



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:24 AM UTC

PDB ID : 1WCM / pdb_00001wcm
Title : Complete 12-Subunit RNA Polymerase II at 3.8 Angstrom
Authors : Armache, K.-J.; Mitterweger, S.; Meinhart, A.; Cramer, P.
Deposited on : 2004-11-17
Resolution : 3.80 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
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

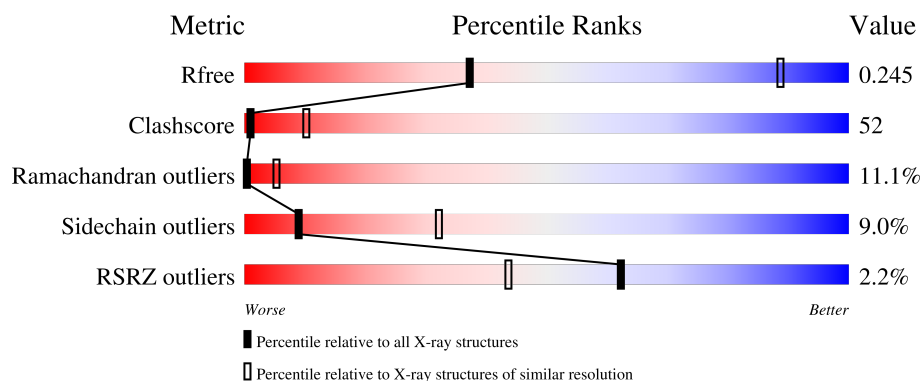
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	1733	2% 23% 44% 13% 18%
2	B	1224	2% 27% 46% 16% 10%
3	C	318	20% 48% 14% 16%
4	D	177	3% 34% 49% 15%
5	E	215	2% 37% 53% 9%

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Mol	Chain	Length	Quality of chain
6	F	155	% 14%30%10%46% .
7	G	171	% 36%50%13% .
8	H	146	8% 30%49%12%9%
9	I	122	2% 36%44%14% . .
10	J	70	17% 49%26% . 7%
11	K	120	% 38%49%8% . .
12	L	70	6% 11%34%20%34%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 30945 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 DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SECOND LARGEST SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8720	5526	1523	1617	54			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 32 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 23

KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 19 KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II AND III 8.3 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		
13	B	1	Total	Zn	0	0
			1	1		
13	C	1	Total	Zn	0	0
			1	1		
13	I	2	Total	Zn	0	0
			2	2		
13	J	1	Total	Zn	0	0
			1	1		
13	L	1	Total	Zn	0	0
			1	1		

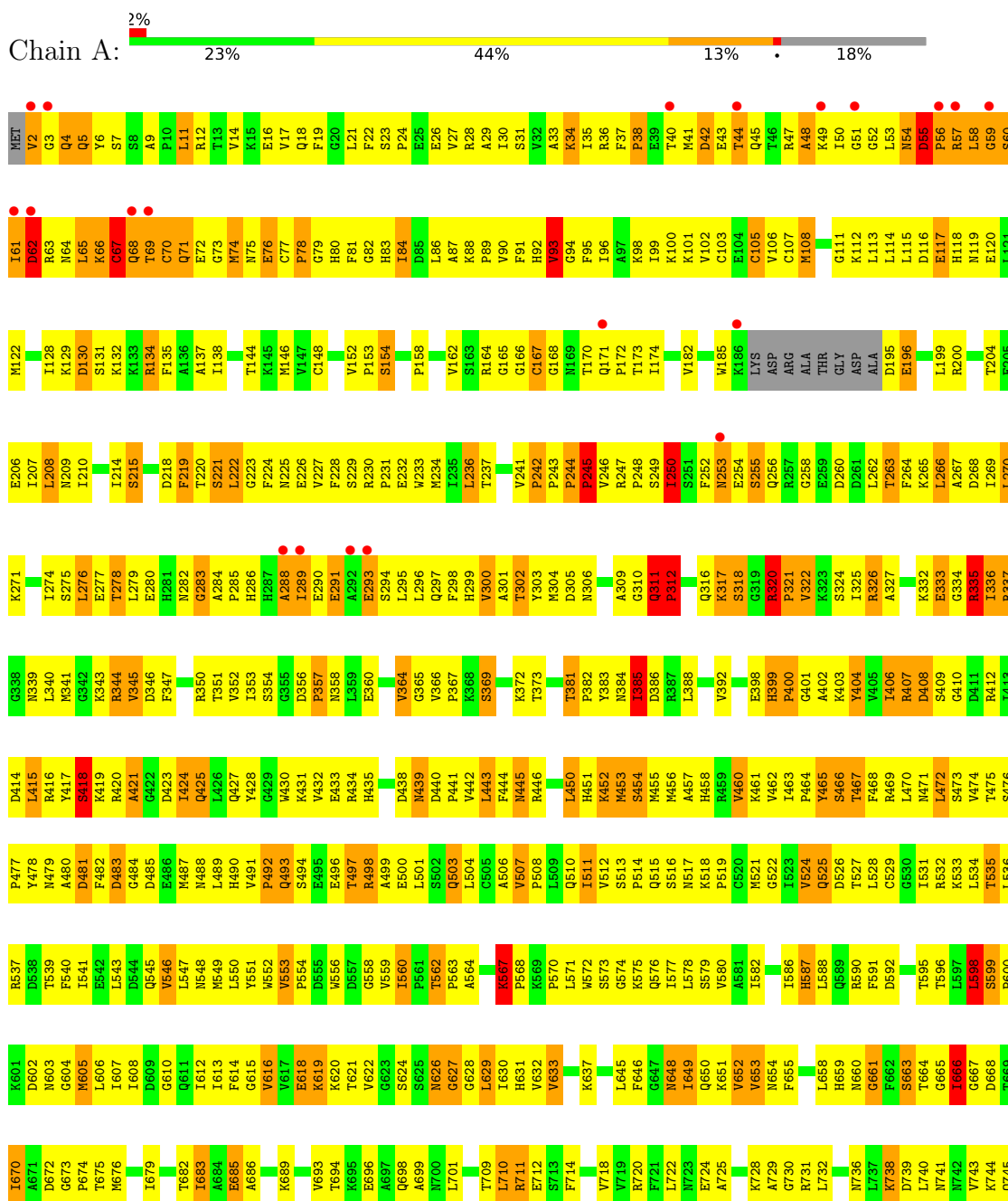
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

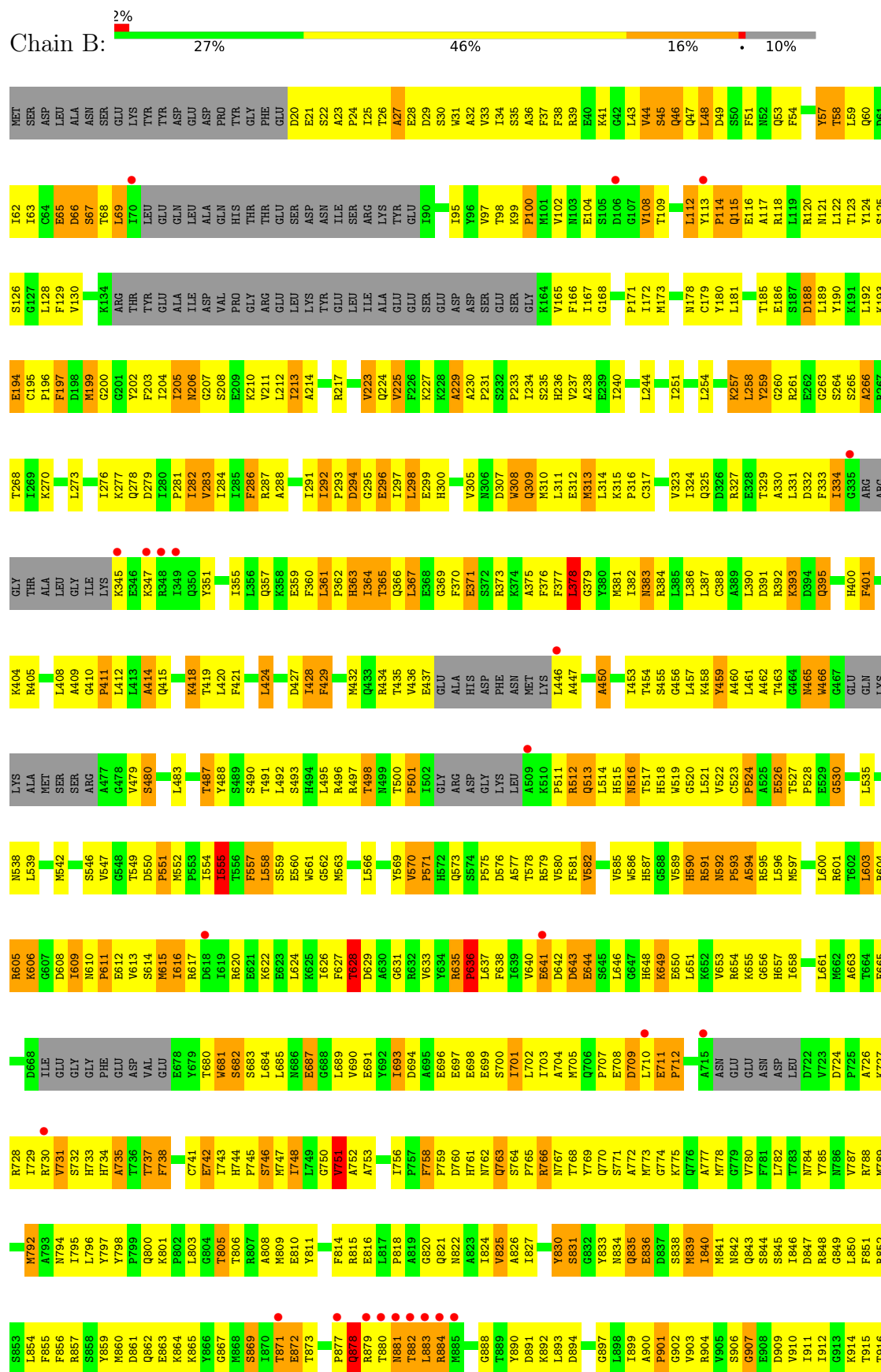
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

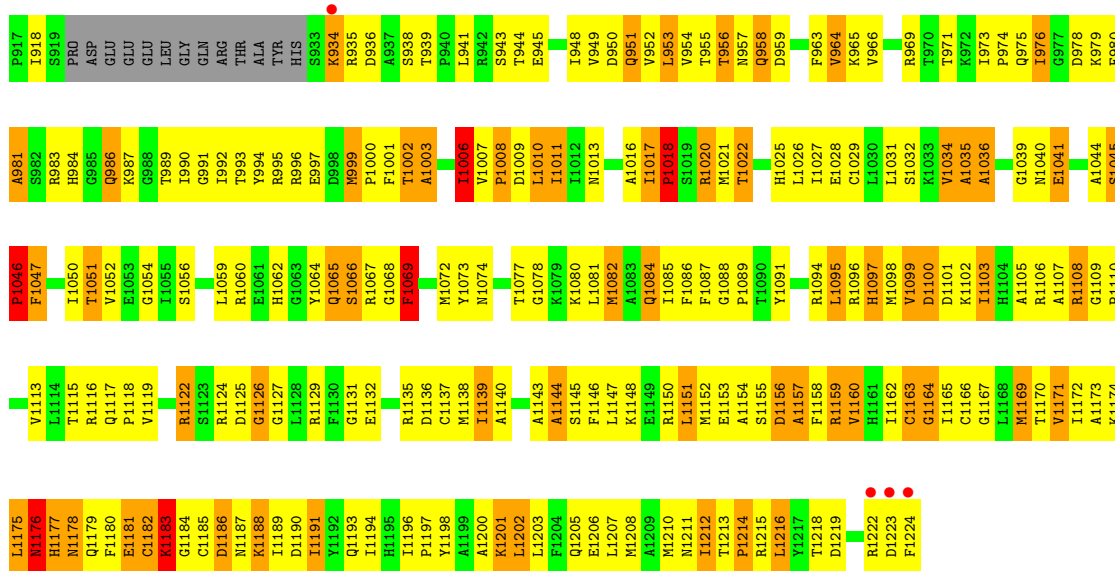
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT



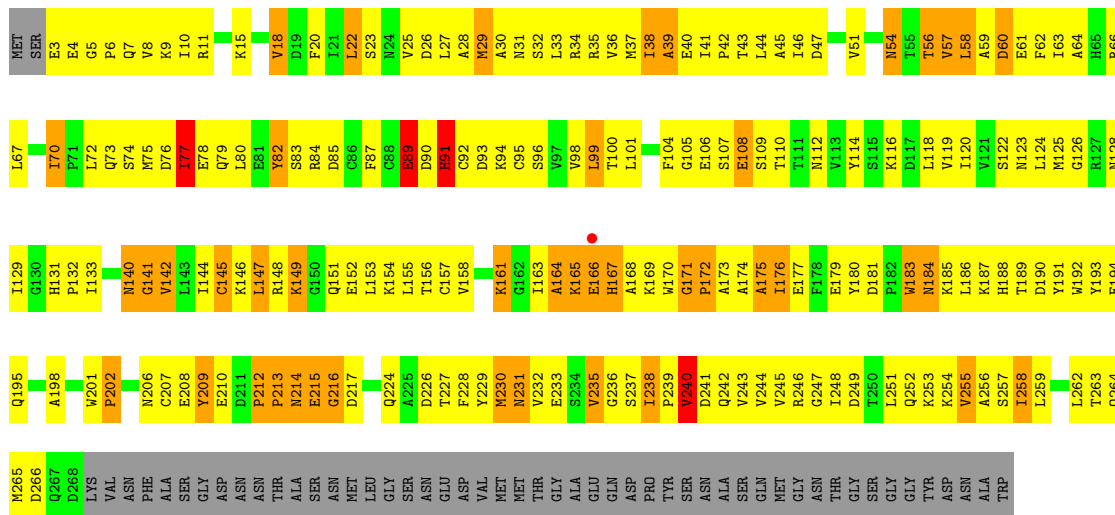
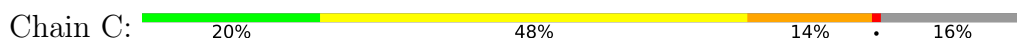


● Molecule 2: DNA-DIRECTED RNA POLYMERASE II SECOND LARGEST SUBUNIT

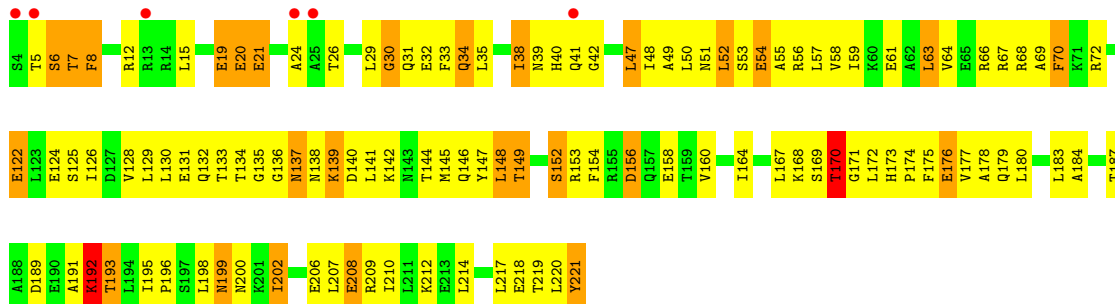




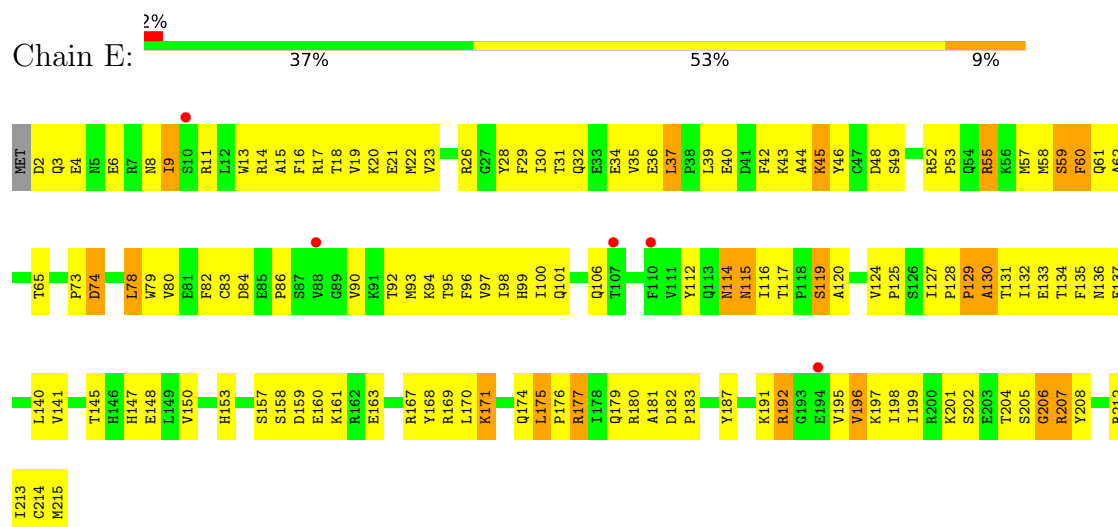
● Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45 KDA POLYPEPTIDE



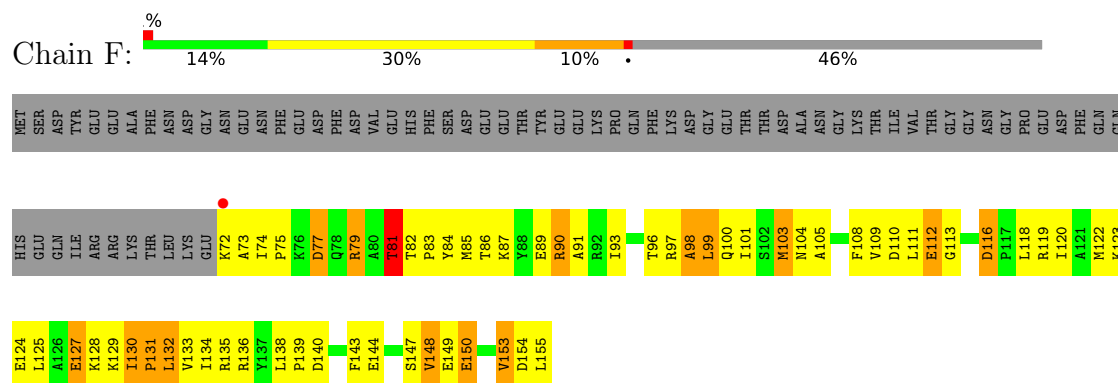
● Molecule 4: DNA-DIRECTED RNA POLYMERASE II 32 KDA POLYPEPTIDE



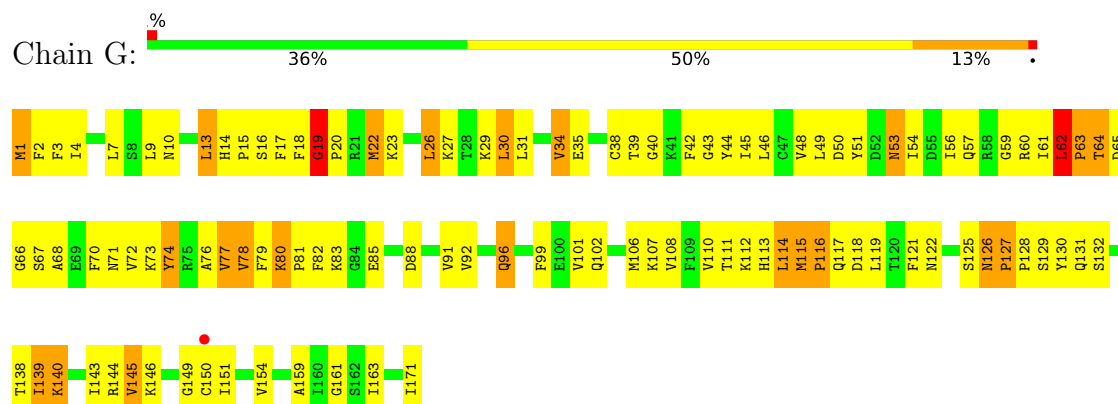
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE



• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE

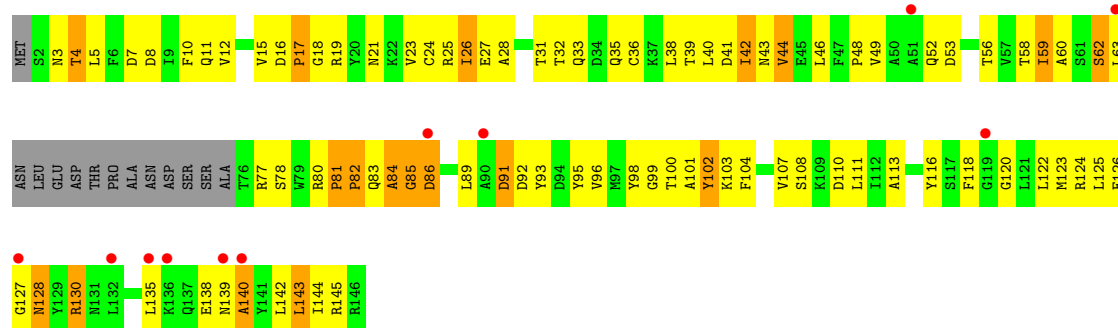


• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 19 KD POLYPEPTIDE

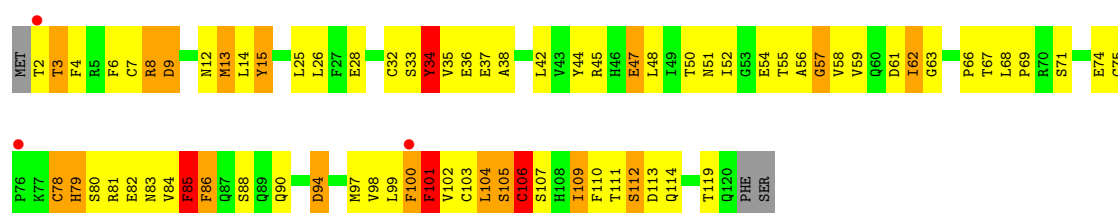


• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE

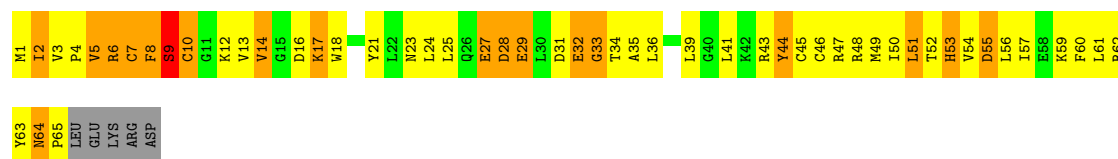
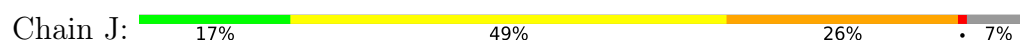




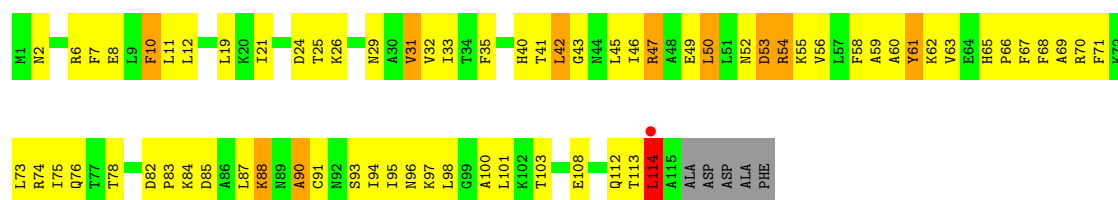
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II 14.2 KDA POLYPEPTIDE



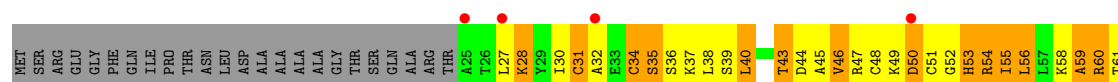
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II AND III 8.3 KDA POLYPEPTIDE



• Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE



• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE



K62	R63	L64	V65	Q66	F67	E68	A69	R70
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.72Å 395.13Å 284.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.80) 99.2 (50.00-3.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.257 , 0.285 0.211 , 0.245	Depositor DCC
R_{free} test set	2439 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	116.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 86.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.021 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30945	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	2/11339 (0.0%)	1.11	89/15334 (0.6%)
2	B	0.55	0/8890	1.04	61/11990 (0.5%)
3	C	0.62	0/2133	1.13	14/2891 (0.5%)
4	D	0.52	0/1365	1.17	13/1837 (0.7%)
5	E	0.48	0/1788	0.99	10/2406 (0.4%)
6	F	0.67	0/691	1.21	10/933 (1.1%)
7	G	0.61	0/1368	1.13	16/1844 (0.9%)
8	H	0.46	0/1086	1.03	7/1470 (0.5%)
9	I	0.58	0/989	1.16	10/1331 (0.8%)
10	J	0.61	0/541	1.12	2/727 (0.3%)
11	K	0.58	1/938 (0.1%)	1.03	3/1267 (0.2%)
12	L	0.68	0/365	1.07	2/485 (0.4%)
All	All	0.57	3/31493 (0.0%)	1.09	237/42515 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	C	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	999	VAL	CA-CB	-5.44	1.50	1.55
11	K	114	LEU	C-N	-5.33	1.25	1.33
1	A	250	ILE	CA-CB	5.04	1.61	1.54

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1185	CYS	N-CA-C	-13.57	96.69	113.38
4	D	54	GLU	N-CA-C	-13.25	97.61	114.04
1	A	452	LYS	N-CA-C	-13.20	96.94	111.07
4	D	26	THR	N-CA-C	-10.66	97.91	112.94
1	A	344	ARG	N-CA-C	-9.76	97.37	110.55
9	I	104	LEU	N-CA-C	-9.59	100.34	112.90
3	C	258	ILE	N-CA-C	-8.93	104.13	111.81
1	A	567	LYS	CA-C-N	-8.73	108.92	119.84
1	A	567	LYS	C-N-CA	-8.73	108.92	119.84
6	F	127	GLU	N-CA-C	-8.64	102.05	112.59
7	G	62	LEU	CA-C-N	-8.51	109.21	119.84
7	G	62	LEU	C-N-CA	-8.51	109.21	119.84
4	D	171	GLY	N-CA-C	-8.45	103.66	115.32
3	C	39	ALA	N-CA-C	8.43	123.70	113.41
4	D	7	THR	N-CA-C	8.24	124.90	107.67
1	A	1261	LYS	N-CA-C	-8.24	105.23	114.62
1	A	320	ARG	CA-C-N	8.03	129.88	119.84
1	A	320	ARG	C-N-CA	8.03	129.88	119.84
1	A	582	ILE	CA-C-N	7.94	127.87	119.85
1	A	582	ILE	C-N-CA	7.94	127.87	119.85
3	C	38	ILE	N-CA-C	7.83	117.94	110.42
1	A	982	THR	N-CA-C	-7.69	99.66	110.50
1	A	466	SER	N-CA-C	7.66	122.38	112.26
1	A	928	LEU	N-CA-C	-7.61	102.67	110.97
1	A	1262	LYS	N-CA-C	-7.61	102.99	111.82
7	G	30	LEU	N-CA-C	-7.59	102.69	110.97
2	B	395	GLN	N-CA-C	-7.58	100.53	110.53
1	A	1422	ARG	N-CA-C	-7.53	103.65	114.12
1	A	564	ALA	N-CA-C	-7.53	103.00	111.14
1	A	288	ALA	N-CA-C	-7.51	102.03	113.89
3	C	40	GLU	N-CA-C	7.44	121.66	112.59
8	H	80	ARG	CA-C-N	7.38	127.98	120.38
8	H	80	ARG	C-N-CA	7.38	127.98	120.38
2	B	1020	ARG	N-CA-C	-7.35	103.35	111.36
2	B	1052	VAL	N-CA-C	-7.30	103.74	110.82
6	F	130	ILE	CA-C-N	7.17	128.80	119.84
6	F	130	ILE	C-N-CA	7.17	128.80	119.84
1	A	440	ASP	N-CA-C	-7.16	100.63	109.65
1	A	729	ALA	N-CA-C	-7.16	103.56	111.36
1	A	454	SER	N-CA-C	-7.15	104.42	113.01
7	G	22	MET	N-CA-C	-7.13	103.19	112.68
1	A	293	GLU	N-CA-C	-7.09	104.67	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	LEU	N-CA-C	-7.03	102.83	111.40
5	E	171	LYS	N-CA-C	-7.01	99.56	110.42
4	D	55	ALA	N-CA-C	-6.99	103.09	111.69
4	D	72	ARG	N-CA-C	-6.98	104.73	113.18
2	B	681	TRP	N-CA-C	-6.97	100.90	111.56
2	B	882	THR	N-CA-C	6.96	119.52	111.02
1	A	539	THR	N-CA-C	6.95	119.44	108.67
2	B	296	GLU	N-CA-C	-6.95	103.47	112.23
1	A	1403	GLU	N-CA-C	6.92	125.53	110.80
4	D	38	ILE	N-CA-C	6.90	117.83	108.17
1	A	950	GLY	N-CA-C	-6.87	105.58	115.27
1	A	1291	VAL	CA-C-N	6.86	128.42	119.84
1	A	1291	VAL	C-N-CA	6.86	128.42	119.84
1	A	291	GLU	N-CA-C	-6.84	105.22	113.97
1	A	425	GLN	N-CA-C	-6.83	98.07	109.07
7	G	129	SER	N-CA-C	6.79	118.11	108.74
4	D	34	GLN	N-CA-C	-6.75	101.81	110.19
1	A	472	LEU	N-CA-C	6.69	118.37	111.14
1	A	738	LYS	N-CA-C	6.67	119.17	110.43
2	B	208	SER	N-CA-C	6.67	119.91	110.50
1	A	1311	VAL	N-CA-C	6.67	118.72	107.18
9	I	112	SER	N-CA-C	-6.63	103.51	112.26
10	J	10	CYS	CA-CB-SG	6.60	129.59	114.40
1	A	30	ILE	N-CA-C	6.56	117.24	110.36
6	F	77	ASP	N-CA-C	-6.55	100.28	110.17
2	B	66	ASP	N-CA-C	-6.54	104.61	112.59
2	B	1151	LEU	N-CA-C	6.49	119.35	111.82
2	B	1173	ALA	N-CA-C	6.47	118.47	109.15
2	B	535	LEU	N-CA-C	-6.47	105.51	113.41
1	A	1138	ILE	CB-CA-C	-6.47	106.21	111.71
1	A	453	MET	N-CA-C	6.45	120.61	112.87
2	B	1009	ASP	N-CA-C	-6.45	105.95	113.88
1	A	1434	ALA	CA-C-N	6.44	127.89	119.84
1	A	1434	ALA	C-N-CA	6.44	127.89	119.84
2	B	292	ILE	N-CA-C	6.44	122.79	108.88
1	A	227	VAL	N-CA-C	6.43	117.34	111.81
1	A	1010	ALA	N-CA-C	-6.41	104.34	111.71
1	A	158	PRO	N-CA-C	-6.39	106.16	114.03
4	D	173	HIS	CA-C-N	6.39	127.83	119.84
4	D	173	HIS	C-N-CA	6.39	127.83	119.84
3	C	165	LYS	N-CA-C	-6.37	102.86	112.04
2	B	872	GLU	N-CA-C	-6.37	102.32	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	363	HIS	N-CA-C	-6.36	101.57	110.35
1	A	360	GLU	N-CA-C	-6.35	102.60	110.41
1	A	337	ARG	N-CA-C	6.33	119.16	111.82
1	A	311	GLN	N-CA-C	6.24	123.61	109.81
1	A	242	PRO	CA-C-N	6.21	126.78	120.38
1	A	242	PRO	C-N-CA	6.21	126.78	120.38
1	A	689	LYS	N-CA-C	-6.21	104.96	112.54
1	A	1413	GLY	N-CA-C	-6.20	106.98	114.66
4	D	8	PHE	N-CA-C	6.18	123.97	110.80
1	A	998	LEU	N-CA-C	6.18	119.59	109.76
5	E	9	ILE	N-CA-C	-6.17	105.81	111.67
1	A	511	ILE	N-CA-C	6.15	117.63	110.62
1	A	199	LEU	N-CA-C	6.12	118.26	108.41
9	I	109	ILE	N-CA-C	6.10	115.13	106.53
12	L	31	CYS	N-CA-C	-6.09	100.83	109.96
1	A	398	GLU	N-CA-C	-6.08	102.92	110.41
5	E	32	GLN	N-CA-C	-6.07	105.36	112.89
2	B	112	LEU	N-CA-C	6.02	119.38	110.48
7	G	64	THR	N-CA-C	-6.01	105.86	113.43
8	H	4	THR	N-CA-C	-6.01	100.20	109.52
1	A	1445	ILE	CB-CA-C	-5.97	104.18	111.88
1	A	56	PRO	N-CA-C	-5.97	100.18	112.47
2	B	805	THR	N-CA-C	5.95	117.25	108.86
2	B	555	ILE	N-CA-C	-5.95	105.05	110.82
1	A	424	ILE	N-CA-C	5.91	121.63	109.34
9	I	79	HIS	N-CA-C	5.88	119.76	112.47
2	B	1201	LYS	N-CA-C	-5.87	103.86	111.02
11	K	8	GLU	N-CA-C	-5.86	106.36	112.93
1	A	415	LEU	N-CA-C	5.84	119.23	111.75
9	I	81	ARG	N-CA-C	5.84	118.35	110.88
2	B	1177	HIS	N-CA-C	-5.83	106.40	112.93
4	D	170	THR	N-CA-C	5.82	117.70	111.36
2	B	687	GLU	N-CA-C	-5.82	104.85	112.41
1	A	1021	LEU	N-CA-C	-5.82	104.85	111.07
10	J	5	VAL	N-CA-C	-5.81	102.08	109.58
2	B	1078	GLY	N-CA-C	-5.81	106.97	115.63
2	B	1163	CYS	N-CA-C	-5.81	100.24	109.59
1	A	562	THR	CA-C-N	5.79	127.08	119.84
1	A	562	THR	C-N-CA	5.79	127.08	119.84
2	B	428	ILE	N-CA-C	-5.78	103.86	111.09
1	A	1098	VAL	CB-CA-C	-5.76	108.23	113.70
1	A	663	SER	N-CA-C	5.73	115.41	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1045	SER	CA-C-N	5.72	126.99	119.84
2	B	1045	SER	C-N-CA	5.72	126.99	119.84
5	E	177	ARG	N-CA-C	5.72	119.01	110.14
9	I	85	PHE	N-CA-C	5.72	118.88	110.59
1	A	683	ILE	N-CA-C	-5.70	105.29	110.82
9	I	105	SER	N-CA-C	5.70	120.00	112.25
2	B	1164	GLY	N-CA-C	-5.68	107.88	115.32
1	A	1444	MET	N-CA-C	5.67	118.31	109.52
2	B	840	ILE	N-CA-C	-5.67	99.58	107.80
2	B	1129	ARG	N-CA-C	5.67	119.48	109.96
1	A	173	THR	N-CA-C	-5.66	103.06	110.53
2	B	934	LYS	N-CA-C	5.64	118.46	108.24
6	F	120	ILE	N-CA-C	-5.64	105.03	110.72
5	E	65	THR	N-CA-C	-5.64	102.14	110.48
1	A	467	THR	N-CA-C	5.64	118.65	109.24
3	C	183	TRP	N-CA-C	-5.64	98.01	107.99
4	D	176	GLU	N-CA-C	-5.62	104.54	111.40
8	H	16	ASP	N-CA-C	5.61	119.41	107.91
2	B	763	GLN	N-CA-C	-5.61	101.75	110.10
7	G	2	PHE	N-CA-C	-5.57	102.65	110.50
2	B	609	ILE	N-CA-C	-5.55	99.75	107.80
2	B	378	LEU	N-CA-C	-5.54	105.14	112.34
6	F	105	ALA	N-CA-C	-5.53	102.09	110.39
2	B	1036	ALA	N-CA-C	-5.53	105.65	112.90
2	B	558	LEU	N-CA-C	5.53	116.99	110.97
3	C	96	SER	N-CA-C	5.53	117.47	109.07
1	A	513	SER	CA-C-N	5.50	125.20	119.64
1	A	513	SER	C-N-CA	5.50	125.20	119.64
1	A	553	VAL	CA-C-N	5.50	125.17	119.56
1	A	553	VAL	C-N-CA	5.50	125.17	119.56
2	B	1139	ILE	N-CA-C	-5.49	105.18	110.72
1	A	637	LYS	N-CA-C	5.47	117.32	111.36
1	A	710	LEU	N-CA-C	-5.46	105.43	111.71
1	A	507	VAL	CB-CA-C	-5.44	108.53	113.70
8	H	12	VAL	N-CA-C	5.40	115.35	108.12
2	B	213	ILE	N-CA-C	5.39	117.06	108.87
1	A	778	GLY	N-CA-C	-5.38	105.88	112.77
8	H	42	ILE	N-CA-C	5.38	115.45	108.35
8	H	85	GLY	N-CA-C	-5.38	108.43	114.40
5	E	119	SER	N-CA-C	-5.37	105.86	112.90
11	K	31	VAL	N-CA-C	5.37	116.43	108.65
2	B	616	ILE	N-CA-C	5.36	115.83	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1213	THR	N-CA-C	5.36	117.18	109.04
7	G	114	LEU	N-CA-C	-5.33	106.46	113.17
2	B	1008	PRO	N-CA-C	5.32	119.06	111.13
1	A	999	VAL	N-CA-C	-5.32	106.48	111.48
7	G	65	ASP	N-CA-C	-5.32	102.30	109.95
7	G	140	LYS	N-CA-C	5.31	119.38	113.01
1	A	55	ASP	N-CA-C	5.30	121.52	109.81
2	B	650	GLU	N-CA-C	5.30	116.58	108.52
6	F	153	VAL	N-CA-C	5.27	113.97	106.53
1	A	60	SER	N-CA-C	5.27	114.99	108.19
7	G	40	GLY	N-CA-C	-5.24	108.16	114.66
1	A	67	CYS	N-CA-C	-5.24	99.64	110.80
2	B	1066	SER	N-CA-C	5.24	119.29	113.01
6	F	112	GLU	N-CA-C	-5.23	106.16	113.37
1	A	1299	VAL	N-CA-C	5.22	117.56	108.95
3	C	91	HIS	N-CA-C	5.21	121.91	110.80
9	I	101	PHE	CA-C-N	-5.21	115.94	123.03
9	I	101	PHE	C-N-CA	-5.21	115.94	123.03
1	A	229	SER	N-CA-C	5.20	115.90	107.32
2	B	628	THR	N-CA-C	-5.20	107.59	114.04
9	I	119	THR	N-CA-C	-5.20	107.32	113.97
2	B	424	LEU	N-CA-C	-5.19	104.56	112.04
1	A	685	GLU	N-CA-C	-5.18	105.81	111.82
1	A	1102	LYS	N-CA-C	-5.18	105.53	111.07
2	B	944	THR	N-CA-C	5.17	117.71	111.40
2	B	606	LYS	N-CA-C	-5.17	107.63	114.04
3	C	148	ARG	N-CA-C	5.17	121.80	110.80
11	K	19	LEU	N-CA-C	5.16	118.00	109.85
1	A	294	SER	N-CA-C	-5.16	105.35	111.69
3	C	193	TYR	N-CA-C	5.15	115.09	108.34
7	G	19	GLY	CA-C-N	5.15	126.28	119.84
7	G	19	GLY	C-N-CA	5.15	126.28	119.84
2	B	964	VAL	N-CA-C	5.15	115.69	108.17
5	E	55	ARG	N-CA-C	5.14	116.57	111.07
2	B	99	LYS	CA-C-N	5.14	126.26	119.84
2	B	99	LYS	C-N-CA	5.14	126.26	119.84
2	B	1113	VAL	CB-CA-C	-5.14	106.37	111.30
7	G	127	PRO	CA-C-N	5.14	125.14	119.90
7	G	127	PRO	C-N-CA	5.14	125.14	119.90
1	A	227	VAL	CB-CA-C	-5.13	105.65	111.55
1	A	990	VAL	N-CA-C	-5.12	105.39	110.62
6	F	108	PHE	N-CA-C	5.12	119.24	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	981	ALA	N-CA-C	5.11	116.29	108.52
1	A	491	VAL	CA-C-N	5.11	126.22	119.84
1	A	491	VAL	C-N-CA	5.11	126.22	119.84
2	B	774	GLY	N-CA-C	-5.11	108.73	114.40
2	B	871	THR	N-CA-C	5.10	117.76	109.24
1	A	1333	ILE	N-CA-C	-5.09	105.02	110.36
3	C	70	ILE	CA-C-N	5.08	125.00	119.76
3	C	70	ILE	C-N-CA	5.08	125.00	119.76
5	E	52	ARG	CA-C-N	5.08	125.23	119.90
5	E	52	ARG	C-N-CA	5.08	125.23	119.90
2	B	693	ILE	N-CA-C	5.07	115.07	107.51
12	L	34	CYS	N-CA-C	-5.07	107.25	112.93
2	B	277	LYS	N-CA-C	5.07	117.54	111.71
2	B	526	GLU	N-CA-C	5.06	116.90	107.99
2	B	825	VAL	N-CA-C	5.06	115.93	110.21
3	C	235	VAL	N-CA-C	-5.06	106.75	111.45
1	A	222	LEU	N-CA-C	-5.05	102.29	110.32
1	A	1310	GLY	N-CA-C	-5.05	102.18	110.56
3	C	38	ILE	CB-CA-C	-5.05	105.50	111.97
2	B	361	LEU	CA-C-N	5.04	126.14	119.84
2	B	361	LEU	C-N-CA	5.04	126.14	119.84
2	B	69	LEU	N-CA-C	5.03	116.32	109.18
6	F	98	ALA	N-CA-C	-5.03	105.49	110.97
7	G	145	VAL	N-CA-C	5.02	116.52	108.89
5	E	6	GLU	N-CA-C	-5.01	106.26	112.38
1	A	134	ARG	N-CA-C	-5.00	107.01	113.01
1	A	237	THR	N-CA-C	-5.00	108.92	114.62

