



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:06 AM UTC

PDB ID : 1K83 / pdb_00001k83
Title : Crystal Structure of Yeast RNA Polymerase II Complexed with the Inhibitor Alpha Amanitin
Authors : Bushnell, D.A.; Cramer, P.; Kornberg, R.D.
Deposited on : 2001-10-22
Resolution : 2.80 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

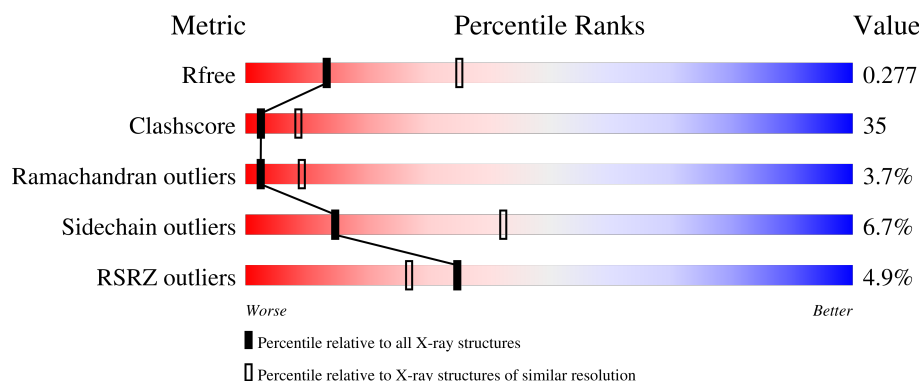
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1733	3% 37% 34% 7% 21%
2	B	1224	4% 45% 38% 5% 12%
3	C	318	% 34% 42% 7% 16%
4	E	215	2% 52% 41% 6% .
5	F	155	% 23% 28% . 46%

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Mol	Chain	Length	Quality of chain
6	H	146	18% 27% 49% 13% • 9%
7	I	122	5% 42% 51% 7%
8	J	70	% 46% 43% • • 7%
9	K	120	% 42% 44% 8% • 5%
10	L	70	17% 13% 37% 14% 36%
11	M	8	25% 12% 50% 38%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 27902 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II LARGEST SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1366	Total	C	N	O	S	0	0	0
			10751	6785	1871	2036	59			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1082	Total	C	N	O	S	0	0	0
			8616	5467	1503	1594	52			

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

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

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1744	1107	308	318	11			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE.

TIDE.

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

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	122	Total	C	N	O	S	0	0	0
			997	613	182	191	11			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	45	Total	C	N	O	S	0	0	0
			359	221	71	63	4			

- Molecule 11 is a protein called ALPHA AMANITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	8	Total	C	N	O	S	0	0	0
			64	39	10	14	1			

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 13 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total 1	Mn 1	0	0

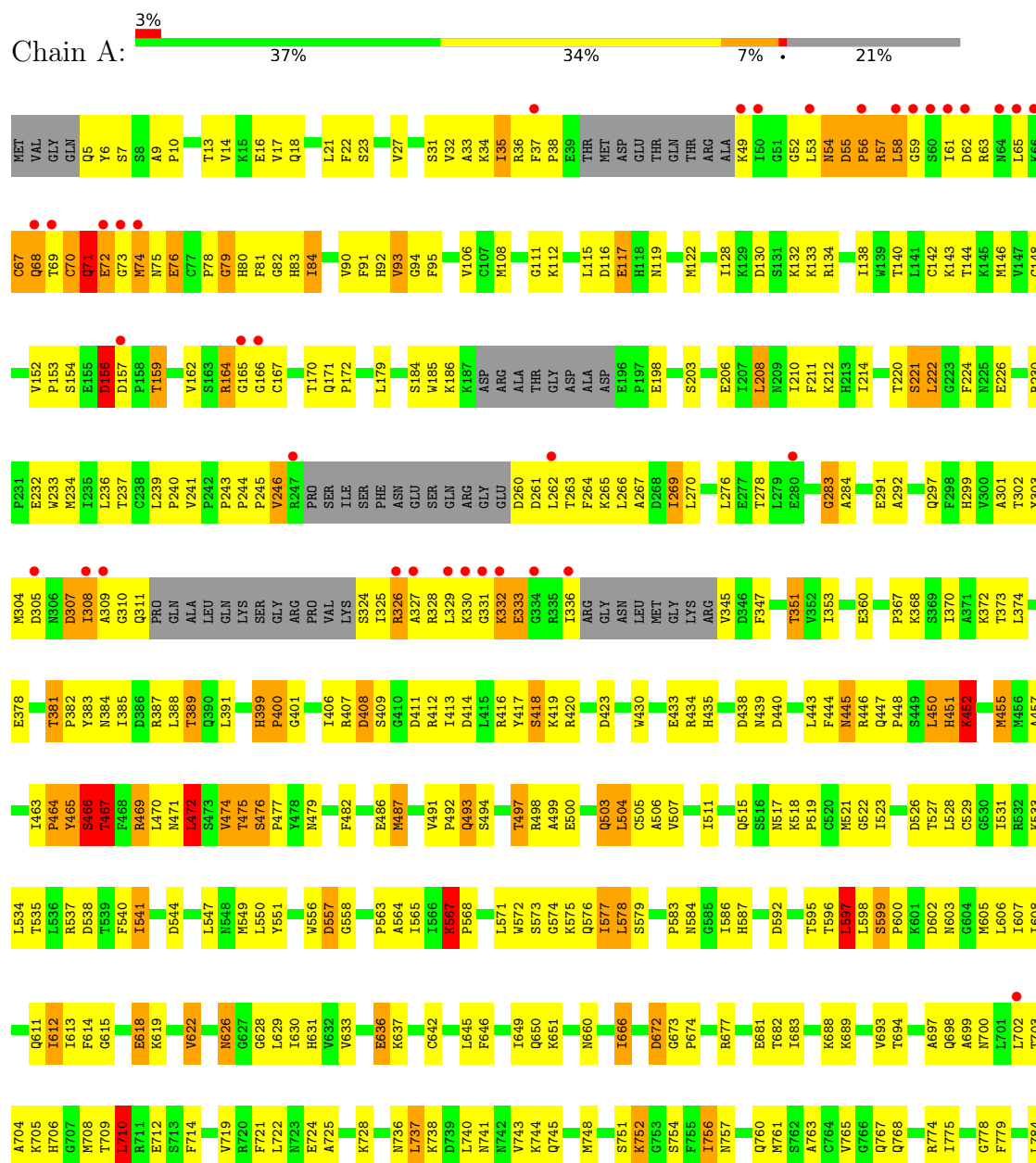
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	31	Total 31	O 31	0	0
14	B	23	Total 23	O 23	0	0
14	C	3	Total 3	O 3	0	0
14	E	6	Total 6	O 6	0	0
14	F	4	Total 4	O 4	0	0
14	J	1	Total 1	O 1	0	0
14	M	1	Total 1	O 1	0	0

3 Residue-property plots

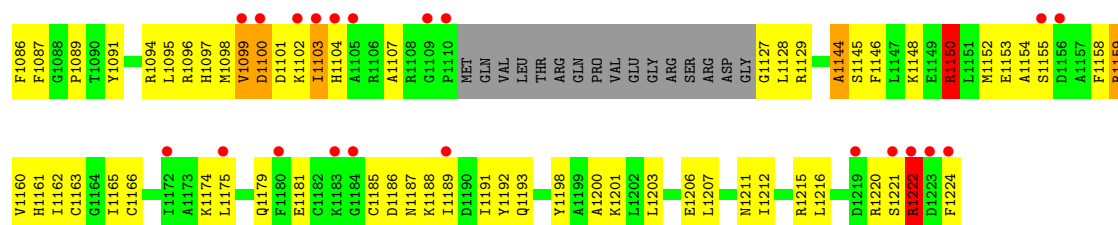
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

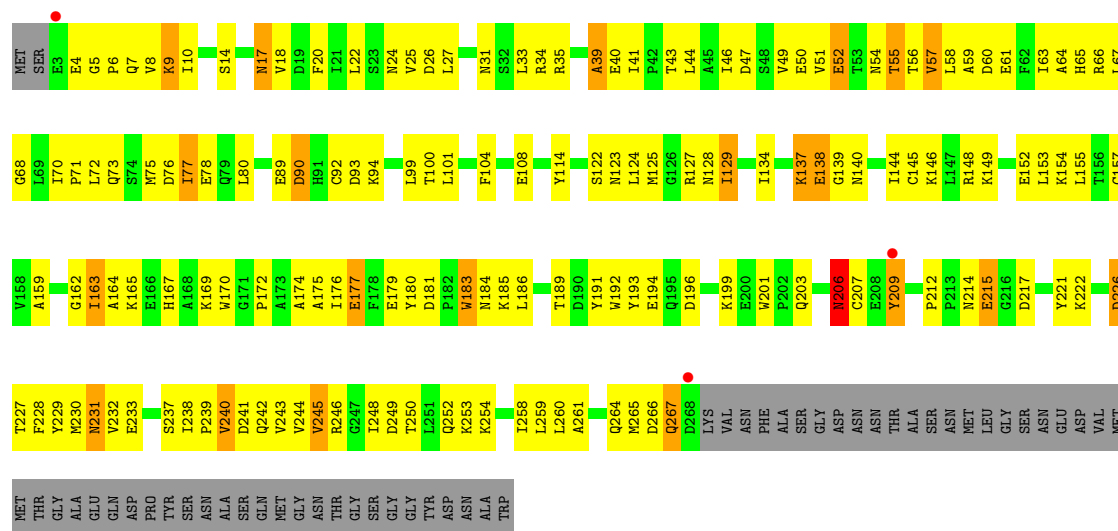




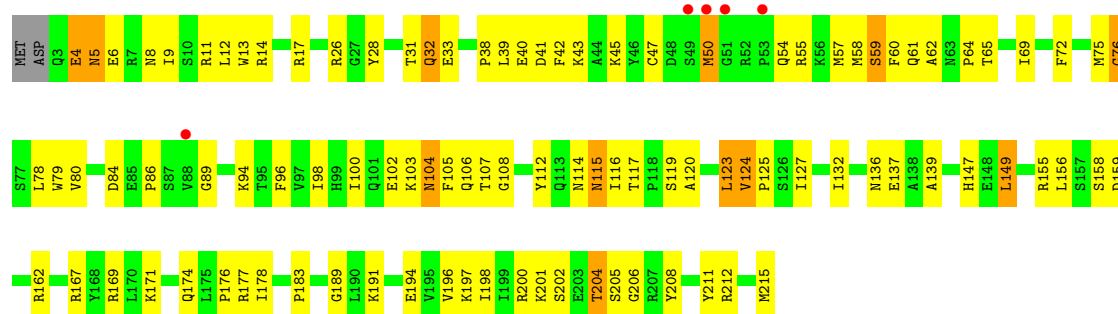




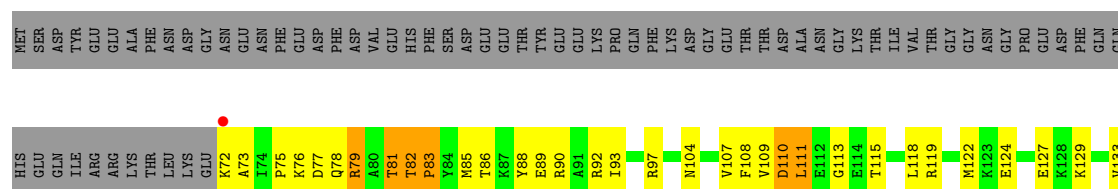
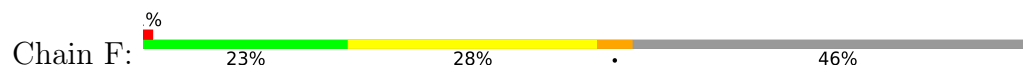
● Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE

