



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:38 AM UTC

PDB ID : 2B63 / pdb_00002b63
Title : Complete RNA Polymerase II-RNA inhibitor complex
Authors : Kettenberger, H.; Eisenfuehr, A.; Brueckner, F.; Theis, M.; Famulok, M.; Cramer, P.
Deposited on : 2005-09-30
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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

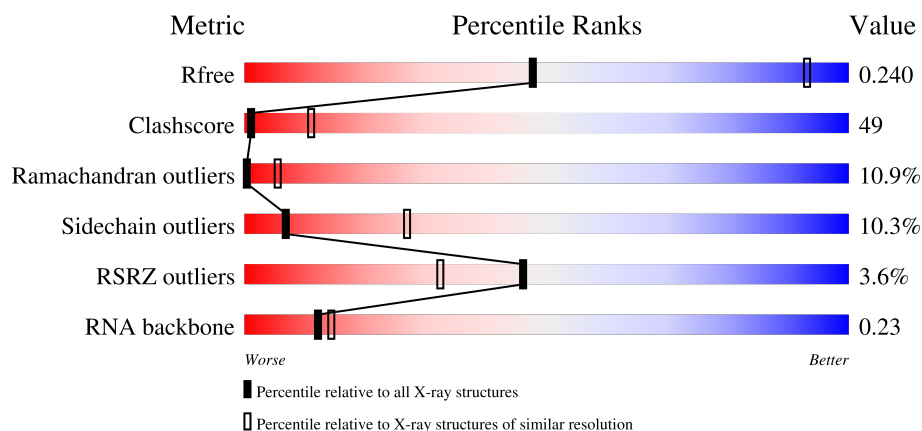
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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)
RNA backbone	3983	1007 (4.50-3.10)

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	R	31	6% 13% 39% 29% 19%
2	A	1733	2% 26% 43% 11% 18%
3	B	1224	4% 27% 46% 16% 9%
4	C	318	0% 24% 46% 12% 16%

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Mol	Chain	Length	Quality of chain
5	D	221	4% 26% 39% 14% 20%
6	E	215	6% 37% 54% 7%
7	F	155	% 18% 27% 9% 46%
8	G	171	% 36% 47% 14%
9	H	146	8% 28% 48% 14% 9%
10	I	122	4% 25% 57% 11%
11	J	70	% 19% 49% 23% 7%
12	K	120	2% 37% 49% 9%
13	L	70	6% 13% 34% 17% 34%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31731 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 RNA chain called 31-MER.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	R	31	Total	Br	C	N	O	P	88	0	0
			666	4	296	119	217	30			

- Molecule 2 is a protein called DNA-directed RNA polymerase II largest subunit.

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

- Molecule 3 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	1112	Total	C	N	O	S	0	0	0
			8836	5594	1548	1639	55			

- Molecule 4 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 5 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

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

- Molecule 8 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	115	Total	C	N	O	S	0	0	0
			924	593	157	172	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

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

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

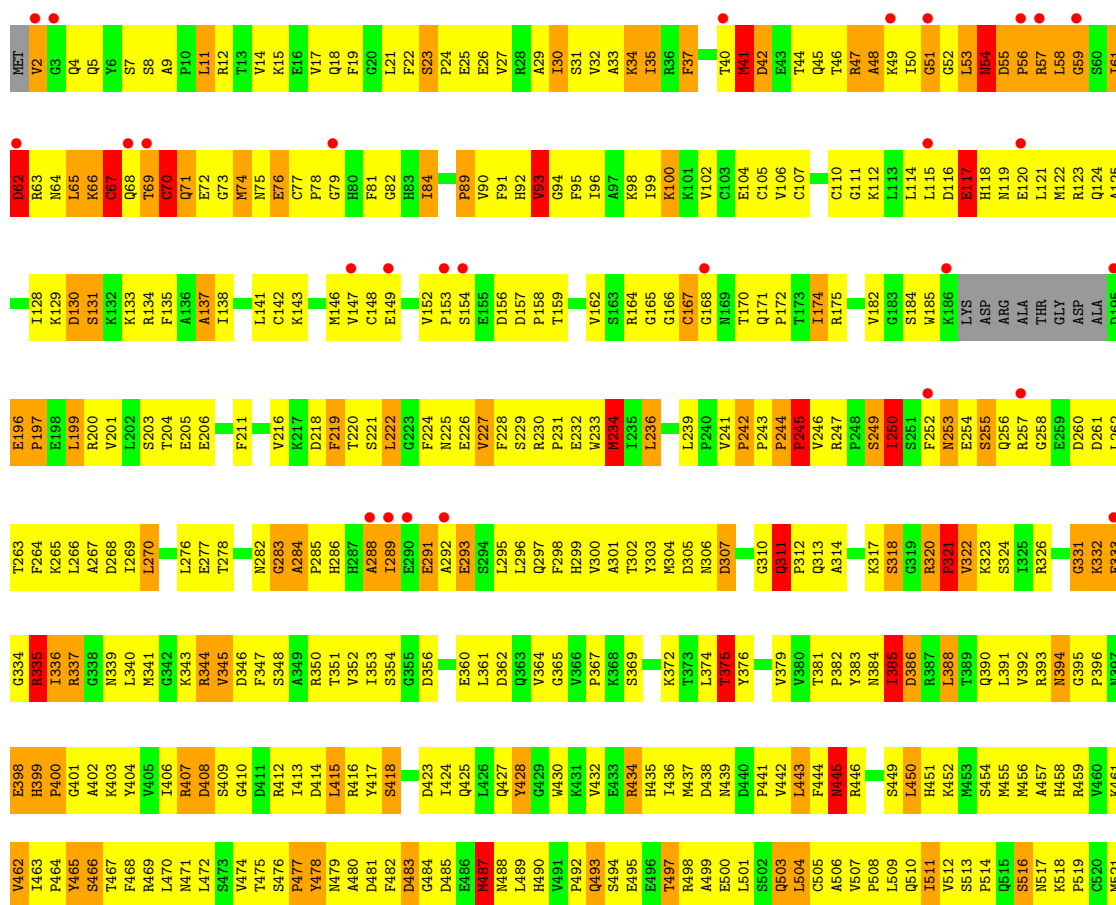
3 Residue-property plots

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.

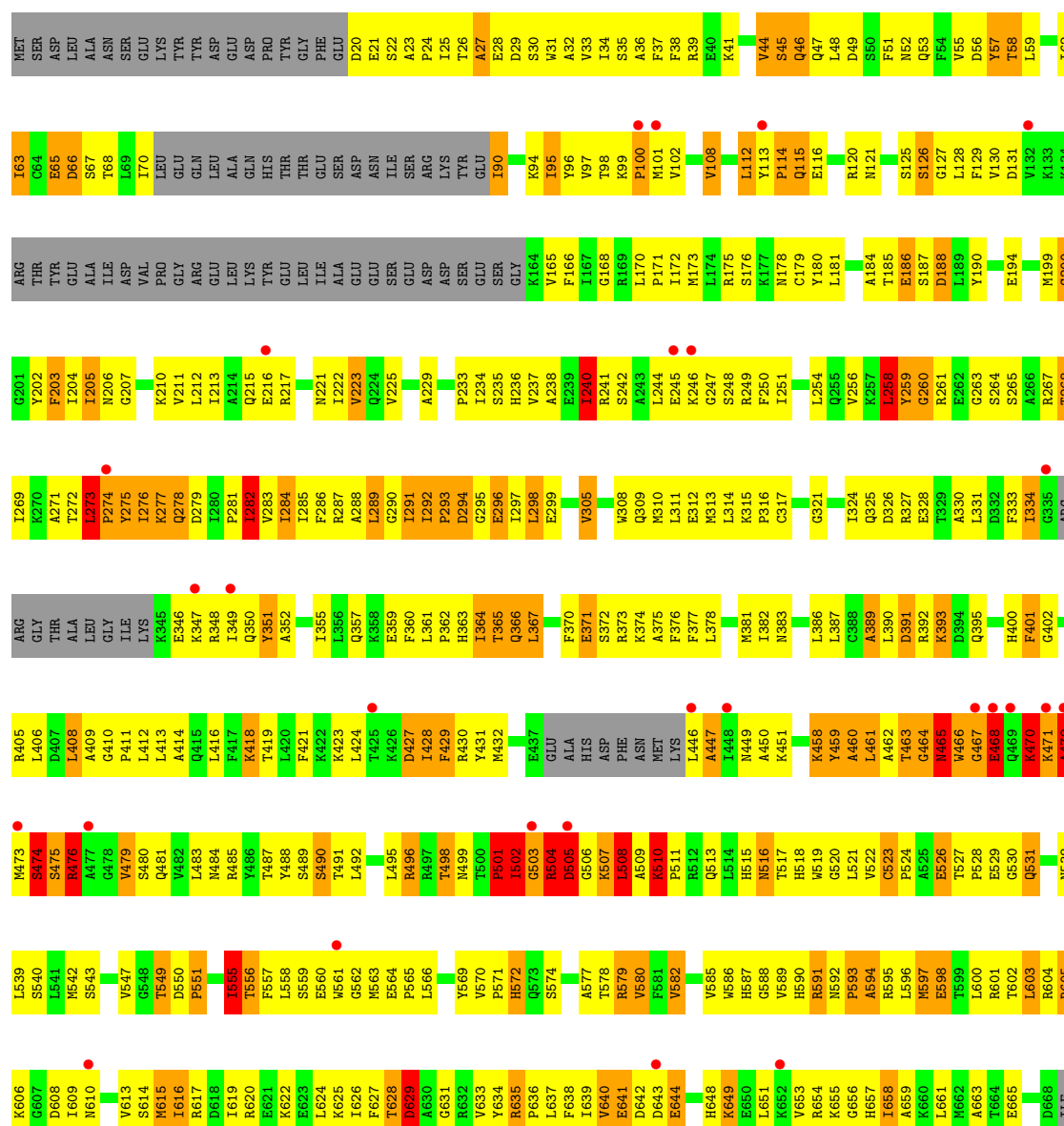
• Molecule 1: 31-MER



• Molecule 2: DNA-directed RNA polymerase II largest subunit

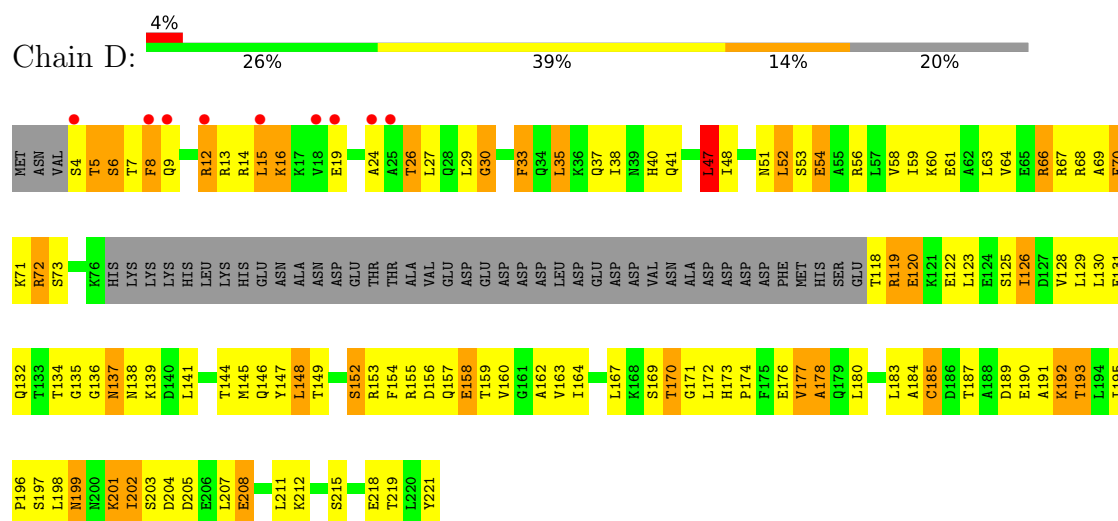




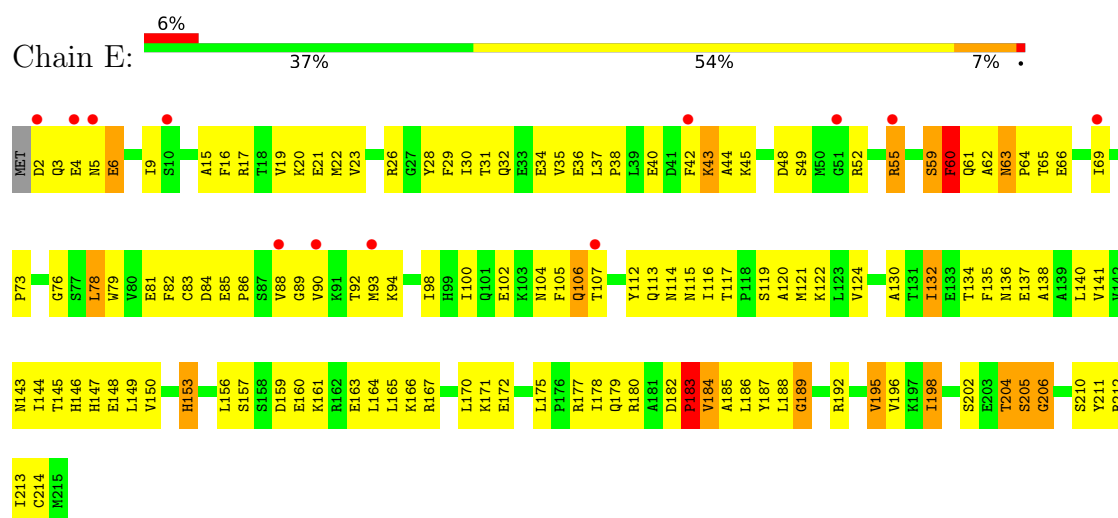




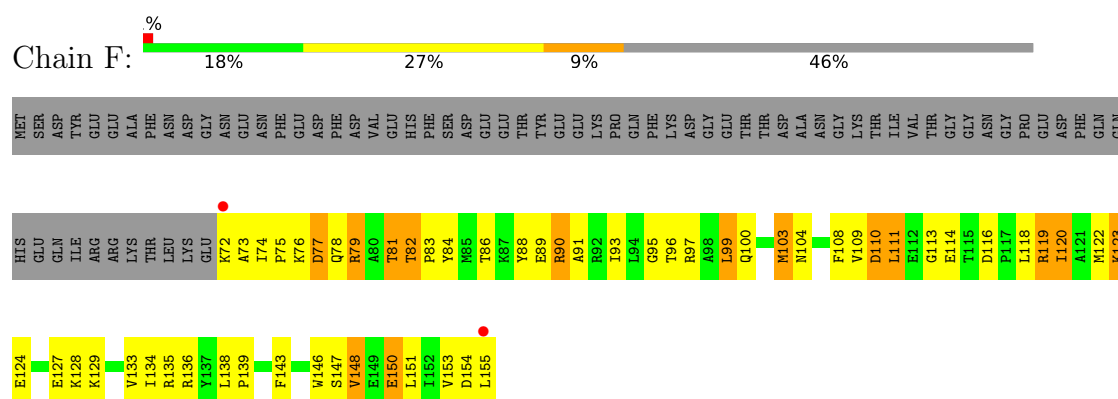
• Molecule 5: DNA-directed RNA polymerase II 32 kDa polypeptide



• Molecule 6: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

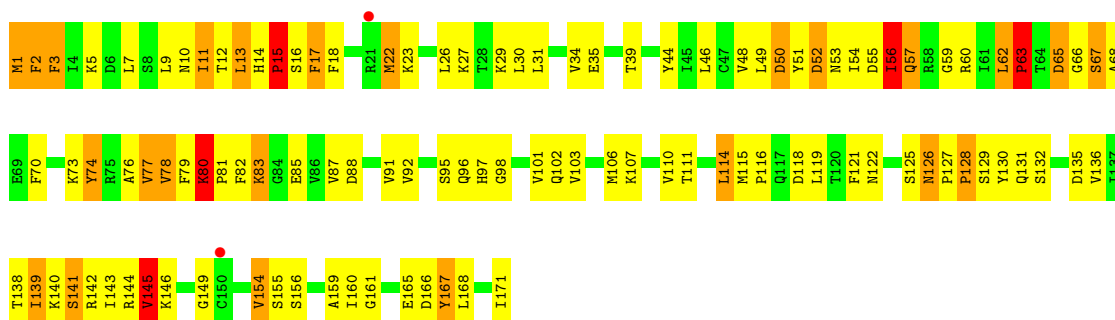


• Molecule 7: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

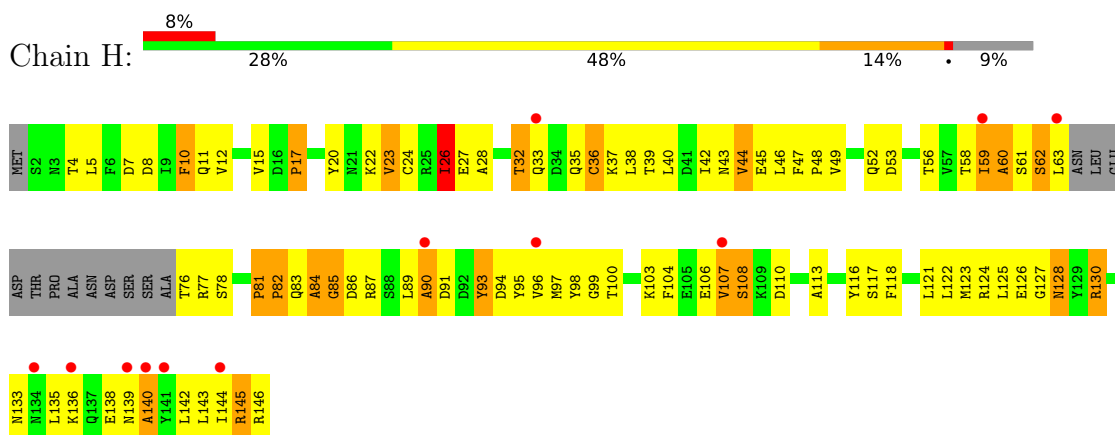


• Molecule 8: DNA-directed RNA polymerase II 19 kDa polypeptide

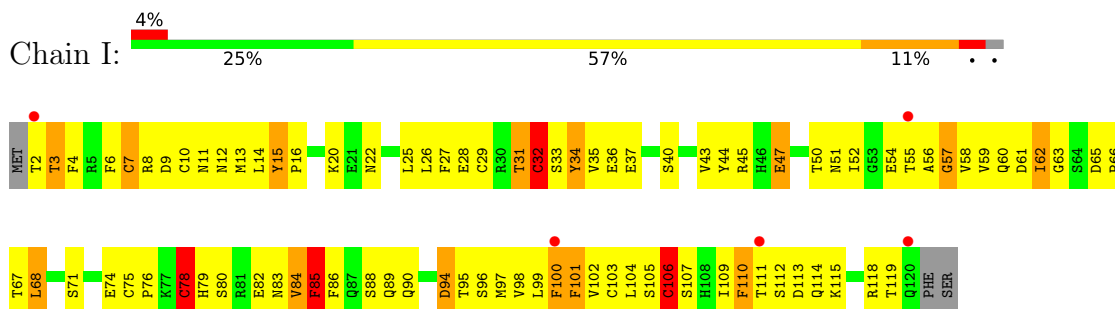




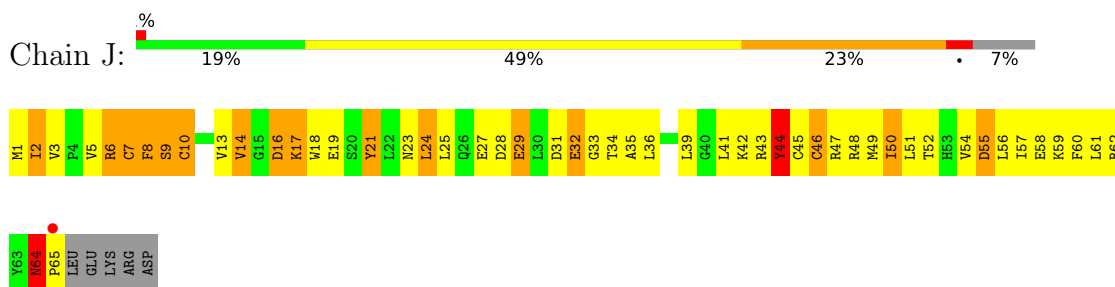
- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



- Molecule 10: DNA-directed RNA polymerase II subunit 9

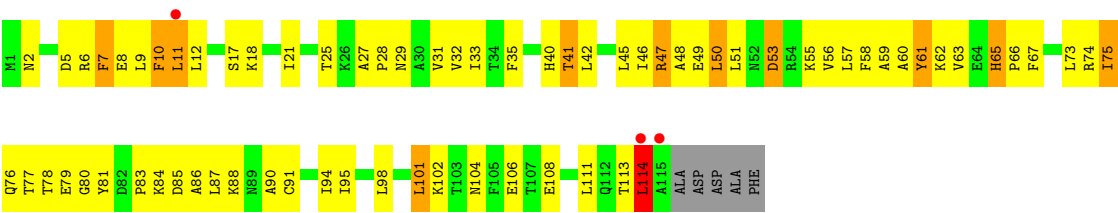


- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10

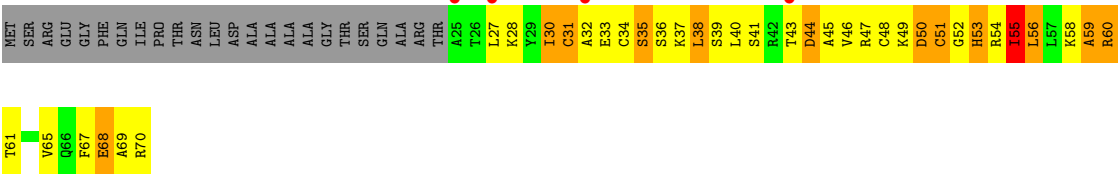


- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide





● Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	224.59Å 399.81Å 286.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.80) 99.8 (50.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.273 0.213 , 0.240	Depositor DCC
R_{free} test set	8121 reflections (3.27%)	wwPDB-VP
Wilson B-factor (Å ²)	121.4	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 84.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.018 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31731	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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, 5BU, 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	R	0.80	3/652 (0.5%)	1.08	3/1017 (0.3%)
2	A	0.59	2/11339 (0.0%)	1.11	86/15334 (0.6%)
3	B	0.57	0/9008	1.16	76/12146 (0.6%)
4	C	0.56	0/2133	1.16	18/2891 (0.6%)
5	D	0.54	0/1365	1.09	13/1837 (0.7%)
6	E	0.51	0/1788	1.09	15/2406 (0.6%)
7	F	0.71	0/691	1.17	6/933 (0.6%)
8	G	0.58	0/1368	1.20	13/1844 (0.7%)
9	H	0.45	0/1086	0.97	4/1470 (0.3%)
10	I	0.43	0/989	1.16	11/1331 (0.8%)
11	J	0.59	0/541	1.14	3/727 (0.4%)
12	K	0.52	0/942	0.98	4/1272 (0.3%)
13	L	0.62	0/365	1.03	3/485 (0.6%)
All	All	0.58	5/32267 (0.0%)	1.12	255/43693 (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	R	0	2
11	J	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	28	5BU	O3'-P	7.88	1.64	1.56
1	R	12	5BU	O3'-P	7.34	1.63	1.56
2	A	1273	LEU	CA-C	5.47	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	17	5BU	O3'-P	5.07	1.61	1.56
2	A	250	ILE	CA-CB	5.02	1.61	1.54

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	508	LEU	N-CA-C	-22.89	86.78	108.75
3	B	275	TYR	N-CA-C	-14.72	95.27	113.23
2	A	56	PRO	N-CA-C	-13.55	100.59	114.68
3	B	1185	CYS	N-CA-C	-13.49	95.36	114.12
3	B	464	GLY	N-CA-C	-11.63	100.04	115.40
3	B	503	GLY	N-CA-C	-11.57	85.76	113.18
3	B	473	MET	N-CA-C	-11.48	95.28	111.81
3	B	681	TRP	N-CA-C	-10.66	99.79	113.12
2	A	344	ARG	N-CA-C	-10.18	95.46	110.52
5	D	26	THR	N-CA-C	-10.15	100.38	113.17
2	A	1403	GLU	N-CA-C	10.13	125.24	113.38
10	I	32	CYS	N-CA-C	10.01	116.99	108.78
2	A	452	LYS	N-CA-C	-9.99	100.38	111.07
3	B	479	VAL	N-CA-C	-9.98	94.11	108.48
3	B	273	LEU	C-N-CD	-9.80	99.03	120.60
8	G	62	LEU	CA-C-N	-9.54	107.92	119.84
8	G	62	LEU	C-N-CA	-9.54	107.92	119.84
8	G	22	MET	N-CA-C	-9.41	100.16	112.68
10	I	109	ILE	N-CA-C	9.34	116.21	106.21
2	A	158	PRO	N-CA-C	-9.25	105.06	114.68
10	I	76	PRO	N-CA-C	-8.97	102.16	114.27
3	B	395	GLN	N-CA-C	-8.95	98.72	110.53
3	B	294	ASP	N-CA-C	-8.57	99.27	110.33
2	A	1262	LYS	N-CA-C	-8.54	101.96	112.38
2	A	466	SER	N-CA-C	8.40	124.63	113.20
11	J	44	TYR	N-CA-C	8.32	121.40	111.33
3	B	296	GLU	N-CA-C	-8.23	102.12	112.90
3	B	468	GLU	N-CA-C	8.00	127.83	110.80
2	A	861	GLY	N-CA-C	-7.98	103.70	114.95
3	B	470	LYS	N-CA-C	7.91	127.64	110.80
3	B	297	ILE	N-CA-C	-7.80	103.19	110.53
3	B	474	SER	N-CA-C	7.80	127.42	110.80
3	B	471	LYS	N-CA-C	-7.79	94.20	110.80
2	A	137	ALA	N-CA-C	-7.77	102.59	112.93
3	B	472	ALA	N-CA-C	7.75	127.31	110.80
6	E	55	ARG	N-CA-C	7.69	119.74	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	183	TRP	N-CA-C	-7.66	97.09	109.96
2	A	954	TRP	N-CA-C	7.65	116.93	108.14
4	C	212	PRO	CA-C-N	7.64	129.39	119.84
4	C	212	PRO	C-N-CA	7.64	129.39	119.84
2	A	143	LYS	N-CA-C	-7.57	102.69	112.23
1	R	5	C	C2'-C3'-O3'	7.52	124.98	113.70
3	B	1145	SER	N-CA-C	7.51	119.11	111.07
3	B	824	ILE	N-CA-C	7.46	114.19	106.21
3	B	502	ILE	N-CA-C	7.42	124.77	109.34
2	A	827	THR	N-CA-C	-7.38	104.80	113.88
4	C	39	ALA	N-CA-C	7.37	124.36	114.12
8	G	80	LYS	CA-C-N	7.35	128.34	120.11
8	G	80	LYS	C-N-CA	7.35	128.34	120.11
5	D	38	ILE	N-CA-C	7.35	120.03	108.87
3	B	427	ASP	N-CA-C	-7.34	103.75	114.39
10	I	119	THR	N-CA-C	-7.32	104.20	113.72
6	E	150	VAL	N-CA-C	7.24	114.15	107.56
6	E	149	LEU	CA-C-N	-7.21	117.70	122.60
6	E	149	LEU	C-N-CA	-7.21	117.70	122.60
8	G	145	VAL	N-CA-C	7.21	119.52	109.29
6	E	60	PHE	N-CA-C	7.19	117.73	108.24
2	A	311	GLN	N-CA-C	7.18	125.67	109.81
2	A	567	LYS	CA-C-N	-7.06	111.01	119.84
2	A	567	LYS	C-N-CA	-7.06	111.01	119.84
8	G	3	PHE	N-CA-C	7.06	120.14	109.41
2	A	1422	ARG	N-CA-C	-7.05	104.33	114.12
3	B	805	THR	N-CA-C	6.99	117.50	108.34
8	G	65	ASP	N-CA-C	-6.94	99.69	109.69
2	A	928	LEU	N-CA-C	-6.91	102.32	111.24
2	A	1444	MET	N-CA-C	6.88	119.90	109.23
2	A	1277	GLU	N-CA-C	6.88	119.83	110.55
2	A	513	SER	CA-C-N	6.84	127.43	120.04
2	A	513	SER	C-N-CA	6.84	127.43	120.04
4	C	165	LYS	N-CA-C	-6.84	103.05	111.40
6	E	9	ILE	N-CA-C	-6.80	105.12	111.45
2	A	539	THR	N-CA-C	6.74	119.67	108.96
3	B	273	LEU	CA-C-N	6.73	143.15	127.00
3	B	273	LEU	C-N-CA	6.73	143.15	127.00
4	C	181	ASP	CA-C-N	6.71	126.22	119.24
4	C	181	ASP	C-N-CA	6.71	126.22	119.24
3	B	112	LEU	N-CA-C	6.71	119.61	110.55
2	A	234	MET	N-CA-C	-6.71	104.96	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	555	ILE	N-CA-C	-6.70	104.12	110.42
3	B	276	ILE	N-CA-C	6.70	120.73	113.43
3	B	507	LYS	N-CA-C	6.67	120.50	108.17
11	J	10	CYS	N-CA-C	6.64	118.60	111.36
2	A	398	GLU	N-CA-C	-6.60	99.77	110.20
6	E	52	ARG	CA-C-N	6.58	126.81	119.90
6	E	52	ARG	C-N-CA	6.58	126.81	119.90
3	B	66	ASP	N-CA-C	-6.56	106.02	112.97
4	C	225	ALA	N-CA-C	6.50	118.25	107.20
2	A	1275	GLY	N-CA-C	6.46	120.00	110.63
11	J	42	LYS	N-CA-C	6.46	119.57	111.24
6	E	63	ASN	CA-C-N	6.44	126.20	119.76
6	E	63	ASN	C-N-CA	6.44	126.20	119.76
3	B	127	GLY	N-CA-C	6.42	120.42	112.14
3	B	366	GLN	N-CA-C	-6.41	105.04	112.92
2	A	887	GLY	N-CA-C	6.40	121.33	112.37
8	G	76	ALA	N-CA-C	6.39	117.56	108.74
2	A	1155	ASP	CA-C-N	6.36	126.91	120.04
2	A	1155	ASP	C-N-CA	6.36	126.91	120.04
12	K	75	ILE	N-CA-C	6.29	116.91	108.11
3	B	640	VAL	N-CA-C	6.27	118.92	112.90
2	A	511	ILE	N-CA-C	6.27	116.94	110.36
7	F	148	VAL	N-CA-C	-6.26	104.24	110.62
2	A	331	GLY	N-CA-C	6.25	128.00	113.18
2	A	30	ILE	N-CA-C	6.24	116.41	110.42
5	D	171	GLY	N-CA-C	-6.23	106.72	115.32
3	B	1135	ARG	N-CA-C	-6.22	104.19	110.97
2	A	1078	GLN	N-CA-C	-6.21	105.68	113.20
3	B	523	CYS	CA-C-N	6.21	126.75	120.04
3	B	523	CYS	C-N-CA	6.21	126.75	120.04
5	D	66	ARG	N-CA-C	-6.19	104.45	111.14
2	A	277	GLU	N-CA-C	-6.16	105.67	113.43
3	B	1181	GLU	N-CA-C	6.15	123.91	110.80
10	I	32	CYS	CA-C-O	6.15	121.51	117.94
3	B	825	VAL	N-CA-C	6.15	117.16	110.21
2	A	776	ALA	N-CA-C	6.13	119.57	109.94
2	A	222	LEU	N-CA-C	-6.12	101.43	110.48
2	A	67	CYS	N-CA-C	-6.11	97.80	110.80
2	A	201	VAL	N-CA-C	6.06	117.50	108.23
8	G	83	LYS	N-CA-C	-6.06	101.31	110.28
2	A	950	GLY	N-CA-C	-6.05	106.58	115.72
10	I	32	CYS	CB-CA-C	-6.05	108.35	117.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1177	HIS	N-CA-C	-6.05	105.48	112.92
3	B	574	SER	CA-C-N	6.03	127.37	119.84
3	B	574	SER	C-N-CA	6.03	127.37	119.84
7	F	150	GLU	N-CA-C	6.03	117.65	111.14
2	A	288	ALA	N-CA-C	-6.02	103.46	112.54
3	B	1223	ASP	CB-CA-C	-6.01	109.62	116.54
2	A	47	ARG	N-CA-C	6.00	118.52	108.73
5	D	8	PHE	N-CA-C	6.00	123.59	110.80
8	G	52	ASP	N-CA-C	6.00	117.69	111.03
2	A	984	LYS	N-CA-C	-6.00	104.08	111.40
3	B	1151	LEU	N-CA-C	5.95	118.53	111.33
2	A	998	LEU	N-CA-C	5.94	119.50	109.76
5	D	70	PHE	N-CA-C	-5.94	105.29	112.54
10	I	28	GLU	N-CA-C	5.94	116.94	108.74
3	B	693	ILE	N-CA-C	5.93	116.40	107.80
2	A	1039	LYS	N-CA-C	-5.93	104.74	111.14
3	B	1168	LEU	N-CA-C	5.92	118.22	109.69
3	B	458	LYS	N-CA-C	-5.91	104.47	111.03
2	A	100	LYS	N-CA-C	-5.87	104.80	111.14
3	B	1182	CYS	N-CA-C	-5.86	96.39	108.53
3	B	1013	ASN	N-CA-C	5.80	117.13	109.93
2	A	738	LYS	N-CA-C	5.80	118.68	110.50
2	A	1293	SER	N-CA-C	-5.80	101.78	110.24
1	R	8	U	N1-C1'-C2'	5.79	120.68	112.00
5	D	72	ARG	N-CA-C	-5.78	105.33	112.38
10	I	85	PHE	N-CA-C	5.78	119.01	110.46
2	A	30	ILE	CB-CA-C	-5.77	104.58	111.97
4	C	211	ASP	CA-C-N	5.75	126.31	120.38
4	C	211	ASP	C-N-CA	5.75	126.31	120.38
2	A	1163	ILE	CA-C-N	5.71	125.08	118.85
2	A	1163	ILE	C-N-CA	5.71	125.08	118.85
7	F	120	ILE	CB-CA-C	-5.70	104.57	112.04
9	H	23	VAL	N-CA-C	5.69	115.86	108.35
4	C	4	GLU	N-CA-C	5.67	120.22	112.68
6	E	6	GLU	N-CA-C	-5.66	106.22	113.01
2	A	432	VAL	CB-CA-C	-5.65	104.81	111.09
3	B	389	ALA	N-CA-C	-5.65	106.23	113.01
6	E	5	ASN	N-CA-C	-5.65	106.06	114.64
2	A	467	THR	N-CA-C	5.63	117.95	109.23
3	B	580	VAL	N-CA-C	5.62	116.57	108.48
2	A	636	GLU	N-CA-C	5.61	118.24	111.40
3	B	978	ASP	N-CA-C	5.61	117.77	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1070	GLU	N-CA-C	-5.59	99.64	108.14
2	A	221	SER	N-CA-C	-5.59	104.41	111.11
2	A	333	GLU	N-CA-C	-5.58	106.42	113.23
3	B	1183	LYS	N-CA-C	-5.57	102.77	110.35
13	L	31	CYS	N-CA-C	-5.57	103.13	110.43
2	A	291	GLU	N-CA-C	-5.55	105.86	113.30
2	A	1291	VAL	CA-C-N	5.52	126.38	119.98
2	A	1291	VAL	C-N-CA	5.52	126.38	119.98
3	B	700	SER	N-CA-C	5.51	117.49	109.71
2	A	289	ILE	N-CA-C	-5.51	107.44	111.90
9	H	26	ILE	N-CA-C	5.51	115.88	108.17
2	A	174	ILE	N-CA-C	5.47	116.61	108.46
2	A	683	ILE	N-CA-C	-5.47	106.36	111.45
2	A	488	ASN	N-CA-C	5.47	118.65	109.95
12	K	65	HIS	CA-C-N	5.47	126.67	119.84
12	K	65	HIS	C-N-CA	5.47	126.67	119.84
2	A	628	GLY	N-CA-C	5.45	119.52	112.54
3	B	872	GLU	N-CA-C	-5.45	103.19	110.55
2	A	81	PHE	N-CA-C	5.45	117.32	110.24
9	H	145	ARG	N-CA-C	5.44	118.05	108.75
6	E	32	GLN	N-CA-C	-5.43	105.38	112.23
3	B	292	ILE	N-CA-C	5.43	120.61	108.88
3	B	428	ILE	N-CA-C	-5.43	105.83	111.58
3	B	572	HIS	N-CA-C	5.43	118.69	111.75
3	B	1088	GLY	CA-C-N	5.42	125.42	119.89
3	B	1088	GLY	C-N-CA	5.42	125.42	119.89
7	F	82	THR	CA-C-N	5.41	125.89	120.04
7	F	82	THR	C-N-CA	5.41	125.89	120.04
2	A	242	PRO	CA-C-N	5.40	125.94	120.38
2	A	242	PRO	C-N-CA	5.40	125.94	120.38
2	A	584	ASN	N-CA-C	5.40	118.14	110.10
5	D	35	LEU	N-CA-C	-5.40	105.40	111.28
2	A	445	ASN	N-CA-C	5.39	116.99	108.96
10	I	68	LEU	CA-C-N	5.38	125.84	120.14
10	I	68	LEU	C-N-CA	5.38	125.84	120.14
5	D	158	GLU	N-CA-C	-5.38	104.76	112.13
3	B	99	LYS	CA-C-N	5.37	126.55	119.84
3	B	99	LYS	C-N-CA	5.37	126.55	119.84
3	B	1109	GLY	CA-C-N	5.37	126.55	119.84
3	B	1109	GLY	C-N-CA	5.37	126.55	119.84
2	A	718	VAL	N-CA-C	-5.35	104.67	110.23
2	A	837	ILE	N-CA-C	-5.33	105.30	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	53	ASP	N-CA-C	-5.33	101.09	109.25
2	A	375	THR	N-CA-C	5.33	117.36	108.99
3	B	841	MET	N-CA-C	5.31	116.85	107.61
2	A	199	LEU	N-CA-C	5.31	118.27	109.46
2	A	487	MET	N-CA-C	5.30	117.74	109.52
2	A	1264	GLU	N-CA-C	-5.30	105.15	111.03
4	C	193	TYR	N-CA-C	5.29	116.33	108.86
2	A	744	LYS	N-CA-C	-5.29	105.42	111.14
2	A	293	GLU	N-CA-C	-5.29	105.18	111.69
3	B	423	LYS	N-CA-C	-5.28	106.79	113.18
2	A	553	VAL	CA-C-N	5.27	124.93	119.56
2	A	553	VAL	C-N-CA	5.27	124.93	119.56
3	B	840	ILE	N-CA-C	-5.25	101.08	109.17
3	B	293	PRO	N-CA-C	5.25	118.72	110.80
4	C	40	GLU	CA-C-N	-5.24	118.82	122.59
4	C	40	GLU	C-N-CA	-5.24	118.82	122.59
2	A	1077	THR	N-CA-C	-5.23	107.57	114.31
9	H	85	GLY	N-CA-C	-5.20	106.43	113.24
10	I	31	THR	N-CA-C	-5.20	105.76	112.68
2	A	1064	VAL	N-CA-C	5.20	118.34	111.17
2	A	982	THR	N-CA-C	-5.20	103.67	110.53
6	E	150	VAL	CA-C-N	5.16	125.61	120.14
6	E	150	VAL	C-N-CA	5.16	125.61	120.14
8	G	56	ILE	N-CA-C	-5.16	107.39	113.42
5	D	33	PHE	N-CA-C	5.15	117.05	110.61
4	C	41	ILE	CA-C-N	5.14	125.38	119.83
4	C	41	ILE	C-N-CA	5.14	125.38	119.83
3	B	703	ILE	N-CA-C	5.13	115.98	108.53
2	A	1440	ALA	N-CA-C	-5.13	106.87	112.72
3	B	602	THR	N-CA-C	-5.13	107.41	113.97
4	C	23	SER	N-CA-C	5.12	116.96	109.24
7	F	77	ASP	N-CA-C	-5.12	103.17	110.59
2	A	229	SER	N-CA-C	5.10	115.87	107.20
3	B	1129	ARG	N-CA-C	5.10	117.28	109.07
1	R	2	C	O4'-C1'-N1	5.09	115.84	108.20
13	L	30	ILE	N-CA-C	5.08	115.05	108.35
2	A	546	VAL	N-CA-C	-5.07	106.41	113.00
3	B	732	SER	N-CA-C	5.06	114.72	108.19
3	B	408	LEU	N-CA-C	5.05	115.98	108.86
13	L	68	GLU	N-CA-C	-5.05	102.22	110.20
3	B	1210	MET	N-CA-C	-5.04	106.38	112.88
3	B	1001	PHE	N-CA-C	5.04	116.84	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	217	ASP	N-CA-C	5.04	115.39	109.60
2	A	478	TYR	N-CA-C	-5.03	106.25	112.38
3	B	915	THR	N-CA-C	5.02	116.82	109.24
5	D	178	ALA	N-CA-C	-5.02	105.25	112.13
2	A	54	ASN	CA-C-N	5.02	134.04	121.80
2	A	54	ASN	C-N-CA	5.02	134.04	121.80
5	D	201	LYS	N-CA-C	5.02	119.65	111.37
8	G	129	SER	N-CA-C	5.01	114.95	107.88
5	D	54	GLU	N-CA-C	-5.01	106.01	111.82

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	J	44	TYR	Sidechain
1	R	2	C	Sidechain
1	R	5	C	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	R	666	0	331	42	0
2	A	11140	0	11217	1183	0
3	B	8836	0	8871	984	0
4	C	2095	0	2051	253	0
5	D	1356	0	1319	127	0
6	E	1752	0	1776	142	0
7	F	679	0	701	60	0
8	G	1340	0	1357	144	0
9	H	1068	0	1040	126	0
10	I	971	0	928	92	0
11	J	532	0	542	93	0
12	K	924	0	934	86	0
13	L	363	0	386	43	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	31731	0	31453	3118	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 49.