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	TYR	Sidechain
3	C	82	TYR	Sidechain

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	11140	0	11217	1296	0
2	B	8720	0	8745	996	0
3	C	2095	0	2051	258	0
4	D	1356	0	1319	125	0
5	E	1752	0	1776	161	0
6	F	679	0	701	86	0
7	G	1340	0	1357	156	0
8	H	1068	0	1040	107	0
9	I	971	0	927	102	0
10	J	532	0	542	101	0
11	K	920	0	929	92	0
12	L	363	0	386	47	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	30945	0	30990	3237	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 52.

All (3237) 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:77:CYS:O	1:A:78:PRO:O	1.65	1.14
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.30	1.11
7:G:138:THR:HG22	7:G:139:ILE:H	1.12	1.09
1:A:53:LEU:HD23	1:A:54:ASN:N	1.69	1.06
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.69	1.06
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.33	1.04
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.37	1.04
8:H:100:THR:HG23	8:H:138:GLU:HA	1.37	1.03
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.21	1.03
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.40	1.03
1:A:855:THR:HG21	1:A:857:ARG:HE	1.22	1.02
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.23	1.02
7:G:15:PRO:HA	7:G:18:PHE:CD1	1.96	1.00
2:B:549:THR:HG22	2:B:550:ASP:H	1.24	0.99
2:B:65:GLU:HG3	2:B:66:ASP:H	1.27	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:806:THR:HG22	2:B:808:ALA:H	1.27	0.98
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.26	0.98
9:I:85:PHE:H	9:I:85:PHE:HD2	1.06	0.98
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.46	0.97
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.00	0.97
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.42	0.97
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.28	0.97
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.45	0.97
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.00	0.97
1:A:1329:THR:HG22	1:A:1331:SER:H	1.30	0.95
1:A:754:SER:H	1:A:757:ASN:HD22	1.11	0.95
1:A:77:CYS:O	1:A:77:CYS:SG	2.24	0.95
2:B:46:GLN:HG3	2:B:47:GLN:H	1.28	0.95
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.45	0.95
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.31	0.95
3:C:142:VAL:H	10:J:16:ASP:HB3	1.31	0.95
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.47	0.95
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.32	0.94
4:D:47:LEU:HD13	4:D:48:ILE:H	1.31	0.94
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.50	0.94
1:A:709:THR:HG22	1:A:711:ARG:H	1.32	0.93
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.50	0.93
1:A:53:LEU:HD23	1:A:54:ASN:H	1.26	0.93
8:H:4:THR:HA	8:H:60:ALA:HB2	1.52	0.92
9:I:34:TYR:HD2	9:I:35:VAL:N	1.67	0.92
1:A:901:LEU:H	1:A:926:GLN:NE2	1.67	0.92
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.50	0.92
1:A:40:THR:HG22	1:A:41:MET:HG3	1.52	0.92
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.50	0.92
6:F:81:THR:HG21	6:F:136:ARG:HD3	1.52	0.91
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.51	0.91
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.31	0.91
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.52	0.91
2:B:999:MET:HA	2:B:999:MET:HE3	1.52	0.90
1:A:55:ASP:C	1:A:57:ARG:H	1.72	0.90
4:D:134:THR:HG22	4:D:136:GLY:H	1.36	0.90
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.53	0.90
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.72	0.89
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.54	0.89
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.38	0.89
1:A:524:VAL:HG12	1:A:525:GLN:H	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.03	0.89
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.54	0.89
11:K:65:HIS:HD2	11:K:67:PHE:H	1.21	0.88
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.55	0.88
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.04	0.88
2:B:98:THR:O	2:B:126:SER:HB2	1.73	0.88
2:B:806:THR:N	2:B:809:MET:HE3	1.89	0.87
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.04	0.87
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.56	0.87
9:I:34:TYR:CD2	9:I:35:VAL:N	2.42	0.87
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.75	0.87
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.53	0.86
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.39	0.86
1:A:903:ASN:HD22	1:A:904:THR:N	1.73	0.86
9:I:75:CYS:SG	9:I:79:HIS:N	2.49	0.86
4:D:40:HIS:HB3	7:G:73:LYS:HZ1	1.38	0.86
4:D:144:THR:O	4:D:148:LEU:HB2	1.75	0.86
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.57	0.86
2:B:589:VAL:HG12	2:B:590:HIS:H	1.40	0.86
7:G:1:MET:SD	7:G:79:PHE:CD1	2.69	0.86
1:A:56:PRO:O	1:A:57:ARG:HG3	1.76	0.86
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.58	0.86
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.41	0.86
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.38	0.86
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.75	0.85
2:B:168:GLY:H	2:B:450:ALA:HB1	1.38	0.85
3:C:33:LEU:HG	3:C:37:MET:HE2	1.56	0.85
3:C:164:ALA:HA	3:C:167:HIS:O	1.76	0.85
3:C:20:PHE:HE1	3:C:22:LEU:HD12	1.42	0.85
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.58	0.85
2:B:1224:PHE:HE2	5:E:171:LYS:HG3	1.40	0.85
3:C:47:ASP:HA	12:L:69:ALA:CB	2.06	0.85
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.57	0.85
2:B:515:HIS:H	2:B:518:HIS:HD2	1.19	0.85
2:B:705:MET:H	2:B:710:LEU:HD12	1.42	0.85
7:G:1:MET:SD	7:G:79:PHE:HD1	2.00	0.84
2:B:955:THR:HG23	12:L:54:ARG:O	1.77	0.84
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.58	0.84
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.58	0.84
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.13	0.84
5:E:19:VAL:O	5:E:23:VAL:HG23	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:THR:HG22	2:B:884:ARG:H	1.44	0.83
1:A:70:CYS:O	1:A:72:GLU:HG2	1.76	0.83
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.60	0.83
3:C:213:PRO:O	3:C:214:ASN:HB2	1.76	0.83
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.58	0.83
2:B:363:HIS:O	2:B:364:ILE:HB	1.77	0.83
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.61	0.83
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.08	0.83
2:B:842:ASN:ND2	2:B:845:SER:H	1.77	0.83
1:A:1329:THR:HG22	1:A:1331:SER:N	1.93	0.83
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.08	0.83
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.61	0.83
8:H:23:VAL:HG22	8:H:43:ASN:HA	1.61	0.83
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.61	0.82
2:B:847:ASP:HB3	3:C:167:HIS:HE2	1.45	0.82
3:C:66:ARG:NH2	10:J:5:VAL:HG23	1.94	0.82
1:A:605:MET:HE2	1:A:607:ILE:HG13	1.61	0.82
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.15	0.82
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	1.94	0.82
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.61	0.82
4:D:130:LEU:C	4:D:132:GLN:H	1.86	0.81
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.45	0.81
7:G:128:PRO:O	7:G:138:THR:HG23	1.78	0.81
1:A:438:ASP:O	1:A:439:ASN:HB2	1.78	0.81
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.25	0.81
2:B:35:SER:HA	2:B:811:TYR:HE2	1.45	0.81
2:B:847:ASP:HB3	3:C:167:HIS:NE2	1.95	0.81
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.79	0.81
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.60	0.81
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.13	0.81
3:C:43:THR:HG22	3:C:44:LEU:N	1.93	0.81
5:E:22:MET:HE3	5:E:26:ARG:HE	1.45	0.81
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.60	0.81
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.63	0.81
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.63	0.81
1:A:709:THR:HG23	9:I:94:ASP:HA	1.63	0.81
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.63	0.81
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.61	0.81
1:A:534:LEU:O	1:A:574:GLY:HA3	1.81	0.81
3:C:98:VAL:C	3:C:99:LEU:HD23	2.05	0.81
3:C:56:THR:HG22	3:C:57:VAL:H	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.64	0.80
1:A:567:LYS:NZ	8:H:46:LEU:HB2	1.96	0.80
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.63	0.80
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.27	0.80
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.62	0.80
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.21	0.80
4:D:170:THR:CG2	4:D:172:LEU:HG	2.11	0.80
1:A:249:SER:O	1:A:250:ILE:HG13	1.81	0.80
1:A:344:ARG:HD2	2:B:1118:PRO:O	1.82	0.80
1:A:1422:ARG:HH22	2:B:1224:PHE:C	1.90	0.80
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	1.80	0.80
7:G:138:THR:HG22	7:G:139:ILE:N	1.92	0.80
1:A:76:GLU:HG3	1:A:76:GLU:O	1.81	0.80
1:A:741:ASN:HD22	1:A:744:LYS:H	1.26	0.80
2:B:401:PHE:HA	2:B:404:LYS:HG3	1.61	0.80
3:C:32:SER:O	3:C:36:VAL:HG23	1.82	0.80
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.63	0.80
2:B:918:ILE:HB	2:B:935:ARG:HD2	1.62	0.80
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.12	0.80
2:B:1162:ILE:HG22	2:B:1163:CYS:H	1.47	0.80
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.62	0.79
2:B:515:HIS:HD2	2:B:517:THR:H	1.27	0.79
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.63	0.79
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.62	0.79
5:E:29:PHE:O	5:E:30:ILE:HG13	1.82	0.79
1:A:67:CYS:O	1:A:70:CYS:HB3	1.82	0.79
3:C:22:LEU:HD13	3:C:230:MET:HE3	1.64	0.79
6:F:111:LEU:C	6:F:113:GLY:H	1.90	0.79
2:B:25:ILE:HD11	2:B:653:VAL:O	1.82	0.79
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.64	0.79
3:C:262:LEU:HD11	11:K:87:LEU:HD23	1.62	0.79
11:K:113:THR:O	11:K:114:LEU:HB2	1.81	0.79
1:A:356:ASP:HB2	1:A:469:ARG:NH1	1.97	0.79
3:C:43:THR:HG22	3:C:44:LEU:H	1.48	0.79
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.62	0.78
2:B:465:ASN:HD22	2:B:465:ASN:N	1.78	0.78
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.64	0.78
1:A:855:THR:HG21	1:A:857:ARG:NE	1.97	0.78
1:A:1336:MET:HE3	1:A:1381:LEU:HG	1.65	0.78
4:D:153:ARG:NH2	4:D:184:ALA:HA	1.98	0.78
1:A:858:ASN:ND2	1:A:860:LEU:H	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.18	0.78
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.64	0.78
2:B:1065:GLN:HE21	2:B:1066:SER:N	1.82	0.78
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.30	0.78
1:A:340:LEU:HD21	2:B:1200:ALA:N	1.99	0.78
8:H:102:TYR:OH	8:H:122:LEU:HD22	1.82	0.78
1:A:265:LYS:HZ3	1:A:322:VAL:HG13	1.49	0.78
2:B:778:MET:HE2	2:B:1094:ARG:HG2	1.67	0.77
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.48	0.77
5:E:175:LEU:HD23	5:E:176:PRO:HD2	1.66	0.77
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.47	0.77
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.65	0.77
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.64	0.77
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.49	0.77
1:A:1341:ILE:HG23	1:A:1342:GLU:N	1.98	0.77
2:B:613:VAL:HG13	2:B:627:PHE:O	1.85	0.77
1:A:388:LEU:O	1:A:392:VAL:HG23	1.85	0.77
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.65	0.77
2:B:1034:VAL:HG12	2:B:1035:ALA:N	1.98	0.77
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.67	0.77
2:B:955:THR:HG22	2:B:956:THR:N	2.00	0.77
7:G:81:PRO:HG3	7:G:106:MET:SD	2.25	0.77
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.67	0.77
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.67	0.77
1:A:1116:LEU:N	1:A:1308:THR:HG22	2.00	0.77
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.67	0.76
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.66	0.76
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.65	0.76
2:B:863:GLU:OE2	2:B:873:THR:HA	1.85	0.76
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.50	0.76
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.67	0.76
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.67	0.76
1:A:590:ARG:HG3	1:A:590:ARG:NH1	2.00	0.76
5:E:117:THR:HG22	5:E:119:SER:H	1.50	0.76
1:A:598:LEU:HD22	8:H:25:ARG:NH1	2.01	0.76
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.19	0.76
1:A:1341:ILE:HD12	1:A:1379:GLY:O	1.85	0.76
2:B:37:PHE:CD1	2:B:41:LYS:HG3	2.20	0.76
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.67	0.76
1:A:528:LEU:O	1:A:531:ILE:HG22	1.86	0.76
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:LEU:O	1:A:606:LEU:HA	1.85	0.76
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.68	0.76
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.49	0.76
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.21	0.75
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.51	0.75
1:A:560:ILE:HG13	8:H:78:SER:HB2	1.68	0.75
2:B:1069:PHE:H	2:B:1069:PHE:HD1	1.34	0.75
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.68	0.75
1:A:91:PHE:HB2	1:A:297:GLN:NE2	2.02	0.75
5:E:90:VAL:HG23	5:E:120:ALA:HA	1.69	0.75
11:K:46:ILE:O	11:K:50:LEU:HB2	1.85	0.75
2:B:879:ARG:HH11	2:B:883:LEU:HD22	1.50	0.75
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.21	0.75
2:B:37:PHE:HE2	2:B:542:MET:HA	1.52	0.75
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.68	0.75
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.69	0.74
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.69	0.74
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.22	0.74
7:G:43:GLY:HA3	7:G:80:LYS:HB3	1.68	0.74
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.67	0.74
1:A:230:ARG:H	1:A:233:TRP:HE3	1.34	0.74
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.17	0.74
2:B:806:THR:H	2:B:809:MET:HE3	1.50	0.74
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.84	0.74
1:A:68:GLN:C	1:A:70:CYS:H	1.95	0.74
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.69	0.74
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.21	0.74
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.18	0.74
1:A:1323:ASP:OD1	1:A:1325:THR:HB	1.88	0.74
2:B:801:LYS:O	10:J:52:THR:HG23	1.86	0.74
2:B:859:TYR:OH	2:B:941:LEU:HD12	1.86	0.74
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.68	0.74
12:L:48:CYS:HB3	12:L:51:CYS:O	1.88	0.74
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.70	0.74
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.88	0.74
2:B:978:ASP:OD2	2:B:1098:MET:HG2	1.88	0.74
4:D:66:ARG:HD2	4:D:133:THR:HB	1.68	0.74
5:E:2:ASP:O	5:E:3:GLN:HG2	1.87	0.74
1:A:590:ARG:NH2	1:A:620:LYS:HB3	2.01	0.74
1:A:1450:LEU:O	1:A:1450:LEU:HG	1.88	0.74
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.68	0.74
1:A:535:THR:HG21	1:A:616:VAL:HA	1.70	0.73
1:A:768:GLN:CG	1:A:816:HIS:HA	2.18	0.73
2:B:806:THR:HG22	2:B:808:ALA:N	2.03	0.73
2:B:955:THR:HG22	2:B:956:THR:H	1.53	0.73
2:B:1183:LYS:N	2:B:1183:LYS:HE3	2.03	0.73
1:A:253:ASN:HB3	2:B:935:ARG:NH2	2.03	0.73
1:A:254:GLU:HB2	2:B:935:ARG:HH12	1.52	0.73
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.24	0.73
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.18	0.73
1:A:1332:PHE:HD2	1:A:1332:PHE:N	1.86	0.73
5:E:202:SER:OG	5:E:204:THR:HG22	1.89	0.73
1:A:321:PRO:O	1:A:322:VAL:HB	1.88	0.73
5:E:192:ARG:HH11	5:E:192:ARG:HG3	1.51	0.73
5:E:213:ILE:HG12	5:E:214:CYS:H	1.54	0.73
8:H:59:ILE:HG22	8:H:60:ALA:N	2.02	0.73
2:B:408:LEU:HG	2:B:409:ALA:H	1.52	0.73
8:H:36:CYS:HA	8:H:126:GLU:O	1.89	0.73
1:A:164:ARG:HG3	1:A:165:GLY:H	1.52	0.73
1:A:754:SER:H	1:A:757:ASN:ND2	1.86	0.73
1:A:858:ASN:C	1:A:858:ASN:HD22	1.94	0.73
7:G:138:THR:CG2	7:G:139:ILE:H	1.95	0.73
1:A:853:ASP:OD1	1:A:855:THR:HB	1.89	0.73
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.69	0.73
12:L:30:ILE:O	12:L:56:LEU:HA	1.88	0.73
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.24	0.73
3:C:263:THR:C	3:C:265:MET:H	1.97	0.73
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.24	0.73
1:A:335:ARG:HH12	2:B:1202:LEU:HD13	1.54	0.72
2:B:871:THR:HG22	2:B:872:GLU:O	1.88	0.72
4:D:5:THR:O	4:D:6:SER:O	2.07	0.72
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.04	0.72
2:B:766:ARG:HH22	2:B:1020:ARG:HH11	1.37	0.72
3:C:73:GLN:HB3	3:C:131:HIS:H	1.55	0.72
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.04	0.72
2:B:378:LEU:HD12	2:B:378:LEU:O	1.88	0.72
2:B:516:ASN:HD22	2:B:516:ASN:N	1.87	0.72
2:B:616:ILE:HG13	2:B:697:GLU:HG3	1.70	0.72
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.18	0.72
2:B:411:PRO:O	2:B:414:ALA:HB3	1.88	0.72
1:A:475:THR:HG23	1:A:476:SER:N	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.20	0.72
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.05	0.72
2:B:1138:MET:HE2	2:B:1146:PHE:HD2	1.54	0.72
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.71	0.72
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.03	0.72
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.72	0.72
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.72	0.72
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.54	0.72
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.71	0.72
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.48	0.72
4:D:130:LEU:O	4:D:132:GLN:N	2.22	0.72
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.25	0.71
1:A:903:ASN:HD22	1:A:903:ASN:C	1.97	0.71
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.05	0.71
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.70	0.71
2:B:745:PRO:O	2:B:748:ILE:HG12	1.89	0.71
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.71	0.71
1:A:1114:PRO:O	1:A:1115:SER:O	2.06	0.71
1:A:808:LEU:HD23	1:A:813:PHE:HA	1.71	0.71
7:G:80:LYS:HD3	7:G:80:LYS:N	2.06	0.71
10:J:5:VAL:HG12	10:J:6:ARG:CG	2.15	0.71
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.72	0.71
1:A:1437:GLY:O	1:A:1439:GLY:N	2.23	0.71
3:C:175:ALA:O	3:C:176:ILE:HG13	1.90	0.71
6:F:138:LEU:HB3	6:F:139:PRO:HD2	1.72	0.71
1:A:1239:ARG:HH22	1:A:1241:ARG:NH2	1.88	0.71
1:A:746:MET:HE3	2:B:1018:PRO:HG2	1.73	0.71
1:A:1152:ILE:HG13	9:I:44:TYR:HB3	1.71	0.71
2:B:1099:VAL:O	2:B:1101:ASP:N	2.24	0.71
8:H:113:ALA:HB2	8:H:126:GLU:HG3	1.72	0.71
1:A:55:ASP:CG	1:A:55:ASP:O	2.32	0.70
1:A:75:ASN:O	1:A:76:GLU:HB3	1.91	0.70
1:A:164:ARG:HG3	1:A:165:GLY:N	2.04	0.70
2:B:365:THR:HG23	2:B:367:LEU:H	1.54	0.70
2:B:708:GLU:O	2:B:710:LEU:N	2.24	0.70
4:D:47:LEU:HD13	4:D:48:ILE:N	2.03	0.70
5:E:48:ASP:CG	5:E:49:SER:H	1.99	0.70
8:H:59:ILE:HG22	8:H:60:ALA:H	1.54	0.70
1:A:69:THR:C	1:A:71:GLN:H	1.98	0.70
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.54	0.70
1:A:384:ASN:OD1	1:A:388:LEU:HD12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.21	0.70
2:B:227:LYS:HB2	2:B:395:GLN:OE1	1.90	0.70
5:E:179:GLN:HB2	5:E:182:ASP:HB2	1.73	0.70
2:B:557:PHE:C	2:B:557:PHE:CD2	2.68	0.70
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.06	0.70
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.92	0.70
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.26	0.70
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.57	0.70
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.27	0.70
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.06	0.70
2:B:211:VAL:O	2:B:480:SER:HA	1.91	0.70
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.22	0.70
3:C:167:HIS:CE1	12:L:70:ARG:HB3	2.27	0.70
4:D:176:GLU:C	4:D:178:ALA:H	1.98	0.70
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.22	0.70
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.74	0.70
2:B:1006:ILE:HD13	10:J:44:TYR:CE2	2.26	0.70
1:A:384:ASN:CG	1:A:388:LEU:HD12	2.17	0.70
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.06	0.70
2:B:1182:CYS:C	2:B:1183:LYS:HE3	2.17	0.70
11:K:47:ARG:HB3	11:K:47:ARG:NH1	2.05	0.70
1:A:92:HIS:O	1:A:94:GLY:N	2.24	0.70
1:A:302:THR:HA	1:A:305:ASP:O	1.92	0.70
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.06	0.70
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.21	0.70
2:B:847:ASP:C	2:B:849:GLY:H	1.98	0.70
1:A:466:SER:O	2:B:1103:ILE:HD11	1.92	0.70
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.74	0.70
7:G:14:HIS:CD2	7:G:16:SER:HB2	2.27	0.70
7:G:18:PHE:HA	7:G:22:MET:CE	2.22	0.70
1:A:14:VAL:HG21	2:B:1216:LEU:HD13	1.75	0.69
1:A:913:LEU:HD12	1:A:914:GLU:N	2.05	0.69
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.74	0.69
5:E:22:MET:HE3	5:E:26:ARG:NE	2.06	0.69
8:H:40:LEU:HD22	8:H:123:MET:HE3	1.74	0.69
11:K:65:HIS:CD2	11:K:67:PHE:H	2.05	0.69
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.57	0.69
4:D:33:PHE:CE1	7:G:80:LYS:HE3	2.27	0.69
1:A:1445:ILE:HG12	7:G:18:PHE:CE2	2.27	0.69
2:B:770:GLN:CD	2:B:983:ARG:HA	2.16	0.69
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:HD22	1:A:228:PHE:H	1.39	0.69
2:B:642:ASP:O	2:B:644:GLU:N	2.22	0.69
4:D:48:ILE:CG2	7:G:4:ILE:HB	2.19	0.69
2:B:737:THR:HG21	9:I:66:PRO:HA	1.74	0.69
2:B:1087:PHE:HD2	2:B:1088:GLY:N	1.90	0.69
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.07	0.69
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.07	0.69
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.28	0.69
2:B:975:GLN:HG2	2:B:976:ILE:H	1.56	0.69
2:B:766:ARG:NH2	2:B:1020:ARG:HH11	1.90	0.69
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.22	0.69
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.74	0.69
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.75	0.69
9:I:71:SER:OG	9:I:83:ASN:HB2	1.92	0.69
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.75	0.69
2:B:654:ARG:H	2:B:657:HIS:HD2	1.39	0.69
2:B:728:ARG:HH12	2:B:1047:PHE:HB3	1.57	0.69
2:B:953:LEU:HD23	2:B:953:LEU:O	1.92	0.69
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.74	0.69
3:C:20:PHE:CE1	3:C:22:LEU:HD12	2.25	0.69
4:D:170:THR:HG21	4:D:172:LEU:HG	1.74	0.69
6:F:82:THR:HG22	6:F:84:TYR:H	1.58	0.69
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.93	0.69
8:H:4:THR:HA	8:H:60:ALA:CB	2.22	0.69
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.73	0.69
1:A:844:ALA:C	1:A:845:LEU:HD23	2.18	0.69
1:A:1120:LEU:O	1:A:1323:ASP:HB2	1.93	0.69
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.74	0.69
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.92	0.69
1:A:78:PRO:HA	2:B:1201:LYS:NZ	2.08	0.69
1:A:1329:THR:CG2	1:A:1331:SER:H	2.03	0.69
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.74	0.69
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.21	0.69
1:A:106:VAL:HG13	1:A:112:LYS:O	1.93	0.68
1:A:463:ILE:HD12	1:A:469:ARG:HD2	1.74	0.68
2:B:333:PHE:O	2:B:334:ILE:HG13	1.92	0.68
1:A:107:CYS:H	1:A:114:LEU:HD21	1.57	0.68
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.40	0.68
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.24	0.68
1:A:115:LEU:HB2	1:A:122:MET:HE2	1.76	0.68
1:A:248:PRO:O	1:A:260:ASP:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:HD12	1:A:667:GLY:H	1.57	0.68
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.74	0.68
3:C:172:PRO:O	3:C:235:VAL:HG23	1.93	0.68
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.74	0.68
8:H:89:LEU:C	8:H:91:ASP:H	2.02	0.68
9:I:111:THR:HG22	9:I:112:SER:N	2.09	0.68
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.24	0.68
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.75	0.68
2:B:65:GLU:HG3	2:B:66:ASP:N	2.05	0.68
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.75	0.68
6:F:97:ARG:O	6:F:101:ILE:HG13	1.93	0.68
1:A:35:ILE:HG22	1:A:35:ILE:O	1.93	0.68
1:A:450:LEU:HD12	1:A:450:LEU:N	2.09	0.68
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.75	0.68
1:A:856:THR:HB	1:A:865:GLN:HB2	1.75	0.68
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.76	0.68
12:L:38:LEU:O	12:L:39:SER:HB3	1.93	0.68
2:B:199:MET:HE2	2:B:492:LEU:HD23	1.76	0.68
1:A:19:PHE:O	1:A:1416:ALA:HA	1.93	0.68
1:A:107:CYS:N	1:A:114:LEU:HD21	2.08	0.68
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.08	0.68
1:A:675:THR:O	1:A:679:ILE:HG13	1.93	0.68
2:B:112:LEU:HD12	2:B:113:TYR:H	1.58	0.68
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.56	0.68
9:I:13:MET:HG3	9:I:14:LEU:N	2.09	0.68
1:A:809:THR:OG1	1:A:812:GLU:HG3	1.94	0.68
1:A:981:LEU:HD21	1:A:1038:THR:C	2.19	0.68
2:B:707:PRO:O	2:B:711:GLU:HG3	1.93	0.68
4:D:34:GLN:O	4:D:47:LEU:HD23	1.94	0.68
11:K:31:VAL:HG12	11:K:32:VAL:N	2.08	0.68
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.59	0.67
1:A:63:ARG:HA	1:A:74:MET:SD	2.35	0.67
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.75	0.67
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.28	0.67
2:B:549:THR:HG22	2:B:550:ASP:N	2.05	0.67
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.29	0.67
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.09	0.67
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.59	0.67
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.29	0.67
2:B:39:ARG:HH21	2:B:665:GLU:HG2	1.59	0.67
4:D:40:HIS:CB	7:G:73:LYS:HZ3	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:TYR:HB3	3:C:140:ASN:O	1.94	0.67
4:D:29:LEU:HD22	7:G:82:PHE:CE2	2.28	0.67
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.09	0.67
9:I:50:THR:HG22	9:I:52:ILE:H	1.60	0.67
1:A:55:ASP:C	1:A:57:ARG:N	2.41	0.67
2:B:217:ARG:HD2	2:B:217:ARG:C	2.19	0.67
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.77	0.67
2:B:1002:THR:HG23	2:B:1006:ILE:HG13	1.77	0.67
5:E:15:ALA:O	5:E:19:VAL:HG23	1.94	0.67
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.59	0.67
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.25	0.67
8:H:93:TYR:HB3	8:H:144:ILE:O	1.93	0.67
9:I:101:PHE:N	9:I:101:PHE:CD1	2.61	0.67
1:A:23:SER:HA	1:A:233:TRP:CD1	2.30	0.67
1:A:388:LEU:HD22	1:A:432:VAL:HG21	1.76	0.67
1:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.59	0.67
2:B:515:HIS:CD2	2:B:517:THR:H	2.11	0.67
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.30	0.67
1:A:567:LYS:HE3	8:H:46:LEU:HB2	1.77	0.67
3:C:186:LEU:HD21	3:C:224:GLN:O	1.95	0.67
6:F:97:ARG:HD3	6:F:130:ILE:HG23	1.77	0.67
8:H:81:PRO:CB	8:H:82:PRO:CD	2.72	0.67
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.24	0.67
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	1.95	0.67
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.59	0.67
4:D:176:GLU:O	4:D:178:ALA:N	2.26	0.67
7:G:1:MET:SD	7:G:1:MET:C	2.78	0.67
7:G:143:ILE:HG22	7:G:144:ARG:N	2.08	0.67
1:A:79:GLY:HA3	1:A:243:PRO:HG2	1.74	0.67
2:B:831:SER:HB3	2:B:994:TYR:OH	1.95	0.67
4:D:53:SER:HB3	4:D:152:SER:CB	2.25	0.67
6:F:125:LEU:HG	6:F:125:LEU:O	1.94	0.67
7:G:1:MET:HE1	7:G:80:LYS:N	2.10	0.67
1:A:311:GLN:HB3	1:A:312:PRO:HD3	1.76	0.66
1:A:567:LYS:HB3	8:H:96:VAL:H	1.60	0.66
2:B:192:LEU:O	2:B:193:LYS:HB2	1.94	0.66
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.76	0.66
6:F:90:ARG:HD3	6:F:155:LEU:CD1	2.24	0.66
7:G:18:PHE:HA	7:G:22:MET:HE2	1.76	0.66
1:A:979:SER:OG	1:A:981:LEU:HG	1.94	0.66
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.76	0.66
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.30	0.66
7:G:91:VAL:HB	7:G:139:ILE:O	1.95	0.66
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.30	0.66
9:I:51:ASN:O	9:I:54:GLU:HG3	1.95	0.66
9:I:52:ILE:HG13	9:I:52:ILE:O	1.95	0.66
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.26	0.66
2:B:1051:THR:HB	2:B:1054:GLY:H	1.61	0.66
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.60	0.66
1:A:18:GLN:HB2	2:B:1215:ARG:HB2	1.77	0.66
1:A:75:ASN:O	1:A:76:GLU:CB	2.43	0.66
2:B:705:MET:HA	2:B:705:MET:HE3	1.78	0.66
2:B:902:GLY:O	12:L:65:VAL:HG11	1.96	0.66
3:C:179:GLU:HG2	3:C:180:TYR:H	1.61	0.66
1:A:2:VAL:HG21	2:B:1158:PHE:N	2.11	0.66
1:A:843:LYS:HD3	1:A:846:GLU:OE2	1.95	0.66
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.58	0.66
2:B:370:PHE:HE2	2:B:373:ARG:HH11	1.42	0.66
2:B:852:ARG:HH22	12:L:70:ARG:C	2.04	0.66
2:B:996:ARG:NH1	3:C:38:ILE:HG23	2.10	0.66
2:B:1223:ASP:O	2:B:1224:PHE:HB2	1.94	0.66
3:C:18:VAL:HG12	3:C:18:VAL:O	1.94	0.66
5:E:157:SER:C	5:E:159:ASP:H	2.04	0.66
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.76	0.66
2:B:952:VAL:HG12	2:B:953:LEU:H	1.61	0.66
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.78	0.66
2:B:1202:LEU:O	2:B:1206:GLU:HG3	1.96	0.66
6:F:90:ARG:HG3	6:F:91:ALA:N	2.11	0.66
1:A:84:ILE:O	1:A:84:ILE:HG23	1.95	0.66
1:A:385:ILE:HG22	1:A:386:ASP:N	2.10	0.66
3:C:179:GLU:HG2	3:C:180:TYR:N	2.09	0.66
7:G:1:MET:HE1	7:G:80:LYS:H	1.60	0.66
8:H:126:GLU:C	8:H:130:ARG:HH22	2.03	0.66
1:A:866:PHE:O	1:A:867:ILE:HG13	1.94	0.66
2:B:378:LEU:O	2:B:382:ILE:HG13	1.96	0.66
2:B:1045:SER:O	2:B:1046:PRO:O	2.14	0.66
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.25	0.66
4:D:130:LEU:C	4:D:132:GLN:N	2.54	0.66
1:A:399:HIS:O	1:A:401:GLY:N	2.28	0.66
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.78	0.66
3:C:152:GLU:OE2	3:C:154:LYS:HE3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:HIS:C	10:J:53:HIS:CD2	2.73	0.66
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.04	0.66
5:E:176:PRO:O	5:E:212:ARG:HA	1.96	0.66
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.77	0.66
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.79	0.65
1:A:1007:ILE:C	1:A:1009:ASN:H	2.02	0.65
1:A:1436:ILE:O	1:A:1437:GLY:C	2.39	0.65
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.78	0.65
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.31	0.65
3:C:189:THR:HG22	3:C:190:ASP:H	1.60	0.65
4:D:122:GLU:HA	4:D:125:SER:OG	1.95	0.65
7:G:30:LEU:HD13	7:G:72:VAL:HG11	1.77	0.65
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.26	0.65
1:A:986:ILE:HG22	1:A:987:VAL:N	2.10	0.65
2:B:604:ARG:NH2	2:B:613:VAL:O	2.29	0.65
2:B:642:ASP:HA	2:B:649:LYS:HA	1.77	0.65
2:B:857:ARG:HD2	2:B:945:GLU:OE1	1.95	0.65
1:A:867:ILE:HD12	5:E:208:TYR:HE1	1.58	0.65
3:C:43:THR:CG2	3:C:44:LEU:H	2.08	0.65
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.78	0.65
12:L:58:LYS:O	12:L:58:LYS:HG2	1.96	0.65
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.11	0.65
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.31	0.65
8:H:56:THR:HB	8:H:145:ARG:HG2	1.79	0.65
9:I:2:THR:O	9:I:3:THR:C	2.39	0.65
1:A:69:THR:O	1:A:71:GLN:N	2.29	0.65
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.32	0.65
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.37	0.65
2:B:197:PHE:CZ	2:B:816:GLU:HG2	2.32	0.65
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.79	0.65
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.31	0.65
1:A:979:SER:OG	1:A:980:ASP:N	2.28	0.65
2:B:563:MET:HE3	2:B:580:VAL:HB	1.77	0.65
2:B:850:LEU:HD12	2:B:851:PHE:H	1.62	0.65
3:C:189:THR:HG22	3:C:190:ASP:N	2.11	0.65
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.61	0.65
8:H:123:MET:HE1	8:H:142:LEU:HD11	1.78	0.65
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.62	0.65
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.10	0.65
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.04	0.65
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:975:GLN:O	2:B:990:ILE:HD12	1.97	0.65
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.79	0.65
5:E:84:ASP:O	5:E:86:PRO:HD3	1.97	0.65
7:G:51:TYR:C	7:G:51:TYR:CD2	2.75	0.65
12:L:39:SER:O	12:L:40:LEU:HG	1.97	0.65
1:A:504:LEU:HD11	6:F:91:ALA:HB1	1.77	0.65
3:C:43:THR:CG2	3:C:44:LEU:N	2.59	0.65
6:F:111:LEU:HD12	6:F:111:LEU:N	2.12	0.65
7:G:7:LEU:HD11	7:G:45:ILE:HD11	1.78	0.65
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.27	0.65
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.79	0.65
1:A:818:MET:HA	2:B:514:LEU:HB3	1.79	0.65
2:B:357:GLN:O	2:B:366:GLN:HA	1.97	0.65
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.27	0.65
3:C:168:ALA:O	3:C:170:TRP:N	2.30	0.65
8:H:38:LEU:HD12	8:H:124:ARG:O	1.96	0.65
10:J:1:MET:HE2	10:J:60:PHE:CE2	2.31	0.65
1:A:1017:LEU:HB3	5:E:205:SER:HA	1.79	0.65
2:B:704:ALA:HB3	2:B:741:CYS:SG	2.37	0.65
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.14	0.65
7:G:110:VAL:HG22	7:G:161:GLY:O	1.97	0.65
10:J:1:MET:H2	10:J:56:LEU:N	1.94	0.65
1:A:869:GLY:O	5:E:204:THR:HG21	1.97	0.64
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.61	0.64
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	1.78	0.64
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.23	0.64
2:B:1172:ILE:HG22	2:B:1172:ILE:O	1.96	0.64
12:L:31:CYS:HB3	12:L:35:SER:N	2.13	0.64
3:C:165:LYS:O	11:K:6:ARG:NH1	2.30	0.64
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.79	0.64
1:A:535:THR:HG23	1:A:575:LYS:HE2	1.79	0.64
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.27	0.64
2:B:999:MET:HA	2:B:999:MET:CE	2.25	0.64
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.80	0.64
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.32	0.64
6:F:135:ARG:HD3	6:F:143:PHE:CD2	2.32	0.64
1:A:50:ILE:O	1:A:52:GLY:N	2.28	0.64
1:A:69:THR:C	1:A:71:GLN:N	2.55	0.64
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.79	0.64
1:A:442:VAL:HB	1:A:489:LEU:HD11	1.77	0.64
1:A:1017:LEU:HB2	5:E:206:GLY:N	2.07	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1115:SER:O	1:A:1116:LEU:HB3	1.96	0.64
1:A:1293:SER:OG	1:A:1294:PRO:HD2	1.97	0.64
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.26	0.64
8:H:91:ASP:C	8:H:93:TYR:H	2.05	0.64
1:A:23:SER:HA	1:A:233:TRP:NE1	2.12	0.64
1:A:665:GLY:HA2	2:B:1026:LEU:HD21	1.78	0.64
1:A:672:ASP:HB2	1:A:736:ASN:OD1	1.98	0.64
1:A:1039:LYS:HG3	1:A:1043:ASP:OD2	1.98	0.64
2:B:601:ARG:O	2:B:605:ARG:HG3	1.97	0.64
2:B:880:THR:O	2:B:881:ASN:HB2	1.96	0.64
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.26	0.64
1:A:743:VAL:O	1:A:747:VAL:HG23	1.96	0.64
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.33	0.64
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.26	0.64
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.33	0.64
1:A:384:ASN:O	1:A:385:ILE:C	2.41	0.64
1:A:1348:LEU:HG	1:A:1372:VAL:CG2	2.27	0.64
2:B:580:VAL:HG22	2:B:624:LEU:CB	2.27	0.64
3:C:66:ARG:NH1	10:J:2:ILE:HG21	2.13	0.64
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.80	0.64
7:G:9:LEU:HD12	7:G:10:ASN:H	1.63	0.64
1:A:88:LYS:HE3	1:A:280:GLU:OE2	1.98	0.64
1:A:503:GLN:HE21	6:F:90:ARG:NH2	1.95	0.64
1:A:670:ILE:HG23	1:A:805:LEU:CD2	2.28	0.64
1:A:720:ARG:O	1:A:724:GLU:HB2	1.97	0.64
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.33	0.64
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.79	0.64
5:E:157:SER:OG	5:E:160:GLU:HG3	1.97	0.64
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.31	0.64
12:L:31:CYS:SG	12:L:34:CYS:N	2.69	0.64
1:A:47:ARG:HH12	1:A:254:GLU:HG2	1.63	0.64
1:A:866:PHE:C	1:A:867:ILE:HG13	2.22	0.64
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.13	0.64
2:B:1085:ILE:N	2:B:1085:ILE:HD12	2.12	0.64
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.13	0.64
2:B:842:ASN:HD22	2:B:845:SER:CB	2.11	0.63
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.80	0.63
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.80	0.63
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.63	0.63
4:D:54:GLU:O	4:D:58:VAL:HG23	1.99	0.63
5:E:22:MET:CE	5:E:26:ARG:HH21	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:47:ARG:HG2	10:J:47:ARG:HH11	1.63	0.63
1:A:404:TYR:HB2	1:A:433:GLU:HB2	1.81	0.63
1:A:500:GLU:OE2	2:B:1145:SER:HB2	1.99	0.63
2:B:731:VAL:HG12	2:B:732:SER:H	1.62	0.63
3:C:99:LEU:HA	3:C:119:VAL:O	1.98	0.63
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.62	0.63
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.60	0.63
9:I:102:VAL:HG12	9:I:103:CYS:N	2.12	0.63
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.80	0.63
1:A:401:GLY:C	1:A:435:HIS:HD2	2.06	0.63
2:B:309:GLN:HG3	9:I:52:ILE:CD1	2.29	0.63
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.79	0.63
4:D:156:ASP:C	4:D:158:GLU:H	2.03	0.63
1:A:4:GLN:O	1:A:5:GLN:O	2.17	0.63
1:A:979:SER:HG	1:A:981:LEU:HG	1.62	0.63
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.62	0.63
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.29	0.63
1:A:591:PHE:HA	1:A:595:THR:HG21	1.80	0.63
2:B:879:ARG:NH1	2:B:883:LEU:HD22	2.13	0.63
4:D:191:ALA:O	4:D:193:THR:N	2.32	0.63
5:E:213:ILE:HG12	5:E:214:CYS:N	2.12	0.63
7:G:74:TYR:H	7:G:74:TYR:HD2	1.46	0.63
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.63	0.63
1:A:1224:LEU:HD12	1:A:1241:ARG:O	1.99	0.63
1:A:295:LEU:O	1:A:298:PHE:HB3	1.97	0.63
1:A:886:ILE:HG22	1:A:887:GLY:N	2.13	0.63
5:E:124:VAL:HG13	5:E:132:ILE:HD12	1.79	0.63
6:F:86:THR:HG23	6:F:89:GLU:OE1	1.98	0.63
9:I:8:ARG:CG	9:I:34:TYR:HE1	2.12	0.63
1:A:567:LYS:CB	8:H:95:TYR:HA	2.28	0.62
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.81	0.62
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.80	0.62
8:H:99:GLY:N	8:H:118:PHE:HD2	1.97	0.62
10:J:23:ASN:C	10:J:25:LEU:H	2.05	0.62
1:A:114:LEU:HD13	1:A:171:GLN:OE1	1.99	0.62
2:B:63:ILE:O	2:B:67:SER:HB3	1.98	0.62
1:A:1261:LYS:O	1:A:1264:GLU:HB3	1.99	0.62
2:B:205:ILE:O	2:B:207:GLY:N	2.32	0.62
2:B:212:LEU:CD2	2:B:480:SER:HB2	2.29	0.62
2:B:906:SER:O	2:B:941:LEU:HD23	1.99	0.62
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.55	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:101:PHE:HD1	9:I:101:PHE:H	1.46	0.62
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.29	0.62
1:A:1206:ASP:HB3	1:A:1274:ARG:HH12	1.64	0.62
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.28	0.62
1:A:77:CYS:O	1:A:78:PRO:C	2.40	0.62
1:A:129:LYS:O	1:A:130:ASP:HB2	1.99	0.62
1:A:714:PHE:HB2	9:I:97:MET:HE1	1.81	0.62
1:A:1445:ILE:HG12	7:G:18:PHE:HE2	1.62	0.62
1:A:1454:MET:O	1:A:1454:MET:HG3	1.98	0.62
6:F:89:GLU:OE2	6:F:134:ILE:HG21	1.98	0.62
1:A:90:VAL:HG13	1:A:297:GLN:HA	1.82	0.62
1:A:366:VAL:HG21	1:A:460:VAL:HG22	1.81	0.62
1:A:1021:LEU:O	1:A:1024:SER:HB3	1.99	0.62
2:B:1152:MET:CE	2:B:1157:ALA:HA	2.29	0.62
9:I:6:PHE:HB3	9:I:12:ASN:O	1.98	0.62
1:A:50:ILE:C	1:A:52:GLY:H	2.06	0.62
1:A:475:THR:CG2	1:A:476:SER:N	2.63	0.62
1:A:646:PHE:O	1:A:650:GLN:HG3	1.99	0.62
1:A:134:ARG:O	1:A:134:ARG:HG2	1.99	0.62
1:A:289:ILE:C	1:A:291:GLU:H	2.07	0.62
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.64	0.62
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.81	0.62
10:J:12:LYS:O	10:J:14:VAL:HG23	2.00	0.62
1:A:481:ASP:OD1	1:A:485:ASP:OD2	2.18	0.62
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.29	0.62
2:B:121:ASN:HA	2:B:207:GLY:CA	2.29	0.62
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.82	0.62
1:A:412:ARG:NH2	2:B:1108:ARG:NH1	2.48	0.62
1:A:590:ARG:HD2	1:A:605:MET:HB3	1.82	0.62
1:A:1120:LEU:HD12	1:A:1120:LEU:N	2.14	0.62
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.47	0.62
