0.41
1:B:813:SER:HA	1:B:814:PRO:HD2	1.90	0.41
1:C:555:LEU:HD11	1:C:914:LEU:CD2	2.49	0.41
1:C:795:ASP:OD1	1:C:797:GLN:HG2	2.20	0.41
1:C:841:MET:HE3	1:C:859:TRP:CD2	2.55	0.41
1:C:987:MET:O	1:C:989:LEU:N	2.53	0.41
1:A:269:GLU:C	1:A:270:LEU:O	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:HD11	1:A:477:ALA:HB1	2.02	0.41
1:A:774:MET:CG	1:A:775:SER:H	2.33	0.41
1:A:781:MET:HE1	1:C:228:GLN:CB	2.50	0.41
1:B:25:LEU:HD12	1:B:25:LEU:O	2.19	0.41
1:B:150:THR:HG23	1:B:153:ASP:CG	2.44	0.41
1:B:254:ASN:ND2	1:B:258:SER:CB	2.69	0.41
1:B:508:GLY:O	1:B:509:LYS:C	2.62	0.41
1:B:938:SER:HB3	1:B:1014:ALA:HB1	2.02	0.41
1:C:177:LEU:HD23	1:C:289:LEU:CD1	2.51	0.41
1:C:199:THR:HB	1:C:200:PRO:CD	2.50	0.41
1:C:513:PHE:C	1:C:515:TRP:N	2.74	0.41
1:C:680:PHE:CZ	1:C:844:MET:HE2	2.55	0.41
2:D:106:VAL:O	2:D:116:PRO:HD2	2.20	0.41
1:A:119:PRO:O	1:A:120:GLN:C	2.61	0.41
1:A:189:ASN:OD1	1:A:779:TYR:CZ	2.73	0.41
1:B:352:PHE:HD2	1:B:353:LEU:CD1	2.31	0.41
1:B:456:MET:CG	1:B:467:TYR:HB3	2.49	0.41
1:C:72:ILE:HG21	1:C:94:PHE:HE2	1.85	0.41
1:C:564:LEU:HA	1:C:565:PRO:HD3	1.86	0.41
1:A:168:ARG:HH22	1:B:820:ASN:C	2.28	0.41
1:A:198:LEU:HD23	1:A:198:LEU:HA	1.86	0.41
1:A:324:VAL:C	1:A:326:PRO:HD3	2.46	0.41
1:A:487:ILE:HG22	1:A:488:LEU:N	2.36	0.41
1:A:535:LEU:HD23	1:A:535:LEU:HA	1.80	0.41
1:C:682:PHE:CE2	1:C:684:LEU:HD23	2.51	0.41
1:A:67:GLN:NE2	1:C:767:ARG:HH11	2.15	0.41
1:B:10:ILE:HD12	1:C:895:TRP:HE1	1.86	0.41
1:B:355:MET:HB2	1:B:355:MET:HE2	1.92	0.41
1:B:876:LEU:H	1:B:876:LEU:HG	1.30	0.41
1:C:572:PHE:CE2	1:C:631:LEU:HD21	2.56	0.41
1:A:331:PRO:O	1:A:335:ILE:HG13	2.20	0.41
1:A:391:ASN:OD1	1:A:391:ASN:C	2.64	0.41
1:A:393:LEU:HD13	1:A:466:ILE:HG23	2.03	0.41
1:A:731:ILE:H	1:A:731:ILE:HG12	1.67	0.41
1:A:949:ALA:O	1:A:953:MET:HG3	2.20	0.41
1:B:540:ARG:O	1:B:544:LEU:CD1	2.69	0.41
1:B:971:ARG:O	1:B:975:ILE:HG13	2.21	0.41
1:C:582:ALA:HB3	1:C:623:ASN:CB	2.48	0.41
1:C:588:GLN:NE2	1:C:613:ASN:HD22	2.17	0.41
1:C:873:ALA:N	1:C:874:PRO:CD	2.83	0.41
1:C:937:LEU:C	1:C:940:LYS:HG2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LYS:O	1:A:295:THR:OG1	2.36	0.41
1:A:330:THR:N	1:A:331:PRO:CD	2.84	0.41
1:A:490:PRO:O	1:A:491:ALA:C	2.58	0.41
1:A:505:HIS:CE1	1:A:973:ARG:HH12	2.39	0.41
1:A:569:GLN:O	1:A:571:VAL:HG23	2.21	0.41
1:A:591:LEU:CD1	1:A:613:ASN:HD22	2.33	0.41
1:A:652:THR:HA	1:A:655:PHE:CD2	2.48	0.41
1:B:197:GLN:HA	1:B:798:MET:HE2	1.74	0.41
1:B:303:ALA:O	1:B:307:ARG:HB2	2.21	0.41
1:B:498:LYS:HA	1:B:499:PRO:HD3	1.85	0.41
1:B:937:LEU:O	1:B:937:LEU:HD23	2.21	0.41
1:C:36:PRO:CD	1:C:393:LEU:HD12	2.51	0.41
1:C:156:ASP:OD1	1:C:182:TYR:CG	2.74	0.41
1:C:927:PHE:O	1:C:928:GLN:C	2.62	0.41
2:D:27:ASP:OD1	2:D:61:GLU:HG3	2.21	0.41
1:A:108:GLN:HE22	1:B:113:LEU:HG	1.85	0.41
1:A:219:LEU:HD13	1:B:783:PRO:HG3	2.02	0.41
1:A:539:GLY:C	1:A:542:LEU:H	2.28	0.41
1:A:685:ILE:HD11	1:A:857:TYR:C	2.46	0.41
1:A:913:LEU:HD23	1:A:913:LEU:HA	1.78	0.41
1:A:946:VAL:HG23	1:A:1026:PHE:CD1	2.56	0.41
1:A:990:VAL:HG11	1:A:1008:MET:HE2	2.03	0.41
1:B:7:ASP:C	1:B:9:PRO:HD3	2.46	0.41
1:B:246:PHE:O	1:B:249:ILE:HG13	2.21	0.41