All (3118) 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)
5:D:40:HIS:HB3	8:G:73:LYS:NZ	1.60	1.16
2:A:1329:THR:HG22	2:A:1331:SER:H	1.01	1.12
3:B:827:ILE:HG12	3:B:1012:ILE:HD11	1.18	1.11
3:B:463:THR:HB	3:B:465:ASN:HB2	1.32	1.10
1:R:3:A:OP2	3:B:531:GLN:HB3	1.50	1.10
3:B:882:THR:HG22	3:B:884:ARG:H	1.14	1.10
9:H:59:ILE:HG22	9:H:60:ALA:H	0.92	1.08
10:I:34:TYR:HD2	10:I:35:VAL:N	1.54	1.06
11:J:5:VAL:HG12	11:J:6:ARG:HG3	1.31	1.05
2:A:53:LEU:HD23	2:A:54:ASN:N	1.71	1.04
2:A:53:LEU:CD2	2:A:54:ASN:H	1.69	1.04
9:H:100:THR:HG23	9:H:138:GLU:HA	1.35	1.04
8:G:13:LEU:HD21	8:G:17:PHE:HB2	1.39	1.04
2:A:779:PHE:CE1	2:A:785:PRO:HD3	1.94	1.03
3:B:254:LEU:HD23	3:B:381:MET:HE1	1.36	1.03
12:K:47:ARG:HB3	12:K:47:ARG:HH11	1.17	1.03
2:A:61:ILE:HG22	2:A:62:ASP:H	1.22	1.03
2:A:107:CYS:H	2:A:114:LEU:HD21	1.22	1.03
2:A:590:ARG:NH2	2:A:620:LYS:HB3	1.74	1.03
3:B:505:ASP:CG	3:B:506:GLY:H	1.68	1.01
4:C:57:VAL:HG11	11:J:60:PHE:HB3	1.41	1.01
2:A:1161:THR:HG22	2:A:1163:ILE:H	1.26	1.01
2:A:53:LEU:HD23	2:A:54:ASN:H	0.87	1.01
9:H:59:ILE:HG22	9:H:60:ALA:N	1.72	1.01
2:A:826:ASP:O	2:A:830:LYS:HB2	1.61	1.01
3:B:509:ALA:O	3:B:511:PRO:HD3	1.61	1.00
6:E:29:PHE:O	6:E:30:ILE:HG13	1.61	1.00
2:A:225:ASN:ND2	2:A:228:PHE:H	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:138:THR:HG22	8:G:139:ILE:H	1.25	0.99
3:B:577:ALA:HB1	3:B:589:VAL:HG11	1.45	0.98
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.43	0.98
11:J:64:ASN:HB3	11:J:65:PRO:CD	1.92	0.98
8:G:143:ILE:HG22	8:G:144:ARG:H	1.28	0.97
3:B:684:LEU:H	3:B:684:LEU:HD12	1.30	0.96
2:A:907:THR:HG22	2:A:908:LEU:H	1.26	0.96
3:B:276:ILE:HD11	3:B:355:ILE:HG21	1.45	0.95
3:B:65:GLU:HG3	3:B:66:ASP:H	1.30	0.95
2:A:767:GLN:HE21	2:A:774:ARG:HB3	1.28	0.95
3:B:365:THR:HG23	3:B:367:LEU:H	1.32	0.94
2:A:249:SER:O	2:A:250:ILE:HG12	1.66	0.94
2:A:1116:LEU:HG	2:A:1308:THR:HG21	1.46	0.94
9:H:59:ILE:CG2	9:H:60:ALA:H	1.79	0.94
6:E:94:LYS:HE2	6:E:98:ILE:HD11	1.49	0.94
3:B:510:LYS:H	3:B:510:LYS:HD2	1.32	0.93
2:A:858:ASN:ND2	2:A:860:LEU:H	1.67	0.93
10:I:85:PHE:H	10:I:85:PHE:HD2	1.08	0.93
2:A:1329:THR:HG22	2:A:1331:SER:N	1.84	0.92
2:A:868:TYR:CE1	2:A:1064:VAL:HG11	2.04	0.92
5:D:40:HIS:HB3	8:G:73:LYS:HZ3	1.18	0.92
3:B:800:GLN:HB3	11:J:52:THR:HG21	1.51	0.92
2:A:783:THR:HG22	2:A:784:LEU:HG	1.51	0.91
2:A:901:LEU:HG	2:A:926:GLN:HE21	1.32	0.91
12:K:21:ILE:HG12	12:K:33:ILE:HG13	1.52	0.91
2:A:567:LYS:HZ1	9:H:46:LEU:HB2	1.36	0.91
2:A:1017:LEU:HB2	6:E:206:GLY:H	1.33	0.91
9:H:23:VAL:HG22	9:H:43:ASN:HA	1.52	0.90
7:F:93:ILE:HD11	7:F:134:ILE:HD11	1.51	0.90
2:A:225:ASN:HD22	2:A:228:PHE:H	0.98	0.90
2:A:567:LYS:CG	2:A:568:PRO:HD2	2.01	0.90
6:E:22:MET:HE3	6:E:26:ARG:HE	1.34	0.90
3:B:1072:MET:CE	3:B:1085:ILE:HB	2.01	0.89
2:A:1094:VAL:HG13	2:A:1113:THR:HG21	1.55	0.89
2:A:605:MET:HE2	2:A:607:ILE:HG13	1.55	0.89
4:C:17:ASN:HD22	4:C:17:ASN:N	1.70	0.89
6:E:22:MET:HE3	6:E:26:ARG:NE	1.88	0.89
3:B:642:ASP:HA	3:B:649:LYS:HA	1.52	0.89
3:B:589:VAL:HG12	3:B:590:HIS:H	1.36	0.89
7:F:82:THR:HG22	7:F:84:TYR:H	1.36	0.89
8:G:143:ILE:HG22	8:G:144:ARG:N	1.84	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1428:VAL:HG13	3:B:1151:LEU:HD21	1.53	0.88
3:B:271:ALA:HB1	3:B:273:LEU:HD11	1.53	0.88
3:B:1065:GLN:HE21	3:B:1067:ARG:N	1.70	0.88
4:C:47:ASP:HA	13:L:69:ALA:HB3	1.55	0.88
9:H:126:GLU:C	9:H:130:ARG:HH22	1.82	0.88
10:I:111:THR:HG22	10:I:113:ASP:H	1.35	0.88
9:H:42:ILE:HG23	9:H:95:TYR:HE1	1.37	0.88
4:C:251:LEU:O	4:C:251:LEU:HD12	1.73	0.88
3:B:953:LEU:HD21	3:B:965:LYS:HB2	1.56	0.87
3:B:705:MET:H	3:B:710:LEU:HD12	1.39	0.87
12:K:47:ARG:HB3	12:K:47:ARG:NH1	1.89	0.87
2:A:369:SER:HB3	12:K:2:ASN:HD21	1.37	0.87
3:B:1007:VAL:HG22	3:B:1008:PRO:HD2	1.54	0.87
3:B:827:ILE:CG1	3:B:1012:ILE:HD11	2.04	0.87
6:E:153:HIS:HB3	6:E:196:VAL:HG11	1.56	0.87
2:A:590:ARG:HH21	2:A:620:LYS:HB3	1.31	0.87
2:A:1242:VAL:HG12	2:A:1243:VAL:H	1.35	0.86
3:B:281:PRO:HG2	3:B:284:ILE:HD13	1.57	0.86
3:B:464:GLY:C	3:B:466:TRP:H	1.83	0.86
3:B:510:LYS:H	3:B:510:LYS:CD	1.87	0.86
4:C:142:VAL:H	11:J:16:ASP:HB3	1.40	0.86
3:B:846:ILE:HG23	3:B:974:PRO:HG2	1.57	0.86
2:A:1312:ASN:O	2:A:1316:VAL:HG23	1.74	0.86
3:B:821:GLN:HE22	3:B:851:PHE:HA	1.40	0.86
11:J:64:ASN:HB3	11:J:65:PRO:HD3	1.55	0.86
2:A:1438:THR:HB	3:B:1144:ALA:HB3	1.55	0.86
3:B:476:ARG:HA	3:B:476:ARG:HH11	1.40	0.86
6:E:156:LEU:HD12	6:E:195:VAL:HB	1.57	0.86
2:A:399:HIS:HB3	2:A:400:PRO:HD3	1.57	0.85
2:A:1364:ASN:HD22	2:A:1365:TYR:N	1.73	0.85
4:C:164:ALA:HA	4:C:167:HIS:O	1.75	0.85
2:A:164:ARG:HG3	2:A:165:GLY:H	1.38	0.85
2:A:821:ARG:HB2	2:A:821:ARG:HH11	1.41	0.85
2:A:605:MET:HE3	2:A:606:LEU:H	1.41	0.85
3:B:800:GLN:HB3	11:J:52:THR:CG2	2.06	0.85
1:R:2:C:O2'	1:R:3:A:OP1	1.95	0.85
2:A:56:PRO:O	2:A:57:ARG:HG3	1.76	0.85
4:C:16:ASP:C	4:C:17:ASN:HD22	1.85	0.85
6:E:144:ILE:HD12	6:E:145:THR:N	1.91	0.84
2:A:527:THR:HG21	2:A:650:GLN:HG2	1.57	0.84
8:G:115:MET:HB2	8:G:116:PRO:HD2	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:29:G:H4'	2:A:1386:ARG:HH12	1.42	0.84
2:A:981:LEU:HD21	2:A:1039:LYS:HA	1.58	0.84
3:B:999:MET:HA	3:B:999:MET:HE3	1.59	0.84
2:A:285:PRO:HG2	2:A:288:ALA:HB3	1.60	0.84
2:A:567:LYS:HG3	2:A:568:PRO:HD2	1.56	0.84
2:A:15:LYS:HB3	3:B:1220:ARG:HH21	1.43	0.83
3:B:980:PHE:HE1	3:B:990:ILE:HD11	1.42	0.83
2:A:628:GLY:O	2:A:632:VAL:HG23	1.78	0.83
2:A:800:VAL:HG22	2:A:812:GLU:HB3	1.60	0.83
2:A:1394:THR:HG21	2:A:1398:MET:SD	2.19	0.83
10:I:8:ARG:HG3	10:I:34:TYR:HE1	1.43	0.83
2:A:54:ASN:HB3	2:A:247:ARG:HH12	1.44	0.83
2:A:768:GLN:HG2	2:A:816:HIS:HA	1.61	0.83
2:A:147:VAL:N	2:A:171:GLN:HE21	1.75	0.83
3:B:463:THR:C	3:B:465:ASN:H	1.85	0.82
3:B:1152:MET:CE	3:B:1157:ALA:HA	2.08	0.82
3:B:120:ARG:HG2	3:B:955:THR:HG21	1.59	0.82
4:C:167:HIS:HA	12:K:6:ARG:HH12	1.43	0.82
2:A:528:LEU:O	2:A:531:ILE:HG22	1.79	0.82
3:B:1072:MET:HE3	3:B:1085:ILE:HB	1.61	0.82
3:B:952:VAL:HG12	3:B:953:LEU:N	1.94	0.82
8:G:145:VAL:HG12	8:G:146:LYS:H	1.43	0.82
2:A:901:LEU:H	2:A:926:GLN:NE2	1.77	0.82
5:D:134:THR:HG22	5:D:136:GLY:H	1.44	0.82
2:A:22:PHE:HB2	3:B:1211:ASN:ND2	1.94	0.82
2:A:744:LYS:HG2	2:A:748:MET:HE2	1.59	0.82
3:B:273:LEU:N	3:B:273:LEU:HD22	1.93	0.82
3:B:1152:MET:HE1	3:B:1157:ALA:HA	1.60	0.82
5:D:144:THR:HG21	8:G:46:LEU:HD13	1.59	0.81
2:A:828:ALA:CB	3:B:530:GLY:HA2	2.09	0.81
3:B:284:ILE:H	3:B:284:ILE:HD12	1.45	0.81
3:B:463:THR:CB	3:B:465:ASN:HB2	2.08	0.81
3:B:579:ARG:HB2	3:B:586:TRP:NE1	1.95	0.81
8:G:14:HIS:ND1	8:G:15:PRO:HD2	1.95	0.81
12:K:113:THR:O	12:K:114:LEU:HB2	1.78	0.81
2:A:254:GLU:O	2:A:256:GLN:N	2.13	0.81
3:B:879:ARG:HH11	3:B:883:LEU:HD22	1.46	0.81
4:C:186:LEU:HD21	4:C:224:GLN:O	1.81	0.81
2:A:907:THR:HG22	2:A:908:LEU:N	1.89	0.81
3:B:25:ILE:HD11	3:B:653:VAL:O	1.80	0.81
3:B:801:LYS:O	11:J:52:THR:HG23	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:59:ILE:HD11	8:G:77:VAL:HG11	1.60	0.81
3:B:254:LEU:CD2	3:B:381:MET:HE1	2.10	0.81
2:A:472:LEU:HD11	3:B:835:GLN:NE2	1.94	0.81
3:B:472:ALA:C	3:B:474:SER:H	1.87	0.81
2:A:877:HIS:C	2:A:878:ILE:HG13	2.03	0.81
8:G:56:ILE:HD12	8:G:56:ILE:H	1.46	0.81
5:D:202:ILE:HG23	5:D:203:SER:N	1.96	0.81
2:A:1329:THR:CG2	2:A:1331:SER:H	1.89	0.80
13:L:60:ARG:HG2	13:L:61:THR:H	1.46	0.80
2:A:67:CYS:O	2:A:70:CYS:HB3	1.82	0.80
2:A:524:VAL:HG12	2:A:525:GLN:H	1.45	0.80
3:B:1201:LYS:HE2	3:B:1205:GLN:OE1	1.81	0.80
3:B:918:ILE:HB	3:B:935:ARG:HD2	1.61	0.80
10:I:34:TYR:CD2	10:I:35:VAL:N	2.45	0.80
3:B:516:ASN:HD22	3:B:516:ASN:N	1.77	0.80
8:G:143:ILE:CG2	8:G:144:ARG:H	1.94	0.80
2:A:598:LEU:HA	9:H:122:LEU:HD13	1.62	0.79
6:E:202:SER:OG	6:E:204:THR:HG22	1.82	0.79
10:I:26:LEU:HD23	10:I:37:GLU:HA	1.64	0.79
2:A:798:GLY:HA2	2:A:815:PHE:CD1	2.17	0.79
3:B:501:PRO:HG2	3:B:502:ILE:HG12	1.64	0.79
2:A:49:LYS:NZ	2:A:61:ILE:HG12	1.98	0.79
3:B:589:VAL:HG12	3:B:590:HIS:N	1.97	0.79
3:B:1187:ASN:O	3:B:1188:LYS:HB2	1.81	0.79
5:D:33:PHE:CE2	8:G:80:LYS:NZ	2.50	0.79
3:B:23:ALA:HB1	3:B:24:PRO:HD2	1.65	0.79
3:B:579:ARG:HB2	3:B:586:TRP:HE1	1.46	0.79
4:C:31:ASN:O	4:C:34:ARG:HB3	1.82	0.79
2:A:1336:MET:HE3	2:A:1381:LEU:HG	1.65	0.79
3:B:247:GLY:H	3:B:418:LYS:NZ	1.79	0.79
2:A:351:THR:HG22	3:B:1103:ILE:HA	1.65	0.79
2:A:907:THR:CG2	2:A:908:LEU:H	1.96	0.79
2:A:1189:SER:O	2:A:1241:ARG:HD3	1.82	0.78
2:A:767:GLN:NE2	2:A:774:ARG:HB3	1.97	0.78
2:A:535:THR:HG21	2:A:616:VAL:HA	1.65	0.78
2:A:1345:ARG:HG3	2:A:1376:THR:HG21	1.63	0.78
2:A:107:CYS:N	2:A:114:LEU:HD21	1.99	0.78
2:A:855:THR:HG23	2:A:857:ARG:HG3	1.63	0.78
2:A:1420:ASP:HB3	2:A:1422:ARG:HG3	1.66	0.78
2:A:1102:LYS:HG2	2:A:1106:ASN:HD21	1.47	0.78
3:B:466:TRP:O	3:B:468:GLU:N	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:172:PRO:O	4:C:235:VAL:HG23	1.83	0.78
2:A:728:LYS:HA	2:A:731:ARG:HB2	1.65	0.77
3:B:293:PRO:HG2	3:B:296:GLU:HB3	1.66	0.77
3:B:613:VAL:HG13	3:B:627:PHE:O	1.85	0.77
2:A:913:LEU:HD12	2:A:914:GLU:N	1.98	0.77
3:B:654:ARG:H	3:B:657:HIS:HD2	1.29	0.77
2:A:56:PRO:HD2	2:A:58:LEU:HG	1.67	0.77
3:B:1172:ILE:HD12	3:B:1172:ILE:N	2.00	0.77
2:A:55:ASP:C	2:A:57:ARG:H	1.90	0.77
2:A:146:MET:HA	2:A:171:GLN:HB2	1.65	0.77
2:A:709:THR:HG23	10:I:94:ASP:HA	1.66	0.77
3:B:37:PHE:CD1	3:B:41:LYS:HG3	2.19	0.77
10:I:34:TYR:HD2	10:I:35:VAL:H	1.32	0.77
5:D:35:LEU:H	5:D:35:LEU:HD12	1.50	0.77
2:A:442:VAL:HB	2:A:489:LEU:HD11	1.67	0.77
8:G:122:ASN:ND2	8:G:125:SER:HB3	1.99	0.77
3:B:199:MET:HE2	3:B:492:LEU:CD2	2.15	0.77
3:B:211:VAL:O	3:B:480:SER:HA	1.83	0.77
2:A:577:ILE:O	2:A:580:VAL:HG23	1.85	0.76
3:B:37:PHE:CE1	3:B:41:LYS:HG3	2.20	0.76
3:B:582:VAL:HG23	3:B:626:ILE:HB	1.65	0.76
3:B:1017:ILE:HB	3:B:1018:PRO:HD3	1.66	0.76
2:A:84:ILE:HG22	2:A:239:LEU:HB3	1.67	0.76
2:A:567:LYS:NZ	9:H:46:LEU:HB2	1.98	0.76
2:A:1428:VAL:HG13	3:B:1151:LEU:CD2	2.16	0.76
9:H:4:THR:HA	9:H:60:ALA:HB2	1.67	0.76
2:A:41:MET:HB3	2:A:49:LYS:HA	1.66	0.76
2:A:341:MET:HE1	3:B:1135:ARG:NH1	2.00	0.76
3:B:955:THR:HG22	3:B:956:THR:N	2.01	0.76
11:J:16:ASP:OD1	11:J:17:LYS:HD2	1.86	0.76
2:A:828:ALA:HB1	3:B:530:GLY:HA2	1.67	0.76
9:H:36:CYS:HA	9:H:126:GLU:O	1.84	0.76
2:A:24:PRO:HD2	2:A:233:TRP:HE1	1.51	0.76
2:A:230:ARG:H	2:A:233:TRP:HE3	1.33	0.76
2:A:438:ASP:O	2:A:439:ASN:HB2	1.86	0.76
3:B:1162:ILE:HG22	3:B:1163:CYS:H	1.50	0.76
6:E:116:ILE:HG22	6:E:117:THR:N	2.01	0.76
11:J:1:MET:H2	11:J:56:LEU:N	1.83	0.76
9:H:23:VAL:HG13	9:H:42:ILE:O	1.85	0.76
2:A:250:ILE:O	2:A:258:GLY:HA3	1.85	0.76
3:B:205:ILE:N	3:B:205:ILE:HD12	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:510:LYS:HD2	3:B:510:LYS:N	1.98	0.76
2:A:1206:ASP:HB3	2:A:1274:ARG:HH12	1.51	0.75
3:B:273:LEU:O	3:B:273:LEU:HD23	1.85	0.75
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.17	0.75
3:B:996:ARG:HH22	4:C:175:ALA:H	1.33	0.75
2:A:382:PRO:HB3	2:A:428:TYR:HE2	1.51	0.75
3:B:463:THR:HB	3:B:465:ASN:CB	2.15	0.75
3:B:841:MET:HG2	3:B:846:ILE:HD11	1.67	0.75
6:E:19:VAL:O	6:E:23:VAL:HG23	1.86	0.75
2:A:1063:MET:SD	2:A:1436:ILE:HG13	2.26	0.75
2:A:1345:ARG:HG2	2:A:1372:VAL:HG13	1.66	0.75
11:J:57:ILE:HA	11:J:60:PHE:HD2	1.51	0.75
2:A:1370:LEU:O	2:A:1374:VAL:HG23	1.87	0.75
3:B:1182:CYS:O	3:B:1182:CYS:SG	2.45	0.75
2:A:438:ASP:OD1	2:A:462:VAL:HG23	1.86	0.75
2:A:858:ASN:C	2:A:858:ASN:HD22	1.95	0.75
3:B:983:ARG:HD2	3:B:1091:TYR:HB3	1.69	0.75
2:A:1444:MET:HG2	8:G:60:ARG:HA	1.69	0.74
2:A:374:LEU:HB3	2:A:436:ILE:HD11	1.69	0.74
2:A:1313:LEU:O	2:A:1315:GLU:N	2.20	0.74
1:R:11:U:H4'	1:R:12:5BU:OP2	1.85	0.74
2:A:339:ASN:HB3	3:B:1117:GLN:HE22	1.51	0.74
3:B:580:VAL:HG13	3:B:624:LEU:HB3	1.69	0.74
4:C:32:SER:O	4:C:36:VAL:HG23	1.88	0.74
4:C:147:LEU:HB2	4:C:151:GLN:HB2	1.68	0.74
4:C:248:ILE:HD12	12:K:101:LEU:HD22	1.69	0.74
3:B:468:GLU:N	3:B:468:GLU:CD	2.45	0.74
3:B:711:GLU:H	3:B:712:PRO:HD2	1.50	0.74
10:I:55:THR:HG22	10:I:58:VAL:HG21	1.69	0.74
9:H:61:SER:O	9:H:62:SER:HB3	1.88	0.74
2:A:1107:VAL:HG12	2:A:1107:VAL:O	1.87	0.74
3:B:125:SER:HA	3:B:171:PRO:HA	1.68	0.74
5:D:63:LEU:HD12	5:D:129:LEU:HG	1.68	0.74
1:R:15:G:OP1	3:B:474:SER:HB3	1.86	0.74
3:B:1096:ARG:O	3:B:1097:HIS:HB2	1.86	0.74
2:A:50:ILE:O	2:A:52:GLY:N	2.19	0.74
2:A:93:VAL:HG13	2:A:301:ALA:HB1	1.69	0.74
2:A:666:ILE:HD12	2:A:667:GLY:H	1.53	0.74
2:A:1261:LYS:O	2:A:1264:GLU:HB3	1.88	0.74
3:B:284:ILE:HD12	3:B:284:ILE:N	2.03	0.74
3:B:882:THR:HG22	3:B:884:ARG:N	1.98	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:14:VAL:H	2:A:1432:GLN:HE22	1.36	0.73
2:A:21:LEU:HD21	2:A:1414:ALA:HA	1.70	0.73
6:E:153:HIS:HB3	6:E:196:VAL:CG1	2.18	0.73
2:A:1057:VAL:HG12	2:A:1058:VAL:N	2.04	0.73
5:D:7:THR:O	5:D:9:GLN:N	2.22	0.73
12:K:56:VAL:HA	12:K:77:THR:HG22	1.68	0.73
2:A:68:GLN:C	2:A:70:CYS:H	1.96	0.73
2:A:853:ASP:OD1	2:A:855:THR:HB	1.88	0.73
2:A:1372:VAL:HG12	2:A:1373:ASP:N	2.03	0.73
8:G:13:LEU:CD2	8:G:17:PHE:HB2	2.18	0.73
2:A:743:VAL:O	2:A:747:VAL:HG23	1.87	0.73
3:B:834:ASN:HB3	3:B:840:ILE:HG13	1.71	0.73
3:B:978:ASP:OD2	3:B:1098:MET:HG2	1.88	0.73
3:B:1099:VAL:O	3:B:1101:ASP:N	2.21	0.73
6:E:124:VAL:HG13	6:E:132:ILE:HD13	1.70	0.73
2:A:541:ILE:HG12	2:A:549:MET:HE1	1.69	0.73
9:H:98:TYR:C	9:H:118:PHE:HD2	1.96	0.73
10:I:111:THR:HG22	10:I:113:ASP:N	2.03	0.73
11:J:57:ILE:HA	11:J:60:PHE:CD2	2.23	0.73
2:A:567:LYS:CD	2:A:568:PRO:HD2	2.19	0.73
2:A:1325:THR:HG23	6:E:146:HIS:O	1.88	0.73
4:C:116:LYS:HD3	4:C:140:ASN:HB3	1.70	0.73
5:D:47:LEU:HD13	5:D:48:ILE:H	1.54	0.73
3:B:1065:GLN:HE21	3:B:1067:ARG:H	1.37	0.73
2:A:1364:ASN:HD22	2:A:1364:ASN:C	1.96	0.73
2:A:524:VAL:HG12	2:A:525:GLN:N	2.02	0.72
2:A:710:LEU:H	2:A:710:LEU:HD12	1.53	0.72
3:B:215:GLN:HE22	3:B:499:ASN:HD22	1.36	0.72
3:B:862:GLN:HG2	3:B:963:PHE:HD1	1.54	0.72
3:B:952:VAL:HG12	3:B:953:LEU:H	1.54	0.72
4:C:77:ILE:HG12	4:C:161:LYS:HE3	1.71	0.72
8:G:56:ILE:HD12	8:G:56:ILE:N	2.04	0.72
8:G:138:THR:HG22	8:G:139:ILE:N	2.00	0.72
3:B:516:ASN:HD22	3:B:516:ASN:H	1.35	0.72
4:C:98:VAL:C	4:C:99:LEU:HD23	2.14	0.72
3:B:1007:VAL:HG22	3:B:1008:PRO:CD	2.19	0.72
2:A:903:ASN:C	2:A:903:ASN:HD22	1.97	0.72
3:B:509:ALA:O	3:B:511:PRO:CD	2.36	0.72
8:G:1:MET:HE1	8:G:80:LYS:H	1.54	0.72
3:B:616:ILE:HD12	3:B:616:ILE:N	2.04	0.72
3:B:622:LYS:HE2	10:I:59:VAL:HG22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1072:MET:HE1	3:B:1085:ILE:HB	1.70	0.72
4:C:148:ARG:HG2	4:C:149:LYS:H	1.54	0.72
12:K:58:PHE:HE2	12:K:74:ARG:HE	1.32	0.72
2:A:1116:LEU:N	2:A:1308:THR:HG22	2.04	0.72
4:C:37:MET:HA	4:C:41:ILE:HD11	1.70	0.72
2:A:70:CYS:O	2:A:72:GLU:HG2	1.90	0.72
2:A:1102:LYS:HG2	2:A:1106:ASN:ND2	2.04	0.72
3:B:1224:PHE:HE2	6:E:171:LYS:HG3	1.55	0.72
2:A:567:LYS:HB3	9:H:96:VAL:H	1.55	0.72
2:A:875:ALA:HA	2:A:878:ILE:HD12	1.72	0.72
2:A:886:ILE:HG22	2:A:887:GLY:N	2.04	0.72
6:E:135:PHE:HD2	6:E:140:LEU:HD21	1.52	0.72
3:B:563:MET:HE3	3:B:580:VAL:HB	1.71	0.72
4:C:77:ILE:HA	4:C:129:ILE:HD11	1.71	0.72
4:C:194:GLU:O	4:C:195:GLN:HG3	1.90	0.72
9:H:93:TYR:HB3	9:H:144:ILE:O	1.90	0.72
5:D:33:PHE:CZ	8:G:80:LYS:NZ	2.59	0.71
8:G:143:ILE:CG2	8:G:144:ARG:N	2.53	0.71
2:A:1283:VAL:HG12	2:A:1284:MET:H	1.55	0.71
4:C:166:GLU:HG3	12:K:10:PHE:HZ	1.55	0.71
13:L:53:HIS:HB3	13:L:55:ILE:HD11	1.71	0.71
2:A:23:SER:HA	2:A:233:TRP:NE1	2.05	0.71
2:A:269:ILE:HG12	2:A:299:HIS:HB3	1.72	0.71
1:R:7:C:H3'	1:R:8:U:H5''	1.71	0.71
4:C:92:CYS:SG	4:C:94:LYS:HB3	2.29	0.71
2:A:117:GLU:H	2:A:117:GLU:CD	1.97	0.71
2:A:886:ILE:HD11	2:A:943:LEU:HB3	1.72	0.71
3:B:827:ILE:HG12	3:B:1012:ILE:CD1	2.10	0.71
2:A:1329:THR:H	2:A:1335:ILE:HD11	1.55	0.71
3:B:1002:THR:HG21	3:B:1006:ILE:HD12	1.72	0.71
2:A:93:VAL:HG22	2:A:301:ALA:HA	1.71	0.71
3:B:291:ILE:HD12	3:B:291:ILE:N	2.04	0.71
3:B:806:THR:HB	3:B:809:MET:HG3	1.71	0.71
3:B:977:GLY:HA3	3:B:1099:VAL:HG21	1.73	0.71
2:A:763:ALA:O	2:A:803:SER:HB3	1.91	0.71
2:A:984:LYS:HB3	2:A:988:LEU:HD12	1.73	0.71
2:A:1155:ASP:OD2	2:A:1161:THR:HG23	1.90	0.71
3:B:357:GLN:HA	3:B:374:LYS:NZ	2.05	0.71
4:C:114:TYR:HB3	4:C:140:ASN:O	1.90	0.71
2:A:225:ASN:HD22	2:A:228:PHE:N	1.82	0.70
3:B:505:ASP:CG	3:B:506:GLY:N	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:865:LYS:HE2	3:B:871:THR:OG1	1.91	0.70
9:H:100:THR:OG1	9:H:138:GLU:HG3	1.91	0.70
2:A:35:ILE:HA	2:A:52:GLY:O	1.90	0.70
2:A:1161:THR:HG22	2:A:1163:ILE:N	2.04	0.70
3:B:1051:THR:HG22	3:B:1052:VAL:N	2.05	0.70
3:B:745:PRO:O	3:B:748:ILE:HG12	1.91	0.70
3:B:859:TYR:OH	3:B:941:LEU:HD12	1.91	0.70
2:A:302:THR:HA	2:A:305:ASP:O	1.90	0.70
2:A:541:ILE:HG21	2:A:549:MET:CE	2.21	0.70
2:A:768:GLN:CG	2:A:816:HIS:HA	2.21	0.70
2:A:1202:MET:HE1	2:A:1212:VAL:HG21	1.74	0.70
3:B:95:ILE:HG12	3:B:130:VAL:HG22	1.72	0.70
3:B:468:GLU:CD	3:B:468:GLU:H	2.00	0.70
4:C:31:ASN:OD1	4:C:34:ARG:HD3	1.92	0.70
8:G:1:MET:SD	8:G:79:PHE:CD1	2.85	0.70
2:A:537:ARG:HD2	9:H:20:TYR:CE1	2.26	0.70
4:C:212:PRO:HB3	4:C:213:PRO:HD2	1.74	0.70
5:D:59:ILE:O	5:D:63:LEU:HB2	1.91	0.70
8:G:119:LEU:HD12	8:G:131:GLN:O	1.90	0.70
2:A:63:ARG:HA	2:A:74:MET:SD	2.31	0.70
2:A:134:ARG:O	2:A:134:ARG:HG2	1.90	0.70
6:E:213:ILE:HG12	6:E:214:CYS:H	1.57	0.70
2:A:565:ILE:C	2:A:566:ILE:HD13	2.17	0.70
3:B:274:PRO:O	3:B:275:TYR:HB2	1.91	0.70
2:A:537:ARG:HD2	9:H:20:TYR:HE1	1.57	0.69
11:J:1:MET:HE2	11:J:60:PHE:CZ	2.26	0.69
1:R:3:A:H2	1:R:15:G:H21	1.37	0.69
2:A:474:VAL:C	2:A:477:PRO:HD2	2.17	0.69
2:A:600:PRO:HG2	2:A:601:LYS:H	1.56	0.69
4:C:258:ILE:HD13	12:K:35:PHE:HE2	1.57	0.69
5:D:195:ILE:O	5:D:195:ILE:HG22	1.91	0.69
2:A:306:ASN:HB2	2:A:324:SER:HB3	1.74	0.69
2:A:381:THR:OG1	2:A:382:PRO:HD2	1.91	0.69
2:A:1409:LEU:HD13	3:B:1207:LEU:HD11	1.74	0.69
3:B:782:LEU:HD12	3:B:788:ARG:HH11	1.56	0.69
3:B:1162:ILE:HD11	3:B:1194:ILE:CG1	2.21	0.69
2:A:1111:MET:HE2	2:A:1330:ASN:OD1	1.92	0.69
2:A:1279:ILE:HD11	2:A:1316:VAL:HG21	1.73	0.69
3:B:240:ILE:HG22	3:B:254:LEU:HB3	1.73	0.69
3:B:737:THR:HG21	10:I:66:PRO:HA	1.74	0.69
2:A:164:ARG:HG3	2:A:165:GLY:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1116:LEU:H	2:A:1308:THR:HG22	1.57	0.69
2:A:1349:TYR:HB2	2:A:1372:VAL:HG21	1.74	0.69
3:B:555:ILE:C	3:B:557:PHE:H	2.00	0.69
10:I:111:THR:HG22	10:I:112:SER:N	2.06	0.69
3:B:364:ILE:HG12	3:B:585:VAL:HG13	1.74	0.69
9:H:4:THR:HG22	9:H:5:LEU:H	1.56	0.69
4:C:33:LEU:HG	4:C:37:MET:HE2	1.73	0.69
11:J:23:ASN:C	11:J:25:LEU:H	2.00	0.69
3:B:274:PRO:O	3:B:276:ILE:HD13	1.93	0.69
3:B:980:PHE:CE1	3:B:990:ILE:HD11	2.25	0.69
1:R:12:5BU:O2'	1:R:13:G:O5'	2.07	0.69
2:A:90:VAL:HG12	2:A:297:GLN:NE2	2.07	0.69
2:A:1166:ASP:OD2	2:A:1239:ARG:HD2	1.93	0.69
4:C:124:LEU:O	4:C:127:ARG:HG2	1.93	0.69
10:I:68:LEU:HB3	10:I:84:VAL:HG23	1.74	0.69
2:A:783:THR:HG21	2:A:815:PHE:CZ	2.28	0.69
3:B:284:ILE:H	3:B:284:ILE:CD1	2.06	0.69
4:C:73:GLN:HB3	4:C:131:HIS:H	1.58	0.69
2:A:55:ASP:CG	2:A:55:ASP:O	2.33	0.68
2:A:567:LYS:HB2	9:H:94:ASP:O	1.93	0.68
3:B:708:GLU:O	3:B:710:LEU:N	2.26	0.68
3:B:847:ASP:HB3	4:C:167:HIS:NE2	2.09	0.68
3:B:1099:VAL:HG13	3:B:1103:ILE:CD1	2.23	0.68
7:F:77:ASP:O	7:F:78:GLN:HB2	1.93	0.68
8:G:11:ILE:HG21	8:G:29:LYS:HG2	1.75	0.68
12:K:12:LEU:H	12:K:12:LEU:HD12	1.58	0.68
12:K:53:ASP:OD1	12:K:55:LYS:HB2	1.93	0.68
3:B:555:ILE:HD11	3:B:587:HIS:CD2	2.27	0.68
6:E:198:ILE:N	6:E:198:ILE:HD12	2.08	0.68
2:A:49:LYS:HZ3	2:A:61:ILE:HG12	1.56	0.68
6:E:61:GLN:HB2	6:E:79:TRP:CE3	2.28	0.68
2:A:701:LEU:HD21	10:I:114:GLN:HB2	1.74	0.68
2:A:1441:PHE:CZ	7:F:89:GLU:HA	2.29	0.68
3:B:758:PHE:HB3	3:B:761:HIS:HD2	1.57	0.68
2:A:69:THR:C	2:A:71:GLN:H	2.02	0.68
2:A:794:PRO:HG2	2:A:795:GLU:OE2	1.93	0.68
2:A:1402:PHE:CE1	2:A:1403:GLU:HG3	2.29	0.68
3:B:378:LEU:O	3:B:382:ILE:HG13	1.93	0.68
6:E:116:ILE:HG22	6:E:117:THR:H	1.59	0.68
2:A:829:VAL:C	2:A:831:THR:H	1.99	0.68
3:B:797:TYR:CD2	3:B:852:ARG:HB2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:130:LEU:C	5:D:132:GLN:H	2.02	0.68
4:C:43:THR:HG22	4:C:44:LEU:N	2.09	0.68
2:A:981:LEU:CD2	2:A:1039:LYS:HA	2.24	0.68
2:A:1341:ILE:HD12	2:A:1379:GLY:O	1.94	0.68
8:G:74:TYR:H	8:G:74:TYR:HD2	1.39	0.68
2:A:244:PRO:O	2:A:246:VAL:N	2.26	0.68
3:B:1099:VAL:C	3:B:1101:ASP:H	2.00	0.68
3:B:1002:THR:HG23	3:B:1006:ILE:HG13	1.76	0.68
5:D:144:THR:O	5:D:148:LEU:HB2	1.94	0.68
2:A:374:LEU:CB	2:A:436:ILE:HD11	2.24	0.67
3:B:363:HIS:O	3:B:364:ILE:HB	1.94	0.67
9:H:81:PRO:CB	9:H:82:PRO:HD2	2.25	0.67
9:H:99:GLY:HA3	9:H:118:PHE:HA	1.76	0.67
2:A:1148:ILE:HD11	2:A:1198:ASP:HB2	1.76	0.67
3:B:479:VAL:O	3:B:480:SER:HB3	1.92	0.67
2:A:463:ILE:HD13	2:A:469:ARG:HD2	1.77	0.67
2:A:1032:LEU:O	2:A:1036:ARG:HD3	1.93	0.67
3:B:464:GLY:C	3:B:466:TRP:N	2.49	0.67
3:B:501:PRO:O	3:B:502:ILE:HG13	1.93	0.67
3:B:899:ILE:HD11	3:B:911:ILE:HA	1.76	0.67
8:G:7:LEU:HB2	8:G:74:TYR:CE2	2.29	0.67
3:B:483:LEU:HD12	3:B:484:ASN:N	2.10	0.67
3:B:1099:VAL:HG12	3:B:1100:ASP:N	2.07	0.67
12:K:65:HIS:HD2	12:K:67:PHE:H	1.43	0.67
2:A:119:ASN:O	2:A:122:MET:HB3	1.95	0.67
2:A:1272:THR:C	2:A:1273:LEU:HD12	2.19	0.67
3:B:217:ARG:HE	3:B:405:ARG:HB2	1.60	0.67
4:C:148:ARG:CG	4:C:149:LYS:H	2.05	0.67
5:D:192:LYS:NZ	5:D:199:ASN:HA	2.10	0.67
2:A:1319:VAL:HG13	2:A:1320:PRO:HD2	1.77	0.67
3:B:955:THR:CG2	3:B:956:THR:N	2.58	0.67
5:D:40:HIS:CB	8:G:73:LYS:HZ3	2.02	0.67
2:A:147:VAL:N	2:A:171:GLN:NE2	2.42	0.67
3:B:310:MET:O	3:B:313:MET:HB2	1.95	0.67
3:B:463:THR:C	3:B:465:ASN:N	2.49	0.67
6:E:132:ILE:HD12	6:E:132:ILE:N	2.10	0.67
2:A:474:VAL:O	2:A:477:PRO:HD2	1.95	0.67
9:H:81:PRO:HB3	9:H:82:PRO:HD2	1.76	0.67
2:A:898:ARG:HB2	2:A:933:TYR:CE1	2.30	0.66
3:B:879:ARG:NH1	3:B:883:LEU:HD22	2.10	0.66
2:A:4:GLN:O	2:A:5:GLN:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:260:GLY:O	3:B:267:ARG:HD3	1.95	0.66
4:C:189:THR:HG22	4:C:190:ASP:N	2.09	0.66
5:D:153:ARG:NH2	5:D:184:ALA:HA	2.10	0.66
5:D:156:ASP:C	5:D:158:GLU:H	2.02	0.66
7:F:111:LEU:C	7:F:113:GLY:H	2.03	0.66
2:A:845:LEU:HD22	2:A:1374:VAL:HG21	1.78	0.66
2:A:965:GLN:HA	2:A:968:GLN:HG3	1.78	0.66
2:A:1114:PRO:HG2	2:A:1115:SER:H	1.60	0.66
2:A:401:GLY:C	2:A:435:HIS:HD2	2.03	0.66
2:A:551:TYR:CE2	12:K:62:LYS:HE2	2.30	0.66
2:A:664:THR:HG22	2:A:665:GLY:N	2.09	0.66
3:B:996:ARG:NH2	4:C:175:ALA:H	1.92	0.66
5:D:192:LYS:HZ3	5:D:199:ASN:HA	1.60	0.66
13:L:31:CYS:SG	13:L:34:CYS:N	2.66	0.66
3:B:515:HIS:H	3:B:518:HIS:HD2	1.44	0.66
8:G:1:MET:HE3	8:G:80:LYS:O	1.96	0.66
12:K:12:LEU:HD12	12:K:12:LEU:N	2.10	0.66
2:A:84:ILE:O	2:A:84:ILE:HG23	1.96	0.66
2:A:147:VAL:H	2:A:171:GLN:HE21	1.42	0.66
3:B:696:GLU:O	3:B:699:GLU:HB2	1.95	0.66
4:C:75:MET:HE2	4:C:239:PRO:HG2	1.76	0.66
2:A:11:LEU:O	2:A:11:LEU:HD23	1.96	0.66
2:A:414:ASP:OD1	2:A:416:ARG:HG2	1.96	0.66
2:A:1149:ALA:HB2	10:I:47:GLU:HA	1.77	0.66
7:F:103:MET:HE1	8:G:65:ASP:HB2	1.78	0.66
2:A:343:LYS:HE2	3:B:1156:ASP:OD2	1.96	0.66
2:A:903:ASN:ND2	2:A:905:ASP:H	1.92	0.66
3:B:483:LEU:HD12	3:B:484:ASN:H	1.61	0.66
3:B:642:ASP:HB3	3:B:649:LYS:HD2	1.78	0.66
3:B:918:ILE:HG21	3:B:935:ARG:NH1	2.11	0.66
2:A:1028:THR:O	2:A:1032:LEU:HD12	1.96	0.66
3:B:465:ASN:O	3:B:466:TRP:C	2.38	0.66
3:B:806:THR:HG22	3:B:808:ALA:N	2.10	0.66
8:G:132:SER:HB3	8:G:135:ASP:H	1.61	0.66
2:A:629:LEU:O	2:A:629:LEU:HD23	1.95	0.66
2:A:825:ILE:C	2:A:827:THR:H	2.03	0.66
3:B:408:LEU:C	3:B:412:LEU:HD12	2.21	0.66
6:E:61:GLN:HG2	6:E:62:ALA:N	2.10	0.66
9:H:89:LEU:C	9:H:91:ASP:H	2.02	0.66
10:I:8:ARG:HG3	10:I:34:TYR:CE1	2.29	0.66
10:I:62:ILE:O	10:I:62:ILE:HG12	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:27:ALA:HB1	12:K:28:PRO:HD2	1.77	0.66
2:A:384:ASN:CG	2:A:388:LEU:HD12	2.20	0.65
2:A:590:ARG:HG3	2:A:590:ARG:NH1	2.09	0.65
3:B:272:THR:C	3:B:273:LEU:HD13	2.21	0.65
9:H:123:MET:HE1	9:H:142:LEU:CD1	2.26	0.65
2:A:1017:LEU:HB3	6:E:205:SER:HA	1.78	0.65
3:B:558:LEU:CD2	3:B:596:LEU:HD11	2.27	0.65
5:D:52:LEU:HD21	5:D:147:TYR:HE2	1.61	0.65
8:G:81:PRO:HB3	8:G:106:MET:HE1	1.77	0.65
8:G:145:VAL:HG12	8:G:146:LYS:N	2.10	0.65
9:H:143:LEU:C	9:H:144:ILE:HG13	2.20	0.65
3:B:390:LEU:O	3:B:392:ARG:HG3	1.96	0.65
3:B:496:ARG:HB3	3:B:496:ARG:HH11	1.61	0.65
11:J:1:MET:HE2	11:J:60:PHE:CE2	2.31	0.65
2:A:61:ILE:HG22	2:A:62:ASP:N	2.03	0.65
2:A:658:LEU:HD13	3:B:831:SER:HA	1.78	0.65
3:B:830:TYR:CE2	3:B:1000:PRO:HD3	2.32	0.65
8:G:110:VAL:HG13	8:G:161:GLY:O	1.97	0.65
9:H:12:VAL:HA	9:H:28:ALA:HB2	1.79	0.65
10:I:52:ILE:HG13	10:I:52:ILE:O	1.96	0.65
3:B:274:PRO:O	3:B:274:PRO:HD2	1.96	0.65
3:B:821:GLN:NE2	3:B:851:PHE:HA	2.09	0.65
3:B:1166:CYS:SG	3:B:1166:CYS:O	2.53	0.65
4:C:35:ARG:HH12	12:K:40:HIS:HB2	1.62	0.65
2:A:42:ASP:HA	2:A:46:THR:O	1.94	0.65
2:A:828:ALA:HB2	3:B:530:GLY:HA2	1.78	0.65
3:B:94:LYS:HG2	3:B:95:ILE:N	2.11	0.65
3:B:501:PRO:C	3:B:502:ILE:HG13	2.21	0.65
4:C:100:THR:HG22	4:C:101:LEU:H	1.60	0.65
5:D:170:THR:HB	5:D:172:LEU:HG	1.77	0.65
6:E:124:VAL:HG13	6:E:132:ILE:HB	1.77	0.65
2:A:1242:VAL:HG12	2:A:1243:VAL:N	2.10	0.65
2:A:1389:PHE:CD1	2:A:1389:PHE:C	2.74	0.65
5:D:56:ARG:HB2	5:D:148:LEU:HD22	1.78	0.65
11:J:50:ILE:H	11:J:50:ILE:HD12	1.60	0.65
2:A:203:SER:OG	2:A:206:GLU:HB2	1.97	0.65
2:A:344:ARG:HB2	3:B:1118:PRO:HD2	1.77	0.65
2:A:356:ASP:HB2	2:A:469:ARG:HH11	1.61	0.65
3:B:504:ARG:HB3	3:B:507:LYS:HE2	1.78	0.65
3:B:948:ILE:HG22	3:B:949:VAL:O	1.96	0.65
5:D:160:VAL:O	5:D:164:ILE:HG13	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:115:LEU:HB2	2:A:122:MET:HE2	1.78	0.65
2:A:783:THR:HG21	2:A:815:PHE:CE2	2.31	0.65
3:B:850:LEU:HD12	3:B:851:PHE:N	2.12	0.65
2:A:114:LEU:HD13	2:A:171:GLN:OE1	1.97	0.65
2:A:547:LEU:HD22	12:K:58:PHE:CE1	2.32	0.65
2:A:1451:VAL:O	2:A:1454:MET:HG2	1.96	0.65
2:A:353:ILE:HG21	2:A:487:MET:HE3	1.78	0.64
3:B:210:LYS:HE2	3:B:462:ALA:O	1.97	0.64
4:C:8:VAL:HG12	4:C:9:LYS:H	1.61	0.64
4:C:177:GLU:HB2	4:C:231:ASN:HB3	1.78	0.64
2:A:901:LEU:H	2:A:926:GLN:HE21	1.45	0.64
3:B:240:ILE:CG2	3:B:254:LEU:HB3	2.27	0.64
6:E:55:ARG:HD2	6:E:83:CYS:O	1.97	0.64
9:H:15:VAL:HG22	9:H:26:ILE:HD11	1.78	0.64
2:A:92:HIS:O	2:A:94:GLY:N	2.29	0.64
2:A:666:ILE:HD11	3:B:1067:ARG:O	1.97	0.64
3:B:95:ILE:HG12	3:B:130:VAL:CG2	2.27	0.64
3:B:466:TRP:C	3:B:468:GLU:H	2.04	0.64
13:L:30:ILE:HG22	13:L:31:CYS:O	1.97	0.64
2:A:782:ARG:NH2	3:B:699:GLU:O	2.28	0.64
2:A:869:GLY:O	2:A:870:GLU:HB2	1.97	0.64
2:A:1015:VAL:HG12	2:A:1019:CYS:SG	2.37	0.64
2:A:1373:ASP:HA	2:A:1376:THR:HG22	1.78	0.64
4:C:5:GLY:O	4:C:7:GLN:HG3	1.98	0.64
4:C:67:LEU:HD11	4:C:155:LEU:CD1	2.28	0.64
5:D:52:LEU:HD21	5:D:147:TYR:CE2	2.32	0.64
9:H:40:LEU:HD13	9:H:123:MET:HB2	1.78	0.64
2:A:979:SER:OG	2:A:980:ASP:N	2.30	0.64
3:B:758:PHE:HB3	3:B:761:HIS:CD2	2.31	0.64
3:B:1162:ILE:HD11	3:B:1194:ILE:HG13	1.80	0.64
4:C:166:GLU:O	4:C:167:HIS:HB2	1.97	0.64
11:J:50:ILE:HD12	11:J:50:ILE:N	2.13	0.64
1:R:3:A:C2	1:R:16:G:H1'	2.33	0.64
1:R:15:G:O2'	1:R:16:G:H5'	1.97	0.64
2:A:808:LEU:HD23	2:A:812:GLU:C	2.22	0.64
3:B:865:LYS:HZ2	3:B:869:SER:HA	1.63	0.64
3:B:1001:PHE:CZ	3:B:1073:TYR:HB2	2.32	0.64
4:C:189:THR:HG22	4:C:190:ASP:H	1.60	0.64
8:G:1:MET:HG3	8:G:85:GLU:OE2	1.98	0.64
2:A:340:LEU:HD21	3:B:1200:ALA:N	2.12	0.64
2:A:341:MET:HE1	2:A:843:LYS:HZ1	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:411:PRO:O	3:B:414:ALA:HB3	1.96	0.64
3:B:644:GLU:HG2	3:B:654:ARG:HH22	1.61	0.64
9:H:35:GLN:O	9:H:37:LYS:HG3	1.96	0.64
2:A:709:THR:HG22	2:A:711:ARG:H	1.62	0.64
2:A:809:THR:HG23	2:A:812:GLU:OE1	1.98	0.64
2:A:1072:ILE:O	2:A:1075:PRO:HG2	1.98	0.64
3:B:428:ILE:HG22	3:B:432:MET:HE2	1.79	0.64
3:B:701:ILE:HD11	3:B:703:ILE:HD11	1.80	0.64
5:D:40:HIS:CB	8:G:73:LYS:NZ	2.52	0.64
2:A:32:VAL:HG21	2:A:68:GLN:NE2	2.12	0.64
3:B:799:PRO:HB3	3:B:818:PRO:HG2	1.80	0.64
9:H:59:ILE:O	9:H:60:ALA:HB3	1.97	0.64
2:A:166:GLY:O	2:A:167:CYS:SG	2.56	0.63
2:A:746:MET:HE3	3:B:1018:PRO:HG2	1.78	0.63
2:A:1364:ASN:C	2:A:1364:ASN:ND2	2.56	0.63
3:B:504:ARG:CB	3:B:507:LYS:HE2	2.28	0.63
3:B:557:PHE:C	3:B:557:PHE:CD2	2.75	0.63
6:E:161:LYS:HD2	6:E:195:VAL:CG2	2.28	0.63
9:H:44:VAL:O	9:H:44:VAL:HG12	1.98	0.63
2:A:1120:LEU:HD12	2:A:1120:LEU:N	2.13	0.63
3:B:770:GLN:OE1	3:B:983:ARG:HA	1.98	0.63
2:A:55:ASP:N	2:A:56:PRO:HD3	2.13	0.63
2:A:881:GLN:NE2	2:A:959:ASN:HA	2.13	0.63
3:B:918:ILE:CB	3:B:935:ARG:HD2	2.27	0.63
4:C:148:ARG:H	4:C:151:GLN:HG3	1.63	0.63
1:R:28:5BU:H2'	1:R:29:G:C8	2.33	0.63
11:J:1:MET:N	11:J:56:LEU:N	2.47	0.63
2:A:172:PRO:HB3	2:A:185:TRP:CE2	2.33	0.63
3:B:273:LEU:N	3:B:273:LEU:CD2	2.62	0.63
3:B:446:LEU:O	3:B:447:ALA:HB3	1.99	0.63
3:B:999:MET:HG3	3:B:1000:PRO:HD2	1.81	0.63
3:B:1085:ILE:N	3:B:1085:ILE:HD12	2.13	0.63
4:C:18:VAL:HG12	4:C:18:VAL:O	1.97	0.63
2:A:332:LYS:HG2	2:A:333:GLU:HG2	1.80	0.63
2:A:1438:THR:HB	3:B:1144:ALA:CB	2.26	0.63
3:B:842:ASN:ND2	3:B:845:SER:OG	2.29	0.63
3:B:1034:VAL:HG12	3:B:1035:ALA:N	2.14	0.63
4:C:56:THR:HG22	4:C:57:VAL:N	2.12	0.63
4:C:67:LEU:HA	4:C:70:ILE:HD13	1.81	0.63
5:D:40:HIS:CE1	5:D:41:GLN:HG3	2.33	0.63
6:E:48:ASP:CG	6:E:49:SER:H	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:262:LEU:HD11	12:K:87:LEU:HD23	1.81	0.63
2:A:1004:ASN:O	2:A:1008:GLN:HB2	1.98	0.63
3:B:359:GLU:O	3:B:362:PRO:HD3	1.98	0.63
3:B:463:THR:HB	3:B:465:ASN:H	1.64	0.63
3:B:952:VAL:CG1	3:B:953:LEU:N	2.62	0.63
3:B:821:GLN:HE22	3:B:851:PHE:CA	2.09	0.63
3:B:1119:VAL:HG23	3:B:1126:GLY:HA2	1.80	0.63
4:C:76:ASP:O	4:C:79:GLN:HG2	1.98	0.63
1:R:8:U:O2	1:R:8:U:H2'	1.99	0.62
2:A:1102:LYS:O	2:A:1106:ASN:ND2	2.32	0.62
3:B:282:ILE:N	3:B:282:ILE:HD13	2.14	0.62
7:F:147:SER:OG	7:F:150:GLU:HG3	1.98	0.62
12:K:63:VAL:HG23	12:K:63:VAL:O	1.98	0.62
2:A:384:ASN:O	2:A:385:ILE:C	2.41	0.62
2:A:563:PRO:HG3	2:A:572:TRP:CZ2	2.34	0.62
2:A:821:ARG:HB2	2:A:821:ARG:NH1	2.14	0.62
2:A:836:TYR:CE2	2:A:840:ARG:HD2	2.34	0.62
2:A:842:VAL:HG11	3:B:1136:ASP:OD2	1.98	0.62
3:B:658:ILE:HG22	3:B:659:ALA:N	2.13	0.62
2:A:567:LYS:HD3	9:H:95:TYR:CD2	2.34	0.62
2:A:1325:THR:O	6:E:148:GLU:HB2	1.99	0.62
3:B:272:THR:O	3:B:273:LEU:HB3	1.99	0.62
2:A:1195:LEU:HD11	2:A:1267:MET:HE1	1.80	0.62
3:B:65:GLU:HG3	3:B:66:ASP:N	2.10	0.62
3:B:466:TRP:C	3:B:468:GLU:N	2.57	0.62
3:B:1096:ARG:O	3:B:1097:HIS:CB	2.47	0.62
7:F:76:LYS:O	7:F:79:ARG:HD3	1.98	0.62
7:F:109:VAL:HG21	7:F:124:GLU:HA	1.81	0.62
2:A:63:ARG:HG2	2:A:74:MET:SD	2.40	0.62
2:A:856:THR:HB	2:A:865:GLN:HB2	1.82	0.62
3:B:1006:ILE:HD13	11:J:44:TYR:CE2	2.34	0.62
4:C:166:GLU:HG3	12:K:10:PHE:CZ	2.34	0.62
5:D:185:CYS:HB3	5:D:211:LEU:HD22	1.81	0.62
2:A:1313:LEU:HD23	2:A:1338:VAL:HG21	1.81	0.62
5:D:66:ARG:O	5:D:70:PHE:HB2	2.00	0.62
7:F:89:GLU:OE2	7:F:134:ILE:HG21	1.99	0.62
9:H:17:PRO:HB3	9:H:24:CYS:SG	2.38	0.62
2:A:1127:ASP:O	2:A:1130:GLN:HB3	1.99	0.62
3:B:95:ILE:HD13	3:B:96:TYR:N	2.15	0.62
5:D:189:ASP:O	5:D:193:THR:HB	2.00	0.62
2:A:79:GLY:HA3	2:A:243:PRO:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:82:GLY:O	2:A:241:VAL:N	2.26	0.62
2:A:506:ALA:HB3	2:A:509:LEU:HD12	1.82	0.62
2:A:1454:MET:O	2:A:1454:MET:HG3	1.99	0.62
3:B:200:GLY:HA2	3:B:202:TYR:CE2	2.35	0.62
2:A:295:LEU:O	2:A:298:PHE:HB3	2.00	0.62
2:A:335:ARG:HA	2:A:339:ASN:HD22	1.65	0.62
2:A:1206:ASP:CB	2:A:1274:ARG:HH12	2.11	0.62
3:B:847:ASP:C	3:B:849:GLY:H	2.07	0.62
6:E:163:GLU:O	6:E:166:LYS:N	2.33	0.62
2:A:225:ASN:ND2	2:A:227:VAL:H	1.98	0.62
2:A:254:GLU:HB2	3:B:935:ARG:HH22	1.65	0.62
3:B:27:ALA:O	3:B:29:ASP:N	2.33	0.62
3:B:526:GLU:HG2	3:B:538:ASN:HD22	1.63	0.62
5:D:33:PHE:CE1	8:G:80:LYS:HD2	2.35	0.62
9:H:84:ALA:HB1	9:H:87:ARG:HB2	1.82	0.62
2:A:129:LYS:O	2:A:130:ASP:HB2	1.99	0.61
3:B:1160:VAL:HG11	3:B:1169:MET:SD	2.40	0.61
6:E:163:GLU:O	6:E:164:LEU:C	2.42	0.61
2:A:446:ARG:HB2	2:A:487:MET:SD	2.40	0.61
2:A:1116:LEU:C	2:A:1116:LEU:HD12	2.25	0.61
3:B:521:LEU:HB3	3:B:633:VAL:HG11	1.82	0.61
3:B:653:VAL:CG2	3:B:689:LEU:HB3	2.31	0.61
6:E:17:ARG:O	6:E:21:GLU:HG3	1.99	0.61
2:A:567:LYS:HZ2	9:H:47:PHE:HB2	1.66	0.61
2:A:645:LEU:O	2:A:646:PHE:C	2.43	0.61
2:A:1130:GLN:NE2	2:A:1134:ILE:HD11	2.15	0.61
3:B:542:MET:HE3	3:B:636:PRO:HG2	1.82	0.61
3:B:556:THR:HG22	3:B:556:THR:O	2.00	0.61
3:B:906:SER:HA	3:B:946:ASN:HB2	1.81	0.61
3:B:1224:PHE:CE2	6:E:171:LYS:HG3	2.34	0.61
6:E:15:ALA:O	6:E:19:VAL:HG23	2.00	0.61
6:E:29:PHE:C	6:E:30:ILE:HG13	2.25	0.61
13:L:46:VAL:O	13:L:46:VAL:HG12	2.00	0.61
2:A:135:PHE:C	2:A:137:ALA:H	2.06	0.61
2:A:573:SER:O	2:A:576:GLN:HB2	2.00	0.61
3:B:637:LEU:HD12	3:B:693:ILE:HD12	1.82	0.61
3:B:984:HIS:CD2	3:B:1025:HIS:HB2	2.35	0.61
3:B:1095:LEU:H	3:B:1095:LEU:HD12	1.65	0.61
13:L:30:ILE:O	13:L:56:LEU:HA	2.00	0.61
3:B:53:GLN:HG2	3:B:547:VAL:HG22	1.83	0.61
2:A:244:PRO:HB2	2:A:245:PRO:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:535:THR:HG21	2:A:617:VAL:H	1.65	0.61
2:A:709:THR:CG2	10:I:94:ASP:HA	2.30	0.61
13:L:39:SER:O	13:L:40:LEU:HG	2.00	0.61
9:H:89:LEU:HB3	9:H:91:ASP:OD1	1.99	0.61
1:R:2:C:C2'	1:R:3:A:OP1	2.49	0.61
2:A:1435:PRO:HA	2:A:1439:GLY:O	2.01	0.61
3:B:51:PHE:CD2	3:B:173:MET:HB3	2.36	0.61
3:B:168:GLY:H	3:B:450:ALA:HB1	1.66	0.61
3:B:240:ILE:HG23	3:B:240:ILE:O	2.00	0.61
3:B:640:VAL:O	3:B:640:VAL:HG12	1.99	0.61
3:B:1183:LYS:HA	3:B:1186:ASP:HA	1.82	0.61
5:D:47:LEU:C	5:D:48:ILE:HD12	2.25	0.61
5:D:195:ILE:HG22	5:D:198:LEU:HG	1.81	0.61
8:G:80:LYS:O	8:G:80:LYS:HG2	2.01	0.61
2:A:147:VAL:H	2:A:171:GLN:NE2	1.97	0.61
2:A:567:LYS:CG	2:A:568:PRO:CD	2.77	0.61
2:A:1004:ASN:ND2	6:E:167:ARG:HD2	2.15	0.61
2:A:1425:SER:O	2:A:1426:GLU:C	2.44	0.61
3:B:862:GLN:HG2	3:B:963:PHE:CD1	2.36	0.61
3:B:1051:THR:HG22	3:B:1052:VAL:H	1.66	0.61
4:C:31:ASN:O	4:C:34:ARG:N	2.34	0.61
5:D:48:ILE:HD12	5:D:48:ILE:N	2.16	0.61
5:D:138:ASN:OD1	5:D:141:LEU:HB2	2.00	0.61
7:F:81:THR:HB	7:F:136:ARG:NH1	2.16	0.61
11:J:27:GLU:C	11:J:29:GLU:H	2.09	0.61
2:A:289:ILE:C	2:A:291:GLU:H	2.08	0.61
2:A:463:ILE:HB	2:A:464:PRO:HD2	1.83	0.61
2:A:605:MET:HE2	2:A:607:ILE:CG1	2.28	0.61
2:A:925:LEU:O	2:A:927:VAL:N	2.34	0.61
2:A:1447:GLU:OE2	8:G:23:LYS:HB2	2.00	0.61
3:B:293:PRO:HG2	3:B:296:GLU:CB	2.30	0.61
3:B:1045:SER:O	3:B:1046:PRO:O	2.19	0.61
4:C:56:THR:HG22	4:C:57:VAL:H	1.64	0.61
12:K:46:ILE:O	12:K:50:LEU:HB2	2.00	0.61
2:A:33:ALA:HB1	2:A:56:PRO:HB2	1.82	0.60
2:A:224:PHE:CE2	2:A:231:PRO:HG3	2.36	0.60
2:A:427:GLN:HB2	2:A:430:TRP:CD2	2.36	0.60
2:A:1124:HIS:HB3	2:A:1130:GLN:HG2	1.83	0.60
3:B:1162:ILE:HG22	3:B:1163:CYS:N	2.16	0.60
4:C:66:ARG:NH2	11:J:3:VAL:O	2.34	0.60
9:H:59:ILE:CG2	9:H:60:ALA:N	2.46	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:858:ASN:ND2	2:A:858:ASN:C	2.58	0.60
9:H:100:THR:HG23	9:H:138:GLU:CA	2.21	0.60
2:A:321:PRO:O	2:A:322:VAL:HB	2.00	0.60
2:A:341:MET:CE	2:A:843:LYS:HZ1	2.14	0.60
2:A:605:MET:HE3	2:A:606:LEU:N	2.14	0.60
8:G:1:MET:SD	8:G:2:PHE:N	2.74	0.60
3:B:825:VAL:CG1	3:B:826:ALA:N	2.63	0.60