1:A:722:LEU:O	1:A:725:ALA:HB3	1.99	0.61
2:B:365:THR:HG23	2:B:367:LEU:HG	1.82	0.61
2:B:549:THR:H	2:B:628:THR:HG23	1.65	0.61
2:B:615:MET:C	2:B:616:ILE:HD12	2.25	0.61
4:D:202:ILE:HG21	4:D:207:LEU:HB2	1.82	0.61
5:E:78:LEU:HD23	5:E:78:LEU:C	2.24	0.61
6:F:111:LEU:HD12	6:F:111:LEU:H	1.65	0.61
1:A:2:VAL:HG21	2:B:1157:ALA:C	2.25	0.61
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.00	0.61
2:B:43:LEU:HD11	2:B:811:TYR:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:244:VAL:O	3:C:248:ILE:HG13	2.00	0.61
8:H:83:GLN:C	8:H:85:GLY:H	2.08	0.61
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.81	0.61
1:A:467:THR:O	1:A:469:ARG:HG3	2.00	0.61
2:B:731:VAL:HG12	2:B:732:SER:N	2.16	0.61
11:K:61:TYR:C	11:K:61:TYR:CD2	2.78	0.61
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.65	0.61
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.84	0.61
3:C:31:ASN:O	3:C:32:SER:C	2.42	0.61
9:I:85:PHE:HD2	9:I:85:PHE:N	1.88	0.61
1:A:135:PHE:C	1:A:137:ALA:H	2.06	0.61
2:B:1099:VAL:C	2:B:1101:ASP:H	2.07	0.61
8:H:100:THR:OG1	8:H:138:GLU:HG3	2.00	0.61
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.15	0.61
2:B:465:ASN:N	2:B:465:ASN:ND2	2.49	0.61
2:B:882:THR:HG22	2:B:884:ARG:N	2.13	0.61
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.16	0.61
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.35	0.61
1:A:1116:LEU:HG	1:A:1308:THR:HB	1.83	0.61
2:B:860:MET:HG2	2:B:861:ASP:N	2.14	0.61
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.29	0.61
1:A:907:THR:CG2	1:A:908:LEU:N	2.63	0.61
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.83	0.61
2:B:314:LEU:O	2:B:317:CYS:HB3	2.00	0.61
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.82	0.61
8:H:98:TYR:C	8:H:118:PHE:HD2	2.08	0.61
1:A:119:ASN:O	1:A:122:MET:HB3	2.01	0.61
1:A:144:THR:O	1:A:146:MET:HG3	2.01	0.61
1:A:1349:TYR:CE1	1:A:1368:MET:HE3	2.34	0.61
1:A:416:ARG:C	1:A:417:TYR:HD2	2.09	0.61
1:A:590:ARG:O	1:A:591:PHE:HB2	2.01	0.61
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.30	0.61
1:A:1097:GLY:O	1:A:1100:ARG:HB3	2.01	0.61
1:A:1151:GLU:OE2	9:I:45:ARG:HD2	2.01	0.61
2:B:287:ARG:NH1	2:B:324:ILE:O	2.34	0.61
2:B:824:ILE:CG2	2:B:1087:PHE:HE2	2.08	0.61
5:E:22:MET:HE3	5:E:26:ARG:NH2	2.15	0.61
1:A:774:ARG:O	1:A:775:ILE:C	2.43	0.60
2:B:542:MET:HE2	2:B:743:ILE:HG13	1.82	0.60
5:E:78:LEU:HD23	5:E:79:TRP:N	2.16	0.60
9:I:111:THR:HG22	9:I:112:SER:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:NZ	1:A:322:VAL:HG22	2.15	0.60
1:A:518:LYS:HE2	1:A:624:SER:O	2.02	0.60
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.83	0.60
2:B:197:PHE:HZ	2:B:816:GLU:HG2	1.65	0.60
2:B:542:MET:HE3	2:B:636:PRO:HG3	1.83	0.60
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.37	0.60
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.83	0.60
5:E:207:ARG:CB	5:E:207:ARG:HH11	2.13	0.60
6:F:111:LEU:C	6:F:113:GLY:N	2.56	0.60
1:A:146:MET:HA	1:A:171:GLN:HB2	1.83	0.60
1:A:728:LYS:O	1:A:732:LEU:HG	2.01	0.60
2:B:745:PRO:C	2:B:747:MET:H	2.09	0.60
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.37	0.60
2:B:980:PHE:HE2	2:B:1094:ARG:CG	2.14	0.60
3:C:45:ALA:HA	3:C:72:LEU:CD1	2.31	0.60
4:D:198:LEU:O	4:D:200:ASN:N	2.33	0.60
6:F:93:ILE:HD11	6:F:134:ILE:CD1	2.26	0.60
9:I:62:ILE:O	9:I:62:ILE:HG12	2.01	0.60
1:A:108:MET:SD	1:A:210:ILE:HD13	2.41	0.60
1:A:590:ARG:HB3	1:A:605:MET:N	2.15	0.60
3:C:22:LEU:HD13	3:C:230:MET:CE	2.32	0.60
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.36	0.60
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.17	0.60
1:A:524:VAL:HG12	1:A:525:GLN:N	2.12	0.60
1:A:1343:ALA:HB2	5:E:150:VAL:CG2	2.31	0.60
2:B:46:GLN:HG3	2:B:47:GLN:N	2.07	0.60
2:B:745:PRO:O	2:B:747:MET:N	2.33	0.60
2:B:949:VAL:HG12	2:B:950:ASP:N	2.15	0.60
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.37	0.60
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.02	0.60
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.02	0.60
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.01	0.60
2:B:822:ASN:O	10:J:48:ARG:NH1	2.34	0.60
7:G:119:LEU:HD12	7:G:131:GLN:O	2.02	0.60
1:A:98:LYS:O	1:A:99:ILE:C	2.45	0.60
1:A:503:GLN:NE2	6:F:90:ARG:HH21	1.97	0.60
3:C:208:GLU:O	3:C:210:GLU:N	2.34	0.60
5:E:29:PHE:C	5:E:30:ILE:HG13	2.26	0.60
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.82	0.60
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.28	0.60
2:B:310:MET:O	2:B:313:MET:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.84	0.60
2:B:1099:VAL:HG12	2:B:1100:ASP:H	1.67	0.60
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.83	0.60
4:D:156:ASP:C	4:D:158:GLU:N	2.60	0.60
12:L:36:SER:O	12:L:37:LYS:C	2.44	0.60
1:A:254:GLU:HB2	2:B:935:ARG:NH1	2.17	0.60
1:A:255:SER:OG	2:B:918:ILE:HG23	2.02	0.60
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.84	0.60
1:A:384:ASN:O	1:A:386:ASP:N	2.34	0.60
2:B:189:LEU:O	2:B:192:LEU:N	2.28	0.60
3:C:56:THR:HG22	3:C:57:VAL:N	2.16	0.60
3:C:146:LYS:C	3:C:147:LEU:HD23	2.26	0.60
4:D:56:ARG:HD3	4:D:149:THR:HA	1.82	0.60
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.29	0.60
11:K:60:ALA:O	11:K:73:LEU:HD12	2.01	0.60
1:A:613:ILE:O	1:A:614:PHE:HB3	2.01	0.60
1:A:854:ASN:HB3	1:A:1000:LEU:HD21	1.83	0.60
1:A:1059:HIS:ND1	6:F:86:THR:HA	2.17	0.60
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.31	0.60
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.83	0.60
2:B:955:THR:CG2	2:B:956:THR:H	2.15	0.60
2:B:1034:VAL:C	2:B:1036:ALA:H	2.09	0.60
6:F:77:ASP:C	6:F:79:ARG:H	2.10	0.60
7:G:17:PHE:C	7:G:19:GLY:H	2.10	0.60
12:L:60:ARG:HG2	12:L:61:THR:H	1.67	0.60
1:A:71:GLN:C	1:A:73:GLY:H	2.09	0.59
1:A:1197:LEU:HD12	1:A:1209:MET:HE1	1.82	0.59
2:B:446:LEU:O	2:B:447:ALA:HB3	2.02	0.59
2:B:1115:THR:O	2:B:1116:ARG:HB2	2.01	0.59
9:I:105:SER:O	9:I:106:CYS:HB3	2.01	0.59
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.83	0.59
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.42	0.59
2:B:557:PHE:C	2:B:557:PHE:HD2	2.09	0.59
2:B:705:MET:N	2:B:710:LEU:HD12	2.16	0.59
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.84	0.59
2:B:1224:PHE:CE2	5:E:171:LYS:HG3	2.30	0.59
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.35	0.59
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.83	0.59
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.30	0.59
3:C:66:ARG:NH1	3:C:144:ILE:O	2.35	0.59
5:E:35:VAL:C	5:E:37:LEU:H	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ARG:NH2	2:B:991:GLY:O	2.36	0.59
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.32	0.59
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.32	0.59
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.37	0.59
3:C:254:LYS:O	3:C:256:ALA:N	2.35	0.59
4:D:220:LEU:O	4:D:221:TYR:HD1	1.85	0.59
9:I:85:PHE:HD1	9:I:99:LEU:HD13	1.67	0.59
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.30	0.59
11:K:10:PHE:N	11:K:10:PHE:CD2	2.71	0.59
1:A:1313:LEU:O	1:A:1315:GLU:N	2.35	0.59
2:B:515:HIS:H	2:B:518:HIS:CD2	2.10	0.59
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.33	0.59
2:B:1099:VAL:HG12	2:B:1100:ASP:N	2.17	0.59
4:D:68:ARG:C	4:D:70:PHE:H	2.09	0.59
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.15	0.59
3:C:263:THR:C	3:C:265:MET:N	2.61	0.59
4:D:128:VAL:O	4:D:132:GLN:HG3	2.03	0.59
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.83	0.59
10:J:14:VAL:O	10:J:14:VAL:HG12	2.03	0.59
1:A:310:GLY:O	1:A:312:PRO:HD2	2.03	0.59
1:A:1115:SER:C	1:A:1308:THR:HG22	2.28	0.59
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.68	0.59
2:B:787:VAL:O	2:B:787:VAL:HG12	2.02	0.59
3:C:124:LEU:O	3:C:125:MET:HB2	2.01	0.59
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.84	0.59
1:A:262:LEU:C	1:A:264:PHE:H	2.11	0.59
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.17	0.59
1:A:913:LEU:HD12	1:A:914:GLU:H	1.66	0.59
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.67	0.59
2:B:1180:PHE:O	2:B:1181:GLU:O	2.20	0.59
1:A:472:LEU:O	1:A:475:THR:HB	2.03	0.59
1:A:1430:LEU:HB2	1:A:1432:GLN:HG3	1.85	0.59
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.85	0.59
8:H:44:VAL:O	8:H:44:VAL:HG12	2.03	0.59
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.85	0.59
1:A:299:HIS:C	1:A:301:ALA:H	2.11	0.59
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.38	0.59
1:A:782:ARG:NH2	2:B:699:GLU:O	2.34	0.59
1:A:1017:LEU:CB	5:E:205:SER:HA	2.33	0.59
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.84	0.59
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:SG	1:A:171:GLN:HG2	2.42	0.58
1:A:855:THR:CG2	1:A:857:ARG:HE	2.07	0.58
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.37	0.58
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.83	0.58
2:B:196:PRO:HG2	2:B:197:PHE:H	1.68	0.58
2:B:205:ILE:N	2:B:205:ILE:HD12	2.17	0.58
5:E:131:THR:HG21	5:E:191:LYS:NZ	2.18	0.58
2:B:180:TYR:HD1	2:B:180:TYR:H	1.51	0.58
2:B:838:SER:HB2	2:B:989:THR:O	2.03	0.58
3:C:254:LYS:O	3:C:258:ILE:HD13	2.04	0.58
11:K:63:VAL:HG23	11:K:63:VAL:O	2.03	0.58
1:A:532:ARG:HH22	1:A:745:GLN:HG2	1.67	0.58
1:A:545:GLN:O	1:A:546:VAL:C	2.46	0.58
1:A:853:ASP:OD1	1:A:855:THR:CB	2.51	0.58
4:D:130:LEU:HD22	4:D:134:THR:OG1	2.03	0.58
7:G:14:HIS:HD2	7:G:16:SER:HB2	1.66	0.58
1:A:605:MET:HE3	1:A:606:LEU:H	1.68	0.58
1:A:658:LEU:HD23	1:A:659:HIS:CE1	2.38	0.58
1:A:800:VAL:HG22	1:A:812:GLU:HB3	1.85	0.58
2:B:265:SER:O	2:B:266:ALA:HB3	2.02	0.58
2:B:359:GLU:O	2:B:362:PRO:HD3	2.04	0.58
4:D:51:ASN:O	4:D:54:GLU:HB3	2.04	0.58
12:L:53:HIS:O	12:L:55:ILE:HG12	2.04	0.58
2:B:616:ILE:HD12	2:B:616:ILE:N	2.18	0.58
2:B:705:MET:H	2:B:710:LEU:CD1	2.14	0.58
2:B:825:VAL:CG1	2:B:826:ALA:N	2.67	0.58
3:C:241:ASP:O	3:C:245:VAL:HG23	2.03	0.58
4:D:33:PHE:CZ	7:G:80:LYS:HE3	2.38	0.58
6:F:103:MET:O	6:F:104:ASN:HB2	2.03	0.58
9:I:102:VAL:CG1	9:I:103:CYS:N	2.65	0.58
1:A:262:LEU:O	1:A:264:PHE:N	2.37	0.58
1:A:325:ILE:HG21	2:B:1210:MET:HG3	1.84	0.58
1:A:341:MET:HE1	2:B:1135:ARG:HH12	1.69	0.58
1:A:567:LYS:CG	1:A:568:PRO:CD	2.79	0.58
2:B:283:VAL:O	2:B:286:PHE:N	2.37	0.58
2:B:811:TYR:N	2:B:811:TYR:CD1	2.71	0.58
5:E:39:LEU:O	5:E:42:PHE:HB3	2.02	0.58
6:F:99:LEU:HD12	6:F:99:LEU:O	2.04	0.58
9:I:61:ASP:C	9:I:63:GLY:H	2.12	0.58
1:A:254:GLU:HG3	2:B:935:ARG:HH22	1.67	0.58
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:957:ASN:O	2:B:959:ASP:N	2.37	0.58
8:H:143:LEU:HD12	8:H:143:LEU:N	2.19	0.58
12:L:43:THR:HG22	12:L:43:THR:O	2.02	0.58
1:A:49:LYS:HZ1	1:A:61:ILE:N	2.02	0.58
1:A:63:ARG:HA	1:A:74:MET:CE	2.34	0.58
1:A:67:CYS:O	1:A:68:GLN:HB2	2.04	0.58
1:A:665:GLY:O	1:A:667:GLY:N	2.37	0.58
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.37	0.58
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.18	0.58
1:A:1155:ASP:OD1	1:A:1161:THR:HA	2.03	0.58
4:D:134:THR:CG2	4:D:135:GLY:N	2.66	0.58
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.38	0.58
11:K:12:LEU:H	11:K:12:LEU:HD12	1.68	0.58
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.38	0.58
1:A:2:VAL:HG21	2:B:1158:PHE:CA	2.34	0.58
1:A:471:ASN:OD1	1:A:472:LEU:N	2.36	0.58
1:A:549:MET:SD	1:A:577:ILE:HD11	2.43	0.58
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	2.03	0.58
2:B:640:VAL:O	2:B:641:GLU:C	2.46	0.58
3:C:27:LEU:O	3:C:28:ALA:C	2.47	0.58
3:C:235:VAL:HG13	10:J:13:VAL:CG2	2.34	0.58
9:I:14:LEU:HA	9:I:28:GLU:O	2.04	0.58
1:A:278:THR:O	1:A:282:ASN:HB2	2.04	0.58
1:A:503:GLN:C	1:A:504:LEU:HD12	2.29	0.58
1:A:965:GLN:O	1:A:968:GLN:HB2	2.04	0.58
1:A:1116:LEU:HD11	1:A:1118:VAL:HG13	1.86	0.58
1:A:1400:CYS:SG	1:A:1409:LEU:HG	2.44	0.58
1:A:1418:LEU:HD23	2:B:1222:ARG:HD2	1.86	0.58
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.34	0.58
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.37	0.58
5:E:14:ARG:HH21	5:E:141:VAL:CG1	2.17	0.58
5:E:114:ASN:O	5:E:115:ASN:HB3	2.03	0.58
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.11	0.58
1:A:35:ILE:HA	1:A:52:GLY:O	2.04	0.57
1:A:265:LYS:NZ	1:A:322:VAL:HG13	2.17	0.57
2:B:117:ALA:HA	2:B:122:LEU:HD12	1.85	0.57
2:B:589:VAL:HG12	2:B:590:HIS:N	2.17	0.57
2:B:1031:LEU:HD23	2:B:1044:ALA:HB2	1.85	0.57
4:D:153:ARG:HH22	4:D:184:ALA:HA	1.68	0.57
8:H:18:GLY:O	8:H:19:ARG:HB2	2.04	0.57
12:L:27:LEU:O	12:L:28:LYS:HG2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HG22	1:A:84:ILE:HD12	1.86	0.57
1:A:81:PHE:CZ	2:B:1208:MET:HE2	2.39	0.57
1:A:446:ARG:HD3	1:A:480:ALA:HB2	1.86	0.57
1:A:853:ASP:O	1:A:854:ASN:HB2	2.04	0.57
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.68	0.57
2:B:460:ALA:HB1	2:B:466:TRP:CZ3	2.38	0.57
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.43	0.57
9:I:55:THR:CG2	9:I:58:VAL:HG21	2.34	0.57
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.86	0.57
1:A:341:MET:HE2	1:A:843:LYS:HZ1	1.67	0.57
1:A:401:GLY:C	1:A:435:HIS:CD2	2.82	0.57
2:B:65:GLU:CG	2:B:66:ASP:H	2.11	0.57
2:B:805:THR:HA	2:B:809:MET:HE1	1.86	0.57
4:D:191:ALA:C	4:D:193:THR:H	2.12	0.57
7:G:3:PHE:CD1	7:G:80:LYS:NZ	2.70	0.57
7:G:7:LEU:CD1	7:G:45:ILE:HD11	2.33	0.57
7:G:106:MET:CG	7:G:107:LYS:N	2.66	0.57
1:A:61:ILE:O	1:A:63:ARG:N	2.38	0.57
1:A:666:ILE:CD1	1:A:667:GLY:H	2.18	0.57
1:A:1051:ALA:O	1:A:1055:ARG:HG3	2.04	0.57
2:B:737:THR:CG2	9:I:66:PRO:HA	2.33	0.57
2:B:785:TYR:CD1	2:B:785:TYR:C	2.82	0.57
4:D:189:ASP:O	4:D:193:THR:HB	2.05	0.57
10:J:27:GLU:C	10:J:29:GLU:H	2.13	0.57
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.85	0.57
1:A:47:ARG:HH12	1:A:254:GLU:CG	2.17	0.57
1:A:698:GLN:HA	9:I:97:MET:O	2.04	0.57
1:A:877:HIS:C	1:A:878:ILE:HG13	2.29	0.57
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.69	0.57
2:B:604:ARG:HH22	2:B:614:SER:HA	1.69	0.57
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.32	0.57
7:G:1:MET:O	7:G:3:PHE:CE1	2.58	0.57
1:A:195:ASP:O	1:A:196:GLU:HB3	2.02	0.57
1:A:207:ILE:O	1:A:208:LEU:C	2.48	0.57
1:A:311:GLN:O	1:A:312:PRO:C	2.47	0.57
1:A:714:PHE:CB	9:I:97:MET:HE1	2.35	0.57
1:A:1323:ASP:C	1:A:1325:THR:H	2.12	0.57
2:B:244:LEU:HD21	2:B:366:GLN:NE2	2.20	0.57
2:B:952:VAL:HG12	2:B:953:LEU:N	2.20	0.57
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.05	0.57
1:A:11:LEU:HB2	2:B:1193:GLN:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PRO:O	1:A:322:VAL:CB	2.53	0.57
1:A:598:LEU:O	1:A:599:SER:C	2.47	0.57
1:A:1029:ARG:HH11	1:A:1029:ARG:HG3	1.70	0.57
2:B:1196:ILE:HB	2:B:1197:PRO:HD2	1.86	0.57
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.86	0.57
1:A:658:LEU:HD13	2:B:831:SER:HA	1.86	0.57
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.73	0.57
2:B:850:LEU:HD12	2:B:851:PHE:N	2.19	0.57
3:C:36:VAL:HG21	3:C:251:LEU:HD22	1.86	0.57
5:E:157:SER:C	5:E:159:ASP:N	2.60	0.57
7:G:7:LEU:O	7:G:73:LYS:HD2	2.05	0.57
7:G:99:PHE:HZ	7:G:163:ILE:HD13	1.70	0.57
8:H:99:GLY:N	8:H:118:PHE:CD2	2.72	0.57
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.34	0.57
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	2.20	0.57
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.39	0.57
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.87	0.57
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.05	0.57
2:B:1001:PHE:CE2	3:C:34:ARG:NE	2.73	0.57
10:J:1:MET:N	10:J:56:LEU:N	2.53	0.57
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.40	0.57
1:A:1396:ALA:O	1:A:1398:MET:N	2.38	0.57
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.70	0.57
2:B:949:VAL:HG12	2:B:950:ASP:H	1.70	0.57
2:B:980:PHE:CD2	2:B:1094:ARG:HA	2.40	0.57
7:G:3:PHE:CE1	7:G:80:LYS:HE2	2.40	0.57
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.40	0.56
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.02	0.56
2:B:309:GLN:HG3	9:I:52:ILE:HD11	1.87	0.56
2:B:899:ILE:HD11	2:B:910:VAL:O	2.04	0.56
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.86	0.56
4:D:59:ILE:HG21	4:D:145:MET:SD	2.45	0.56
7:G:1:MET:HG3	7:G:85:GLU:OE2	2.05	0.56
1:A:21:LEU:HG	1:A:1413:GLY:O	2.05	0.56
1:A:663:SER:OG	1:A:664:THR:N	2.36	0.56
1:A:844:ALA:O	1:A:845:LEU:HD23	2.05	0.56
1:A:958:VAL:O	1:A:958:VAL:HG12	2.05	0.56
1:A:998:LEU:H	1:A:998:LEU:HD12	1.69	0.56
2:B:847:ASP:C	2:B:849:GLY:N	2.61	0.56
2:B:955:THR:CG2	2:B:956:THR:N	2.67	0.56
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ASN:O	1:A:65:LEU:C	2.48	0.56
1:A:252:PHE:O	1:A:256:GLN:NE2	2.39	0.56
1:A:311:GLN:HB3	1:A:312:PRO:CD	2.33	0.56
1:A:886:ILE:HD11	1:A:943:LEU:CB	2.35	0.56
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.21	0.56
2:B:54:PHE:HA	2:B:58:THR:HB	1.86	0.56
2:B:114:PRO:O	2:B:116:GLU:N	2.38	0.56
2:B:224:GLN:O	2:B:238:ALA:HA	2.05	0.56
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.23	0.56
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.06	0.56
2:B:1001:PHE:HE2	3:C:34:ARG:CZ	2.17	0.56
2:B:1034:VAL:CG1	2:B:1035:ALA:N	2.67	0.56
2:B:1102:LYS:O	2:B:1103:ILE:C	2.47	0.56
3:C:252:GLN:HG3	11:K:95:ILE:HG23	1.87	0.56
5:E:180:ARG:HH21	5:E:192:ARG:CB	2.15	0.56
6:F:109:VAL:HG11	6:F:123:LYS:HG2	1.85	0.56
6:F:130:ILE:O	6:F:148:VAL:HG21	2.06	0.56
7:G:35:GLU:OE2	7:G:48:VAL:HG23	2.05	0.56
10:J:3:VAL:HA	10:J:53:HIS:CE1	2.39	0.56
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.87	0.56
1:A:265:LYS:HE2	1:A:322:VAL:CG1	2.35	0.56
1:A:482:PHE:C	1:A:484:GLY:H	2.13	0.56
1:A:605:MET:HE2	1:A:607:ILE:CG1	2.34	0.56
1:A:714:PHE:O	1:A:718:VAL:HG23	2.05	0.56
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.34	0.56
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.30	0.56
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.86	0.56
1:A:185:TRP:HZ3	1:A:200:ARG:HG2	1.71	0.56
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.40	0.56
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.41	0.56
1:A:1409:LEU:HD13	2:B:1207:LEU:CD2	2.36	0.56
2:B:984:HIS:CG	2:B:1025:HIS:HB2	2.41	0.56
3:C:60:ASP:OD2	12:L:60:ARG:NH2	2.39	0.56
7:G:26:LEU:O	7:G:27:LYS:C	2.48	0.56
11:K:21:ILE:HG23	11:K:31:VAL:CG1	2.36	0.56
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.41	0.56
1:A:940:ARG:HG2	1:A:940:ARG:HH11	1.71	0.56
1:A:1035:TYR:O	1:A:1037:LEU:N	2.37	0.56
2:B:190:TYR:CE2	10:J:62:ARG:HB3	2.40	0.56
2:B:351:TYR:O	2:B:355:ILE:HG13	2.05	0.56
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:GLY:O	3:C:7:GLN:HG3	2.06	0.56
7:G:111:THR:HB	7:G:114:LEU:HB2	1.88	0.56
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.34	0.56
1:A:586:ILE:HG22	1:A:587:HIS:N	2.21	0.56
1:A:840:ARG:O	1:A:841:LEU:C	2.47	0.56
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.40	0.56
1:A:963:ILE:HD13	1:A:1049:ILE:HG12	1.87	0.56
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.40	0.56
2:B:295:GLY:H	2:B:298:LEU:HD23	1.70	0.56
2:B:465:ASN:HD22	2:B:465:ASN:H	1.53	0.56
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.87	0.56
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.88	0.56
4:D:192:LYS:HZ3	4:D:199:ASN:HA	1.71	0.56
5:E:93:MET:SD	5:E:97:VAL:HG23	2.46	0.56
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.31	0.56
6:F:75:PRO:O	6:F:77:ASP:O	2.23	0.56
6:F:90:ARG:HD3	6:F:155:LEU:HD11	1.88	0.56
6:F:109:VAL:HG12	6:F:110:ASP:N	2.20	0.56
11:K:82:ASP:OD1	11:K:84:LYS:N	2.38	0.56
11:K:90:ALA:O	11:K:94:ILE:HG13	2.04	0.56
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.88	0.56
1:A:492:PRO:O	1:A:493:GLN:NE2	2.38	0.56
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.66	0.56
2:B:526:GLU:OE2	2:B:752:ALA:HB2	2.06	0.56
2:B:877:PRO:C	2:B:878:GLN:HG3	2.31	0.56
4:D:176:GLU:C	4:D:178:ALA:N	2.63	0.56
7:G:1:MET:SD	7:G:1:MET:O	2.64	0.56
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.88	0.56
10:J:53:HIS:CD2	10:J:54:VAL:N	2.74	0.56
1:A:817:ALA:O	1:A:818:MET:C	2.48	0.56
1:A:858:ASN:ND2	1:A:858:ASN:C	2.59	0.56
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.87	0.56
1:A:1127:ASP:HB3	1:A:1130:GLN:CB	2.35	0.56
2:B:833:TYR:N	2:B:833:TYR:CD1	2.73	0.56
12:L:47:ARG:HH11	12:L:47:ARG:HG3	1.70	0.56
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.41	0.56
1:A:1007:ILE:C	1:A:1009:ASN:N	2.62	0.56
2:B:604:ARG:NH2	2:B:614:SER:HA	2.20	0.56
3:C:76:ASP:O	3:C:77:ILE:C	2.48	0.56
4:D:192:LYS:HZ3	4:D:192:LYS:HB3	1.70	0.56
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:N	1:A:265:LYS:HD2	2.20	0.55
1:A:632:VAL:O	1:A:633:VAL:C	2.48	0.55
2:B:114:PRO:HG2	2:B:115:GLN:H	1.71	0.55
2:B:893:LEU:HD11	2:B:910:VAL:HG11	1.88	0.55
3:C:168:ALA:C	3:C:170:TRP:N	2.64	0.55
1:A:23:SER:O	1:A:24:PRO:C	2.47	0.55
1:A:60:SER:C	1:A:61:ILE:HG13	2.30	0.55
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.68	0.55
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.87	0.55
1:A:1010:ALA:HA	1:A:1013:ASP:OD2	2.06	0.55
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.88	0.55
2:B:44:VAL:O	2:B:45:SER:C	2.48	0.55
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.37	0.55
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.36	0.55
2:B:258:LEU:HG	2:B:258:LEU:O	2.05	0.55
2:B:376:PHE:HB3	2:B:586:TRP:CZ3	2.42	0.55
5:E:128:PRO:HA	5:E:129:PRO:C	2.32	0.55
7:G:145:VAL:HG12	7:G:146:LYS:N	2.21	0.55
12:L:40:LEU:HD22	12:L:44:ASP:CG	2.31	0.55
1:A:265:LYS:HD2	1:A:265:LYS:H	1.72	0.55
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.41	0.55
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.07	0.55
1:A:504:LEU:HD12	1:A:504:LEU:N	2.21	0.55
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.89	0.55
1:A:907:THR:HG22	1:A:908:LEU:N	2.20	0.55
1:A:1157:ASP:C	1:A:1159:ARG:H	2.14	0.55
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.05	0.55
1:A:1364:ASN:O	1:A:1365:TYR:C	2.50	0.55
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.36	0.55
2:B:129:PHE:HA	2:B:165:VAL:O	2.06	0.55
2:B:377:PHE:C	2:B:379:GLY:N	2.62	0.55
3:C:174:ALA:O	3:C:175:ALA:HB2	2.05	0.55
5:E:3:GLN:HG3	5:E:4:GLU:N	2.20	0.55
5:E:23:VAL:O	5:E:28:TYR:HB2	2.07	0.55
8:H:123:MET:HE1	8:H:142:LEU:CD1	2.36	0.55
9:I:68:LEU:HB3	9:I:84:VAL:HG23	1.87	0.55
1:A:90:VAL:HG12	1:A:91:PHE:N	2.22	0.55
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.21	0.55
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.89	0.55
1:A:857:ARG:HD3	1:A:861:GLY:O	2.06	0.55
2:B:235:SER:C	2:B:236:HIS:HD2	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:ILE:HD13	2:B:330:ALA:HA	1.88	0.55
1:A:666:ILE:HD12	1:A:666:ILE:N	2.21	0.55
1:A:730:GLY:O	1:A:732:LEU:N	2.40	0.55
1:A:1242:VAL:O	1:A:1243:VAL:HB	2.07	0.55
2:B:997:GLU:CD	2:B:997:GLU:H	2.13	0.55
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.37	0.55
3:C:31:ASN:OD1	3:C:34:ARG:NH1	2.40	0.55
3:C:258:ILE:HD12	3:C:258:ILE:N	2.22	0.55
7:G:117:GLN:C	7:G:119:LEU:H	2.15	0.55
9:I:74:GLU:HA	9:I:80:SER:O	2.06	0.55
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.37	0.55
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.41	0.55
2:B:360:PHE:C	2:B:360:PHE:CD2	2.85	0.55
2:B:696:GLU:O	2:B:699:GLU:HB2	2.07	0.55
2:B:843:GLN:O	2:B:846:ILE:HB	2.07	0.55
2:B:882:THR:HB	2:B:934:LYS:O	2.06	0.55
4:D:51:ASN:O	4:D:52:LEU:O	2.25	0.55
1:A:56:PRO:O	1:A:57:ARG:CG	2.51	0.55
1:A:658:LEU:HD23	1:A:659:HIS:HE1	1.72	0.55
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.71	0.55
2:B:97:VAL:HG12	2:B:178:ASN:ND2	2.22	0.55
2:B:311:LEU:O	2:B:312:GLU:C	2.48	0.55
3:C:76:ASP:O	3:C:79:GLN:HG2	2.06	0.55
3:C:215:GLU:O	3:C:216:GLY:C	2.50	0.55
7:G:27:LYS:O	7:G:30:LEU:HB3	2.07	0.55
7:G:81:PRO:HB3	7:G:106:MET:HE1	1.89	0.55
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.31	0.55
1:A:353:ILE:HG21	1:A:487:MET:CE	2.37	0.55
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.42	0.55
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.55	0.55
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.37	0.55
2:B:205:ILE:N	2:B:205:ILE:CD1	2.68	0.55
2:B:552:MET:C	2:B:554:ILE:H	2.15	0.55
2:B:1082:MET:O	3:C:189:THR:HG23	2.07	0.55
3:C:3:GLU:HG2	3:C:4:GLU:N	2.22	0.55
4:D:64:VAL:C	4:D:66:ARG:H	2.14	0.55
7:G:51:TYR:O	7:G:54:ILE:HG13	2.06	0.55
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.22	0.55
1:A:92:HIS:HB3	1:A:95:PHE:HB2	1.89	0.55
1:A:114:LEU:O	1:A:115:LEU:HG	2.07	0.55
1:A:738:LYS:C	1:A:740:LEU:H	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.07	0.55
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.06	0.55
2:B:35:SER:O	2:B:39:ARG:HG3	2.05	0.55
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.72	0.55
2:B:579:ARG:N	2:B:589:VAL:HG13	2.22	0.55
3:C:235:VAL:HG13	10:J:13:VAL:HG23	1.89	0.55
7:G:125:SER:OG	7:G:128:PRO:HA	2.07	0.55
7:G:150:CYS:C	7:G:151:ILE:HG13	2.31	0.55
1:A:166:GLY:O	1:A:167:CYS:SG	2.64	0.54
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.88	0.54
1:A:416:ARG:C	1:A:417:TYR:CD2	2.85	0.54
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.37	0.54
2:B:558:LEU:C	2:B:560:GLU:H	2.15	0.54
2:B:710:LEU:O	2:B:711:GLU:HG2	2.06	0.54
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.47	0.54
1:A:3:GLY:O	1:A:4:GLN:HB2	2.06	0.54
1:A:816:HIS:HE2	2:B:764:SER:H	1.55	0.54
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.47	0.54
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.89	0.54
2:B:654:ARG:H	2:B:657:HIS:CD2	2.23	0.54
3:C:18:VAL:CG2	3:C:240:VAL:HB	2.37	0.54
3:C:226:ASP:O	3:C:227:THR:HB	2.07	0.54
1:A:939:ASP:O	1:A:943:LEU:HG	2.07	0.54
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.72	0.54
2:B:223:VAL:HG11	2:B:381:MET:HG2	1.88	0.54
3:C:98:VAL:O	3:C:99:LEU:HD23	2.08	0.54
6:F:73:ALA:HA	6:F:143:PHE:CE1	2.43	0.54
6:F:90:ARG:HD3	6:F:155:LEU:HD12	1.88	0.54
1:A:265:LYS:CE	1:A:322:VAL:HG13	2.37	0.54
1:A:546:VAL:O	1:A:550:LEU:HG	2.08	0.54
1:A:794:PRO:C	1:A:796:SER:H	2.15	0.54
1:A:845:LEU:HB3	1:A:848:ILE:HD12	1.88	0.54
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.24	0.54
2:B:746:SER:HB2	2:B:1046:PRO:HG2	1.89	0.54
3:C:168:ALA:C	3:C:170:TRP:H	2.16	0.54
8:H:95:TYR:HB3	8:H:144:ILE:HB	1.89	0.54
1:A:316:GLN:O	1:A:317:LYS:C	2.50	0.54
1:A:381:THR:HG23	1:A:383:TYR:H	1.73	0.54
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.08	0.54
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.89	0.54
2:B:516:ASN:N	2:B:516:ASN:ND2	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.07	0.54
2:B:1115:THR:CG2	2:B:1117:GLN:HG3	2.36	0.54
11:K:12:LEU:HD12	11:K:12:LEU:N	2.22	0.54
1:A:108:MET:SD	1:A:108:MET:N	2.79	0.54
1:A:814:PHE:O	1:A:817:ALA:HB3	2.08	0.54
1:A:873:MET:C	1:A:1058:VAL:CG2	2.80	0.54
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.90	0.54
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.34	0.54
2:B:872:GLU:HA	2:B:915:THR:O	2.08	0.54
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.73	0.54
3:C:254:LYS:C	3:C:256:ALA:H	2.15	0.54
4:D:153:ARG:C	4:D:154:PHE:CD1	2.86	0.54
5:E:207:ARG:HH11	5:E:207:ARG:HB3	1.73	0.54
8:H:89:LEU:HB3	8:H:91:ASP:OD1	2.06	0.54
8:H:100:THR:HG22	8:H:101:ALA:N	2.21	0.54
10:J:1:MET:HE2	10:J:60:PHE:CZ	2.42	0.54
1:A:534:LEU:O	1:A:534:LEU:HG	2.07	0.54
1:A:829:VAL:C	1:A:831:THR:H	2.14	0.54
1:A:847:ASP:OD1	1:A:848:ILE:HG13	2.07	0.54
8:H:139:ASN:O	8:H:140:ALA:HB2	2.08	0.54
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.38	0.54
10:J:44:TYR:HA	10:J:47:ARG:CB	2.37	0.54
1:A:71:GLN:O	1:A:73:GLY:N	2.38	0.54
1:A:244:PRO:O	1:A:247:ARG:N	2.41	0.54
1:A:666:ILE:H	2:B:1026:LEU:HD22	1.72	0.54
2:B:234:ILE:HD12	2:B:234:ILE:N	2.23	0.54
2:B:315:LYS:N	2:B:316:PRO:HD2	2.23	0.54
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.89	0.54
8:H:84:ALA:C	8:H:86:ASP:H	2.15	0.54
9:I:99:LEU:C	9:I:100:PHE:HD1	2.16	0.54
10:J:23:ASN:C	10:J:25:LEU:N	2.64	0.54
1:A:262:LEU:C	1:A:264:PHE:N	2.66	0.54
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.37	0.54
1:A:845:LEU:O	1:A:846:GLU:C	2.49	0.54
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.90	0.54
2:B:57:TYR:CD1	2:B:57:TYR:N	2.74	0.54
2:B:833:TYR:N	2:B:833:TYR:HD1	2.06	0.54
3:C:181:ASP:OD2	3:C:185:LYS:N	2.41	0.54
4:D:56:ARG:HD2	4:D:149:THR:OG1	2.08	0.54
5:E:55:ARG:HD2	5:E:83:CYS:O	2.08	0.54
11:K:47:ARG:O	11:K:47:ARG:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:ALA:O	1:A:819:GLY:N	2.41	0.54
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.33	0.54
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.08	0.54
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.08	0.54
1:A:1377:THR:O	1:A:1379:GLY:N	2.41	0.54
2:B:125:SER:HA	2:B:171:PRO:HA	1.89	0.54
2:B:360:PHE:O	2:B:361:LEU:C	2.51	0.54
2:B:773:MET:C	2:B:775:LYS:H	2.13	0.54
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.38	0.54
3:C:8:VAL:HG12	3:C:9:LYS:N	2.23	0.54
5:E:46:TYR:CE2	5:E:58:MET:HA	2.43	0.54
6:F:96:THR:O	6:F:100:GLN:HG3	2.07	0.54
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.90	0.54
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.90	0.53
1:A:694:THR:O	1:A:698:GLN:HG3	2.08	0.53
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.23	0.53
2:B:803:LEU:CD1	2:B:1032:SER:HB3	2.38	0.53
2:B:806:THR:HA	2:B:1045:SER:OG	2.07	0.53
2:B:1068:GLY:O	2:B:1069:PHE:O	2.27	0.53
2:B:1074:ASN:HB2	2:B:1081:LEU:HD21	1.90	0.53
4:D:24:ALA:HA	7:G:83:LYS:O	2.08	0.53
4:D:202:ILE:CG2	4:D:207:LEU:HB2	2.38	0.53
6:F:118:LEU:HD12	6:F:118:LEU:O	2.07	0.53
9:I:32:CYS:SG	9:I:33:SER:N	2.81	0.53
10:J:44:TYR:CD2	10:J:44:TYR:N	2.76	0.53
1:A:1279:ILE:HD11	1:A:1316:VAL:CG2	2.37	0.53
1:A:1372:VAL:O	1:A:1376:THR:HG22	2.08	0.53
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.90	0.53
7:G:56:ILE:O	7:G:57:GLN:HB2	2.06	0.53
11:K:65:HIS:HD2	11:K:67:PHE:N	1.98	0.53
12:L:34:CYS:O	12:L:35:SER:C	2.52	0.53
1:A:47:ARG:O	1:A:48:ALA:HB2	2.08	0.53
1:A:417:TYR:CD2	1:A:417:TYR:N	2.75	0.53
1:A:475:THR:CG2	1:A:476:SER:H	2.19	0.53
1:A:567:LYS:CB	1:A:568:PRO:CD	2.85	0.53
2:B:763:GLN:HG2	2:B:765:PRO:CD	2.35	0.53
2:B:865:LYS:NZ	2:B:869:SER:HA	2.22	0.53
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.33	0.53
2:B:1152:MET:HE3	2:B:1157:ALA:HA	1.90	0.53
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.28	0.53
5:E:9:ILE:HD11	5:E:53:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:13:MET:O	9:I:14:LEU:HD23	2.08	0.53
1:A:366:VAL:CG2	1:A:460:VAL:HG22	2.39	0.53
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.43	0.53
1:A:528:LEU:HD23	1:A:751:SER:HA	1.91	0.53
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.39	0.53
2:B:235:SER:OG	2:B:236:HIS:CD2	2.61	0.53
4:D:29:LEU:HD22	7:G:82:PHE:CD2	2.44	0.53
10:J:44:TYR:H	10:J:44:TYR:HD2	1.55	0.53
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.90	0.53
2:B:1040:ASN:O	2:B:1041:GLU:C	2.50	0.53
4:D:64:VAL:C	4:D:66:ARG:N	2.67	0.53
5:E:192:ARG:HG3	5:E:192:ARG:NH1	2.21	0.53
10:J:3:VAL:HA	10:J:53:HIS:ND1	2.24	0.53
1:A:306:ASN:HD21	1:A:322:VAL:HB	1.74	0.53
1:A:356:ASP:O	1:A:358:ASN:N	2.42	0.53
1:A:1053:PHE:C	1:A:1055:ARG:H	2.15	0.53
2:B:181:LEU:HD22	2:B:189:LEU:HD22	1.91	0.53
2:B:773:MET:C	2:B:775:LYS:N	2.65	0.53
2:B:841:MET:SD	2:B:846:ILE:HD11	2.49	0.53
4:D:63:LEU:HD13	4:D:133:THR:OG1	2.08	0.53
5:E:90:VAL:O	5:E:90:VAL:HG22	2.08	0.53
11:K:47:ARG:HD3	11:K:59:ALA:O	2.08	0.53
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.73	0.53
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.44	0.53
4:D:53:SER:HB3	4:D:152:SER:CA	2.38	0.53
5:E:116:ILE:HG22	5:E:117:THR:N	2.23	0.53
12:L:52:GLY:O	12:L:53:HIS:C	2.52	0.53
1:A:43:GLU:O	1:A:44:THR:HB	2.09	0.53
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.39	0.53
2:B:880:THR:HB	2:B:934:LYS:HD2	1.90	0.53
7:G:62:LEU:HB3	7:G:63:PRO:CD	2.39	0.53
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.90	0.53
1:A:673:GLY:O	1:A:676:MET:HB2	2.09	0.53
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.24	0.53
1:A:960:ILE:O	1:A:961:ARG:C	2.50	0.53
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.91	0.53
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.37	0.53
2:B:205:ILE:O	2:B:206:ASN:C	2.52	0.53
2:B:281:PRO:O	2:B:283:VAL:N	2.41	0.53
2:B:333:PHE:C	2:B:334:ILE:HG13	2.34	0.53
2:B:493:SER:HA	2:B:751:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:GLU:O	3:C:167:HIS:HB2	2.08	0.53
8:H:4:THR:CA	8:H:60:ALA:HB2	2.34	0.53
1:A:548:ASN:OD1	11:K:60:ALA:HB1	2.09	0.53
1:A:577:ILE:HA	1:A:580:VAL:HG23	1.91	0.53
1:A:618:GLU:O	1:A:620:LYS:N	2.41	0.53
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.90	0.53
1:A:867:ILE:HD12	5:E:208:TYR:CE1	2.41	0.53
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.91	0.53
1:A:1094:VAL:HG12	1:A:1095:THR:N	2.24	0.53
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.74	0.53
2:B:459:TYR:C	2:B:459:TYR:CD2	2.86	0.53
2:B:555:ILE:HD11	2:B:587:HIS:CE1	2.44	0.53
3:C:254:LYS:C	3:C:256:ALA:N	2.67	0.53
8:H:84:ALA:C	8:H:86:ASP:N	2.67	0.53
8:H:113:ALA:HB1	8:H:125:LEU:O	2.09	0.53
10:J:44:TYR:N	10:J:44:TYR:HD2	2.07	0.53
1:A:34:LYS:HB3	1:A:36:ARG:HE	1.73	0.52
1:A:55:ASP:N	1:A:56:PRO:HD3	2.24	0.52
1:A:818:MET:N	2:B:514:LEU:HD23	2.24	0.52
1:A:1164:PRO:O	1:A:1166:ASP:N	2.43	0.52
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.10	0.52
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.90	0.52
2:B:1107:ALA:O	2:B:1108:ARG:HG2	2.09	0.52
3:C:147:LEU:HD12	3:C:151:GLN:O	2.09	0.52
5:E:22:MET:HE3	5:E:26:ARG:CZ	2.39	0.52
1:A:50:ILE:C	1:A:52:GLY:N	2.64	0.52
1:A:277:GLU:C	1:A:279:LEU:H	2.17	0.52
1:A:364:VAL:O	1:A:364:VAL:HG13	2.08	0.52
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.30	0.52
1:A:420:ARG:O	1:A:421:ALA:C	2.51	0.52
1:A:567:LYS:HB3	8:H:96:VAL:N	2.23	0.52
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	2.09	0.52
2:B:496:ARG:HB3	2:B:496:ARG:HH11	1.73	0.52
2:B:778:MET:HE2	2:B:1094:ARG:CG	2.37	0.52
2:B:810:GLU:HB2	2:B:815:ARG:HH22	1.74	0.52
2:B:843:GLN:HB2	2:B:993:THR:HB	1.91	0.52
3:C:73:GLN:NE2	3:C:74:SER:H	2.07	0.52
7:G:1:MET:SD	7:G:79:PHE:CE1	3.02	0.52
9:I:8:ARG:HG2	9:I:34:TYR:HE1	1.73	0.52
1:A:1004:ASN:OD1	1:A:1005:GLU:N	2.42	0.52
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:137:ASN:C	4:D:137:ASN:HD22	2.17	0.52
8:H:41:ASP:OD2	8:H:122:LEU:N	2.41	0.52
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.45	0.52
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.39	0.52
1:A:874:ASP:N	1:A:1058:VAL:HG22	2.24	0.52
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.91	0.52
1:A:1120:LEU:HD13	1:A:1304:TRP:O	2.09	0.52
1:A:1365:TYR:O	1:A:1367:HIS:N	2.42	0.52
2:B:240:ILE:HG23	2:B:240:ILE:O	2.09	0.52
2:B:370:PHE:HE2	2:B:373:ARG:NH1	2.08	0.52
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.24	0.52
2:B:1208:MET:O	2:B:1211:ASN:N	2.40	0.52
3:C:107:SER:C	3:C:109:SER:H	2.17	0.52
4:D:33:PHE:CZ	7:G:80:LYS:CE	2.92	0.52
5:E:161:LYS:C	5:E:163:GLU:H	2.17	0.52
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.40	0.52
1:A:306:ASN:ND2	1:A:322:VAL:HB	2.24	0.52
1:A:325:ILE:HG22	2:B:1210:MET:HE2	1.92	0.52
1:A:903:ASN:C	1:A:903:ASN:ND2	2.64	0.52
1:A:1451:VAL:C	1:A:1453:TYR:H	2.15	0.52
2:B:35:SER:HA	2:B:811:TYR:CE2	2.35	0.52
2:B:615:MET:CB	2:B:626:ILE:HG12	2.39	0.52
2:B:750:GLY:O	2:B:751:VAL:C	2.53	0.52
2:B:798:TYR:CE2	3:C:62:PHE:CE2	2.97	0.52
5:E:168:TYR:HB2	5:E:170:LEU:HG	1.90	0.52
7:G:1:MET:O	7:G:1:MET:HE2	2.10	0.52
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.75	0.52
1:A:921:GLY:O	1:A:922:ASP:C	2.53	0.52
1:A:1007:ILE:O	1:A:1009:ASN:N	2.41	0.52
2:B:57:TYR:N	2:B:57:TYR:HD1	2.08	0.52
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.92	0.52
2:B:862:GLN:HG2	2:B:963:PHE:CD1	2.44	0.52
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.45	0.52
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.92	0.52
6:F:109:VAL:HG13	6:F:127:GLU:OE1	2.09	0.52
7:G:80:LYS:O	7:G:80:LYS:HG2	2.09	0.52
8:H:127:GLY:O	8:H:128:ASN:HB2	2.10	0.52
1:A:42:ASP:HB3	1:A:45:GLN:H	1.73	0.52
1:A:95:PHE:O	1:A:96:ILE:C	2.53	0.52
1:A:757:ASN:HA	2:B:1021:MET:SD	2.50	0.52
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:597:MET:HA	2:B:597:MET:HE3	1.91	0.52
6:F:101:ILE:HD11	6:F:124:GLU:OE1	2.09	0.52
7:G:111:THR:HG22	7:G:113:HIS:H	1.74	0.52
11:K:31:VAL:CG1	11:K:32:VAL:N	2.72	0.52
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.45	0.52
1:A:730:GLY:C	1:A:732:LEU:H	2.17	0.52
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.25	0.52
2:B:383:ASN:O	2:B:384:ARG:C	2.53	0.52
2:B:948:ILE:HG22	2:B:949:VAL:O	2.09	0.52
2:B:1107:ALA:O	2:B:1108:ARG:O	2.28	0.52
4:D:167:LEU:O	4:D:170:THR:OG1	2.23	0.52
6:F:79:ARG:HG3	6:F:144:GLU:OE1	2.10	0.52
6:F:140:ASP:C	6:F:140:ASP:OD1	2.52	0.52
8:H:33:GLN:C	8:H:35:GLN:H	2.18	0.52
10:J:13:VAL:C	10:J:14:VAL:HG23	2.34	0.52
11:K:85:ASP:O	11:K:88:LYS:HB2	2.10	0.52
1:A:78:PRO:HA	2:B:1201:LYS:HZ1	1.74	0.52
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.92	0.52
1:A:231:PRO:HA	1:A:234:MET:HE2	1.92	0.52
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.91	0.52
1:A:628:GLY:O	1:A:632:VAL:HG23	2.10	0.52
1:A:871:ASP:HB3	5:E:204:THR:HG23	1.91	0.52
1:A:901:LEU:H	1:A:926:GLN:HE21	1.56	0.52
1:A:901:LEU:HD22	1:A:919:ILE:HG21	1.92	0.52
1:A:1141:THR:OG1	1:A:1205:LYS:HD3	2.10	0.52
5:E:14:ARG:HH21	5:E:141:VAL:HG12	1.73	0.52
1:A:18:GLN:HB3	2:B:1215:ARG:HG3	1.91	0.52
1:A:605:MET:HE3	1:A:606:LEU:N	2.25	0.52
1:A:648:ASN:O	1:A:649:ILE:C	2.53	0.52
1:A:853:ASP:OD1	1:A:855:THR:N	2.43	0.52
1:A:1325:THR:O	5:E:148:GLU:HB2	2.10	0.52
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.45	0.52
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.34	0.52
8:H:138:GLU:O	8:H:139:ASN:C	2.52	0.52
10:J:45:CYS:O	10:J:48:ARG:HG3	2.10	0.52
1:A:996:ASN:O	1:A:998:LEU:HD12	2.10	0.51
2:B:455:SER:O	2:B:456:GLY:C	2.51	0.51
2:B:984:HIS:CD2	2:B:1025:HIS:HB2	2.45	0.51
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.09	0.51
3:C:263:THR:O	3:C:265:MET:N	2.43	0.51
4:D:210:ILE:O	4:D:214:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:81:THR:HB	6:F:136:ARG:HH11	1.75	0.51
8:H:31:THR:O	8:H:31:THR:HG22	2.10	0.51
9:I:100:PHE:N	9:I:100:PHE:CD1	2.78	0.51
10:J:53:HIS:HD2	10:J:54:VAL:N	2.08	0.51
11:K:69:ALA:O	11:K:70:ARG:HB3	2.11	0.51
1:A:58:LEU:HD22	1:A:80:HIS:O	2.11	0.51
1:A:89:PRO:C	1:A:204:THR:HG21	2.36	0.51
1:A:115:LEU:CB	1:A:122:MET:HE2	2.41	0.51
1:A:365:GLY:O	1:A:468:PHE:HA	2.11	0.51
1:A:630:ILE:HD13	1:A:646:PHE:CZ	2.45	0.51
3:C:54:ASN:HB2	3:C:153:LEU:HD12	1.93	0.51
3:C:215:GLU:O	3:C:217:ASP:N	2.43	0.51
4:D:206:GLU:C	4:D:208:GLU:N	2.68	0.51
6:F:81:THR:HG21	6:F:136:ARG:CD	2.33	0.51
9:I:102:VAL:CG1	9:I:103:CYS:H	2.24	0.51
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.09	0.51
1:A:89:PRO:HB2	1:A:204:THR:HG22	1.92	0.51
1:A:231:PRO:C	1:A:233:TRP:H	2.18	0.51