1:B:408:ASP:O	1:B:412:VAL:HG23	2.20	0.41
1:B:420:MET:O	1:B:423:GLU:O	2.38	0.41
1:B:511:GLY:HA2	1:B:513:PHE:C	2.43	0.41
1:B:578:LEU:HD13	1:B:578:LEU:HA	1.96	0.41
1:B:681:ASP:HB3	1:B:863:SER:O	2.20	0.41
1:B:693:GLU:HA	1:B:696:THR:HG22	2.03	0.41
1:B:851:LEU:HD12	1:B:851:LEU:H	1.85	0.41
1:C:9:PRO:CD	1:C:10:ILE:H	2.34	0.41
1:C:158:VAL:HG12	1:C:159:ALA:N	2.27	0.41
1:C:180:SER:CB	1:C:274:ASN:H	2.33	0.41
1:C:569:GLN:HE21	1:C:569:GLN:HB3	1.47	0.41
2:D:123:ILE:O	2:D:123:ILE:HG12	2.21	0.41
2:E:46:VAL:CG1	2:E:47:GLY:N	2.56	0.41
2:E:133:LEU:HD23	2:E:137:ALA:HA	2.02	0.41
2:E:154:ILE:HG13	2:E:155:ASP:N	2.30	0.41
1:A:454:VAL:N	1:A:455:PRO:HD2	2.35	0.41
1:A:519:MET:HG3	1:A:520:PHE:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:ILE:HD12	1:A:910:ILE:HA	1.88	0.41
1:A:991:ILE:HD12	1:A:991:ILE:HA	1.81	0.41
1:B:187:TRP:O	1:B:266:ALA:HA	2.21	0.41
1:B:193:LEU:H	1:B:193:LEU:CD2	2.06	0.41
1:B:249:ILE:O	1:B:262:LEU:N	2.48	0.41
1:B:255:GLN:C	1:B:257:GLY:H	2.29	0.41
1:C:115:MET:N	1:C:116:PRO:CD	2.84	0.41
1:C:138:MET:HE3	1:C:138:MET:HB2	1.88	0.41
1:C:774:MET:HE2	1:C:774:MET:HB2	1.33	0.41
1:C:879:ILE:O	1:C:880:SER:C	2.62	0.41
2:E:121:ALA:CB	2:E:152:ILE:HG12	2.50	0.41
1:A:293:LEU:HD11	1:A:299:ALA:HA	2.03	0.40
1:B:537:SER:O	1:B:541:TYR:CD1	2.73	0.40
1:B:582:ALA:HB3	1:B:623:ASN:HB3	2.02	0.40
1:B:649:MET:HA	1:B:649:MET:HE2	1.90	0.40
1:B:919:ARG:HD3	1:B:1005:THR:HG21	2.03	0.40
1:B:987:MET:N	1:B:988:PRO:CD	2.83	0.40
1:B:1021:PHE:O	1:B:1024:VAL:HB	2.20	0.40
1:C:80:SER:HB3	1:C:90:ILE:HG23	2.02	0.40
1:C:632:LYS:O	1:C:633:ASP:O	2.38	0.40
2:D:112:ASN:HB3	2:D:114:PHE:CD2	2.56	0.40
1:A:310:LEU:HA	1:A:313:MET:HE2	2.02	0.40
1:A:542:LEU:O	1:A:545:TYR:N	2.48	0.40
1:A:637:ARG:N	1:A:638:PRO:HD3	2.36	0.40
1:B:420:MET:HE2	1:B:420:MET:HB3	1.85	0.40
1:B:459:PHE:C	1:B:464:GLY:HA3	2.45	0.40
1:B:543:VAL:O	1:B:547:ILE:HG13	2.21	0.40
1:B:841:MET:O	1:B:842:GLU:C	2.64	0.40
1:B:869:SER:OG	1:B:870:GLY:N	2.54	0.40
1:C:742:SER:O	1:C:743:ILE:C	2.60	0.40
1:A:150:THR:OG1	1:A:151:GLN:N	2.55	0.40
1:A:158:VAL:HG12	1:A:289:LEU:HD21	2.03	0.40
1:A:188:MET:HE2	1:A:188:MET:HB3	1.78	0.40
1:A:306:ILE:HD13	1:A:306:ILE:HG23	1.71	0.40
1:A:489:THR:HB	1:A:490:PRO:HD2	1.99	0.40
1:A:693:GLU:CD	1:A:693:GLU:N	2.79	0.40
1:B:621:GLY:C	1:B:623:ASN:H	2.29	0.40
1:C:213:GLN:HE22	1:C:238:THR:HG22	1.86	0.40
1:C:483:LEU:O	1:C:487:ILE:HB	2.21	0.40
1:C:502:LYS:CG	1:C:503:GLY:N	2.77	0.40
1:C:568:ASP:HA	1:C:644:VAL:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:ASP:HA	2:D:45:HIS:HA	1.53	0.40
2:E:79:LEU:HD22	2:E:111:HIS:NE2	2.36	0.40
2:E:100:LEU:O	2:E:101:LYS:C	2.64	0.40
1:A:109:ASN:O	1:A:113:LEU:HD12	2.21	0.40
1:A:197:GLN:HA	1:A:798:MET:HE2	2.03	0.40
1:A:605:ASN:OD1	1:A:642:ASN:CG	2.65	0.40
1:B:104:GLN:NE2	1:B:129:VAL:O	2.54	0.40
1:B:142:VAL:HG13	1:B:321:LEU:HD11	2.03	0.40
1:B:184:MET:HE3	1:B:268:ILE:HG22	2.04	0.40
1:B:353:LEU:C	1:B:355:MET:N	2.78	0.40
1:B:790:TYR:CD1	1:B:800:PRO:CA	3.04	0.40
1:C:180:SER:HG	1:C:273:GLU:H	1.70	0.40
1:C:457:ALA:CB	1:C:468:ARG:HG2	2.49	0.40
1:C:497:LEU:CD2	1:C:497:LEU:C	2.85	0.40