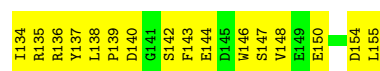


● Molecule 4: DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE

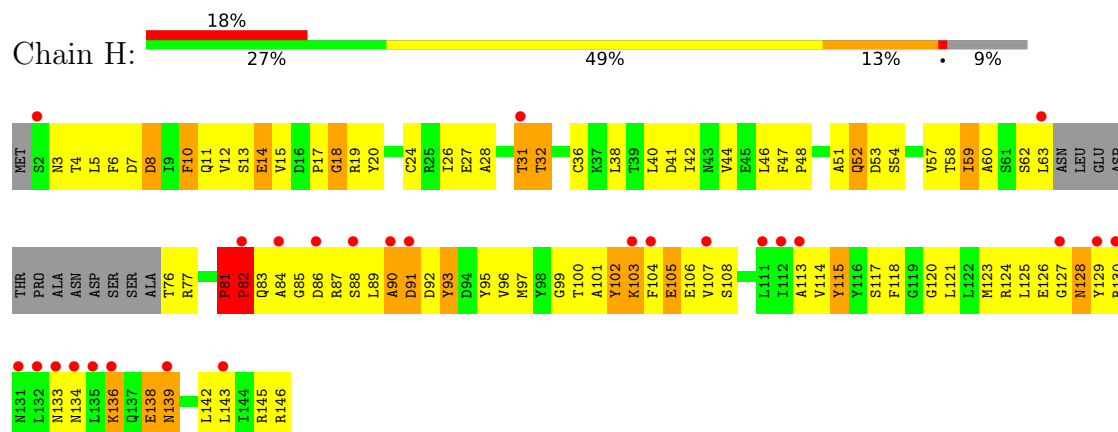


● Molecule 5: DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE

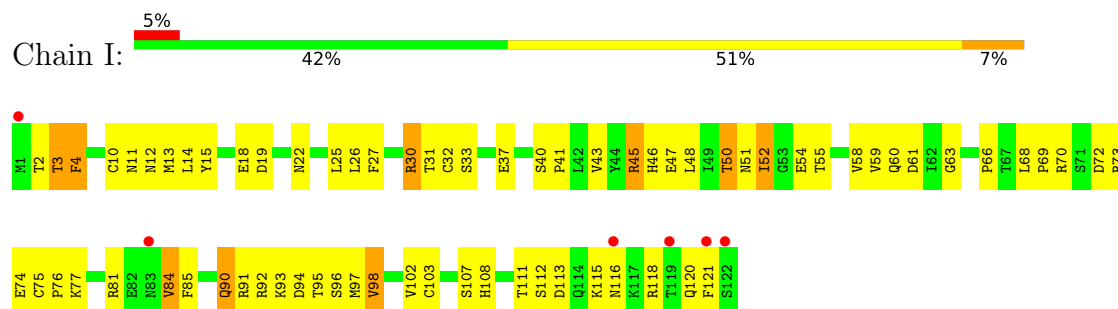




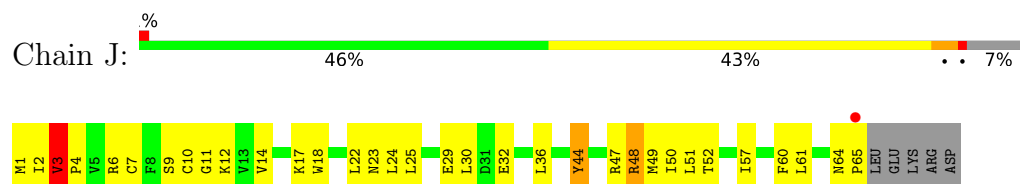
● Molecule 6: DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE



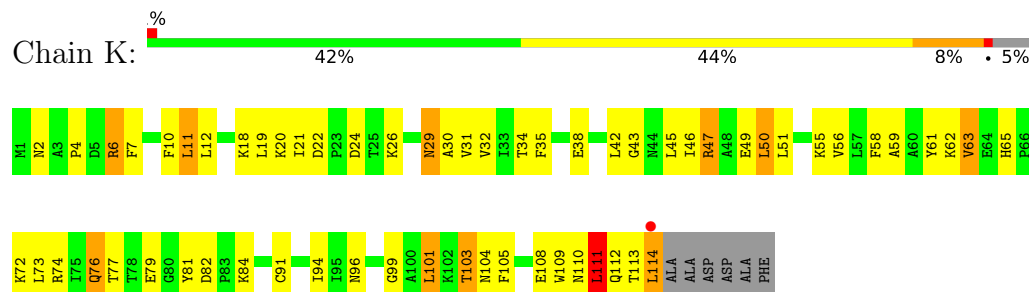
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE



• Molecule 8: DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE

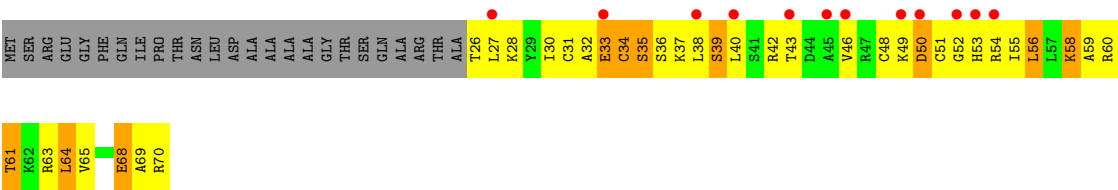


● Molecule 9: DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE

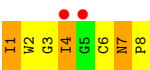
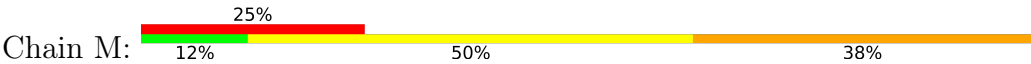


• Molecule 10: DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE





● Molecule 11: ALPHA AMANITIN



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.51Å 222.48Å 374.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 92.7 (20.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.280 0.227 , 0.277	Depositor DCC
R_{free} test set	3507 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27902	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: TRX, MN, ZN, HYP, ILX, CSX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	1/10940 (0.0%)	1.05	57/14792 (0.4%)
2	B	0.53	0/8786	1.02	47/11847 (0.4%)
3	C	0.50	0/2133	1.03	7/2891 (0.2%)
4	E	0.49	0/1780	1.00	5/2395 (0.2%)
5	F	0.56	0/691	1.05	1/933 (0.1%)
6	H	0.42	0/1086	1.04	11/1470 (0.7%)
7	I	0.52	0/1016	1.03	5/1365 (0.4%)
8	J	0.51	0/541	1.05	4/727 (0.6%)
9	K	0.45	0/937	0.88	0/1265
10	L	0.49	0/361	0.99	2/478 (0.4%)
11	M	3.44	3/22 (13.6%)	2.31	1/26 (3.8%)
All	All	0.53	4/28293 (0.0%)	1.03	140/38189 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	4	ILE	CA-C	9.28	1.62	1.52
11	M	7	ASN	CA-C	6.51	1.66	1.52
1	A	487	MET	SD-CE	-6.30	1.63	1.79
11	M	4	ILE	C-O	6.20	1.31	1.24

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	333	GLU	N-CA-C	-10.85	100.59	114.04
1	A	827	THR	N-CA-C	-10.25	99.31	112.23
1	A	1155	ASP	CA-C-N	9.81	129.17	118.97
1	A	1155	ASP	C-N-CA	9.81	129.17	118.97
6	H	31	THR	N-CA-C	-8.92	98.75	110.53
1	A	452	LYS	N-CA-C	-8.67	101.54	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	171	LYS	N-CA-C	-8.65	97.72	110.52
1	A	798	GLY	N-CA-C	8.30	126.98	115.27
6	H	136	LYS	N-CA-C	-8.30	101.24	112.94
4	E	80	VAL	N-CA-C	-8.03	101.30	110.05
2	B	825	VAL	N-CA-C	7.76	119.03	108.17
8	J	9	SER	N-CA-C	7.75	119.50	111.14
3	C	40	GLU	N-CA-C	7.70	122.73	111.87
2	B	1078	GLY	N-CA-C	-7.65	105.26	115.21
6	H	92	ASP	N-CA-C	-7.52	104.15	112.72
2	B	736	THR	N-CA-C	-7.44	103.52	112.59
6	H	102	TYR	N-CA-C	-7.41	102.48	112.26
6	H	81	PRO	N-CA-C	7.40	119.73	110.70
7	I	10	CYS	N-CA-C	7.39	122.33	113.16
10	L	58	LYS	N-CA-C	7.37	121.96	113.19
2	B	732	SER	N-CA-C	7.35	120.01	110.53
2	B	609	ILE	N-CA-C	-7.32	97.94	108.48
1	A	222	LEU	N-CA-C	-7.31	98.39	109.79
2	B	710	LEU	N-CA-C	-7.23	102.74	112.94
2	B	1085	ILE	N-CA-C	7.08	118.07	108.17
1	A	491	VAL	N-CA-C	6.88	114.36	107.55
1	A	779	PHE	N-CA-C	-6.86	101.68	110.53
1	A	1341	ILE	N-CA-C	6.85	117.60	110.62
3	C	39	ALA	N-CA-C	6.76	122.19	113.88
5	F	83	PRO	N-CA-C	-6.75	105.15	114.27
2	B	111	ALA	N-CA-C	-6.72	100.53	110.48
2	B	292	ILE	N-CA-C	6.71	123.37	108.88
1	A	1032	LEU	N-CA-C	6.60	118.27	111.14
1	A	660	ASN	N-CA-C	-6.59	103.91	112.68
1	A	564	ALA	N-CA-C	-6.57	104.75	112.89
2	B	280	ILE	N-CA-C	6.52	115.75	108.05
1	A	234	MET	N-CA-C	-6.51	105.31	113.18
1	A	797	LYS	N-CA-C	6.47	120.65	113.21
2	B	172	ILE	N-CA-C	6.45	117.19	108.17
1	A	1405	THR	N-CA-C	-6.42	104.15	112.23
3	C	183	TRP	N-CA-C	-6.41	98.28	108.73
6	H	115	TYR	N-CA-C	6.32	119.70	109.40
6	H	134	ASN	N-CA-C	6.32	118.68	110.53
1	A	567	LYS	CA-C-N	-6.30	113.65	119.82
1	A	567	LYS	C-N-CA	-6.30	113.65	119.82
3	C	55	THR	N-CA-C	-6.27	104.94	112.59
8	J	44	TYR	N-CA-C	6.20	120.40	112.34
1	A	326	ARG	N-CA-C	-6.18	103.86	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1086	PHE	N-CA-C	-6.17	100.51	109.59
2	B	606	LYS	N-CA-C	-6.17	102.12	111.56
2	B	851	PHE	N-CA-C	6.15	122.11	113.56
1	A	54	ASN	N-CA-C	6.15	120.11	112.24
1	A	1154	TYR	N-CA-C	-6.13	97.72	108.20
1	A	472	LEU	N-CA-C	6.12	119.85	112.38
1	A	931	GLU	N-CA-C	-6.11	104.70	111.36
2	B	200	GLY	N-CA-C	6.10	127.64	113.18
2	B	703	ILE	N-CA-C	6.10	116.71	108.17
1	A	1434	ALA	N-CA-C	6.07	117.36	109.64
1	A	156	ASP	CA-C-O	6.06	121.46	117.94
2	B	894	ASP	N-CA-C	-6.03	101.27	110.14
1	A	1130	GLN	N-CA-C	-6.02	105.43	112.89
2	B	1066	SER	N-CA-C	6.00	123.57	110.80
1	A	507	VAL	CB-CA-C	-5.96	108.04	113.70
1	A	81	PHE	N-CA-C	5.93	119.92	109.96
2	B	343	ILE	N-CA-C	5.92	116.69	109.30
3	C	191	TYR	N-CA-C	5.91	118.82	109.96
1	A	332	LYS	N-CA-C	-5.89	105.85	114.39
2	B	264	SER	N-CA-C	-5.88	101.81	110.52
1	A	710	LEU	N-CA-C	-5.88	103.85	111.02
1	A	688	LYS	N-CA-C	-5.80	103.69	112.04
10	L	33	GLU	N-CA-C	5.78	119.95	111.34
2	B	99	LYS	N-CA-C	-5.76	101.65	110.07
2	B	829	CYS	N-CA-C	-5.75	99.15	108.41
1	A	1156	PRO	N-CA-C	5.74	121.68	113.47
2	B	743	ILE	N-CA-C	-5.74	105.14	110.53
7	I	84	VAL	N-CA-C	-5.73	99.88	108.12
2	B	591	ARG	N-CA-C	-5.72	102.83	110.55
2	B	232	SER	CA-C-N	5.71	125.81	119.87
2	B	232	SER	C-N-CA	5.71	125.81	119.87
1	A	76	GLU	N-CA-C	-5.70	106.96	114.31
1	A	864	ILE	N-CA-C	-5.69	106.91	111.81
2	B	1146	PHE	N-CA-C	-5.65	105.20	111.36
2	B	1009	ASP	N-CA-C	-5.64	106.24	113.23
1	A	828	ALA	N-CA-C	-5.62	105.07	111.14
7	I	31	THR	N-CA-C	-5.60	102.51	111.02
1	A	156	ASP	CB-CA-C	-5.59	109.02	117.07
1	A	884	ASP	N-CA-C	5.59	117.82	111.11
2	B	56	ASP	N-CA-C	5.58	117.03	111.07
2	B	136	THR	N-CA-C	5.58	117.18	109.15
1	A	1209	MET	N-CA-C	-5.56	105.22	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	72	PHE	CA-C-N	5.55	125.22	119.05
4	E	72	PHE	C-N-CA	5.55	125.22	119.05
1	A	998	LEU	N-CA-C	5.52	118.81	109.76
7	I	90	GLN	N-CA-C	-5.50	103.22	110.43
2	B	1001	PHE	N-CA-C	5.49	117.41	109.07
1	A	1311	VAL	N-CA-C	5.48	116.63	108.46
2	B	227	LYS	N-CA-C	-5.47	102.80	110.35
3	C	226	ASP	N-CA-C	-5.47	101.44	109.81
2	B	837	ASP	N-CA-C	5.46	121.15	113.56
2	B	232	SER	N-CA-C	5.46	115.88	109.60
1	A	221	SER	N-CA-C	-5.44	105.50	111.82
1	A	1403	GLU	N-CA-C	-5.44	106.71	113.19
3	C	177	GLU	N-CA-C	-5.44	102.95	110.35
1	A	1098	VAL	CB-CA-C	-5.44	108.53	113.70
6	H	10	PHE	N-CA-C	5.43	118.58	109.95
2	B	955	THR	N-CA-C	5.41	115.53	108.07
2	B	1150	ARG	N-CA-C	5.41	118.34	111.69
6	H	86	ASP	N-CA-C	-5.40	106.83	113.41
2	B	857	ARG	N-CA-C	-5.39	100.61	109.40
1	A	117	GLU	N-CA-C	-5.35	106.72	113.20
6	H	57	VAL	N-CA-C	5.35	115.78	107.28
1	A	567	LYS	N-CA-C	5.33	121.59	109.81
2	B	1000	PRO	N-CA-C	-5.32	103.48	111.57
1	A	597	LEU	N-CA-C	-5.32	106.82	113.15
2	B	1166	CYS	N-CA-C	-5.32	101.04	109.76
1	A	474	VAL	N-CA-C	-5.32	106.69	112.80
2	B	1144	ALA	N-CA-C	5.29	117.12	111.36
1	A	471	ASN	N-CA-C	-5.28	102.46	110.28
1	A	1121	GLU	CA-C-N	5.26	126.41	119.84
1	A	1121	GLU	C-N-CA	5.26	126.41	119.84
6	H	103	LYS	N-CA-C	5.24	118.40	110.64
2	B	619	ILE	N-CA-C	5.22	115.43	110.42
1	A	578	LEU	N-CA-C	-5.21	105.60	111.28
1	A	269	ILE	N-CA-C	-5.18	105.33	110.62
1	A	802	ASN	N-CA-C	5.18	117.37	110.53
1	A	898	ARG	N-CA-C	5.16	117.17	109.59
1	A	1066	VAL	N-CA-C	-5.14	105.37	110.62
7	I	25	LEU	N-CA-C	5.13	117.98	109.46
4	E	32	GLN	N-CA-C	-5.13	105.67	112.34
11	M	4	ILE	CA-C-O	5.13	126.89	121.04
8	J	3	VAL	CA-C-N	-5.13	114.50	119.78
8	J	3	VAL	C-N-CA	-5.13	114.50	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	202	TYR	N-CA-C	5.12	116.45	109.18
2	B	526	GLU	N-CA-C	5.08	117.56	108.17
2	B	748	ILE	N-CA-C	-5.08	105.44	112.50
2	B	774	GLY	N-CA-C	-5.08	106.59	113.24
2	B	864	LYS	N-CA-C	5.07	121.61	110.80
1	A	224	PHE	N-CA-C	5.07	118.02	110.52
2	B	378	LEU	N-CA-C	-5.06	105.85	111.36
1	A	493	GLN	N-CA-C	5.02	119.49	113.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10751	0	10819	796	0
2	B	8616	0	8645	605	0
3	C	2095	0	2051	178	0
4	E	1744	0	1772	96	0
5	F	679	0	701	60	0
6	H	1068	0	1040	119	0
7	I	997	0	953	83	0
8	J	532	0	542	60	0
9	K	919	0	929	70	0
10	L	359	0	382	65	1
11	M	64	0	51	7	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	I	2	0	0	0	0
12	J	1	0	0	0	0
12	L	1	0	0	0	0
13	A	1	0	0	0	0
14	A	31	0	0	1	0
14	B	23	0	0	5	0
14	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	E	6	0	0	1	0
14	F	4	0	0	0	0
14	J	1	0	0	0	0
14	M	1	0	0	0	0
All	All	27902	0	27885	1926	1