1:A:299:HIS:C	1:A:301:ALA:N	2.67	0.51
1:A:483:ASP:O	2:B:979:LYS:HE3	2.11	0.51
1:A:730:GLY:C	1:A:732:LEU:N	2.67	0.51
1:A:984:LYS:O	1:A:985:ASP:C	2.54	0.51
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.43	0.51
2:B:108:VAL:HG12	2:B:109:THR:H	1.74	0.51
2:B:637:LEU:O	2:B:690:VAL:HG13	2.10	0.51
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.38	0.51
2:B:1183:LYS:N	2:B:1183:LYS:CE	2.71	0.51
3:C:239:PRO:O	3:C:241:ASP:N	2.43	0.51
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.46	0.51
1:A:600:PRO:C	1:A:602:ASP:H	2.19	0.51
1:A:746:MET:CE	2:B:1018:PRO:HG2	2.40	0.51
2:B:230:ALA:N	2:B:231:PRO:HD2	2.25	0.51
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.92	0.51
3:C:242:GLN:C	3:C:244:VAL:N	2.68	0.51
5:E:55:ARG:C	5:E:57:MET:N	2.69	0.51
5:E:55:ARG:C	5:E:57:MET:H	2.17	0.51
6:F:99:LEU:HD12	6:F:99:LEU:C	2.36	0.51
6:F:130:ILE:O	6:F:148:VAL:CG2	2.58	0.51
9:I:50:THR:HG22	9:I:51:ASN:N	2.26	0.51
12:L:34:CYS:SG	12:L:51:CYS:SG	3.08	0.51
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:CG	1:A:926:GLN:HE21	2.22	0.51
1:A:1161:THR:OG1	1:A:1239:ARG:NH2	2.44	0.51
2:B:327:ARG:O	2:B:331:LEU:HD13	2.11	0.51
2:B:900:ALA:HB3	12:L:61:THR:OG1	2.10	0.51
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.11	0.51
7:G:117:GLN:O	7:G:119:LEU:N	2.43	0.51
1:A:335:ARG:O	1:A:336:ILE:C	2.52	0.51
1:A:399:HIS:CG	1:A:400:PRO:N	2.78	0.51
1:A:809:THR:H	1:A:812:GLU:HB2	1.76	0.51
1:A:1369:ALA:O	1:A:1370:LEU:C	2.52	0.51
2:B:492:LEU:O	2:B:495:LEU:N	2.40	0.51
2:B:879:ARG:HH11	2:B:883:LEU:CD2	2.20	0.51
2:B:953:LEU:HD23	2:B:965:LYS:H	1.76	0.51
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.69	0.51
8:H:27:GLU:HA	8:H:38:LEU:O	2.11	0.51
1:A:241:VAL:HG13	1:A:266:LEU:HD13	1.91	0.51
1:A:418:SER:O	1:A:420:ARG:N	2.43	0.51
1:A:535:THR:CG2	1:A:616:VAL:HA	2.40	0.51
1:A:577:ILE:C	1:A:579:SER:N	2.65	0.51
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.17	0.51
1:A:1334:ASP:O	1:A:1336:MET:N	2.43	0.51
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.92	0.51
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.89	0.51
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.28	0.51
5:E:92:THR:O	5:E:95:THR:HB	2.11	0.51
7:G:17:PHE:N	7:G:17:PHE:CD2	2.78	0.51
7:G:79:PHE:CZ	7:G:106:MET:HE2	2.45	0.51
8:H:142:LEU:C	8:H:143:LEU:HD12	2.36	0.51
9:I:4:PHE:HE1	9:I:6:PHE:HE2	1.58	0.51
1:A:37:PHE:N	1:A:37:PHE:CD1	2.79	0.51
1:A:134:ARG:O	1:A:138:ILE:HG13	2.11	0.51
1:A:263:THR:HG22	1:A:263:THR:O	2.09	0.51
1:A:265:LYS:HE2	1:A:322:VAL:HG13	1.93	0.51
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.53	0.51
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.93	0.51
3:C:82:TYR:O	3:C:83:SER:C	2.54	0.51
4:D:66:ARG:O	4:D:70:PHE:HB2	2.10	0.51
6:F:131:PRO:C	6:F:132:LEU:HD23	2.35	0.51
6:F:143:PHE:C	6:F:143:PHE:CD1	2.89	0.51
7:G:49:LEU:HG	7:G:76:ALA:HA	1.93	0.51
8:H:59:ILE:O	8:H:60:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PRO:CB	1:A:245:PRO:CD	2.89	0.51
1:A:388:LEU:HD22	1:A:432:VAL:CG2	2.41	0.51
1:A:614:PHE:CD1	1:A:614:PHE:C	2.89	0.51
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.41	0.51
2:B:594:ALA:HA	2:B:617:ARG:HH12	1.76	0.51
2:B:745:PRO:C	2:B:747:MET:N	2.68	0.51
2:B:780:VAL:HG12	2:B:782:LEU:O	2.10	0.51
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.59	0.51
2:B:1087:PHE:HD2	2:B:1088:GLY:H	1.58	0.51
3:C:39:ALA:HA	3:C:164:ALA:CB	2.31	0.51
3:C:142:VAL:N	10:J:16:ASP:HB3	2.14	0.51
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.75	0.51
1:A:763:ALA:O	1:A:803:SER:HB3	2.11	0.51
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.46	0.51
1:A:1153:TYR:CE1	9:I:42:LEU:HD13	2.46	0.51
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.93	0.51
3:C:47:ASP:CA	12:L:69:ALA:CB	2.87	0.51
7:G:1:MET:O	7:G:3:PHE:CD1	2.64	0.51
8:H:82:PRO:O	8:H:84:ALA:N	2.35	0.51
1:A:24:PRO:HD2	1:A:233:TRP:CD1	2.45	0.50
1:A:68:GLN:O	1:A:70:CYS:N	2.43	0.50
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.52	0.50
1:A:1116:LEU:C	1:A:1116:LEU:HD12	2.36	0.50
1:A:1342:GLU:HG3	5:E:198:ILE:HD13	1.93	0.50
2:B:1174:LYS:O	2:B:1175:LEU:C	2.53	0.50
3:C:33:LEU:O	3:C:34:ARG:C	2.54	0.50
3:C:258:ILE:N	3:C:258:ILE:CD1	2.74	0.50
1:A:14:VAL:CG2	2:B:1216:LEU:HD13	2.40	0.50
1:A:76:GLU:O	1:A:76:GLU:CG	2.57	0.50
1:A:525:GLN:CD	2:B:836:GLU:HG2	2.36	0.50
2:B:168:GLY:HA2	2:B:454:THR:HG1	1.76	0.50
2:B:364:ILE:HG22	2:B:365:THR:N	2.26	0.50
2:B:843:GLN:O	2:B:844:SER:C	2.54	0.50
2:B:1174:LYS:O	2:B:1176:ASN:N	2.44	0.50
3:C:91:HIS:HD2	3:C:91:HIS:O	1.94	0.50
5:E:168:TYR:CB	5:E:170:LEU:HG	2.40	0.50
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.26	0.50
7:G:53:ASN:HD22	7:G:53:ASN:N	2.09	0.50
1:A:28:ARG:O	1:A:29:ALA:C	2.55	0.50
1:A:218:ASP:HA	1:A:221:SER:OG	2.11	0.50
1:A:269:ILE:CG1	1:A:299:HIS:HB3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:O	1:A:457:ALA:HA	2.12	0.50
1:A:577:ILE:O	1:A:580:VAL:HG23	2.11	0.50
1:A:823:GLY:O	1:A:825:ILE:N	2.44	0.50
1:A:885:THR:O	1:A:940:ARG:HD2	2.10	0.50
1:A:909:ASP:O	1:A:911:SER:N	2.45	0.50
1:A:1028:THR:O	1:A:1032:LEU:HD12	2.12	0.50
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	2.12	0.50
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.37	0.50
2:B:309:GLN:OE1	9:I:52:ILE:HD11	2.11	0.50
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.93	0.50
2:B:1022:THR:HG23	2:B:1022:THR:O	2.10	0.50
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.91	0.50
3:C:98:VAL:HG23	3:C:122:SER:HB3	1.93	0.50
4:D:134:THR:HG22	4:D:135:GLY:N	2.27	0.50
5:E:96:PHE:CZ	5:E:100:ILE:HD11	2.46	0.50
10:J:7:CYS:SG	10:J:49:MET:HE3	2.51	0.50
1:A:71:GLN:C	1:A:73:GLY:N	2.69	0.50
1:A:406:ILE:HG13	1:A:431:LYS:HB2	1.93	0.50
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.93	0.50
1:A:881:GLN:NE2	1:A:958:VAL:O	2.38	0.50
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.42	0.50
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.52	0.50
2:B:300:HIS:CE1	2:B:376:PHE:CE1	2.99	0.50
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.95	0.50
2:B:893:LEU:HD22	2:B:897:GLY:C	2.36	0.50
2:B:1186:ASP:C	2:B:1186:ASP:OD1	2.54	0.50
3:C:145:CYS:HA	10:J:2:ILE:HD11	1.92	0.50
6:F:77:ASP:C	6:F:79:ARG:N	2.67	0.50
7:G:26:LEU:O	7:G:29:LYS:N	2.43	0.50
8:H:128:ASN:CG	8:H:128:ASN:O	2.54	0.50
1:A:283:GLY:O	1:A:285:PRO:HD3	2.10	0.50
1:A:325:ILE:CG2	2:B:1210:MET:HE2	2.42	0.50
1:A:367:PRO:HA	1:A:463:ILE:O	2.10	0.50
1:A:784:LEU:HB3	1:A:785:PRO:HD2	1.94	0.50
1:A:1120:LEU:CD1	1:A:1120:LEU:H	2.24	0.50
1:A:1377:THR:O	1:A:1378:GLN:C	2.54	0.50
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.46	0.50
2:B:435:THR:CG2	2:B:437:GLU:HB2	2.41	0.50
2:B:511:PRO:O	2:B:512:ARG:C	2.54	0.50
2:B:765:PRO:O	2:B:768:THR:N	2.44	0.50
2:B:1034:VAL:HG12	2:B:1035:ALA:H	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1182:CYS:O	2:B:1183:LYS:C	2.54	0.50
3:C:63:ILE:O	3:C:64:ALA:C	2.55	0.50
3:C:256:ALA:C	3:C:258:ILE:H	2.19	0.50
4:D:56:ARG:NH2	4:D:57:LEU:HD21	2.26	0.50
1:A:120:GLU:C	1:A:122:MET:N	2.70	0.50
1:A:399:HIS:CB	1:A:400:PRO:CD	2.88	0.50
1:A:408:ASP:C	1:A:410:GLY:H	2.18	0.50
1:A:755:PHE:O	1:A:756:ILE:C	2.55	0.50
2:B:882:THR:O	2:B:883:LEU:HB2	2.11	0.50
3:C:242:GLN:C	3:C:244:VAL:H	2.18	0.50
7:G:80:LYS:O	7:G:82:PHE:CE1	2.65	0.50
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.92	0.50
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.41	0.50
1:A:443:LEU:O	1:A:489:LEU:HD12	2.12	0.50
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.27	0.50
1:A:874:ASP:CA	1:A:1058:VAL:HG22	2.42	0.50
1:A:1005:GLU:O	1:A:1009:ASN:HB2	2.12	0.50
1:A:135:PHE:C	1:A:137:ALA:N	2.70	0.50
1:A:215:SER:HB3	1:A:218:ASP:OD2	2.12	0.50
1:A:1265:ASN:C	1:A:1267:MET:N	2.67	0.50
2:B:642:ASP:CB	2:B:649:LYS:HA	2.42	0.50
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.41	0.50
2:B:890:TYR:O	2:B:892:LYS:N	2.45	0.50
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.42	0.50
8:H:62:SER:O	8:H:63:LEU:C	2.54	0.50
8:H:82:PRO:C	8:H:84:ALA:H	2.17	0.50
9:I:100:PHE:HD1	9:I:100:PHE:N	2.09	0.50
9:I:111:THR:HG22	9:I:113:ASP:N	2.27	0.50
12:L:27:LEU:HD13	12:L:37:LYS:HE2	1.94	0.50
1:A:466:SER:HB3	2:B:1103:ILE:HG12	1.93	0.50
1:A:873:MET:HE3	1:A:957:PRO:HG3	1.94	0.50
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.94	0.50
2:B:642:ASP:CA	2:B:649:LYS:HA	2.41	0.50
7:G:81:PRO:HA	7:G:85:GLU:OE1	2.12	0.50
2:B:284:ILE:HG12	2:B:324:ILE:HD12	1.92	0.49
2:B:521:LEU:HD13	2:B:633:VAL:HB	1.93	0.49
2:B:806:THR:HG22	2:B:808:ALA:HB3	1.94	0.49
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.94	0.49
3:C:18:VAL:O	3:C:20:PHE:HD2	1.95	0.49
7:G:15:PRO:O	7:G:16:SER:C	2.55	0.49
12:L:48:CYS:SG	12:L:49:LYS:N	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:VAL:HA	1:A:519:PRO:HA	1.93	0.49
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.12	0.49
1:A:1410:PHE:HA	2:B:1212:ILE:CD1	2.41	0.49
2:B:204:ILE:C	2:B:205:ILE:HD12	2.36	0.49
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.24	0.49
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.92	0.49
2:B:995:ARG:NH1	3:C:165:LYS:HG2	2.27	0.49
2:B:1006:ILE:HD13	10:J:44:TYR:HE2	1.72	0.49
3:C:29:MET:HE2	11:K:98:LEU:CD2	2.42	0.49
3:C:77:ILE:C	3:C:79:GLN:H	2.20	0.49
10:J:32:GLU:O	10:J:34:THR:N	2.44	0.49
1:A:58:LEU:O	1:A:59:GLY:O	2.30	0.49
1:A:504:LEU:HD11	6:F:91:ALA:CB	2.41	0.49
1:A:982:THR:HB	1:A:985:ASP:H	1.76	0.49
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.12	0.49
2:B:199:MET:HE2	2:B:492:LEU:CD2	2.42	0.49
2:B:299:GLU:HB3	2:B:571:PRO:HG3	1.94	0.49
3:C:140:ASN:O	3:C:141:GLY:O	2.30	0.49
3:C:243:VAL:O	3:C:243:VAL:HG12	2.11	0.49
5:E:22:MET:CE	5:E:26:ARG:NH2	2.74	0.49
8:H:27:GLU:HG2	8:H:39:THR:HG23	1.93	0.49
8:H:102:TYR:N	8:H:102:TYR:CD2	2.80	0.49
1:A:402:ALA:CB	1:A:434:ARG:HA	2.43	0.49
1:A:783:THR:HG22	1:A:784:LEU:HG	1.93	0.49
1:A:852:TYR:HA	1:A:1060:PRO:HB3	1.94	0.49
1:A:873:MET:HG2	1:A:957:PRO:HB3	1.95	0.49
1:A:1004:ASN:O	1:A:1008:GLN:HB2	2.12	0.49
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.27	0.49
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.13	0.49
2:B:980:PHE:HE2	2:B:1094:ARG:CB	2.24	0.49
2:B:1002:THR:HG21	2:B:1006:ILE:HD12	1.93	0.49
2:B:1081:LEU:O	2:B:1082:MET:C	2.55	0.49
1:A:84:ILE:HD11	1:A:270:LEU:CD1	2.34	0.49
1:A:116:ASP:O	1:A:118:HIS:N	2.45	0.49
1:A:311:GLN:CB	1:A:312:PRO:HD3	2.42	0.49
1:A:317:LYS:O	1:A:318:SER:CB	2.60	0.49
1:A:325:ILE:O	1:A:326:ARG:C	2.55	0.49
1:A:573:SER:O	1:A:576:GLN:HB2	2.12	0.49
1:A:765:VAL:HG12	1:A:766:GLY:N	2.26	0.49
1:A:877:HIS:O	1:A:878:ILE:CG1	2.60	0.49
1:A:1349:TYR:HB2	1:A:1372:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:MET:N	2:B:199:MET:SD	2.79	0.49
2:B:1174:LYS:O	2:B:1176:ASN:HB2	2.11	0.49
3:C:99:LEU:HD23	3:C:99:LEU:N	2.26	0.49
1:A:61:ILE:HG22	1:A:62:ASP:H	1.78	0.49
1:A:903:ASN:ND2	1:A:905:ASP:H	2.09	0.49
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.37	0.49
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.92	0.49
2:B:661:LEU:C	2:B:663:ALA:N	2.71	0.49
2:B:728:ARG:NH1	2:B:1047:PHE:HB3	2.26	0.49
2:B:916:THR:O	2:B:935:ARG:HG3	2.12	0.49
2:B:1178:ASN:O	2:B:1179:GLN:C	2.56	0.49
3:C:30:ALA:O	3:C:33:LEU:HB3	2.11	0.49
3:C:66:ARG:NH2	10:J:3:VAL:O	2.45	0.49
4:D:68:ARG:C	4:D:70:PHE:N	2.70	0.49
5:E:161:LYS:C	5:E:163:GLU:N	2.68	0.49
8:H:41:ASP:O	8:H:42:ILE:HG13	2.13	0.49
1:A:41:MET:O	1:A:42:ASP:C	2.56	0.49
1:A:311:GLN:CB	1:A:312:PRO:CD	2.91	0.49
1:A:340:LEU:HD21	2:B:1200:ALA:CA	2.43	0.49
1:A:414:ASP:OD1	1:A:416:ARG:HG3	2.11	0.49
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.95	0.49
1:A:545:GLN:O	1:A:548:ASN:N	2.45	0.49
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.95	0.49
1:A:622:VAL:O	1:A:622:VAL:HG22	2.13	0.49
1:A:1120:LEU:N	1:A:1120:LEU:CD1	2.76	0.49
1:A:1451:VAL:C	1:A:1453:TYR:N	2.70	0.49
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.94	0.49
7:G:80:LYS:HD3	7:G:80:LYS:H	1.77	0.49
12:L:49:LYS:O	12:L:50:ASP:CB	2.60	0.49
1:A:299:HIS:O	1:A:301:ALA:N	2.46	0.49
1:A:1280:GLU:O	1:A:1281:ARG:O	2.30	0.49
2:B:210:LYS:HG3	2:B:461:LEU:O	2.13	0.49
2:B:661:LEU:C	2:B:663:ALA:H	2.19	0.49
2:B:785:TYR:C	2:B:787:VAL:N	2.71	0.49
2:B:1197:PRO:HG2	2:B:1200:ALA:HB3	1.92	0.49
3:C:90:ASP:O	3:C:91:HIS:CB	2.60	0.49
9:I:34:TYR:CD2	9:I:34:TYR:C	2.90	0.49
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.95	0.49
1:A:244:PRO:O	1:A:246:VAL:N	2.46	0.49
1:A:244:PRO:HG2	1:A:245:PRO:CD	2.43	0.49
1:A:854:ASN:CB	1:A:1000:LEU:HD21	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.43	0.49
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.41	0.49
1:A:1388:GLY:O	1:A:1390:ASN:N	2.46	0.49
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.93	0.49
2:B:734:HIS:O	2:B:735:ALA:HB2	2.12	0.49
2:B:831:SER:CB	2:B:994:TYR:OH	2.60	0.49
5:E:48:ASP:CG	5:E:49:SER:N	2.69	0.49
6:F:116:ASP:C	6:F:116:ASP:OD1	2.55	0.49
10:J:27:GLU:O	10:J:29:GLU:N	2.45	0.49
1:A:26:GLU:O	1:A:27:VAL:C	2.54	0.49
1:A:218:ASP:O	1:A:219:PHE:C	2.56	0.49
1:A:243:PRO:O	1:A:244:PRO:C	2.55	0.49
1:A:450:LEU:HD12	1:A:450:LEU:H	1.78	0.49
1:A:629:LEU:O	1:A:633:VAL:HG23	2.12	0.49
1:A:652:VAL:O	1:A:653:VAL:C	2.56	0.49
1:A:1327:ILE:HG22	5:E:147:HIS:CE1	2.48	0.49
2:B:189:LEU:O	2:B:192:LEU:HB2	2.13	0.49
3:C:163:ILE:O	3:C:165:LYS:N	2.45	0.49
5:E:169:ARG:HH12	6:F:74:ILE:HD11	1.78	0.49
7:G:9:LEU:HG	7:G:10:ASN:N	2.27	0.49
8:H:99:GLY:HA3	8:H:118:PHE:HA	1.95	0.49
1:A:966:ASN:O	1:A:967:ALA:C	2.56	0.48
2:B:251:ILE:O	2:B:251:ILE:HG22	2.13	0.48
2:B:563:MET:HA	2:B:589:VAL:O	2.13	0.48
2:B:1034:VAL:O	2:B:1036:ALA:N	2.46	0.48
5:E:202:SER:HB3	5:E:205:SER:O	2.12	0.48
11:K:108:GLU:O	11:K:112:GLN:HG2	2.12	0.48
1:A:82:GLY:O	1:A:241:VAL:N	2.42	0.48
1:A:335:ARG:CA	1:A:339:ASN:HB2	2.40	0.48
1:A:552:TRP:O	1:A:554:PRO:HD3	2.13	0.48
1:A:1045:VAL:O	1:A:1049:ILE:HG13	2.13	0.48
2:B:361:LEU:N	2:B:362:PRO:CD	2.75	0.48
2:B:653:VAL:HG23	2:B:689:LEU:HB3	1.94	0.48
2:B:950:ASP:O	2:B:951:GLN:HB2	2.14	0.48
3:C:90:ASP:O	3:C:90:ASP:CG	2.57	0.48
7:G:117:GLN:C	7:G:119:LEU:N	2.69	0.48
11:K:47:ARG:HD2	11:K:47:ARG:C	2.38	0.48
12:L:46:VAL:CG1	12:L:56:LEU:HD12	2.43	0.48
1:A:369:SER:CB	11:K:2:ASN:OD1	2.60	0.48
1:A:1120:LEU:HD12	1:A:1120:LEU:H	1.78	0.48
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:PHE:CD1	2:B:811:TYR:CD2	3.01	0.48
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.48	0.48
2:B:642:ASP:CB	2:B:649:LYS:HG3	2.42	0.48
3:C:99:LEU:HD12	3:C:118:LEU:HD13	1.94	0.48
3:C:147:LEU:HD23	3:C:147:LEU:N	2.28	0.48
3:C:167:HIS:CD2	3:C:168:ALA:H	2.31	0.48
3:C:170:TRP:O	3:C:171:GLY:C	2.57	0.48
4:D:192:LYS:HB3	4:D:192:LYS:NZ	2.28	0.48
10:J:32:GLU:O	10:J:35:ALA:N	2.47	0.48
1:A:300:VAL:O	1:A:300:VAL:HG12	2.12	0.48
1:A:500:GLU:OE1	2:B:1143:ALA:C	2.57	0.48
1:A:626:ASN:C	1:A:628:GLY:H	2.21	0.48
1:A:1369:ALA:O	1:A:1373:ASP:OD2	2.31	0.48
2:B:744:HIS:HD2	2:B:746:SER:OG	1.95	0.48
2:B:794:ASN:C	2:B:795:ILE:HD12	2.37	0.48
4:D:138:ASN:C	4:D:140:ASP:N	2.70	0.48
7:G:96:GLN:HA	7:G:121:PHE:CE2	2.48	0.48
8:H:89:LEU:C	8:H:91:ASP:N	2.68	0.48
9:I:13:MET:HG3	9:I:14:LEU:H	1.74	0.48
9:I:85:PHE:CD1	9:I:99:LEU:HD13	2.45	0.48
10:J:53:HIS:CD2	10:J:54:VAL:C	2.92	0.48
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.95	0.48
1:A:40:THR:HG22	1:A:41:MET:CG	2.32	0.48
1:A:41:MET:HB3	1:A:48:ALA:O	2.13	0.48
1:A:174:ILE:HG23	1:A:182:VAL:O	2.13	0.48
1:A:340:LEU:HD13	1:A:1429:ILE:CG2	2.38	0.48
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.95	0.48
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.78	0.48
1:A:849:MET:HE3	1:A:1061:GLY:O	2.13	0.48
1:A:977:LYS:HB3	1:A:978:PRO:HD2	1.95	0.48
1:A:1209:MET:HE1	1:A:1236:LEU:HB3	1.94	0.48
1:A:1280:GLU:O	1:A:1281:ARG:C	2.55	0.48
2:B:414:ALA:O	2:B:415:GLN:C	2.57	0.48
2:B:785:TYR:C	2:B:787:VAL:H	2.19	0.48
3:C:25:VAL:HG23	3:C:228:PHE:CE1	2.48	0.48
3:C:255:VAL:O	3:C:255:VAL:HG12	2.14	0.48
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.95	0.48
7:G:43:GLY:CA	7:G:80:LYS:HB3	2.42	0.48
7:G:99:PHE:CE2	7:G:115:MET:HE2	2.49	0.48
8:H:143:LEU:C	8:H:144:ILE:HG13	2.38	0.48
1:A:65:LEU:O	1:A:66:LYS:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.46	0.48
1:A:351:THR:HG21	2:B:1103:ILE:HG13	1.95	0.48
1:A:357:PRO:HD2	2:B:833:TYR:CE1	2.48	0.48
1:A:551:TYR:CE2	11:K:62:LYS:HE2	2.49	0.48
1:A:626:ASN:O	1:A:628:GLY:N	2.44	0.48
1:A:1340:GLY:O	1:A:1343:ALA:N	2.43	0.48
2:B:180:TYR:CD1	2:B:180:TYR:N	2.82	0.48
2:B:223:VAL:CG1	2:B:381:MET:HG2	2.42	0.48
2:B:842:ASN:ND2	2:B:845:SER:OG	2.44	0.48
2:B:1177:HIS:C	2:B:1179:GLN:H	2.21	0.48
4:D:20:GLU:O	4:D:21:GLU:O	2.32	0.48
4:D:35:LEU:HD12	4:D:35:LEU:N	2.29	0.48
4:D:135:GLY:C	4:D:137:ASN:H	2.21	0.48
5:E:13:TRP:O	5:E:16:PHE:HB3	2.14	0.48
6:F:89:GLU:HB3	6:F:134:ILE:HD13	1.95	0.48
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.94	0.48
11:K:24:ASP:OD1	11:K:26:LYS:HB2	2.14	0.48
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.95	0.48
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.76	0.48
2:B:125:SER:HA	2:B:172:ILE:H	1.78	0.48
2:B:520:GLY:HA2	2:B:748:ILE:HG22	1.95	0.48
2:B:542:MET:HG2	2:B:747:MET:HB3	1.96	0.48
2:B:847:ASP:O	2:B:849:GLY:N	2.47	0.48
3:C:11:ARG:HD3	3:C:209:TYR:CE2	2.48	0.48
3:C:91:HIS:O	3:C:91:HIS:CD2	2.67	0.48
3:C:105:GLY:O	3:C:149:LYS:O	2.32	0.48
7:G:1:MET:O	7:G:1:MET:CE	2.61	0.48
7:G:66:GLY:O	7:G:67:SER:C	2.56	0.48
10:J:16:ASP:O	10:J:18:TRP:N	2.47	0.48
1:A:78:PRO:HA	2:B:1201:LYS:HZ2	1.77	0.48
1:A:166:GLY:O	1:A:167:CYS:CB	2.62	0.48
1:A:901:LEU:HG	1:A:926:GLN:NE2	2.25	0.48
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.13	0.48
1:A:1220:PHE:CD1	1:A:1224:LEU:HD23	2.49	0.48
2:B:387:LEU:O	2:B:392:ARG:HB2	2.13	0.48
2:B:519:TRP:C	2:B:519:TRP:CD1	2.91	0.48
2:B:591:ARG:O	2:B:592:ASN:C	2.56	0.48
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.43	0.48
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.94	0.48
2:B:803:LEU:HD12	2:B:1032:SER:HB3	1.95	0.48
2:B:893:LEU:HD11	2:B:910:VAL:CG1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:CD2	1:A:54:ASN:N	2.61	0.48
1:A:381:THR:CG2	1:A:383:TYR:H	2.27	0.48
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.93	0.48
1:A:1015:VAL:O	1:A:1016:THR:C	2.57	0.48
1:A:1327:ILE:HG22	5:E:147:HIS:HE1	1.77	0.48
1:A:1344:GLY:O	1:A:1345:ARG:C	2.56	0.48
2:B:461:LEU:N	2:B:461:LEU:HD12	2.29	0.48
2:B:542:MET:HE3	2:B:636:PRO:CG	2.42	0.48
2:B:954:VAL:O	12:L:55:ILE:O	2.31	0.48
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.79	0.48
3:C:77:ILE:CG2	3:C:161:LYS:HE3	2.39	0.48
3:C:209:TYR:HD1	3:C:209:TYR:H	1.60	0.48
4:D:51:ASN:O	4:D:52:LEU:C	2.57	0.48
5:E:18:THR:O	5:E:19:VAL:C	2.55	0.48
7:G:13:LEU:CD2	7:G:17:PHE:HB2	2.38	0.48
1:A:62:ASP:HB3	1:A:64:ASN:ND2	2.28	0.48
1:A:332:LYS:O	1:A:334:GLY:N	2.46	0.48
1:A:427:GLN:O	1:A:428:TYR:C	2.56	0.48
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.96	0.48
1:A:942:PHE:C	1:A:942:PHE:CD2	2.91	0.48
1:A:1001:ARG:O	1:A:1002:GLY:O	2.31	0.48
3:C:194:GLU:O	3:C:195:GLN:HG3	2.14	0.48
3:C:208:GLU:C	3:C:210:GLU:H	2.22	0.48
4:D:138:ASN:OD1	4:D:141:LEU:HB2	2.13	0.48
5:E:129:PRO:O	5:E:130:ALA:C	2.57	0.48
2:B:234:ILE:HD12	2:B:234:ILE:H	1.79	0.47
2:B:844:SER:O	2:B:847:ASP:HB2	2.14	0.47
3:C:35:ARG:NH1	11:K:41:THR:H	2.12	0.47
6:F:99:LEU:HD21	7:G:64:THR:O	2.14	0.47
7:G:26:LEU:HD12	7:G:56:ILE:HD13	1.95	0.47
7:G:77:VAL:O	7:G:77:VAL:HG12	2.14	0.47
7:G:91:VAL:HG12	7:G:92:VAL:N	2.28	0.47
11:K:93:SER:O	11:K:97:LYS:HG3	2.14	0.47
1:A:236:LEU:N	1:A:236:LEU:HD23	2.30	0.47
1:A:265:LYS:HZ1	1:A:322:VAL:HG22	1.77	0.47
1:A:326:ARG:HH22	1:A:1407:GLU:HG3	1.77	0.47
1:A:863:VAL:HG11	1:A:866:PHE:CE2	2.49	0.47
1:A:1101:LEU:O	1:A:1101:LEU:HD12	2.14	0.47
1:A:1446:ASP:HB2	6:F:133:VAL:CG2	2.44	0.47
2:B:806:THR:HG22	2:B:808:ALA:CB	2.44	0.47
2:B:864:LYS:N	2:B:872:GLU:OE1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:CYS:C	3:C:94:LYS:N	2.72	0.47
3:C:214:ASN:HB3	3:C:217:ASP:OD2	2.15	0.47
6:F:132:LEU:HD23	6:F:132:LEU:N	2.28	0.47
7:G:44:TYR:O	7:G:78:VAL:HA	2.14	0.47
7:G:143:ILE:CG2	7:G:144:ARG:N	2.75	0.47
8:H:58:THR:HG22	8:H:59:ILE:H	1.79	0.47
10:J:2:ILE:HG12	10:J:57:ILE:HD12	1.95	0.47
10:J:64:ASN:CB	10:J:65:PRO:CD	2.88	0.47
1:A:35:ILE:CG2	1:A:84:ILE:HD12	2.44	0.47
1:A:741:ASN:ND2	1:A:743:VAL:HB	2.24	0.47
1:A:768:GLN:NE2	1:A:816:HIS:ND1	2.62	0.47
1:A:1162:VAL:O	1:A:1162:VAL:HG12	2.14	0.47
1:A:1291:VAL:HG13	1:A:1292:PRO:N	2.29	0.47
1:A:1333:ILE:HG22	1:A:1334:ASP:N	2.29	0.47
2:B:27:ALA:O	2:B:29:ASP:N	2.47	0.47
2:B:523:CYS:SG	2:B:524:PRO:HD2	2.54	0.47
2:B:552:MET:C	2:B:554:ILE:N	2.72	0.47
2:B:865:LYS:HZ2	2:B:869:SER:HA	1.79	0.47
2:B:903:VAL:HG12	2:B:904:ARG:N	2.28	0.47
2:B:1034:VAL:C	2:B:1036:ALA:N	2.72	0.47
5:E:35:VAL:C	5:E:37:LEU:N	2.72	0.47
6:F:127:GLU:O	6:F:129:LYS:HG3	2.14	0.47
8:H:91:ASP:O	8:H:93:TYR:N	2.46	0.47
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.37	0.47
1:A:309:ALA:C	1:A:311:GLN:H	2.21	0.47
1:A:444:PHE:HB2	1:A:458:HIS:HD2	1.80	0.47
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.49	0.47
1:A:1006:ILE:HD12	5:E:163:GLU:HG3	1.95	0.47
1:A:1431:GLY:HA3	2:B:1152:MET:SD	2.55	0.47
2:B:235:SER:C	2:B:236:HIS:CD2	2.93	0.47
2:B:855:PHE:CD1	2:B:855:PHE:C	2.90	0.47
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.96	0.47
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.97	0.47
8:H:58:THR:HB	8:H:143:LEU:HD13	1.97	0.47
1:A:92:HIS:HB2	1:A:236:LEU:HD21	1.96	0.47
1:A:167:CYS:SG	1:A:167:CYS:O	2.72	0.47
2:B:373:ARG:CG	2:B:566:LEU:HD23	2.45	0.47
2:B:882:THR:HG21	2:B:935:ARG:HA	1.95	0.47
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.30	0.47
5:E:157:SER:HG	5:E:160:GLU:HG3	1.78	0.47
1:A:456:MET:HE1	1:A:474:VAL:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:ASP:HB3	1:A:1130:GLN:HB2	1.96	0.47
1:A:1227:ILE:CG2	1:A:1228:TRP:N	2.78	0.47
1:A:1265:ASN:O	1:A:1268:LEU:N	2.41	0.47
1:A:1441:PHE:HB2	6:F:135:ARG:O	2.15	0.47
2:B:654:ARG:C	2:B:656:GLY:H	2.23	0.47
2:B:708:GLU:O	2:B:709:ASP:C	2.58	0.47
2:B:918:ILE:HD12	2:B:935:ARG:HD3	1.97	0.47
4:D:40:HIS:CE1	4:D:41:GLN:HG3	2.49	0.47
7:G:81:PRO:C	7:G:82:PHE:CD1	2.93	0.47
1:A:324:SER:O	1:A:325:ILE:C	2.56	0.47
1:A:496:GLU:O	1:A:499:ALA:HB3	2.15	0.47
1:A:547:LEU:HD22	11:K:58:PHE:HD1	1.78	0.47
1:A:872:GLY:O	1:A:1058:VAL:HG23	2.13	0.47
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.49	0.47
1:A:1053:PHE:C	1:A:1055:ARG:N	2.70	0.47
1:A:1265:ASN:C	1:A:1267:MET:H	2.23	0.47
1:A:1451:VAL:O	1:A:1454:MET:HG2	2.15	0.47
2:B:205:ILE:HG22	2:B:206:ASN:N	2.30	0.47
2:B:225:VAL:HA	2:B:237:VAL:O	2.14	0.47
2:B:305:VAL:O	2:B:305:VAL:HG12	2.15	0.47
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.95	0.47
2:B:999:MET:HE3	2:B:999:MET:CA	2.35	0.47
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.55	0.47
2:B:1214:PRO:O	2:B:1214:PRO:HG2	2.14	0.47
3:C:6:PRO:HB3	3:C:25:VAL:CG1	2.45	0.47
3:C:183:TRP:O	3:C:185:LYS:N	2.48	0.47
7:G:99:PHE:CD1	7:G:99:PHE:C	2.93	0.47
9:I:61:ASP:O	9:I:63:GLY:N	2.47	0.47
9:I:111:THR:CG2	9:I:112:SER:N	2.77	0.47
10:J:16:ASP:OD1	10:J:17:LYS:N	2.42	0.47
10:J:47:ARG:NH1	10:J:47:ARG:HG2	2.29	0.47
10:J:48:ARG:HD2	10:J:49:MET:N	2.29	0.47
12:L:46:VAL:O	12:L:46:VAL:HG12	2.14	0.47
1:A:279:LEU:O	1:A:284:ALA:HB2	2.15	0.47
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.45	0.47
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.18	0.47
1:A:699:ALA:HB3	1:A:701:LEU:HG	1.95	0.47
1:A:823:GLY:C	1:A:825:ILE:N	2.72	0.47
1:A:1261:LYS:HA	1:A:1264:GLU:HB3	1.96	0.47
2:B:230:ALA:N	2:B:231:PRO:CD	2.77	0.47
2:B:333:PHE:O	2:B:334:ILE:CG1	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:GLU:O	3:C:90:ASP:HB3	2.15	0.47
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.95	0.47
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.50	0.47
7:G:143:ILE:HG22	7:G:144:ARG:H	1.76	0.47
9:I:75:CYS:SG	9:I:80:SER:N	2.85	0.47
10:J:31:ASP:O	10:J:32:GLU:C	2.58	0.47
1:A:402:ALA:HB1	1:A:433:GLU:O	2.15	0.47
1:A:553:VAL:HG22	1:A:652:VAL:CG2	2.44	0.47
1:A:570:PRO:C	1:A:571:LEU:HD12	2.40	0.47
1:A:786:HIS:HE1	2:B:705:MET:HE1	1.80	0.47
2:B:552:MET:HA	2:B:555:ILE:HB	1.96	0.47
2:B:999:MET:HE2	2:B:1000:PRO:HD2	1.97	0.47
2:B:1131:GLY:O	2:B:1132:GLU:C	2.58	0.47
2:B:1187:ASN:OD1	2:B:1188:LYS:N	2.40	0.47
2:B:1198:TYR:C	2:B:1198:TYR:CD2	2.93	0.47
3:C:90:ASP:O	3:C:90:ASP:OD1	2.33	0.47
3:C:133:ILE:HD12	3:C:237:SER:HA	1.96	0.47
3:C:236:GLY:C	3:C:238:ILE:N	2.72	0.47
4:D:146:GLN:O	4:D:147:TYR:C	2.57	0.47
5:E:157:SER:O	5:E:159:ASP:N	2.48	0.47
8:H:83:GLN:C	8:H:85:GLY:N	2.73	0.47
8:H:111:LEU:HD23	8:H:127:GLY:O	2.15	0.47
11:K:52:ASN:O	11:K:54:ARG:N	2.48	0.47
11:K:59:ALA:HA	11:K:74:ARG:O	2.15	0.47
1:A:2:VAL:CG2	2:B:1158:PHE:HA	2.45	0.47
1:A:326:ARG:HG2	1:A:327:ALA:N	2.29	0.47
1:A:347:PHE:H	2:B:1107:ALA:HA	1.80	0.47
1:A:877:HIS:C	1:A:878:ILE:CG1	2.88	0.47
2:B:298:LEU:HD13	2:B:314:LEU:HD13	1.97	0.47
2:B:558:LEU:O	2:B:560:GLU:N	2.47	0.47
2:B:865:LYS:HE2	2:B:871:THR:OG1	2.15	0.47
2:B:1050:ILE:CG2	2:B:1051:THR:N	2.78	0.47
3:C:77:ILE:O	3:C:79:GLN:N	2.46	0.47
3:C:253:LYS:O	3:C:256:ALA:HB3	2.15	0.47
3:C:257:SER:C	3:C:258:ILE:HD12	2.40	0.47
4:D:191:ALA:C	4:D:193:THR:N	2.73	0.47
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.37	0.47
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.44	0.47
6:F:128:LYS:HD3	6:F:149:GLU:O	2.15	0.47
7:G:13:LEU:O	7:G:67:SER:HA	2.15	0.47
7:G:121:PHE:HB2	7:G:130:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:VAL:HG22	8:H:26:ILE:HD11	1.96	0.47
10:J:56:LEU:O	10:J:59:LYS:N	2.45	0.47
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.14	0.46
1:A:510:GLN:OE1	1:A:510:GLN:HA	2.14	0.46
2:B:582:VAL:HG12	2:B:587:HIS:NE2	2.30	0.46
2:B:710:LEU:C	2:B:711:GLU:HG2	2.40	0.46
2:B:769:TYR:C	2:B:771:SER:N	2.73	0.46
2:B:1017:ILE:CB	2:B:1018:PRO:HD3	2.44	0.46
4:D:38:ILE:HG22	4:D:39:ASN:O	2.14	0.46
6:F:132:LEU:O	6:F:148:VAL:HG22	2.15	0.46
9:I:56:ALA:O	9:I:57:GLY:O	2.34	0.46
9:I:85:PHE:N	9:I:85:PHE:CD2	2.60	0.46
1:A:7:SER:C	1:A:9:ALA:H	2.23	0.46
1:A:105:CYS:O	1:A:114:LEU:HG	2.14	0.46
1:A:608:ILE:C	1:A:610:GLY:N	2.72	0.46
1:A:935:GLN:C	1:A:937:VAL:N	2.72	0.46
1:A:1147:THR:HG22	9:I:48:LEU:HD12	1.97	0.46
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.14	0.46
1:A:1435:PRO:O	1:A:1436:ILE:HG13	2.15	0.46
2:B:307:ASP:O	2:B:308:TRP:C	2.58	0.46
2:B:376:PHE:HE2	2:B:569:TYR:HD2	1.62	0.46
2:B:681:TRP:O	2:B:683:SER:N	2.49	0.46
3:C:133:ILE:CD1	3:C:237:SER:HA	2.45	0.46
4:D:154:PHE:HB2	4:D:160:VAL:HG22	1.97	0.46
7:G:14:HIS:HD2	7:G:16:SER:CB	2.28	0.46
7:G:18:PHE:HA	7:G:22:MET:HE3	1.95	0.46
10:J:8:PHE:H	10:J:49:MET:CE	2.28	0.46
1:A:77:CYS:C	1:A:78:PRO:O	2.45	0.46
1:A:116:ASP:O	1:A:117:GLU:C	2.57	0.46
1:A:277:GLU:C	1:A:279:LEU:N	2.73	0.46
1:A:761:MET:HA	1:A:804:TYR:HB2	1.97	0.46
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.29	0.46
2:B:39:ARG:HH21	2:B:665:GLU:CG	2.26	0.46
2:B:756:ILE:O	2:B:759:PRO:HD3	2.14	0.46
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.77	0.46
3:C:179:GLU:O	3:C:180:TYR:HB3	2.14	0.46
4:D:47:LEU:CD1	4:D:48:ILE:N	2.77	0.46
5:E:124:VAL:CG1	5:E:132:ILE:HB	2.43	0.46
10:J:7:CYS:CA	10:J:49:MET:HE3	2.45	0.46
1:A:254:GLU:O	1:A:256:GLN:N	2.47	0.46
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ASP:O	1:A:854:ASN:CB	2.64	0.46
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	2.13	0.46
1:A:1019:CYS:O	1:A:1022:LEU:N	2.48	0.46
1:A:1044:TRP:O	1:A:1045:VAL:C	2.59	0.46
2:B:638:PHE:HB2	2:B:741:CYS:O	2.16	0.46
2:B:653:VAL:HG22	2:B:689:LEU:HD13	1.97	0.46
2:B:654:ARG:O	2:B:656:GLY:N	2.48	0.46
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.96	0.46
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.70	0.46
2:B:820:GLY:C	2:B:1091:TYR:CE1	2.94	0.46
3:C:112:ASN:HB2	3:C:114:TYR:CE1	2.50	0.46
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.97	0.46
6:F:111:LEU:O	6:F:113:GLY:N	2.48	0.46
7:G:115:MET:HB3	7:G:116:PRO:CD	2.42	0.46
1:A:356:ASP:C	1:A:358:ASN:H	2.24	0.46
1:A:498:ARG:O	1:A:501:LEU:N	2.47	0.46
1:A:1150:SER:O	1:A:1151:GLU:HG3	2.15	0.46
2:B:104:GLU:OE1	12:L:54:ARG:NH2	2.49	0.46
2:B:400:HIS:ND1	2:B:517:THR:HG21	2.31	0.46
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.79	0.46
2:B:435:THR:C	2:B:437:GLU:H	2.23	0.46
2:B:603:LEU:HD13	2:B:608:ASP:CB	2.43	0.46
2:B:613:VAL:HG22	2:B:628:THR:HA	1.96	0.46
2:B:834:ASN:HA	2:B:838:SER:O	2.15	0.46
4:D:19:GLU:O	4:D:21:GLU:N	2.49	0.46
9:I:106:CYS:O	9:I:107:SER:HB2	2.16	0.46
10:J:7:CYS:HA	10:J:49:MET:HE3	1.98	0.46
12:L:27:LEU:HD23	12:L:27:LEU:N	2.29	0.46
1:A:17:VAL:HA	2:B:1215:ARG:O	2.15	0.46
1:A:500:GLU:OE2	2:B:1145:SER:CB	2.63	0.46
1:A:626:ASN:O	1:A:631:HIS:CD2	2.69	0.46
1:A:1369:ALA:O	1:A:1372:VAL:HG12	2.14	0.46
2:B:981:ALA:HB3	2:B:1095:LEU:HD21	1.97	0.46
2:B:999:MET:HG2	2:B:1007:VAL:HG22	1.97	0.46
2:B:1002:THR:O	2:B:1003:ALA:C	2.59	0.46
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.53	0.46
2:B:1197:PRO:O	2:B:1200:ALA:N	2.48	0.46
4:D:206:GLU:C	4:D:208:GLU:H	2.23	0.46
1:A:7:SER:CB	2:B:1175:LEU:HD22	2.45	0.46
1:A:34:LYS:HD3	1:A:34:LYS:N	2.31	0.46
1:A:1132:LYS:O	1:A:1134:ILE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1283:VAL:HG12	1:A:1284:MET:H	1.81	0.46
2:B:284:ILE:HG23	2:B:324:ILE:CD1	2.45	0.46
2:B:465:ASN:ND2	2:B:465:ASN:H	2.12	0.46
2:B:948:ILE:C	2:B:949:VAL:O	2.56	0.46
2:B:990:ILE:HG22	2:B:991:GLY:N	2.31	0.46
2:B:1034:VAL:HG23	2:B:1059:LEU:HD13	1.98	0.46
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.51	0.46
2:B:1152:MET:O	2:B:1154:ALA:N	2.49	0.46
3:C:29:MET:HE2	11:K:98:LEU:HD21	1.97	0.46
3:C:66:ARG:CZ	10:J:2:ILE:HG21	2.46	0.46
3:C:100:THR:HG22	3:C:101:LEU:N	2.31	0.46
3:C:259:LEU:CD1	11:K:91:CYS:HB2	2.45	0.46
5:E:205:SER:O	5:E:206:GLY:C	2.58	0.46
8:H:25:ARG:HA	8:H:41:ASP:HA	1.98	0.46
8:H:58:THR:HG22	8:H:59:ILE:N	2.31	0.46
8:H:123:MET:HG2	8:H:124:ARG:N	2.31	0.46
10:J:56:LEU:O	10:J:57:ILE:C	2.58	0.46
1:A:553:VAL:HG13	1:A:648:ASN:HB3	1.97	0.46
1:A:655:PHE:O	1:A:658:LEU:HB3	2.16	0.46
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.31	0.46
2:B:563:MET:CE	2:B:580:VAL:HB	2.43	0.46
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.31	0.46
3:C:104:PHE:HD2	3:C:105:GLY:N	2.14	0.46
3:C:181:ASP:OD1	3:C:186:LEU:HD13	2.16	0.46
4:D:192:LYS:NZ	4:D:199:ASN:HA	2.30	0.46
5:E:35:VAL:O	5:E:37:LEU:N	2.48	0.46
1:A:134:ARG:HD3	1:A:221:SER:O	2.16	0.46
1:A:344:ARG:HG2	1:A:344:ARG:HH11	1.80	0.46
1:A:524:VAL:HG12	1:A:525:GLN:HE21	1.81	0.46
1:A:971:PHE:HE2	1:A:1040:GLN:HG2	1.80	0.46
1:A:1173:HIS:C	1:A:1174:PHE:CD1	2.94	0.46
1:A:1334:ASP:C	1:A:1336:MET:H	2.23	0.46
2:B:118:ARG:HG2	2:B:204:ILE:HD13	1.97	0.46
2:B:185:THR:H	2:B:188:ASP:HB2	1.80	0.46
2:B:560:GLU:O	2:B:561:TRP:CD1	2.69	0.46
2:B:711:GLU:H	2:B:712:PRO:HD2	1.80	0.46
5:E:98:ILE:O	5:E:99:HIS:C	2.59	0.46
7:G:108:VAL:HG13	7:G:159:ALA:O	2.15	0.46
9:I:61:ASP:C	9:I:63:GLY:N	2.73	0.46
11:K:58:PHE:HB3	11:K:76:GLN:HE21	1.81	0.46
1:A:231:PRO:C	1:A:233:TRP:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:HB3	2:B:935:ARG:CZ	2.45	0.46
1:A:779:PHE:CE1	1:A:785:PRO:CD	2.93	0.46
1:A:829:VAL:C	1:A:831:THR:N	2.74	0.46
1:A:1135:ARG:C	1:A:1137:ALA:H	2.24	0.46
2:B:345:LYS:O	2:B:347:LYS:HG2	2.16	0.46
2:B:405:ARG:HA	2:B:631:GLY:O	2.16	0.46
2:B:435:THR:C	2:B:437:GLU:N	2.74	0.46
2:B:492:LEU:O	2:B:493:SER:C	2.60	0.46
2:B:729:ILE:O	2:B:729:ILE:HG22	2.15	0.46
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.46	0.46
4:D:196:PRO:C	4:D:198:LEU:H	2.23	0.46
6:F:81:THR:HB	6:F:136:ARG:NH1	2.30	0.46
7:G:14:HIS:CD2	7:G:16:SER:CB	2.98	0.46
8:H:7:ASP:O	8:H:8:ASP:HB2	2.15	0.46
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.46	0.46
10:J:23:ASN:O	10:J:25:LEU:N	2.49	0.46
12:L:62:LYS:O	12:L:63:ARG:C	2.59	0.46
1:A:43:GLU:O	1:A:44:THR:CB	2.64	0.45
1:A:608:ILE:HG13	1:A:613:ILE:HD12	1.97	0.45
1:A:645:LEU:O	1:A:646:PHE:C	2.59	0.45
1:A:1213:GLY:O	1:A:1214:GLU:C	2.59	0.45
1:A:1297:GLU:H	1:A:1297:GLU:HG3	1.51	0.45
1:A:1410:PHE:C	1:A:1412:ALA:H	2.23	0.45
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.15	0.45
2:B:595:ARG:O	2:B:596:LEU:C	2.59	0.45
3:C:75:MET:O	3:C:246:ARG:NH2	2.49	0.45
5:E:161:LYS:O	5:E:163:GLU:N	2.49	0.45
7:G:115:MET:CB	7:G:116:PRO:HD2	2.41	0.45
8:H:110:ASP:O	8:H:128:ASN:ND2	2.48	0.45
9:I:4:PHE:HE1	9:I:6:PHE:CE2	2.34	0.45
11:K:40:HIS:O	11:K:41:THR:C	2.59	0.45
1:A:116:ASP:C	1:A:118:HIS:N	2.71	0.45
1:A:332:LYS:C	1:A:334:GLY:H	2.25	0.45
1:A:474:VAL:C	1:A:477:PRO:HD2	2.41	0.45
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.50	0.45
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.17	0.45
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.31	0.45
1:A:1313:LEU:C	1:A:1315:GLU:H	2.24	0.45
1:A:1444:MET:CG	7:G:60:ARG:HA	2.46	0.45
2:B:114:PRO:O	2:B:117:ALA:N	2.48	0.45
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1068:GLY:O	2:B:1069:PHE:C	2.59	0.45
2:B:1162:ILE:CG2	2:B:1163:CYS:H	2.25	0.45
3:C:67:LEU:HD11	3:C:155:LEU:HD12	1.97	0.45
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.98	0.45
8:H:93:TYR:N	8:H:93:TYR:CD1	2.84	0.45
11:K:31:VAL:HG12	11:K:32:VAL:H	1.79	0.45
1:A:95:PHE:CD1	1:A:234:MET:HG2	2.51	0.45
1:A:250:ILE:O	1:A:258:GLY:HA3	2.16	0.45
1:A:298:PHE:O	1:A:301:ALA:HB3	2.15	0.45
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.98	0.45
1:A:577:ILE:O	1:A:578:LEU:C	2.56	0.45
1:A:673:GLY:N	1:A:674:PRO:HD2	2.30	0.45
1:A:874:ASP:O	1:A:876:ALA:N	2.50	0.45
1:A:935:GLN:O	1:A:936:LEU:C	2.59	0.45
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.97	0.45
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.81	0.45
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.74	0.45
2:B:879:ARG:O	2:B:880:THR:HB	2.15	0.45
3:C:90:ASP:O	3:C:91:HIS:HB3	2.16	0.45
3:C:112:ASN:HD22	3:C:112:ASN:N	2.12	0.45
4:D:53:SER:HB3	4:D:152:SER:HA	1.98	0.45
7:G:106:MET:HG2	7:G:107:LYS:N	2.31	0.45
7:G:139:ILE:HG22	7:G:140:LYS:N	2.31	0.45
1:A:33:ALA:O	1:A:83:HIS:HD2	1.99	0.45
1:A:41:MET:HB2	1:A:42:ASP:H	1.46	0.45
1:A:474:VAL:HG22	1:A:474:VAL:O	2.16	0.45
1:A:1156:PRO:HA	1:A:1190:PRO:CB	2.46	0.45
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.16	0.45
2:B:130:VAL:HG23	2:B:167:ILE:HD12	1.98	0.45
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.98	0.45
2:B:899:ILE:O	2:B:952:VAL:HG21	2.16	0.45
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.42	0.45
4:D:54:GLU:OE1	4:D:164:ILE:HD11	2.16	0.45
5:E:17:ARG:O	5:E:20:LYS:HB2	2.16	0.45
6:F:147:SER:OG	6:F:150:GLU:HG3	2.15	0.45
7:G:73:LYS:HE3	7:G:74:TYR:O	2.17	0.45
10:J:34:THR:O	10:J:35:ALA:C	2.59	0.45
12:L:30:ILE:HG22	12:L:31:CYS:N	2.32	0.45
1:A:2:VAL:HG21	2:B:1158:PHE:HA	1.98	0.45
1:A:70:CYS:O	1:A:71:GLN:C	2.59	0.45
1:A:289:ILE:O	1:A:291:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:LEU:HD21	9:I:114:GLN:HB2	1.98	0.45
1:A:1001:ARG:HG2	1:A:1001:ARG:HH11	1.82	0.45
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.46	0.45
1:A:1389:PHE:CD1	1:A:1389:PHE:C	2.94	0.45
2:B:46:GLN:CG	2:B:47:GLN:H	2.10	0.45
2:B:410:GLY:O	2:B:412:LEU:N	2.50	0.45
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.46	0.45
2:B:784:ASN:O	2:B:788:ARG:HG3	2.17	0.45
2:B:826:ALA:HB2	2:B:1008:PRO:HB3	1.98	0.45
2:B:936:ASP:OD1	2:B:938:SER:N	2.43	0.45
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.49	0.45
4:D:51:ASN:ND2	4:D:54:GLU:OE2	2.50	0.45
5:E:136:ASN:OD1	5:E:137:GLU:N	2.50	0.45
6:F:123:LYS:O	6:F:124:GLU:C	2.58	0.45
7:G:50:ASP:O	7:G:51:TYR:C	2.58	0.45
10:J:51:LEU:O	10:J:51:LEU:HD12	2.17	0.45
1:A:84:ILE:O	1:A:84:ILE:CG2	2.63	0.45
1:A:332:LYS:HG3	1:A:333:GLU:N	2.30	0.45
1:A:399:HIS:O	1:A:400:PRO:C	2.58	0.45
1:A:432:VAL:O	1:A:433:GLU:C	2.60	0.45
1:A:514:PRO:C	1:A:516:SER:N	2.75	0.45
1:A:767:GLN:HB2	1:A:799:PHE:HD1	1.82	0.45
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.16	0.45
2:B:237:VAL:HG12	2:B:238:ALA:N	2.31	0.45
2:B:840:ILE:CG2	2:B:994:TYR:HD1	2.30	0.45
2:B:854:LEU:HB3	2:B:856:PHE:HE1	1.81	0.45
2:B:873:THR:O	2:B:914:LYS:HA	2.16	0.45
2:B:1065:GLN:HE21	2:B:1066:SER:CA	2.30	0.45
3:C:105:GLY:HA3	3:C:149:LYS:O	2.17	0.45
3:C:146:LYS:HB2	10:J:61:LEU:HD11	1.97	0.45
4:D:51:ASN:C	4:D:52:LEU:O	2.59	0.45
4:D:153:ARG:HB3	4:D:154:PHE:CE1	2.52	0.45
5:E:16:PHE:O	5:E:17:ARG:C	2.59	0.45
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.78	0.45
12:L:58:LYS:O	12:L:59:ALA:O	2.34	0.45
1:A:44:THR:O	1:A:45:GLN:HB2	2.17	0.45
1:A:253:ASN:CB	2:B:935:ARG:CZ	2.94	0.45
1:A:296:LEU:O	1:A:297:GLN:C	2.58	0.45
1:A:415:LEU:HA	1:A:415:LEU:HD23	1.75	0.45
1:A:499:ALA:O	1:A:503:GLN:HB2	2.16	0.45
1:A:524:VAL:CG1	1:A:525:GLN:H	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HG22	1:A:710:LEU:N	2.32	0.45
1:A:982:THR:O	1:A:985:ASP:HB2	2.16	0.45
1:A:1053:PHE:O	1:A:1055:ARG:N	2.50	0.45
1:A:1161:THR:CG2	1:A:1163:ILE:HG13	2.46	0.45
2:B:115:GLN:HG2	2:B:193:LYS:CB	2.46	0.45
2:B:294:ASP:OD2	2:B:294:ASP:N	2.50	0.45
2:B:593:PRO:O	2:B:594:ALA:C	2.60	0.45
2:B:603:LEU:HD22	2:B:603:LEU:HA	1.86	0.45
2:B:979:LYS:HG3	2:B:989:THR:HG22	1.98	0.45
3:C:76:ASP:OD2	3:C:128:ASN:N	2.49	0.45
5:E:129:PRO:O	5:E:130:ALA:O	2.34	0.45
5:E:212:ARG:HG3	5:E:212:ARG:HH11	1.82	0.45
6:F:143:PHE:C	6:F:143:PHE:HD1	2.23	0.45
8:H:4:THR:O	8:H:5:LEU:HD23	2.17	0.45
9:I:15:TYR:N	9:I:15:TYR:CD1	2.84	0.45
10:J:1:MET:HE2	10:J:60:PHE:HE2	1.78	0.45
1:A:244:PRO:HG2	1:A:245:PRO:HD2	1.99	0.45
1:A:252:PHE:HB2	1:A:256:GLN:CD	2.42	0.45
1:A:353:ILE:HB	1:A:470:LEU:CD2	2.47	0.45
1:A:666:ILE:CD1	1:A:667:GLY:N	2.80	0.45
1:A:1019:CYS:O	1:A:1020:CYS:C	2.60	0.45
1:A:1205:LYS:O	1:A:1206:ASP:C	2.59	0.45
2:B:769:TYR:O	2:B:772:ALA:N	2.50	0.45
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.84	0.45
4:D:153:ARG:C	4:D:154:PHE:CG	2.95	0.45
9:I:110:PHE:CD2	9:I:110:PHE:N	2.85	0.45
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.46	0.45
1:A:418:SER:C	1:A:420:ARG:H	2.24	0.45
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.47	0.45
1:A:841:LEU:O	1:A:845:LEU:HG	2.16	0.45
1:A:947:PHE:CD2	1:A:954:TRP:CZ2	3.04	0.45
1:A:1215:ARG:HD2	1:A:1215:ARG:HA	1.72	0.45
1:A:1445:ILE:HD11	7:G:61:ILE:HG12	1.99	0.45
2:B:48:LEU:O	2:B:49:ASP:C	2.59	0.45
2:B:307:ASP:O	2:B:309:GLN:N	2.50	0.45
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.99	0.45
6:F:85:MET:HE2	6:F:93:ILE:HD12	1.99	0.45
11:K:46:ILE:O	11:K:46:ILE:HG22	2.16	0.45
11:K:53:ASP:O	11:K:55:LYS:N	2.50	0.45
1:A:590:ARG:HH21	1:A:620:LYS:CB	2.28	0.45
1:A:665:GLY:C	1:A:666:ILE:HD12	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:ASP:HA	1:A:741:ASN:OD1	2.17	0.45