1:C:733:GLN:HE22	1:C:743:ILE:HD13	1.85	0.40
2:D:52:HIS:NE2	2:D:83:PRO:HD3	2.37	0.40
1:A:309:GLU:O	1:A:309:GLU:HG3	2.22	0.40
1:A:314:GLU:HA	1:A:317:PHE:CE2	2.56	0.40
1:A:390:ILE:H	1:A:390:ILE:HG12	1.73	0.40
1:A:422:GLU:C	1:A:502:LYS:HG3	2.46	0.40
1:A:699:ARG:O	1:A:702:LEU:HB3	2.22	0.40
1:A:800:PRO:C	1:A:802:SER:H	2.28	0.40
1:B:379:THR:O	1:B:383:LEU:HG	2.21	0.40
1:B:699:ARG:C	1:B:701:GLN:N	2.78	0.40
1:B:799:VAL:CG1	1:B:804:PHE:HE1	2.35	0.40
1:B:851:LEU:HD12	1:B:851:LEU:N	2.36	0.40
1:C:668:LEU:C	1:C:669:PRO:O	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1004/1049 (96%)	919 (92%)	78 (8%)	7 (1%)	18	49
1	B	1022/1049 (97%)	941 (92%)	73 (7%)	8 (1%)	16	46
1	C	1038/1049 (99%)	954 (92%)	80 (8%)	4 (0%)	30	59
2	D	152/169 (90%)	141 (93%)	10 (7%)	1 (1%)	18	49
2	E	147/169 (87%)	136 (92%)	10 (7%)	1 (1%)	18	49
All	All	3363/3485 (96%)	3091 (92%)	251 (8%)	21 (1%)	21	51

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	638	PRO
1	B	671	ILE
1	C	224	PRO
1	B	1014	ALA
1	A	315	PRO
1	C	633	ASP
2	D	70	GLY
1	A	184	MET
1	B	200	PRO
1	B	747	ASN
1	B	864	TYR
1	C	36	PRO
1	B	448	VAL
2	E	50	PRO
1	A	746	ILE
1	A	852	PRO
1	A	998	GLY
1	A	560	PRO
1	B	436	GLY
1	A	988	PRO
1	C	771	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	770/854 (90%)	657 (85%)	113 (15%)	3	14
1	B	772/854 (90%)	633 (82%)	139 (18%)	2	8
1	C	802/854 (94%)	686 (86%)	116 (14%)	3	14
2	D	103/133 (77%)	87 (84%)	16 (16%)	2	12
2	E	88/133 (66%)	82 (93%)	6 (7%)	14	43
All	All	2535/2828 (90%)	2145 (85%)	390 (15%)	2	12

All (390) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	25	LEU
1	A	30	LEU
1	A	32	VAL
1	A	46	SER
1	A	48	SER
1	A	65	ILE
1	A	74	ASN
1	A	75	LEU
1	A	78	MET
1	A	79	SER
1	A	82	SER
1	A	121	GLU
1	A	127	VAL
1	A	140	VAL
1	A	143	ILE
1	A	169	THR
1	A	180	SER
1	A	188	MET
1	A	197	GLN
1	A	201	VAL
1	A	205	THR
1	A	235	ILE
1	A	237	GLN
1	A	241	THR
1	A	244	GLU
1	A	262	LEU
1	A	264	ASP
1	A	269	GLU
1	A	277	ILE
1	A	278	ILE

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Mol	Chain	Res	Type
1	A	292	LYS
1	A	295	THR
1	A	306	ILE
1	A	312	LYS
1	A	321	LEU
1	A	330	THR
1	A	340	VAL
1	A	390	ILE
1	A	445	ILE
1	A	482	VAL
1	A	486	LEU
1	A	487	ILE
1	A	488	LEU
1	A	489	THR
1	A	495	THR
1	A	497	LEU
1	A	498	LYS
1	A	504	ASP
1	A	519	MET
1	A	520	PHE
1	A	531	VAL
1	A	543	VAL
1	A	558	ARG
1	A	571	VAL
1	A	583	THR
1	A	586	ARG
1	A	587	THR
1	A	589	LYS
1	A	601	LYS
1	A	602	GLU
1	A	604	ASN
1	A	605	ASN
1	A	612	VAL
1	A	622	GLN
1	A	640	GLU
1	A	648	THR
1	A	650	ARG
1	A	658	ILE
1	A	685	ILE
1	A	687	GLN
1	A	696	THR
1	A	716	VAL

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Mol	Chain	Res	Type
1	A	717	ARG
1	A	754	TRP
1	A	757	SER
1	A	758	TYR
1	A	759	VAL
1	A	775	SER
1	A	780	ARG
1	A	784	ASP
1	A	786	ILE
1	A	795	ASP
1	A	799	VAL
1	A	807	SER
1	A	808	ARG
1	A	811	TYR
1	A	813	SER
1	A	815	ARG
1	A	822	LEU
1	A	823	PRO
1	A	825	MET
1	A	827	ILE
1	A	830	GLN
1	A	847	LEU
1	A	860	THR
1	A	893	GLU
1	A	894	SER
1	A	900	SER
1	A	917	THR
1	A	932	LEU
1	A	935	ILE
1	A	946	VAL
1	A	950	LYS
1	A	953	MET
1	A	956	GLU
1	A	961	ILE
1	A	971	ARG