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 35.

All (1926) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.09	1.15
1:A:974:ASP:HB2	6:H:136:LYS:HZ3	1.15	1.12
1:A:470:LEU:HD11	1:A:487:MET:HE1	1.21	1.10
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.17	1.09
2:B:871:THR:HG22	2:B:872:GLU:H	1.09	1.09
1:A:855:THR:HG21	1:A:857:ARG:HE	1.10	1.08
3:C:265:MET:HE1	9:K:19:LEU:HB2	1.31	1.08
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.33	1.07
1:A:1394:THR:HG22	1:A:1395:GLY:H	1.10	1.06
2:B:800:GLN:HB3	8:J:52:THR:CG2	1.86	1.05
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.36	1.04
2:B:955:THR:HG22	2:B:956:THR:H	1.23	1.04
9:K:47:ARG:HB3	9:K:47:ARG:HH11	1.23	1.02
3:C:56:THR:HG23	3:C:58:LEU:H	1.15	1.02
1:A:672:ASP:HB2	1:A:736:ASN:ND2	1.73	1.02
2:B:29:ASP:HB3	2:B:658:ILE:CD1	1.88	1.02
1:A:308:ILE:HG22	1:A:309:ALA:H	1.25	1.01
1:A:450:LEU:H	1:A:450:LEU:HD12	1.27	0.99
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.45	0.99
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.28	0.99
1:A:901:LEU:N	1:A:926:GLN:HE21	1.61	0.98
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.45	0.98
1:A:55:ASP:H	1:A:56:PRO:HD2	1.28	0.97
1:A:849:MET:HE1	1:A:1436:ILE:HA	1.46	0.97
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.46	0.97
7:I:111:THR:HG22	7:I:113:ASP:H	1.28	0.97
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.46	0.97
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.43	0.97
1:A:1336:MET:HE3	1:A:1381:LEU:HG	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:65:HIS:HD2	9:K:67:PHE:H	1.04	0.96
1:A:470:LEU:HD11	1:A:487:MET:CE	1.95	0.96
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.80	0.96
2:B:542:MET:HG3	2:B:747:MET:HE3	1.46	0.95
1:A:80:HIS:O	1:A:243:PRO:HB3	1.66	0.95
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.94	0.95
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.45	0.95
1:A:345:VAL:HG21	2:B:1129:ARG:HA	1.46	0.95
1:A:901:LEU:H	1:A:926:GLN:NE2	1.64	0.94
2:B:392:ARG:NH2	7:I:52:ILE:HD11	1.81	0.94
5:F:111:LEU:HD12	5:F:111:LEU:H	1.30	0.94
2:B:1153:GLU:HG2	2:B:1154:ALA:H	1.30	0.94
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.47	0.94
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.65	0.94
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.48	0.94
2:B:244:LEU:HD11	2:B:366:GLN:HE21	1.29	0.94
2:B:205:ILE:HD13	2:B:461:LEU:HB3	1.48	0.93
2:B:654:ARG:H	2:B:657:HIS:HD2	1.12	0.93
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.51	0.93
1:A:597:LEU:H	1:A:597:LEU:HD12	1.34	0.92
2:B:542:MET:HE2	2:B:747:MET:HG3	1.50	0.92
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	0.94	0.92
1:A:49:LYS:HD3	1:A:55:ASP:HB2	1.49	0.92
1:A:399:HIS:O	1:A:401:GLY:N	2.02	0.92
8:J:44:TYR:HA	8:J:47:ARG:HG3	1.52	0.92
1:A:903:ASN:HD22	1:A:905:ASP:H	1.14	0.91
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.32	0.91
1:A:704:ALA:HB2	1:A:710:LEU:HD12	1.52	0.91
1:A:1446:ASP:HB2	5:F:133:VAL:HG23	1.50	0.91
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.53	0.91
2:B:103:ASN:HB2	2:B:169:ARG:NH2	1.86	0.90
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.51	0.90
8:J:64:ASN:HB3	8:J:65:PRO:HD3	1.53	0.90
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.36	0.90
2:B:365:THR:HG22	2:B:367:LEU:H	1.35	0.90
1:A:672:ASP:HB2	1:A:736:ASN:HD21	1.31	0.90
1:A:374:LEU:HD23	2:B:1107:ALA:HB2	1.53	0.90
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.53	0.90
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	1.69	0.89
1:A:567:LYS:HB3	6:H:96:VAL:N	1.88	0.89
2:B:205:ILE:HD11	2:B:461:LEU:HD23	1.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	1.69	0.89
1:A:714:PHE:HB2	7:I:97:MET:HE1	1.54	0.88
1:A:705:LYS:HB2	1:A:708:MET:HE3	1.52	0.88
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.55	0.88
1:A:33:ALA:O	1:A:83:HIS:HB3	1.74	0.88
2:B:879:ARG:HE	2:B:885:MET:HE2	1.36	0.88
1:A:179:LEU:HD21	1:A:308:ILE:HD13	1.56	0.87
3:C:148:ARG:NH1	8:J:64:ASN:HA	1.89	0.87
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.56	0.87
2:B:563:MET:CE	2:B:580:VAL:HB	2.05	0.87
6:H:100:THR:OG1	6:H:138:GLU:HG3	1.73	0.87
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.54	0.87
1:A:1161:THR:HG22	1:A:1163:ILE:N	1.90	0.87
5:F:81:THR:CG2	5:F:136:ARG:HH11	1.88	0.87
1:A:112:LYS:NZ	1:A:165:GLY:H	1.73	0.87
4:E:78:LEU:HD23	4:E:107:THR:HB	1.56	0.87
2:B:806:THR:HG22	2:B:808:ALA:H	1.39	0.86
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.54	0.86
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.56	0.86
1:A:587:HIS:CE1	1:A:969:GLN:HG2	2.10	0.86
2:B:130:VAL:HG12	2:B:131:ASP:H	1.41	0.86
2:B:205:ILE:CD1	2:B:461:LEU:HB3	2.06	0.86
4:E:159:ASP:HA	4:E:162:ARG:NH1	1.91	0.86
1:A:1383:SER:HB3	1:A:1387:HIS:NE2	1.91	0.86
9:K:113:THR:O	9:K:114:LEU:HB2	1.74	0.85
2:B:705:MET:HE3	2:B:742:GLU:HG3	1.57	0.85
1:A:305:ASP:HB3	1:A:326:ARG:CZ	2.06	0.85
10:L:61:THR:HB	10:L:63:ARG:HG2	1.58	0.85
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.59	0.85
3:C:73:GLN:HE21	3:C:75:MET:H	1.24	0.84
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.11	0.84
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.57	0.84
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.57	0.84
1:A:122:MET:HE1	1:A:138:ILE:HG23	1.60	0.84
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	1.58	0.84
2:B:268:THR:HG21	2:B:270:LYS:HE3	1.60	0.83
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.60	0.83
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.77	0.83
2:B:1051:THR:HG22	2:B:1053:GLU:N	1.92	0.83
1:A:500:GLU:OE2	1:A:1438:THR:HG21	1.77	0.83
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.61	0.83
6:H:130:ARG:HA	6:H:133:ASN:HD22	1.41	0.83
1:A:444:PHE:CE2	1:A:470:LEU:HD21	2.13	0.83
2:B:651:LEU:HD11	2:B:707:PRO:HB3	1.59	0.83
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.61	0.83
1:A:132:LYS:HZ1	1:A:1411:GLU:HB3	1.44	0.82
1:A:901:LEU:H	1:A:926:GLN:HE21	0.85	0.82
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.44	0.82
2:B:324:ILE:HD11	2:B:333:PHE:CD1	2.15	0.82
1:A:587:HIS:NE2	1:A:969:GLN:HG2	1.94	0.81
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.62	0.81
1:A:709:THR:HG21	7:I:93:LYS:O	1.79	0.81
1:A:1394:THR:HG22	1:A:1395:GLY:N	1.92	0.81
6:H:130:ARG:HA	6:H:133:ASN:ND2	1.95	0.81
7:I:47:GLU:OE1	7:I:50:THR:HG23	1.79	0.81
1:A:32:VAL:HG11	1:A:68:GLN:HE22	1.44	0.81
3:C:174:ALA:O	8:J:10:CYS:HB2	1.79	0.81
1:A:982:THR:HG22	1:A:984:LYS:H	1.46	0.81
2:B:531:GLN:CD	2:B:531:GLN:H	1.87	0.81
2:B:914:LYS:HB3	2:B:937:ALA:O	1.81	0.81
1:A:38:PRO:HA	1:A:270:LEU:HD13	1.63	0.80
1:A:1198:ASP:O	1:A:1202:MET:HG2	1.81	0.80
3:C:25:VAL:HG23	3:C:228:PHE:HE1	1.46	0.80
1:A:63:ARG:HA	1:A:74:MET:HE2	1.62	0.80
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.61	0.80
1:A:444:PHE:HE2	1:A:470:LEU:HD21	1.47	0.80
10:L:26:THR:HG22	10:L:27:LEU:H	1.47	0.80
1:A:503:GLN:HE21	5:F:90:ARG:NH2	1.80	0.80
5:F:109:VAL:HG12	5:F:110:ASP:N	1.96	0.80
5:F:109:VAL:HG12	5:F:110:ASP:H	1.46	0.80
1:A:913:LEU:HD11	1:A:981:LEU:O	1.81	0.79
1:A:55:ASP:O	1:A:57:ARG:N	2.14	0.79
3:C:51:VAL:HG22	3:C:155:LEU:HD12	1.64	0.79
2:B:254:LEU:CD2	2:B:381:MET:HE1	2.12	0.79
9:K:65:HIS:CD2	9:K:67:PHE:H	1.96	0.79
1:A:567:LYS:NZ	6:H:46:LEU:HB2	1.98	0.79
2:B:244:LEU:HD11	2:B:366:GLN:NE2	1.96	0.79
1:A:55:ASP:N	1:A:56:PRO:HD2	1.97	0.79
1:A:347:PHE:H	2:B:1107:ALA:HA	1.47	0.79
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.12	0.79
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:THR:HG23	3:C:58:LEU:N	1.94	0.79
9:K:29:ASN:HD21	9:K:79:GLU:HA	1.48	0.79
2:B:63:ILE:HB	2:B:95:ILE:HD11	1.65	0.79
2:B:889:THR:HG22	2:B:891:ASP:H	1.44	0.78
1:A:328:ARG:HD3	1:A:332:LYS:NZ	1.97	0.78
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.13	0.78
6:H:105:GLU:O	6:H:107:VAL:HG23	1.84	0.78
2:B:871:THR:HG22	2:B:872:GLU:N	1.92	0.78
3:C:148:ARG:HH12	8:J:64:ASN:HA	1.45	0.78