1:A:853:ASP:OD1	1:A:853:ASP:C	2.60	0.45
1:A:909:ASP:C	1:A:911:SER:H	2.25	0.45
1:A:1349:TYR:CA	1:A:1372:VAL:HG21	2.47	0.45
1:A:1388:GLY:C	1:A:1390:ASN:H	2.25	0.45
1:A:1409:LEU:O	1:A:1412:ALA:HB3	2.17	0.45
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.51	0.45
2:B:329:THR:O	2:B:332:ASP:HB3	2.16	0.45
2:B:758:PHE:N	2:B:759:PRO:CD	2.80	0.45
2:B:1008:PRO:HB2	2:B:1010:LEU:O	2.17	0.45
2:B:1177:HIS:O	2:B:1179:GLN:N	2.50	0.45
5:E:43:LYS:O	5:E:45:LYS:N	2.48	0.45
1:A:63:ARG:HA	1:A:74:MET:HE2	1.99	0.44
1:A:1401:SER:O	1:A:1402:PHE:HB2	2.18	0.44
2:B:294:ASP:O	2:B:296:GLU:N	2.48	0.44
2:B:730:ARG:O	2:B:731:VAL:O	2.36	0.44
3:C:38:ILE:HA	3:C:173:ALA:HB2	1.98	0.44
3:C:144:ILE:O	3:C:145:CYS:HB3	2.17	0.44
7:G:31:LEU:HD22	7:G:48:VAL:HG21	1.99	0.44
8:H:82:PRO:C	8:H:84:ALA:N	2.75	0.44
1:A:407:ARG:HG2	1:A:430:TRP:CZ3	2.52	0.44
1:A:418:SER:C	1:A:420:ARG:N	2.75	0.44
1:A:809:THR:O	1:A:810:PRO:C	2.59	0.44
1:A:929:LEU:CD2	1:A:983:ILE:HG21	2.47	0.44
1:A:1027:ALA:O	1:A:1028:THR:C	2.59	0.44
1:A:1265:ASN:O	1:A:1267:MET:N	2.50	0.44
1:A:1334:ASP:C	1:A:1336:MET:N	2.73	0.44
2:B:410:GLY:O	2:B:411:PRO:C	2.60	0.44
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.53	0.44
2:B:570:VAL:HG23	2:B:573:GLN:HB3	1.99	0.44
2:B:640:VAL:O	2:B:640:VAL:HG12	2.16	0.44
2:B:789:MET:HE2	2:B:953:LEU:HD22	1.98	0.44
3:C:44:LEU:HD23	3:C:45:ALA:N	2.32	0.44
3:C:123:ASN:ND2	3:C:125:MET:SD	2.90	0.44
3:C:262:LEU:HD23	3:C:262:LEU:HA	1.75	0.44
4:D:141:LEU:O	4:D:142:LYS:C	2.61	0.44
5:E:124:VAL:HB	5:E:125:PRO:HD3	2.00	0.44
5:E:134:THR:C	5:E:135:PHE:HD1	2.26	0.44
7:G:48:VAL:HG13	7:G:74:TYR:HD1	1.82	0.44
10:J:2:ILE:C	10:J:53:HIS:CE1	2.95	0.44
1:A:215:SER:O	1:A:218:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:VAL:HG12	1:A:353:ILE:N	2.32	0.44
1:A:709:THR:HB	1:A:712:GLU:HG3	1.99	0.44
1:A:964:ILE:O	1:A:965:GLN:C	2.59	0.44
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.31	0.44
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.99	0.44
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.47	0.44
2:B:546:SER:OG	2:B:631:GLY:N	2.39	0.44
2:B:1001:PHE:HD2	3:C:34:ARG:HH21	1.66	0.44
3:C:27:LEU:O	3:C:30:ALA:N	2.50	0.44
3:C:163:ILE:C	3:C:165:LYS:H	2.25	0.44
7:G:9:LEU:CD1	7:G:10:ASN:H	2.30	0.44
9:I:8:ARG:CG	9:I:34:TYR:CE1	2.94	0.44
11:K:42:LEU:O	11:K:46:ILE:HG13	2.17	0.44
11:K:53:ASP:C	11:K:55:LYS:H	2.26	0.44
11:K:87:LEU:O	11:K:88:LYS:C	2.60	0.44
1:A:92:HIS:O	1:A:95:PHE:N	2.34	0.44
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.48	0.44
1:A:595:THR:O	1:A:596:THR:HG23	2.18	0.44
1:A:666:ILE:HD12	1:A:667:GLY:N	2.30	0.44
1:A:901:LEU:O	1:A:921:GLY:N	2.48	0.44
1:A:1349:TYR:O	1:A:1350:LYS:C	2.60	0.44
2:B:108:VAL:HG12	2:B:109:THR:N	2.33	0.44
2:B:432:MET:C	2:B:434:ARG:H	2.26	0.44
2:B:558:LEU:C	2:B:560:GLU:N	2.74	0.44
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.99	0.44
2:B:753:ALA:HA	2:B:756:ILE:HD12	2.00	0.44
3:C:245:VAL:C	3:C:247:GLY:N	2.74	0.44
4:D:170:THR:HB	4:D:172:LEU:H	1.83	0.44
6:F:89:GLU:HB3	6:F:134:ILE:CD1	2.48	0.44
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.98	0.44
11:K:35:PHE:CD1	11:K:71:PHE:CE1	3.05	0.44
11:K:95:ILE:O	11:K:98:LEU:HB2	2.17	0.44
1:A:33:ALA:HB1	1:A:35:ILE:HG13	2.00	0.44
1:A:103:CYS:O	1:A:106:VAL:O	2.35	0.44
1:A:401:GLY:O	1:A:435:HIS:CD2	2.71	0.44
1:A:874:ASP:O	1:A:875:ALA:C	2.59	0.44
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.57	0.44
2:B:258:LEU:O	2:B:259:TYR:O	2.36	0.44
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.99	0.44
2:B:436:VAL:O	2:B:436:VAL:HG12	2.18	0.44
2:B:460:ALA:C	2:B:462:ALA:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:581:PHE:HA	2:B:585:VAL:O	2.17	0.44
2:B:604:ARG:C	2:B:606:LYS:H	2.26	0.44
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.53	0.44
2:B:862:GLN:O	2:B:914:LYS:HE3	2.18	0.44
2:B:1084:GLN:N	2:B:1084:GLN:NE2	2.66	0.44
2:B:1181:GLU:O	2:B:1182:CYS:HB2	2.18	0.44
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.98	0.44
3:C:83:SER:O	3:C:85:ASP:N	2.51	0.44
3:C:91:HIS:CD2	3:C:91:HIS:C	2.95	0.44
3:C:246:ARG:HA	3:C:249:ASP:HB3	1.99	0.44
3:C:248:ILE:HG23	11:K:98:LEU:HD22	2.00	0.44
7:G:34:VAL:HG12	7:G:45:ILE:CG2	2.41	0.44
8:H:11:GLN:HA	8:H:53:ASP:O	2.18	0.44
10:J:1:MET:H2	10:J:55:ASP:C	2.26	0.44
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.49	0.44
1:A:18:GLN:H	2:B:1215:ARG:HB2	1.83	0.44
1:A:278:THR:O	1:A:278:THR:HG22	2.17	0.44
1:A:282:ASN:O	1:A:284:ALA:N	2.51	0.44
1:A:336:ILE:HG22	1:A:337:ARG:N	2.32	0.44
1:A:573:SER:O	1:A:574:GLY:C	2.61	0.44
1:A:618:GLU:O	1:A:619:LYS:C	2.60	0.44
1:A:779:PHE:O	1:A:780:VAL:C	2.59	0.44
1:A:883:LEU:CD2	1:A:1021:LEU:HB2	2.48	0.44
1:A:1153:TYR:CD2	1:A:1163:ILE:HD11	2.52	0.44
1:A:1335:ILE:O	1:A:1335:ILE:CG2	2.65	0.44
1:A:1364:ASN:HD22	1:A:1364:ASN:C	2.24	0.44
1:A:1368:MET:HE3	1:A:1368:MET:HB2	1.74	0.44
2:B:172:ILE:CG2	2:B:173:MET:N	2.81	0.44
2:B:189:LEU:O	2:B:190:TYR:C	2.61	0.44
2:B:312:GLU:O	2:B:315:LYS:N	2.50	0.44
2:B:641:GLU:C	2:B:643:ASP:H	2.25	0.44
2:B:680:THR:O	2:B:684:LEU:HD12	2.18	0.44
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.99	0.44
4:D:49:ALA:HB2	4:D:174:PRO:HB3	1.99	0.44
5:E:114:ASN:O	5:E:115:ASN:CB	2.65	0.44
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.99	0.44
10:J:53:HIS:NE2	10:J:55:ASP:HA	2.33	0.44
1:A:51:GLY:HA2	1:A:56:PRO:HA	2.00	0.44
1:A:335:ARG:HB3	1:A:336:ILE:H	1.65	0.44
1:A:494:SER:H	1:A:497:THR:HB	1.82	0.44
1:A:738:LYS:HZ1	3:C:194:GLU:C	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:CD1	1:A:1118:VAL:HG13	2.48	0.44
1:A:1142:THR:O	1:A:1143:LEU:C	2.61	0.44
1:A:1193:LEU:HD12	1:A:1193:LEU:C	2.41	0.44
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.17	0.44
1:A:1438:THR:O	1:A:1438:THR:HG22	2.17	0.44
2:B:203:PHE:N	2:B:203:PHE:CD1	2.86	0.44
2:B:265:SER:O	2:B:266:ALA:CB	2.65	0.44
2:B:286:PHE:CD1	2:B:297:ILE:HG23	2.53	0.44
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.53	0.44
2:B:390:LEU:O	2:B:391:ASP:C	2.58	0.44
2:B:418:LYS:C	2:B:420:LEU:N	2.75	0.44
2:B:424:LEU:O	2:B:428:ILE:HG13	2.18	0.44
2:B:1031:LEU:CD2	2:B:1044:ALA:HB2	2.48	0.44
3:C:161:LYS:O	3:C:170:TRP:NE1	2.51	0.44
7:G:9:LEU:CG	7:G:10:ASN:N	2.81	0.44
8:H:10:PHE:N	8:H:10:PHE:CD1	2.85	0.44
8:H:11:GLN:O	8:H:28:ALA:HB1	2.17	0.44
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.30	0.44
10:J:13:VAL:O	10:J:14:VAL:CG2	2.66	0.44
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.48	0.44
1:A:47:ARG:HH22	1:A:254:GLU:HA	1.83	0.44
1:A:334:GLY:O	1:A:335:ARG:C	2.60	0.44
1:A:344:ARG:C	1:A:345:VAL:CG1	2.91	0.44
1:A:350:ARG:HH11	1:A:350:ARG:HG3	1.83	0.44
1:A:427:GLN:HB2	1:A:430:TRP:NE1	2.32	0.44
1:A:659:HIS:C	1:A:661:GLY:H	2.26	0.44
1:A:791:ASP:C	1:A:791:ASP:OD1	2.60	0.44
1:A:1115:SER:C	1:A:1308:THR:CG2	2.90	0.44
2:B:181:LEU:CD2	2:B:189:LEU:HD22	2.47	0.44
2:B:882:THR:O	2:B:883:LEU:CB	2.65	0.44
2:B:1110:PRO:HG3	2:B:1124:ARG:O	2.18	0.44
3:C:22:LEU:HD23	3:C:25:VAL:HG21	2.00	0.44
3:C:44:LEU:HD23	3:C:44:LEU:C	2.42	0.44
4:D:66:ARG:O	4:D:67:ARG:C	2.61	0.44
7:G:3:PHE:CD1	7:G:80:LYS:HE2	2.53	0.44
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.48	0.44
1:A:373:THR:HG21	2:B:1105:ALA:HB3	1.98	0.44
1:A:556:TRP:CZ2	1:A:558:GLY:HA2	2.53	0.44
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.66	0.44
1:A:963:ILE:HD13	1:A:1049:ILE:CG1	2.47	0.44
1:A:1011:GLN:O	1:A:1012:ARG:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1015:VAL:O	1:A:1018:PHE:N	2.49	0.44
1:A:1132:LYS:O	1:A:1135:ARG:N	2.51	0.44
2:B:794:ASN:O	2:B:795:ILE:HD12	2.17	0.44
2:B:906:SER:O	2:B:907:GLY:O	2.34	0.44
3:C:259:LEU:HD11	11:K:91:CYS:HB2	1.99	0.44
5:E:94:LYS:HE2	5:E:98:ILE:CD1	2.38	0.44
5:E:135:PHE:CB	5:E:140:LEU:HD11	2.47	0.44
7:G:18:PHE:HZ	7:G:68:ALA:HB2	1.83	0.44
7:G:22:MET:O	7:G:23:LYS:C	2.60	0.44
10:J:8:PHE:O	10:J:9:SER:C	2.60	0.44
1:A:18:GLN:O	2:B:1215:ARG:CG	2.66	0.43
1:A:40:THR:CG2	1:A:41:MET:HG3	2.36	0.43
1:A:456:MET:HB2	1:A:478:TYR:OH	2.18	0.43
1:A:526:ASP:OD1	2:B:1013:ASN:ND2	2.49	0.43
1:A:528:LEU:O	1:A:529:CYS:C	2.60	0.43
1:A:1226:VAL:HG22	1:A:1240:CYS:HB3	2.00	0.43
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.43	0.43
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.47	0.43
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.18	0.43
2:B:45:SER:O	2:B:46:GLN:C	2.60	0.43
2:B:693:ILE:HD13	2:B:701:ILE:HD13	2.00	0.43
2:B:763:GLN:HG2	2:B:765:PRO:CG	2.48	0.43
2:B:838:SER:CB	2:B:989:THR:O	2.64	0.43
2:B:839:MET:HG3	2:B:1010:LEU:CD1	2.44	0.43
2:B:1169:MET:HE1	2:B:1201:LYS:CA	2.45	0.43
3:C:73:GLN:HE21	3:C:74:SER:H	1.65	0.43
8:H:10:PHE:HE2	8:H:36:CYS:HG	1.65	0.43
1:A:42:ASP:HB3	1:A:45:GLN:HA	2.00	0.43
1:A:48:ALA:C	1:A:49:LYS:HG3	2.43	0.43
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.83	0.43
1:A:73:GLY:O	1:A:74:MET:C	2.61	0.43
1:A:152:VAL:HG12	1:A:153:PRO:CD	2.47	0.43
1:A:559:VAL:O	1:A:559:VAL:HG12	2.17	0.43
1:A:846:GLU:HB2	1:A:847:ASP:H	1.66	0.43
1:A:932:GLU:O	1:A:936:LEU:HG	2.18	0.43
1:A:1164:PRO:C	1:A:1166:ASP:N	2.76	0.43
2:B:51:PHE:HB2	2:B:173:MET:CE	2.48	0.43
2:B:579:ARG:HA	2:B:589:VAL:HG13	1.99	0.43
2:B:1207:LEU:HB3	2:B:1212:ILE:HG22	1.99	0.43
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.18	0.43
1:A:93:VAL:HG23	1:A:304:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLU:O	1:A:207:ILE:C	2.60	0.43
1:A:224:PHE:CZ	1:A:231:PRO:HG3	2.52	0.43
1:A:522:GLY:O	1:A:646:PHE:HE2	2.01	0.43
1:A:575:LYS:NZ	1:A:615:GLY:H	2.16	0.43
1:A:1148:ILE:HB	1:A:1196:GLU:O	2.18	0.43
2:B:60:GLN:O	2:B:63:ILE:HG22	2.18	0.43
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.99	0.43
2:B:113:TYR:HB3	2:B:114:PRO:HD2	2.00	0.43
2:B:460:ALA:C	2:B:462:ALA:N	2.76	0.43
2:B:765:PRO:O	2:B:767:ASN:N	2.51	0.43
2:B:825:VAL:HG12	2:B:826:ALA:N	2.32	0.43
2:B:1072:MET:HE3	2:B:1085:ILE:HD13	2.00	0.43
2:B:1072:MET:HE1	2:B:1085:ILE:HB	1.92	0.43
4:D:33:PHE:CE2	7:G:80:LYS:NZ	2.72	0.43
7:G:115:MET:CB	7:G:116:PRO:CD	2.96	0.43
11:K:58:PHE:CB	11:K:76:GLN:HE21	2.31	0.43
11:K:58:PHE:HE2	11:K:74:ARG:HE	1.57	0.43
1:A:269:ILE:HD11	1:A:300:VAL:HA	2.01	0.43
1:A:508:PRO:O	1:A:511:ILE:HG13	2.18	0.43
1:A:752:LYS:HA	1:A:752:LYS:HD3	1.83	0.43
1:A:839:ARG:O	1:A:840:ARG:C	2.59	0.43
2:B:25:ILE:HD11	2:B:653:VAL:C	2.42	0.43
2:B:58:THR:O	2:B:62:ILE:HG13	2.18	0.43
2:B:1137:CYS:O	2:B:1140:ALA:HB3	2.17	0.43
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.84	0.43
3:C:238:ILE:HD11	3:C:246:ARG:HH11	1.83	0.43
4:D:51:ASN:OD1	4:D:52:LEU:O	2.37	0.43
9:I:99:LEU:C	9:I:100:PHE:CD1	2.96	0.43
10:J:41:LEU:HD11	10:J:50:ILE:HG13	2.00	0.43
1:A:106:VAL:HG13	1:A:112:LYS:C	2.43	0.43
1:A:578:LEU:HD23	1:A:612:ILE:HD11	1.99	0.43
1:A:1208:THR:O	1:A:1209:MET:C	2.62	0.43
2:B:32:ALA:O	2:B:35:SER:HB2	2.19	0.43
3:C:31:ASN:O	3:C:35:ARG:HG3	2.18	0.43
4:D:138:ASN:O	4:D:140:ASP:N	2.52	0.43
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.52	0.43
8:H:40:LEU:HD21	8:H:142:LEU:HD21	2.00	0.43
10:J:16:ASP:C	10:J:18:TRP:H	2.26	0.43
1:A:247:ARG:O	1:A:247:ARG:HG3	2.18	0.43
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.84	0.43
1:A:1111:MET:H	1:A:1111:MET:HG2	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	2.00	0.43
2:B:20:ASP:C	2:B:22:SER:H	2.27	0.43
2:B:418:LYS:O	2:B:420:LEU:N	2.51	0.43
2:B:458:LYS:O	2:B:459:TYR:C	2.61	0.43
2:B:859:TYR:CE1	2:B:941:LEU:HD12	2.53	0.43
3:C:80:LEU:HD22	3:C:129:ILE:HD13	2.01	0.43
3:C:226:ASP:O	3:C:227:THR:CB	2.66	0.43
5:E:29:PHE:O	5:E:30:ILE:CG1	2.59	0.43
7:G:88:ASP:OD2	7:G:88:ASP:N	2.49	0.43
7:G:119:LEU:HD13	7:G:132:SER:HB2	2.00	0.43
9:I:4:PHE:CD1	9:I:4:PHE:C	2.97	0.43
10:J:28:ASP:O	10:J:29:GLU:C	2.61	0.43
11:K:31:VAL:CG1	11:K:32:VAL:H	2.31	0.43
11:K:100:ALA:O	11:K:103:THR:HB	2.18	0.43
12:L:61:THR:HG22	12:L:63:ARG:HG2	2.01	0.43
1:A:120:GLU:C	1:A:122:MET:H	2.26	0.43
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.41	0.43
1:A:1131:ALA:O	1:A:1132:LYS:C	2.62	0.43
1:A:1209:MET:O	1:A:1210:GLY:C	2.61	0.43
1:A:1315:GLU:C	1:A:1317:MET:N	2.75	0.43
2:B:26:THR:O	2:B:29:ASP:HB2	2.17	0.43
2:B:824:ILE:CD1	10:J:48:ARG:NH1	2.81	0.43
2:B:900:ALA:O	2:B:903:VAL:HG23	2.19	0.43
3:C:70:ILE:HD11	3:C:144:ILE:CG1	2.49	0.43
5:E:147:HIS:O	5:E:148:GLU:C	2.61	0.43
7:G:10:ASN:OD1	7:G:71:ASN:HA	2.19	0.43
8:H:103:LYS:HG2	8:H:104:PHE:N	2.34	0.43
9:I:8:ARG:HG3	9:I:34:TYR:CD1	2.54	0.43
10:J:2:ILE:HG22	10:J:3:VAL:O	2.18	0.43
1:A:23:SER:CB	1:A:233:TRP:NE1	2.82	0.43
1:A:58:LEU:HD13	1:A:243:PRO:HA	2.00	0.43
1:A:270:LEU:O	1:A:271:LYS:C	2.60	0.43
1:A:382:PRO:CB	1:A:428:TYR:HE2	2.30	0.43
1:A:552:TRP:HE3	1:A:651:LYS:HB3	1.83	0.43
1:A:679:ILE:O	1:A:682:THR:N	2.52	0.43
1:A:682:THR:HG23	1:A:728:LYS:HE3	2.00	0.43
1:A:817:ALA:HA	2:B:764:SER:OG	2.17	0.43
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	2.00	0.43
1:A:1376:THR:O	1:A:1377:THR:C	2.62	0.43
3:C:99:LEU:HD22	3:C:120:ILE:HG12	2.01	0.43
4:D:52:LEU:CD2	4:D:147:TYR:HE2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.45	0.43
8:H:38:LEU:HD13	8:H:125:LEU:CD1	2.49	0.43
1:A:86:LEU:HD13	1:A:90:VAL:HG23	2.00	0.43
1:A:224:PHE:CZ	1:A:234:MET:HE2	2.53	0.43
1:A:477:PRO:HG2	1:A:521:MET:HG2	2.00	0.43
1:A:590:ARG:HD3	1:A:604:GLY:C	2.44	0.43
2:B:31:TRP:O	2:B:32:ALA:C	2.62	0.43
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.53	0.43
2:B:237:VAL:HG22	2:B:257:LYS:HA	2.00	0.43
2:B:324:ILE:CG2	2:B:325:GLN:N	2.79	0.43
2:B:351:TYR:CD1	2:B:355:ILE:HD11	2.53	0.43
2:B:737:THR:O	2:B:738:PHE:C	2.62	0.43
2:B:814:PHE:C	2:B:816:GLU:N	2.77	0.43
2:B:911:ILE:HG22	2:B:912:ILE:HG13	2.00	0.43
2:B:1106:ARG:NH2	2:B:1109:GLY:H	2.17	0.43
3:C:183:TRP:CE2	3:C:207:CYS:HB3	2.54	0.43
7:G:126:ASN:HD22	7:G:126:ASN:HA	1.56	0.43
8:H:15:VAL:HG22	8:H:26:ILE:CG1	2.49	0.43
9:I:34:TYR:C	9:I:35:VAL:HG23	2.44	0.43
9:I:86:PHE:CD1	9:I:86:PHE:C	2.97	0.43
11:K:101:LEU:O	11:K:101:LEU:HD23	2.19	0.43
1:A:73:GLY:O	1:A:75:ASN:N	2.52	0.43
1:A:148:CYS:O	1:A:168:GLY:HA2	2.19	0.43
1:A:268:ASP:O	1:A:269:ILE:C	2.62	0.43
1:A:320:ARG:HA	1:A:321:PRO:HD3	1.89	0.43
1:A:574:GLY:O	1:A:575:LYS:C	2.62	0.43
1:A:596:THR:C	1:A:598:LEU:N	2.73	0.43
1:A:693:VAL:HA	1:A:696:GLU:HB3	2.01	0.43
2:B:192:LEU:O	2:B:193:LYS:CB	2.62	0.43
2:B:593:PRO:O	2:B:596:LEU:N	2.52	0.43
2:B:1029:CYS:HA	2:B:1089:PRO:O	2.19	0.43
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.33	0.43
8:H:3:ASN:HB3	8:H:4:THR:H	1.63	0.43
9:I:103:CYS:HB3	9:I:107:SER:H	1.83	0.43
12:L:47:ARG:HG3	12:L:47:ARG:NH1	2.33	0.43
1:A:62:ASP:O	1:A:63:ARG:C	2.61	0.42
1:A:100:LYS:O	1:A:102:VAL:N	2.52	0.42
1:A:473:SER:C	1:A:475:THR:H	2.27	0.42
1:A:685:GLU:HG3	1:A:686:ALA:N	2.34	0.42
1:A:1279:ILE:HG23	1:A:1308:THR:OG1	2.19	0.42
2:B:200:GLY:HA2	2:B:202:TYR:HE2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:GLY:O	2:B:264:SER:C	2.62	0.42
2:B:694:ASP:O	2:B:698:GLU:HB2	2.18	0.42
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.54	0.42
2:B:769:TYR:C	2:B:771:SER:H	2.26	0.42
2:B:792:MET:HA	2:B:856:PHE:O	2.19	0.42
2:B:1085:ILE:N	2:B:1085:ILE:CD1	2.81	0.42
3:C:58:LEU:N	3:C:58:LEU:CD2	2.81	0.42
6:F:98:ALA:O	6:F:99:LEU:C	2.62	0.42
9:I:84:VAL:HG13	9:I:84:VAL:O	2.19	0.42
11:K:53:ASP:C	11:K:55:LYS:N	2.76	0.42
1:A:41:MET:O	1:A:50:ILE:HG13	2.20	0.42
1:A:241:VAL:O	1:A:242:PRO:C	2.61	0.42
1:A:475:THR:HG23	1:A:476:SER:H	1.76	0.42
1:A:535:THR:O	1:A:575:LYS:HG3	2.19	0.42
1:A:537:ARG:NH1	8:H:120:GLY:O	2.49	0.42
1:A:682:THR:HA	1:A:685:GLU:HG2	2.00	0.42
1:A:861:GLY:HA3	5:E:174:GLN:NE2	2.34	0.42
1:A:1036:ARG:HG2	1:A:1036:ARG:HH11	1.83	0.42
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.19	0.42
1:A:1209:MET:SD	1:A:1236:LEU:HD22	2.59	0.42
1:A:1425:SER:O	1:A:1426:GLU:C	2.61	0.42
2:B:123:THR:O	2:B:125:SER:N	2.47	0.42
2:B:377:PHE:C	2:B:379:GLY:H	2.27	0.42
2:B:762:ASN:OD1	2:B:1022:THR:HA	2.19	0.42
2:B:765:PRO:C	2:B:767:ASN:N	2.77	0.42
5:E:31:THR:OG1	5:E:34:GLU:N	2.50	0.42
5:E:117:THR:O	5:E:120:ALA:N	2.44	0.42
5:E:177:ARG:C	5:E:212:ARG:HD3	2.44	0.42
5:E:191:LYS:O	5:E:192:ARG:C	2.62	0.42
6:F:154:ASP:HB3	6:F:155:LEU:H	1.64	0.42
9:I:75:CYS:SG	9:I:79:HIS:CA	3.07	0.42
11:K:49:GLU:HG3	11:K:94:ILE:HG13	2.00	0.42
1:A:277:GLU:O	1:A:279:LEU:N	2.52	0.42
1:A:298:PHE:HD2	1:A:299:HIS:CD2	2.37	0.42
1:A:339:ASN:O	1:A:343:LYS:HG2	2.19	0.42
1:A:481:ASP:OD1	1:A:483:ASP:CG	2.62	0.42
1:A:1115:SER:O	1:A:1116:LEU:CB	2.67	0.42
1:A:1409:LEU:CD1	2:B:1207:LEU:HD21	2.42	0.42
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.54	0.42
2:B:257:LYS:N	2:B:270:LYS:O	2.52	0.42
2:B:258:LEU:O	2:B:258:LEU:CG	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:466:TRP:CE3	2:B:466:TRP:HA	2.53	0.42
2:B:575:PRO:C	2:B:577:ALA:H	2.27	0.42
3:C:92:CYS:O	3:C:94:LYS:N	2.52	0.42
5:E:22:MET:O	5:E:26:ARG:HG3	2.19	0.42
5:E:112:TYR:CZ	5:E:136:ASN:HB2	2.54	0.42
12:L:40:LEU:HD13	12:L:44:ASP:CB	2.49	0.42
1:A:29:ALA:HB1	2:B:1184:GLY:HA2	2.00	0.42
1:A:244:PRO:O	1:A:245:PRO:C	2.61	0.42
1:A:266:LEU:O	1:A:267:ALA:C	2.63	0.42
1:A:274:ILE:O	1:A:275:SER:C	2.62	0.42
1:A:482:PHE:C	1:A:484:GLY:N	2.77	0.42
1:A:603:ASN:O	1:A:604:GLY:C	2.60	0.42
1:A:660:ASN:O	1:A:661:GLY:O	2.37	0.42
1:A:741:ASN:HD22	1:A:744:LYS:N	2.07	0.42
1:A:901:LEU:N	1:A:926:GLN:NE2	2.50	0.42
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	2.19	0.42
1:A:1147:THR:HA	1:A:1197:LEU:HD23	2.00	0.42
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.49	0.42
1:A:1437:GLY:C	1:A:1439:GLY:N	2.76	0.42
2:B:298:LEU:N	2:B:298:LEU:CD2	2.83	0.42
2:B:651:LEU:HD11	2:B:707:PRO:CB	2.49	0.42
2:B:834:ASN:ND2	2:B:1013:ASN:HB2	2.34	0.42
2:B:957:ASN:O	2:B:958:GLN:C	2.63	0.42
2:B:986:GLN:O	2:B:987:LYS:C	2.62	0.42
2:B:1032:SER:O	2:B:1036:ALA:HB2	2.19	0.42
2:B:1115:THR:CG2	2:B:1117:GLN:CG	2.97	0.42
4:D:180:LEU:HD23	4:D:180:LEU:HA	1.75	0.42
5:E:42:PHE:CE1	5:E:58:MET:HE3	2.55	0.42
5:E:101:GLN:NE2	5:E:127:ILE:HG21	2.34	0.42
5:E:114:ASN:HD22	5:E:114:ASN:HA	1.62	0.42
9:I:58:VAL:O	9:I:58:VAL:HG12	2.19	0.42
11:K:96:ASN:O	11:K:97:LYS:C	2.62	0.42
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	2.02	0.42
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.54	0.42
1:A:367:PRO:HB3	1:A:465:TYR:O	2.19	0.42
1:A:453:MET:C	1:A:455:MET:N	2.76	0.42
1:A:804:TYR:OH	1:A:816:HIS:NE2	2.53	0.42
1:A:1157:ASP:C	1:A:1159:ARG:N	2.77	0.42
1:A:1170:ILE:H	1:A:1170:ILE:HG13	1.62	0.42
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.67	0.42
1:A:1422:ARG:NH2	2:B:1224:PHE:C	2.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:582:VAL:HA	2:B:626:ILE:O	2.19	0.42
2:B:753:ALA:HA	2:B:756:ILE:CD1	2.48	0.42
2:B:1006:ILE:HG22	10:J:45:CYS:HB3	2.02	0.42
2:B:1084:GLN:NE2	2:B:1084:GLN:H	2.17	0.42
2:B:1152:MET:HE1	2:B:1157:ALA:HA	1.99	0.42
3:C:67:LEU:HD11	3:C:155:LEU:HD13	2.01	0.42
5:E:127:ILE:O	5:E:130:ALA:HB3	2.20	0.42
7:G:145:VAL:CG1	7:G:146:LYS:N	2.81	0.42
9:I:56:ALA:O	9:I:57:GLY:C	2.63	0.42
9:I:101:PHE:HD1	9:I:110:PHE:O	2.02	0.42
1:A:31:SER:OG	1:A:82:GLY:HA2	2.19	0.42
1:A:53:LEU:HD22	1:A:54:ASN:HD22	1.85	0.42
1:A:210:ILE:O	1:A:214:ILE:HG13	2.19	0.42
1:A:264:PHE:O	1:A:267:ALA:HB3	2.20	0.42
1:A:472:LEU:HD11	2:B:835:GLN:CD	2.44	0.42
1:A:765:VAL:HG23	1:A:802:ASN:O	2.20	0.42
1:A:807:GLY:HA2	2:B:760:ASP:O	2.19	0.42
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.17	0.42
1:A:873:MET:C	1:A:1058:VAL:HG23	2.43	0.42
1:A:940:ARG:O	1:A:941:LYS:C	2.62	0.42
1:A:1029:ARG:HG3	1:A:1029:ARG:NH1	2.34	0.42
1:A:1031:VAL:O	1:A:1031:VAL:HG12	2.20	0.42
1:A:1115:SER:OG	1:A:1116:LEU:N	2.53	0.42
1:A:1129:GLU:O	1:A:1130:GLN:C	2.61	0.42
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	2.02	0.42
1:A:1362:TYR:CD1	1:A:1362:TYR:C	2.96	0.42
2:B:281:PRO:C	2:B:283:VAL:N	2.76	0.42
2:B:314:LEU:O	2:B:315:LYS:C	2.62	0.42
2:B:654:ARG:C	2:B:656:GLY:N	2.77	0.42
2:B:992:ILE:HD11	11:K:66:PRO:HB2	2.01	0.42
2:B:1106:ARG:HD3	2:B:1127:GLY:CA	2.49	0.42
3:C:62:PHE:O	3:C:63:ILE:C	2.62	0.42
3:C:80:LEU:HD11	3:C:95:CYS:CA	2.49	0.42
3:C:123:ASN:HD22	3:C:125:MET:CG	2.29	0.42
3:C:131:HIS:HA	3:C:132:PRO:HD3	1.92	0.42
3:C:256:ALA:C	3:C:258:ILE:N	2.77	0.42
10:J:41:LEU:CD1	10:J:50:ILE:HG13	2.49	0.42
10:J:52:THR:O	10:J:53:HIS:C	2.63	0.42
1:A:67:CYS:O	1:A:68:GLN:CB	2.67	0.42
1:A:231:PRO:O	1:A:233:TRP:N	2.52	0.42
1:A:337:ARG:CZ	1:A:839:ARG:HH12	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.55	0.42
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.33	0.42
1:A:481:ASP:OD1	1:A:483:ASP:OD2	2.38	0.42
1:A:535:THR:CG2	1:A:575:LYS:HE2	2.49	0.42
1:A:1010:ALA:O	1:A:1013:ASP:HB2	2.20	0.42
1:A:1409:LEU:O	1:A:1410:PHE:C	2.62	0.42
1:A:1434:ALA:HA	1:A:1435:PRO:HD3	1.76	0.42
2:B:654:ARG:N	2:B:657:HIS:HD2	2.13	0.42
2:B:796:LEU:HD12	2:B:852:ARG:O	2.19	0.42
2:B:1162:ILE:CG2	2:B:1163:CYS:N	2.79	0.42
3:C:229:TYR:CD1	3:C:229:TYR:N	2.88	0.42
4:D:29:LEU:O	4:D:30:GLY:C	2.62	0.42
5:E:20:LYS:O	5:E:21:GLU:C	2.62	0.42
5:E:177:ARG:O	5:E:212:ARG:CD	2.68	0.42
7:G:125:SER:HG	7:G:128:PRO:HA	1.83	0.42
8:H:40:LEU:CD2	8:H:142:LEU:HD21	2.50	0.42
9:I:111:THR:CG2	9:I:113:ASP:HB2	2.49	0.42
1:A:68:GLN:C	1:A:70:CYS:N	2.65	0.42
1:A:249:SER:HB2	1:A:250:ILE:H	1.66	0.42
1:A:275:SER:O	1:A:279:LEU:HG	2.19	0.42
1:A:306:ASN:ND2	1:A:322:VAL:CG1	2.82	0.42
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.34	0.42
1:A:466:SER:HB2	2:B:1099:VAL:HG11	2.02	0.42
1:A:497:THR:HG22	1:A:498:ARG:N	2.34	0.42
1:A:818:MET:H	2:B:514:LEU:HD23	1.83	0.42
1:A:1067:LEU:O	1:A:1068:ALA:C	2.62	0.42
1:A:1072:ILE:O	1:A:1075:PRO:HD2	2.20	0.42
1:A:1313:LEU:C	1:A:1315:GLU:N	2.78	0.42
2:B:167:ILE:HG22	2:B:453:ILE:HD12	2.01	0.42
2:B:644:GLU:C	2:B:646:LEU:N	2.77	0.42
2:B:860:MET:HE2	2:B:965:LYS:HE2	2.02	0.42
2:B:1060:ARG:C	2:B:1062:HIS:N	2.78	0.42
4:D:7:THR:CB	7:G:42:PHE:CZ	3.03	0.42
1:A:23:SER:HB3	1:A:233:TRP:NE1	2.35	0.42
1:A:526:ASP:O	1:A:527:THR:C	2.63	0.42
1:A:817:ALA:O	1:A:820:GLY:N	2.52	0.42
1:A:867:ILE:O	1:A:868:TYR:C	2.63	0.42
1:A:1206:ASP:HB3	1:A:1274:ARG:NH1	2.34	0.42
2:B:213:ILE:HD13	2:B:213:ILE:HA	1.88	0.42
2:B:312:GLU:O	2:B:313:MET:C	2.63	0.42
2:B:700:SER:C	2:B:701:ILE:CG2	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:702:LEU:HD12	2:B:703:ILE:H	1.84	0.42
2:B:986:GLN:HA	2:B:986:GLN:OE1	2.20	0.42
2:B:1064:TYR:O	2:B:1065:GLN:C	2.63	0.42
2:B:1216:LEU:N	2:B:1216:LEU:HD23	2.35	0.42
2:B:1219:ASP:OD1	2:B:1219:ASP:O	2.38	0.42
3:C:8:VAL:HG12	3:C:9:LYS:H	1.83	0.42
3:C:15:LYS:O	3:C:240:VAL:HG22	2.20	0.42
4:D:167:LEU:C	4:D:169:SER:H	2.28	0.42
5:E:133:GLU:HB3	5:E:135:PHE:HE1	1.84	0.42
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.55	0.42
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.49	0.42
1:A:606:LEU:HB3	1:A:614:PHE:CE2	2.54	0.42
1:A:825:ILE:HG22	1:A:826:ASP:N	2.34	0.42
1:A:852:TYR:CD2	1:A:1060:PRO:CB	3.03	0.42
1:A:901:LEU:HA	1:A:907:THR:OG1	2.20	0.42
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	2.01	0.42
1:A:1340:GLY:O	1:A:1341:ILE:C	2.62	0.42
2:B:33:VAL:O	2:B:34:ILE:C	2.63	0.42
2:B:366:GLN:O	2:B:367:LEU:O	2.38	0.42
2:B:386:LEU:O	2:B:387:LEU:C	2.61	0.42
2:B:610:ASN:C	2:B:612:GLU:H	2.28	0.42
2:B:624:LEU:HD12	2:B:624:LEU:HA	1.84	0.42
2:B:1029:CYS:HB3	2:B:1086:PHE:CZ	2.55	0.42
2:B:1069:PHE:CD1	2:B:1069:PHE:N	2.78	0.42
3:C:174:ALA:O	3:C:175:ALA:CB	2.67	0.42
4:D:179:GLN:O	4:D:183:LEU:HB2	2.20	0.42
5:E:61:GLN:HG2	5:E:62:ALA:N	2.35	0.42
6:F:82:THR:HA	6:F:83:PRO:HD3	1.80	0.42
8:H:48:PRO:O	8:H:49:VAL:HG23	2.20	0.42
9:I:12:ASN:HB3	9:I:13:MET:H	1.57	0.42
10:J:32:GLU:O	10:J:33:GLY:C	2.62	0.42
1:A:254:GLU:CG	2:B:935:ARG:HH22	2.31	0.41
1:A:472:LEU:O	1:A:475:THR:CB	2.68	0.41
1:A:794:PRO:C	1:A:796:SER:N	2.78	0.41
1:A:1070:GLN:O	1:A:1071:SER:C	2.62	0.41
1:A:1111:MET:CE	1:A:1330:ASN:OD1	2.68	0.41
1:A:1125:ALA:C	1:A:1127:ASP:H	2.28	0.41
1:A:1217:LYS:O	1:A:1221:LYS:N	2.52	0.41
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.55	0.41
1:A:1437:GLY:O	1:A:1438:THR:C	2.63	0.41
2:B:205:ILE:CG2	2:B:206:ASN:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:373:ARG:HG3	2:B:566:LEU:HD23	2.01	0.41
2:B:515:HIS:O	2:B:518:HIS:HB2	2.20	0.41
2:B:593:PRO:O	2:B:595:ARG:N	2.53	0.41
2:B:596:LEU:O	2:B:600:LEU:HG	2.19	0.41
2:B:604:ARG:HG3	2:B:611:PRO:HA	2.02	0.41
2:B:610:ASN:O	2:B:612:GLU:N	2.53	0.41
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.34	0.41
2:B:1182:CYS:O	2:B:1183:LYS:O	2.37	0.41
3:C:92:CYS:C	3:C:94:LYS:H	2.27	0.41
4:D:206:GLU:O	4:D:208:GLU:N	2.53	0.41
4:D:209:ARG:O	4:D:212:LYS:HB2	2.20	0.41
4:D:217:LEU:O	4:D:219:THR:N	2.53	0.41
5:E:201:LYS:HA	5:E:206:GLY:O	2.19	0.41
6:F:72:LYS:O	6:F:73:ALA:HB3	2.20	0.41
6:F:97:ARG:NH1	6:F:100:GLN:OE1	2.53	0.41
8:H:91:ASP:C	8:H:93:TYR:N	2.72	0.41
9:I:83:ASN:HA	9:I:102:VAL:O	2.19	0.41
1:A:760:GLN:OE1	2:B:1021:MET:HE1	2.19	0.41
1:A:825:ILE:O	1:A:826:ASP:C	2.62	0.41
1:A:843:LYS:HD3	1:A:843:LYS:HA	1.82	0.41
1:A:1074:GLU:C	1:A:1076:ALA:H	2.28	0.41
2:B:193:LYS:HD3	2:B:787:VAL:HG11	2.01	0.41
2:B:233:PRO:HG2	2:B:234:ILE:CD1	2.40	0.41
2:B:278:GLN:HG2	2:B:279:ASP:H	1.85	0.41
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.83	0.41
2:B:954:VAL:HA	2:B:964:VAL:HG22	2.01	0.41
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.34	0.41
2:B:1187:ASN:OD1	2:B:1189:ILE:N	2.52	0.41
2:B:1197:PRO:O	2:B:1200:ALA:HB3	2.20	0.41
3:C:94:LYS:HB2	3:C:94:LYS:HE3	1.86	0.41
4:D:53:SER:CB	4:D:153:ARG:H	2.32	0.41
4:D:66:ARG:CD	4:D:133:THR:HB	2.43	0.41
5:E:198:ILE:HD11	5:E:212:ARG:CG	2.46	0.41
6:F:93:ILE:HD13	6:F:148:VAL:HG13	2.02	0.41
8:H:127:GLY:HA3	8:H:130:ARG:NH2	2.35	0.41
1:A:55:ASP:N	1:A:56:PRO:CD	2.83	0.41
1:A:414:ASP:OD1	1:A:416:ARG:CG	2.68	0.41
1:A:525:GLN:O	1:A:526:ASP:C	2.62	0.41
1:A:626:ASN:HB3	1:A:627:GLY:H	1.71	0.41
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.84	0.41
1:A:1059:HIS:CE1	6:F:86:THR:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.51	0.41
1:A:1372:VAL:CG1	1:A:1373:ASP:N	2.82	0.41
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.84	0.41
2:B:34:ILE:O	2:B:35:SER:C	2.63	0.41
2:B:365:THR:HG23	2:B:367:LEU:N	2.27	0.41
2:B:827:ILE:O	2:B:827:ILE:HG22	2.20	0.41
2:B:918:ILE:HG21	2:B:935:ARG:NH1	2.36	0.41
2:B:1068:GLY:C	2:B:1069:PHE:O	2.63	0.41
3:C:252:GLN:CG	11:K:95:ILE:HG23	2.50	0.41
5:E:82:PHE:CD1	5:E:82:PHE:N	2.88	0.41
6:F:74:ILE:HG23	6:F:75:PRO:HD2	2.01	0.41
9:I:98:VAL:C	9:I:99:LEU:HD23	2.45	0.41
10:J:48:ARG:HD2	10:J:48:ARG:C	2.45	0.41
11:K:7:PHE:CD1	11:K:7:PHE:C	2.98	0.41
11:K:68:PHE:CD2	11:K:68:PHE:N	2.86	0.41
1:A:70:CYS:O	1:A:70:CYS:SG	2.78	0.41
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.20	0.41
1:A:443:LEU:HD11	1:A:455:MET:SD	2.59	0.41
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.01	0.41
1:A:532:ARG:O	1:A:533:LYS:C	2.64	0.41
1:A:683:ILE:O	1:A:686:ALA:HB3	2.20	0.41
1:A:836:TYR:O	1:A:837:ILE:C	2.63	0.41
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.55	0.41
1:A:940:ARG:HG2	1:A:940:ARG:NH1	2.35	0.41
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.20	0.41
1:A:1450:LEU:HD21	7:G:19:GLY:O	2.20	0.41
2:B:29:ASP:O	2:B:30:SER:C	2.64	0.41
2:B:214:ALA:HB3	2:B:498:THR:HA	2.01	0.41
2:B:235:SER:O	2:B:236:HIS:HD2	2.04	0.41
2:B:603:LEU:HB3	2:B:609:ILE:CG1	2.50	0.41
2:B:638:PHE:HD2	2:B:690:VAL:HG22	1.86	0.41
2:B:778:MET:CE	2:B:1094:ARG:CD	2.96	0.41
2:B:821:GLN:NE2	2:B:851:PHE:HA	2.35	0.41
2:B:822:ASN:HD22	10:J:52:THR:HG21	1.85	0.41
3:C:116:LYS:HD3	3:C:140:ASN:HB3	2.03	0.41
3:C:123:ASN:HD21	3:C:125:MET:HA	1.85	0.41
4:D:138:ASN:O	4:D:141:LEU:N	2.54	0.41
4:D:153:ARG:O	4:D:154:PHE:CG	2.73	0.41
6:F:111:LEU:N	6:F:111:LEU:CD1	2.83	0.41
1:A:220:THR:O	1:A:221:SER:C	2.64	0.41
1:A:444:PHE:CB	1:A:458:HIS:CD2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:VAL:O	1:A:654:ASN:C	2.64	0.41
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.56	0.41
1:A:1127:ASP:O	1:A:1130:GLN:HB3	2.20	0.41
1:A:1365:TYR:O	1:A:1366:ARG:C	2.63	0.41
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.56	0.41
2:B:371:GLU:CD	2:B:371:GLU:N	2.77	0.41
2:B:552:MET:O	2:B:554:ILE:N	2.53	0.41
2:B:579:ARG:CA	2:B:589:VAL:HG13	2.51	0.41
2:B:1164:GLY:HA3	2:B:1190:ASP:OD2	2.21	0.41
2:B:1183:LYS:HE3	2:B:1183:LYS:O	2.20	0.41
2:B:1200:ALA:O	2:B:1201:LYS:C	2.63	0.41
3:C:116:LYS:HD3	3:C:140:ASN:HA	2.03	0.41
3:C:241:ASP:CG	3:C:242:GLN:N	2.77	0.41
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.86	0.41
5:E:98:ILE:C	5:E:100:ILE:N	2.78	0.41
6:F:96:THR:O	6:F:99:LEU:HB3	2.21	0.41
7:G:149:GLY:O	7:G:159:ALA:HB1	2.20	0.41
9:I:34:TYR:O	9:I:35:VAL:CG2	2.69	0.41
11:K:10:PHE:CD1	11:K:11:LEU:CD2	3.04	0.41
1:A:93:VAL:CG2	1:A:304:MET:HE3	2.50	0.41
1:A:296:LEU:C	1:A:298:PHE:N	2.78	0.41
1:A:356:ASP:OD2	11:K:65:HIS:CE1	2.71	0.41
1:A:599:SER:HB2	1:A:603:ASN:H	1.84	0.41
1:A:621:THR:O	1:A:629:LEU:HB2	2.21	0.41
1:A:822:GLU:O	1:A:825:ILE:HB	2.21	0.41
1:A:958:VAL:HG22	1:A:1052:GLN:HB3	2.03	0.41
1:A:1157:ASP:O	1:A:1159:ARG:N	2.54	0.41
1:A:1406:VAL:O	1:A:1407:GLU:C	2.63	0.41
2:B:130:VAL:CG2	2:B:167:ILE:HD12	2.50	0.41
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.36	0.41
2:B:575:PRO:HG2	2:B:576:ASP:H	1.86	0.41
2:B:687:GLU:O	2:B:689:LEU:HG	2.20	0.41
2:B:918:ILE:HD12	2:B:935:ARG:CD	2.51	0.41
2:B:952:VAL:O	2:B:953:LEU:HB3	2.21	0.41
2:B:1162:ILE:O	2:B:1171:VAL:HG21	2.20	0.41
3:C:9:LYS:O	3:C:10:ILE:C	2.62	0.41
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.56	0.41
5:E:171:LYS:HA	5:E:171:LYS:HD3	1.89	0.41
6:F:75:PRO:C	6:F:77:ASP:N	2.78	0.41
1:A:343:LYS:HE2	2:B:1156:ASP:OD2	2.21	0.41
1:A:446:ARG:NH1	1:A:479:ASN:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LYS:HE2	1:A:452:LYS:HB3	1.74	0.41
1:A:464:PRO:HG2	1:A:465:TYR:CD1	2.54	0.41
1:A:738:LYS:C	1:A:740:LEU:N	2.78	0.41
1:A:789:LYS:HE3	9:I:67:THR:HB	2.03	0.41
1:A:1425:SER:O	1:A:1429:ILE:HG13	2.21	0.41
2:B:168:GLY:N	2:B:450:ALA:HB1	2.19	0.41
2:B:446:LEU:O	2:B:447:ALA:CB	2.66	0.41
2:B:496:ARG:HB3	2:B:496:ARG:NH1	2.36	0.41
3:C:26:ASP:O	3:C:27:LEU:C	2.64	0.41
3:C:240:VAL:O	3:C:244:VAL:HG23	2.21	0.41
5:E:60:PHE:CE2	5:E:80:VAL:HB	2.56	0.41
8:H:56:THR:O	8:H:144:ILE:HA	2.21	0.41
9:I:88:SER:C	9:I:90:GLN:H	2.29	0.41
11:K:12:LEU:H	11:K:12:LEU:CD1	2.32	0.41
11:K:113:THR:O	11:K:114:LEU:CB	2.63	0.41
1:A:774:ARG:CZ	1:A:797:LYS:CB	2.98	0.41
2:B:20:ASP:O	2:B:22:SER:N	2.45	0.41
2:B:487:THR:O	2:B:490:SER:HB3	2.21	0.41
2:B:522:VAL:HG12	2:B:523:CYS:N	2.36	0.41
2:B:578:THR:O	2:B:579:ARG:C	2.62	0.41
2:B:589:VAL:CG1	2:B:590:HIS:H	2.11	0.41
2:B:637:LEU:HD23	2:B:742:GLU:HA	2.02	0.41
2:B:681:TRP:C	2:B:683:SER:N	2.78	0.41
2:B:912:ILE:HD11	2:B:966:VAL:HG23	2.03	0.41
2:B:1080:LYS:HD2	3:C:188:HIS:HB2	2.03	0.41
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.54	0.41
4:D:156:ASP:O	4:D:158:GLU:N	2.54	0.41
5:E:9:ILE:C	5:E:11:ARG:N	2.78	0.41
5:E:116:ILE:CG2	5:E:117:THR:N	2.83	0.41
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.97	0.41
1:A:209:ASN:O	1:A:210:ILE:C	2.62	0.41
1:A:242:PRO:O	1:A:247:ARG:NE	2.52	0.41
1:A:527:THR:O	1:A:531:ILE:HB	2.21	0.41
1:A:541:ILE:CG2	1:A:546:VAL:HG23	2.50	0.41
1:A:586:ILE:CG2	1:A:587:HIS:N	2.83	0.41
1:A:744:LYS:O	1:A:747:VAL:N	2.54	0.41
1:A:1059:HIS:CE1	6:F:87:LYS:H	2.39	0.41
1:A:1150:SER:C	1:A:1151:GLU:HG3	2.45	0.41
1:A:1164:PRO:C	1:A:1166:ASP:H	2.28	0.41
1:A:1299:VAL:CG1	1:A:1300:LYS:N	2.83	0.41
1:A:1323:ASP:C	1:A:1325:THR:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:GLY:C	1:A:1439:GLY:H	2.29	0.41
1:A:1444:MET:O	6:F:132:LEU:HA	2.20	0.41
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.41	0.41
2:B:288:ALA:HA	2:B:331:LEU:HD12	2.02	0.41
2:B:479:VAL:O	2:B:480:SER:HB3	2.20	0.41
2:B:593:PRO:C	2:B:595:ARG:N	2.79	0.41
2:B:842:ASN:HD21	2:B:845:SER:H	1.60	0.41
2:B:1208:MET:HA	2:B:1212:ILE:O	2.20	0.41
3:C:73:GLN:HE21	3:C:74:SER:N	2.19	0.41
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.86	0.41
4:D:30:GLY:O	4:D:31:GLN:C	2.64	0.41
4:D:52:LEU:C	4:D:54:GLU:H	2.29	0.41
5:E:23:VAL:O	5:E:28:TYR:HD1	2.03	0.41
5:E:90:VAL:CA	5:E:120:ALA:HB2	2.49	0.41
5:E:98:ILE:O	5:E:100:ILE:N	2.53	0.41
5:E:117:THR:C	5:E:119:SER:H	2.27	0.41
6:F:99:LEU:O	6:F:103:MET:CG	2.69	0.41
7:G:101:VAL:HG12	7:G:102:GLN:N	2.35	0.41
11:K:43:GLY:HA3	11:K:61:TYR:CE1	2.56	0.41
1:A:7:SER:HB2	2:B:1175:LEU:HD22	2.03	0.41
1:A:42:ASP:C	1:A:44:THR:N	2.77	0.41
1:A:276:LEU:O	1:A:277:GLU:C	2.65	0.41
1:A:373:THR:HG21	2:B:1105:ALA:CB	2.51	0.41
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.39	0.41
1:A:659:HIS:C	1:A:661:GLY:N	2.79	0.41
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	2.03	0.41
1:A:1019:CYS:O	1:A:1023:ARG:N	2.45	0.41
1:A:1152:ILE:CG1	9:I:44:TYR:HB3	2.46	0.41
1:A:1369:ALA:C	1:A:1373:ASP:OD2	2.64	0.41
2:B:54:PHE:CE2	2:B:59:LEU:HD13	2.55	0.41
2:B:65:GLU:HG3	2:B:66:ASP:OD1	2.21	0.41
2:B:400:HIS:O	2:B:401:PHE:C	2.64	0.41
2:B:759:PRO:C	2:B:761:HIS:H	2.29	0.41
2:B:800:GLN:CA	10:J:52:THR:HG22	2.51	0.41
2:B:910:VAL:HG12	2:B:911:ILE:N	2.35	0.41
2:B:1147:LEU:CD2	2:B:1151:LEU:HD22	2.51	0.41
2:B:1200:ALA:O	2:B:1203:LEU:HB3	2.21	0.41
4:D:128:VAL:C	4:D:130:LEU:N	2.78	0.41
5:E:181:ALA:O	5:E:182:ASP:C	2.64	0.41
7:G:74:TYR:N	7:G:74:TYR:CD2	2.88	0.41
7:G:111:THR:O	7:G:112:LYS:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:52:ASN:O	11:K:53:ASP:C	2.64	0.41
1:A:289:ILE:C	1:A:291:GLU:N	2.73	0.40
1:A:416:ARG:O	1:A:417:TYR:HD2	2.03	0.40
1:A:445:ASN:CB	1:A:455:MET:HG2	2.44	0.40
1:A:823:GLY:O	1:A:824:LEU:C	2.64	0.40
1:A:1048:ASN:O	1:A:1049:ILE:C	2.64	0.40
1:A:1120:LEU:CD1	1:A:1304:TRP:O	2.69	0.40
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.56	0.40
2:B:487:THR:CG2	2:B:488:TYR:N	2.84	0.40
2:B:801:LYS:N	10:J:52:THR:HG22	2.36	0.40
2:B:810:GLU:CB	2:B:815:ARG:HH22	2.33	0.40
2:B:838:SER:CA	2:B:989:THR:O	2.69	0.40
2:B:1147:LEU:O	2:B:1148:LYS:C	2.62	0.40
3:C:62:PHE:O	3:C:66:ARG:HG3	2.21	0.40
3:C:80:LEU:CD1	3:C:95:CYS:HA	2.51	0.40
3:C:247:GLY:C	3:C:249:ASP:N	2.77	0.40
4:D:128:VAL:O	4:D:129:LEU:C	2.64	0.40
7:G:138:THR:O	7:G:139:ILE:C	2.64	0.40
8:H:96:VAL:HA	8:H:142:LEU:O	2.21	0.40
9:I:50:THR:HG22	9:I:52:ILE:N	2.32	0.40
11:K:83:PRO:O	11:K:84:LYS:C	2.64	0.40
1:A:6:TYR:CD1	1:A:7:SER:N	2.89	0.40
1:A:57:ARG:C	1:A:58:LEU:O	2.62	0.40
1:A:306:ASN:HB2	1:A:324:SER:HB3	2.02	0.40
1:A:532:ARG:O	1:A:535:THR:HB	2.22	0.40
1:A:877:HIS:O	1:A:878:ILE:HG12	2.21	0.40
1:A:1333:ILE:O	1:A:1337:GLU:HG3	2.21	0.40
1:A:1392:SER:C	1:A:1394:THR:H	2.29	0.40
2:B:211:VAL:HG23	2:B:483:LEU:HB2	2.03	0.40
2:B:388:CYS:C	2:B:390:LEU:H	2.28	0.40
2:B:814:PHE:C	2:B:816:GLU:H	2.27	0.40
2:B:841:MET:O	2:B:993:THR:HA	2.21	0.40
2:B:1027:ILE:O	2:B:1028:GLU:C	2.64	0.40
2:B:1087:PHE:CD2	2:B:1088:GLY:N	2.80	0.40
7:G:31:LEU:CD2	7:G:48:VAL:HG21	2.51	0.40
12:L:38:LEU:O	12:L:39:SER:CB	2.63	0.40
1:A:24:PRO:O	1:A:28:ARG:HG3	2.21	0.40
1:A:103:CYS:C	1:A:105:CYS:N	2.78	0.40
1:A:255:SER:O	1:A:256:GLN:HG3	2.20	0.40
1:A:326:ARG:NH2	1:A:1407:GLU:HG3	2.36	0.40
1:A:344:ARG:HG2	1:A:344:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:GLU:HB2	5:E:204:THR:HG21	2.03	0.40
1:A:913:LEU:HD23	1:A:919:ILE:HD12	2.04	0.40
1:A:1163:ILE:HG22	1:A:1164:PRO:HD2	2.04	0.40
1:A:1215:ARG:O	1:A:1216:ILE:C	2.64	0.40
1:A:1332:PHE:HA	1:A:1335:ILE:HB	2.03	0.40
1:A:1434:ALA:CB	1:A:1436:ILE:HD12	2.52	0.40
2:B:286:PHE:HE2	2:B:375:ALA:HB1	1.87	0.40
2:B:309:GLN:CG	9:I:52:ILE:HD11	2.51	0.40
2:B:500:THR:HA	2:B:501:PRO:HD2	1.87	0.40
2:B:519:TRP:HE1	2:B:635:ARG:NH2	2.19	0.40
2:B:520:GLY:H	2:B:748:ILE:HG22	1.87	0.40
2:B:770:GLN:CD	2:B:983:ARG:CA	2.92	0.40
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	2.02	0.40
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.46	0.40
2:B:1135:ARG:O	2:B:1138:MET:N	2.54	0.40
2:B:1178:ASN:O	2:B:1180:PHE:CD1	2.74	0.40
3:C:59:ALA:O	3:C:60:ASP:C	2.64	0.40
3:C:206:ASN:OD1	3:C:229:TYR:CD2	2.74	0.40
4:D:196:PRO:C	4:D:198:LEU:N	2.79	0.40
7:G:82:PHE:CD1	7:G:82:PHE:N	2.90	0.40
1:A:130:ASP:O	1:A:132:LYS:N	2.55	0.40
1:A:172:PRO:HD3	1:A:185:TRP:HE1	1.86	0.40
1:A:514:PRO:C	1:A:516:SER:H	2.29	0.40
1:A:696:GLU:O	1:A:696:GLU:HG2	2.21	0.40
1:A:795:GLU:CD	1:A:795:GLU:H	2.30	0.40
1:A:811:GLN:O	1:A:812:GLU:C	2.65	0.40
1:A:1066:VAL:O	1:A:1067:LEU:C	2.65	0.40
1:A:1067:LEU:HD12	1:A:1071:SER:OG	2.21	0.40
1:A:1227:ILE:CG2	1:A:1228:TRP:H	2.35	0.40
1:A:1370:LEU:O	1:A:1373:ASP:HB2	2.21	0.40
2:B:701:ILE:HG13	2:B:702:LEU:N	2.35	0.40
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.86	0.40
2:B:758:PHE:O	2:B:760:ASP:N	2.54	0.40
2:B:901:PRO:O	2:B:949:VAL:HB	2.21	0.40
2:B:1124:ARG:O	2:B:1125:ASP:CB	2.68	0.40
3:C:107:SER:C	3:C:109:SER:N	2.80	0.40
4:D:40:HIS:C	4:D:42:GLY:N	2.78	0.40
10:J:3:VAL:HA	10:J:4:PRO:HD3	1.88	0.40
10:J:13:VAL:C	10:J:14:VAL:CG2	2.94	0.40
12:L:66:GLN:C	12:L:67:PHE:CD1	2.99	0.40
1:A:69:THR:O	1:A:71:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:O	1:A:224:PHE:N	2.55	0.40
1:A:403:LYS:O	1:A:404:TYR:CG	2.74	0.40
1:A:472:LEU:CD1	2:B:835:GLN:CD	2.95	0.40
1:A:630:ILE:O	1:A:631:HIS:C	2.63	0.40
1:A:874:ASP:HA	1:A:1058:VAL:HG22	2.03	0.40
1:A:878:ILE:HG23	1:A:956:LEU:C	2.47	0.40
1:A:1001:ARG:O	1:A:1002:GLY:C	2.64	0.40
1:A:1118:VAL:O	1:A:1118:VAL:HG23	2.20	0.40
1:A:1211:GLN:O	1:A:1212:VAL:C	2.65	0.40
1:A:1381:LEU:HA	1:A:1381:LEU:HD23	1.77	0.40
2:B:166:PHE:C	2:B:167:ILE:HG13	2.45	0.40
2:B:283:VAL:O	2:B:284:ILE:C	2.64	0.40
2:B:386:LEU:O	2:B:388:CYS:N	2.55	0.40
2:B:798:TYR:CE2	3:C:62:PHE:HE2	2.38	0.40
2:B:839:MET:HE3	2:B:1010:LEU:HD21	2.03	0.40
2:B:1215:ARG:C	2:B:1216:LEU:HD23	2.47	0.40
5:E:8:ASN:OD1	5:E:8:ASN:O	2.40	0.40
5:E:23:VAL:HG13	5:E:78:LEU:CD1	2.49	0.40
5:E:23:VAL:O	5:E:23:VAL:HG12	2.21	0.40
5:E:58:MET:O	5:E:59:SER:C	2.63	0.40
7:G:49:LEU:HD23	7:G:49:LEU:N	2.35	0.40
10:J:2:ILE:H	10:J:57:ILE:HG22	1.87	0.40
11:K:65:HIS:CG	11:K:66:PRO:HD2	2.56	0.40
12:L:43:THR:C	12:L:45:ALA:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1406/1733 (81%)	949 (68%)	293 (21%)	164 (12%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1077/1224 (88%)	735 (68%)	221 (20%)	121 (11%)	0	5
3	C	264/318 (83%)	159 (60%)	66 (25%)	39 (15%)	0	2
4	D	173/177 (98%)	122 (70%)	34 (20%)	17 (10%)	0	7
5	E	212/215 (99%)	148 (70%)	49 (23%)	15 (7%)	1	12
6	F	82/155 (53%)	64 (78%)	14 (17%)	4 (5%)	1	17
7	G	169/171 (99%)	131 (78%)	26 (15%)	12 (7%)	1	12
8	H	129/146 (88%)	84 (65%)	29 (22%)	16 (12%)	0	4
9	I	117/122 (96%)	80 (68%)	29 (25%)	8 (7%)	1	12
10	J	63/70 (90%)	37 (59%)	10 (16%)	16 (25%)	0	0
11	K	113/120 (94%)	89 (79%)	18 (16%)	6 (5%)	1	16
12	L	44/70 (63%)	19 (43%)	14 (32%)	11 (25%)	0	0
All	All	3849/4521 (85%)	2617 (68%)	803 (21%)	429 (11%)	0	5