1	A	972	LEU
1	A	976	LEU
1	A	978	THR
1	A	991	ILE
1	A	1030	ARG
1	B	21	LEU
1	B	46	SER

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Mol	Chain	Res	Type
1	B	53	ASP
1	B	55	LYS
1	B	58	GLN
1	B	60	THR
1	B	69	MET
1	B	75	LEU
1	B	79	SER
1	B	80	SER
1	B	82	SER
1	B	87	THR
1	B	95	GLU
1	B	99	ASP
1	B	107	VAL
1	B	108	GLN
1	B	111	LEU
1	B	117	LEU
1	B	121	GLU
1	B	128	SER
1	B	143	ILE
1	B	150	THR
1	B	153	ASP
1	B	161	ASN
1	B	162	MET
1	B	163	LYS
1	B	166	ILE
1	B	170	SER
1	B	172	VAL
1	B	189	ASN
1	B	193	LEU
1	B	197	GLN
1	B	207	ILE
1	B	213	GLN
1	B	218	GLN
1	B	222	THR
1	B	229	GLN
1	B	230	LEU
1	B	231	ASN
1	B	233	SER
1	B	234	ILE
1	B	235	ILE
1	B	237	GLN
1	B	250	LEU

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Mol	Chain	Res	Type
1	B	253	VAL
1	B	259	ARG
1	B	270	LEU
1	B	274	ASN
1	B	278	ILE
1	B	284	GLN
1	B	289	LEU
1	B	306	ILE
1	B	321	LEU
1	B	323	ILE
1	B	329	THR
1	B	361	ASN
1	B	365	THR
1	B	366	LEU
1	B	369	THR
1	B	377	LEU
1	B	382	VAL
1	B	399	VAL
1	B	405	LEU
1	B	410	ILE
1	B	423	GLU
1	B	425	LEU
1	B	462	SER
1	B	493	CYS
1	B	495	THR
1	B	497	LEU
1	B	500	ILE
1	B	507	GLU
1	B	513	PHE
1	B	519	MET
1	B	540	ARG
1	B	555	LEU
1	B	557	VAL
1	B	564	LEU
1	B	574	THR
1	B	577	GLN
1	B	578	LEU
1	B	587	THR
1	B	623	ASN
1	B	628	PHE
1	B	647	ILE
1	B	649	MET

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Mol	Chain	Res	Type
1	B	658	ILE
1	B	669	PRO
1	B	671	ILE
1	B	674	LEU
1	B	676	THR
1	B	687	GLN
1	B	695	LEU
1	B	705	GLU
1	B	712	MET
1	B	713	LEU
1	B	714	THR
1	B	717	ARG
1	B	721	LEU
1	B	723	ASP
1	B	730	ASP
1	B	731	ILE
1	B	732	ASP
1	B	757	SER
1	B	759	VAL
1	B	763	ILE
1	B	765	ARG
1	B	771	VAL
1	B	780	ARG
1	B	786	ILE
1	B	808	ARG
1	B	815	ARG
1	B	822	LEU
1	B	824	SER
1	B	825	MET
1	B	844	MET
1	B	853	THR
1	B	859	TRP
1	B	862	MET
1	B	867	ARG
1	B	871	ASN
1	B	874	PRO
1	B	876	LEU
1	B	881	LEU
1	B	886	LEU
1	B	888	LEU
1	B	894	SER
1	B	914	LEU

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Mol	Chain	Res	Type
1	B	919	ARG
1	B	921	LEU
1	B	960	LEU
1	B	968	VAL
1	B	971	ARG
1	B	972	LEU
1	B	987	MET
1	B	989	LEU
1	B	990	VAL
1	B	991	ILE
1	B	1028	VAL
1	C	4	PHE
1	C	11	PHE
1	C	15	ILE
1	C	56	THR
1	C	58	GLN
1	C	69	MET
1	C	81	ASN
1	C	85	THR
1	C	88	VAL
1	C	98	THR
1	C	127	VAL
1	C	133	SER
1	C	143	ILE
1	C	145	THR
1	C	148	THR
1	C	150	THR
1	C	154	ILE
1	C	157	TYR
1	C	161	ASN
1	C	167	SER
1	C	175	VAL
1	C	197	GLN
1	C	218	GLN
1	C	225	VAL
1	C	226	LYS
1	C	233	SER
1	C	241	THR
1	C	261	LEU
1	C	263	ARG
1	C	268	ILE
1	C	278	ILE

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Mol	Chain	Res	Type
1	C	289	LEU
1	C	310	LEU
1	C	321	LEU
1	C	325	TYR
1	C	329	THR
1	C	330	THR
1	C	372	VAL
1	C	404	LEU
1	C	411	VAL
1	C	425	LEU
1	C	429	GLU
1	C	435	MET
1	C	437	GLN
1	C	439	GLN
1	C	452	VAL
1	C	466	ILE
1	C	473	THR
1	C	482	VAL
1	C	497	LEU
1	C	507	GLU
1	C	510	LYS
1	C	512	PHE
1	C	528	THR
1	C	538	THR
1	C	542	LEU
1	C	544	LEU
1	C	561	SER
1	C	567	GLU
1	C	569	GLN
1	C	571	VAL
1	C	575	MET
1	C	587	THR
1	C	604	ASN
1	C	623	ASN
1	C	626	ILE
1	C	629	VAL
1	C	631	LEU
1	C	640	GLU
1	C	641	GLU
1	C	671	ILE
1	C	674	LEU
1	C	684	LEU