4:C:237:SER:C	4:C:238:ILE:HD12	2.25	0.60
9:H:40:LEU:CD1	9:H:123:MET:HB2	2.31	0.60
2:A:340:LEU:HD13	2:A:1429:ILE:HG23	1.84	0.60
3:B:199:MET:HE2	3:B:492:LEU:HD23	1.84	0.60
2:A:629:LEU:HD23	2:A:629:LEU:C	2.27	0.60
2:A:914:GLU:HB2	2:A:979:SER:O	2.01	0.60
3:B:44:VAL:O	3:B:45:SER:C	2.45	0.60
6:E:61:GLN:HB2	6:E:79:TRP:HE3	1.66	0.60
8:G:138:THR:CG2	8:G:139:ILE:H	2.07	0.60
10:I:26:LEU:CD2	10:I:37:GLU:HA	2.31	0.60
2:A:148:CYS:HB3	2:A:168:GLY:HA2	1.83	0.60
2:A:388:LEU:HA	2:A:391:LEU:HD12	1.82	0.60
2:A:464:PRO:HG2	2:A:465:TYR:HD1	1.65	0.60
3:B:33:VAL:HG21	3:B:638:PHE:HZ	1.67	0.60
3:B:247:GLY:H	3:B:418:LYS:HZ1	1.50	0.60
3:B:521:LEU:HD13	3:B:633:VAL:HB	1.84	0.60
3:B:642:ASP:HB3	3:B:649:LYS:CD	2.31	0.60
3:B:710:LEU:HA	3:B:733:HIS:HB3	1.82	0.60
9:H:38:LEU:HD12	9:H:124:ARG:O	2.00	0.60
9:H:126:GLU:C	9:H:130:ARG:NH2	2.57	0.60
3:B:387:LEU:H	3:B:387:LEU:HD12	1.66	0.60
3:B:789:MET:HE3	3:B:965:LYS:HB3	1.83	0.60
8:G:91:VAL:HG12	8:G:92:VAL:N	2.16	0.60
1:R:16:G:C4	1:R:17:5BU:BR	3.10	0.60
2:A:61:ILE:CG2	2:A:62:ASP:H	2.01	0.60
2:A:896:ARG:HD3	2:A:897:TYR:CE1	2.37	0.60
3:B:515:HIS:HD2	3:B:517:THR:H	1.50	0.60
6:E:182:ASP:O	6:E:185:ALA:N	2.35	0.60
9:H:58:THR:C	9:H:59:ILE:HD12	2.26	0.60
10:I:7:CYS:HB3	10:I:14:LEU:HD21	1.84	0.60
2:A:1094:VAL:HG13	2:A:1113:THR:CG2	2.30	0.59
2:A:1120:LEU:CD1	2:A:1120:LEU:H	2.14	0.59
2:A:1334:ASP:C	2:A:1336:MET:N	2.58	0.59
4:C:161:LYS:O	4:C:170:TRP:NE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:161:LYS:HD2	6:E:195:VAL:HG23	1.84	0.59
6:E:178:ILE:HG22	6:E:213:ILE:O	2.02	0.59
10:I:101:PHE:N	10:I:101:PHE:CD1	2.70	0.59
2:A:720:ARG:O	2:A:724:GLU:HB2	2.02	0.59
2:A:734:GLU:HG2	2:A:734:GLU:O	2.02	0.59
3:B:217:ARG:HD2	3:B:217:ARG:C	2.27	0.59
3:B:527:THR:OG1	3:B:528:PRO:HD2	2.02	0.59
3:B:1130:PHE:CE1	3:B:1150:ARG:HG3	2.37	0.59
3:B:1162:ILE:HD11	3:B:1194:ILE:HG12	1.83	0.59
4:C:147:LEU:N	4:C:147:LEU:HD23	2.17	0.59
8:G:15:PRO:HA	8:G:18:PHE:CD1	2.38	0.59
8:G:87:VAL:HG21	8:G:103:VAL:HG11	1.85	0.59
2:A:41:MET:O	2:A:50:ILE:HG13	2.01	0.59
2:A:92:HIS:HB2	2:A:236:LEU:HD21	1.83	0.59
2:A:534:LEU:O	2:A:574:GLY:HA3	2.02	0.59
2:A:965:GLN:O	2:A:968:GLN:HB2	2.02	0.59
3:B:589:VAL:CG1	3:B:590:HIS:H	2.12	0.59
3:B:882:THR:CG2	3:B:884:ARG:HB2	2.32	0.59
4:C:73:GLN:HE21	4:C:75:MET:H	1.48	0.59
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.83	0.59
2:A:7:SER:C	2:A:9:ALA:H	2.10	0.59
2:A:24:PRO:HD2	2:A:233:TRP:NE1	2.16	0.59
2:A:1209:MET:SD	2:A:1236:LEU:HD22	2.42	0.59
3:B:952:VAL:CG1	3:B:953:LEU:H	2.15	0.59
2:A:475:THR:HG23	2:A:476:SER:N	2.17	0.59
2:A:567:LYS:HB3	9:H:95:TYR:HA	1.83	0.59
3:B:213:ILE:HD11	3:B:481:GLN:OE1	2.02	0.59
3:B:350:GLN:O	3:B:352:ALA:N	2.35	0.59
3:B:472:ALA:C	3:B:474:SER:N	2.55	0.59
3:B:1002:THR:HG21	3:B:1006:ILE:CD1	2.31	0.59
2:A:84:ILE:HD11	2:A:270:LEU:HD13	1.84	0.59
3:B:288:ALA:HB2	3:B:330:ALA:HB1	1.83	0.59
4:C:133:ILE:CD1	4:C:237:SER:HA	2.32	0.59
9:H:142:LEU:C	9:H:143:LEU:HD12	2.28	0.59
11:J:41:LEU:HD13	11:J:50:ILE:HD13	1.83	0.59
2:A:388:LEU:O	2:A:392:VAL:HG23	2.02	0.59
3:B:113:TYR:HB3	3:B:114:PRO:HD2	1.85	0.59
3:B:282:ILE:N	3:B:282:ILE:CD1	2.66	0.59
3:B:521:LEU:HD22	3:B:633:VAL:HG12	1.84	0.59
3:B:542:MET:HE3	3:B:636:PRO:CG	2.33	0.59
4:C:8:VAL:HG12	4:C:9:LYS:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:186:LEU:N	4:C:186:LEU:HD12	2.17	0.59
6:E:157:SER:OG	6:E:160:GLU:HG3	2.02	0.59
8:G:143:ILE:HD12	8:G:143:ILE:N	2.18	0.59
2:A:30:ILE:HG23	3:B:1170:THR:CG2	2.33	0.59
2:A:455:MET:HE3	3:B:1134:GLU:HG3	1.85	0.59
2:A:590:ARG:HG3	2:A:590:ARG:HH11	1.67	0.59
2:A:666:ILE:CD1	2:A:667:GLY:H	2.16	0.59
4:C:148:ARG:HG2	4:C:149:LYS:N	2.17	0.59
6:E:16:PHE:CE2	6:E:20:LYS:HE2	2.37	0.59
9:H:127:GLY:O	9:H:128:ASN:HB2	2.03	0.59
10:I:111:THR:CG2	10:I:112:SER:N	2.65	0.59
2:A:130:ASP:O	2:A:131:SER:C	2.45	0.59
2:A:650:GLN:O	2:A:654:ASN:HB2	2.03	0.59
2:A:1332:PHE:H	2:A:1332:PHE:HD2	1.51	0.59
3:B:247:GLY:H	3:B:418:LYS:HZ3	1.51	0.59
3:B:276:ILE:HG23	3:B:276:ILE:O	2.02	0.59
3:B:314:LEU:O	3:B:317:CYS:HB3	2.03	0.59
3:B:606:LYS:HD2	3:B:608:ASP:OD2	2.03	0.59
8:G:15:PRO:HA	8:G:18:PHE:CE1	2.38	0.59
10:I:50:THR:CG2	10:I:52:ILE:HG12	2.33	0.59
2:A:504:LEU:HD12	2:A:504:LEU:N	2.18	0.59
2:A:598:LEU:O	2:A:599:SER:C	2.46	0.59
2:A:1115:SER:HA	2:A:1308:THR:HG23	1.84	0.59
2:A:1208:THR:HG22	2:A:1210:GLY:H	1.68	0.59
3:B:505:ASP:O	3:B:507:LYS:N	2.35	0.59
3:B:579:ARG:HG2	3:B:579:ARG:HH11	1.67	0.59
3:B:797:TYR:HD2	3:B:852:ARG:HB2	1.66	0.59
3:B:880:THR:O	3:B:881:ASN:HB2	2.02	0.59
3:B:1002:THR:CG2	3:B:1006:ILE:HG13	2.32	0.59
3:B:1069:PHE:H	3:B:1069:PHE:HD1	1.51	0.59
4:C:22:LEU:HD21	12:K:101:LEU:HD11	1.85	0.59
10:I:82:GLU:HB3	10:I:104:LEU:HD12	1.85	0.59
2:A:154:SER:HB3	2:A:162:VAL:HG21	1.84	0.58
2:A:1144:LYS:HB2	2:A:1268:LEU:O	2.03	0.58
2:A:1212:VAL:O	2:A:1216:ILE:HG13	2.03	0.58
3:B:39:ARG:NH2	3:B:665:GLU:HG2	2.18	0.58
4:C:226:ASP:O	4:C:227:THR:HB	2.03	0.58
1:R:19:G:H1	1:R:28:5BU:H3	1.51	0.58
1:R:29:G:C4'	2:A:1386:ARG:HH12	2.15	0.58
2:A:219:PHE:O	2:A:222:LEU:O	2.19	0.58
2:A:471:ASN:O	2:A:474:VAL:HG12	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:858:ASN:HD21	2:A:860:LEU:H	1.46	0.58
3:B:773:MET:HE2	3:B:985:GLY:HA2	1.84	0.58
3:B:1169:MET:HE1	3:B:1201:LYS:HA	1.85	0.58
4:C:208:GLU:O	4:C:210:GLU:N	2.36	0.58
9:H:107:VAL:HG21	9:H:126:GLU:OE2	2.03	0.58
2:A:711:ARG:NH1	10:I:95:THR:HB	2.19	0.58
2:A:866:PHE:C	2:A:867:ILE:HG13	2.28	0.58
2:A:903:ASN:HD22	2:A:904:THR:N	2.00	0.58
3:B:526:GLU:HG2	3:B:538:ASN:ND2	2.18	0.58
3:B:1023:VAL:O	3:B:1026:LEU:HB2	2.03	0.58
6:E:177:ARG:C	6:E:212:ARG:HD3	2.28	0.58
2:A:115:LEU:CB	2:A:122:MET:HE2	2.33	0.58
2:A:252:PHE:O	2:A:253:ASN:HB2	2.03	0.58
2:A:1102:LYS:CG	2:A:1106:ASN:HD21	2.13	0.58
2:A:1299:VAL:HG12	2:A:1300:LYS:N	2.18	0.58
2:A:1356:ILE:HG22	2:A:1361:SER:HB2	1.84	0.58
3:B:365:THR:CG2	3:B:367:LEU:H	2.11	0.58
8:G:139:ILE:HG22	8:G:140:LYS:N	2.17	0.58
1:R:10:A:O2'	1:R:12:5BU:C6	2.51	0.58
2:A:351:THR:HB	3:B:1103:ILE:HD12	1.85	0.58
2:A:816:HIS:CD2	3:B:764:SER:HB2	2.39	0.58
2:A:1118:VAL:O	2:A:1305:VAL:HG13	2.03	0.58
2:A:1198:ASP:O	2:A:1202:MET:HG2	2.03	0.58
3:B:429:PHE:HA	3:B:432:MET:HE3	1.84	0.58
8:G:91:VAL:HB	8:G:139:ILE:O	2.03	0.58
2:A:57:ARG:O	2:A:58:LEU:O	2.21	0.58
2:A:567:LYS:HB3	9:H:96:VAL:N	2.18	0.58
2:A:1402:PHE:CD1	2:A:1403:GLU:HG3	2.37	0.58
2:A:22:PHE:CB	3:B:1211:ASN:ND2	2.66	0.58
2:A:823:GLY:O	2:A:825:ILE:N	2.37	0.58
2:A:838:GLN:O	2:A:842:VAL:HG23	2.03	0.58
2:A:1224:LEU:HD12	2:A:1241:ARG:O	2.03	0.58
3:B:360:PHE:O	3:B:361:LEU:C	2.45	0.58
3:B:1099:VAL:HG13	3:B:1103:ILE:HD13	1.85	0.58
10:I:29:CYS:SG	10:I:32:CYS:N	2.64	0.58
2:A:317:LYS:O	2:A:318:SER:HB3	2.02	0.58
3:B:95:ILE:CG1	3:B:130:VAL:HG22	2.34	0.58
3:B:400:HIS:O	3:B:402:GLY:N	2.37	0.58
3:B:503:GLY:O	3:B:504:ARG:HB2	2.04	0.58
3:B:1099:VAL:HG13	3:B:1103:ILE:HD11	1.86	0.58
8:G:1:MET:CE	8:G:80:LYS:H	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:32:GLU:O	11:J:34:THR:N	2.37	0.58
2:A:710:LEU:HD12	2:A:710:LEU:N	2.17	0.58
2:A:1057:VAL:HG12	2:A:1058:VAL:H	1.68	0.58
2:A:1206:ASP:O	2:A:1274:ARG:NH1	2.35	0.58
2:A:1372:VAL:CG1	2:A:1373:ASP:N	2.67	0.58
3:B:94:LYS:O	3:B:130:VAL:HG13	2.04	0.58
3:B:504:ARG:HB3	3:B:507:LYS:CE	2.33	0.58
4:C:37:MET:HA	4:C:41:ILE:CD1	2.33	0.58
9:H:130:ARG:H	9:H:130:ARG:HD2	1.68	0.58
11:J:8:PHE:H	11:J:49:MET:CE	2.17	0.58
13:L:49:LYS:O	13:L:50:ASP:CB	2.51	0.58
1:R:27:5BU:BR	1:R:28:5BU:BR	3.32	0.58
2:A:663:SER:OG	2:A:664:THR:N	2.37	0.58
2:A:774:ARG:CZ	2:A:797:LYS:HG3	2.33	0.58
2:A:1334:ASP:C	2:A:1336:MET:H	2.11	0.58
3:B:866:TYR:O	3:B:868:MET:N	2.37	0.58
3:B:955:THR:CG2	3:B:956:THR:H	2.17	0.58
2:A:41:MET:O	2:A:42:ASP:C	2.47	0.57
2:A:224:PHE:CZ	2:A:231:PRO:HG3	2.39	0.57
2:A:590:ARG:HH11	2:A:590:ARG:CG	2.17	0.57
2:A:754:SER:H	2:A:757:ASN:HD22	1.52	0.57
2:A:1195:LEU:HD11	2:A:1267:MET:CE	2.34	0.57
3:B:773:MET:SD	3:B:987:LYS:HD3	2.44	0.57
3:B:1073:TYR:OH	4:C:179:GLU:HG3	2.04	0.57
5:D:29:LEU:HD22	8:G:82:PHE:CE2	2.39	0.57
10:I:110:PHE:H	10:I:110:PHE:HD2	1.51	0.57
2:A:50:ILE:C	2:A:52:GLY:H	2.10	0.57
3:B:309:GLN:OE1	10:I:52:ILE:HD11	2.03	0.57
3:B:640:VAL:O	3:B:641:GLU:C	2.48	0.57
4:C:6:PRO:HB2	12:K:101:LEU:HD12	1.86	0.57
4:C:175:ALA:O	4:C:176:ILE:HG13	2.04	0.57
6:E:165:LEU:HD23	6:E:170:LEU:HB2	1.85	0.57
2:A:546:VAL:HG13	2:A:577:ILE:HG21	1.86	0.57
3:B:282:ILE:HD13	3:B:283:VAL:H	1.68	0.57
3:B:373:ARG:HA	3:B:566:LEU:HD23	1.85	0.57
3:B:1065:GLN:NE2	3:B:1066:SER:N	2.53	0.57
7:F:74:ILE:HG23	7:F:75:PRO:HD2	1.86	0.57
12:K:47:ARG:HH11	12:K:47:ARG:CB	2.05	0.57
2:A:1291:VAL:HG13	2:A:1292:PRO:HD2	1.87	0.57
3:B:210:LYS:HA	3:B:481:GLN:O	2.04	0.57
3:B:504:ARG:HB3	3:B:507:LYS:NZ	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:43:THR:CG2	4:C:44:LEU:N	2.67	0.57
7:F:99:LEU:HD12	7:F:99:LEU:O	2.04	0.57
1:R:7:C:N3	3:B:465:ASN:ND2	2.53	0.57
2:A:730:GLY:C	2:A:732:LEU:H	2.12	0.57
3:B:846:ILE:CG2	3:B:974:PRO:HG2	2.33	0.57
3:B:997:GLU:CD	3:B:997:GLU:H	2.10	0.57
3:B:1178:ASN:O	3:B:1179:GLN:C	2.48	0.57
12:K:42:LEU:O	12:K:46:ILE:HG12	2.04	0.57
2:A:75:ASN:O	2:A:76:GLU:HB2	2.05	0.57
2:A:89:PRO:HB2	2:A:204:THR:HG22	1.87	0.57
2:A:745:GLN:HA	2:A:748:MET:HE3	1.86	0.57
2:A:963:ILE:HD11	2:A:1048:ASN:HB3	1.87	0.57
2:A:1345:ARG:HD2	2:A:1373:ASP:OD1	2.05	0.57
2:A:1378:GLN:O	6:E:177:ARG:HB2	2.04	0.57
3:B:185:THR:O	3:B:186:GLU:C	2.47	0.57
3:B:778:MET:CE	3:B:1094:ARG:HD3	2.35	0.57
7:F:111:LEU:HD12	7:F:111:LEU:H	1.69	0.57
2:A:868:TYR:CE1	2:A:1064:VAL:CG1	2.83	0.57
3:B:274:PRO:O	3:B:274:PRO:CD	2.52	0.57
3:B:515:HIS:CD2	3:B:517:THR:H	2.21	0.57
3:B:778:MET:HE1	3:B:1094:ARG:HD3	1.87	0.57
4:C:174:ALA:O	4:C:175:ALA:HB3	2.05	0.57
7:F:138:LEU:HB3	7:F:139:PRO:HD2	1.87	0.57
9:H:42:ILE:HG23	9:H:95:TYR:CE1	2.29	0.57
12:K:58:PHE:HE2	12:K:74:ARG:NE	2.02	0.57
2:A:1094:VAL:CG1	2:A:1113:THR:HG21	2.32	0.57
3:B:57:TYR:CD1	3:B:57:TYR:N	2.72	0.57
9:H:123:MET:HE1	9:H:142:LEU:HD13	1.86	0.57
10:I:16:PRO:HB3	10:I:27:PHE:CE2	2.40	0.57
2:A:500:GLU:OE2	2:A:1438:THR:HG21	2.05	0.57
2:A:1116:LEU:N	2:A:1308:THR:CG2	2.67	0.57
3:B:504:ARG:HB3	3:B:507:LYS:HZ1	1.70	0.57
3:B:549:THR:H	3:B:628:THR:HG23	1.70	0.57
7:F:86:THR:OG1	7:F:89:GLU:HG3	2.05	0.57
1:R:7:C:N4	1:R:13:G:H21	2.02	0.57
2:A:1214:GLU:O	2:A:1218:GLN:HG2	2.05	0.57
3:B:789:MET:HE2	3:B:953:LEU:HD22	1.87	0.57
7:F:81:THR:HB	7:F:136:ARG:HH11	1.69	0.57
8:G:53:ASN:HD22	8:G:53:ASN:N	2.03	0.57
9:H:98:TYR:C	9:H:118:PHE:CD2	2.80	0.57
12:K:55:LYS:HB3	12:K:81:TYR:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1385:THR:HG22	2:A:1386:ARG:N	2.20	0.56
2:A:1420:ASP:O	2:A:1421:CYS:HB2	2.05	0.56
3:B:563:MET:CE	3:B:580:VAL:HB	2.34	0.56
6:E:116:ILE:CG2	6:E:117:THR:H	2.18	0.56
6:E:116:ILE:CG2	6:E:117:THR:N	2.67	0.56
2:A:499:ALA:O	2:A:503:GLN:HB2	2.04	0.56
3:B:408:LEU:O	3:B:411:PRO:HD2	2.04	0.56
3:B:1120:GLU:HG2	3:B:1121:GLY:N	2.19	0.56
4:C:47:ASP:HA	13:L:69:ALA:CB	2.31	0.56
4:C:249:ASP:O	4:C:252:GLN:HB3	2.06	0.56
2:A:336:ILE:HG22	2:A:337:ARG:N	2.20	0.56
2:A:369:SER:HB3	12:K:2:ASN:ND2	2.16	0.56
2:A:445:ASN:HB2	2:A:455:MET:HG2	1.88	0.56
2:A:586:ILE:CD1	2:A:633:VAL:HG22	2.34	0.56
2:A:849:MET:HE3	2:A:1061:GLY:O	2.04	0.56
2:A:855:THR:HG21	2:A:857:ARG:HE	1.69	0.56
2:A:919:ILE:HG23	2:A:925:LEU:HD12	1.85	0.56
2:A:1114:PRO:O	2:A:1115:SER:O	2.23	0.56
2:A:1323:ASP:OD1	2:A:1325:THR:HB	2.04	0.56
2:A:1353:TYR:HD1	2:A:1368:MET:HE1	1.69	0.56
2:A:1398:MET:C	2:A:1400:CYS:H	2.11	0.56
4:C:167:HIS:CD2	4:C:168:ALA:H	2.23	0.56
5:D:134:THR:HG22	5:D:135:GLY:N	2.18	0.56
8:G:7:LEU:O	8:G:73:LYS:HD2	2.06	0.56
9:H:91:ASP:C	9:H:93:TYR:H	2.13	0.56
2:A:498:ARG:O	2:A:501:LEU:N	2.38	0.56
2:A:805:LEU:HD11	3:B:1052:VAL:HG21	1.87	0.56
2:A:935:GLN:HE21	2:A:1023:ARG:NH1	2.04	0.56
2:A:1313:LEU:C	2:A:1315:GLU:H	2.13	0.56
3:B:185:THR:H	3:B:188:ASP:HB2	1.70	0.56
3:B:1115:THR:O	3:B:1116:ARG:HB2	2.05	0.56
2:A:67:CYS:O	2:A:68:GLN:HB2	2.05	0.56
2:A:1450:LEU:O	2:A:1450:LEU:HG	2.05	0.56
3:B:299:GLU:OE2	3:B:572:HIS:HE1	1.88	0.56
3:B:357:GLN:O	3:B:366:GLN:HA	2.06	0.56
3:B:558:LEU:C	3:B:560:GLU:H	2.13	0.56
3:B:828:ALA:HB2	3:B:1085:ILE:HG23	1.87	0.56
4:C:184:ASN:ND2	4:C:187:LYS:HA	2.21	0.56
6:E:85:GLU:HB2	6:E:88:VAL:HG22	1.86	0.56
2:A:55:ASP:C	2:A:57:ARG:N	2.58	0.56
2:A:361:LEU:HA	2:A:471:ASN:HD22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:103:MET:CE	8:G:66:GLY:H	2.19	0.56
2:A:53:LEU:O	2:A:54:ASN:C	2.48	0.56
2:A:146:MET:CA	2:A:171:GLN:HB2	2.34	0.56
2:A:384:ASN:OD1	2:A:388:LEU:HD12	2.06	0.56
3:B:569:TYR:CE1	3:B:589:VAL:HG21	2.41	0.56
3:B:777:ALA:HA	3:B:1095:LEU:HA	1.87	0.56
3:B:803:LEU:HD12	3:B:1032:SER:HB3	1.87	0.56
4:C:181:ASP:CG	4:C:186:LEU:HD13	2.30	0.56
5:D:137:ASN:C	5:D:137:ASN:HD22	2.13	0.56
5:D:155:ARG:HG2	5:D:155:ARG:O	2.05	0.56
8:G:34:VAL:HG11	8:G:74:TYR:HE1	1.71	0.56
2:A:547:LEU:HD22	12:K:58:PHE:CD1	2.41	0.56
2:A:746:MET:HE3	3:B:1018:PRO:CG	2.36	0.56
2:A:849:MET:CE	2:A:1061:GLY:HA2	2.36	0.56
3:B:401:PHE:CE2	3:B:633:VAL:HG21	2.39	0.56
3:B:758:PHE:CE1	3:B:1027:ILE:HG22	2.41	0.56
4:C:31:ASN:O	4:C:32:SER:C	2.48	0.56
5:D:170:THR:CG2	5:D:172:LEU:HG	2.36	0.56
10:I:75:CYS:SG	10:I:103:CYS:SG	3.03	0.56
11:J:1:MET:N	11:J:56:LEU:H	2.03	0.56
2:A:738:LYS:C	2:A:740:LEU:H	2.14	0.56
2:A:1120:LEU:HD12	2:A:1120:LEU:H	1.70	0.56
2:A:1315:GLU:C	2:A:1317:MET:H	2.13	0.56
2:A:1444:MET:O	7:F:133:VAL:N	2.38	0.56
3:B:240:ILE:C	3:B:240:ILE:HD13	2.31	0.56
3:B:284:ILE:HD11	3:B:321:GLY:HA2	1.88	0.56
3:B:1000:PRO:O	3:B:1007:VAL:HG23	2.06	0.56
10:I:61:ASP:C	10:I:63:GLY:H	2.13	0.56
2:A:399:HIS:CB	2:A:400:PRO:HD3	2.33	0.56
2:A:903:ASN:C	2:A:903:ASN:ND2	2.61	0.56
2:A:1398:MET:C	2:A:1400:CYS:N	2.62	0.56
3:B:464:GLY:O	3:B:466:TRP:N	2.39	0.56
3:B:614:SER:C	3:B:615:MET:HG3	2.30	0.56
3:B:1182:CYS:O	3:B:1186:ASP:N	2.39	0.56
2:A:524:VAL:HG12	2:A:525:GLN:HG2	1.88	0.55
2:A:626:ASN:O	2:A:631:HIS:CD2	2.58	0.55
2:A:1334:ASP:O	2:A:1336:MET:N	2.38	0.55
3:B:467:GLY:O	3:B:470:LYS:HG3	2.06	0.55
3:B:822:ASN:ND2	11:J:52:THR:HG21	2.21	0.55
4:C:26:ASP:O	4:C:27:LEU:C	2.49	0.55
4:C:66:ARG:O	4:C:69:LEU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:128:PRO:O	8:G:138:THR:HG23	2.05	0.55
10:I:7:CYS:HB2	10:I:34:TYR:CD1	2.41	0.55
10:I:50:THR:HG22	10:I:51:ASN:N	2.19	0.55
2:A:69:THR:C	2:A:71:GLN:N	2.63	0.55
3:B:661:LEU:C	3:B:663:ALA:H	2.14	0.55
4:C:36:VAL:HG21	4:C:251:LEU:HD22	1.88	0.55
7:F:103:MET:O	7:F:104:ASN:HB2	2.06	0.55
9:H:22:LYS:O	9:H:23:VAL:HG23	2.05	0.55
2:A:843:LYS:HD3	2:A:846:GLU:OE2	2.06	0.55
2:A:855:THR:HG21	2:A:857:ARG:NE	2.22	0.55
2:A:1094:VAL:HG22	2:A:1113:THR:HG21	1.88	0.55
3:B:591:ARG:O	3:B:593:PRO:HD3	2.06	0.55
3:B:1172:ILE:N	3:B:1172:ILE:CD1	2.68	0.55
5:D:51:ASN:O	5:D:54:GLU:HB3	2.06	0.55
7:F:119:ARG:HH11	7:F:119:ARG:HG3	1.71	0.55
2:A:72:GLU:OE2	3:B:1175:LEU:HB2	2.07	0.55
2:A:964:ILE:HD13	2:A:1045:VAL:HG21	1.89	0.55
4:C:74:SER:O	4:C:238:ILE:HD11	2.07	0.55
5:D:134:THR:HG22	5:D:136:GLY:N	2.19	0.55
2:A:231:PRO:C	2:A:233:TRP:H	2.14	0.55
2:A:321:PRO:O	2:A:322:VAL:CB	2.54	0.55
2:A:503:GLN:HE21	7:F:90:ARG:HH21	1.53	0.55
2:A:590:ARG:O	2:A:591:PHE:HB2	2.05	0.55
2:A:741:ASN:HD22	2:A:744:LYS:H	1.54	0.55
2:A:1410:PHE:HA	3:B:1212:ILE:HD11	1.88	0.55
4:C:86:CYS:O	4:C:88:CYS:N	2.39	0.55
4:C:88:CYS:SG	4:C:92:CYS:HB3	2.46	0.55
2:A:543:LEU:C	2:A:545:GLN:H	2.15	0.55
2:A:901:LEU:HG	2:A:926:GLN:NE2	2.11	0.55
2:A:929:LEU:HD23	2:A:983:ILE:HG21	1.88	0.55
2:A:1121:GLU:CG	2:A:1122:PRO:HD2	2.37	0.55
3:B:293:PRO:C	3:B:294:ASP:O	2.45	0.55
3:B:503:GLY:O	3:B:507:LYS:HG3	2.06	0.55
3:B:839:MET:CE	3:B:980:PHE:HB2	2.37	0.55
3:B:1202:LEU:O	3:B:1206:GLU:HG3	2.06	0.55
4:C:69:LEU:N	4:C:69:LEU:HD12	2.20	0.55
2:A:583:PRO:HG2	2:A:586:ILE:HD11	1.88	0.55
2:A:823:GLY:C	2:A:825:ILE:H	2.15	0.55
2:A:1443:VAL:C	2:A:1444:MET:HG3	2.31	0.55
3:B:681:TRP:HA	3:B:684:LEU:HD13	1.88	0.55
3:B:778:MET:HE2	3:B:1094:ARG:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:55:ASP:H	2:A:56:PRO:HD3	1.71	0.55
2:A:196:GLU:HG2	2:A:197:PRO:HD2	1.88	0.55
2:A:722:LEU:O	2:A:725:ALA:HB3	2.06	0.55
2:A:1093:LYS:O	2:A:1094:VAL:HG23	2.06	0.55
2:A:1213:GLY:O	2:A:1214:GLU:C	2.49	0.55
2:A:50:ILE:C	2:A:52:GLY:N	2.61	0.55
2:A:93:VAL:CG2	2:A:301:ALA:HA	2.37	0.55
2:A:541:ILE:HG21	2:A:549:MET:HE3	1.88	0.55
3:B:130:VAL:HG12	3:B:131:ASP:N	2.21	0.55
3:B:204:ILE:C	3:B:205:ILE:HD12	2.32	0.55
3:B:233:PRO:HG2	3:B:234:ILE:CD1	2.37	0.55
3:B:365:THR:HG23	3:B:367:LEU:N	2.12	0.55
3:B:831:SER:CB	3:B:994:TYR:OH	2.54	0.55
3:B:1110:PRO:O	3:B:1119:VAL:HG22	2.07	0.55
2:A:218:ASP:O	2:A:219:PHE:C	2.50	0.55
2:A:317:LYS:O	2:A:318:SER:CB	2.54	0.55
3:B:223:VAL:HG11	3:B:381:MET:HG2	1.87	0.55
3:B:346:GLU:CA	3:B:349:ILE:HD13	2.37	0.55
3:B:558:LEU:O	3:B:560:GLU:N	2.40	0.55
3:B:844:SER:O	3:B:847:ASP:HB2	2.07	0.55
8:G:15:PRO:O	8:G:16:SER:C	2.50	0.55
9:H:15:VAL:HG22	9:H:26:ILE:CD1	2.36	0.55
2:A:90:VAL:CG1	2:A:297:GLN:NE2	2.70	0.54
2:A:225:ASN:ND2	2:A:228:PHE:N	2.43	0.54
2:A:613:ILE:HG22	2:A:614:PHE:HD2	1.72	0.54
2:A:639:PRO:CD	2:A:640:GLN:H	2.19	0.54
3:B:465:ASN:O	3:B:466:TRP:O	2.25	0.54
3:B:1166:CYS:O	3:B:1168:LEU:N	2.36	0.54
4:C:82:TYR:O	4:C:83:SER:C	2.49	0.54
5:D:37:GLN:OE1	8:G:5:LYS:NZ	2.34	0.54
1:R:29:G:H4'	2:A:1386:ARG:NH1	2.17	0.54
2:A:482:PHE:C	2:A:484:GLY:H	2.16	0.54
2:A:630:ILE:HD13	2:A:645:LEU:HD23	1.88	0.54
2:A:675:THR:O	2:A:679:ILE:HG12	2.08	0.54
2:A:1436:ILE:O	2:A:1437:GLY:C	2.49	0.54
3:B:34:ILE:O	3:B:37:PHE:HB3	2.07	0.54
3:B:373:ARG:HG2	3:B:566:LEU:HD23	1.89	0.54
3:B:642:ASP:O	3:B:644:GLU:N	2.40	0.54
3:B:705:MET:HE2	3:B:745:PRO:HB3	1.90	0.54
3:B:850:LEU:HD12	3:B:851:PHE:H	1.70	0.54
3:B:1023:VAL:O	3:B:1026:LEU:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1187:ASN:O	3:B:1188:LYS:CB	2.53	0.54
4:C:22:LEU:HD13	4:C:230:MET:HE1	1.88	0.54
5:D:47:LEU:HD13	5:D:48:ILE:N	2.21	0.54
6:E:88:VAL:HG12	6:E:89:GLY:N	2.20	0.54
1:R:7:C:H41	1:R:13:G:H21	1.53	0.54
2:A:40:THR:HG23	2:A:54:ASN:HD21	1.71	0.54
2:A:401:GLY:C	2:A:435:HIS:CD2	2.83	0.54
2:A:518:LYS:HG3	2:A:519:PRO:O	2.08	0.54
2:A:567:LYS:NZ	9:H:47:PHE:HB2	2.20	0.54
2:A:567:LYS:CB	2:A:568:PRO:CD	2.84	0.54
2:A:577:ILE:HD13	2:A:577:ILE:N	2.22	0.54
2:A:869:GLY:O	6:E:204:THR:HG21	2.07	0.54
3:B:798:TYR:HE2	4:C:62:PHE:CZ	2.25	0.54
4:C:75:MET:HE2	4:C:239:PRO:CG	2.37	0.54
6:E:114:ASN:O	6:E:115:ASN:HB3	2.08	0.54
9:H:56:THR:O	9:H:144:ILE:HA	2.08	0.54
9:H:82:PRO:C	9:H:84:ALA:H	2.15	0.54
2:A:49:LYS:HD3	2:A:55:ASP:HB3	1.88	0.54
2:A:269:ILE:HD11	2:A:300:VAL:HA	1.89	0.54
2:A:853:ASP:OD1	2:A:853:ASP:C	2.49	0.54
3:B:254:LEU:HD11	3:B:273:LEU:HG	1.88	0.54
3:B:949:VAL:HG12	3:B:950:ASP:N	2.23	0.54
4:C:73:GLN:NE2	4:C:75:MET:H	2.05	0.54
5:D:198:LEU:O	5:D:199:ASN:C	2.50	0.54
8:G:126:ASN:HD22	8:G:127:PRO:HA	1.70	0.54
11:J:51:LEU:O	11:J:51:LEU:HD12	2.08	0.54
2:A:588:LEU:O	2:A:606:LEU:HA	2.07	0.54
2:A:650:GLN:O	2:A:654:ASN:ND2	2.37	0.54
2:A:942:PHE:C	2:A:942:PHE:CD2	2.86	0.54
2:A:1341:ILE:HB	6:E:182:ASP:OD2	2.08	0.54
3:B:20:ASP:C	3:B:22:SER:H	2.16	0.54
3:B:114:PRO:HG2	3:B:115:GLN:H	1.71	0.54
3:B:945:GLU:O	3:B:946:ASN:HB3	2.08	0.54
4:C:241:ASP:CG	4:C:242:GLN:N	2.65	0.54
8:G:154:VAL:HG12	8:G:155:SER:N	2.22	0.54
2:A:12:ARG:O	3:B:1194:ILE:HG22	2.08	0.54
2:A:382:PRO:CB	2:A:428:TYR:HE2	2.18	0.54
3:B:258:LEU:HG	3:B:258:LEU:O	2.07	0.54
3:B:274:PRO:HD2	3:B:276:ILE:HD13	1.89	0.54
3:B:387:LEU:H	3:B:387:LEU:CD1	2.21	0.54
4:C:253:LYS:O	4:C:256:ALA:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:52:LEU:O	5:D:54:GLU:N	2.37	0.54
10:I:85:PHE:CD2	10:I:85:PHE:N	2.61	0.54
2:A:1341:ILE:CG2	2:A:1342:GLU:N	2.71	0.54
2:A:1444:MET:HE1	7:F:135:ARG:NE	2.23	0.54
3:B:94:LYS:HG2	3:B:95:ILE:H	1.73	0.54
3:B:558:LEU:C	3:B:560:GLU:N	2.66	0.54
3:B:954:VAL:O	13:L:55:ILE:O	2.25	0.54
3:B:1156:ASP:O	3:B:1157:ALA:O	2.26	0.54
5:D:162:ALA:O	5:D:163:VAL:C	2.51	0.54
5:D:208:GLU:O	5:D:212:LYS:HG3	2.07	0.54
8:G:1:MET:HE2	8:G:3:PHE:CE1	2.43	0.54
11:J:8:PHE:H	11:J:49:MET:HE3	1.71	0.54
2:A:492:PRO:O	2:A:493:GLN:NE2	2.41	0.54
2:A:541:ILE:HD12	2:A:541:ILE:N	2.23	0.54
2:A:825:ILE:C	2:A:827:THR:N	2.65	0.54
2:A:1001:ARG:O	2:A:1002:GLY:O	2.26	0.54
2:A:1007:ILE:C	2:A:1009:ASN:H	2.15	0.54
2:A:1265:ASN:HD21	3:B:265:SER:HB3	1.73	0.54
2:A:1359:ASP:C	2:A:1361:SER:H	2.15	0.54
2:A:1420:ASP:CB	2:A:1422:ARG:HG3	2.37	0.54
3:B:1065:GLN:HG3	3:B:1067:ARG:H	1.71	0.54
5:D:130:LEU:O	5:D:132:GLN:N	2.41	0.54
7:F:90:ARG:HG3	7:F:91:ALA:N	2.23	0.54
7:F:128:LYS:HE2	7:F:151:LEU:O	2.08	0.54
8:G:91:VAL:CG2	8:G:143:ILE:HD13	2.37	0.54
2:A:37:PHE:N	2:A:37:PHE:CD1	2.76	0.54
2:A:120:GLU:C	2:A:122:MET:H	2.15	0.54
2:A:441:PRO:HD2	2:A:498:ARG:NH2	2.22	0.54
2:A:921:GLY:O	2:A:922:ASP:C	2.50	0.54
3:B:272:THR:O	3:B:273:LEU:CB	2.55	0.54
3:B:1208:MET:O	3:B:1211:ASN:N	2.31	0.54
4:C:167:HIS:HA	12:K:6:ARG:NH1	2.19	0.54
8:G:1:MET:O	8:G:3:PHE:CE1	2.61	0.54
2:A:70:CYS:O	2:A:70:CYS:SG	2.65	0.54
2:A:157:ASP:C	2:A:159:THR:H	2.15	0.54
2:A:407:ARG:HA	2:A:430:TRP:CD1	2.43	0.54
2:A:563:PRO:HB3	2:A:571:LEU:O	2.08	0.54
2:A:853:ASP:OD1	2:A:855:THR:CB	2.56	0.54
3:B:918:ILE:CG1	3:B:935:ARG:HD2	2.38	0.54
3:B:1022:THR:HG23	3:B:1022:THR:O	2.08	0.54
4:C:66:ARG:NH1	11:J:2:ILE:HG21	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:64:VAL:O	5:D:67:ARG:N	2.41	0.54
5:D:122:GLU:HA	5:D:125:SER:OG	2.09	0.54
12:K:31:VAL:HG12	12:K:32:VAL:N	2.23	0.54
1:R:2:C:H1'	1:R:3:A:OP1	2.08	0.53
2:A:147:VAL:C	2:A:171:GLN:HE21	2.16	0.53
2:A:322:VAL:HG12	2:A:323:LYS:N	2.23	0.53
2:A:472:LEU:HD11	3:B:835:GLN:CD	2.33	0.53
2:A:490:HIS:HB3	3:B:1150:ARG:NH1	2.23	0.53
2:A:535:THR:CG2	2:A:616:VAL:HA	2.37	0.53
2:A:1116:LEU:O	2:A:1308:THR:HG22	2.07	0.53
3:B:90:ILE:HD11	3:B:432:MET:SD	2.48	0.53
3:B:508:LEU:HD13	3:B:508:LEU:N	2.23	0.53
3:B:953:LEU:HD23	3:B:953:LEU:O	2.08	0.53
9:H:4:THR:HG22	9:H:5:LEU:N	2.22	0.53
10:I:43:VAL:O	10:I:43:VAL:HG12	2.07	0.53
12:K:90:ALA:O	12:K:94:ILE:HG12	2.08	0.53
2:A:450:LEU:O	2:A:1070:GLN:HB3	2.08	0.53
2:A:829:VAL:C	2:A:831:THR:N	2.66	0.53
2:A:1017:LEU:CB	6:E:205:SER:HA	2.38	0.53
2:A:1118:VAL:CG2	2:A:1306:LEU:HB2	2.38	0.53
3:B:282:ILE:HD11	3:B:317:CYS:SG	2.47	0.53
3:B:287:ARG:NH1	3:B:324:ILE:O	2.40	0.53
3:B:1065:GLN:NE2	3:B:1067:ARG:HG2	2.23	0.53
9:H:58:THR:O	9:H:59:ILE:HD12	2.09	0.53
11:J:2:ILE:HG22	11:J:3:VAL:O	2.08	0.53
11:J:48:ARG:HH21	11:J:49:MET:HE1	1.73	0.53
2:A:427:GLN:HG3	2:A:430:TRP:CZ2	2.43	0.53
2:A:751:SER:OG	3:B:1015:HIS:CE1	2.61	0.53
2:A:1027:ALA:O	2:A:1031:VAL:HG23	2.07	0.53
2:A:1030:ARG:HG3	2:A:1034:GLU:OE2	2.07	0.53
2:A:1116:LEU:HD12	2:A:1116:LEU:O	2.09	0.53
3:B:259:TYR:HD1	3:B:259:TYR:H	1.57	0.53
3:B:269:ILE:HD12	3:B:269:ILE:N	2.23	0.53
3:B:1031:LEU:CD2	3:B:1044:ALA:HB2	2.39	0.53
5:D:146:GLN:O	5:D:149:THR:HG22	2.08	0.53
9:H:56:THR:HB	9:H:145:ARG:HG2	1.91	0.53
9:H:59:ILE:O	9:H:60:ALA:CB	2.56	0.53
2:A:563:PRO:HG3	2:A:572:TRP:CE2	2.43	0.53
2:A:877:HIS:C	2:A:878:ILE:CG1	2.80	0.53
2:A:1057:VAL:CG1	2:A:1058:VAL:N	2.70	0.53
2:A:1265:ASN:ND2	3:B:265:SER:HB3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1291:VAL:HG13	2:A:1292:PRO:CD	2.39	0.53
3:B:258:LEU:O	3:B:258:LEU:CG	2.56	0.53
3:B:1060:ARG:CZ	4:C:202:PRO:HG3	2.38	0.53
4:C:237:SER:O	4:C:238:ILE:HD12	2.08	0.53
4:C:260:LEU:O	4:C:264:GLN:HG3	2.08	0.53
2:A:265:LYS:HE2	2:A:302:THR:CG2	2.38	0.53
2:A:269:ILE:HD13	2:A:300:VAL:HG22	1.90	0.53
2:A:345:VAL:HG23	2:A:346:ASP:O	2.09	0.53
2:A:629:LEU:HD23	2:A:633:VAL:HG23	1.91	0.53
2:A:645:LEU:HG	2:A:649:ILE:HD12	1.90	0.53
3:B:35:SER:O	3:B:39:ARG:HG3	2.08	0.53
3:B:120:ARG:CG	3:B:955:THR:HG21	2.34	0.53
3:B:785:TYR:CD1	3:B:785:TYR:C	2.87	0.53
3:B:1115:THR:HG22	3:B:1117:GLN:HG3	1.91	0.53
7:F:118:LEU:O	7:F:122:MET:HG3	2.09	0.53
2:A:683:ILE:HG21	2:A:801:GLU:HG3	1.90	0.53
2:A:808:LEU:HD23	2:A:813:PHE:N	2.23	0.53
2:A:1031:VAL:O	2:A:1031:VAL:HG12	2.08	0.53
3:B:245:GLU:O	3:B:246:LYS:HG3	2.08	0.53
3:B:562:GLY:HA3	3:B:590:HIS:CE1	2.43	0.53
8:G:149:GLY:O	8:G:159:ALA:HB1	2.08	0.53
9:H:27:GLU:HG2	9:H:39:THR:HG23	1.91	0.53
11:J:21:TYR:HB2	11:J:39:LEU:CD1	2.39	0.53
2:A:56:PRO:O	2:A:57:ARG:CG	2.53	0.53
2:A:352:VAL:HG12	2:A:353:ILE:N	2.23	0.53
2:A:382:PRO:HB3	2:A:428:TYR:CE2	2.38	0.53
2:A:456:MET:HB2	2:A:478:TYR:OH	2.08	0.53
2:A:963:ILE:HD11	2:A:1048:ASN:CB	2.39	0.53
2:A:1207:LEU:HA	2:A:1211:GLN:OE1	2.09	0.53
3:B:121:ASN:HA	3:B:207:GLY:HA3	1.91	0.53
5:D:202:ILE:CG2	5:D:203:SER:N	2.68	0.53
11:J:44:TYR:H	11:J:44:TYR:HD2	1.57	0.53
2:A:68:GLN:O	2:A:70:CYS:N	2.36	0.53
2:A:1283:VAL:HG12	2:A:1284:MET:N	2.22	0.53
4:C:146:LYS:C	4:C:147:LEU:HD23	2.34	0.53
2:A:322:VAL:CG1	2:A:323:LYS:N	2.71	0.53
2:A:466:SER:HB3	3:B:1103:ILE:HG12	1.91	0.53
2:A:686:ALA:O	2:A:690:VAL:HG23	2.09	0.53
2:A:1259:MET:C	2:A:1261:LYS:H	2.17	0.53
3:B:773:MET:C	3:B:775:LYS:H	2.17	0.53
3:B:880:THR:HB	3:B:934:LYS:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:979:LYS:HG2	3:B:1095:LEU:HD13	1.90	0.53
4:C:167:HIS:CD2	4:C:168:ALA:N	2.77	0.53
4:C:179:GLU:HG2	4:C:180:TYR:N	2.24	0.53
5:D:14:ARG:O	5:D:16:LYS:N	2.42	0.53
5:D:153:ARG:C	5:D:154:PHE:CD1	2.87	0.53
1:R:17:5BU:O2'	1:R:18:C:H5'	2.09	0.53
2:A:2:VAL:HG21	3:B:1157:ALA:HB1	1.89	0.53
2:A:49:LYS:HZ1	2:A:61:ILE:H	1.55	0.53
2:A:71:GLN:HG3	2:A:72:GLU:N	2.24	0.53
2:A:1339:LEU:HD13	6:E:147:HIS:CD2	2.44	0.53
3:B:62:ILE:HG23	3:B:418:LYS:HG2	1.91	0.53
3:B:387:LEU:HD12	3:B:387:LEU:N	2.24	0.53
3:B:593:PRO:O	3:B:596:LEU:N	2.42	0.53
3:B:973:ILE:HG23	3:B:974:PRO:HD2	1.90	0.53
4:C:184:ASN:HD21	4:C:187:LYS:HA	1.72	0.53
6:E:22:MET:HE3	6:E:26:ARG:CZ	2.38	0.53
9:H:32:THR:HG22	9:H:33:GLN:OE1	2.09	0.53
2:A:84:ILE:CG2	2:A:239:LEU:HB3	2.37	0.52
2:A:1007:ILE:C	2:A:1009:ASN:N	2.67	0.52
2:A:1280:GLU:O	2:A:1282:VAL:HG23	2.08	0.52
3:B:58:THR:O	3:B:62:ILE:HG12	2.09	0.52
3:B:421:PHE:O	3:B:424:LEU:HB3	2.09	0.52
3:B:1201:LYS:HE2	3:B:1205:GLN:CD	2.33	0.52
9:H:110:ASP:O	9:H:128:ASN:ND2	2.42	0.52
2:A:49:LYS:HZ1	2:A:61:ILE:N	2.07	0.52
2:A:567:LYS:HB2	2:A:568:PRO:CD	2.39	0.52
2:A:1373:ASP:O	2:A:1376:THR:HG22	2.09	0.52
3:B:516:ASN:N	3:B:516:ASN:ND2	2.50	0.52
3:B:542:MET:HE2	3:B:743:ILE:HG13	1.91	0.52
3:B:1073:TYR:CE2	3:B:1080:LYS:HG2	2.44	0.52
3:B:1102:LYS:O	3:B:1103:ILE:C	2.51	0.52
5:D:167:LEU:O	5:D:170:THR:OG1	2.28	0.52
6:E:202:SER:C	6:E:204:THR:H	2.16	0.52
9:H:83:GLN:C	9:H:85:GLY:H	2.16	0.52
10:I:83:ASN:HA	10:I:102:VAL:O	2.09	0.52
2:A:276:LEU:HG	2:A:276:LEU:O	2.09	0.52
2:A:340:LEU:HD13	2:A:1429:ILE:CG2	2.38	0.52
2:A:512:VAL:HA	2:A:519:PRO:HA	1.90	0.52
2:A:586:ILE:HD13	2:A:633:VAL:HG22	1.91	0.52
2:A:590:ARG:HH21	2:A:620:LYS:CB	2.13	0.52
2:A:590:ARG:NH1	2:A:590:ARG:CG	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:873:MET:C	2:A:1058:VAL:HG23	2.34	0.52
2:A:1094:VAL:CG1	2:A:1095:THR:N	2.72	0.52
3:B:203:PHE:CB	3:B:205:ILE:HD11	2.39	0.52
3:B:287:ARG:HA	3:B:291:ILE:O	2.09	0.52
3:B:603:LEU:HB3	3:B:609:ILE:HG13	1.91	0.52
3:B:847:ASP:HB3	4:C:167:HIS:CD2	2.44	0.52
6:E:2:ASP:O	6:E:3:GLN:HG2	2.09	0.52
6:E:112:TYR:CE1	6:E:136:ASN:HA	2.44	0.52
8:G:1:MET:HE1	8:G:80:LYS:N	2.23	0.52
13:L:32:ALA:HB2	13:L:55:ILE:HG13	1.91	0.52
2:A:68:GLN:C	2:A:70:CYS:N	2.67	0.52
2:A:442:VAL:O	2:A:457:ALA:HA	2.10	0.52
2:A:590:ARG:HG2	2:A:591:PHE:N	2.23	0.52
2:A:920:LEU:HD23	2:A:920:LEU:C	2.34	0.52
2:A:1074:GLU:C	2:A:1076:ALA:H	2.18	0.52
3:B:285:ILE:HG21	3:B:378:LEU:CD2	2.39	0.52
3:B:984:HIS:NE2	3:B:1025:HIS:HA	2.24	0.52
4:C:259:LEU:HD13	12:K:91:CYS:HB2	1.91	0.52
4:C:263:THR:C	4:C:265:MET:H	2.17	0.52
6:E:145:THR:HG21	6:E:187:TYR:CD2	2.44	0.52
2:A:877:HIS:O	2:A:878:ILE:HG13	2.09	0.52
2:A:1254:ALA:O	2:A:1255:GLU:HB2	2.10	0.52
3:B:251:ILE:O	3:B:251:ILE:HG22	2.10	0.52
3:B:429:PHE:C	3:B:431:TYR:H	2.18	0.52
3:B:843:GLN:HA	3:B:846:ILE:HD13	1.91	0.52
5:D:156:ASP:HB2	5:D:159:THR:HG23	1.91	0.52
6:E:205:SER:O	6:E:206:GLY:C	2.52	0.52
8:G:35:GLU:OE2	8:G:48:VAL:HG23	2.09	0.52
13:L:27:LEU:HD13	13:L:37:LYS:HE2	1.92	0.52
2:A:710:LEU:H	2:A:710:LEU:CD1	2.19	0.52
2:A:857:ARG:NH1	7:F:139:PRO:HB2	2.25	0.52
3:B:235:SER:OG	3:B:236:HIS:CD2	2.62	0.52
3:B:349:ILE:HD12	3:B:349:ILE:N	2.25	0.52
3:B:466:TRP:O	3:B:467:GLY:C	2.52	0.52
3:B:582:VAL:CG2	3:B:626:ILE:HB	2.36	0.52
3:B:840:ILE:HG22	3:B:841:MET:N	2.25	0.52
3:B:969:ARG:NH1	4:C:61:GLU:OE1	2.43	0.52
3:B:1051:THR:CG2	3:B:1052:VAL:N	2.72	0.52
3:B:1183:LYS:O	3:B:1183:LYS:HE3	2.09	0.52
4:C:83:SER:C	4:C:85:ASP:H	2.18	0.52
4:C:244:VAL:O	4:C:248:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:95:SER:C	8:G:97:HIS:H	2.17	0.52
2:A:69:THR:O	2:A:71:GLN:N	2.43	0.52
2:A:524:VAL:CG1	2:A:525:GLN:N	2.72	0.52
2:A:1074:GLU:N	2:A:1075:PRO:HD2	2.24	0.52
3:B:309:GLN:HG3	10:I:52:ILE:CD1	2.40	0.52
4:C:191:TYR:HB3	4:C:201:TRP:CD1	2.45	0.52
5:D:118:THR:O	5:D:119:ARG:C	2.53	0.52
8:G:101:VAL:CG1	8:G:102:GLN:N	2.73	0.52
11:J:34:THR:O	11:J:35:ALA:C	2.53	0.52
1:R:20:A:H2'	1:R:21:G:C8	2.45	0.52
2:A:134:ARG:O	2:A:138:ILE:HG12	2.08	0.52
2:A:244:PRO:HG2	2:A:245:PRO:CD	2.38	0.52
2:A:465:TYR:CD2	3:B:976:ILE:HG13	2.44	0.52
2:A:765:VAL:HG23	2:A:802:ASN:O	2.10	0.52
2:A:1237:ILE:HG22	2:A:1238:ILE:N	2.25	0.52
2:A:1345:ARG:HG2	2:A:1372:VAL:CG1	2.39	0.52
3:B:796:LEU:HD12	3:B:797:TYR:N	2.24	0.52
3:B:810:GLU:HB2	3:B:815:ARG:HH22	1.75	0.52
3:B:899:ILE:CD1	3:B:911:ILE:HA	2.40	0.52
5:D:191:ALA:C	5:D:193:THR:H	2.17	0.52
7:F:75:PRO:O	7:F:77:ASP:O	2.27	0.52
2:A:446:ARG:CD	2:A:480:ALA:HB2	2.40	0.52
2:A:829:VAL:O	2:A:831:THR:N	2.38	0.52
2:A:899:VAL:HB	2:A:929:LEU:HD11	1.91	0.52
3:B:843:GLN:O	3:B:844:SER:C	2.51	0.52
4:C:235:VAL:HG13	11:J:13:VAL:HG23	1.91	0.52
5:D:153:ARG:HB3	5:D:154:PHE:CE1	2.45	0.52
2:A:98:LYS:O	2:A:102:VAL:HG23	2.10	0.52
2:A:276:LEU:HD13	2:A:292:ALA:C	2.35	0.52
2:A:532:ARG:O	2:A:533:LYS:C	2.52	0.52
2:A:867:ILE:O	2:A:868:TYR:C	2.51	0.52
2:A:1072:ILE:HD11	2:A:1368:MET:HG2	1.91	0.52
3:B:172:ILE:HG22	3:B:173:MET:N	2.23	0.52
3:B:237:VAL:HG12	3:B:238:ALA:N	2.24	0.52
3:B:615:MET:C	3:B:616:ILE:HD12	2.35	0.52
3:B:842:ASN:HB2	3:B:1008:PRO:O	2.10	0.52
5:D:144:THR:O	5:D:144:THR:HG22	2.10	0.52
7:F:79:ARG:HH21	7:F:146:TRP:HA	1.75	0.52
1:R:15:G:H2'	1:R:16:G:H8	1.75	0.51
2:A:35:ILE:HG12	2:A:56:PRO:HG2	1.91	0.51
2:A:709:THR:HG22	2:A:710:LEU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:982:THR:HG22	2:A:984:LYS:H	1.75	0.51
2:A:1193:LEU:HB2	2:A:1260:LEU:HD11	1.92	0.51
3:B:880:THR:O	3:B:934:LYS:HG3	2.09	0.51
4:C:73:GLN:NE2	4:C:75:MET:N	2.58	0.51
4:C:101:LEU:HD12	4:C:102:GLN:N	2.25	0.51
7:F:127:GLU:O	7:F:129:LYS:HG3	2.09	0.51
8:G:91:VAL:HG23	8:G:143:ILE:HD13	1.91	0.51
2:A:73:GLY:O	2:A:75:ASN:N	2.43	0.51
2:A:339:ASN:HB3	3:B:1117:GLN:NE2	2.23	0.51
3:B:57:TYR:O	3:B:59:LEU:N	2.43	0.51
3:B:112:LEU:HG	3:B:113:TYR:N	2.25	0.51
3:B:824:ILE:HG12	11:J:48:ARG:HH12	1.74	0.51
3:B:839:MET:HE1	3:B:980:PHE:HB2	1.93	0.51
7:F:109:VAL:HG11	7:F:123:LYS:HG2	1.92	0.51
13:L:43:THR:HG22	13:L:43:THR:O	2.10	0.51
2:A:133:LYS:C	2:A:135:PHE:H	2.19	0.51
2:A:939:ASP:OD1	2:A:1023:ARG:NH1	2.43	0.51
2:A:986:ILE:HG22	2:A:987:VAL:N	2.23	0.51
3:B:865:LYS:NZ	3:B:869:SER:HA	2.24	0.51
4:C:27:LEU:O	4:C:30:ALA:HB3	2.10	0.51
5:D:156:ASP:O	5:D:158:GLU:N	2.43	0.51
8:G:15:PRO:HD3	8:G:67:SER:HA	1.91	0.51
12:K:91:CYS:O	12:K:95:ILE:HG12	2.11	0.51
2:A:450:LEU:HD12	2:A:450:LEU:N	2.25	0.51
2:A:997:LEU:HD13	2:A:1018:PHE:HE2	1.76	0.51
2:A:1313:LEU:HD23	2:A:1338:VAL:CG2	2.40	0.51
3:B:936:ASP:OD1	3:B:937:ALA:N	2.43	0.51
3:B:1045:SER:HB3	3:B:1046:PRO:HD2	1.91	0.51
3:B:1068:GLY:O	3:B:1069:PHE:O	2.28	0.51
4:C:167:HIS:HD2	4:C:168:ALA:H	1.58	0.51
5:D:156:ASP:C	5:D:158:GLU:N	2.67	0.51
9:H:47:PHE:CD2	9:H:47:PHE:O	2.63	0.51
11:J:48:ARG:HD2	11:J:48:ARG:C	2.36	0.51
13:L:48:CYS:SG	13:L:49:LYS:N	2.84	0.51
2:A:21:LEU:HD21	2:A:1414:ALA:CA	2.40	0.51
2:A:401:GLY:O	2:A:435:HIS:CD2	2.63	0.51
2:A:1227:ILE:HG22	2:A:1228:TRP:N	2.24	0.51
3:B:383:ASN:O	3:B:387:LEU:HD13	2.09	0.51
3:B:464:GLY:HA3	3:B:479:VAL:O	2.11	0.51
3:B:601:ARG:O	3:B:605:ARG:HG3	2.09	0.51
3:B:661:LEU:C	3:B:663:ALA:N	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:896:ASP:C	3:B:896:ASP:OD1	2.54	0.51
4:C:31:ASN:HA	4:C:34:ARG:HB3	1.91	0.51
8:G:102:GLN:HG3	8:G:106:MET:O	2.10	0.51
2:A:344:ARG:C	2:A:345:VAL:CG1	2.84	0.51
2:A:1149:ALA:CB	10:I:47:GLU:HA	2.41	0.51
2:A:1437:GLY:O	2:A:1439:GLY:N	2.44	0.51
3:B:1183:LYS:N	3:B:1183:LYS:CE	2.74	0.51
4:C:18:VAL:HG23	4:C:240:VAL:CG1	2.40	0.51
5:D:170:THR:CB	5:D:172:LEU:HG	2.40	0.51
8:G:106:MET:CG	8:G:107:LYS:N	2.73	0.51
9:H:62:SER:O	9:H:63:LEU:C	2.53	0.51
2:A:98:LYS:HB3	2:A:234:MET:HE1	1.92	0.51
2:A:196:GLU:CG	2:A:197:PRO:HD2	2.41	0.51
3:B:205:ILE:C	3:B:207:GLY:N	2.69	0.51
3:B:233:PRO:HG2	3:B:234:ILE:HD12	1.92	0.51
3:B:558:LEU:HD22	3:B:596:LEU:HD11	1.93	0.51
3:B:1183:LYS:CE	3:B:1183:LYS:H	2.24	0.51
4:C:241:ASP:CG	4:C:242:GLN:H	2.18	0.51
8:G:9:LEU:HG	8:G:10:ASN:N	2.26	0.51
11:J:2:ILE:HD11	11:J:57:ILE:HD13	1.92	0.51
2:A:42:ASP:O	2:A:44:THR:N	2.44	0.51
2:A:89:PRO:C	2:A:204:THR:HG21	2.36	0.51
2:A:768:GLN:HG2	2:A:816:HIS:CA	2.38	0.51
2:A:996:ASN:HB3	2:A:1050:GLU:OE2	2.09	0.51
3:B:48:LEU:O	3:B:51:PHE:N	2.43	0.51
3:B:305:VAL:O	3:B:305:VAL:HG12	2.10	0.51
3:B:393:LYS:HA	3:B:393:LYS:HE3	1.92	0.51
3:B:635:ARG:NH2	3:B:742:GLU:OE2	2.44	0.51
3:B:798:TYR:HE2	4:C:62:PHE:HZ	1.59	0.51
4:C:16:ASP:C	4:C:17:ASN:ND2	2.63	0.51
6:E:23:VAL:HG13	6:E:28:TYR:HD1	1.76	0.51
7:F:82:THR:HG22	7:F:84:TYR:N	2.17	0.51
9:H:42:ILE:CG2	9:H:43:ASN:N	2.73	0.51
2:A:34:LYS:CD	2:A:34:LYS:N	2.74	0.51
2:A:54:ASN:CB	2:A:247:ARG:HH12	2.19	0.51
2:A:539:THR:C	2:A:540:PHE:CD1	2.89	0.51
2:A:567:LYS:CE	9:H:46:LEU:HB2	2.41	0.51
2:A:757:ASN:O	2:A:761:MET:HG3	2.11	0.51
2:A:1450:LEU:HD11	7:F:108:PHE:CZ	2.45	0.51
3:B:616:ILE:HG13	3:B:697:GLU:HG3	1.91	0.51
4:C:38:ILE:HD11	4:C:176:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:91:HIS:CD2	4:C:91:HIS:O	2.64	0.51
6:E:186:LEU:C	6:E:189:GLY:H	2.18	0.51
2:A:1430:LEU:O	3:B:1197:PRO:HD2	2.10	0.51
3:B:638:PHE:HB2	3:B:741:CYS:O	2.11	0.51
3:B:705:MET:HA	3:B:705:MET:HE3	1.93	0.51
5:D:202:ILE:HG21	5:D:207:LEU:HB2	1.93	0.51
6:E:157:SER:C	6:E:159:ASP:H	2.19	0.51
9:H:143:LEU:O	9:H:144:ILE:HG13	2.11	0.51
13:L:33:GLU:C	13:L:35:SER:H	2.19	0.51
13:L:53:HIS:HB3	13:L:55:ILE:CD1	2.41	0.51
2:A:116:ASP:O	2:A:118:HIS:N	2.44	0.50
2:A:587:HIS:O	2:A:588:LEU:HB2	2.11	0.50