All (429) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	48	ALA
1	A	54	ASN
1	A	55	ASP
1	A	57	ARG
1	A	62	ASP
1	A	65	LEU
1	A	74	MET
1	A	76	GLU
1	A	78	PRO
1	A	93	VAL
1	A	130	ASP
1	A	154	SER
1	A	167	CYS
1	A	250	ILE
1	A	255	SER
1	A	286	HIS
1	A	311	GLN
1	A	322	VAL
1	A	333	GLU
1	A	335	ARG
1	A	385	ILE

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Mol	Chain	Res	Type
1	A	418	SER
1	A	423	ASP
1	A	424	ILE
1	A	536	LEU
1	A	567	LYS
1	A	619	LYS
1	A	626	ASN
1	A	666	ILE
1	A	775	ILE
1	A	968	GLN
1	A	1002	GLY
1	A	1036	ARG
1	A	1115	SER
1	A	1122	PRO
1	A	1223	ASP
1	A	1281	ARG
1	A	1314	SER
1	A	1341	ILE
1	A	1365	TYR
1	A	1366	ARG
1	A	1378	GLN
1	A	1397	LEU
1	A	1403	GLU
1	A	1405	THR
1	A	1438	THR
2	B	108	VAL
2	B	115	GLN
2	B	186	GLU
2	B	206	ASN
2	B	258	LEU
2	B	259	TYR
2	B	334	ILE
2	B	367	LEU
2	B	629	ASP
2	B	643	ASP
2	B	709	ASP
2	B	727	LYS
2	B	731	VAL
2	B	746	SER
2	B	751	VAL
2	B	881	ASN
2	B	891	ASP