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Mol	Chain	Res	Type
1	C	690	LEU
1	C	695	LEU
1	C	715	SER
1	C	717	ARG
1	C	721	LEU
1	C	723	ASP
1	C	730	ASP
1	C	732	ASP
1	C	739	LEU
1	C	742	SER
1	C	743	ILE
1	C	749	THR
1	C	750	LEU
1	C	757	SER
1	C	774	MET
1	C	782	LEU
1	C	805	SER
1	C	815	ARG
1	C	816	LEU
1	C	830	GLN
1	C	862	MET
1	C	867	ARG
1	C	869	SER
1	C	875	SER
1	C	876	LEU
1	C	879	ILE
1	C	880	SER
1	C	891	LEU
1	C	910	ILE
1	C	917	THR
1	C	922	THR
1	C	924	ASP
1	C	947	GLU
1	C	952	LEU
1	C	956	GLU
1	C	960	LEU
1	C	976	LEU
1	C	978	THR
1	C	979	SER
1	C	990	VAL
1	C	993	THR
1	C	1011	MET

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Mol	Chain	Res	Type
1	C	1019	ILE
2	D	18	LEU
2	D	27	ASP
2	D	41	ASN
2	D	45	HIS
2	D	46	VAL
2	D	53	LEU
2	D	63	VAL
2	D	73	VAL
2	D	77	ASP
2	D	78	SER
2	D	83	PRO
2	D	84	LEU
2	D	129	VAL
2	D	132	LEU
2	D	133	LEU
2	D	154	ILE
2	E	99	LEU
2	E	102	ASN
2	E	123	ILE
2	E	152	ILE
2	E	154	ILE
2	E	155	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	67	GLN
1	A	123	GLN
1	A	176	GLN
1	A	181	GLN
1	A	189	ASN
1	A	191	ASN
1	A	194	ASN
1	A	197	GLN
1	A	228	GLN
1	A	231	ASN
1	A	274	ASN
1	A	284	GLN
1	A	298	ASN
1	A	361	ASN

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Mol	Chain	Res	Type
1	A	439	GLN
1	A	577	GLN
1	A	613	ASN
1	A	687	GLN
1	A	700	ASN
1	A	701	GLN
1	A	709	HIS
1	A	737	GLN
1	A	760	ASN
1	A	1000	GLN
1	B	81	ASN
1	B	104	GLN
1	B	108	GLN
1	B	123	GLN
1	B	124	GLN
1	B	125	GLN
1	B	161	ASN
1	B	176	GLN
1	B	197	GLN
1	B	218	GLN
1	B	231	ASN
1	B	254	ASN
1	B	284	GLN
1	B	361	ASN
1	B	569	GLN
1	B	577	GLN
1	B	592	ASN
1	B	596	HIS
1	B	605	ASN
1	B	687	GLN
1	B	701	GLN
1	B	709	HIS
1	B	726	GLN
1	B	733	GLN
1	B	760	ASN
1	B	830	GLN
1	B	941	ASN
1	C	3	ASN
1	C	34	GLN
1	C	67	GLN
1	C	68	ASN
1	C	104	GLN

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Mol	Chain	Res	Type
1	C	125	GLN
1	C	144	ASN
1	C	181	GLN
1	C	197	GLN
1	C	213	GLN
1	C	274	ASN
1	C	298	ASN
1	C	360	GLN
1	C	517	ASN
1	C	525	HIS
1	C	569	GLN
1	C	577	GLN
1	C	588	GLN
1	C	604	ASN
1	C	623	ASN
1	C	701	GLN
1	C	719	ASN
1	C	760	ASN
1	C	830	GLN
1	C	865	GLN
1	C	928	GLN
2	D	45	HIS
2	D	52	HIS
2	D	118	HIS
2	E	69	ASN
2	E	118	HIS
2	E	156	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	A	1	1	8,9,10	0.34	0	8,9,11	0.81	0
1	FME	B	1	1	8,9,10	0.56	0	8,9,11	0.94	0
1	FME	C	1	1	8,9,10	0.56	0	8,9,11	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	2/7/9/11	-
1	FME	B	1	1	-	4/7/9/11	-
1	FME	C	1	1	-	3/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	B	1	FME	O1-CN-N-CA
1	B	1	FME	CB-CA-N-CN
1	C	1	FME	CB-CG-SD-CE
1	A	1	FME	CB-CG-SD-CE
1	C	1	FME	N-CA-CB-CG
1	C	1	FME	C-CA-CB-CG
1	B	1	FME	N-CA-CB-CG
1	B	1	FME	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	5	0
1	B	1	FME	10	0
1	C	1	FME	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	1007/1049 (95%)	0.82	137 (13%) 7 6	30, 72, 138, 274	1 (0%)
1	B	1027/1049 (97%)	0.75	148 (14%) 6 6	26, 71, 142, 330	0
1	C	1037/1049 (98%)	0.62	137 (13%) 7 7	26, 63, 126, 198	0
2	D	154/169 (91%)	0.81	20 (12%) 7 7	11, 85, 134, 207	1 (0%)
2	E	148/169 (87%)	2.35	66 (44%) 0 0	26, 147, 256, 372	1 (0%)