2:B:294:ASP:H	7:I:12:ASN:ND2	1.82	0.78
5:F:147:SER:OG	5:F:150:GLU:HG3	1.84	0.77
1:A:112:LYS:HZ2	1:A:165:GLY:H	1.30	0.77
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.67	0.77
1:A:974:ASP:HB2	6:H:136:LYS:NZ	1.98	0.77
2:B:871:THR:CG2	2:B:872:GLU:H	1.91	0.77
10:L:26:THR:HG22	10:L:27:LEU:N	2.00	0.77
2:B:652:LYS:HE3	2:B:688:GLY:O	1.85	0.77
6:H:97:MET:HE3	6:H:142:LEU:HD23	1.67	0.77
1:A:1094:VAL:HG12	1:A:1095:THR:H	1.49	0.77
7:I:50:THR:H	7:I:92:ARG:HH12	1.33	0.76
3:C:258:ILE:HD13	9:K:35:PHE:HE2	1.50	0.76
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.65	0.76
4:E:100:ILE:HD13	4:E:108:GLY:HA3	1.66	0.76
3:C:22:LEU:HD21	9:K:101:LEU:HD21	1.64	0.76
1:A:596:THR:HG22	1:A:597:LEU:H	1.51	0.76
1:A:677:ARG:O	1:A:681:GLU:HG3	1.85	0.76
1:A:1400:CYS:HB3	1:A:1405:THR:OG1	1.85	0.76
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.66	0.76
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.67	0.76
1:A:276:LEU:HD13	1:A:292:ALA:HB3	1.67	0.76
1:A:849:MET:HE3	1:A:1063:MET:SD	2.26	0.76
2:B:705:MET:CE	2:B:742:GLU:HG3	2.17	0.76
4:E:94:LYS:HG3	4:E:123:LEU:HD11	1.65	0.75
6:H:15:VAL:HG22	6:H:26:ILE:HG12	1.68	0.75
6:H:101:ALA:H	6:H:138:GLU:HA	1.50	0.75
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.67	0.75
6:H:103:LYS:HZ2	6:H:114:VAL:HB	1.51	0.75
4:E:155:ARG:HD2	4:E:194:GLU:OE2	1.86	0.75
1:A:55:ASP:C	1:A:57:ARG:H	1.95	0.75
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.51	0.75
1:A:855:THR:HG21	1:A:857:ARG:NE	1.96	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.67	0.75
1:A:901:LEU:HA	1:A:907:THR:HG23	1.67	0.74
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.68	0.74
3:C:261:ALA:O	3:C:265:MET:HB2	1.86	0.74
7:I:45:ARG:HG2	7:I:45:ARG:HH11	1.53	0.74
9:K:18:LYS:HZ2	9:K:38:GLU:HG2	1.53	0.74
1:A:760:GLN:HE22	11:M:1:ILX:HG23	1.53	0.74
2:B:345:LYS:HA	2:B:348:ARG:NH1	2.03	0.74
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.69	0.74
8:J:2:ILE:HD11	8:J:57:ILE:CD1	2.18	0.74
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.68	0.74
1:A:567:LYS:HB3	6:H:96:VAL:H	1.52	0.73
8:J:48:ARG:HG2	8:J:48:ARG:HH11	1.51	0.73
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.70	0.73
10:L:32:ALA:HB2	10:L:55:ILE:HB	1.70	0.73
1:A:666:ILE:HD12	2:B:1030:LEU:HD22	1.69	0.73
7:I:98:VAL:HG21	7:I:113:ASP:HB2	1.69	0.73
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.03	0.73
9:K:47:ARG:HB3	9:K:47:ARG:NH1	2.01	0.73
3:C:137:LYS:H	3:C:137:LYS:HD2	1.53	0.73
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.18	0.73
6:H:104:PHE:O	6:H:106:GLU:N	2.21	0.73
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.24	0.73
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.24	0.73
1:A:170:THR:HG21	1:A:186:LYS:O	1.89	0.73
2:B:654:ARG:H	2:B:657:HIS:CD2	2.03	0.73
6:H:36:CYS:HB2	6:H:129:TYR:OH	1.88	0.73
2:B:709:ASP:HB2	2:B:733:HIS:HB3	1.71	0.73
6:H:125:LEU:C	6:H:130:ARG:HH12	1.97	0.72
1:A:1128:GLN:O	1:A:1132:LYS:HG3	1.87	0.72
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.54	0.72
3:C:196:ASP:OD2	3:C:199:LYS:HG3	1.90	0.72
1:A:329:LEU:O	1:A:333:GLU:N	2.22	0.72
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.72	0.72
1:A:974:ASP:CB	6:H:136:LYS:HZ3	1.99	0.72
6:H:11:GLN:NE2	6:H:52:GLN:HA	2.04	0.72
1:A:108:MET:HG2	1:A:171:GLN:HE22	1.53	0.72
1:A:903:ASN:ND2	1:A:905:ASP:H	1.86	0.72
3:C:196:ASP:CG	3:C:199:LYS:HG3	2.14	0.72
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.72	0.72
2:B:999:MET:HA	2:B:999:MET:HE3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:VAL:HG12	2:B:131:ASP:N	2.02	0.71
2:B:680:THR:HG22	2:B:681:TRP:N	2.05	0.71
1:A:523:ILE:HD12	1:A:622:VAL:HG22	1.70	0.71
2:B:997:GLU:HG2	3:C:39:ALA:HB2	1.72	0.71
1:A:526:ASP:HB2	2:B:835:GLN:OE1	1.91	0.71
3:C:250:THR:O	3:C:254:LYS:HG3	1.90	0.71
5:F:81:THR:HG22	5:F:136:ARG:HH11	1.54	0.71
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.38	0.71
1:A:5:GLN:HG2	1:A:6:TYR:H	1.55	0.71
1:A:132:LYS:NZ	1:A:1411:GLU:HB3	2.04	0.71
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.25	0.71
2:B:879:ARG:HB3	2:B:883:LEU:CD2	2.21	0.71
3:C:66:ARG:NH2	8:J:3:VAL:O	2.23	0.71
1:A:907:THR:HG22	1:A:908:LEU:H	1.56	0.71
2:B:277:LYS:N	2:B:277:LYS:HD2	2.06	0.71
9:K:30:ALA:HB2	9:K:76:GLN:HG3	1.73	0.71
2:B:243:ALA:HB2	2:B:251:ILE:HG12	1.73	0.71
2:B:1097:HIS:HB3	2:B:1102:LYS:NZ	2.06	0.70
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.21	0.70
1:A:1398:MET:HG3	1:A:1426:GLU:OE2	1.92	0.70
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.30	0.70
1:A:567:LYS:CB	1:A:568:PRO:CD	2.69	0.70
1:A:308:ILE:HG22	1:A:309:ALA:N	2.04	0.70
1:A:573:SER:HB3	1:A:576:GLN:HG3	1.74	0.70
1:A:1394:THR:HG23	1:A:1398:MET:HE3	1.73	0.70
2:B:955:THR:HG23	10:L:54:ARG:O	1.92	0.70
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.73	0.70
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.56	0.70
3:C:5:GLY:C	3:C:24:ASN:HD22	2.00	0.70
10:L:46:VAL:HG13	10:L:56:LEU:HD12	1.74	0.70
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.07	0.70
1:A:329:LEU:HA	1:A:332:LYS:HB2	1.74	0.69
2:B:899:ILE:HG22	2:B:900:ALA:N	2.05	0.69
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.73	0.69
1:A:672:ASP:CB	1:A:736:ASN:HD21	2.03	0.69
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.07	0.69
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.73	0.69
2:B:890:TYR:HB3	2:B:893:LEU:HD12	1.73	0.69
2:B:1181:GLU:HG3	2:B:1188:LYS:HE2	1.73	0.69
6:H:130:ARG:HA	6:H:133:ASN:HB2	1.74	0.69
1:A:855:THR:CG2	1:A:857:ARG:HE	1.98	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:954:VAL:O	10:L:55:ILE:O	2.11	0.69
3:C:22:LEU:HD12	3:C:230:MET:HE3	1.72	0.69
1:A:1398:MET:HG2	1:A:1425:SER:HB2	1.73	0.69
3:C:25:VAL:HG23	3:C:228:PHE:CE1	2.28	0.69
8:J:36:LEU:HB2	8:J:47:ARG:HH21	1.57	0.69
1:A:56:PRO:O	1:A:57:ARG:HG3	1.93	0.69
1:A:262:LEU:O	1:A:266:LEU:HG	1.93	0.69
2:B:542:MET:CE	2:B:747:MET:HG3	2.23	0.69
2:B:801:LYS:O	8:J:52:THR:HG23	1.93	0.69
10:L:38:LEU:HG	10:L:39:SER:H	1.58	0.69
1:A:1147:THR:HB	7:I:48:LEU:HD12	1.75	0.69
5:F:76:LYS:O	5:F:79:ARG:HD2	1.93	0.69
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.74	0.68
1:A:1395:GLY:C	1:A:1397:LEU:H	2.01	0.68
2:B:1198:TYR:CE1	2:B:1201:LYS:HD3	2.28	0.68
7:I:111:THR:HG22	7:I:112:SER:N	2.07	0.68
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.74	0.68
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.57	0.68
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.75	0.68
2:B:737:THR:HG21	7:I:66:PRO:HA	1.76	0.68
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.28	0.68
1:A:714:PHE:CB	7:I:97:MET:HE1	2.23	0.68
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.75	0.68
1:A:1341:ILE:HD12	1:A:1379:GLY:HA2	1.76	0.68
2:B:120:ARG:NH2	10:L:54:ARG:HD2	2.09	0.68
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.74	0.68
1:A:140:THR:HA	1:A:143:LYS:HE2	1.76	0.67
1:A:725:ALA:HA	1:A:728:LYS:HE2	1.74	0.67
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.75	0.67
1:A:445:ASN:CB	1:A:455:MET:HG2	2.19	0.67
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.28	0.67
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.77	0.67
1:A:465:TYR:HA	9:K:2:ASN:HB3	1.76	0.67
1:A:1077:THR:HG22	1:A:1077:THR:O	1.94	0.67
2:B:118:ARG:NH1	2:B:204:ILE:HD11	2.09	0.67
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.24	0.67
6:H:103:LYS:NZ	6:H:114:VAL:HB	2.09	0.67
1:A:1341:ILE:HD11	1:A:1376:THR:HG23	1.77	0.67
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.41	0.67
7:I:4:PHE:HE1	7:I:13:MET:HE2	1.60	0.67
10:L:34:CYS:HB3	10:L:51:CYS:SG	2.34	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1181:GLU:CG	2:B:1188:LYS:HE2	2.25	0.67
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.30	0.67
1:A:1394:THR:CG2	1:A:1395:GLY:H	1.93	0.67
2:B:130:VAL:CG2	2:B:167:ILE:HD12	2.25	0.67
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.25	0.67
5:F:77:ASP:O	5:F:78:GLN:HB2	1.94	0.67