2:A:1027:ALA:HB3	2:A:1030:ARG:HB2	1.93	0.50
3:B:1017:ILE:HB	3:B:1018:PRO:CD	2.39	0.50
4:C:86:CYS:C	4:C:88:CYS:H	2.19	0.50
5:D:51:ASN:O	5:D:52:LEU:O	2.28	0.50
6:E:35:VAL:C	6:E:37:LEU:H	2.18	0.50
8:G:81:PRO:HG3	8:G:106:MET:SD	2.51	0.50
8:G:101:VAL:HG12	8:G:102:GLN:N	2.26	0.50
2:A:567:LYS:CB	9:H:95:TYR:HA	2.40	0.50
2:A:913:LEU:HD12	2:A:913:LEU:C	2.36	0.50
2:A:1436:ILE:O	2:A:1436:ILE:HG22	2.11	0.50
3:B:276:ILE:O	3:B:276:ILE:CG2	2.59	0.50
3:B:292:ILE:N	3:B:293:PRO:HD2	2.26	0.50
4:C:35:ARG:HA	4:C:38:ILE:HG12	1.93	0.50
4:C:36:VAL:HG21	4:C:251:LEU:HB2	1.92	0.50
12:K:6:ARG:O	12:K:9:LEU:HG	2.11	0.50
2:A:346:ASP:CG	3:B:1108:ARG:HA	2.37	0.50
2:A:437:MET:O	2:A:438:ASP:C	2.54	0.50
2:A:524:VAL:CG1	2:A:525:GLN:H	2.17	0.50
2:A:618:GLU:O	2:A:619:LYS:C	2.54	0.50
2:A:907:THR:CG2	2:A:908:LEU:N	2.58	0.50
2:A:1127:ASP:HB3	2:A:1130:GLN:CB	2.42	0.50
3:B:212:LEU:HD23	3:B:480:SER:HB2	1.93	0.50
3:B:957:ASN:O	3:B:959:ASP:N	2.45	0.50
6:E:23:VAL:O	6:E:28:TYR:HB2	2.11	0.50
13:L:53:HIS:O	13:L:55:ILE:HG12	2.11	0.50
2:A:84:ILE:O	2:A:84:ILE:CG2	2.59	0.50
2:A:106:VAL:HG13	2:A:112:LYS:O	2.12	0.50
2:A:244:PRO:CB	2:A:245:PRO:HD3	2.42	0.50
2:A:666:ILE:HD12	2:A:666:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1120:LEU:N	2:A:1120:LEU:CD1	2.73	0.50
3:B:496:ARG:NH1	3:B:539:LEU:HB2	2.26	0.50
3:B:508:LEU:O	3:B:509:ALA:C	2.50	0.50
3:B:1133:MET:O	3:B:1136:ASP:HB2	2.11	0.50
11:J:44:TYR:CD2	11:J:44:TYR:N	2.80	0.50
12:K:48:ALA:O	12:K:51:LEU:N	2.40	0.50
13:L:59:ALA:O	13:L:60:ARG:O	2.29	0.50
2:A:622:VAL:O	2:A:622:VAL:HG13	2.12	0.50
2:A:908:LEU:O	2:A:909:ASP:C	2.54	0.50
3:B:57:TYR:N	3:B:57:TYR:HD1	2.10	0.50
3:B:333:PHE:C	3:B:334:ILE:HG12	2.35	0.50
3:B:1006:ILE:HD13	11:J:44:TYR:HE2	1.77	0.50
4:C:38:ILE:CD1	4:C:176:ILE:HD12	2.41	0.50
4:C:84:ARG:NE	12:K:11:LEU:HD11	2.27	0.50
4:C:133:ILE:HD11	4:C:237:SER:HA	1.93	0.50
5:D:51:ASN:O	5:D:52:LEU:C	2.53	0.50
9:H:15:VAL:HG22	9:H:26:ILE:CG1	2.40	0.50
2:A:332:LYS:HB2	2:A:337:ARG:CZ	2.42	0.50
2:A:337:ARG:HD3	3:B:1132:GLU:OE2	2.11	0.50
2:A:767:GLN:NE2	2:A:774:ARG:HD2	2.26	0.50
2:A:1211:GLN:O	2:A:1212:VAL:C	2.55	0.50
2:A:1409:LEU:HD13	3:B:1207:LEU:CD1	2.41	0.50
3:B:470:LYS:HE2	3:B:471:LYS:H	1.77	0.50
3:B:590:HIS:NE2	3:B:592:ASN:O	2.44	0.50
3:B:955:THR:HG22	3:B:956:THR:O	2.12	0.50
4:C:67:LEU:HD11	4:C:155:LEU:HD12	1.93	0.50
4:C:239:PRO:HB2	4:C:241:ASP:OD1	2.12	0.50
9:H:139:ASN:O	9:H:140:ALA:HB2	2.12	0.50
2:A:70:CYS:O	2:A:71:GLN:C	2.53	0.50
2:A:343:LYS:NZ	3:B:1151:LEU:O	2.30	0.50
3:B:776:GLN:O	3:B:1095:LEU:HB3	2.11	0.50
3:B:800:GLN:HB3	11:J:52:THR:HG22	1.89	0.50
3:B:1015:HIS:C	3:B:1017:ILE:H	2.20	0.50
5:D:5:THR:O	5:D:6:SER:O	2.29	0.50
8:G:136:VAL:O	8:G:136:VAL:HG12	2.10	0.50
2:A:99:ILE:HG12	2:A:234:MET:HE3	1.93	0.50
2:A:236:LEU:N	2:A:236:LEU:HD23	2.26	0.50
2:A:307:ASP:N	2:A:307:ASP:OD2	2.44	0.50
2:A:503:GLN:HE21	7:F:90:ARG:NH2	2.09	0.50
2:A:507:VAL:N	2:A:508:PRO:CD	2.75	0.50
2:A:840:ARG:O	2:A:841:LEU:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:971:PHE:CE2	2:A:1040:GLN:HG2	2.47	0.50
3:B:295:GLY:H	3:B:298:LEU:HD23	1.77	0.50
3:B:648:HIS:CG	3:B:649:LYS:N	2.79	0.50
4:C:175:ALA:HB1	11:J:43:ARG:HH12	1.76	0.50
6:E:78:LEU:HD23	6:E:78:LEU:C	2.36	0.50
7:F:86:THR:HG23	7:F:89:GLU:OE1	2.12	0.50
2:A:356:ASP:HB2	2:A:469:ARG:NH1	2.25	0.50
2:A:868:TYR:CD1	2:A:1064:VAL:HG11	2.47	0.50
2:A:1356:ILE:CG2	2:A:1361:SER:HB2	2.41	0.50
3:B:190:TYR:CE2	11:J:62:ARG:HB3	2.46	0.50
3:B:487:THR:CG2	3:B:488:TYR:N	2.75	0.50
3:B:695:ALA:O	3:B:698:GLU:HB3	2.12	0.50
3:B:841:MET:CG	3:B:846:ILE:HD11	2.41	0.50
4:C:147:LEU:HD12	4:C:151:GLN:O	2.11	0.50
6:E:213:ILE:HG12	6:E:214:CYS:N	2.25	0.50
13:L:60:ARG:HG2	13:L:61:THR:N	2.21	0.50
2:A:26:GLU:O	2:A:27:VAL:C	2.54	0.49
2:A:51:GLY:HA2	2:A:56:PRO:HA	1.94	0.49
2:A:546:VAL:O	2:A:550:LEU:HG	2.12	0.49
3:B:460:ALA:O	3:B:462:ALA:N	2.45	0.49
3:B:508:LEU:HD22	3:B:508:LEU:H	1.76	0.49
3:B:653:VAL:HG22	3:B:689:LEU:HB3	1.94	0.49
4:C:56:THR:HG22	4:C:58:LEU:H	1.76	0.49
4:C:70:ILE:H	4:C:70:ILE:HD12	1.76	0.49
4:C:243:VAL:O	4:C:243:VAL:HG12	2.12	0.49
5:D:134:THR:CG2	5:D:135:GLY:N	2.75	0.49
6:E:16:PHE:CZ	6:E:20:LYS:HE2	2.47	0.49
10:I:16:PRO:HB3	10:I:27:PHE:CD2	2.46	0.49
10:I:50:THR:HG22	10:I:52:ILE:H	1.77	0.49
2:A:1148:ILE:HD11	2:A:1198:ASP:CB	2.41	0.49
2:A:1279:ILE:HG23	2:A:1308:THR:OG1	2.13	0.49
3:B:97:VAL:HG12	3:B:178:ASN:HD21	1.77	0.49
3:B:315:LYS:N	3:B:316:PRO:HD2	2.26	0.49
3:B:459:TYR:C	3:B:459:TYR:CD2	2.90	0.49
3:B:705:MET:N	3:B:710:LEU:HD12	2.19	0.49
4:C:70:ILE:HD12	4:C:70:ILE:N	2.27	0.49
5:D:120:GLU:HA	5:D:123:LEU:HD12	1.94	0.49
5:D:137:ASN:HD22	5:D:138:ASN:N	2.10	0.49
6:E:79:TRP:CD1	6:E:100:ILE:HD11	2.47	0.49
9:H:63:LEU:C	9:H:90:ALA:HB3	2.37	0.49
11:J:21:TYR:HA	11:J:39:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:44:TYR:HD2	11:J:44:TYR:N	2.11	0.49
2:A:1130:GLN:HE21	2:A:1134:ILE:HD11	1.76	0.49
2:A:1330:ASN:OD1	2:A:1330:ASN:C	2.55	0.49
2:A:1364:ASN:O	2:A:1365:TYR:C	2.55	0.49
3:B:234:ILE:HD12	3:B:234:ILE:N	2.27	0.49
3:B:1183:LYS:H	3:B:1183:LYS:HE2	1.78	0.49
4:C:60:ASP:OD2	13:L:60:ARG:NH2	2.45	0.49
4:C:242:GLN:C	4:C:244:VAL:H	2.19	0.49
5:D:52:LEU:C	5:D:54:GLU:H	2.19	0.49
12:K:10:PHE:N	12:K:10:PHE:CD2	2.79	0.49
2:A:1005:GLU:O	2:A:1009:ASN:HB2	2.12	0.49
2:A:1227:ILE:HG22	2:A:1228:TRP:H	1.75	0.49
3:B:34:ILE:O	3:B:37:PHE:N	2.44	0.49
3:B:363:HIS:CD2	3:B:585:VAL:HG22	2.47	0.49
3:B:761:HIS:HB2	3:B:1024:ALA:HB2	1.94	0.49
3:B:821:GLN:HE22	3:B:851:PHE:N	2.11	0.49
6:E:136:ASN:OD1	6:E:137:GLU:N	2.45	0.49
6:E:165:LEU:HD22	6:E:170:LEU:O	2.12	0.49
9:H:76:THR:O	9:H:76:THR:HG22	2.12	0.49
10:I:34:TYR:CD2	10:I:34:TYR:C	2.87	0.49
10:I:50:THR:HG23	10:I:52:ILE:HG12	1.94	0.49
12:K:61:TYR:CD2	12:K:61:TYR:C	2.90	0.49
2:A:96:ILE:H	2:A:96:ILE:HD12	1.76	0.49
2:A:335:ARG:NH1	3:B:1202:LEU:HD13	2.27	0.49
2:A:381:THR:HG23	2:A:383:TYR:H	1.76	0.49
2:A:401:GLY:O	2:A:435:HIS:HD2	1.94	0.49
2:A:1121:GLU:HG3	2:A:1122:PRO:HD2	1.95	0.49
2:A:1444:MET:HG2	8:G:60:ARG:CA	2.39	0.49
3:B:503:GLY:O	3:B:504:ARG:CB	2.59	0.49
3:B:506:GLY:O	3:B:508:LEU:HD22	2.13	0.49
3:B:515:HIS:O	3:B:518:HIS:HB2	2.12	0.49
3:B:684:LEU:HD12	3:B:684:LEU:N	2.13	0.49
3:B:798:TYR:CE2	4:C:62:PHE:CZ	3.00	0.49
3:B:971:THR:OG1	4:C:61:GLU:HG3	2.12	0.49
3:B:1214:PRO:O	3:B:1214:PRO:HG2	2.13	0.49
11:J:5:VAL:O	11:J:6:ARG:O	2.30	0.49
1:R:16:G:C5	1:R:17:5BU:BR	3.20	0.49
2:A:608:ILE:C	2:A:610:GLY:H	2.21	0.49
3:B:180:TYR:HD1	3:B:180:TYR:H	1.59	0.49
3:B:350:GLN:C	3:B:352:ALA:N	2.69	0.49
2:A:1011:GLN:NE2	2:A:1015:VAL:HG21	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:653:VAL:HG22	3:B:689:LEU:HD22	1.93	0.49
4:C:27:LEU:O	4:C:30:ALA:N	2.46	0.49
6:E:65:THR:O	6:E:69:ILE:HG13	2.12	0.49
10:I:25:LEU:HD12	10:I:26:LEU:H	1.76	0.49
2:A:269:ILE:CG1	2:A:299:HIS:HB3	2.42	0.49
2:A:353:ILE:HD13	2:A:487:MET:HE2	1.95	0.49
2:A:399:HIS:O	2:A:401:GLY:N	2.46	0.49
2:A:1304:TRP:O	2:A:1305:VAL:HG23	2.13	0.49
2:A:1315:GLU:C	2:A:1317:MET:N	2.70	0.49
2:A:1327:ILE:HG22	6:E:147:HIS:CE1	2.48	0.49
3:B:185:THR:H	3:B:188:ASP:CB	2.24	0.49
3:B:781:PHE:O	3:B:782:LEU:HG	2.13	0.49
4:C:163:ILE:C	4:C:165:LYS:H	2.21	0.49
6:E:198:ILE:N	6:E:210:SER:O	2.44	0.49
8:G:51:TYR:C	8:G:51:TYR:CD2	2.91	0.49
2:A:289:ILE:C	2:A:291:GLU:N	2.71	0.49
2:A:567:LYS:HD3	9:H:95:TYR:CG	2.48	0.49
2:A:925:LEU:C	2:A:927:VAL:H	2.21	0.49
2:A:1059:HIS:ND1	7:F:86:THR:HA	2.27	0.49
2:A:1094:VAL:HG12	2:A:1095:THR:N	2.26	0.49
3:B:38:PHE:HD1	3:B:811:TYR:CD2	2.31	0.49
4:C:239:PRO:O	4:C:241:ASP:N	2.46	0.49
11:J:23:ASN:O	11:J:25:LEU:N	2.46	0.49
2:A:71:GLN:HG3	2:A:72:GLU:H	1.78	0.49
2:A:705:LYS:HB2	2:A:708:MET:HE3	1.94	0.49
2:A:1197:LEU:HD12	2:A:1209:MET:HE1	1.95	0.49
3:B:363:HIS:O	3:B:364:ILE:CB	2.61	0.49
3:B:990:ILE:HG22	3:B:991:GLY:N	2.28	0.49
5:D:56:ARG:HA	5:D:148:LEU:HD13	1.95	0.49
5:D:69:ALA:HA	5:D:72:ARG:HG3	1.94	0.49
5:D:190:GLU:HG3	8:G:167:TYR:CD2	2.48	0.49
11:J:7:CYS:CA	11:J:49:MET:HE3	2.43	0.49
11:J:14:VAL:O	11:J:14:VAL:CG1	2.61	0.49
13:L:38:LEU:O	13:L:39:SER:HB3	2.13	0.49
2:A:96:ILE:H	2:A:96:ILE:CD1	2.27	0.48
2:A:100:LYS:O	2:A:104:GLU:HG3	2.12	0.48
2:A:768:GLN:NE2	2:A:816:HIS:ND1	2.61	0.48
2:A:1206:ASP:CB	2:A:1274:ARG:NH1	2.76	0.48
2:A:1265:ASN:O	2:A:1267:MET:N	2.46	0.48
2:A:1410:PHE:C	2:A:1412:ALA:H	2.20	0.48
3:B:33:VAL:O	3:B:36:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:203:PHE:N	3:B:203:PHE:CD1	2.81	0.48
3:B:272:THR:O	3:B:273:LEU:HD13	2.12	0.48
4:C:6:PRO:HB3	4:C:25:VAL:HG12	1.95	0.48
5:D:54:GLU:O	5:D:58:VAL:HG23	2.13	0.48
13:L:44:ASP:O	13:L:45:ALA:HB3	2.13	0.48
2:A:40:THR:HG22	2:A:41:MET:CG	2.42	0.48
2:A:117:GLU:CD	2:A:117:GLU:N	2.69	0.48
2:A:376:TYR:OH	2:A:498:ARG:HD2	2.13	0.48
2:A:1118:VAL:HG23	2:A:1306:LEU:HB2	1.95	0.48
3:B:20:ASP:O	3:B:22:SER:N	2.37	0.48
3:B:550:ASP:OD1	3:B:551:PRO:HD2	2.13	0.48
4:C:226:ASP:O	4:C:227:THR:CB	2.60	0.48
4:C:238:ILE:HG22	4:C:243:VAL:HG23	1.94	0.48
13:L:28:LYS:HB2	13:L:39:SER:HA	1.95	0.48
2:A:541:ILE:HG21	2:A:549:MET:HE1	1.92	0.48
2:A:1329:THR:CG2	2:A:1330:ASN:N	2.76	0.48
3:B:129:PHE:CD2	3:B:166:PHE:HA	2.49	0.48
3:B:205:ILE:O	3:B:207:GLY:N	2.46	0.48
3:B:582:VAL:O	3:B:582:VAL:HG12	2.13	0.48
3:B:796:LEU:HD12	3:B:797:TYR:H	1.77	0.48
3:B:1219:ASP:OD1	3:B:1219:ASP:O	2.31	0.48
8:G:1:MET:SD	8:G:79:PHE:CE1	3.06	0.48
9:H:116:TYR:HB2	9:H:123:MET:HB3	1.95	0.48
2:A:475:THR:CG2	2:A:476:SER:N	2.77	0.48
2:A:664:THR:CG2	2:A:665:GLY:N	2.76	0.48
3:B:491:THR:O	3:B:492:LEU:C	2.55	0.48
3:B:507:LYS:HD3	3:B:507:LYS:HA	1.53	0.48
3:B:763:GLN:O	3:B:764:SER:C	2.57	0.48
4:C:10:ILE:HG13	12:K:108:GLU:HB3	1.95	0.48
5:D:185:CYS:HB3	5:D:211:LEU:CD2	2.43	0.48
6:E:28:TYR:CE1	6:E:78:LEU:HD13	2.49	0.48
6:E:117:THR:HG22	6:E:119:SER:H	1.77	0.48
6:E:180:ARG:HH21	6:E:192:ARG:HB2	1.78	0.48
8:G:26:LEU:HD12	8:G:56:ILE:HG21	1.93	0.48
9:H:10:PHE:N	9:H:10:PHE:CD1	2.81	0.48
12:K:57:LEU:N	12:K:76:GLN:O	2.38	0.48
2:A:500:GLU:OE1	3:B:1143:ALA:C	2.56	0.48
2:A:1384:VAL:O	2:A:1384:VAL:HG12	2.13	0.48
3:B:33:VAL:HG21	3:B:638:PHE:CZ	2.48	0.48
3:B:405:ARG:HA	3:B:631:GLY:O	2.13	0.48
3:B:563:MET:HE2	3:B:588:GLY:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:593:PRO:O	3:B:594:ALA:C	2.55	0.48
3:B:648:HIS:CG	3:B:649:LYS:H	2.32	0.48
3:B:1177:HIS:HB2	3:B:1179:GLN:HE21	1.77	0.48
4:C:35:ARG:NH1	12:K:41:THR:H	2.12	0.48
4:C:53:THR:O	4:C:153:LEU:HA	2.14	0.48
5:D:40:HIS:HB3	8:G:73:LYS:HZ2	1.65	0.48
5:D:51:ASN:OD1	5:D:52:LEU:O	2.32	0.48
5:D:176:GLU:C	5:D:178:ALA:H	2.21	0.48
6:E:55:ARG:NH1	6:E:113:GLN:NE2	2.61	0.48
6:E:179:GLN:HB2	6:E:182:ASP:HB2	1.96	0.48
10:I:100:PHE:N	10:I:100:PHE:CD1	2.81	0.48
2:A:17:VAL:HA	3:B:1215:ARG:O	2.13	0.48
2:A:264:PHE:O	2:A:265:LYS:C	2.56	0.48
2:A:901:LEU:CG	2:A:926:GLN:HE21	2.17	0.48
2:A:966:ASN:O	2:A:967:ALA:C	2.57	0.48
3:B:515:HIS:HB3	3:B:518:HIS:CD2	2.48	0.48
3:B:1180:PHE:O	3:B:1181:GLU:HB2	2.13	0.48
4:C:27:LEU:O	4:C:28:ALA:C	2.57	0.48
4:C:66:ARG:NH2	11:J:5:VAL:HG23	2.29	0.48
4:C:101:LEU:HD12	4:C:101:LEU:C	2.38	0.48
4:C:179:GLU:HG2	4:C:180:TYR:H	1.78	0.48
6:E:120:ALA:O	6:E:122:LYS:N	2.46	0.48
8:G:31:LEU:CD2	8:G:48:VAL:HG21	2.44	0.48
8:G:140:LYS:O	8:G:141:SER:C	2.56	0.48
13:L:58:LYS:O	13:L:59:ALA:O	2.32	0.48
2:A:120:GLU:C	2:A:122:MET:N	2.69	0.48
2:A:450:LEU:HD12	2:A:450:LEU:H	1.78	0.48
2:A:831:THR:HG23	2:A:832:ALA:N	2.28	0.48
2:A:1116:LEU:HG	2:A:1308:THR:CG2	2.32	0.48
2:A:1341:ILE:HG23	2:A:1342:GLU:N	2.27	0.48
3:B:642:ASP:CA	3:B:649:LYS:HA	2.35	0.48
3:B:863:GLU:HG3	3:B:962:LYS:HB2	1.96	0.48
4:C:47:ASP:CA	13:L:69:ALA:HB3	2.37	0.48
5:D:40:HIS:CG	5:D:41:GLN:N	2.82	0.48
9:H:128:ASN:OD1	9:H:128:ASN:O	2.31	0.48
10:I:100:PHE:N	10:I:100:PHE:HD1	2.11	0.48
11:J:2:ILE:HD11	11:J:57:ILE:CD1	2.44	0.48
2:A:591:PHE:HA	2:A:595:THR:HG21	1.95	0.48
2:A:664:THR:HG22	2:A:665:GLY:H	1.75	0.48
2:A:831:THR:CG2	2:A:832:ALA:N	2.76	0.48
2:A:858:ASN:ND2	2:A:859:SER:N	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:929:LEU:HD23	2:A:983:ILE:CG2	2.44	0.48
2:A:1021:LEU:O	2:A:1024:SER:HB3	2.14	0.48
2:A:1127:ASP:HB3	2:A:1130:GLN:HB2	1.96	0.48
2:A:1242:VAL:CG1	2:A:1243:VAL:H	2.18	0.48
2:A:1336:MET:HE3	2:A:1381:LEU:CG	2.38	0.48
3:B:980:PHE:CE2	3:B:1094:ARG:HG3	2.49	0.48
3:B:1060:ARG:NE	4:C:202:PRO:HG3	2.29	0.48
3:B:1197:PRO:O	3:B:1200:ALA:N	2.47	0.48
11:J:64:ASN:HB3	11:J:65:PRO:HD2	1.91	0.48
2:A:543:LEU:O	2:A:545:GLN:N	2.46	0.48
2:A:566:ILE:HD13	2:A:566:ILE:N	2.29	0.48
2:A:629:LEU:C	2:A:629:LEU:CD2	2.87	0.48
2:A:774:ARG:HB2	2:A:797:LYS:O	2.13	0.48
2:A:1128:GLN:HG3	2:A:1129:GLU:N	2.29	0.48
2:A:1336:MET:CE	2:A:1381:LEU:HG	2.41	0.48
2:A:1450:LEU:O	2:A:1450:LEU:CG	2.61	0.48
3:B:290:GLY:C	3:B:291:ILE:HD12	2.39	0.48
3:B:327:ARG:O	3:B:330:ALA:HB3	2.14	0.48
3:B:615:MET:HB2	3:B:615:MET:HE3	1.84	0.48
3:B:731:VAL:HG12	3:B:732:SER:N	2.29	0.48
4:C:183:TRP:CZ2	4:C:207:CYS:HB3	2.49	0.48
6:E:198:ILE:HD12	6:E:198:ILE:H	1.78	0.48
9:H:15:VAL:HG22	9:H:26:ILE:HG12	1.96	0.48
9:H:123:MET:HE1	9:H:142:LEU:HD11	1.96	0.48
11:J:23:ASN:C	11:J:25:LEU:N	2.65	0.48
12:K:87:LEU:O	12:K:88:LYS:C	2.56	0.48
2:A:26:GLU:O	2:A:29:ALA:N	2.46	0.48
2:A:135:PHE:C	2:A:137:ALA:N	2.70	0.48
2:A:269:ILE:CD1	2:A:300:VAL:HA	2.43	0.48
2:A:313:GLN:O	2:A:314:ALA:HB3	2.14	0.48
2:A:583:PRO:HG2	2:A:586:ILE:CD1	2.43	0.48
3:B:476:ARG:HA	3:B:476:ARG:NH1	2.19	0.48
3:B:806:THR:CG2	3:B:808:ALA:HB3	2.44	0.48
3:B:1038:SER:C	3:B:1040:ASN:H	2.22	0.48
4:C:39:ALA:HA	4:C:164:ALA:HB3	1.95	0.48
8:G:59:GLY:HA3	8:G:70:PHE:CE2	2.49	0.48
9:H:89:LEU:C	9:H:91:ASP:N	2.69	0.48
11:J:47:ARG:C	11:J:49:MET:N	2.72	0.48
2:A:166:GLY:O	2:A:167:CYS:CB	2.62	0.47
2:A:276:LEU:HD21	2:A:293:GLU:HG3	1.95	0.47
2:A:372:LYS:HA	2:A:435:HIS:ND1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:939:ASP:O	2:A:940:ARG:C	2.54	0.47
2:A:1002:GLY:HA3	2:A:1007:ILE:HG21	1.96	0.47
2:A:1265:ASN:C	2:A:1267:MET:N	2.70	0.47
3:B:773:MET:C	3:B:775:LYS:N	2.70	0.47
3:B:1183:LYS:HE3	3:B:1183:LYS:N	2.29	0.47
2:A:14:VAL:HG21	3:B:1216:LEU:HD12	1.96	0.47
2:A:249:SER:O	2:A:250:ILE:CG1	2.52	0.47
2:A:1226:VAL:C	2:A:1227:ILE:HG13	2.39	0.47
2:A:1226:VAL:HG12	2:A:1227:ILE:N	2.29	0.47
3:B:272:THR:N	3:B:273:LEU:HD13	2.28	0.47
3:B:595:ARG:O	3:B:596:LEU:C	2.57	0.47
3:B:878:GLN:OE1	3:B:878:GLN:O	2.33	0.47
3:B:955:THR:HG23	13:L:54:ARG:O	2.13	0.47
3:B:955:THR:OG1	13:L:55:ILE:HA	2.14	0.47
3:B:977:GLY:HA3	3:B:1099:VAL:CG2	2.43	0.47
3:B:1001:PHE:CD2	4:C:34:ARG:NH2	2.82	0.47
3:B:1208:MET:C	3:B:1210:MET:H	2.22	0.47
4:C:7:GLN:HG2	12:K:104:ASN:HD22	1.78	0.47
4:C:73:GLN:N	4:C:131:HIS:O	2.47	0.47
4:C:79:GLN:O	4:C:127:ARG:NH1	2.47	0.47
4:C:206:ASN:OD1	4:C:229:TYR:CD2	2.67	0.47
4:C:242:GLN:C	4:C:244:VAL:N	2.72	0.47
5:D:185:CYS:CB	5:D:211:LEU:HD22	2.44	0.47
9:H:117:SER:HA	9:H:121:LEU:O	2.14	0.47
2:A:62:ASP:HB3	2:A:64:ASN:ND2	2.29	0.47
2:A:925:LEU:C	2:A:927:VAL:N	2.72	0.47
2:A:1423:GLY:HA3	2:A:1426:GLU:HG2	1.95	0.47
3:B:27:ALA:C	3:B:29:ASP:N	2.73	0.47
3:B:285:ILE:O	3:B:289:LEU:HB2	2.14	0.47
3:B:428:ILE:O	3:B:432:MET:HE2	2.14	0.47
3:B:446:LEU:O	3:B:447:ALA:CB	2.62	0.47
4:C:114:TYR:OH	11:J:19:GLU:OE2	2.32	0.47
6:E:186:LEU:C	6:E:188:LEU:N	2.71	0.47
10:I:68:LEU:HB3	10:I:84:VAL:CG2	2.43	0.47
2:A:61:ILE:O	2:A:63:ARG:N	2.48	0.47
2:A:347:PHE:HE2	2:A:375:THR:HG22	1.78	0.47
2:A:364:VAL:O	2:A:364:VAL:HG13	2.14	0.47
2:A:472:LEU:O	2:A:475:THR:HG22	2.15	0.47
2:A:527:THR:CG2	2:A:650:GLN:HA	2.45	0.47
2:A:774:ARG:NH2	2:A:797:LYS:HG3	2.30	0.47
2:A:960:ILE:O	2:A:961:ARG:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1143:LEU:HB2	2:A:1271:ILE:CG2	2.44	0.47
2:A:1385:THR:O	2:A:1387:HIS:N	2.48	0.47
3:B:205:ILE:N	3:B:205:ILE:CD1	2.71	0.47
3:B:555:ILE:C	3:B:557:PHE:N	2.65	0.47
3:B:763:GLN:HG2	3:B:765:PRO:HD2	1.96	0.47
3:B:831:SER:HB3	3:B:994:TYR:OH	2.14	0.47
3:B:1072:MET:CE	3:B:1087:PHE:HD1	2.27	0.47
4:C:65:HIS:O	4:C:69:LEU:HD13	2.13	0.47
5:D:185:CYS:SG	5:D:191:ALA:HB2	2.55	0.47
11:J:7:CYS:HA	11:J:49:MET:HE3	1.97	0.47
12:K:50:LEU:HD13	12:K:75:ILE:HD11	1.96	0.47
12:K:55:LYS:HB2	12:K:81:TYR:CE1	2.49	0.47
12:K:65:HIS:CD2	12:K:67:PHE:H	2.26	0.47
1:R:30:A:H2'	1:R:31:U:O4'	2.15	0.47
2:A:15:LYS:HB3	3:B:1220:ARG:NH2	2.21	0.47
2:A:89:PRO:HB2	2:A:204:THR:CG2	2.44	0.47
2:A:567:LYS:HG3	2:A:568:PRO:CD	2.35	0.47
2:A:600:PRO:C	2:A:602:ASP:H	2.22	0.47
2:A:823:GLY:C	2:A:825:ILE:N	2.71	0.47
2:A:1403:GLU:O	2:A:1404:GLU:HG3	2.14	0.47
3:B:609:ILE:O	3:B:610:ASN:C	2.56	0.47
3:B:821:GLN:HE22	3:B:851:PHE:H	1.62	0.47
3:B:1007:VAL:CG2	3:B:1008:PRO:HD2	2.35	0.47
3:B:1050:ILE:HG22	3:B:1051:THR:N	2.28	0.47
8:G:106:MET:HG2	8:G:107:LYS:N	2.28	0.47
12:K:42:LEU:HD23	12:K:46:ILE:HG13	1.96	0.47
13:L:38:LEU:HD12	13:L:38:LEU:C	2.40	0.47
1:R:20:A:H2'	1:R:21:G:H8	1.79	0.47
2:A:19:PHE:HB3	2:A:1413:GLY:HA2	1.95	0.47
2:A:96:ILE:HD12	2:A:96:ILE:N	2.28	0.47
2:A:184:SER:HB3	2:A:199:LEU:HD23	1.96	0.47
2:A:382:PRO:HD3	2:A:428:TYR:CD2	2.49	0.47
2:A:427:GLN:HB2	2:A:430:TRP:CE2	2.50	0.47
2:A:698:GLN:HA	10:I:97:MET:O	2.15	0.47
3:B:410:GLY:O	3:B:413:LEU:N	2.47	0.47
3:B:644:GLU:HG2	3:B:654:ARG:NH2	2.26	0.47
3:B:1110:PRO:HG2	3:B:1119:VAL:CG2	2.45	0.47
4:C:189:THR:CG2	4:C:190:ASP:H	2.27	0.47
4:C:255:VAL:HG21	12:K:94:ILE:HG21	1.97	0.47
5:D:195:ILE:O	5:D:198:LEU:HG	2.14	0.47
6:E:3:GLN:HG3	6:E:4:GLU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:22:MET:O	8:G:23:LYS:C	2.57	0.47
8:G:115:MET:HB2	8:G:116:PRO:CD	2.36	0.47
9:H:81:PRO:CB	9:H:82:PRO:CD	2.91	0.47
13:L:60:ARG:CG	13:L:61:THR:H	2.23	0.47
2:A:95:PHE:O	2:A:96:ILE:C	2.56	0.47
2:A:501:LEU:HA	2:A:505:CYS:HB2	1.96	0.47
2:A:516:SER:O	2:A:518:LYS:N	2.47	0.47
2:A:578:LEU:HD23	2:A:612:ILE:CD1	2.44	0.47
2:A:608:ILE:C	2:A:610:GLY:N	2.71	0.47
2:A:715:GLU:O	2:A:716:ASP:C	2.57	0.47
2:A:728:LYS:O	2:A:729:ALA:C	2.56	0.47
2:A:897:TYR:HB3	2:A:936:LEU:HD12	1.95	0.47
2:A:1057:VAL:CG1	2:A:1058:VAL:H	2.28	0.47
2:A:1189:SER:OG	2:A:1190:PRO:HD2	2.15	0.47
2:A:1449:SER:C	2:A:1451:VAL:H	2.22	0.47
3:B:184:ALA:HB1	3:B:188:ASP:HB3	1.97	0.47
3:B:386:LEU:O	3:B:389:ALA:N	2.48	0.47
3:B:487:THR:HG22	3:B:488:TYR:N	2.29	0.47
3:B:529:GLU:O	3:B:531:GLN:HG2	2.15	0.47
3:B:579:ARG:CB	3:B:586:TRP:HE1	2.22	0.47
3:B:825:VAL:HG13	3:B:826:ALA:N	2.30	0.47
3:B:847:ASP:C	3:B:849:GLY:N	2.72	0.47
3:B:896:ASP:OD1	3:B:898:LEU:HG	2.14	0.47
3:B:1135:ARG:O	3:B:1136:ASP:C	2.56	0.47
5:D:64:VAL:C	5:D:66:ARG:N	2.72	0.47
6:E:60:PHE:C	6:E:60:PHE:CD2	2.92	0.47
6:E:88:VAL:CG1	6:E:89:GLY:N	2.78	0.47
7:F:109:VAL:HG23	7:F:124:GLU:HG2	1.97	0.47
9:H:33:GLN:C	9:H:35:GLN:H	2.23	0.47
9:H:93:TYR:CD1	9:H:93:TYR:N	2.82	0.47
12:K:40:HIS:ND1	12:K:61:TYR:OH	2.29	0.47
2:A:456:MET:HE3	2:A:478:TYR:CZ	2.50	0.47
2:A:595:THR:O	2:A:596:THR:HG23	2.15	0.47
2:A:1434:ALA:O	2:A:1436:ILE:N	2.44	0.47
3:B:48:LEU:O	3:B:49:ASP:C	2.58	0.47
3:B:225:VAL:HA	3:B:237:VAL:O	2.14	0.47
3:B:244:LEU:HD21	3:B:366:GLN:NE2	2.29	0.47
3:B:794:ASN:C	3:B:795:ILE:HD12	2.40	0.47
3:B:842:ASN:ND2	3:B:845:SER:H	2.13	0.47
3:B:882:THR:HG21	3:B:884:ARG:HB2	1.96	0.47
3:B:1171:VAL:C	3:B:1172:ILE:HD12	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:208:GLU:C	4:C:210:GLU:H	2.23	0.47
8:G:13:LEU:HD21	8:G:17:PHE:CB	2.27	0.47
8:G:27:LYS:O	8:G:30:LEU:HB3	2.15	0.47
2:A:1152:ILE:HG23	2:A:1192:LEU:O	2.14	0.47
2:A:1445:ILE:HD13	8:G:18:PHE:CE2	2.50	0.47
3:B:271:ALA:HB1	3:B:273:LEU:CD1	2.34	0.47
3:B:357:GLN:HA	3:B:374:LYS:HZ3	1.80	0.47
3:B:526:GLU:HG2	3:B:526:GLU:O	2.14	0.47
3:B:635:ARG:HH11	3:B:635:ARG:HG3	1.80	0.47
3:B:658:ILE:O	3:B:661:LEU:HB2	2.14	0.47
3:B:750:GLY:O	3:B:751:VAL:C	2.58	0.47
3:B:1060:ARG:C	3:B:1062:HIS:H	2.23	0.47
3:B:1156:ASP:HB3	3:B:1198:TYR:N	2.30	0.47
4:C:112:ASN:HB2	4:C:114:TYR:HE1	1.80	0.47
4:C:144:ILE:HG22	4:C:145:CYS:HB3	1.95	0.47
4:C:254:LYS:C	4:C:256:ALA:N	2.73	0.47
5:D:4:SER:O	5:D:5:THR:CB	2.62	0.47
9:H:24:CYS:HB2	9:H:44:VAL:HG21	1.97	0.47
12:K:21:ILE:HG23	12:K:31:VAL:HG11	1.97	0.47
2:A:122:MET:O	2:A:123:ARG:C	2.58	0.47
2:A:476:SER:N	2:A:477:PRO:CD	2.78	0.47
2:A:997:LEU:HD13	2:A:1018:PHE:CE2	2.50	0.47
2:A:1073:GLY:O	2:A:1076:ALA:HB3	2.14	0.47
3:B:63:ILE:HD13	3:B:63:ILE:O	2.15	0.47
3:B:361:LEU:HD21	3:B:377:PHE:CD2	2.50	0.47
3:B:763:GLN:C	3:B:765:PRO:HD2	2.40	0.47
3:B:912:ILE:O	3:B:938:SER:HB3	2.16	0.47
4:C:70:ILE:HG13	4:C:142:VAL:HG11	1.96	0.47
4:C:213:PRO:O	4:C:214:ASN:HB2	2.14	0.47
8:G:53:ASN:N	8:G:53:ASN:ND2	2.62	0.47
9:H:143:LEU:HD12	9:H:143:LEU:N	2.30	0.47
11:J:14:VAL:O	11:J:14:VAL:HG12	2.13	0.47
2:A:474:VAL:O	2:A:474:VAL:HG22	2.15	0.46
2:A:730:GLY:O	2:A:732:LEU:N	2.48	0.46
2:A:853:ASP:O	2:A:854:ASN:HB2	2.13	0.46
2:A:974:ASP:C	2:A:976:THR:H	2.23	0.46
2:A:1004:ASN:C	2:A:1004:ASN:OD1	2.58	0.46
2:A:1214:GLU:C	2:A:1218:GLN:HE21	2.23	0.46
3:B:47:GLN:O	3:B:173:MET:HE1	2.16	0.46
3:B:185:THR:O	3:B:188:ASP:N	2.48	0.46
3:B:203:PHE:HB2	3:B:205:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:460:ALA:O	3:B:461:LEU:C	2.59	0.46
3:B:501:PRO:C	3:B:502:ILE:CG1	2.87	0.46
3:B:635:ARG:HG3	3:B:635:ARG:NH1	2.30	0.46
3:B:773:MET:CE	3:B:985:GLY:HA2	2.44	0.46
3:B:992:ILE:HG13	3:B:993:THR:N	2.29	0.46
4:C:234:SER:OG	4:C:235:VAL:N	2.47	0.46
6:E:23:VAL:HG13	6:E:78:LEU:HD13	1.97	0.46
9:H:99:GLY:N	9:H:118:PHE:CD2	2.84	0.46
10:I:71:SER:OG	10:I:83:ASN:HB2	2.15	0.46
1:R:7:C:H41	1:R:13:G:N2	2.12	0.46
2:A:42:ASP:HB3	2:A:45:GLN:H	1.81	0.46
2:A:730:GLY:C	2:A:732:LEU:N	2.73	0.46
2:A:808:LEU:CD2	2:A:813:PHE:HA	2.45	0.46
2:A:852:TYR:CZ	7:F:136:ARG:HG2	2.51	0.46
2:A:867:ILE:O	2:A:870:GLU:N	2.42	0.46
2:A:1017:LEU:HB2	6:E:206:GLY:N	2.15	0.46
2:A:1041:ALA:O	2:A:1044:TRP:HB3	2.16	0.46
2:A:1161:THR:C	2:A:1163:ILE:H	2.22	0.46
2:A:1329:THR:HG22	2:A:1330:ASN:N	2.29	0.46
3:B:263:GLY:O	3:B:264:SER:C	2.58	0.46
3:B:593:PRO:O	3:B:595:ARG:N	2.48	0.46
3:B:653:VAL:HG22	3:B:689:LEU:HD13	1.97	0.46
3:B:878:GLN:O	3:B:879:ARG:C	2.57	0.46
3:B:899:ILE:HG22	3:B:900:ALA:N	2.30	0.46
3:B:999:MET:HB3	3:B:1007:VAL:HG21	1.96	0.46
4:C:235:VAL:HG13	11:J:13:VAL:CG2	2.45	0.46
6:E:20:LYS:O	6:E:23:VAL:N	2.47	0.46
11:J:8:PHE:N	11:J:49:MET:HE3	2.30	0.46
12:K:85:ASP:O	12:K:88:LYS:HB2	2.14	0.46
2:A:79:GLY:HA3	2:A:243:PRO:CG	2.43	0.46
2:A:196:GLU:HG2	2:A:197:PRO:CD	2.44	0.46
2:A:898:ARG:HD3	2:A:933:TYR:CD1	2.50	0.46
4:C:11:ARG:O	4:C:12:GLU:C	2.58	0.46
4:C:77:ILE:C	4:C:79:GLN:H	2.23	0.46
4:C:112:ASN:CB	4:C:114:TYR:CE1	2.98	0.46
4:C:238:ILE:HG22	4:C:243:VAL:CG2	2.45	0.46
6:E:124:VAL:HG13	6:E:132:ILE:CD1	2.41	0.46
8:G:119:LEU:HD12	8:G:131:GLN:C	2.41	0.46
9:H:11:GLN:HA	9:H:53:ASP:O	2.15	0.46
11:J:6:ARG:HG2	11:J:13:VAL:HA	1.97	0.46
2:A:784:LEU:C	2:A:786:HIS:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1115:SER:OG	2:A:1116:LEU:N	2.49	0.46
3:B:114:PRO:O	3:B:116:GLU:N	2.47	0.46
3:B:519:TRP:C	3:B:519:TRP:CD1	2.93	0.46
3:B:903:VAL:HG12	3:B:904:ARG:N	2.30	0.46
4:C:3:GLU:HG2	4:C:4:GLU:N	2.30	0.46
9:H:43:ASN:C	9:H:45:GLU:H	2.23	0.46
12:K:33:ILE:HD12	12:K:33:ILE:N	2.30	0.46
2:A:260:ASP:O	2:A:261:ASP:C	2.57	0.46
2:A:532:ARG:NH1	2:A:532:ARG:HG2	2.30	0.46
2:A:913:LEU:HD11	2:A:915:SER:OG	2.15	0.46
2:A:1151:GLU:HA	10:I:44:TYR:O	2.16	0.46
3:B:95:ILE:HA	3:B:129:PHE:O	2.14	0.46
3:B:179:CYS:SG	3:B:181:LEU:HB2	2.55	0.46
3:B:258:LEU:C	3:B:258:LEU:HD12	2.40	0.46
3:B:331:LEU:HD12	3:B:331:LEU:N	2.31	0.46
3:B:496:ARG:HH12	3:B:539:LEU:HB2	1.79	0.46
3:B:1051:THR:HG22	3:B:1053:GLU:H	1.81	0.46
4:C:44:LEU:HD23	4:C:44:LEU:C	2.41	0.46
4:C:148:ARG:O	4:C:149:LYS:C	2.59	0.46
8:G:166:ASP:C	8:G:168:LEU:H	2.24	0.46
2:A:23:SER:O	2:A:24:PRO:C	2.58	0.46
2:A:49:LYS:CD	2:A:55:ASP:HB3	2.44	0.46
2:A:244:PRO:HG2	2:A:245:PRO:HD2	1.98	0.46
2:A:381:THR:HG23	2:A:383:TYR:N	2.31	0.46
2:A:537:ARG:O	2:A:540:PHE:CE1	2.69	0.46
2:A:871:ASP:OD2	2:A:873:MET:HB2	2.16	0.46
2:A:898:ARG:HB2	2:A:933:TYR:HE1	1.77	0.46
2:A:1036:ARG:HG2	2:A:1036:ARG:HH11	1.80	0.46
2:A:1205:LYS:O	2:A:1206:ASP:C	2.59	0.46
3:B:466:TRP:CD1	3:B:468:GLU:OE2	2.69	0.46
3:B:489:SER:OG	3:B:490:SER:N	2.49	0.46
3:B:654:ARG:O	3:B:656:GLY:N	2.49	0.46
3:B:729:ILE:O	3:B:729:ILE:HG22	2.15	0.46
3:B:816:GLU:O	3:B:817:LEU:HD23	2.16	0.46
3:B:1163:CYS:SG	3:B:1165:ILE:N	2.74	0.46
5:D:144:THR:O	5:D:144:THR:CG2	2.64	0.46
9:H:43:ASN:OD1	9:H:46:LEU:HG	2.16	0.46
10:I:54:GLU:OE2	10:I:118:ARG:NH1	2.48	0.46
1:R:5:C:H4'	1:R:6:A:OP1	2.14	0.46
2:A:174:ILE:HG23	2:A:182:VAL:O	2.16	0.46
2:A:219:PHE:CE2	2:A:231:PRO:HD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:809:THR:H	2:A:812:GLU:HB2	1.81	0.46
3:B:822:ASN:HD22	11:J:52:THR:HG21	1.80	0.46
3:B:911:ILE:HD11	3:B:941:LEU:HD13	1.98	0.46
4:C:46:ILE:HD12	4:C:67:LEU:HB3	1.97	0.46
4:C:66:ARG:O	4:C:67:LEU:C	2.58	0.46
6:E:55:ARG:H	6:E:84:ASP:CG	2.22	0.46
6:E:78:LEU:HB2	6:E:107:THR:HB	1.98	0.46
6:E:143:ASN:OD1	6:E:187:TYR:CE1	2.69	0.46
7:F:114:GLU:OE2	7:F:119:ARG:HG2	2.16	0.46
8:G:111:THR:HB	8:G:114:LEU:HB2	1.96	0.46
2:A:90:VAL:HG12	2:A:297:GLN:HE22	1.77	0.46
2:A:385:ILE:HG22	2:A:386:ASP:N	2.31	0.46
2:A:463:ILE:HD12	2:A:464:PRO:O	2.16	0.46
2:A:608:ILE:HD12	2:A:613:ILE:HG13	1.98	0.46
2:A:767:GLN:HE21	2:A:774:ARG:HD2	1.81	0.46
2:A:836:TYR:CZ	2:A:840:ARG:HD2	2.51	0.46
2:A:860:LEU:HB3	2:A:862:ASN:OD1	2.16	0.46
2:A:1409:LEU:CD1	3:B:1207:LEU:HD11	2.44	0.46
3:B:94:LYS:O	3:B:130:VAL:HA	2.15	0.46
3:B:95:ILE:HD13	3:B:95:ILE:C	2.41	0.46
3:B:639:ILE:HD13	3:B:690:VAL:HA	1.97	0.46
4:C:43:THR:CG2	4:C:44:LEU:H	2.29	0.46
4:C:58:LEU:HD22	4:C:58:LEU:N	2.31	0.46
4:C:112:ASN:HB3	4:C:114:TYR:CE1	2.51	0.46
5:D:215:SER:HA	5:D:218:GLU:HB2	1.98	0.46
6:E:81:GLU:C	6:E:82:PHE:HD1	2.24	0.46
6:E:102:GLU:C	6:E:104:ASN:N	2.73	0.46
6:E:153:HIS:ND1	6:E:153:HIS:N	2.64	0.46
2:A:1155:ASP:OD2	2:A:1162:VAL:N	2.39	0.46
2:A:1261:LYS:C	2:A:1264:GLU:H	2.23	0.46
2:A:1273:LEU:HD12	2:A:1273:LEU:N	2.31	0.46
2:A:1327:ILE:HG22	6:E:147:HIS:HE1	1.81	0.46
2:A:1359:ASP:C	2:A:1361:SER:N	2.74	0.46
3:B:1208:MET:C	3:B:1210:MET:N	2.74	0.46
6:E:100:ILE:HG23	6:E:105:PHE:HB2	1.98	0.46
2:A:23:SER:HA	2:A:233:TRP:CD1	2.51	0.46
2:A:399:HIS:CB	2:A:400:PRO:CD	2.94	0.46
2:A:626:ASN:O	2:A:631:HIS:HD2	1.98	0.46
2:A:897:TYR:HB3	2:A:936:LEU:CD1	2.46	0.46
2:A:1021:LEU:O	2:A:1021:LEU:HD12	2.16	0.46
3:B:240:ILE:CG2	3:B:240:ILE:O	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:275:TYR:C	3:B:276:ILE:HD12	2.41	0.46
3:B:644:GLU:CG	3:B:654:ARG:HH22	2.28	0.46
3:B:680:THR:O	3:B:683:SER:OG	2.32	0.46
3:B:980:PHE:HD2	3:B:1094:ARG:HA	1.81	0.46
3:B:1031:LEU:HD23	3:B:1044:ALA:HB2	1.98	0.46
4:C:104:PHE:HD2	4:C:105:GLY:N	2.13	0.46
11:J:24:LEU:N	11:J:24:LEU:HD23	2.30	0.46
1:R:9:G:H5'	1:R:10:A:OP1	2.14	0.45
2:A:350:ARG:O	2:A:351:THR:HG22	2.16	0.45
2:A:417:TYR:O	2:A:418:SER:C	2.59	0.45
2:A:1333:ILE:O	2:A:1337:GLU:HG3	2.16	0.45
3:B:203:PHE:HB3	3:B:205:ILE:HD11	1.97	0.45
3:B:296:GLU:O	3:B:299:GLU:HB2	2.16	0.45
3:B:400:HIS:O	3:B:401:PHE:C	2.58	0.45
3:B:542:MET:HB3	3:B:636:PRO:HD2	1.98	0.45
3:B:563:MET:HE2	3:B:588:GLY:C	2.41	0.45
3:B:806:THR:HA	3:B:1045:SER:OG	2.16	0.45
5:D:123:LEU:HD23	5:D:149:THR:HG21	1.98	0.45
9:H:42:ILE:CG2	9:H:95:TYR:HE1	2.19	0.45
10:I:99:LEU:O	10:I:111:THR:HG23	2.16	0.45
2:A:57:ARG:O	2:A:68:GLN:NE2	2.48	0.45
2:A:84:ILE:HD11	2:A:270:LEU:HD22	1.98	0.45
2:A:442:VAL:CB	2:A:489:LEU:HD11	2.42	0.45
2:A:463:ILE:HD13	2:A:469:ARG:CD	2.46	0.45
2:A:737:LEU:HA	2:A:737:LEU:HD23	1.65	0.45
2:A:807:GLY:HA2	3:B:760:ASP:O	2.16	0.45
2:A:1097:GLY:C	2:A:1099:PRO:HD2	2.41	0.45
3:B:125:SER:O	3:B:126:SER:HB3	2.17	0.45
3:B:376:PHE:HB3	3:B:586:TRP:CZ3	2.51	0.45
3:B:865:LYS:HD3	3:B:870:ILE:O	2.16	0.45
3:B:1131:GLY:N	3:B:1134:GLU:OE1	2.48	0.45
4:C:77:ILE:CG2	4:C:78:GLU:N	2.79	0.45
5:D:51:ASN:C	5:D:52:LEU:O	2.58	0.45
7:F:96:THR:O	7:F:100:GLN:HG3	2.16	0.45
7:F:109:VAL:HG12	7:F:110:ASP:N	2.32	0.45
8:G:121:PHE:HB2	8:G:130:TYR:CE2	2.51	0.45
9:H:113:ALA:HA	9:H:125:LEU:O	2.16	0.45
12:K:53:ASP:HB3	12:K:56:VAL:HG23	1.99	0.45
2:A:244:PRO:CB	2:A:245:PRO:CD	2.94	0.45
2:A:523:ILE:HG22	2:A:528:LEU:HB2	1.99	0.45
2:A:897:TYR:N	2:A:897:TYR:CD1	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1064:VAL:O	2:A:1064:VAL:HG12	2.15	0.45
2:A:1170:ILE:H	2:A:1170:ILE:HG13	1.60	0.45
2:A:1431:GLY:HA3	3:B:1197:PRO:HD3	1.98	0.45
3:B:593:PRO:HG2	3:B:617:ARG:NH2	2.31	0.45
3:B:797:TYR:CD2	3:B:852:ARG:CB	2.99	0.45
3:B:846:ILE:HG23	3:B:974:PRO:CG	2.38	0.45
4:C:40:GLU:OE1	4:C:254:LYS:NZ	2.49	0.45
5:D:29:LEU:O	5:D:30:GLY:O	2.35	0.45
5:D:37:GLN:HE22	8:G:5:LYS:HD2	1.79	0.45
8:G:160:ILE:H	8:G:160:ILE:HD12	1.82	0.45
10:I:34:TYR:O	10:I:35:VAL:HG23	2.17	0.45
2:A:92:HIS:O	2:A:95:PHE:N	2.46	0.45
2:A:98:LYS:O	2:A:102:VAL:N	2.47	0.45
2:A:494:SER:O	2:A:497:THR:N	2.48	0.45
2:A:1342:GLU:OE2	6:E:212:ARG:NH1	2.43	0.45
2:A:1409:LEU:O	2:A:1412:ALA:HB3	2.16	0.45
3:B:37:PHE:HE2	3:B:542:MET:HA	1.82	0.45
3:B:240:ILE:HD13	3:B:241:ARG:N	2.32	0.45
3:B:556:THR:O	3:B:556:THR:CG2	2.63	0.45
3:B:604:ARG:O	3:B:606:LYS:N	2.50	0.45
3:B:616:ILE:N	3:B:616:ILE:CD1	2.74	0.45
4:C:111:THR:C	4:C:112:ASN:HD22	2.24	0.45
6:E:59:SER:HB3	6:E:81:GLU:HA	1.99	0.45
6:E:161:LYS:C	6:E:163:GLU:N	2.72	0.45
13:L:49:LYS:O	13:L:50:ASP:HB2	2.17	0.45
2:A:875:ALA:HA	2:A:878:ILE:CD1	2.44	0.45
2:A:1263:ILE:O	2:A:1267:MET:HG3	2.16	0.45
2:A:1280:GLU:O	2:A:1281:ARG:C	2.59	0.45
2:A:1394:THR:CG2	2:A:1398:MET:SD	2.98	0.45
3:B:44:VAL:O	3:B:46:GLN:HG3	2.17	0.45
3:B:872:GLU:HA	3:B:915:THR:O	2.17	0.45
3:B:873:THR:O	3:B:914:LYS:HA	2.16	0.45
3:B:981:ALA:HB2	3:B:987:LYS:HA	1.98	0.45
4:C:35:ARG:NH1	12:K:40:HIS:HB2	2.30	0.45
4:C:41:ILE:HD12	4:C:41:ILE:N	2.30	0.45
6:E:144:ILE:HD12	6:E:145:THR:H	1.78	0.45
9:H:127:GLY:N	9:H:130:ARG:HH22	2.12	0.45
9:H:128:ASN:O	9:H:128:ASN:CG	2.59	0.45
10:I:8:ARG:O	10:I:10:CYS:N	2.49	0.45
12:K:31:VAL:CG1	12:K:32:VAL:N	2.79	0.45
2:A:22:PHE:CB	3:B:1211:ASN:HD21	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:90:VAL:HG13	2:A:297:GLN:CD	2.41	0.45
2:A:236:LEU:N	2:A:236:LEU:CD2	2.79	0.45
2:A:264:PHE:O	2:A:267:ALA:N	2.49	0.45
2:A:350:ARG:O	2:A:351:THR:CG2	2.64	0.45
2:A:443:LEU:HD23	2:A:501:LEU:HD22	1.99	0.45
2:A:970:THR:O	2:A:970:THR:HG22	2.16	0.45
2:A:1385:THR:HG22	2:A:1386:ARG:H	1.80	0.45
3:B:347:LYS:HG3	3:B:348:ARG:H	1.81	0.45
3:B:467:GLY:O	3:B:470:LYS:CG	2.64	0.45
3:B:820:GLY:N	3:B:1091:TYR:OH	2.50	0.45
3:B:903:VAL:CG1	3:B:904:ARG:N	2.80	0.45
4:C:258:ILE:HD13	12:K:35:PHE:CE2	2.46	0.45
6:E:92:THR:HG22	6:E:92:THR:O	2.17	0.45
6:E:157:SER:C	6:E:159:ASP:N	2.73	0.45
7:F:97:ARG:HD2	7:F:97:ARG:HA	1.69	0.45
8:G:88:ASP:HB3	8:G:144:ARG:HG3	1.99	0.45
11:J:64:ASN:CB	11:J:65:PRO:CD	2.80	0.45
2:A:65:LEU:O	2:A:66:LYS:C	2.59	0.45
2:A:123:ARG:O	2:A:125:ALA:N	2.50	0.45
2:A:268:ASP:HB3	2:A:299:HIS:CE1	2.52	0.45
2:A:283:GLY:O	2:A:285:PRO:CD	2.65	0.45
2:A:335:ARG:NH1	3:B:1206:GLU:OE2	2.50	0.45
2:A:543:LEU:C	2:A:545:GLN:N	2.74	0.45
2:A:881:GLN:HE22	2:A:960:ILE:H	1.64	0.45
2:A:1349:TYR:O	2:A:1350:LYS:C	2.60	0.45
3:B:26:THR:O	3:B:29:ASP:HB2	2.16	0.45
3:B:113:TYR:CB	3:B:114:PRO:HD2	2.46	0.45
3:B:199:MET:HE2	3:B:492:LEU:HD21	1.95	0.45
3:B:258:LEU:O	3:B:259:TYR:O	2.35	0.45
3:B:327:ARG:HH22	3:B:371:GLU:HG2	1.82	0.45
3:B:801:LYS:N	11:J:52:THR:CG2	2.79	0.45
3:B:953:LEU:CD2	3:B:965:LYS:HB2	2.35	0.45
3:B:1013:ASN:OD1	3:B:1015:HIS:N	2.47	0.45
4:C:6:PRO:HB3	4:C:25:VAL:CG1	2.47	0.45
5:D:153:ARG:HB3	5:D:154:PHE:CD1	2.52	0.45
6:E:136:ASN:OD1	6:E:136:ASN:C	2.60	0.45
7:F:81:THR:HG1	7:F:146:TRP:NE1	2.14	0.45
12:K:56:VAL:HG22	12:K:77:THR:HG22	1.99	0.45
2:A:7:SER:C	2:A:9:ALA:N	2.73	0.45
2:A:532:ARG:HG2	2:A:532:ARG:HH11	1.82	0.45
2:A:901:LEU:N	2:A:926:GLN:NE2	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1388:GLY:O	2:A:1390:ASN:N	2.50	0.45
3:B:238:ALA:HB3	3:B:256:VAL:HB	1.99	0.45
3:B:248:SER:O	3:B:249:ARG:HB2	2.16	0.45
3:B:840:ILE:HD13	3:B:994:TYR:HE1	1.81	0.45
4:C:37:MET:SD	4:C:232:VAL:HG21	2.56	0.45
7:F:72:LYS:O	7:F:73:ALA:HB3	2.17	0.45
7:F:99:LEU:HD12	7:F:99:LEU:C	2.41	0.45
8:G:17:PHE:N	8:G:17:PHE:CD2	2.85	0.45
10:I:6:PHE:HB3	10:I:12:ASN:O	2.16	0.45
12:K:49:GLU:HG3	12:K:94:ILE:HG12	1.99	0.45
2:A:58:LEU:O	2:A:59:GLY:O	2.35	0.45
2:A:89:PRO:O	2:A:204:THR:HG21	2.17	0.45
2:A:1069:ALA:O	2:A:1070:GLN:C	2.58	0.45
2:A:1433:MET:CE	8:G:63:PRO:HB2	2.46	0.45
3:B:429:PHE:HA	3:B:432:MET:CE	2.47	0.45
3:B:821:GLN:NE2	3:B:851:PHE:CD2	2.85	0.45
3:B:843:GLN:O	3:B:846:ILE:N	2.49	0.45
4:C:29:MET:CE	12:K:98:LEU:HG	2.46	0.45
4:C:77:ILE:HA	4:C:129:ILE:CD1	2.44	0.45
4:C:123:ASN:ND2	4:C:125:MET:SD	2.90	0.45
8:G:1:MET:O	8:G:3:PHE:CD1	2.70	0.45
8:G:34:VAL:HG11	8:G:74:TYR:CE1	2.52	0.45
12:K:42:LEU:HD23	12:K:46:ILE:CG1	2.46	0.45
2:A:446:ARG:HD2	2:A:480:ALA:HB2	1.99	0.45
2:A:738:LYS:HB2	2:A:740:LEU:CD2	2.46	0.45
2:A:808:LEU:HD22	2:A:813:PHE:HA	1.98	0.45
2:A:1059:HIS:O	2:A:1060:PRO:C	2.57	0.45
2:A:1291:VAL:HG13	2:A:1292:PRO:N	2.32	0.45
2:A:1299:VAL:HG12	2:A:1300:LYS:H	1.81	0.45
2:A:1345:ARG:CG	2:A:1372:VAL:HG13	2.43	0.45
3:B:205:ILE:C	3:B:207:GLY:H	2.24	0.45
3:B:324:ILE:CG2	3:B:325:GLN:N	2.80	0.45
3:B:726:ALA:HB1	3:B:1051:THR:HG21	1.99	0.45
4:C:175:ALA:HB1	11:J:43:ARG:NH1	2.31	0.45
6:E:136:ASN:OD1	6:E:138:ALA:N	2.49	0.45
8:G:1:MET:HE2	8:G:3:PHE:CD1	2.51	0.45
2:A:40:THR:HG22	2:A:41:MET:HG2	1.98	0.44
2:A:565:ILE:O	2:A:570:PRO:HA	2.17	0.44
2:A:728:LYS:O	2:A:732:LEU:HG	2.17	0.44
2:A:783:THR:CG2	2:A:815:PHE:CE2	2.99	0.44
2:A:1278:ASN:O	2:A:1280:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:289:LEU:HD13	3:B:375:ALA:HB2	1.99	0.44
3:B:313:MET:O	3:B:316:PRO:HD2	2.17	0.44
3:B:1065:GLN:HB2	4:C:201:TRP:CZ3	2.52	0.44
4:C:17:ASN:N	4:C:17:ASN:ND2	2.43	0.44
4:C:114:TYR:C	4:C:116:LYS:H	2.23	0.44
5:D:205:ASP:O	5:D:208:GLU:N	2.50	0.44
7:F:90:ARG:HD3	7:F:155:LEU:CD1	2.47	0.44
9:H:104:PHE:CZ	9:H:136:LYS:HG2	2.53	0.44
10:I:101:PHE:N	10:I:101:PHE:HD1	2.15	0.44
2:A:92:HIS:HB2	2:A:236:LEU:CD2	2.48	0.44
2:A:244:PRO:O	2:A:247:ARG:N	2.40	0.44
2:A:1385:THR:C	2:A:1387:HIS:N	2.76	0.44
3:B:292:ILE:HD12	3:B:326:ASP:HA	1.99	0.44
3:B:520:GLY:HA2	3:B:748:ILE:HG22	2.00	0.44
3:B:549:THR:HG22	3:B:550:ASP:H	1.82	0.44
3:B:800:GLN:CB	11:J:52:THR:HG22	2.47	0.44
3:B:1023:VAL:O	3:B:1024:ALA:C	2.60	0.44
3:B:1051:THR:CG2	3:B:1052:VAL:H	2.29	0.44
4:C:99:LEU:HD23	4:C:99:LEU:N	2.32	0.44
5:D:126:ILE:HD13	5:D:126:ILE:HA	1.87	0.44
5:D:135:GLY:C	5:D:137:ASN:H	2.25	0.44