All	All	3373/3485 (96%)	0.81	508 (15%) 5 5	11, 71, 152, 372	3 (0%)

All (508) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	158	ASN	15.1
2	E	45	HIS	13.4
2	D	158	ASN	12.2
1	A	462	SER	11.5
2	E	48	TRP	11.0
2	E	44	ASP	11.0
1	B	674	LEU	10.9
1	A	123	GLN	10.6
1	B	858	ASP	9.7
2	E	57	PHE	8.3
1	B	675	GLY	8.3
1	A	124	GLN	8.2
1	A	617	PHE	7.6
2	E	43	SER	7.4
2	E	49	THR	7.2
1	C	120	GLN	7.2
2	E	56	TYR	7.1
1	B	859	TRP	6.8
2	E	58	GLY	6.7
1	A	36	PRO	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	959	GLY	6.4
2	E	76	ASP	6.4
1	A	37	THR	6.4
1	A	812	GLY	6.3
1	C	86	GLY	6.3
1	A	256	ASP	6.2
1	B	509	LYS	6.1
1	B	676	THR	6.0
1	B	563	PHE	6.0
1	A	461	GLY	5.8
1	A	671	ILE	5.8
1	B	510	LYS	5.7
2	E	46	VAL	5.7
1	B	996	GLY	5.7
1	A	860	THR	5.6
1	C	733	GLN	5.6
1	B	407	ASP	5.6
1	C	50	PRO	5.6
1	C	125	GLN	5.5
2	E	53	LEU	5.5
1	B	678	THR	5.4
2	E	86	LEU	5.4
1	A	811	TYR	5.4
1	A	463	THR	5.3
1	A	995	ALA	5.3
2	E	151	ASP	5.3
1	A	938	SER	5.3
2	D	37	GLY	5.3
1	A	681	ASP	5.3
1	B	511	GLY	5.2
1	A	670	ALA	5.2
1	C	951	ASP	5.2
2	D	35	ALA	5.2
1	C	513	PHE	5.1
1	B	134	SER	5.1
1	A	859	TRP	5.0
1	B	216	ALA	4.9
2	D	36	ASN	4.9
2	E	16	LYS	4.9
1	C	872	GLN	4.9
2	E	145	PHE	4.9
1	B	561	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	962	GLU	4.9
2	E	90	ARG	4.9
1	A	723	ASP	4.9
1	B	271	GLY	4.8
1	C	96	SER	4.8
1	A	254	ASN	4.8
1	A	719	ASN	4.8
1	B	677	ALA	4.7
2	E	137	ALA	4.7
1	B	559	LEU	4.6
1	B	133	SER	4.6
1	B	599	LEU	4.6
1	C	1032	ARG	4.5
2	E	93	LEU	4.5
1	C	918	PHE	4.5
1	A	120	GLN	4.5
1	B	120	GLN	4.5
2	D	140	ASN	4.5
1	B	516	PHE	4.5
1	A	711	ASP	4.4
1	B	301	ASP	4.4
2	E	82	THR	4.4
2	D	33	LEU	4.4
1	A	607	GLU	4.3
1	C	723	ASP	4.3
1	A	96	SER	4.3
1	B	164	ASP	4.2
1	B	635	ALA	4.2
1	C	48	SER	4.2
1	C	123	GLN	4.2
1	A	966	ASP	4.2
1	B	853	THR	4.2
1	A	620	ARG	4.2
1	C	49	TYR	4.2
1	C	428	LYS	4.1
2	E	153	SER	4.1
1	C	563	PHE	4.1
1	A	586	ARG	4.1
1	C	760	ASN	4.1
1	B	633	ASP	4.0
1	A	35	TYR	4.0
1	A	125	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	630	SER	4.0
1	C	170	SER	4.0
1	B	124	GLN	4.0
1	A	958	LYS	4.0
1	B	672	VAL	4.0
1	C	994	GLY	4.0
1	A	121	GLU	4.0
1	B	274	ASN	4.0
1	B	361	ASN	4.0
1	B	600	THR	4.0
1	B	993	THR	4.0
1	C	564	LEU	4.0
1	A	904	VAL	3.9
2	D	70	GLY	3.9
2	E	54	ALA	3.9
1	A	408	ASP	3.9
1	A	606	VAL	3.9
1	B	857	TYR	3.9
1	A	53	ASP	3.9
1	B	1031	ARG	3.9
1	B	506	GLY	3.9
1	B	560	PRO	3.9
1	B	512	PHE	3.9
1	B	771	VAL	3.9
1	B	617	PHE	3.9
1	C	124	GLN	3.9
2	E	92	HIS	3.9
1	B	224	PRO	3.8
1	C	1038	GLU	3.8
1	B	985	GLY	3.8
2	E	47	GLY	3.8
1	A	464	GLY	3.8
2	E	17	LYS	3.8
1	A	797	GLN	3.8
1	B	871	ASN	3.8
1	A	208	LYS	3.8
1	A	608	SER	3.8
1	C	121	GLU	3.8
1	A	1014	ALA	3.7
1	C	501	ALA	3.7
1	C	505	HIS	3.7
2	E	55	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	218	GLN	3.7
1	C	1034	SER	3.7
1	B	660	ASP	3.7
1	C	7	ASP	3.7
1	B	507	GLU	3.7
1	A	963	ALA	3.7
1	C	87	THR	3.7
1	A	672	VAL	3.7
1	A	679	GLY	3.7
1	A	836	SER	3.7
1	A	872	GLN	3.7
1	C	496	MET	3.7
2	E	87	ALA	3.6
2	E	159	GLU	3.6
1	B	39	ALA	3.6
1	B	673	GLU	3.6
1	C	515	TRP	3.6
1	C	955	LYS	3.6
1	C	362	PHE	3.5
1	C	146	ASP	3.5
1	B	223	PRO	3.5
2	E	50	PRO	3.5