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.19	0.67
5:F:138:LEU:HD12	5:F:142:SER:OG	1.94	0.67
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.24	0.66
1:A:858:ASN:C	1:A:858:ASN:HD22	2.02	0.66
2:B:876:LYS:HE2	2:B:893:LEU:O	1.94	0.66
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.76	0.66
2:B:979:LYS:HE3	2:B:987:LYS:HD2	1.77	0.66
1:A:67:CYS:O	1:A:68:GLN:HB2	1.93	0.66
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.76	0.66
2:B:62:ILE:O	2:B:65:GLU:HG2	1.95	0.66
1:A:49:LYS:HD3	1:A:55:ASP:CB	2.22	0.66
1:A:1191:TRP:HZ3	7:I:43:VAL:HG21	1.60	0.66
3:C:134:ILE:HG21	3:C:139:GLY:HA2	1.77	0.66
1:A:503:GLN:NE2	5:F:90:ARG:NH2	2.44	0.66
1:A:597:LEU:HD12	1:A:597:LEU:N	2.07	0.66
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.78	0.66
5:F:81:THR:HG22	5:F:136:ARG:NH1	2.10	0.66
8:J:2:ILE:HD11	8:J:57:ILE:HD13	1.78	0.66
1:A:263:THR:HA	1:A:266:LEU:HD12	1.78	0.66
1:A:834:THR:HG21	1:A:1077:THR:HA	1.78	0.66
1:A:689:LYS:O	1:A:693:VAL:HG23	1.96	0.66
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.56	0.66
1:A:567:LYS:HZ1	6:H:46:LEU:HB2	1.60	0.66
1:A:1269:GLU:OE2	2:B:263:GLY:HA3	1.95	0.66
1:A:1431:GLY:HA2	2:B:1152:MET:HE2	1.78	0.66
2:B:874:PHE:O	2:B:875:GLU:HG3	1.95	0.66
6:H:89:LEU:C	6:H:91:ASP:H	2.03	0.66
7:I:50:THR:CG2	7:I:52:ILE:HG23	2.26	0.66
1:A:464:PRO:O	1:A:465:TYR:O	2.14	0.66
3:C:148:ARG:HD2	8:J:61:LEU:O	1.96	0.66
1:A:23:SER:O	1:A:27:VAL:HG23	1.95	0.65
1:A:768:GLN:NE2	1:A:816:HIS:ND1	2.44	0.65
2:B:737:THR:HG21	7:I:66:PRO:O	1.96	0.65
3:C:249:ASP:OD1	3:C:253:LYS:HE3	1.96	0.65
5:F:81:THR:HG21	5:F:136:ARG:HH11	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ILE:HD12	1:A:541:ILE:N	2.11	0.65
5:F:79:ARG:HH22	5:F:150:GLU:CD	2.03	0.65
8:J:1:MET:HG3	8:J:60:PHE:CE2	2.24	0.65
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.26	0.65
1:A:901:LEU:O	1:A:920:LEU:HD23	1.95	0.65
2:B:408:LEU:HD11	2:B:545:ILE:HD12	1.79	0.65
2:B:726:ALA:CB	2:B:1051:THR:HG21	2.23	0.65
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.26	0.65
3:C:22:LEU:HD12	3:C:230:MET:CE	2.26	0.65
4:E:5:ASN:O	4:E:9:ILE:HG13	1.97	0.65
1:A:537:ARG:NH1	6:H:120:GLY:O	2.30	0.65
1:A:693:VAL:HG21	1:A:721:PHE:CE1	2.26	0.65
1:A:1390:ASN:O	1:A:1391:ARG:HB2	1.96	0.65
2:B:737:THR:CG2	7:I:66:PRO:HA	2.27	0.65
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.76	0.65
5:F:81:THR:HB	5:F:144:GLU:OE1	1.95	0.65
6:H:42:ILE:HG23	6:H:95:TYR:CE1	2.32	0.65
1:A:65:LEU:O	1:A:71:GLN:HA	1.97	0.65
2:B:806:THR:HG22	2:B:808:ALA:N	2.08	0.65
2:B:957:ASN:OD1	2:B:958:GLN:N	2.28	0.65
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.62	0.65
1:A:63:ARG:CA	1:A:74:MET:HE2	2.26	0.65
1:A:760:GLN:HB2	2:B:1021:MET:HE1	1.78	0.65
1:A:387:ARG:O	1:A:391:LEU:HG	1.96	0.65
2:B:731:VAL:HG12	2:B:732:SER:N	2.12	0.65
2:B:1099:VAL:HG12	2:B:1103:ILE:HD11	1.78	0.65
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.79	0.65
1:A:353:ILE:HG21	1:A:487:MET:CE	2.26	0.65
1:A:1140:HIS:CE1	1:A:1272:THR:HG23	2.32	0.65
2:B:296:GLU:O	2:B:300:HIS:HD2	1.79	0.65
2:B:515:HIS:HD2	2:B:517:THR:H	1.43	0.65
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.79	0.64
1:A:998:LEU:HD12	1:A:1001:ARG:NH1	2.11	0.64
1:A:666:ILE:HG12	2:B:1026:LEU:HB3	1.77	0.64
1:A:768:GLN:HE21	1:A:816:HIS:HA	1.63	0.64
2:B:680:THR:CG2	2:B:681:TRP:N	2.61	0.64
2:B:864:LYS:CG	2:B:871:THR:HG23	2.25	0.64
6:H:103:LYS:HB3	6:H:105:GLU:OE2	1.97	0.64
1:A:754:SER:OG	1:A:756:ILE:HG22	1.97	0.64
6:H:82:PRO:O	6:H:84:ALA:N	2.28	0.64
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLU:CD	1:A:387:ARG:HH22	2.05	0.64
1:A:826:ASP:O	1:A:830:LYS:HB2	1.97	0.64
6:H:5:LEU:HD22	6:H:133:ASN:O	1.97	0.64
3:C:73:GLN:HE21	3:C:75:MET:N	1.95	0.64
5:F:109:VAL:CG1	5:F:110:ASP:H	2.11	0.64
9:K:24:ASP:OD2	9:K:74:ARG:NH1	2.29	0.64
2:B:864:LYS:HB3	2:B:871:THR:HA	1.79	0.64
2:B:898:LEU:HD22	2:B:964:VAL:HG11	1.79	0.64
2:B:1022:THR:HG23	2:B:1022:THR:O	1.97	0.64
3:C:67:LEU:HD13	3:C:155:LEU:HD21	1.80	0.64
1:A:1376:THR:HG22	4:E:212:ARG:HH22	1.62	0.64
1:A:1111:MET:HE2	1:A:1331:SER:HB2	1.79	0.64
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.63	0.64
10:L:38:LEU:HD22	10:L:56:LEU:HD21	1.78	0.64
1:A:1336:MET:HE2	1:A:1380:GLY:HA2	1.79	0.64
1:A:1375:MET:HE3	1:A:1384:VAL:HG23	1.78	0.64
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.11	0.64
2:B:239:GLU:HG2	2:B:255:GLN:HG2	1.79	0.64
2:B:1159:ARG:CG	2:B:1193:GLN:HE21	2.11	0.64
1:A:70:CYS:O	1:A:72:GLU:HG3	1.98	0.63
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.79	0.63
1:A:595:THR:OG1	1:A:603:ASN:HB3	1.97	0.63
1:A:469:ARG:NH2	2:B:991:GLY:O	2.31	0.63
2:B:235:SER:HA	2:B:261:ARG:NH2	2.14	0.63
3:C:239:PRO:O	3:C:242:GLN:HB2	1.97	0.63
9:K:38:GLU:OE1	9:K:42:LEU:HD22	1.98	0.63
9:K:103:THR:HG22	9:K:104:ASN:N	2.13	0.63
2:B:956:THR:HA	2:B:961:LEU:O	1.97	0.63
3:C:214:ASN:HB2	3:C:217:ASP:OD2	1.98	0.63
6:H:11:GLN:HE21	6:H:52:GLN:HA	1.61	0.63
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.24	0.63
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.81	0.63
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.80	0.63
6:H:85:GLY:O	6:H:89:LEU:HD21	1.98	0.63
1:A:203:SER:OG	1:A:206:GLU:HG3	1.98	0.63
1:A:1265:ASN:HD21	2:B:263:GLY:C	2.06	0.63
2:B:606:LYS:HD2	2:B:608:ASP:OD2	1.98	0.63
1:A:79:GLY:HA3	1:A:245:PRO:HG3	1.81	0.63
1:A:869:GLY:O	4:E:204:THR:HG21	1.97	0.63
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	1.99	0.63
4:E:204:THR:HG22	4:E:205:SER:N	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:4:GLU:O	4:E:6:GLU:N	2.32	0.63
1:A:596:THR:HG22	1:A:597:LEU:N	2.13	0.63
1:A:1447:GLU:OE1	1:A:1447:GLU:HA	1.97	0.63
2:B:284:ILE:HG12	2:B:324:ILE:HD12	1.81	0.63
2:B:339:THR:HG21	2:B:348:ARG:HG2	1.80	0.63
2:B:995:ARG:HD3	9:K:6:ARG:HH12	1.63	0.63
3:C:52:GLU:HA	10:L:64:LEU:CD2	2.29	0.63
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.79	0.62
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.81	0.62
2:B:103:ASN:CB	2:B:169:ARG:HH22	2.10	0.62
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.80	0.62
2:B:542:MET:HE2	2:B:747:MET:CE	2.30	0.62
2:B:43:LEU:HD11	2:B:811:TYR:O	1.98	0.62
2:B:229:ALA:C	2:B:231:PRO:HD2	2.23	0.62
2:B:969:ARG:HB3	2:B:969:ARG:HH11	1.64	0.62
4:E:120:ALA:O	4:E:123:LEU:HB2	2.00	0.62
1:A:208:LEU:HD22	1:A:212:LYS:HE3	1.81	0.62
1:A:929:LEU:HD11	1:A:983:ILE:HD13	1.80	0.62
1:A:58:LEU:HD22	1:A:80:HIS:O	2.00	0.62
10:L:51:CYS:O	10:L:53:HIS:N	2.31	0.62
1:A:535:THR:O	1:A:535:THR:HG22	1.98	0.62
1:A:565:ILE:HG23	1:A:567:LYS:HG3	1.82	0.62
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.82	0.62
9:K:56:VAL:HA	9:K:77:THR:HG22	1.81	0.62
1:A:682:THR:HG21	1:A:728:LYS:HG3	1.80	0.62
1:A:878:ILE:CG2	1:A:955:PRO:HB2	2.29	0.62
2:B:25:ILE:HD13	2:B:658:ILE:HD11	1.81	0.62
10:L:26:THR:CG2	10:L:27:LEU:H	2.11	0.62
10:L:38:LEU:O	10:L:39:SER:HB2	2.00	0.62
1:A:871:ASP:HB3	4:E:204:THR:HG22	1.80	0.62
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.46	0.62
2:B:680:THR:HG22	2:B:682:SER:H	1.63	0.62
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.97	0.62
1:A:446:ARG:HB2	1:A:487:MET:SD	2.39	0.62
4:E:28:TYR:CZ	4:E:78:LEU:HG	2.35	0.62
10:L:55:ILE:O	10:L:56:LEU:HB2	1.99	0.62
1:A:704:ALA:HB2	1:A:710:LEU:CD1	2.27	0.61
3:C:258:ILE:CD1	9:K:42:LEU:HD21	2.30	0.61
4:E:40:GLU:OE1	4:E:43:LYS:HD2	2.00	0.61
1:A:332:LYS:HD3	2:B:1206:GLU:OE2	2.00	0.61
1:A:1394:THR:CG2	1:A:1398:MET:HB2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1159:ARG:HG3	2:B:1193:GLN:HE21	1.65	0.61
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.65	0.61
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.82	0.61
6:H:130:ARG:CA	6:H:133:ASN:HD22	2.12	0.61
9:K:18:LYS:NZ	9:K:38:GLU:HG2	2.15	0.61
1:A:912:LEU:HD22	1:A:1033:GLN:HA	1.82	0.61
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.82	0.61
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.32	0.61
1:A:697:ALA:HB1	7:I:97:MET:HE3	1.83	0.61
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.15	0.61