6:E:48:ASP:CG	6:E:49:SER:N	2.74	0.44
8:G:88:ASP:HB3	8:G:144:ARG:CB	2.47	0.44
10:I:7:CYS:SG	10:I:8:ARG:O	2.75	0.44
10:I:32:CYS:HB2	10:I:33:SER:H	1.46	0.44
10:I:74:GLU:HA	10:I:80:SER:O	2.18	0.44
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.52	0.44
2:A:116:ASP:C	2:A:118:HIS:N	2.72	0.44
2:A:836:TYR:O	2:A:840:ARG:HD3	2.17	0.44
2:A:877:HIS:O	2:A:878:ILE:CG1	2.65	0.44
2:A:1372:VAL:HG12	2:A:1373:ASP:H	1.81	0.44
3:B:274:PRO:C	3:B:276:ILE:N	2.66	0.44
3:B:766:ARG:HH22	3:B:1020:ARG:HH11	1.65	0.44
3:B:792:MET:HA	3:B:856:PHE:O	2.18	0.44
3:B:814:PHE:C	3:B:816:GLU:N	2.75	0.44
8:G:126:ASN:HA	8:G:127:PRO:C	2.40	0.44
10:I:74:GLU:HB2	10:I:79:HIS:HA	2.00	0.44
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.99	0.44
2:A:365:GLY:O	2:A:468:PHE:HA	2.18	0.44
2:A:404:TYR:N	2:A:415:LEU:HD12	2.33	0.44
2:A:474:VAL:HG22	2:A:478:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:507:VAL:HG13	2:A:521:MET:HE1	1.99	0.44
2:A:599:SER:HA	2:A:600:PRO:HD2	1.84	0.44
2:A:809:THR:O	2:A:810:PRO:C	2.59	0.44
2:A:1058:VAL:CG1	2:A:1059:HIS:N	2.81	0.44
2:A:1260:LEU:O	2:A:1260:LEU:HG	2.16	0.44
3:B:235:SER:C	3:B:236:HIS:CD2	2.96	0.44
3:B:766:ARG:HD3	3:B:766:ARG:HA	1.83	0.44
3:B:1064:TYR:O	3:B:1065:GLN:C	2.61	0.44
3:B:1120:GLU:CG	3:B:1121:GLY:N	2.79	0.44
4:C:89:GLU:O	4:C:90:ASP:CB	2.65	0.44
5:D:47:LEU:HD11	8:G:3:PHE:CD2	2.52	0.44
5:D:47:LEU:HD11	8:G:3:PHE:CE2	2.51	0.44
5:D:177:VAL:O	5:D:177:VAL:HG12	2.18	0.44
6:E:84:ASP:O	6:E:86:PRO:HD3	2.18	0.44
7:F:74:ILE:CG2	7:F:75:PRO:HD2	2.46	0.44
7:F:111:LEU:C	7:F:113:GLY:N	2.68	0.44
8:G:49:LEU:O	8:G:50:ASP:C	2.60	0.44
9:H:42:ILE:HG23	9:H:43:ASN:N	2.32	0.44
1:R:6:A:OP1	3:B:210:LYS:HE3	2.17	0.44
2:A:408:ASP:C	2:A:410:GLY:H	2.26	0.44
2:A:668:ASP:HA	2:A:741:ASN:OD1	2.17	0.44
2:A:919:ILE:O	2:A:920:LEU:C	2.61	0.44
2:A:1313:LEU:C	2:A:1315:GLU:N	2.75	0.44
3:B:98:THR:O	3:B:126:SER:HB2	2.18	0.44
3:B:489:SER:O	3:B:490:SER:C	2.60	0.44
3:B:654:ARG:HH11	3:B:654:ARG:HG3	1.82	0.44
3:B:708:GLU:O	3:B:709:ASP:C	2.60	0.44
3:B:737:THR:HG22	10:I:66:PRO:HB3	2.00	0.44
3:B:859:TYR:CZ	3:B:941:LEU:HD12	2.53	0.44
4:C:193:TYR:C	4:C:193:TYR:CD1	2.96	0.44
5:D:192:LYS:NZ	5:D:192:LYS:HB3	2.32	0.44
8:G:142:ARG:C	8:G:143:ILE:HD12	2.43	0.44
9:H:56:THR:HG21	9:H:145:ARG:HE	1.81	0.44
2:A:91:PHE:HD2	2:A:96:ILE:HG13	1.82	0.44
2:A:255:SER:OG	3:B:918:ILE:HG23	2.18	0.44
2:A:1130:GLN:O	2:A:1134:ILE:HG12	2.18	0.44
3:B:97:VAL:HG12	3:B:178:ASN:ND2	2.32	0.44
3:B:287:ARG:HG2	3:B:292:ILE:HA	1.99	0.44
3:B:408:LEU:HD12	3:B:408:LEU:HA	1.82	0.44
3:B:737:THR:O	3:B:738:PHE:C	2.60	0.44
3:B:794:ASN:O	3:B:795:ILE:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:801:LYS:O	11:J:52:THR:CG2	2.60	0.44
4:C:60:ASP:HB3	13:L:67:PHE:CZ	2.53	0.44
4:C:174:ALA:O	4:C:175:ALA:CB	2.66	0.44
5:D:71:LYS:C	5:D:73:SER:N	2.73	0.44
8:G:1:MET:SD	8:G:1:MET:C	3.00	0.44
9:H:4:THR:HA	9:H:60:ALA:CB	2.44	0.44
9:H:98:TYR:HE1	9:H:139:ASN:HA	1.83	0.44
12:K:55:LYS:CB	12:K:81:TYR:CE1	3.01	0.44
1:R:2:C:C1'	1:R:3:A:OP1	2.65	0.44
2:A:93:VAL:C	2:A:96:ILE:HD13	2.42	0.44
2:A:120:GLU:O	2:A:122:MET:N	2.51	0.44
2:A:252:PHE:HB2	2:A:256:GLN:CD	2.42	0.44
2:A:899:VAL:HB	2:A:929:LEU:CD1	2.48	0.44
2:A:899:VAL:CG2	2:A:1029:ARG:HG2	2.48	0.44
3:B:268:THR:C	3:B:269:ILE:HD12	2.42	0.44
3:B:635:ARG:HB2	3:B:636:PRO:HD2	1.99	0.44
3:B:800:GLN:CA	11:J:52:THR:HG22	2.48	0.44
4:C:44:LEU:HB2	4:C:77:ILE:HD12	2.00	0.44
4:C:77:ILE:HG23	4:C:78:GLU:N	2.32	0.44
5:D:146:GLN:O	5:D:147:TYR:C	2.60	0.44
6:E:61:GLN:HB2	6:E:79:TRP:CZ3	2.52	0.44
8:G:13:LEU:O	8:G:67:SER:HA	2.17	0.44
8:G:50:ASP:C	8:G:50:ASP:OD1	2.60	0.44
8:G:80:LYS:HA	8:G:81:PRO:HD2	1.78	0.44
10:I:61:ASP:C	10:I:63:GLY:N	2.75	0.44
10:I:111:THR:CG2	10:I:112:SER:H	2.31	0.44
12:K:79:GLU:HG2	12:K:80:GLY:N	2.31	0.44
2:A:374:LEU:HB2	2:A:436:ILE:CD1	2.48	0.44
2:A:767:GLN:OE1	2:A:799:PHE:HB2	2.18	0.44
2:A:779:PHE:HE1	2:A:785:PRO:HD3	1.66	0.44
2:A:964:ILE:CD1	2:A:1045:VAL:HG21	2.48	0.44
2:A:1329:THR:HB	2:A:1335:ILE:HD11	1.99	0.44
3:B:221:ASN:OD1	3:B:242:SER:HA	2.18	0.44
3:B:458:LYS:O	3:B:459:TYR:C	2.60	0.44
3:B:578:THR:O	3:B:579:ARG:C	2.61	0.44
3:B:579:ARG:HB2	3:B:586:TRP:CE2	2.53	0.44
9:H:89:LEU:O	9:H:91:ASP:N	2.49	0.44
10:I:15:TYR:N	10:I:15:TYR:CD1	2.86	0.44
11:J:1:MET:H2	11:J:55:ASP:C	2.26	0.44
12:K:45:LEU:C	12:K:47:ARG:N	2.75	0.44
2:A:23:SER:O	2:A:26:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:75:ASN:O	2:A:76:GLU:CB	2.66	0.44
2:A:525:GLN:O	2:A:526:ASP:C	2.60	0.44
2:A:530:GLY:O	2:A:531:ILE:C	2.61	0.44
2:A:567:LYS:NZ	9:H:47:PHE:CB	2.81	0.44
2:A:849:MET:HE3	2:A:1061:GLY:C	2.43	0.44
2:A:868:TYR:OH	2:A:1366:ARG:HD3	2.18	0.44
2:A:1192:LEU:HG	2:A:1193:LEU:N	2.33	0.44
3:B:51:PHE:O	3:B:55:VAL:HG23	2.17	0.44
3:B:405:ARG:HE	3:B:629:ASP:HB3	1.82	0.44
3:B:604:ARG:C	3:B:606:LYS:H	2.25	0.44
3:B:758:PHE:CE1	3:B:1044:ALA:HB1	2.53	0.44
4:C:56:THR:CG2	4:C:57:VAL:N	2.80	0.44
6:E:138:ALA:HA	6:E:141:VAL:HG23	2.00	0.44
6:E:184:VAL:C	6:E:186:LEU:H	2.24	0.44
2:A:57:ARG:C	2:A:58:LEU:O	2.61	0.43
2:A:652:VAL:O	2:A:653:VAL:C	2.60	0.43
2:A:700:ASN:HB2	10:I:98:VAL:HG22	2.00	0.43
2:A:1220:PHE:O	2:A:1221:LYS:HB2	2.17	0.43
3:B:39:ARG:HH21	3:B:665:GLU:CD	2.26	0.43
3:B:560:GLU:O	3:B:561:TRP:CD1	2.71	0.43
3:B:578:THR:O	3:B:578:THR:HG22	2.17	0.43
3:B:620:ARG:NH2	10:I:89:GLN:NE2	2.66	0.43
3:B:654:ARG:C	3:B:656:GLY:H	2.26	0.43
5:D:191:ALA:C	5:D:193:THR:N	2.76	0.43
6:E:89:GLY:HA2	6:E:117:THR:OG1	2.17	0.43
2:A:443:LEU:HD11	2:A:455:MET:HB3	2.00	0.43
2:A:587:HIS:HA	2:A:607:ILE:O	2.18	0.43
2:A:852:TYR:HA	2:A:1060:PRO:HB3	2.00	0.43
2:A:1162:VAL:O	2:A:1162:VAL:HG12	2.18	0.43
2:A:1276:VAL:HG12	2:A:1277:GLU:N	2.33	0.43
3:B:102:VAL:HG23	3:B:112:LEU:HB2	1.99	0.43
3:B:129:PHE:CE2	3:B:166:PHE:HA	2.52	0.43
3:B:225:VAL:HG12	3:B:238:ALA:HA	2.01	0.43
3:B:558:LEU:O	3:B:561:TRP:N	2.51	0.43
4:C:44:LEU:HB2	4:C:77:ILE:CD1	2.48	0.43
4:C:152:GLU:HG2	4:C:153:LEU:H	1.82	0.43
6:E:184:VAL:C	6:E:186:LEU:N	2.76	0.43
7:F:90:ARG:HD3	7:F:155:LEU:HD12	1.98	0.43
8:G:87:VAL:CG2	8:G:103:VAL:HG11	2.48	0.43
11:J:31:ASP:O	11:J:32:GLU:C	2.61	0.43
13:L:70:ARG:HG2	13:L:70:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:28:5BU:H2'	1:R:29:G:H8	1.81	0.43
2:A:751:SER:OG	3:B:1015:HIS:HE1	2.00	0.43
2:A:774:ARG:H	2:A:774:ARG:HG2	1.55	0.43
2:A:964:ILE:HD13	2:A:1045:VAL:CG2	2.48	0.43
3:B:96:TYR:N	3:B:129:PHE:O	2.40	0.43
3:B:496:ARG:HB3	3:B:496:ARG:NH1	2.29	0.43
6:E:6:GLU:HG3	6:E:6:GLU:O	2.18	0.43
9:H:116:TYR:O	9:H:122:LEU:HA	2.18	0.43
10:I:60:GLN:NE2	10:I:107:SER:OG	2.51	0.43
10:I:88:SER:C	10:I:90:GLN:H	2.27	0.43
11:J:36:LEU:O	11:J:39:LEU:N	2.51	0.43
11:J:49:MET:HB3	11:J:50:ILE:HD12	2.00	0.43
12:K:83:PRO:O	12:K:84:LYS:C	2.61	0.43
2:A:19:PHE:O	2:A:1416:ALA:HA	2.18	0.43
2:A:344:ARG:O	2:A:345:VAL:HG12	2.18	0.43
2:A:443:LEU:O	2:A:489:LEU:HD12	2.19	0.43
2:A:464:PRO:HG2	2:A:465:TYR:CD1	2.50	0.43
2:A:510:GLN:OE1	2:A:510:GLN:HA	2.19	0.43
2:A:954:TRP:HB3	2:A:955:PRO:HD2	2.00	0.43
2:A:1376:THR:HA	2:A:1380:GLY:O	2.19	0.43
2:A:1388:GLY:O	2:A:1389:PHE:C	2.61	0.43
3:B:27:ALA:C	3:B:29:ASP:H	2.26	0.43
3:B:56:ASP:C	3:B:57:TYR:HD1	2.26	0.43
3:B:221:ASN:O	3:B:222:ILE:HD13	2.19	0.43
3:B:245:GLU:C	3:B:246:LYS:HG3	2.43	0.43
3:B:272:THR:OG1	3:B:279:ASP:OD1	2.36	0.43
3:B:515:HIS:H	3:B:518:HIS:CD2	2.31	0.43
3:B:530:GLY:C	3:B:531:GLN:HG2	2.44	0.43
3:B:619:ILE:HD12	10:I:65:ASP:HB2	1.99	0.43
3:B:743:ILE:H	3:B:743:ILE:HG12	1.49	0.43
4:C:29:MET:HE2	12:K:98:LEU:CD2	2.48	0.43
4:C:58:LEU:N	4:C:58:LEU:CD2	2.81	0.43
4:C:183:TRP:CE2	4:C:207:CYS:HB3	2.53	0.43
4:C:187:LYS:C	4:C:189:THR:H	2.26	0.43
7:F:81:THR:HG21	7:F:136:ARG:HD3	1.99	0.43
9:H:47:PHE:CD2	9:H:95:TYR:HD1	2.36	0.43
12:K:7:PHE:HA	12:K:10:PHE:CE2	2.54	0.43
2:A:166:GLY:C	2:A:167:CYS:SG	3.02	0.43
2:A:244:PRO:HG2	2:A:245:PRO:HD3	2.01	0.43
2:A:353:ILE:HD13	2:A:487:MET:CE	2.48	0.43
2:A:935:GLN:O	2:A:936:LEU:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1076:ALA:HA	2:A:1079:MET:CE	2.48	0.43
2:A:1332:PHE:CD2	2:A:1332:PHE:N	2.84	0.43
3:B:45:SER:O	3:B:48:LEU:HB2	2.19	0.43
3:B:215:GLN:NE2	3:B:499:ASN:HD22	2.11	0.43
3:B:273:LEU:O	3:B:273:LEU:CD2	2.63	0.43
3:B:564:GLU:O	3:B:565:PRO:C	2.60	0.43
3:B:639:ILE:HD11	3:B:691:GLU:HB2	2.00	0.43
3:B:681:TRP:C	3:B:683:SER:N	2.71	0.43
3:B:999:MET:HA	3:B:999:MET:CE	2.39	0.43
4:C:35:ARG:O	4:C:36:VAL:C	2.62	0.43
4:C:254:LYS:O	4:C:256:ALA:N	2.52	0.43
5:D:60:LYS:O	5:D:61:GLU:C	2.61	0.43
11:J:13:VAL:O	11:J:14:VAL:HG23	2.18	0.43
12:K:49:GLU:C	12:K:51:LEU:H	2.25	0.43
13:L:51:CYS:HB2	13:L:53:HIS:HD2	1.82	0.43
2:A:511:ILE:HD13	2:A:521:MET:HE3	2.00	0.43
2:A:1005:GLU:O	2:A:1006:ILE:C	2.61	0.43
2:A:1334:ASP:O	2:A:1335:ILE:C	2.62	0.43
3:B:309:GLN:CD	10:I:52:ILE:HD11	2.44	0.43
3:B:365:THR:HG23	3:B:367:LEU:CB	2.48	0.43
3:B:464:GLY:CA	3:B:479:VAL:O	2.67	0.43
3:B:526:GLU:HB2	3:B:752:ALA:HB3	2.01	0.43
3:B:684:LEU:HA	3:B:689:LEU:HD12	2.00	0.43
3:B:1030:LEU:HD12	3:B:1030:LEU:HA	1.80	0.43
4:C:131:HIS:HA	4:C:132:PRO:HD3	1.86	0.43
4:C:229:TYR:CD1	4:C:229:TYR:N	2.86	0.43
5:D:26:THR:O	5:D:27:LEU:HB2	2.19	0.43
6:E:157:SER:HG	6:E:160:GLU:HG3	1.83	0.43
8:G:78:VAL:HG12	8:G:79:PHE:H	1.84	0.43
11:J:1:MET:N	11:J:54:VAL:O	2.51	0.43
12:K:85:ASP:O	12:K:86:ALA:C	2.61	0.43
1:R:2:C:N3	1:R:16:G:C2	2.87	0.43
2:A:23:SER:O	2:A:25:GLU:N	2.52	0.43
2:A:90:VAL:CG1	2:A:297:GLN:CD	2.91	0.43
2:A:1434:ALA:HA	2:A:1435:PRO:HD3	1.91	0.43
3:B:758:PHE:O	3:B:760:ASP:N	2.51	0.43
3:B:1026:LEU:HD23	3:B:1086:PHE:CE2	2.54	0.43
4:C:19:ASP:HA	4:C:231:ASN:HA	2.00	0.43
4:C:186:LEU:N	4:C:186:LEU:CD1	2.81	0.43
6:E:31:THR:O	6:E:35:VAL:HG23	2.18	0.43
7:F:74:ILE:HG22	7:F:75:PRO:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:21:TYR:CD2	11:J:21:TYR:C	2.96	0.43
13:L:30:ILE:HD11	13:L:59:ALA:HB2	2.00	0.43
1:R:13:G:H4'	2:A:320:ARG:HD3	2.01	0.43
2:A:472:LEU:CD1	3:B:835:GLN:CD	2.91	0.43
2:A:494:SER:O	2:A:495:GLU:C	2.61	0.43
2:A:632:VAL:O	2:A:633:VAL:C	2.62	0.43
2:A:755:PHE:O	2:A:756:ILE:C	2.62	0.43
2:A:902:LEU:O	2:A:903:ASN:HB2	2.19	0.43
3:B:311:LEU:O	3:B:312:GLU:C	2.62	0.43
3:B:557:PHE:C	3:B:557:PHE:HD2	2.23	0.43
3:B:634:TYR:CD1	3:B:692:TYR:HB3	2.53	0.43
3:B:1178:ASN:O	3:B:1179:GLN:O	2.36	0.43
4:C:163:ILE:C	4:C:165:LYS:N	2.76	0.43
6:E:104:ASN:C	6:E:104:ASN:HD22	2.25	0.43
8:G:49:LEU:HD21	8:G:77:VAL:HG23	1.99	0.43
10:I:4:PHE:CD1	10:I:4:PHE:C	2.97	0.43
11:J:1:MET:HA	11:J:57:ILE:H	1.83	0.43
2:A:157:ASP:C	2:A:159:THR:N	2.75	0.43
2:A:265:LYS:HG2	2:A:303:TYR:HA	2.00	0.43
2:A:348:SER:HB2	3:B:1128:LEU:HD12	1.99	0.43
2:A:497:THR:O	2:A:498:ARG:C	2.60	0.43
2:A:567:LYS:HZ2	9:H:46:LEU:C	2.26	0.43
2:A:1202:MET:HE1	2:A:1212:VAL:CG2	2.47	0.43
2:A:1206:ASP:O	2:A:1207:LEU:HG	2.19	0.43
2:A:1289:ARG:NH1	2:A:1326:ARG:NH1	2.66	0.43
2:A:1401:SER:O	2:A:1402:PHE:HB2	2.18	0.43
3:B:57:TYR:O	3:B:58:THR:C	2.61	0.43
3:B:449:ASN:ND2	3:B:451:LYS:HB3	2.34	0.43
3:B:737:THR:CG2	10:I:66:PRO:HA	2.44	0.43
3:B:1013:ASN:CG	3:B:1014:PRO:HD2	2.44	0.43
3:B:1190:ASP:O	3:B:1191:ILE:HD12	2.18	0.43
4:C:83:SER:O	4:C:85:ASP:N	2.47	0.43
5:D:203:SER:O	5:D:204:ASP:C	2.62	0.43
8:G:1:MET:O	8:G:2:PHE:C	2.61	0.43
2:A:471:ASN:OD1	2:A:471:ASN:C	2.62	0.43
2:A:586:ILE:HD11	2:A:633:VAL:HG22	2.01	0.43
2:A:648:ASN:OD1	2:A:648:ASN:N	2.52	0.43
2:A:714:PHE:O	2:A:718:VAL:HG23	2.19	0.43
2:A:1151:GLU:OE2	10:I:45:ARG:NH1	2.52	0.43
3:B:277:LYS:HB2	3:B:278:GLN:H	1.58	0.43
3:B:431:TYR:CE1	3:B:447:ALA:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:505:ASP:C	3:B:507:LYS:N	2.76	0.43
3:B:683:SER:C	3:B:685:LEU:N	2.77	0.43
3:B:778:MET:HE2	3:B:1094:ARG:CG	2.49	0.43
3:B:782:LEU:HB3	3:B:784:ASN:OD1	2.18	0.43
3:B:806:THR:CG2	3:B:808:ALA:H	2.32	0.43
3:B:983:ARG:CD	3:B:1091:TYR:HB3	2.45	0.43
3:B:1066:SER:O	3:B:1067:ARG:HD3	2.18	0.43
5:D:176:GLU:C	5:D:178:ALA:N	2.76	0.43
6:E:90:VAL:HA	6:E:120:ALA:HB2	2.01	0.43
6:E:164:LEU:HD11	6:E:211:TYR:CE1	2.54	0.43
9:H:82:PRO:C	9:H:84:ALA:N	2.77	0.43
10:I:8:ARG:H	10:I:34:TYR:HE1	1.66	0.43
2:A:244:PRO:C	2:A:246:VAL:N	2.77	0.42
2:A:276:LEU:HD13	2:A:292:ALA:O	2.19	0.42
2:A:682:THR:HA	2:A:685:GLU:HG2	2.00	0.42
2:A:901:LEU:O	2:A:921:GLY:N	2.42	0.42
2:A:971:PHE:HE2	2:A:1040:GLN:HG2	1.84	0.42
2:A:1007:ILE:O	2:A:1009:ASN:N	2.52	0.42
3:B:45:SER:O	3:B:46:GLN:C	2.61	0.42
3:B:522:VAL:HG12	3:B:523:CYS:N	2.33	0.42
3:B:758:PHE:C	3:B:760:ASP:H	2.26	0.42
4:C:160:LYS:O	4:C:161:LYS:O	2.36	0.42
6:E:34:GLU:O	6:E:34:GLU:HG2	2.19	0.42
7:F:127:GLU:O	7:F:128:LYS:C	2.62	0.42
9:H:107:VAL:O	9:H:108:SER:O	2.38	0.42
9:H:116:TYR:HE2	9:H:140:ALA:CB	2.31	0.42
9:H:123:MET:HG2	9:H:124:ARG:N	2.32	0.42
11:J:27:GLU:C	11:J:29:GLU:N	2.77	0.42
2:A:135:PHE:CE1	2:A:222:LEU:HD22	2.53	0.42
2:A:332:LYS:O	2:A:333:GLU:HB2	2.19	0.42
2:A:578:LEU:HD23	2:A:612:ILE:HD11	2.02	0.42
2:A:814:PHE:O	2:A:818:MET:HG3	2.19	0.42
2:A:1100:ARG:HH21	2:A:1351:GLU:CD	2.27	0.42
3:B:95:ILE:CB	3:B:130:VAL:HG22	2.48	0.42
3:B:121:ASN:HA	3:B:207:GLY:CA	2.49	0.42
3:B:236:HIS:CE1	3:B:389:ALA:HA	2.55	0.42
3:B:487:THR:HB	3:B:490:SER:HB3	2.00	0.42
3:B:785:TYR:CD1	3:B:786:ASN:N	2.87	0.42
3:B:812:LEU:O	3:B:813:LYS:C	2.63	0.42
10:I:95:THR:HG22	10:I:96:SER:N	2.34	0.42
11:J:7:CYS:CB	11:J:46:CYS:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:17:SER:O	12:K:18:LYS:C	2.62	0.42
12:K:102:LYS:O	12:K:106:GLU:HG3	2.18	0.42
1:R:7:C:H3'	1:R:8:U:C5'	2.46	0.42
2:A:374:LEU:HB2	2:A:436:ILE:HD11	2.01	0.42
2:A:481:ASP:OD1	2:A:485:ASP:OD2	2.37	0.42
2:A:738:LYS:C	2:A:740:LEU:N	2.77	0.42
2:A:811:GLN:O	2:A:812:GLU:C	2.63	0.42
2:A:870:GLU:HB2	6:E:204:THR:HG21	2.01	0.42
3:B:510:LYS:HB3	3:B:513:GLN:HB2	2.01	0.42
3:B:806:THR:HG21	3:B:808:ALA:HB3	2.01	0.42
3:B:899:ILE:HD12	3:B:911:ILE:HG23	2.02	0.42
3:B:1034:VAL:O	3:B:1036:ALA:N	2.52	0.42
4:C:258:ILE:CD1	12:K:42:LEU:HD21	2.48	0.42
5:D:183:LEU:O	5:D:184:ALA:C	2.62	0.42
6:E:42:PHE:O	6:E:43:LYS:C	2.61	0.42
7:F:143:PHE:C	7:F:143:PHE:CD1	2.97	0.42
9:H:82:PRO:O	9:H:84:ALA:N	2.41	0.42
9:H:145:ARG:O	9:H:146:ARG:HB2	2.18	0.42
2:A:362:ASP:OD1	2:A:459:ARG:HD2	2.19	0.42
2:A:523:ILE:CD1	2:A:649:ILE:HG21	2.50	0.42
2:A:630:ILE:CD1	2:A:645:LEU:HD23	2.49	0.42
2:A:1444:MET:HE3	2:A:1444:MET:HB2	1.95	0.42
2:A:1445:ILE:HD11	8:G:68:ALA:HB2	2.01	0.42
3:B:235:SER:C	3:B:236:HIS:HD2	2.27	0.42
3:B:299:GLU:CD	3:B:572:HIS:HE1	2.28	0.42
3:B:350:GLN:C	3:B:352:ALA:H	2.28	0.42
3:B:370:PHE:C	3:B:372:SER:N	2.76	0.42
3:B:558:LEU:HD21	3:B:596:LEU:HD11	2.01	0.42
3:B:797:TYR:HE1	3:B:854:LEU:HD21	1.84	0.42
3:B:1001:PHE:CE2	3:B:1073:TYR:HB2	2.54	0.42
3:B:1024:ALA:O	3:B:1025:HIS:C	2.61	0.42
6:E:20:LYS:O	6:E:21:GLU:C	2.60	0.42
6:E:120:ALA:C	6:E:122:LYS:H	2.27	0.42
12:K:60:ALA:O	12:K:73:LEU:HD12	2.19	0.42
2:A:37:PHE:N	2:A:37:PHE:HD1	2.17	0.42
2:A:92:HIS:O	2:A:93:VAL:C	2.62	0.42
2:A:282:ASN:O	2:A:284:ALA:N	2.53	0.42
2:A:352:VAL:HG13	2:A:485:ASP:O	2.20	0.42
2:A:668:ASP:CG	2:A:742:ASN:HD22	2.26	0.42
2:A:784:LEU:C	2:A:786:HIS:N	2.77	0.42
2:A:845:LEU:CD2	2:A:1374:VAL:HG21	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1279:ILE:CD1	2:A:1316:VAL:HG21	2.45	0.42
2:A:1335:ILE:HG23	2:A:1339:LEU:HD12	2.00	0.42
2:A:1349:TYR:CB	2:A:1372:VAL:HG21	2.46	0.42
3:B:186:GLU:HB3	3:B:187:SER:H	1.68	0.42
3:B:276:ILE:HD11	3:B:355:ILE:HD13	2.02	0.42
3:B:492:LEU:O	3:B:495:LEU:N	2.48	0.42
3:B:501:PRO:HB2	3:B:502:ILE:H	1.64	0.42
3:B:683:SER:OG	3:B:684:LEU:HD12	2.19	0.42
3:B:882:THR:O	3:B:883:LEU:CB	2.67	0.42
3:B:1115:THR:CG2	3:B:1117:GLN:HG3	2.49	0.42
4:C:143:LEU:HD21	4:C:146:LYS:HE2	2.01	0.42
4:C:191:TYR:CD2	4:C:201:TRP:CD1	3.07	0.42
4:C:251:LEU:HD12	4:C:251:LEU:C	2.41	0.42
6:E:171:LYS:O	6:E:172:GLU:C	2.62	0.42
11:J:60:PHE:C	11:J:62:ARG:H	2.28	0.42
2:A:63:ARG:HA	2:A:74:MET:CE	2.50	0.42
2:A:90:VAL:CG1	2:A:297:GLN:HA	2.48	0.42
2:A:93:VAL:HG23	2:A:304:MET:HE3	2.00	0.42
2:A:283:GLY:O	2:A:285:PRO:HD2	2.20	0.42
2:A:393:ARG:O	2:A:394:ASN:C	2.62	0.42
2:A:1074:GLU:C	2:A:1076:ALA:N	2.77	0.42
2:A:1329:THR:N	2:A:1335:ILE:HD11	2.28	0.42
3:B:390:LEU:O	3:B:391:ASP:C	2.62	0.42
3:B:555:ILE:O	3:B:557:PHE:N	2.52	0.42
3:B:615:MET:HA	3:B:625:LYS:O	2.20	0.42
3:B:823:ALA:O	3:B:1089:PRO:HA	2.20	0.42
3:B:975:GLN:O	3:B:990:ILE:HG13	2.20	0.42
4:C:248:ILE:O	4:C:252:GLN:HB2	2.19	0.42
5:D:145:MET:O	5:D:149:THR:N	2.53	0.42
6:E:198:ILE:N	6:E:198:ILE:CD1	2.77	0.42
7:F:95:GLY:O	7:F:96:THR:C	2.62	0.42
12:K:50:LEU:HD13	12:K:75:ILE:CD1	2.50	0.42
13:L:47:ARG:HH11	13:L:47:ARG:HG3	1.84	0.42
1:R:2:C:H1'	1:R:3:A:P	2.60	0.42
2:A:134:ARG:NH1	2:A:220:THR:O	2.52	0.42
2:A:244:PRO:C	2:A:246:VAL:H	2.28	0.42
2:A:296:LEU:C	2:A:298:PHE:N	2.76	0.42
2:A:393:ARG:O	2:A:395:GLY:N	2.53	0.42
2:A:791:ASP:C	2:A:791:ASP:OD1	2.62	0.42
2:A:826:ASP:HB2	2:A:830:LYS:HD3	2.02	0.42
2:A:1131:ALA:O	2:A:1132:LYS:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1225:PHE:O	2:A:1240:CYS:HA	2.18	0.42
2:A:1373:ASP:CA	2:A:1376:THR:HG22	2.48	0.42
3:B:408:LEU:O	3:B:410:GLY:N	2.53	0.42
3:B:597:MET:O	3:B:600:LEU:N	2.52	0.42
3:B:653:VAL:CG2	3:B:689:LEU:HD22	2.50	0.42
3:B:936:ASP:OD1	3:B:938:SER:N	2.46	0.42
3:B:996:ARG:HH12	4:C:174:ALA:HA	1.85	0.42
5:D:35:LEU:HD21	5:D:173:HIS:HB3	2.02	0.42
5:D:40:HIS:NE2	5:D:41:GLN:HG3	2.34	0.42
5:D:63:LEU:O	5:D:66:ARG:HB3	2.20	0.42
5:D:146:GLN:O	5:D:149:THR:N	2.48	0.42
8:G:98:GLY:HA3	8:G:110:VAL:O	2.19	0.42
10:I:95:THR:HG22	10:I:96:SER:O	2.20	0.42
2:A:334:GLY:O	2:A:335:ARG:C	2.63	0.42
2:A:573:SER:O	2:A:574:GLY:C	2.61	0.42
2:A:714:PHE:HB2	10:I:97:MET:HE1	2.01	0.42
2:A:1308:THR:HG23	2:A:1309:ASP:N	2.34	0.42
2:A:1437:GLY:C	2:A:1439:GLY:N	2.78	0.42
3:B:34:ILE:O	3:B:35:SER:C	2.63	0.42
3:B:190:TYR:CD2	11:J:62:ARG:HB3	2.55	0.42
3:B:873:THR:HG22	3:B:874:PHE:N	2.35	0.42
3:B:1165:ILE:HG22	5:D:15:LEU:HA	2.01	0.42
8:G:125:SER:OG	8:G:128:PRO:HA	2.18	0.42
11:J:16:ASP:C	11:J:18:TRP:H	2.28	0.42
2:A:285:PRO:CG	2:A:288:ALA:HB3	2.39	0.42
2:A:552:TRP:O	2:A:554:PRO:HD3	2.19	0.42
2:A:590:ARG:HD3	2:A:604:GLY:HA2	2.02	0.42
2:A:605:MET:HE1	2:A:612:ILE:HG23	2.02	0.42
2:A:860:LEU:HD23	2:A:860:LEU:HA	1.88	0.42
3:B:63:ILE:HD13	3:B:421:PHE:CZ	2.55	0.42
4:C:102:GLN:HG2	4:C:154:LYS:HG2	2.01	0.42
8:G:56:ILE:C	8:G:57:GLN:O	2.63	0.42
2:A:23:SER:HB3	2:A:233:TRP:CZ2	2.55	0.42
2:A:123:ARG:C	2:A:125:ALA:H	2.28	0.42
2:A:231:PRO:C	2:A:233:TRP:N	2.76	0.42
2:A:311:GLN:O	2:A:312:PRO:C	2.59	0.42
2:A:427:GLN:O	2:A:428:TYR:C	2.62	0.42
2:A:789:LYS:HE3	10:I:67:THR:OG1	2.20	0.42
2:A:1062:GLU:OE2	7:F:88:TYR:OH	2.34	0.42
2:A:1076:ALA:HA	2:A:1079:MET:HE3	2.02	0.42
3:B:843:GLN:N	3:B:994:TYR:O	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:866:TYR:O	3:B:867:GLY:C	2.63	0.42
4:C:166:GLU:O	4:C:167:HIS:CB	2.66	0.42
5:D:63:LEU:CD1	5:D:129:LEU:HG	2.45	0.42
11:J:47:ARG:HG2	11:J:47:ARG:HH11	1.85	0.42
2:A:18:GLN:HG2	2:A:1418:LEU:HD13	2.01	0.41
2:A:44:THR:O	2:A:45:GLN:HB2	2.20	0.41
2:A:47:ARG:HH12	2:A:254:GLU:HG2	1.84	0.41
2:A:55:ASP:O	2:A:55:ASP:OD2	2.37	0.41
2:A:76:GLU:O	2:A:78:PRO:HD3	2.20	0.41
2:A:500:GLU:OE2	3:B:1145:SER:HB2	2.20	0.41
2:A:560:ILE:HG13	9:H:78:SER:HB2	2.02	0.41
2:A:576:GLN:O	2:A:577:ILE:C	2.63	0.41
2:A:896:ARG:HB3	2:A:897:TYR:CD1	2.55	0.41
2:A:933:TYR:C	2:A:935:GLN:H	2.27	0.41
2:A:1377:THR:O	2:A:1378:GLN:C	2.63	0.41
3:B:170:LEU:HA	3:B:171:PRO:HD2	1.94	0.41
3:B:785:TYR:C	3:B:787:VAL:N	2.77	0.41
3:B:1034:VAL:HG23	3:B:1059:LEU:HD13	2.02	0.41
8:G:9:LEU:CG	8:G:10:ASN:N	2.83	0.41
8:G:50:ASP:OD1	8:G:50:ASP:O	2.38	0.41
8:G:145:VAL:CG1	8:G:146:LYS:H	2.23	0.41
9:H:48:PRO:C	9:H:49:VAL:HG23	2.45	0.41
1:R:11:U:HO2'	1:R:12:5BU:P	2.43	0.41
2:A:53:LEU:CD2	2:A:54:ASN:N	2.53	0.41
2:A:185:TRP:CZ3	2:A:200:ARG:HG2	2.55	0.41
2:A:403:LYS:O	2:A:404:TYR:CG	2.73	0.41
2:A:444:PHE:HB3	2:A:458:HIS:CD2	2.55	0.41
2:A:526:ASP:O	2:A:527:THR:C	2.63	0.41
2:A:1028:THR:O	2:A:1029:ARG:C	2.63	0.41
2:A:1125:ALA:C	2:A:1127:ASP:H	2.29	0.41
2:A:1444:MET:CE	7:F:135:ARG:HB2	2.49	0.41
3:B:31:TRP:O	3:B:32:ALA:C	2.62	0.41
3:B:63:ILE:CD1	3:B:421:PHE:CZ	3.03	0.41
3:B:70:ILE:O	3:B:70:ILE:HG22	2.19	0.41
3:B:276:ILE:CD1	3:B:355:ILE:HG21	2.33	0.41
3:B:459:TYR:C	3:B:459:TYR:HD2	2.28	0.41
3:B:769:TYR:O	3:B:772:ALA:N	2.53	0.41
3:B:911:ILE:HD11	3:B:941:LEU:HB2	2.02	0.41
3:B:1081:LEU:O	3:B:1082:MET:C	2.64	0.41
3:B:1216:LEU:C	3:B:1217:TYR:HD1	2.28	0.41
4:C:56:THR:CG2	4:C:57:VAL:H	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:194:GLU:C	4:C:195:GLN:HG3	2.45	0.41
6:E:140:LEU:O	6:E:141:VAL:C	2.63	0.41
10:I:2:THR:O	10:I:3:THR:C	2.63	0.41
12:K:6:ARG:O	12:K:8:GLU:N	2.53	0.41
2:A:600:PRO:CG	2:A:601:LYS:H	2.29	0.41
2:A:926:GLN:O	2:A:930:ASP:HB2	2.20	0.41
3:B:488:TYR:O	3:B:489:SER:C	2.62	0.41
3:B:523:CYS:SG	3:B:524:PRO:HD2	2.59	0.41
3:B:773:MET:O	3:B:775:LYS:N	2.53	0.41
3:B:1137:CYS:O	3:B:1140:ALA:HB3	2.20	0.41
4:C:189:THR:CG2	4:C:190:ASP:N	2.77	0.41
5:D:198:LEU:O	5:D:201:LYS:HB2	2.20	0.41
6:E:61:GLN:HG2	6:E:62:ALA:H	1.80	0.41
8:G:44:TYR:O	8:G:78:VAL:CG1	2.68	0.41
8:G:122:ASN:HD22	8:G:125:SER:HB3	1.80	0.41
11:J:58:GLU:O	11:J:59:LYS:C	2.61	0.41
12:K:27:ALA:HB1	12:K:28:PRO:CD	2.45	0.41
1:R:5:C:O2'	3:B:463:THR:HA	2.21	0.41
2:A:242:PRO:HA	2:A:243:PRO:HD2	1.86	0.41
2:A:470:LEU:HD21	2:A:487:MET:HE3	2.02	0.41
2:A:541:ILE:HG22	2:A:546:VAL:HG23	2.01	0.41
2:A:574:GLY:O	2:A:575:LYS:C	2.62	0.41
2:A:1077:THR:C	2:A:1079:MET:H	2.28	0.41
2:A:1216:ILE:HA	2:A:1219:THR:OG1	2.19	0.41
2:A:1281:ARG:C	2:A:1282:VAL:HG23	2.45	0.41
2:A:1435:PRO:O	2:A:1436:ILE:HD12	2.20	0.41
3:B:498:THR:O	3:B:498:THR:HG22	2.21	0.41
3:B:542:MET:HG2	3:B:747:MET:HB3	2.02	0.41
3:B:563:MET:HE2	3:B:588:GLY:CA	2.51	0.41
5:D:176:GLU:O	5:D:178:ALA:N	2.53	0.41
8:G:23:LYS:HE2	8:G:27:LYS:NZ	2.34	0.41
8:G:51:TYR:O	8:G:54:ILE:HG13	2.21	0.41
12:K:5:ASP:O	12:K:6:ARG:C	2.62	0.41
12:K:6:ARG:C	12:K:8:GLU:H	2.28	0.41
12:K:10:PHE:CD1	12:K:11:LEU:CD2	3.04	0.41
2:A:18:GLN:O	3:B:1215:ARG:HG2	2.20	0.41
2:A:34:LYS:HD3	2:A:34:LYS:H	1.84	0.41
2:A:48:ALA:C	2:A:49:LYS:HG3	2.46	0.41
2:A:489:LEU:HD12	2:A:490:HIS:N	2.35	0.41
2:A:774:ARG:NE	2:A:797:LYS:CB	2.83	0.41
2:A:779:PHE:CD1	2:A:785:PRO:HD3	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:913:LEU:HD12	2:A:914:GLU:H	1.81	0.41
2:A:1015:VAL:CG1	2:A:1019:CYS:SG	3.08	0.41
2:A:1143:LEU:HB2	2:A:1271:ILE:HG21	2.01	0.41
2:A:1265:ASN:O	2:A:1268:LEU:N	2.53	0.41
2:A:1437:GLY:O	2:A:1438:THR:C	2.63	0.41
3:B:202:TYR:CE1	3:B:204:ILE:HD11	2.56	0.41
3:B:579:ARG:HD2	3:B:586:TRP:CZ2	2.56	0.41
3:B:798:TYR:CE2	4:C:62:PHE:HZ	2.36	0.41
3:B:801:LYS:N	11:J:52:THR:HG22	2.35	0.41
3:B:1060:ARG:C	3:B:1062:HIS:N	2.75	0.41
3:B:1109:GLY:HA3	3:B:1110:PRO:HD2	1.80	0.41
3:B:1160:VAL:HG12	3:B:1161:HIS:H	1.86	0.41
3:B:1169:MET:HE2	3:B:1204:PHE:HD1	1.84	0.41
5:D:12:ARG:O	5:D:14:ARG:N	2.54	0.41
6:E:63:ASN:HA	6:E:64:PRO:HD3	1.87	0.41
6:E:186:LEU:C	6:E:188:LEU:H	2.29	0.41
8:G:59:GLY:HA3	8:G:70:PHE:CD2	2.55	0.41
9:H:76:THR:O	9:H:77:ARG:HB2	2.20	0.41
9:H:103:LYS:HG2	9:H:104:PHE:N	2.35	0.41
10:I:50:THR:CG2	10:I:51:ASN:N	2.82	0.41
13:L:52:GLY:O	13:L:53:HIS:C	2.64	0.41
2:A:71:GLN:C	2:A:73:GLY:H	2.27	0.41
2:A:116:ASP:O	2:A:117:GLU:C	2.63	0.41
2:A:262:LEU:O	2:A:263:THR:C	2.61	0.41
2:A:381:THR:HG22	2:A:384:ASN:ND2	2.36	0.41
2:A:402:ALA:HA	2:A:434:ARG:HA	2.01	0.41
2:A:455:MET:HE3	3:B:1134:GLU:CG	2.50	0.41
2:A:506:ALA:HB1	2:A:508:PRO:HD2	2.03	0.41
2:A:1405:THR:HB	2:A:1406:VAL:H	1.76	0.41
3:B:45:SER:O	3:B:48:LEU:N	2.50	0.41
3:B:240:ILE:C	3:B:240:ILE:CD1	2.93	0.41
3:B:274:PRO:N	3:B:276:ILE:HB	2.36	0.41
3:B:386:LEU:O	3:B:387:LEU:C	2.62	0.41
3:B:418:LYS:O	3:B:419:THR:C	2.64	0.41
3:B:980:PHE:CD2	3:B:1094:ARG:HA	2.55	0.41
3:B:1084:GLN:NE2	3:B:1084:GLN:H	2.19	0.41
4:C:41:ILE:HA	4:C:42:PRO:HD3	1.82	0.41
5:D:53:SER:CB	5:D:152:SER:HB3	2.50	0.41
8:G:126:ASN:HD22	8:G:126:ASN:HA	1.56	0.41
9:H:93:TYR:CD2	9:H:143:LEU:HB3	2.55	0.41
10:I:78:CYS:SG	10:I:103:CYS:SG	3.12	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:65:HIS:CD2	12:K:66:PRO:HD2	2.56	0.41
13:L:36:SER:O	13:L:37:LYS:C	2.63	0.41
13:L:40:LEU:HB3	13:L:41:SER:H	1.72	0.41
2:A:152:VAL:HG13	2:A:153:PRO:HD2	2.03	0.41
2:A:390:GLN:O	2:A:394:ASN:ND2	2.53	0.41
2:A:406:ILE:HG22	2:A:412:ARG:HA	2.03	0.41
2:A:639:PRO:CD	2:A:640:GLN:N	2.84	0.41
2:A:851:HIS:O	2:A:854:ASN:N	2.44	0.41
3:B:25:ILE:HD11	3:B:653:VAL:C	2.44	0.41
3:B:172:ILE:CG2	3:B:173:MET:N	2.83	0.41
3:B:314:LEU:O	3:B:317:CYS:CB	2.68	0.41
3:B:378:LEU:O	3:B:378:LEU:HD12	2.20	0.41
3:B:504:ARG:HB2	3:B:507:LYS:HE2	2.03	0.41
3:B:582:VAL:O	3:B:582:VAL:CG1	2.67	0.41
3:B:595:ARG:C	3:B:597:MET:N	2.74	0.41
3:B:616:ILE:CG1	3:B:697:GLU:HA	2.51	0.41
3:B:918:ILE:HG21	3:B:935:ARG:HH11	1.81	0.41
3:B:976:ILE:CD1	3:B:992:ILE:HA	2.51	0.41
3:B:1096:ARG:HH11	3:B:1096:ARG:HG2	1.85	0.41
6:E:66:GLU:HA	6:E:69:ILE:HD12	2.01	0.41
6:E:93:MET:O	6:E:94:LYS:C	2.64	0.41
6:E:132:ILE:N	6:E:132:ILE:CD1	2.78	0.41
9:H:7:ASP:O	9:H:8:ASP:HB2	2.21	0.41
10:I:56:ALA:O	10:I:57:GLY:C	2.64	0.41
13:L:27:LEU:HD23	13:L:27:LEU:N	2.35	0.41
2:A:99:ILE:HG23	2:A:211:PHE:CZ	2.56	0.41
2:A:463:ILE:HB	2:A:464:PRO:CD	2.50	0.41
2:A:478:TYR:O	2:A:479:ASN:HB3	2.21	0.41
2:A:606:LEU:HD23	2:A:614:PHE:CE2	2.55	0.41
2:A:754:SER:O	2:A:755:PHE:C	2.64	0.41
2:A:764:CYS:SG	2:A:801:GLU:O	2.79	0.41
2:A:1001:ARG:O	2:A:1002:GLY:C	2.63	0.41
3:B:130:VAL:CG1	3:B:131:ASP:N	2.83	0.41
3:B:580:VAL:O	3:B:586:TRP:HD1	2.04	0.41
3:B:683:SER:O	3:B:685:LEU:N	2.54	0.41
3:B:798:TYR:CE2	4:C:62:PHE:CE2	3.09	0.41
3:B:1068:GLY:O	3:B:1069:PHE:C	2.64	0.41
4:C:45:ALA:HA	4:C:72:LEU:HD12	2.02	0.41
4:C:100:THR:HG22	4:C:101:LEU:N	2.29	0.41
5:D:24:ALA:HA	8:G:83:LYS:O	2.20	0.41
5:D:159:THR:O	5:D:160:VAL:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:78:LEU:HA	6:E:107:THR:HB	2.03	0.41
8:G:166:ASP:C	8:G:168:LEU:N	2.79	0.41
9:H:12:VAL:HA	9:H:28:ALA:CB	2.50	0.41
9:H:127:GLY:N	9:H:130:ARG:NH2	2.68	0.41
2:A:7:SER:O	2:A:9:ALA:N	2.54	0.41
2:A:12:ARG:CZ	3:B:1192:TYR:HE2	2.34	0.41
2:A:18:GLN:HB2	3:B:1215:ARG:HB2	2.02	0.41
2:A:77:CYS:C	2:A:78:PRO:O	2.60	0.41
2:A:337:ARG:HD3	3:B:1132:GLU:CD	2.46	0.41
2:A:407:ARG:HD2	2:A:413:ILE:HD11	2.03	0.41
2:A:464:PRO:O	2:A:465:TYR:O	2.39	0.41
2:A:481:ASP:OD1	2:A:483:ASP:OD2	2.38	0.41
2:A:507:VAL:C	2:A:509:LEU:N	2.79	0.41
2:A:528:LEU:HD23	2:A:751:SER:HA	2.03	0.41
2:A:575:LYS:O	2:A:576:GLN:O	2.38	0.41
2:A:621:THR:O	2:A:621:THR:HG22	2.21	0.41
2:A:666:ILE:HD12	2:A:667:GLY:N	2.29	0.41
2:A:711:ARG:O	2:A:714:PHE:N	2.53	0.41
2:A:794:PRO:C	2:A:796:SER:H	2.28	0.41
2:A:1059:HIS:O	2:A:1061:GLY:N	2.54	0.41
2:A:1242:VAL:O	2:A:1243:VAL:HB	2.21	0.41
2:A:1261:LYS:C	2:A:1263:ILE:N	2.74	0.41
2:A:1279:ILE:HD11	2:A:1316:VAL:CG2	2.45	0.41
2:A:1397:LEU:HB2	2:A:1426:GLU:OE1	2.20	0.41
3:B:53:GLN:HG2	3:B:547:VAL:CG2	2.50	0.41
3:B:101:MET:C	3:B:102:VAL:HG23	2.46	0.41
3:B:129:PHE:HA	3:B:165:VAL:O	2.20	0.41
3:B:496:ARG:HH11	3:B:496:ARG:CB	2.31	0.41
3:B:615:MET:HB3	3:B:626:ILE:HG12	2.03	0.41
3:B:654:ARG:C	3:B:656:GLY:N	2.79	0.41
3:B:840:ILE:HG23	3:B:992:ILE:HG23	2.03	0.41
3:B:841:MET:HE3	3:B:1010:LEU:HD11	2.03	0.41
3:B:882:THR:O	3:B:883:LEU:HB2	2.21	0.41
3:B:918:ILE:HG13	3:B:935:ARG:HD2	2.02	0.41
3:B:948:ILE:HD12	3:B:948:ILE:N	2.36	0.41
3:B:949:VAL:HG12	3:B:950:ASP:H	1.84	0.41
3:B:1012:ILE:N	3:B:1012:ILE:HD13	2.35	0.41
3:B:1034:VAL:HA	3:B:1037:LEU:HD12	2.03	0.41
5:D:52:LEU:C	5:D:54:GLU:N	2.77	0.41
6:E:105:PHE:O	6:E:106:GLN:HB2	2.21	0.41
6:E:112:TYR:CE1	6:E:136:ASN:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:117:THR:O	6:E:120:ALA:HB3	2.21	0.41
6:E:138:ALA:HA	6:E:141:VAL:CG2	2.51	0.41
6:E:144:ILE:HD12	6:E:144:ILE:C	2.44	0.41
7:F:103:MET:O	7:F:104:ASN:CB	2.68	0.41
8:G:1:MET:HE1	8:G:79:PHE:HA	2.03	0.41
8:G:51:TYR:CD2	8:G:51:TYR:O	2.74	0.41
8:G:79:PHE:CZ	8:G:106:MET:HE2	2.55	0.41
10:I:8:ARG:HE	10:I:8:ARG:HB2	1.63	0.41
10:I:85:PHE:HD1	10:I:99:LEU:HD13	1.86	0.41
13:L:60:ARG:HH21	13:L:65:VAL:HG21	1.85	0.41
2:A:123:ARG:C	2:A:125:ALA:N	2.76	0.41
2:A:226:GLU:O	2:A:226:GLU:HG2	2.21	0.41
2:A:310:GLY:O	2:A:312:PRO:HD2	2.21	0.41
2:A:514:PRO:CB	2:A:875:ALA:HB3	2.51	0.41
2:A:600:PRO:C	2:A:602:ASP:N	2.77	0.41
2:A:603:ASN:HB3	2:A:604:GLY:H	1.62	0.41
2:A:714:PHE:CB	10:I:97:MET:HE1	2.50	0.41
2:A:1094:VAL:HG13	2:A:1113:THR:CB	2.51	0.41
2:A:1142:THR:O	2:A:1145:SER:OG	2.37	0.41
2:A:1198:ASP:HB3	2:A:1201:ALA:HB3	2.03	0.41
3:B:216:GLU:HA	3:B:406:LEU:HD23	2.03	0.41
3:B:370:PHE:C	3:B:372:SER:H	2.29	0.41
3:B:628:THR:O	3:B:629:ASP:C	2.64	0.41
3:B:654:ARG:H	3:B:657:HIS:CD2	2.20	0.41
3:B:734:HIS:O	3:B:735:ALA:HB2	2.21	0.41
3:B:1045:SER:HB3	3:B:1046:PRO:CD	2.50	0.41
3:B:1086:PHE:O	3:B:1086:PHE:CG	2.71	0.41
4:C:85:ASP:O	4:C:86:CYS:C	2.64	0.41
4:C:163:ILE:O	4:C:165:LYS:N	2.54	0.41
5:D:27:LEU:HD13	5:D:173:HIS:HD2	1.86	0.41
5:D:128:VAL:O	5:D:129:LEU:C	2.63	0.41
7:F:82:THR:HA	7:F:83:PRO:HD3	1.80	0.41
7:F:116:ASP:O	7:F:120:ILE:HG13	2.21	0.41
2:A:7:SER:HA	3:B:1175:LEU:HD22	2.02	0.40
2:A:41:MET:HB3	2:A:48:ALA:O	2.21	0.40
2:A:871:ASP:HB3	6:E:204:THR:HG23	2.03	0.40
2:A:928:LEU:O	2:A:931:GLU:N	2.55	0.40
3:B:350:GLN:O	3:B:351:TYR:C	2.63	0.40
3:B:976:ILE:O	3:B:976:ILE:HG22	2.20	0.40
3:B:1110:PRO:HG2	3:B:1119:VAL:HG21	2.02	0.40
4:C:77:ILE:O	4:C:79:GLN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:142:VAL:N	11:J:16:ASP:HB3	2.21	0.40
4:C:238:ILE:HA	4:C:239:PRO:HD3	1.91	0.40
5:D:48:ILE:N	5:D:48:ILE:CD1	2.84	0.40
6:E:120:ALA:C	6:E:122:LYS:N	2.77	0.40
6:E:182:ASP:O	6:E:183:PRO:C	2.64	0.40
8:G:14:HIS:O	8:G:15:PRO:C	2.64	0.40
8:G:83:LYS:HG2	8:G:149:GLY:HA2	2.03	0.40
10:I:99:LEU:C	10:I:100:PHE:HD1	2.28	0.40
2:A:40:THR:HG22	2:A:41:MET:HG3	2.03	0.40
2:A:91:PHE:N	2:A:91:PHE:CD1	2.90	0.40
2:A:184:SER:HB3	2:A:199:LEU:CD2	2.51	0.40
2:A:255:SER:O	2:A:256:GLN:HG3	2.21	0.40
2:A:278:THR:O	2:A:278:THR:HG22	2.21	0.40
2:A:341:MET:CE	2:A:843:LYS:NZ	2.82	0.40
2:A:744:LYS:CG	2:A:748:MET:HE2	2.41	0.40
2:A:1142:THR:O	2:A:1143:LEU:C	2.64	0.40
2:A:1194:ARG:HH11	2:A:1194:ARG:HG2	1.87	0.40
2:A:1348:LEU:O	2:A:1349:TYR:C	2.64	0.40
3:B:52:ASN:O	3:B:53:GLN:C	2.64	0.40
3:B:346:GLU:N	3:B:349:ILE:HD13	2.36	0.40
3:B:640:VAL:HG22	3:B:651:LEU:HD23	2.03	0.40
3:B:680:THR:HB	3:B:681:TRP:H	1.59	0.40
3:B:952:VAL:O	3:B:953:LEU:HB3	2.21	0.40
3:B:957:ASN:O	3:B:958:GLN:C	2.64	0.40
3:B:986:GLN:HE22	3:B:1022:THR:HG21	1.85	0.40
4:C:94:LYS:HB2	4:C:94:LYS:HE3	1.80	0.40
4:C:200:GLU:O	4:C:202:PRO:HD3	2.22	0.40
6:E:23:VAL:CG1	6:E:28:TYR:HD1	2.34	0.40
7:F:103:MET:CE	8:G:65:ASP:HB2	2.50	0.40
8:G:95:SER:O	8:G:97:HIS:N	2.54	0.40
8:G:149:GLY:O	8:G:159:ALA:CB	2.69	0.40
9:H:5:LEU:HD22	9:H:133:ASN:O	2.22	0.40
9:H:95:TYR:CE2	9:H:97:MET:HG3	2.56	0.40
9:H:106:GLU:O	9:H:108:SER:N	2.52	0.40
11:J:59:LYS:H	11:J:59:LYS:HG2	1.62	0.40
2:A:30:ILE:HG23	3:B:1170:THR:HG23	2.02	0.40
2:A:32:VAL:HG21	2:A:68:GLN:HE22	1.84	0.40
2:A:174:ILE:HG22	2:A:175:ARG:N	2.36	0.40
2:A:470:LEU:CD2	2:A:487:MET:HE3	2.51	0.40
2:A:489:LEU:HD12	2:A:490:HIS:H	1.87	0.40
3:B:215:GLN:NE2	3:B:215:GLN:HA	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:542:MET:HE3	3:B:636:PRO:HG3	2.03	0.40
3:B:824:ILE:O	3:B:824:ILE:HG22	2.22	0.40
3:B:1094:ARG:HH21	3:B:1098:MET:HG2	1.86	0.40
4:C:143:LEU:HD21	4:C:146:LYS:CE	2.51	0.40
4:C:204:SER:C	4:C:206:ASN:N	2.79	0.40
6:E:134:THR:C	6:E:135:PHE:HD1	2.30	0.40
8:G:87:VAL:HG23	8:G:103:VAL:HG21	2.03	0.40
11:J:21:TYR:HB2	11:J:39:LEU:HD13	2.04	0.40
11:J:45:CYS:O	11:J:48:ARG:HG3	2.20	0.40
1:R:8:U:O2	1:R:8:U:C2'	2.69	0.40
2:A:2:VAL:HG21	3:B:1157:ALA:CB	2.50	0.40
2:A:246:VAL:O	2:A:246:VAL:HG12	2.19	0.40
2:A:266:LEU:HD21	2:A:303:TYR:CZ	2.56	0.40
2:A:352:VAL:CG1	2:A:353:ILE:N	2.84	0.40
2:A:367:PRO:HB3	2:A:465:TYR:O	2.20	0.40
2:A:442:VAL:HB	2:A:489:LEU:CD1	2.45	0.40
2:A:444:PHE:HB3	2:A:458:HIS:HD2	1.87	0.40
2:A:1039:LYS:HE3	2:A:1043:ASP:OD2	2.22	0.40
2:A:1390:ASN:ND2	2:A:1390:ASN:O	2.55	0.40
3:B:53:GLN:HB2	3:B:547:VAL:HG21	2.03	0.40
3:B:308:TRP:CH2	10:I:45:ARG:HD3	2.56	0.40
3:B:911:ILE:O	3:B:911:ILE:HG22	2.21	0.40
4:C:35:ARG:NH1	12:K:41:THR:N	2.68	0.40
4:C:84:ARG:O	4:C:85:ASP:OD1	2.40	0.40
4:C:112:ASN:HD22	4:C:112:ASN:N	2.17	0.40
4:C:212:PRO:CB	4:C:213:PRO:HD2	2.41	0.40
5:D:195:ILE:O	5:D:195:ILE:CG2	2.62	0.40
8:G:126:ASN:ND2	8:G:127:PRO:HA	2.35	0.40
10:I:34:TYR:HE2	10:I:36:GLU:HB3	1.85	0.40
10:I:105:SER:O	10:I:106:CYS:HB3	2.19	0.40
12:K:47:ARG:HD3	12:K:59:ALA:O	2.22	0.40
13:L:28:LYS:HB2	13:L:39:SER:CA	2.52	0.40
2:A:106:VAL:HG13	2:A:112:LYS:H	1.86	0.40
2:A:141:LEU:O	2:A:142:CYS:SG	2.71	0.40
2:A:254:GLU:HB2	3:B:935:ARG:NH2	2.35	0.40
2:A:298:PHE:CZ	2:A:314:ALA:HB2	2.56	0.40
2:A:498:ARG:O	2:A:499:ALA:C	2.64	0.40
2:A:562:THR:HA	2:A:563:PRO:HD3	1.82	0.40
2:A:574:GLY:O	2:A:577:ILE:HD13	2.22	0.40
2:A:613:ILE:HG22	2:A:614:PHE:CD2	2.55	0.40
2:A:809:THR:OG1	2:A:812:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:962:ARG:O	2:A:963:ILE:C	2.64	0.40
2:A:1299:VAL:CG1	2:A:1300:LYS:N	2.84	0.40
2:A:1335:ILE:O	2:A:1335:ILE:HG22	2.22	0.40
3:B:190:TYR:HD2	11:J:62:ARG:O	2.05	0.40
3:B:254:LEU:HG	3:B:273:LEU:HD12	2.03	0.40
3:B:283:VAL:O	3:B:286:PHE:HB2	2.20	0.40
3:B:906:SER:O	3:B:941:LEU:HD23	2.22	0.40
3:B:1017:ILE:CB	3:B:1018:PRO:CD	3.00	0.40
3:B:1207:LEU:HA	3:B:1207:LEU:HD23	1.85	0.40
8:G:114:LEU:HD12	8:G:114:LEU:HA	1.88	0.40
8:G:143:ILE:N	8:G:143:ILE:CD1	2.85	0.40
10:I:55:THR:HG22	10:I:58:VAL:CG2	2.43	0.40
10:I:110:PHE:CD2	10:I:110:PHE:N	2.83	0.40
12:K:7:PHE:CD1	12:K:7:PHE:C	2.99	0.40
13:L:47:ARG:HB3	13:L:48:CYS:H	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	1406/1733 (81%)	973 (69%)	278 (20%)	155 (11%)	0	5
3	B	1096/1224 (90%)	754 (69%)	214 (20%)	128 (12%)	0	4
4	C	264/318 (83%)	172 (65%)	62 (24%)	30 (11%)	0	5
5	D	173/221 (78%)	116 (67%)	36 (21%)	21 (12%)	0	4
6	E	212/215 (99%)	155 (73%)	42 (20%)	15 (7%)	1	12
7	F	82/155 (53%)	72 (88%)	9 (11%)	1 (1%)	10	40
8	G	169/171 (99%)	133 (79%)	19 (11%)	17 (10%)	0	7
9	H	129/146 (88%)	89 (69%)	23 (18%)	17 (13%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	I	117/122 (96%)	83 (71%)	23 (20%)	11 (9%)	0	8
11	J	63/70 (90%)	35 (56%)	14 (22%)	14 (22%)	0	1
12	K	113/120 (94%)	83 (74%)	25 (22%)	5 (4%)	2	19
13	L	44/70 (63%)	19 (43%)	16 (36%)	9 (20%)	0	1
All	All	3868/4565 (85%)	2684 (69%)	761 (20%)	423 (11%)	0	5