1	A	660	ASP	3.5
2	D	137	ALA	3.5
1	A	743	ILE	3.5
1	B	225	VAL	3.5
1	B	53	ASP	3.5
1	C	126	GLY	3.4
1	B	634	TRP	3.4
1	B	169	THR	3.4
1	B	706	ALA	3.4
1	C	831	ALA	3.4
1	C	776	GLU	3.4
1	A	506	GLY	3.4
1	B	232	ALA	3.4
1	B	558	ARG	3.4
1	B	360	GLN	3.4
1	B	226	LYS	3.4
1	C	161	ASN	3.4
1	C	83	ASP	3.4
2	E	156	ASN	3.3
1	C	423	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	755	GLY	3.3
2	E	105	ASP	3.3
1	C	582	ALA	3.3
1	C	788	ASP	3.3
2	D	160	ASP	3.3
1	A	116	PRO	3.3
1	C	85	THR	3.3
1	C	619	GLY	3.3
1	A	951	ASP	3.3
1	C	426	PRO	3.3
1	B	284	GLN	3.3
1	B	519	MET	3.3
1	C	617	PHE	3.2
2	E	59	HIS	3.2
2	E	140	ASN	3.2
1	C	51	GLY	3.2
1	C	436	GLY	3.2
1	C	926	TYR	3.2
1	A	563	PHE	3.2
1	C	811	TYR	3.2
1	C	134	SER	3.2
1	C	868	LEU	3.1
1	A	680	PHE	3.1
1	B	997	SER	3.1
1	B	954	ASP	3.1
1	C	761	ASP	3.1
1	C	1033	PHE	3.1
1	A	541	TYR	3.1
1	B	123	GLN	3.1
1	C	360	GLN	3.1
1	C	657	GLN	3.1
2	E	91	GLY	3.1
1	A	515	TRP	3.1
1	A	649	MET	3.1
1	B	117	LEU	3.1
1	B	805	SER	3.1
1	A	730	ASP	3.1
1	B	332	PHE	3.1
2	E	147	LYS	3.1
1	A	667	ASN	3.1
2	E	26	GLN	3.1
1	A	634	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1033	PHE	3.1
1	A	969	ARG	3.0
1	C	586	ARG	3.0
1	C	993	THR	3.0
1	C	319	SER	3.0
1	C	678	THR	3.0
1	C	512	PHE	3.0
1	C	558	ARG	3.0
1	C	581	GLY	3.0
1	C	754	TRP	3.0
1	B	562	SER	3.0
2	E	89	ASP	3.0
1	B	221	GLY	3.0
1	B	604	ASN	3.0
1	C	70	ASN	3.0
2	E	144	LYS	3.0
1	B	60	THR	3.0
1	C	1030	ARG	2.9
1	B	961	ILE	2.9
1	B	3	ASN	2.9
1	C	3	ASN	2.9
1	B	233	SER	2.9
1	A	71	GLY	2.9
1	A	669	PRO	2.9
1	A	809	TRP	2.9
1	B	166	ILE	2.9
1	B	229	GLN	2.9
1	B	189	ASN	2.9
1	B	649	MET	2.9
1	C	509	LYS	2.9
1	C	584	GLN	2.9
1	B	636	ASP	2.9
1	C	148	THR	2.9
2	E	70	GLY	2.9
1	C	736	ALA	2.8
1	A	629	VAL	2.8
1	C	1029	VAL	2.8
1	A	971	ARG	2.8
1	B	344	LEU	2.8
1	A	678	THR	2.8
2	E	146	GLY	2.8
1	B	96	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	251	LEU	2.8
1	C	621	GLY	2.8
1	C	670	ALA	2.8
1	C	814	PRO	2.8
1	B	191	ASN	2.8
2	D	122	ASN	2.8
1	B	792	ARG	2.8
1	A	846	GLN	2.8
2	D	54	ALA	2.8
1	A	117	LEU	2.8
1	B	730	ASP	2.7
1	A	582	ALA	2.7
1	C	516	PHE	2.7
2	E	123	ILE	2.7
2	E	106	VAL	2.7
1	C	116	PRO	2.7
1	A	826	GLU	2.7
1	B	607	GLU	2.7
1	A	238	THR	2.7
1	A	581	GLY	2.7
2	D	13	ASP	2.7
1	C	47	ALA	2.7
2	E	75	ALA	2.7
1	C	921	LEU	2.7
1	B	222	THR	2.7
1	A	760	ASN	2.7
1	A	207	ILE	2.7
1	A	1021	PHE	2.7
1	B	273	GLU	2.7
1	C	756	GLY	2.7
1	A	48	SER	2.7
1	B	671	ILE	2.6
1	A	429	GLU	2.6
1	C	507	GLU	2.6
1	A	118	LEU	2.6
1	B	287	SER	2.6
1	A	517	ASN	2.6
1	A	778	LYS	2.6
1	A	1011	MET	2.6
1	B	252	LYS	2.6
1	B	808	ARG	2.6
1	A	130	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	731	ILE	2.6
1	A	428	LYS	2.6
1	A	31	PRO	2.6
1	B	513	PHE	2.6
2	E	77	ASP	2.6
1	B	148	THR	2.6
1	B	688	ALA	2.6
1	B	116	PRO	2.6
1	B	106	GLN	2.6
2	E	74	ASN	2.6
2	E	143	ASP	2.6
1	B	214	VAL	2.6
1	A	505	HIS	2.5
1	C	82	SER	2.5
1	C	562	SER	2.5
1	C	737	GLN	2.5
2	E	166	GLN	2.5
1	B	923	ASN	2.5
1	A	209	ALA	2.5
1	A	978	THR	2.5
1	C	517	ASN	2.5
1	C	956	GLU	2.5
2	E	130	GLU	2.5
1	A	583	THR	2.5
2	E	60	LEU	2.5
1	C	133	SER	2.5
1	C	122	VAL	2.5
1	B	38	ILE	2.5
1	C	229	GLN	2.5
1	C	618	ALA	2.5
1	A	828	LEU	2.5