2:B:886:LYS:HB3	2:B:886:LYS:NZ	2.16	0.61
2:B:957:ASN:CG	2:B:958:GLN:H	2.08	0.61
1:A:693:VAL:CG2	1:A:721:PHE:HE1	2.10	0.61
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.83	0.61
7:I:2:THR:O	7:I:3:THR:C	2.43	0.61
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.49	0.61
1:A:597:LEU:H	1:A:597:LEU:CD1	2.11	0.61
1:A:825:ILE:CD1	2:B:512:ARG:HG3	2.30	0.61
2:B:63:ILE:O	2:B:67:SER:HB3	2.01	0.61
2:B:879:ARG:HB3	2:B:883:LEU:HD22	1.81	0.61
3:C:67:LEU:CD1	3:C:155:LEU:HD21	2.31	0.61
7:I:51:ASN:O	7:I:54:GLU:HG3	2.00	0.61
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.83	0.61
2:B:164:LYS:O	2:B:165:VAL:HB	2.01	0.61
2:B:882:THR:HG22	2:B:884:ARG:HB2	1.83	0.61
3:C:51:VAL:HG22	3:C:155:LEU:CD1	2.30	0.61
7:I:50:THR:HG22	7:I:52:ILE:HG23	1.82	0.61
1:A:724:GLU:O	1:A:728:LYS:HG2	2.01	0.60
1:A:32:VAL:HG11	1:A:68:GLN:NE2	2.16	0.60
1:A:834:THR:HG21	1:A:1077:THR:CA	2.30	0.60
1:A:1111:MET:CE	1:A:1331:SER:HB2	2.31	0.60
7:I:95:THR:HG22	7:I:96:SER:N	2.15	0.60
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.83	0.60
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.16	0.60
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.82	0.60
10:L:58:LYS:O	10:L:58:LYS:HD3	2.01	0.60
1:A:825:ILE:HD13	2:B:512:ARG:HG3	1.83	0.60
1:A:903:ASN:HD22	1:A:905:ASP:N	1.94	0.60
2:B:731:VAL:HG12	2:B:732:SER:H	1.65	0.60
7:I:63:GLY:O	7:I:70:ARG:NH2	2.35	0.60
1:A:540:PHE:C	1:A:541:ILE:HD12	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.37	0.60
1:A:760:GLN:HB2	2:B:1021:MET:CE	2.31	0.60
1:A:1139:GLU:HG3	1:A:1280:GLU:O	2.02	0.60
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.31	0.60
2:B:544:CYS:HB2	2:B:634:TYR:CE1	2.37	0.60
2:B:798:TYR:CD2	8:J:4:PRO:HG3	2.37	0.60
2:B:800:GLN:CB	8:J:52:THR:HG22	2.26	0.60
5:F:154:ASP:O	5:F:155:LEU:HD23	2.01	0.60
7:I:98:VAL:HG21	7:I:113:ASP:CB	2.31	0.60
9:K:46:ILE:O	9:K:50:LEU:HB2	2.01	0.60
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.01	0.60
2:B:103:ASN:HB2	2:B:169:ARG:CZ	2.30	0.60
10:L:33:GLU:HB2	10:L:53:HIS:CD2	2.37	0.60
1:A:673:GLY:N	1:A:674:PRO:HD2	2.17	0.60
1:A:1259:MET:O	1:A:1263:ILE:HG13	2.02	0.60
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.01	0.60
1:A:283:GLY:O	1:A:284:ALA:HB2	2.02	0.60
1:A:303:TYR:CZ	1:A:325:ILE:HD11	2.37	0.60
1:A:1113:THR:O	1:A:1113:THR:HG22	2.02	0.60
2:B:120:ARG:HG3	2:B:955:THR:HG21	1.84	0.60
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.01	0.60
4:E:124:VAL:HB	4:E:125:PRO:CD	2.32	0.60
1:A:831:THR:HG22	1:A:832:ALA:N	2.17	0.59
2:B:1103:ILE:HG22	2:B:1103:ILE:O	2.02	0.59
4:E:127:ILE:HD11	4:E:132:ILE:HD11	1.83	0.59
6:H:130:ARG:CA	6:H:133:ASN:HB2	2.32	0.59
6:H:76:THR:O	6:H:76:THR:HG22	2.02	0.59
2:B:915:THR:HG21	2:B:934:LYS:HG2	1.84	0.59
1:A:276:LEU:HD13	1:A:292:ALA:CB	2.33	0.59
1:A:523:ILE:HD13	1:A:649:ILE:HG21	1.83	0.59
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.36	0.59
1:A:328:ARG:HD3	1:A:332:LYS:HZ1	1.67	0.59
3:C:8:VAL:HG12	3:C:9:LYS:N	2.16	0.59
1:A:57:ARG:HB3	1:A:68:GLN:NE2	2.18	0.59
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.32	0.59
1:A:840:ARG:HG3	1:A:1385:THR:HG22	1.85	0.59
1:A:1094:VAL:HG12	1:A:1095:THR:N	2.18	0.59
1:A:1277:GLU:H	1:A:1277:GLU:CD	2.10	0.59
2:B:1097:HIS:HB3	2:B:1102:LYS:HZ2	1.66	0.59
5:F:81:THR:HG21	5:F:136:ARG:CD	2.32	0.59
6:H:103:LYS:CD	6:H:114:VAL:HB	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:THR:HG22	2:B:99:LYS:N	2.17	0.59
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.17	0.59
10:L:48:CYS:SG	10:L:49:LYS:N	2.75	0.59
1:A:157:ASP:C	1:A:159:THR:H	2.09	0.59
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.33	0.59
1:A:741:ASN:HD22	1:A:744:LYS:H	1.50	0.59
3:C:6:PRO:HB2	9:K:101:LEU:HB2	1.85	0.59
8:J:2:ILE:HD11	8:J:57:ILE:HD12	1.84	0.59
1:A:1336:MET:HE1	1:A:1381:LEU:H	1.67	0.59
2:B:134:LYS:NZ	2:B:446:LEU:HD13	2.17	0.59
3:C:31:ASN:O	3:C:35:ARG:HG3	2.03	0.59
1:A:108:MET:HG2	1:A:171:GLN:NE2	2.16	0.58
1:A:399:HIS:O	1:A:400:PRO:C	2.44	0.58
1:A:608:ILE:HD12	1:A:613:ILE:HD12	1.84	0.58
1:A:57:ARG:C	1:A:68:GLN:HE21	2.11	0.58
1:A:1080:THR:O	1:A:1081:LEU:HG	2.03	0.58
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.85	0.58
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.18	0.58
10:L:51:CYS:HB3	10:L:53:HIS:CD2	2.38	0.58
2:B:35:SER:O	2:B:39:ARG:HG3	2.02	0.58
2:B:563:MET:HE2	2:B:580:VAL:HB	1.81	0.58
3:C:93:ASP:O	3:C:127:ARG:NH2	2.37	0.58
9:K:12:LEU:HD11	9:K:18:LYS:HE2	1.86	0.58
10:L:34:CYS:O	10:L:36:SER:N	2.36	0.58
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.28	0.58
1:A:381:THR:CG2	1:A:383:TYR:H	2.16	0.58
1:A:567:LYS:HZ2	6:H:46:LEU:HB2	1.68	0.58
1:A:763:ALA:O	1:A:803:SER:HB3	2.04	0.58
5:F:85:MET:HE2	5:F:93:ILE:HD12	1.84	0.58
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.03	0.58
1:A:208:LEU:CD2	1:A:212:LYS:HE3	2.33	0.58
3:C:39:ALA:O	3:C:163:ILE:HG23	2.03	0.58
6:H:87:ARG:O	6:H:89:LEU:HG	2.04	0.58
10:L:51:CYS:C	10:L:53:HIS:H	2.10	0.58
1:A:736:ASN:O	1:A:737:LEU:C	2.46	0.58
2:B:515:HIS:CD2	2:B:517:THR:H	2.22	0.58
4:E:158:SER:O	4:E:162:ARG:HG3	2.04	0.58
6:H:40:LEU:HD12	6:H:41:ASP:H	1.69	0.58
8:J:14:VAL:CG1	8:J:50:ILE:HD11	2.33	0.58
1:A:494:SER:OG	1:A:497:THR:HB	2.04	0.58
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1099:VAL:C	2:B:1101:ASP:H	2.12	0.58
2:B:1153:GLU:CG	2:B:1154:ALA:H	2.07	0.58
10:L:30:ILE:HG22	10:L:31:CYS:N	2.19	0.58
1:A:975:HIS:ND1	1:A:1036:ARG:HG3	2.19	0.58
1:A:1015:VAL:HG13	1:A:1019:CYS:SG	2.44	0.58
1:A:1341:ILE:HD12	1:A:1379:GLY:CA	2.34	0.58
2:B:879:ARG:HB3	2:B:883:LEU:HD23	1.84	0.58
6:H:87:ARG:O	6:H:89:LEU:N	2.37	0.58
9:K:29:ASN:ND2	9:K:79:GLU:HA	2.18	0.58
1:A:243:PRO:C	1:A:245:PRO:HD2	2.29	0.58
1:A:666:ILE:HD11	2:B:1030:LEU:HB2	1.85	0.58
2:B:25:ILE:CD1	2:B:653:VAL:HB	2.34	0.58
2:B:889:THR:HG21	2:B:891:ASP:OD2	2.04	0.58
10:L:27:LEU:HD13	10:L:37:LYS:HG2	1.85	0.58
2:B:25:ILE:HD12	2:B:653:VAL:HB	1.85	0.57
2:B:1148:LYS:HG3	2:B:1152:MET:HE1	1.85	0.57
3:C:49:VAL:CG1	3:C:155:LEU:HD11	2.34	0.57
4:E:117:THR:HG22	4:E:119:SER:H	1.69	0.57
8:J:12:LYS:NZ	8:J:17:LYS:NZ	2.52	0.57
1:A:184:SER:HA	1:A:198:GLU:O	2.04	0.57
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.86	0.57
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.04	0.57
2:B:98:THR:O	2:B:126:SER:HB3	2.04	0.57
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.39	0.57
2:B:341:LEU:HG	2:B:341:LEU:O	2.04	0.57
2:B:826:ALA:HB2	2:B:1087:PHE:CD1	2.39	0.57
2:B:860:MET:HG2	2:B:861:ASP:H	1.68	0.57
2:B:1153:GLU:HG2	2:B:1154:ALA:N	2.12	0.57
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.29	0.57
9:K:47:ARG:HH11	9:K:47:ARG:CB	2.06	0.57
1:A:567:LYS:CB	6:H:96:VAL:H	2.16	0.57
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.69	0.57
4:E:38:PRO:HG2	4:E:41:ASP:OD2	2.04	0.57
5:F:107:VAL:HG12	5:F:109:VAL:H	1.69	0.57
8:J:32:GLU:CD	8:J:32:GLU:H	2.13	0.57
1:A:738:LYS:HZ1	3:C:194:GLU:C	2.13	0.57
8:J:64:ASN:HB3	8:J:65:PRO:CD	2.29	0.57
1:A:68:GLN:C	1:A:70:CYS:H	2.13	0.57
1:A:244:PRO:N	1:A:245:PRO:HD2	2.19	0.57
2:B:955:THR:HG22	2:B:956:THR:N	2.05	0.57
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:ASN:OD1	3:C:56:THR:HG22	2.05	0.57
1:A:381:THR:HG23	1:A:383:TYR:H	1.70	0.57
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.86	0.57
2:B:130:VAL:CG1	2:B:131:ASP:H	2.15	0.57
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.86	0.57
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.34	0.57
1:A:32:VAL:CG2	1:A:58:LEU:HD23	2.34	0.57
1:A:329:LEU:HB3	1:A:333:GLU:HB3	1.87	0.57
1:A:522:GLY:HA2	1:A:630:ILE:CD1	2.35	0.57
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.86	0.57
2:B:616:ILE:HD13	2:B:696:GLU:HG3	1.86	0.57
1:A:345:VAL:HG11	2:B:1128:LEU:O	2.05	0.57
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.87	0.57
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.40	0.57
2:B:906:SER:O	2:B:907:GLY:C	2.47	0.57
4:E:58:MET:O	4:E:59:SER:O	2.23	0.57