All (423) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	31	SER
2	A	48	ALA
2	A	55	ASP
2	A	57	ARG
2	A	58	LEU
2	A	62	ASP
2	A	65	LEU
2	A	66	LYS
2	A	71	GLN
2	A	74	MET
2	A	93	VAL
2	A	128	ILE
2	A	130	ASP
2	A	167	CYS
2	A	170	THR
2	A	250	ILE
2	A	255	SER
2	A	286	HIS
2	A	311	GLN
2	A	318	SER
2	A	321	PRO
2	A	322	VAL
2	A	336	ILE
2	A	418	SER
2	A	423	ASP
2	A	517	ASN
2	A	536	LEU
2	A	567	LYS
2	A	576	GLN
2	A	1002	GLY
2	A	1115	SER
2	A	1314	SER

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Mol	Chain	Res	Type
2	A	1365	TYR
2	A	1377	THR
2	A	1392	SER
2	A	1405	THR
3	B	21	GLU
3	B	27	ALA
3	B	28	GLU
3	B	45	SER
3	B	58	THR
3	B	100	PRO
3	B	186	GLU
3	B	259	TYR
3	B	274	PRO
3	B	351	TYR
3	B	364	ILE
3	B	401	PHE
3	B	466	TRP
3	B	467	GLY
3	B	468	GLU
3	B	470	LYS
3	B	472	ALA
3	B	474	SER
3	B	502	ILE
3	B	504	ARG
3	B	510	LYS
3	B	571	PRO
3	B	643	ASP
3	B	709	ASP
3	B	727	LYS
3	B	731	VAL
3	B	751	VAL
3	B	867	GLY
3	B	943	SER
3	B	958	GLN
3	B	1046	PRO
3	B	1069	PHE
3	B	1097	HIS
3	B	1100	ASP
3	B	1157	ALA
3	B	1186	ASP
4	C	87	PHE
4	C	141	GLY