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Mol	Chain	Res	Type
2	B	907	GLY
2	B	958	GLN
2	B	1006	ILE
2	B	1046	PRO
2	B	1069	PHE
2	B	1100	ASP
2	B	1108	ARG
2	B	1156	ASP
2	B	1171	VAL
2	B	1175	LEU
2	B	1181	GLU
2	B	1182	CYS
2	B	1183	LYS
2	B	1186	ASP
2	B	1188	LYS
3	C	56	THR
3	C	78	GLU
3	C	91	HIS
3	C	141	GLY
3	C	149	LYS
3	C	156	THR
3	C	161	LYS
3	C	184	ASN
3	C	202	PRO
3	C	209	TYR
3	C	213	PRO
3	C	214	ASN
3	C	215	GLU
3	C	231	ASN
3	C	240	VAL
4	D	6	SER
4	D	8	PHE
4	D	12	ARG
4	D	19	GLU
4	D	20	GLU
4	D	21	GLU
4	D	52	LEU
4	D	131	GLU
4	D	177	VAL
4	D	192	LYS
4	D	199	ASN
5	E	106	GLN

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Mol	Chain	Res	Type
5	E	130	ALA
7	G	62	LEU
7	G	63	PRO
7	G	139	ILE
8	H	81	PRO
8	H	128	ASN
8	H	140	ALA
9	I	3	THR
9	I	9	ASP
9	I	106	CYS
10	J	2	ILE
10	J	6	ARG
10	J	8	PHE
10	J	9	SER
10	J	17	LYS
10	J	28	ASP
10	J	32	GLU
10	J	64	ASN
11	K	114	LEU
12	L	50	ASP
12	L	53	HIS
12	L	59	ALA
1	A	4	GLN
1	A	42	ASP
1	A	44	THR
1	A	59	GLY
1	A	61	ILE
1	A	66	LYS
1	A	70	CYS
1	A	101	LYS
1	A	111	GLY
1	A	113	LEU
1	A	244	PRO
1	A	263	THR
1	A	290	GLU
1	A	312	PRO
1	A	318	SER
1	A	336	ILE
1	A	364	VAL
1	A	409	SER
1	A	421	ALA
1	A	483	ASP