4:E:116:ILE:HG22	4:E:117:THR:N	2.20	0.57
6:H:7:ASP:O	6:H:8:ASP:HB2	2.05	0.57
6:H:103:LYS:HG2	6:H:115:TYR:N	2.19	0.57
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.40	0.56
1:A:479:ASN:C	1:A:479:ASN:HD22	2.12	0.56
1:A:682:THR:CG2	1:A:728:LYS:HG3	2.34	0.56
1:A:862:ASN:OD1	4:E:174:GLN:HA	2.05	0.56
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.53	0.56
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.05	0.56
2:B:103:ASN:CB	2:B:169:ARG:HH12	2.18	0.56
2:B:955:THR:CG2	2:B:956:THR:H	2.03	0.56
1:A:32:VAL:HB	1:A:57:ARG:HB3	1.85	0.56
1:A:537:ARG:HD2	6:H:20:TYR:CE1	2.41	0.56
1:A:598:LEU:HG	6:H:115:TYR:HE2	1.69	0.56
1:A:613:ILE:HD13	6:H:102:TYR:HB3	1.87	0.56
1:A:971:PHE:O	1:A:972:HIS:C	2.46	0.56
1:A:1390:ASN:O	1:A:1391:ARG:CB	2.52	0.56
2:B:114:PRO:HD3	2:B:124:TYR:CE1	2.40	0.56
2:B:172:ILE:CD1	2:B:178:ASN:HD22	2.18	0.56
2:B:284:ILE:CG1	2:B:324:ILE:HD12	2.35	0.56
2:B:654:ARG:N	2:B:657:HIS:HD2	1.93	0.56
2:B:1072:MET:HE1	2:B:1087:PHE:CD1	2.40	0.56
1:A:112:LYS:NZ	1:A:164:ARG:HB2	2.20	0.56
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.40	0.56
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:737:THR:O	2:B:737:THR:HG22	2.04	0.56
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.87	0.56
1:A:92:HIS:CD2	1:A:94:GLY:H	2.23	0.56
1:A:768:GLN:HG3	1:A:816:HIS:HA	1.87	0.56
1:A:1295:THR:HB	1:A:1297:GLU:OE1	2.06	0.56
1:A:1383:SER:HB3	1:A:1387:HIS:CD2	2.40	0.56
1:A:1395:GLY:C	1:A:1397:LEU:N	2.64	0.56
2:B:234:ILE:HD13	2:B:257:LYS:HD3	1.85	0.56
4:E:114:ASN:O	4:E:115:ASN:HB3	2.05	0.56
10:L:68:GLU:H	10:L:68:GLU:CD	2.12	0.56
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.84	0.56
1:A:636:GLU:OE1	1:A:966:ASN:ND2	2.38	0.56
1:A:1376:THR:CG2	4:E:212:ARG:HH22	2.19	0.56
2:B:899:ILE:HG22	2:B:900:ALA:H	1.70	0.56
6:H:62:SER:O	6:H:63:LEU:C	2.48	0.56
6:H:123:MET:HE1	6:H:142:LEU:HD13	1.86	0.56
9:K:22:ASP:O	9:K:31:VAL:HG13	2.06	0.56
1:A:61:ILE:HG22	1:A:62:ASP:H	1.70	0.56
1:A:534:LEU:O	1:A:574:GLY:HA3	2.05	0.56
1:A:774:ARG:HB2	1:A:797:LYS:HG2	1.87	0.56
2:B:860:MET:HG2	2:B:861:ASP:N	2.21	0.56
2:B:864:LYS:CB	2:B:871:THR:HA	2.36	0.56
2:B:884:ARG:O	2:B:936:ASP:HB2	2.06	0.56
3:C:57:VAL:HG11	8:J:60:PHE:HB2	1.86	0.56
6:H:103:LYS:HZ1	6:H:114:VAL:CG2	2.18	0.56
10:L:34:CYS:C	10:L:36:SER:H	2.12	0.56
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.94	0.56
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.88	0.56
2:B:648:HIS:CD2	2:B:648:HIS:N	2.72	0.56
1:A:382:PRO:HD2	5:F:104:ASN:OD1	2.06	0.56
2:B:542:MET:HE2	2:B:747:MET:CG	2.29	0.56
5:F:93:ILE:HD13	5:F:148:VAL:HG22	1.88	0.56
6:H:138:GLU:HG2	6:H:139:ASN:N	2.21	0.56
1:A:465:TYR:CA	9:K:2:ASN:HB3	2.36	0.56
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.87	0.56
2:B:35:SER:HA	2:B:811:TYR:HE2	1.70	0.56
2:B:104:GLU:OE2	10:L:54:ARG:HD3	2.06	0.56
2:B:794:ASN:C	2:B:795:ILE:HD12	2.30	0.56
1:A:35:ILE:HG23	1:A:52:GLY:O	2.06	0.55
1:A:329:LEU:HD21	2:B:1203:LEU:HD13	1.87	0.55
1:A:388:LEU:HD23	1:A:391:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:THR:O	1:A:698:GLN:HG3	2.06	0.55
2:B:953:LEU:HD21	2:B:955:THR:OG1	2.06	0.55
1:A:69:THR:O	1:A:71:GLN:HG3	2.06	0.55
1:A:725:ALA:HA	1:A:728:LYS:CE	2.36	0.55
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.87	0.55
7:I:111:THR:HG22	7:I:112:SER:H	1.70	0.55
2:B:119:LEU:HD22	2:B:953:LEU:CD1	2.37	0.55
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.38	0.55
2:B:726:ALA:HB1	2:B:1051:THR:CG2	2.29	0.55
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.20	0.55
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.89	0.55
7:I:103:CYS:O	7:I:107:SER:HA	2.07	0.55
8:J:48:ARG:NH2	8:J:49:MET:HE1	2.22	0.55
1:A:329:LEU:C	1:A:331:GLY:H	2.13	0.55
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.33	0.55
2:B:181:LEU:HD22	2:B:189:LEU:HD23	1.87	0.55
2:B:839:MET:CE	2:B:1010:LEU:HD11	2.29	0.55
4:E:31:THR:C	4:E:33:GLU:N	2.58	0.55
1:A:500:GLU:O	1:A:504:LEU:HB2	2.06	0.55
1:A:629:LEU:O	1:A:633:VAL:HG23	2.07	0.55
1:A:858:ASN:C	1:A:858:ASN:ND2	2.65	0.55
1:A:1216:ILE:O	1:A:1219:THR:HB	2.07	0.55
5:F:93:ILE:CD1	5:F:134:ILE:HD11	2.31	0.55
1:A:73:GLY:C	1:A:75:ASN:H	2.15	0.55
2:B:365:THR:HG22	2:B:366:GLN:N	2.20	0.55
2:B:651:LEU:HD11	2:B:707:PRO:CB	2.32	0.55
1:A:1169:ILE:O	1:A:1173:HIS:HD2	1.89	0.55
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.89	0.55
4:E:13:TRP:CE3	4:E:39:LEU:HD13	2.42	0.55
4:E:156:LEU:HD21	4:E:197:LYS:HB2	1.89	0.55
7:I:4:PHE:CE1	7:I:13:MET:HE2	2.41	0.55
1:A:1167:GLU:O	1:A:1171:GLN:HG3	2.07	0.55
1:A:1265:ASN:HD21	2:B:263:GLY:HA2	1.71	0.55
3:C:137:LYS:C	3:C:138:GLU:HG2	2.32	0.55
1:A:418:SER:O	1:A:420:ARG:N	2.40	0.55
1:A:1146:VAL:HG11	1:A:1202:MET:SD	2.47	0.55
6:H:13:SER:O	6:H:14:GLU:HB2	2.05	0.55
1:A:108:MET:HA	1:A:210:ILE:HD13	1.87	0.55
2:B:824:ILE:HG12	8:J:48:ARG:NH1	2.22	0.55
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.39	0.55
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:26:ARG:O	4:E:75:MET:HE1	2.07	0.55
7:I:111:THR:HG22	7:I:113:ASP:N	2.11	0.54
1:A:246:VAL:C	1:A:328:ARG:HH12	2.14	0.54
1:A:595:THR:HG23	1:A:599:SER:HB3	1.88	0.54
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.36	0.54
1:A:82:GLY:HA3	1:A:241:VAL:HB	1.89	0.54
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.42	0.54
1:A:919:ILE:HG12	1:A:925:LEU:HD12	1.89	0.54
1:A:1336:MET:CE	1:A:1380:GLY:HA2	2.37	0.54
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.89	0.54
2:B:514:LEU:HD12	2:B:518:HIS:HD2	1.72	0.54
2:B:1003:ALA:O	3:C:177:GLU:HA	2.06	0.54
10:L:39:SER:O	10:L:40:LEU:HD23	2.07	0.54
1:A:551:TYR:CE2	9:K:62:LYS:HE2	2.42	0.54
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.08	0.54
1:A:579:SER:OG	1:A:612:ILE:HG23	2.07	0.54
1:A:1147:THR:HB	7:I:48:LEU:CD1	2.37	0.54
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.23	0.54
1:A:267:ALA:O	1:A:270:LEU:HB2	2.07	0.54
2:B:843:GLN:N	2:B:994:TYR:O	2.35	0.54
5:F:93:ILE:HD11	5:F:134:ILE:CD1	2.32	0.54
6:H:103:LYS:HD3	6:H:114:VAL:HB	1.88	0.54
1:A:450:LEU:HD12	1:A:450:LEU:N	2.08	0.54
1:A:767:GLN:O	11:M:3:GLY:HA2	2.07	0.54
2:B:861:ASP:OD2	2:B:914:LYS:HD2	2.08	0.54
2:B:1148:LYS:HG3	2:B:1152:MET:CE	2.38	0.54
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.89	0.54
9:K:20:LYS:HB2	9:K:34:THR:HB	1.88	0.54
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.88	0.54
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.23	0.54
2:B:89:GLU:N	2:B:135:ARG:O	2.40	0.54
2:B:103:ASN:HB2	2:B:169:ARG:NH1	2.23	0.54
3:C:55:THR:O	3:C:55:THR:HG22	2.08	0.54
3:C:258:ILE:HD11	9:K:42:LEU:HD21	1.90	0.54
6:H:107:VAL:O	6:H:107:VAL:HG12	2.08	0.54
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.88	0.54
1:A:994:GLN:NE2	1:A:1023:ARG:HE	2.06	0.54
1:A:1433:MET:HE1	1:A:1438:THR:HG23	1.89	0.54
2:B:272:THR:O	2:B:272:THR:HG22	2.08	0.54
4:E:4:GLU:O	4:E:5:ASN:C	2.51	0.54
1:A:598:LEU:O	1:A:599:SER:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:MET:O	1:A:803:SER:HB2	2.08	0.54
2:B:63:ILE:CB	2:B:95:ILE:HD11	2.38	0.54
2:B:550:ASP:OD2	2:B:552:MET:HE2	2.08	0.54
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.72	0.54
1:A:112:LYS:HZ1	1:A:165:GLY:H	1.54	0.53
1:A:239:LEU:HD23	1:A:240:PRO:N	2.22	0.53
1:A:1265:ASN:HD21	2:B:263:GLY:CA	2.20	0.53
5:F:75:PRO:O	5:F:77:ASP:O	2.25	0.53
1:A:134:ARG:HD2	1:A:221:SER:O	2.09	0.53
1:A:327:ALA:HA	1:A:330:LYS:HD2	1.89	0.53
1:A:1318:THR:HG21	4:E:11:ARG:HH12	1.72	0.53
2:B:899:ILE:CG2	2:B:900:ALA:N	2.71	0.53
8:J:7:CYS:SG	8:J:49:MET:HE3	2.48	0.53
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.91	0.53
1:A:911:SER:O	1:A:978:PRO:HG3	2.09	0.53
2:B:230:ALA:N	2:B:231:PRO:HD2	2.24	0.53
2:B:952:VAL:HB	10:L:58:LYS:CB	2.36	0.53
4:E:5:ASN:HA	4:E:8:ASN:HB3	1.90	0.53
6:H:59:ILE:O	6:H:60:ALA:HB3	2.09	0.53
1:A:709:THR:HG23	7:I:94:ASP:HA	1.90	0.53
1:A:1328:TYR:CG	1:A:1329:THR:N	2.75	0.53
1:A:1394:THR:HA	1:A:1398:MET:HE3	1.90	0.53
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.44	0.53