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Mol	Chain	Res	Type
4	C	149	LYS
4	C	161	LYS
4	C	167	HIS
4	C	209	TYR
4	C	212	PRO
4	C	231	ASN
5	D	5	THR
5	D	6	SER
5	D	8	PHE
5	D	15	LEU
5	D	19	GLU
5	D	30	GLY
5	D	169	SER
5	D	199	ASN
6	E	59	SER
6	E	106	GLN
6	E	206	GLY
8	G	2	PHE
8	G	62	LEU
8	G	63	PRO
8	G	139	ILE
9	H	36	CYS
9	H	62	SER
9	H	82	PRO
9	H	108	SER
9	H	128	ASN
10	I	9	ASP
10	I	47	GLU
10	I	106	CYS
11	J	6	ARG
11	J	32	GLU
11	J	33	GLY
11	J	55	ASP
11	J	64	ASN
12	K	114	LEU
13	L	50	ASP
13	L	56	LEU
13	L	59	ALA
13	L	60	ARG
2	A	42	ASP
2	A	54	ASN
2	A	59	GLY

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Mol	Chain	Res	Type
2	A	69	THR
2	A	70	CYS
2	A	76	GLU
2	A	111	GLY
2	A	117	GLU
2	A	124	GLN
2	A	131	SER
2	A	149	GLU
2	A	156	ASP
2	A	245	PRO
2	A	249	SER
2	A	257	ARG
2	A	331	GLY
2	A	332	LYS
2	A	335	ARG
2	A	415	LEU
2	A	424	ILE
2	A	544	ASP
2	A	626	ASN
2	A	731	ARG
2	A	789	LYS
2	A	808	LEU
2	A	824	LEU
2	A	875	ALA
2	A	926	GLN
2	A	975	HIS
2	A	1016	THR
2	A	1036	ARG
2	A	1120	LEU
2	A	1122	PRO
2	A	1128	GLN
2	A	1136	SER
2	A	1223	ASP
2	A	1266	THR
2	A	1297	GLU
2	A	1378	GLN
2	A	1386	ARG
2	A	1389	PHE
2	A	1438	THR
2	A	1448	GLU
3	B	108	VAL
3	B	114	PRO