1	A	621	GLY	2.5
1	B	508	GLY	2.5
1	C	691	GLY	2.5
1	B	556	PHE	2.4
1	C	599	LEU	2.4
2	D	14	LEU	2.4
1	B	498	LYS	2.4
1	B	25	LEU	2.4
2	D	69	ASN	2.4
1	A	407	ASP	2.4
1	A	784	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	751	GLY	2.4
1	C	503	GLY	2.4
2	E	71	ALA	2.4
1	C	948	PHE	2.4
1	B	921	LEU	2.4
1	A	579	PRO	2.4
1	C	495	THR	2.4
1	C	799	VAL	2.4
2	E	28	ASP	2.4
1	A	998	GLY	2.4
1	C	834	GLY	2.4
2	D	55	ALA	2.4
1	B	577	GLN	2.4
1	A	516	PHE	2.4
1	C	734	GLU	2.4
2	E	126	LEU	2.4
1	B	796	GLY	2.4
1	C	506	GLY	2.4
1	C	740	GLY	2.4
2	E	122	ASN	2.4
2	E	108	ALA	2.4
1	A	11	PHE	2.4
1	A	513	PHE	2.4
1	B	564	LEU	2.4
2	D	126	LEU	2.4
1	A	339	GLU	2.4
1	C	673	GLU	2.4
1	B	217	GLY	2.3
1	B	59	ASP	2.3
1	A	115	MET	2.3
1	B	956	GLU	2.3
1	A	119	PRO	2.3
1	B	37	THR	2.3
1	A	33	ALA	2.3
1	C	54	ALA	2.3
1	B	289	LEU	2.3
1	A	961	ILE	2.3
1	B	553	ALA	2.3
1	C	52	ALA	2.3
2	D	71	ALA	2.3
2	E	24	ALA	2.3
1	A	628	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	645	GLU	2.3
1	C	616	GLY	2.3
1	A	206	ALA	2.3
1	A	172	VAL	2.3
2	E	81	VAL	2.3
1	A	332	PHE	2.3
1	A	802	SER	2.3
2	E	107	ASN	2.3
1	C	732	ASP	2.3
1	C	514	GLY	2.2
1	C	963	ALA	2.2
2	E	21	ALA	2.2
1	B	868	LEU	2.2
1	B	275	TYR	2.2
2	E	20	GLU	2.2
1	B	402	ILE	2.2
1	A	440	GLY	2.2
1	A	691	GLY	2.2
1	A	994	GLY	2.2
1	A	842	GLU	2.2
1	C	357	LEU	2.2
1	C	424	GLY	2.2
1	B	1028	VAL	2.2
1	A	980	LEU	2.2
1	A	858	ASP	2.2
1	B	131	LYS	2.2
1	A	432	ARG	2.2
1	C	432	ARG	2.2
1	C	927	PHE	2.2
1	A	759	VAL	2.2
1	C	112	GLN	2.2
1	B	28	LEU	2.2
2	E	117	LEU	2.2
1	B	606	VAL	2.1
2	E	40	VAL	2.1
1	A	657	GLN	2.1
1	C	28	LEU	2.1
2	D	142	GLN	2.1
1	A	915	ALA	2.1
1	B	742	SER	2.1
1	B	862	MET	2.1
1	C	836	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	444	GLY	2.1
1	C	511	GLY	2.1
1	C	920	GLY	2.1
2	D	57	PHE	2.1
1	C	256	ASP	2.1
1	B	643	LYS	2.1
1	A	808	ARG	2.1
1	C	787	GLY	2.1
1	A	282	ASN	2.1
1	C	871	ASN	2.1
1	C	954	ASP	2.1
1	A	713	LEU	2.1
1	B	860	THR	2.1
1	B	917	THR	2.1
1	A	953	MET	2.1
1	B	363	ARG	2.1
1	A	34	GLN	2.1
1	A	494	ALA	2.1
1	A	569	GLN	2.1
1	B	670	ALA	2.1
1	B	499	PRO	2.1
1	C	693	GLU	2.1
1	B	505	HIS	2.1
2	E	27	ASP	2.1
2	E	39	ASP	2.1
1	C	363	ARG	2.1
1	B	541	TYR	2.1
1	B	873	ALA	2.1
2	D	38	ALA	2.1
1	B	569	GLN	2.1
1	A	217	GLY	2.1
1	B	403	GLY	2.1
1	A	718	PRO	2.1
1	C	481	SER	2.1
1	B	109	ASN	2.1
1	B	760	ASN	2.1
1	B	721	LEU	2.1
1	C	497	LEU	2.1
2	E	19	LEU	2.1
1	A	566	ASP	2.1
1	C	60	THR	2.1
1	C	494	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	67	GLN	2.1
1	B	814	PRO	2.1
1	B	955	LYS	2.0
1	B	656	SER	2.0
1	B	270	LEU	2.0
1	C	6	ILE	2.0
1	C	307	ARG	2.0
2	E	112	ASN	2.0
1	A	205	THR	2.0
1	A	636	ASP	2.0
1	B	793	ALA	2.0
1	B	71	GLY	2.0
1	B	657	GLN	2.0
1	C	63	GLN	2.0
1	C	320	GLY	2.0
1	C	458	PHE	2.0
1	A	521	GLU	2.0
1	A	564	LEU	2.0
1	C	674	LEU	2.0
1	A	709	HIS	2.0
1	C	164	ASP	2.0
1	B	362	PHE	2.0
1	B	29	LYS	2.0
1	B	737	GLN	2.0
1	C	498	LYS	2.0
2	E	18	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	FME	B	1	10/11	0.85	0.14	68,71,78,80	0
1	FME	A	1	10/11	0.86	0.14	87,88,108,109	0
1	FME	C	1	10/11	0.86	0.17	62,64,181,181	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.