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Mol	Chain	Res	Type
1	A	661	GLY
1	A	753	GLY
1	A	765	VAL
1	A	780	VAL
1	A	789	LYS
1	A	818	MET
1	A	824	LEU
1	A	846	GLU
1	A	847	ASP
1	A	875	ALA
1	A	986	ILE
1	A	1008	GLN
1	A	1016	THR
1	A	1116	LEU
1	A	1120	LEU
1	A	1133	LEU
1	A	1165	GLU
1	A	1212	VAL
1	A	1221	LYS
1	A	1233	ASP
1	A	1335	ILE
1	A	1377	THR
1	A	1386	ARG
1	A	1389	PHE
1	A	1393	ASN
2	B	21	GLU
2	B	28	GLU
2	B	45	SER
2	B	46	GLN
2	B	114	PRO
2	B	229	ALA
2	B	260	GLY
2	B	266	ALA
2	B	282	ILE
2	B	308	TRP
2	B	513	GLN
2	B	559	SER
2	B	641	GLU
2	B	655	LYS
2	B	869	SER
2	B	888	GLY
2	B	1003	ALA

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Mol	Chain	Res	Type
2	B	1035	ALA
2	B	1041	GLU
2	B	1126	GLY
2	B	1153	GLU
2	B	1155	SER
2	B	1157	ALA
2	B	1167	GLY
2	B	1176	ASN
2	B	1178	ASN
3	C	84	ARG
3	C	87	PHE
3	C	110	THR
3	C	142	VAL
3	C	164	ALA
3	C	169	LYS
3	C	175	ALA
3	C	216	GLY
3	C	255	VAL
3	C	264	GLN
4	D	15	LEU
4	D	218	GLU
5	E	36	GLU
5	E	44	ALA
5	E	59	SER
5	E	73	PRO
5	E	74	ASP
5	E	192	ARG
5	E	206	GLY
6	F	81	THR
7	G	118	ASP
7	G	154	VAL
8	H	32	THR
8	H	59	ILE
8	H	82	PRO
8	H	84	ALA
8	H	92	ASP
8	H	107	VAL
9	I	57	GLY
9	I	62	ILE
10	J	14	VAL
10	J	29	GLU
10	J	33	GLY

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Mol	Chain	Res	Type
11	K	53	ASP
12	L	35	SER
1	A	58	LEU
1	A	71	GLN
1	A	117	GLU
1	A	131	SER
1	A	170	THR
1	A	219	PHE
1	A	223	GLY
1	A	232	GLU
1	A	253	ASN
1	A	278	THR
1	A	317	LYS
1	A	357	PRO
1	A	399	HIS
1	A	419	LYS
1	A	439	ASN
1	A	465	TYR
1	A	517	ASN
1	A	543	LEU
1	A	592	ASP
1	A	605	MET
1	A	731	ARG
1	A	817	ALA
1	A	940	ARG
1	A	1164	PRO
1	A	1309	ASP
1	A	1395	GLY
1	A	1411	GLU
2	B	58	THR
2	B	383	ASN
2	B	450	ALA
2	B	459	TYR
2	B	512	ARG
2	B	571	PRO
2	B	590	HIS
2	B	591	ARG
2	B	605	ARG
2	B	648	HIS
2	B	682	SER
2	B	711	GLU
2	B	738	PHE

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Mol	Chain	Res	Type
2	B	792	MET
2	B	797	TYR
2	B	848	ARG
2	B	878	GLN
2	B	884	ARG
2	B	943	SER
2	B	1017	ILE
3	C	60	ASP
3	C	89	GLU
3	C	93	ASP
3	C	167	HIS
5	E	115	ASN
7	G	53	ASN
8	H	17	PRO
8	H	77	ARG
8	H	108	SER
8	H	135	LEU
9	I	78	CYS
10	J	24	LEU
10	J	51	LEU
10	J	55	ASP
11	K	54	ARG
11	K	88	LYS
12	L	40	LEU
12	L	54	ARG
1	A	69	THR
1	A	276	LEU
1	A	283	GLY
1	A	400	PRO
1	A	756	ILE
1	A	795	GLU
1	A	910	PRO
1	A	958	VAL
1	A	1011	GLN
1	A	1028	THR
1	A	1114	PRO
1	A	1240	CYS
1	A	1242	VAL
1	A	1297	GLU
2	B	67	SER
2	B	68	THR
2	B	100	PRO

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Mol	Chain	Res	Type
2	B	124	TYR
2	B	257	LYS
2	B	369	GLY
2	B	419	THR
2	B	594	ALA
2	B	620	ARG
2	B	735	ALA
2	B	883	LEU
2	B	951	GLN
2	B	1011	ILE
2	B	1082	MET
2	B	1097	HIS
2	B	1144	ALA
3	C	77	ILE
3	C	198	ALA
4	D	30	GLY
7	G	19	GLY
7	G	26	LEU
8	H	44	VAL
8	H	52	GLN
9	I	47	GLU
10	J	27	GLU
11	K	29	ASN
12	L	43	THR
12	L	56	LEU
12	L	60	ARG
1	A	68	GLN
1	A	128	ILE
1	A	226	GLU
1	A	598	LEU
1	A	599	SER
1	A	633	VAL
1	A	648	ASN
1	A	649	ILE
1	A	739	ASP
1	A	755	PHE
1	A	841	LEU
1	A	871	ASP
1	A	969	GLN
1	A	1054	LEU
1	A	1266	THR
2	B	27	ALA

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Mol	Chain	Res	Type
2	B	48	LEU
2	B	65	GLU
2	B	197	PHE
2	B	309	GLN
2	B	414	ALA
2	B	418	LYS
2	B	530	GLY
2	B	636	PRO
2	B	758	PHE
2	B	766	ARG
2	B	867	GLY
2	B	1016	ALA
3	C	108	GLU
4	D	168	LYS
5	E	40	GLU
5	E	45	LYS
6	F	112	GLU
6	F	150	GLU
7	G	34	VAL
7	G	115	MET
1	A	84	ILE
1	A	245	PRO
1	A	492	PRO
1	A	525	GLN
1	A	1158	PRO
1	A	1396	ALA
2	B	313	MET
2	B	364	ILE
2	B	480	SER
2	B	836	GLU
2	B	1214	PRO
3	C	18	VAL
3	C	176	ILE
3	C	230	MET
4	D	69	ALA
4	D	139	LYS
5	E	158	SER
8	H	21	ASN
9	I	34	TYR
10	J	63	TYR
11	K	90	ALA
12	L	28	LYS

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Mol	Chain	Res	Type
12	L	46	VAL
1	A	196	GLU
1	A	300	VAL
1	A	627	GLY
1	A	1057	VAL
2	B	611	PRO
2	B	712	PRO
3	C	172	PRO
3	C	212	PRO
1	A	652	VAL
1	A	653	VAL
2	B	501	PRO
2	B	551	PRO
5	E	37	LEU
1	A	546	VAL
1	A	825	ILE
1	A	1379	GLY
1	A	1454	MET
2	B	411	PRO
2	B	818	PRO
2	B	1018	PRO
3	C	171	GLY
2	B	524	PRO
3	C	126	GLY
6	F	131	PRO
7	G	20	PRO
7	G	116	PRO
2	B	592	ASN
5	E	129	PRO

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	1239/1520 (82%)	1127 (91%)	112 (9%)	9	32
2	B	952/1061 (90%)	862 (90%)	90 (10%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	234/274 (85%)	213 (91%)	21 (9%)	9	32
4	D	140/159 (88%)	119 (85%)	21 (15%)	3	16
5	E	196/197 (100%)	187 (95%)	9 (5%)	24	48
6	F	74/137 (54%)	64 (86%)	10 (14%)	4	19
7	G	152/152 (100%)	141 (93%)	11 (7%)	13	39
8	H	117/128 (91%)	110 (94%)	7 (6%)	17	43
9	I	113/116 (97%)	101 (89%)	12 (11%)	6	26
10	J	60/65 (92%)	54 (90%)	6 (10%)	7	28
11	K	99/102 (97%)	92 (93%)	7 (7%)	13	39
12	L	40/57 (70%)	38 (95%)	2 (5%)	22	47
All	All	3416/3968 (86%)	3108 (91%)	308 (9%)	9	32

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

Mol	Chain	Res	Type
1	A	2	VAL
1	A	11	LEU
1	A	22	PHE
1	A	34	LYS
1	A	38	PRO
1	A	62	ASP
1	A	67	CYS
1	A	93	VAL
1	A	105	CYS
1	A	108	MET
1	A	208	LEU
1	A	215	SER
1	A	221	SER
1	A	236	LEU
1	A	245	PRO
1	A	270	LEU
1	A	289	ILE
1	A	293	GLU
1	A	302	THR
1	A	312	PRO
1	A	320	ARG
1	A	321	PRO
1	A	326	ARG

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Mol	Chain	Res	Type
1	A	335	ARG
1	A	345	VAL
1	A	354	SER
1	A	369	SER
1	A	381	THR
1	A	385	ILE
1	A	404	TYR
1	A	406	ILE
1	A	407	ARG
1	A	408	ASP
1	A	418	SER
1	A	425	GLN
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	460	VAL
1	A	461	LYS
1	A	462	VAL
1	A	481	ASP
1	A	493	GLN
1	A	497	THR
1	A	498	ARG
1	A	503	GLN
1	A	515	GLN
1	A	524	VAL
1	A	535	THR
1	A	560	ILE
1	A	562	THR
1	A	587	HIS
1	A	598	LEU
1	A	616	VAL
1	A	618	GLU
1	A	629	LEU
1	A	666	ILE
1	A	670	ILE
1	A	711	ARG
1	A	774	ARG
1	A	779	PHE
1	A	821	ARG
1	A	827	THR

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Mol	Chain	Res	Type
1	A	831	THR
1	A	834	THR
1	A	845	LEU
1	A	854	ASN
1	A	858	ASN
1	A	886	ILE
1	A	890	ASP
1	A	907	THR
1	A	919	ILE
1	A	929	LEU
1	A	937	VAL
1	A	940	ARG
1	A	949	ASP
1	A	969	GLN
1	A	1006	ILE
1	A	1016	THR
1	A	1029	ARG
1	A	1035	TYR
1	A	1052	GLN
1	A	1067	LEU
1	A	1110	ASN
1	A	1111	MET
1	A	1116	LEU
1	A	1122	PRO
1	A	1127	ASP
1	A	1152	ILE
1	A	1155	ASP
1	A	1170	ILE
1	A	1173	HIS
1	A	1264	GLU
1	A	1271	ILE
1	A	1276	VAL
1	A	1291	VAL
1	A	1295	THR
1	A	1309	ASP
1	A	1325	THR
1	A	1332	PHE
1	A	1333	ILE
1	A	1359	ASP
1	A	1372	VAL
1	A	1400	CYS
1	A	1405	THR

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Mol	Chain	Res	Type
1	A	1428	VAL
1	A	1432	GLN
1	A	1443	VAL
1	A	1445	ILE
1	A	1447	GLU
2	B	44	VAL
2	B	57	TYR
2	B	128	LEU
2	B	188	ASP
2	B	194	GLU
2	B	199	MET
2	B	205	ILE
2	B	223	VAL
2	B	225	VAL
2	B	261	ARG
2	B	268	THR
2	B	283	VAL
2	B	286	PHE
2	B	294	ASP
2	B	298	LEU
2	B	323	VAL
2	B	365	THR
2	B	371	GLU
2	B	378	LEU
2	B	393	LYS
2	B	401	PHE
2	B	427	ASP
2	B	429	PHE
2	B	463	THR
2	B	465	ASN
2	B	466	TRP
2	B	487	THR
2	B	498	THR
2	B	513	GLN
2	B	516	ASN
2	B	555	ILE
2	B	557	PHE
2	B	570	VAL
2	B	582	VAL
2	B	593	PRO
2	B	603	LEU
2	B	615	MET

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Mol	Chain	Res	Type
2	B	628	THR
2	B	635	ARG
2	B	636	PRO
2	B	644	GLU
2	B	649	LYS
2	B	682	SER
2	B	701	ILE
2	B	724	ASP
2	B	737	THR
2	B	742	GLU
2	B	748	ILE
2	B	751	VAL
2	B	830	TYR
2	B	831	SER
2	B	835	GLN
2	B	839	MET
2	B	878	GLN
2	B	894	ASP
2	B	901	PRO
2	B	909	ASP
2	B	939	THR
2	B	953	LEU
2	B	956	THR
2	B	976	ILE
2	B	986	GLN
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1010	LEU
2	B	1018	PRO
2	B	1022	THR
2	B	1034	VAL
2	B	1046	PRO
2	B	1047	PHE
2	B	1051	THR
2	B	1065	GLN
2	B	1069	PHE
2	B	1077	THR
2	B	1084	GLN
2	B	1095	LEU
2	B	1099	VAL
2	B	1103	ILE

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Mol	Chain	Res	Type
2	B	1122	ARG
2	B	1159	ARG
2	B	1160	VAL
2	B	1169	MET
2	B	1170	THR
2	B	1176	ASN
2	B	1183	LYS
2	B	1191	ILE
2	B	1202	LEU
2	B	1212	ILE
2	B	1216	LEU
3	C	22	LEU
3	C	23	SER
3	C	29	MET
3	C	54	ASN
3	C	57	VAL
3	C	58	LEU
3	C	77	ILE
3	C	89	GLU
3	C	91	HIS
3	C	99	LEU
3	C	106	GLU
3	C	108	GLU
3	C	140	ASN
3	C	145	CYS
3	C	147	LEU
3	C	166	GLU
3	C	202	PRO
3	C	233	GLU
3	C	238	ILE
3	C	240	VAL
3	C	266	ASP
4	D	32	GLU
4	D	47	LEU
4	D	61	GLU
4	D	63	LEU
4	D	70	PHE
4	D	122	GLU
4	D	124	GLU
4	D	126	ILE
4	D	137	ASN
4	D	139	LYS

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Mol	Chain	Res	Type
4	D	148	LEU
4	D	149	THR
4	D	152	SER
4	D	156	ASP
4	D	170	THR
4	D	187	THR
4	D	192	LYS
4	D	193	THR
4	D	202	ILE
4	D	208	GLU
4	D	221	TYR
5	E	60	PHE
5	E	74	ASP
5	E	78	LEU
5	E	114	ASN
5	E	175	LEU
5	E	183	PRO
5	E	196	VAL
5	E	207	ARG
5	E	215	MET
6	F	79	ARG
6	F	81	THR
6	F	90	ARG
6	F	99	LEU
6	F	103	MET
6	F	116	ASP
6	F	122	MET
6	F	132	LEU
6	F	148	VAL
6	F	153	VAL
7	G	1	MET
7	G	13	LEU
7	G	38	CYS
7	G	39	THR
7	G	74	TYR
7	G	77	VAL
7	G	78	VAL
7	G	80	LYS
7	G	96	GLN
7	G	126	ASN
7	G	171	ILE
8	H	26	ILE

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Mol	Chain	Res	Type
8	H	62	SER
8	H	86	ASP
8	H	91	ASP
8	H	102	TYR
8	H	130	ARG
8	H	143	LEU
9	I	8	ARG
9	I	9	ASP
9	I	13	MET
9	I	15	TYR
9	I	34	TYR
9	I	78	CYS
9	I	85	PHE
9	I	86	PHE
9	I	94	ASP
9	I	100	PHE
9	I	101	PHE
9	I	106	CYS
10	J	7	CYS
10	J	9	SER
10	J	10	CYS
10	J	44	TYR
10	J	46	CYS
10	J	53	HIS
11	K	10	PHE
11	K	25	THR
11	K	42	LEU
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR
11	K	78	THR
12	L	55	ILE
12	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	54	ASN
1	A	64	ASN
1	A	68	GLN
1	A	71	GLN

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Mol	Chain	Res	Type
1	A	119	ASN
1	A	209	ASN
1	A	213	HIS
1	A	225	ASN
1	A	256	GLN
1	A	287	HIS
1	A	299	HIS
1	A	306	ASN
1	A	339	ASN
1	A	427	GLN
1	A	435	HIS
1	A	445	ASN
1	A	479	ASN
1	A	493	GLN
1	A	503	GLN
1	A	517	ASN
1	A	525	GLN
1	A	611	GLN
1	A	631	HIS
1	A	654	ASN
1	A	698	GLN
1	A	741	ASN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	865	GLN
1	A	877	HIS
1	A	903	ASN
1	A	926	GLN
1	A	1009	ASN
1	A	1040	GLN
1	A	1070	GLN
1	A	1106	ASN
1	A	1140	HIS
1	A	1188	GLN
1	A	1265	ASN
1	A	1364	ASN
1	A	1378	GLN
2	B	60	GLN
2	B	121	ASN
2	B	178	ASN

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Mol	Chain	Res	Type
2	B	215	GLN
2	B	236	HIS
2	B	350	GLN
2	B	363	HIS
2	B	449	ASN
2	B	465	ASN
2	B	484	ASN
2	B	515	HIS
2	B	518	HIS
2	B	538	ASN
2	B	734	HIS
2	B	744	HIS
2	B	821	GLN
2	B	842	ASN
2	B	975	GLN
2	B	1015	HIS
2	B	1062	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
3	C	54	ASN
3	C	65	HIS
3	C	73	GLN
3	C	91	HIS
3	C	112	ASN
3	C	123	ASN
3	C	135	GLN
3	C	167	HIS
3	C	231	ASN
3	C	252	GLN
4	D	40	HIS
4	D	132	GLN
4	D	137	ASN
4	D	157	GLN
4	D	179	GLN
4	D	216	ASN
5	E	8	ASN
5	E	99	HIS
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN

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Mol	Chain	Res	Type
5	E	147	HIS
6	F	104	ASN
7	G	14	HIS
7	G	53	ASN
7	G	57	GLN
7	G	102	GLN
7	G	122	ASN
7	G	126	ASN
7	G	131	GLN
8	H	52	GLN
8	H	131	ASN
9	I	11	ASN
9	I	12	ASN
9	I	89	GLN
11	K	29	ASN
11	K	65	HIS
11	K	76	GLN
12	L	53	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	76:LYS	C	118:THR	N	35.50

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	1416/1733 (81%)	-0.08	26 (1%) 67 46	19, 87, 162, 200	0
2	B	1097/1224 (89%)	0.03	28 (2%) 57 39	23, 97, 166, 194	0
3	C	266/318 (83%)	-0.18	1 (0%) 88 74	37, 81, 139, 160	0
4	D	177/177 (100%)	0.24	6 (3%) 48 33	52, 108, 147, 165	0
5	E	214/215 (99%)	0.22	5 (2%) 61 42	57, 142, 187, 193	0
6	F	84/155 (54%)	-0.41	1 (1%) 76 54	25, 59, 105, 124	0
7	G	171/171 (100%)	-0.02	1 (0%) 85 68	57, 84, 114, 138	0
8	H	133/146 (91%)	0.60	11 (8%) 17 17	101, 138, 175, 184	0
9	I	119/122 (97%)	0.24	3 (2%) 58 40	74, 130, 159, 200	0
10	J	65/70 (92%)	-0.07	0 100 100	42, 79, 120, 127	0
11	K	115/120 (95%)	-0.31	1 (0%) 81 60	42, 83, 114, 123	0
12	L	46/70 (65%)	0.76	4 (8%) 16 16	76, 137, 168, 177	0
All	All	3903/4521 (86%)	0.01	87 (2%) 62 44	19, 94, 166, 200	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	6.2
1	A	3	GLY	5.4
1	A	1081	LEU	5.4
8	H	63	LEU	4.7
8	H	140	ALA	4.5
8	H	139	ASN	4.1
2	B	335	GLY	4.0
2	B	934	LYS	4.0
4	D	25	ALA	3.8
6	F	72	LYS	3.7
2	B	509	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
8	H	90	ALA	3.7
1	A	1257	ASP	3.5
1	A	1254	ALA	3.5
2	B	1224	PHE	3.5
2	B	879	ARG	3.4
1	A	253	ASN	3.3
4	D	24	ALA	3.2
1	A	56	PRO	3.2
1	A	171	GLN	3.2
12	L	50	ASP	3.1
11	K	114	LEU	3.1
4	D	5	THR	3.0
8	H	136	LYS	3.0
1	A	1176	LEU	2.9
2	B	710	LEU	2.9
5	E	88	VAL	2.9
8	H	119	GLY	2.9
1	A	186	LYS	2.9
9	I	2	THR	2.9
1	A	51	GLY	2.8
1	A	59	GLY	2.8
2	B	641	GLU	2.8
1	A	69	THR	2.8
1	A	1205	LYS	2.7
2	B	884	ARG	2.7
1	A	68	GLN	2.6
8	H	135	LEU	2.6
1	A	49	LYS	2.6
1	A	2	VAL	2.6
9	I	76	PRO	2.6
2	B	885	MET	2.6
4	D	4	SER	2.6
2	B	730	ARG	2.5
2	B	1223	ASP	2.5
2	B	880	THR	2.5
1	A	292	ALA	2.4
2	B	883	LEU	2.4
2	B	348	ARG	2.4
1	A	62	ASP	2.4
2	B	106	ASP	2.4
4	D	41	GLN	2.4
8	H	127	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	2.4
1	A	288	ALA	2.4
8	H	51	ALA	2.4
1	A	293	GLU	2.3
1	A	44	THR	2.3
2	B	113	TYR	2.3
12	L	32	ALA	2.3
2	B	349	ILE	2.3
2	B	881	ASN	2.3
5	E	10	SER	2.3
3	C	166	GLU	2.3
2	B	1222	ARG	2.3
2	B	871	THR	2.2
9	I	100	PHE	2.2
4	D	13	ARG	2.2
2	B	446	LEU	2.2
2	B	877	PRO	2.2
1	A	61	ILE	2.2
12	L	25	ALA	2.2
5	E	107	THR	2.2
2	B	70	ILE	2.1
5	E	110	PHE	2.1
1	A	1175	SER	2.1
7	G	150	CYS	2.1
1	A	57	ARG	2.1
8	H	86	ASP	2.1
8	H	132	LEU	2.1
1	A	289	ILE	2.1
2	B	715	ALA	2.0
1	A	40	THR	2.0
5	E	194	GLU	2.0
2	B	345	LYS	2.0
2	B	347	LYS	2.0
2	B	618	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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($\text{\AA}^2$)	Q<0.9
13	ZN	I	1122	1/1	0.91	0.10	156,156,156,156	0
13	ZN	A	2456	1/1	0.98	0.03	86,86,86,86	0
14	MG	A	2458	1/1	0.98	0.07	56,56,56,56	0
13	ZN	L	1071	1/1	0.99	0.07	115,115,115,115	0
13	ZN	J	1066	1/1	0.99	0.06	65,65,65,65	0
13	ZN	A	2457	1/1	1.00	0.02	44,44,44,44	0
13	ZN	B	2225	1/1	1.00	0.02	44,44,44,44	0
13	ZN	C	1269	1/1	1.00	0.01	39,39,39,39	0
13	ZN	I	1121	1/1	1.00	0.03	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.