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Mol	Chain	Res	Type
3	B	126	SER
3	B	176	SER
3	B	206	ASN
3	B	282	ILE
3	B	334	ILE
3	B	409	ALA
3	B	430	ARG
3	B	460	ALA
3	B	461	LEU
3	B	475	SER
3	B	476	ARG
3	B	543	SER
3	B	591	ARG
3	B	594	ALA
3	B	605	ARG
3	B	629	ASP
3	B	655	LYS
3	B	688	GLY
3	B	708	GLU
3	B	842	ASN
3	B	881	ASN
3	B	888	GLY
3	B	891	ASP
3	B	901	PRO
3	B	907	GLY
3	B	1016	ALA
3	B	1167	GLY
3	B	1175	LEU
3	B	1179	GLN
3	B	1188	LYS
4	C	78	GLU
4	C	84	ARG
4	C	90	ASP
4	C	240	VAL
5	D	12	ARG
5	D	13	ARG
5	D	16	LYS
5	D	47	LEU
5	D	52	LEU
5	D	131	GLU
5	D	157	GLN
6	E	36	GLU

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Mol	Chain	Res	Type
6	E	38	PRO
6	E	45	LYS
6	E	121	MET
6	E	189	GLY
7	F	154	ASP
8	G	50	ASP
8	G	67	SER
8	G	96	GLN
8	G	154	VAL
8	G	167	TYR
9	H	81	PRO
9	H	140	ALA
10	I	57	GLY
11	J	2	ILE
11	J	8	PHE
11	J	9	SER
11	J	17	LYS
11	J	24	LEU
11	J	28	ASP
11	J	29	GLU
12	K	7	PHE
13	L	35	SER
13	L	53	HIS
2	A	8	SER
2	A	253	ASN
2	A	283	GLY
2	A	360	GLU
2	A	394	ASN
2	A	409	SER
2	A	465	TYR
2	A	516	SER
2	A	592	ASP
2	A	598	LEU
2	A	603	ASN
2	A	716	ASP
2	A	739	ASP
2	A	830	LYS
2	A	846	GLU
2	A	852	TYR
2	A	903	ASN
2	A	968	GLN
2	A	1114	PRO

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Mol	Chain	Res	Type
2	A	1139	GLU
2	A	1224	LEU
2	A	1255	GLU
3	B	65	GLU
3	B	115	GLN
3	B	258	LEU
3	B	278	GLN
3	B	328	GLU
3	B	418	LYS
3	B	465	ASN
3	B	501	PRO
3	B	526	GLU
3	B	540	SER
3	B	556	THR
3	B	559	SER
3	B	641	GLU
3	B	711	GLU
3	B	764	SER
3	B	792	MET
3	B	818	PRO
3	B	869	SER
3	B	1017	ILE
3	B	1035	ALA
3	B	1065	GLN
3	B	1108	ARG
3	B	1153	GLU
3	B	1155	SER
4	C	28	ALA
4	C	77	ILE
4	C	153	LEU
4	C	156	THR
4	C	215	GLU
4	C	216	GLY
5	D	68	ARG
5	D	119	ARG
5	D	120	GLU
6	E	43	LYS
6	E	73	PRO
6	E	205	SER
8	G	17	PHE
8	G	118	ASP
8	G	141	SER

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Mol	Chain	Res	Type
9	H	32	THR
9	H	60	ALA
9	H	84	ALA
9	H	135	LEU
10	I	3	THR
10	I	11	ASN
13	L	51	CYS
2	A	89	PRO
2	A	197	PRO
2	A	219	PHE
2	A	483	ASP
2	A	526	ASP
2	A	543	LEU
2	A	577	ILE
2	A	591	PHE
2	A	605	MET
2	A	639	PRO
2	A	719	VAL
2	A	727	ASP
2	A	759	ALA
2	A	843	LYS
2	A	847	ASP
2	A	958	VAL
2	A	1211	GLN
2	A	1221	LYS
2	A	1281	ARG
2	A	1309	ASP
2	A	1313	LEU
2	A	1395	GLY
3	B	67	SER
3	B	229	ALA
3	B	367	LEU
3	B	447	ALA
3	B	505	ASP
3	B	579	ARG
3	B	597	MET
3	B	712	PRO
3	B	738	PHE
3	B	752	ALA
3	B	758	PHE
3	B	879	ARG
3	B	906	SER

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Mol	Chain	Res	Type
3	B	1144	ALA
3	B	1181	GLU
4	C	110	THR
4	C	142	VAL
4	C	164	ALA
5	D	174	PRO
6	E	44	ALA
8	G	57	GLN
8	G	156	SER
8	G	165	GLU
9	H	17	PRO
9	H	52	GLN
9	H	90	ALA
9	H	107	VAL
10	I	78	CYS
12	K	29	ASN
12	K	41	THR
13	L	44	ASP
2	A	41	MET
2	A	84	ILE
2	A	121	LEU
2	A	386	ASP
2	A	428	TYR
2	A	829	VAL
2	A	842	VAL
2	A	904	THR
2	A	1069	ALA
2	A	1335	ILE
2	A	1341	ILE
2	A	1379	GLY
2	A	1437	GLY
3	B	68	THR
3	B	240	ILE
3	B	260	GLY
3	B	459	TYR
3	B	593	PRO
3	B	598	GLU
3	B	803	LEU
3	B	813	LYS
3	B	848	ARG
3	B	1018	PRO
3	B	1041	GLU

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Mol	Chain	Res	Type
4	C	12	GLU
4	C	18	VAL
4	C	60	ASP
4	C	172	PRO
4	C	175	ALA
6	E	130	ALA
6	E	183	PRO
9	H	59	ILE
10	I	20	LYS
10	I	34	TYR
11	J	14	VAL
11	J	61	LEU
12	K	111	LEU
2	A	232	GLU
2	A	244	PRO
2	A	399	HIS
2	A	599	SER
2	A	1242	VAL
3	B	200	GLY
3	B	305	VAL
3	B	391	ASP
3	B	759	PRO
3	B	942	ARG
3	B	992	ILE
4	C	126	GLY
4	C	176	ILE
5	D	177	VAL
6	E	76	GLY
10	I	62	ILE
10	I	115	LYS
2	A	196	GLU
3	B	729	ILE
4	C	202	PRO
5	D	196	PRO
8	G	15	PRO
9	H	44	VAL
2	A	35	ILE
2	A	51	GLY
2	A	284	ALA
2	A	385	ILE
2	A	1212	VAL
13	L	55	ILE

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Mol	Chain	Res	Type
2	A	396	PRO
2	A	400	PRO
2	A	753	GLY
2	A	986	ILE
8	G	128	PRO
2	A	477	PRO
2	A	652	VAL
2	A	1302	PRO
3	B	551	PRO
2	A	61	ILE
3	B	658	ILE
3	B	1165	ILE
4	C	139	GLY

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	
2	A	1239/1520 (82%)	1133 (91%)	106 (9%)	10	33
3	B	964/1061 (91%)	840 (87%)	124 (13%)	4	20
4	C	234/274 (85%)	211 (90%)	23 (10%)	7	29
5	D	140/200 (70%)	123 (88%)	17 (12%)	5	21
6	E	196/197 (100%)	185 (94%)	11 (6%)	19	45
7	F	74/137 (54%)	63 (85%)	11 (15%)	3	16
8	G	152/152 (100%)	134 (88%)	18 (12%)	5	22
9	H	117/128 (91%)	112 (96%)	5 (4%)	26	50
10	I	113/116 (97%)	97 (86%)	16 (14%)	3	17
11	J	60/65 (92%)	51 (85%)	9 (15%)	3	16
12	K	99/102 (97%)	90 (91%)	9 (9%)	9	32
13	L	40/57 (70%)	37 (92%)	3 (8%)	12	38
All	All	3428/4009 (86%)	3076 (90%)	352 (10%)	7	27

All (352) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	VAL
2	A	11	LEU
2	A	23	SER
2	A	34	LYS
2	A	37	PHE
2	A	41	MET
2	A	53	LEU
2	A	62	ASP
2	A	67	CYS
2	A	70	CYS
2	A	93	VAL
2	A	105	CYS
2	A	110	CYS
2	A	117	GLU
2	A	205	GLU
2	A	216	VAL
2	A	227	VAL
2	A	234	MET
2	A	236	LEU
2	A	245	PRO
2	A	270	LEU
2	A	307	ASP
2	A	320	ARG
2	A	321	PRO
2	A	326	ARG
2	A	335	ARG
2	A	337	ARG
2	A	345	VAL
2	A	354	SER
2	A	375	THR
2	A	379	VAL
2	A	385	ILE
2	A	388	LEU
2	A	398	GLU
2	A	407	ARG
2	A	408	ASP
2	A	425	GLN
2	A	434	ARG
2	A	443	LEU
2	A	445	ASN
2	A	449	SER
2	A	450	LEU

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Mol	Chain	Res	Type
2	A	451	HIS
2	A	454	SER
2	A	461	LYS
2	A	462	VAL
2	A	487	MET
2	A	493	GLN
2	A	497	THR
2	A	503	GLN
2	A	504	LEU
2	A	527	THR
2	A	560	ILE
2	A	566	ILE
2	A	577	ILE
2	A	590	ARG
2	A	598	LEU
2	A	599	SER
2	A	666	ILE
2	A	676	MET
2	A	710	LEU
2	A	711	ARG
2	A	740	LEU
2	A	768	GLN
2	A	774	ARG
2	A	810	PRO
2	A	821	ARG
2	A	830	LYS
2	A	834	THR
2	A	849	MET
2	A	858	ASN
2	A	886	ILE
2	A	903	ASN
2	A	913	LEU
2	A	929	LEU
2	A	930	ASP
2	A	941	LYS
2	A	948	VAL
2	A	963	ILE
2	A	998	LEU
2	A	1001	ARG
2	A	1029	ARG
2	A	1035	TYR
2	A	1037	LEU

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Mol	Chain	Res	Type
2	A	1046	LEU
2	A	1050	GLU
2	A	1067	LEU
2	A	1111	MET
2	A	1113	THR
2	A	1116	LEU
2	A	1120	LEU
2	A	1122	PRO
2	A	1127	ASP
2	A	1146	VAL
2	A	1170	ILE
2	A	1291	VAL
2	A	1295	THR
2	A	1300	LYS
2	A	1336	MET
2	A	1359	ASP
2	A	1372	VAL
2	A	1389	PHE
2	A	1393	ASN
2	A	1405	THR
2	A	1436	ILE
2	A	1443	VAL
3	B	30	SER
3	B	44	VAL
3	B	46	GLN
3	B	57	TYR
3	B	63	ILE
3	B	90	ILE
3	B	95	ILE
3	B	100	PRO
3	B	108	VAL
3	B	128	LEU
3	B	175	ARG
3	B	188	ASP
3	B	194	GLU
3	B	203	PHE
3	B	205	ILE
3	B	223	VAL
3	B	240	ILE
3	B	250	PHE
3	B	258	LEU
3	B	261	ARG

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Mol	Chain	Res	Type
3	B	268	THR
3	B	273	LEU
3	B	277	LYS
3	B	282	ILE
3	B	284	ILE
3	B	289	LEU
3	B	291	ILE
3	B	298	LEU
3	B	365	THR
3	B	371	GLU
3	B	393	LYS
3	B	416	LEU
3	B	427	ASP
3	B	429	PHE
3	B	463	THR
3	B	465	ASN
3	B	474	SER
3	B	475	SER
3	B	476	ARG
3	B	485	ARG
3	B	490	SER
3	B	496	ARG
3	B	498	THR
3	B	501	PRO
3	B	502	ILE
3	B	504	ARG
3	B	505	ASP
3	B	508	LEU
3	B	510	LYS
3	B	516	ASN
3	B	531	GLN
3	B	549	THR
3	B	555	ILE
3	B	570	VAL
3	B	582	VAL
3	B	598	GLU
3	B	603	LEU
3	B	615	MET
3	B	616	ILE
3	B	628	THR
3	B	629	ASP
3	B	635	ARG

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Mol	Chain	Res	Type
3	B	644	GLU
3	B	649	LYS
3	B	682	SER
3	B	684	LEU
3	B	694	ASP
3	B	724	ASP
3	B	737	THR
3	B	742	GLU
3	B	743	ILE
3	B	778	MET
3	B	787	VAL
3	B	796	LEU
3	B	797	TYR
3	B	806	THR
3	B	831	SER
3	B	835	GLN
3	B	839	MET
3	B	845	SER
3	B	854	LEU
3	B	858	SER
3	B	878	GLN
3	B	894	ASP
3	B	901	PRO
3	B	906	SER
3	B	909	ASP
3	B	939	THR
3	B	953	LEU
3	B	964	VAL
3	B	986	GLN
3	B	992	ILE
3	B	997	GLU
3	B	1002	THR
3	B	1004	GLU
3	B	1006	ILE
3	B	1010	LEU
3	B	1011	ILE
3	B	1012	ILE
3	B	1018	PRO
3	B	1022	THR
3	B	1034	VAL
3	B	1037	LEU
3	B	1046	PRO

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Mol	Chain	Res	Type
3	B	1047	PHE
3	B	1077	THR
3	B	1084	GLN
3	B	1095	LEU
3	B	1099	VAL
3	B	1103	ILE
3	B	1108	ARG
3	B	1112	GLN
3	B	1160	VAL
3	B	1163	CYS
3	B	1170	THR
3	B	1172	ILE
3	B	1182	CYS
3	B	1183	LYS
3	B	1185	CYS
3	B	1193	GLN
3	B	1202	LEU
3	B	1211	ASN
3	B	1212	ILE
3	B	1214	PRO
4	C	17	ASN
4	C	22	LEU
4	C	46	ILE
4	C	54	ASN
4	C	57	VAL
4	C	58	LEU
4	C	74	SER
4	C	77	ILE
4	C	89	GLU
4	C	99	LEU
4	C	108	GLU
4	C	129	ILE
4	C	145	CYS
4	C	147	LEU
4	C	163	ILE
4	C	166	GLU
4	C	176	ILE
4	C	202	PRO
4	C	212	PRO
4	C	233	GLU
4	C	240	VAL
4	C	251	LEU

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Mol	Chain	Res	Type
4	C	266	ASP
5	D	47	LEU
5	D	126	ILE
5	D	137	ASN
5	D	139	LYS
5	D	148	LEU
5	D	152	SER
5	D	170	THR
5	D	180	LEU
5	D	185	CYS
5	D	187	THR
5	D	192	LYS
5	D	193	THR
5	D	197	SER
5	D	202	ILE
5	D	208	GLU
5	D	219	THR
5	D	221	TYR
6	E	40	GLU
6	E	60	PHE
6	E	78	LEU
6	E	132	ILE
6	E	153	HIS
6	E	175	LEU
6	E	183	PRO
6	E	184	VAL
6	E	195	VAL
6	E	198	ILE
6	E	204	THR
7	F	79	ARG
7	F	81	THR
7	F	90	ARG
7	F	99	LEU
7	F	103	MET
7	F	110	ASP
7	F	111	LEU
7	F	119	ARG
7	F	123	LYS
7	F	148	VAL
7	F	153	VAL
8	G	1	MET
8	G	11	ILE

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Mol	Chain	Res	Type
8	G	12	THR
8	G	13	LEU
8	G	15	PRO
8	G	39	THR
8	G	52	ASP
8	G	55	ASP
8	G	56	ILE
8	G	63	PRO
8	G	74	TYR
8	G	77	VAL
8	G	78	VAL
8	G	80	LYS
8	G	114	LEU
8	G	126	ASN
8	G	145	VAL
8	G	171	ILE
9	H	10	PHE
9	H	26	ILE
9	H	86	ASP
9	H	93	TYR
9	H	130	ARG
10	I	7	CYS
10	I	13	MET
10	I	15	TYR
10	I	22	ASN
10	I	31	THR
10	I	32	CYS
10	I	40	SER
10	I	78	CYS
10	I	84	VAL
10	I	85	PHE
10	I	86	PHE
10	I	94	ASP
10	I	100	PHE
10	I	101	PHE
10	I	106	CYS
10	I	110	PHE
11	J	7	CYS
11	J	9	SER
11	J	10	CYS
11	J	16	ASP
11	J	21	TYR

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Mol	Chain	Res	Type
11	J	44	TYR
11	J	46	CYS
11	J	50	ILE
11	J	64	ASN
12	K	10	PHE
12	K	11	LEU
12	K	25	THR
12	K	47	ARG
12	K	50	LEU
12	K	61	TYR
12	K	78	THR
12	K	101	LEU
12	K	114	LEU
13	L	38	LEU
13	L	55	ILE
13	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
2	A	5	GLN
2	A	54	ASN
2	A	64	ASN
2	A	92	HIS
2	A	171	GLN
2	A	225	ASN
2	A	256	GLN
2	A	273	ASN
2	A	287	HIS
2	A	299	HIS
2	A	306	ASN
2	A	313	GLN
2	A	339	ASN
2	A	394	ASN
2	A	435	HIS
2	A	451	HIS
2	A	490	HIS
2	A	493	GLN
2	A	503	GLN
2	A	576	GLN
2	A	631	HIS
2	A	650	GLN

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Mol	Chain	Res	Type
2	A	659	HIS
2	A	698	GLN
2	A	742	ASN
2	A	757	ASN
2	A	768	GLN
2	A	786	HIS
2	A	858	ASN
2	A	881	GLN
2	A	903	ASN
2	A	926	GLN
2	A	935	GLN
2	A	994	GLN
2	A	1106	ASN
2	A	1128	GLN
2	A	1130	GLN
2	A	1188	GLN
2	A	1218	GLN
2	A	1393	ASN
2	A	1427	ASN
2	A	1432	GLN
3	B	60	GLN
3	B	121	ASN
3	B	178	ASN
3	B	215	GLN
3	B	236	HIS
3	B	363	HIS
3	B	366	GLN
3	B	449	ASN
3	B	469	GLN
3	B	499	ASN
3	B	513	GLN
3	B	515	HIS
3	B	516	ASN
3	B	518	HIS
3	B	531	GLN
3	B	538	ASN
3	B	572	HIS
3	B	587	HIS
3	B	734	HIS
3	B	767	ASN
3	B	776	GLN
3	B	821	GLN

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Mol	Chain	Res	Type
3	B	842	ASN
3	B	975	GLN
3	B	1015	HIS
3	B	1065	GLN
3	B	1084	GLN
3	B	1112	GLN
3	B	1117	GLN
3	B	1179	GLN
3	B	1193	GLN
3	B	1211	ASN
4	C	17	ASN
4	C	65	HIS
4	C	73	GLN
4	C	112	ASN
4	C	123	ASN
4	C	151	GLN
4	C	167	HIS
4	C	231	ASN
5	D	39	ASN
5	D	40	HIS
5	D	132	GLN
5	D	137	ASN
5	D	173	HIS
5	D	216	ASN
6	E	5	ASN
6	E	101	GLN
6	E	104	ASN
6	E	113	GLN
6	E	114	ASN
7	F	104	ASN
8	G	53	ASN
8	G	57	GLN
8	G	126	ASN
9	H	3	ASN
9	H	133	ASN
10	I	11	ASN
10	I	12	ASN
10	I	46	HIS
10	I	60	GLN
10	I	89	GLN
12	K	29	ASN
12	K	65	HIS

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Mol	Chain	Res	Type
13	L	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	31/31 (100%)	16 (51%)	3 (9%)

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	3	A
1	R	6	A
1	R	7	C
1	R	8	U
1	R	9	G
1	R	10	A
1	R	12	5BU
1	R	13	G
1	R	24	A
1	R	25	G
1	R	26	C
1	R	27	5BU
1	R	28	5BU
1	R	29	G
1	R	31	U
1	R	32	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	2	C
1	R	5	C
1	R	6	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5BU	R	27	1	19,22,23	0.50	0	27,32,35	1.43	4 (14%)
1	5BU	R	17	1	19,22,23	0.40	0	27,32,35	1.16	1 (3%)
1	5BU	R	12	1	19,22,23	1.31	1 (5%)	27,32,35	1.59	6 (22%)
1	5BU	R	28	1	19,22,23	1.93	1 (5%)	27,32,35	1.57	4 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5BU	R	27	1	-	2/7/25/26	0/2/2/2
1	5BU	R	17	1	-	0/7/25/26	0/2/2/2
1	5BU	R	12	1	-	0/7/25/26	0/2/2/2
1	5BU	R	28	1	-	4/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	28	5BU	BR-C5	7.53	2.06	1.88
1	R	12	5BU	BR-C5	4.89	1.99	1.88

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	27	5BU	BR-C5-C4	4.75	123.49	118.02
1	R	28	5BU	C6-C5-C4	-4.15	116.46	120.67
1	R	28	5BU	O3'-C3'-C2'	4.09	124.92	111.82
1	R	17	5BU	BR-C5-C4	3.70	122.28	118.02
1	R	12	5BU	C1'-N1-C6	3.50	126.92	121.15
1	R	12	5BU	C6-C5-C4	-3.13	117.50	120.67
1	R	12	5BU	C1'-N1-C2	-3.00	112.20	117.59
1	R	27	5BU	C6-C5-C4	-2.88	117.75	120.67
1	R	28	5BU	BR-C5-C6	2.86	124.64	120.64
1	R	28	5BU	C2'-C1'-N1	2.61	120.51	113.25
1	R	12	5BU	O4'-C1'-N1	2.58	114.22	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	12	5BU	O3'-C3'-C2'	2.51	119.88	111.82
1	R	12	5BU	BR-C5-C6	2.45	124.07	120.64
1	R	27	5BU	C1'-N1-C6	-2.39	117.22	121.15
1	R	27	5BU	C1'-N1-C2	2.16	121.48	117.59

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	R	27	5BU	O4'-C4'-C5'-O5'
1	R	28	5BU	O4'-C4'-C5'-O5'
1	R	28	5BU	C3'-C4'-C5'-O5'
1	R	27	5BU	C3'-C4'-C5'-O5'
1	R	28	5BU	C4'-C5'-O5'-P
1	R	28	5BU	C2'-C1'-N1-C2

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	R	27	5BU	1	0
1	R	17	5BU	3	0
1	R	12	5BU	4	0
1	R	28	5BU	4	0

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

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	R	23/31 (74%)	0.51	2 (8%) 16 16	86, 105, 133, 157	0
2	A	1416/1733 (81%)	0.01	42 (2%) 52 36	22, 86, 159, 180	0
3	B	1112/1224 (90%)	0.22	45 (4%) 42 30	26, 95, 168, 180	0
4	C	266/318 (83%)	-0.10	4 (1%) 72 50	47, 82, 139, 156	0
5	D	177/221 (80%)	0.40	9 (5%) 33 25	56, 108, 156, 177	0
6	E	214/215 (99%)	0.52	12 (5%) 30 23	56, 141, 179, 180	0
7	F	84/155 (54%)	-0.34	2 (2%) 59 41	28, 59, 98, 122	0
8	G	171/171 (100%)	-0.05	2 (1%) 76 54	54, 82, 124, 133	0
9	H	133/146 (91%)	0.79	12 (9%) 15 16	105, 144, 178, 180	0
10	I	119/122 (97%)	0.36	5 (4%) 40 29	82, 135, 166, 180	0
11	J	65/70 (92%)	-0.13	1 (1%) 72 50	48, 78, 125, 133	0
12	K	115/120 (95%)	-0.27	3 (2%) 57 39	45, 83, 113, 143	0
13	L	46/70 (65%)	0.76	4 (8%) 16 16	73, 139, 174, 179	0
All	All	3941/4596 (85%)	0.13	143 (3%) 46 32	22, 92, 168, 180	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	56	PRO	7.1
3	B	882	THR	7.1
2	A	1081	LEU	6.2
9	H	63	LEU	5.7
2	A	1205	LYS	5.5
5	D	25	ALA	5.2
3	B	335	GLY	4.9
9	H	90	ALA	4.7
5	D	24	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
3	B	883	LEU	4.4
3	B	505	ASP	4.4
3	B	877	PRO	4.4
3	B	934	LYS	4.2
5	D	18	VAL	4.2
3	B	113	TYR	3.9
9	H	140	ALA	3.9
3	B	467	GLY	3.9
2	A	830	LYS	3.8
5	D	4	SER	3.8
3	B	468	GLU	3.8
2	A	69	THR	3.7
2	A	49	LYS	3.7
1	R	2	C	3.5
9	H	139	ASN	3.5
9	H	107	VAL	3.5
2	A	1254	ALA	3.5
2	A	1176	LEU	3.5
5	D	15	LEU	3.4
2	A	79	GLY	3.4
3	B	446	LEU	3.4
3	B	472	ALA	3.3
3	B	1224	PHE	3.3
6	E	5	ASN	3.3
2	A	3	GLY	3.2
10	I	100	PHE	3.2
3	B	730	ARG	3.2
9	H	59	ILE	3.2
2	A	1173	HIS	3.2
3	B	471	LYS	3.1
3	B	879	ARG	3.0
3	B	469	GLN	3.0
2	A	252	PHE	3.0
3	B	473	MET	3.0
1	R	32	G	3.0
10	I	120	GLN	3.0
10	I	2	THR	2.9
3	B	245	GLU	2.9
2	A	149	GLU	2.8
3	B	477	ALA	2.8
6	E	2	ASP	2.8
13	L	43	THR	2.8

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Mol	Chain	Res	Type	RSRZ
8	G	21	ARG	2.8
7	F	155	LEU	2.8
2	A	1125	ALA	2.8
2	A	68	GLN	2.7
2	A	705	LYS	2.7
2	A	168	GLY	2.7
2	A	289	ILE	2.7
3	B	425	THR	2.7
2	A	57	ARG	2.7
10	I	111	THR	2.7
3	B	1184	GLY	2.7
8	G	150	CYS	2.7
2	A	195	ASP	2.6
3	B	643	ASP	2.6
9	H	144	ILE	2.6
6	E	51	GLY	2.6
3	B	933	SER	2.6
6	E	88	VAL	2.6
2	A	292	ALA	2.6
6	E	107	THR	2.6
2	A	120	GLU	2.6
6	E	4	GLU	2.6
2	A	147	VAL	2.6
7	F	72	LYS	2.6
3	B	349	ILE	2.5
2	A	62	ASP	2.5
6	E	93	MET	2.5
12	K	115	ALA	2.5
4	C	222	LYS	2.5
12	K	114	LEU	2.5
3	B	246	LYS	2.5
12	K	11	LEU	2.5
3	B	652	LYS	2.5
2	A	2	VAL	2.5
13	L	32	ALA	2.4
9	H	136	LYS	2.4
2	A	288	ALA	2.4
6	E	55	ARG	2.4
13	L	27	LEU	2.4
4	C	224	GLN	2.4
3	B	561	TRP	2.4
2	A	40	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	257	ARG	2.4
2	A	1393	ASN	2.4
3	B	731	VAL	2.4
3	B	448	ILE	2.3
2	A	1257	ASP	2.3
2	A	333	GLU	2.3
2	A	115	LEU	2.3
3	B	100	PRO	2.3
2	A	186	LYS	2.3
3	B	726	ALA	2.3
9	H	141	TYR	2.3
6	E	10	SER	2.3
3	B	132	VAL	2.3
3	B	216	GLU	2.2
4	C	232	VAL	2.2
9	H	33	GLN	2.2
6	E	42	PHE	2.2
2	A	832	ALA	2.2
3	B	954	VAL	2.2
2	A	59	GLY	2.2
6	E	69	ILE	2.2
2	A	760	GLN	2.2
5	D	12	ARG	2.2
3	B	875	GLU	2.2
4	C	3	GLU	2.2
6	E	90	VAL	2.1
3	B	101	MET	2.1
2	A	1166	ASP	2.1
2	A	153	PRO	2.1
3	B	503	GLY	2.1
13	L	25	ALA	2.1
2	A	1258	HIS	2.1
2	A	51	GLY	2.1
2	A	290	GLU	2.1
10	I	55	THR	2.1
3	B	274	PRO	2.1
3	B	728	ARG	2.1
9	H	134	ASN	2.1
9	H	96	VAL	2.1
3	B	734	HIS	2.1
5	D	8	PHE	2.1
5	D	9	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
3	B	884	ARG	2.0
3	B	876	LYS	2.0
3	B	610	ASN	2.0
11	J	65	PRO	2.0
3	B	709	ASP	2.0
5	D	19	GLU	2.0
2	A	154	SER	2.0
3	B	347	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	5BU	R	27	21/22	0.76	0.12	140,148,161,171	0
1	5BU	R	28	21/22	0.77	0.11	130,138,155,167	0
1	5BU	R	12	21/22	0.86	0.10	96,112,134,153	0
1	5BU	R	17	21/22	0.90	0.10	88,105,129,149	0

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(Å ²)	Q<0.9
14	ZN	I	1122	1/1	0.97	0.05	176,176,176,176	0
14	ZN	A	2456	1/1	0.98	0.06	73,73,73,73	0
14	ZN	L	1071	1/1	0.98	0.04	114,114,114,114	0
14	ZN	B	2225	1/1	0.99	0.02	66,66,66,66	0
14	ZN	I	1121	1/1	0.99	0.05	85,85,85,85	0
15	MG	A	2458	1/1	0.99	0.07	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	ZN	J	1066	1/1	1.00	0.05	65,65,65,65	0
14	ZN	A	2457	1/1	1.00	0.01	46,46,46,46	0
14	ZN	C	1269	1/1	1.00	0.02	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.