4:E:89:GLY:HA2	4:E:117:THR:OG1	2.08	0.53
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.90	0.53
1:A:567:LYS:CG	6:H:96:VAL:H	2.21	0.53
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.90	0.53
2:B:311:LEU:HB3	7:I:4:PHE:CE2	2.44	0.53
6:H:89:LEU:O	6:H:91:ASP:N	2.39	0.53
8:J:48:ARG:CZ	8:J:49:MET:HE1	2.39	0.53
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.44	0.53
1:A:146:MET:HA	1:A:171:GLN:HB3	1.91	0.53
1:A:345:VAL:CG1	2:B:1150:ARG:HH22	2.21	0.53
1:A:907:THR:HG22	1:A:908:LEU:N	2.21	0.53
2:B:496:ARG:NH2	2:B:541:LEU:HA	2.23	0.53
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.34	0.53
2:B:69:LEU:HD21	2:B:425:THR:HG23	1.91	0.53
3:C:124:LEU:O	3:C:127:ARG:HG2	2.09	0.53
3:C:167:HIS:HD2	3:C:169:LYS:H	1.57	0.53
9:K:47:ARG:HD3	9:K:59:ALA:O	2.08	0.53
1:A:579:SER:HB3	1:A:611:GLN:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.90	0.53
1:A:1392:SER:O	1:A:1393:ASN:HB2	2.09	0.53
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.50	0.53
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.07	0.53
5:F:111:LEU:HD12	5:F:111:LEU:N	2.11	0.53
1:A:503:GLN:NE2	5:F:90:ARG:HH22	2.06	0.53
1:A:531:ILE:HD11	1:A:578:LEU:HD21	1.89	0.53
1:A:630:ILE:HD13	1:A:646:PHE:CZ	2.44	0.53
1:A:1132:LYS:HE2	1:A:1284:MET:HE1	1.91	0.53
1:A:1199:ARG:O	1:A:1202:MET:HB2	2.09	0.53
6:H:63:LEU:C	6:H:90:ALA:CB	2.82	0.53
7:I:45:ARG:HG2	7:I:45:ARG:NH1	2.20	0.53
1:A:1405:THR:HG23	1:A:1408:ILE:HD12	1.89	0.53
2:B:882:THR:C	2:B:884:ARG:H	2.17	0.53
2:B:1127:GLY:O	2:B:1128:LEU:HB3	2.08	0.53
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.07	0.53
4:E:112:TYR:CE1	4:E:115:ASN:HA	2.44	0.53
1:A:10:PRO:HG2	2:B:1192:TYR:HD2	1.74	0.52
1:A:606:LEU:HD11	1:A:608:ILE:HD11	1.91	0.52
1:A:901:LEU:N	1:A:926:GLN:NE2	2.37	0.52
2:B:273:LEU:HD12	2:B:280:ILE:HD12	1.91	0.52
4:E:31:THR:C	4:E:33:GLU:H	2.16	0.52
10:L:27:LEU:HD22	10:L:37:LYS:HD3	1.91	0.52
1:A:17:VAL:HA	2:B:1215:ARG:O	2.09	0.52
1:A:406:ILE:HA	1:A:411:ASP:O	2.10	0.52
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.91	0.52
1:A:1127:ASP:C	1:A:1129:GLU:N	2.67	0.52
2:B:284:ILE:CD1	2:B:324:ILE:HD12	2.39	0.52
2:B:326:ASP:C	2:B:326:ASP:OD2	2.52	0.52
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.74	0.52
3:C:49:VAL:HG11	3:C:155:LEU:HD11	1.90	0.52
1:A:834:THR:CG2	1:A:1077:THR:OG1	2.57	0.52
1:A:1206:ASP:HB2	1:A:1274:ARG:HH12	1.73	0.52
1:A:1341:ILE:CD1	1:A:1376:THR:HG23	2.40	0.52
2:B:65:GLU:HG3	2:B:65:GLU:O	2.10	0.52
2:B:164:LYS:O	2:B:165:VAL:CB	2.57	0.52
2:B:735:ALA:HB3	2:B:738:PHE:CE1	2.44	0.52
2:B:884:ARG:O	2:B:936:ASP:CB	2.57	0.52
2:B:997:GLU:CG	3:C:39:ALA:HB2	2.39	0.52
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.40	0.52
2:B:1099:VAL:O	2:B:1103:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:VAL:HG13	2:B:1150:ARG:HH12	1.74	0.52
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.23	0.52
2:B:167:ILE:HG22	2:B:167:ILE:O	2.09	0.52
2:B:563:MET:HE3	2:B:580:VAL:HB	1.89	0.52
4:E:176:PRO:O	4:E:212:ARG:HA	2.10	0.52
1:A:472:LEU:HD13	2:B:835:GLN:NE2	2.24	0.52
2:B:105:SER:O	2:B:106:ASP:HB2	2.10	0.52
3:C:237:SER:O	3:C:238:ILE:HG13	2.10	0.52
6:H:125:LEU:HB3	6:H:130:ARG:CZ	2.40	0.52
8:J:48:ARG:O	8:J:52:THR:HB	2.10	0.52
1:A:418:SER:C	1:A:420:ARG:H	2.18	0.52
1:A:1386:ARG:HG3	1:A:1386:ARG:O	2.10	0.52
2:B:344:LYS:H	2:B:347:LYS:HZ1	1.57	0.52
2:B:1165:ILE:HG13	2:B:1187:ASN:HD21	1.75	0.52
6:H:97:MET:CE	6:H:142:LEU:HD23	2.38	0.52
1:A:157:ASP:C	1:A:159:THR:N	2.64	0.52
1:A:899:VAL:HG12	1:A:929:LEU:HD13	1.90	0.52
2:B:824:ILE:CG1	8:J:48:ARG:HH12	2.23	0.52
3:C:137:LYS:H	3:C:137:LYS:CD	2.21	0.52
6:H:103:LYS:HG2	6:H:115:TYR:H	1.74	0.52
1:A:1146:VAL:O	1:A:1146:VAL:CG1	2.57	0.52
1:A:1220:PHE:O	1:A:1221:LYS:C	2.53	0.52
2:B:98:THR:HG22	2:B:99:LYS:H	1.74	0.52
2:B:130:VAL:CG1	2:B:131:ASP:N	2.73	0.52
2:B:484:ASN:ND2	2:B:486:TYR:HE1	2.08	0.52
5:F:77:ASP:O	5:F:78:GLN:CB	2.57	0.52
1:A:262:LEU:HD11	1:A:328:ARG:HD2	1.92	0.52
2:B:272:THR:OG1	2:B:279:ASP:OD1	2.26	0.52
6:H:18:GLY:O	6:H:20:TYR:N	2.42	0.52
1:A:72:GLU:HB3	1:A:76:GLU:HB2	1.90	0.52
1:A:768:GLN:NE2	1:A:816:HIS:HA	2.23	0.52
1:A:1128:GLN:O	1:A:1128:GLN:HG3	2.07	0.52
2:B:416:LEU:HD11	2:B:466:TRP:CZ2	2.45	0.52
3:C:77:ILE:CA	3:C:129:ILE:HD11	2.38	0.52
9:K:111:LEU:N	9:K:111:LEU:HD23	2.24	0.52
10:L:26:THR:CG2	10:L:27:LEU:N	2.67	0.52
1:A:606:LEU:HG	1:A:613:ILE:HB	1.92	0.51
2:B:130:VAL:HG21	2:B:167:ILE:HD12	1.92	0.51
3:C:18:VAL:O	3:C:20:PHE:HD2	1.93	0.51
4:E:59:SER:O	4:E:60:PHE:HB3	2.09	0.51
1:A:32:VAL:HB	1:A:57:ARG:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:O	1:A:79:GLY:C	2.52	0.51
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.75	0.51
1:A:751:SER:O	1:A:752:LYS:O	2.29	0.51
1:A:901:LEU:HD23	1:A:907:THR:HG23	1.92	0.51
1:A:998:LEU:HD12	1:A:1001:ARG:HH12	1.74	0.51
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.74	0.51
2:B:830:TYR:CE1	2:B:1000:PRO:HB3	2.46	0.51
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.92	0.51
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.26	0.51
6:H:113:ALA:HB1	6:H:124:ARG:HE	1.74	0.51
6:H:125:LEU:HB3	6:H:130:ARG:NH1	2.24	0.51
7:I:72:ASP:O	7:I:81:ARG:HD2	2.10	0.51
1:A:1318:THR:CG2	4:E:11:ARG:HH12	2.24	0.51
1:A:1336:MET:O	1:A:1336:MET:HG2	2.09	0.51
2:B:227:LYS:NZ	2:B:236:HIS:HE1	2.09	0.51
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.39	0.51
2:B:737:THR:HG21	7:I:66:PRO:CA	2.41	0.51
4:E:61:GLN:HG2	4:E:62:ALA:N	2.25	0.51
1:A:328:ARG:HB3	1:A:332:LYS:NZ	2.25	0.51
1:A:540:PHE:HB3	1:A:571:LEU:HG	1.93	0.51
1:A:1191:TRP:CE2	1:A:1257:ASP:OD1	2.64	0.51
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.44	0.51
3:C:75:MET:HE1	3:C:239:PRO:HG2	1.92	0.51
6:H:130:ARG:HA	6:H:133:ASN:CB	2.40	0.51
7:I:51:ASN:HB2	7:I:118:ARG:NH1	2.26	0.51
1:A:775:ILE:O	1:A:797:LYS:HE3	2.10	0.51
2:B:210:LYS:HE3	2:B:480:SER:OG	2.11	0.51
2:B:763:GLN:HB2	2:B:1021:MET:HB2	1.91	0.51
2:B:776:GLN:O	2:B:1095:LEU:HA	2.10	0.51
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.10	0.51
2:B:1002:THR:HG21	2:B:1006:ILE:HB	1.93	0.51
2:B:1006:ILE:HD12	14:B:2021:HOH:O	2.09	0.51
2:B:1096:ARG:HA	2:B:1098:MET:HE2	1.93	0.51
1:A:605:MET:HE1	1:A:612:ILE:HD12	1.91	0.51
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.09	0.51
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.76	0.51
4:E:55:ARG:HG3	4:E:55:ARG:HH11	1.75	0.51
4:E:65:THR:O	4:E:69:ILE:HG13	2.09	0.51
1:A:857:ARG:HD3	1:A:861:GLY:O	2.11	0.51
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.51	0.51
2:B:1034:VAL:CG2	2:B:1059:LEU:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:63:LEU:C	6:H:90:ALA:HB3	2.35	0.51
8:J:12:LYS:NZ	8:J:17:LYS:HZ1	2.09	0.51
9:K:21:ILE:CG2	9:K:31:VAL:HG11	2.40	0.51
9:K:43:GLY:O	9:K:47:ARG:HB2	2.11	0.51
1:A:549:MET:SD	1:A:577:ILE:HD12	2.51	0.51
1:A:756:ILE:O	1:A:756:ILE:HD13	2.11	0.51
2:B:54:PHE:HA	2:B:58:THR:HB	1.92	0.51
8:J:12:LYS:HZ1	8:J:17:LYS:HZ1	1.59	0.51
10:L:33:GLU:C	10:L:35:SER:H	2.18	0.51
10:L:46:VAL:O	10:L:54:ARG:HA	2.11	0.51
1:A:871:ASP:OD2	4:E:204:THR:HG23	2.10	0.51
1:A:961:ARG:O	1:A:965:GLN:HG3	2.10	0.51
2:B:174:LEU:HD22	2:B:202:TYR:CZ	2.46	0.51
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.92	0.51
2:B:847:ASP:O	3:C:65:HIS:HE1	1.93	0.51
2:B:1002:THR:CG2	2:B:1006:ILE:H	2.23	0.51
9:K:45:LEU:HG	9:K:94:ILE:HD13	1.92	0.51
1:A:78:PRO:HA	2:B:1201:LYS:NZ	2.26	0.51
1:A:307:ASP:C	1:A:308:ILE:HG13	2.36	0.51
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.92	0.51
2:B:1051:THR:HG22	2:B:1052:VAL:N	2.25	0.51
2:B:1165:ILE:HD12	2:B:1187:ASN:ND2	2.26	0.51
6:H:93:TYR:CD1	6:H:93:TYR:N	2.79	0.51
10:L:38:LEU:O	10:L:39:SER:CB	2.59	0.51
1:A:61:ILE:O	1:A:62:ASP:HB2	2.11	0.50
1:A:754:SER:H	1:A:757:ASN:HD22	1.59	0.50
1:A:869:GLY:O	1:A:870:GLU:HB2	2.12	0.50
3:C:89:GLU:O	3:C:90:ASP:HB3	2.10	0.50
4:E:45:LYS:HG2	4:E:45:LYS:O	2.11	0.50
1:A:327:ALA:HA	1:A:330:LYS:CD	2.41	0.50
2:B:737:THR:CG2	7:I:66:PRO:CA	2.89	0.50
6:H:10:PHE:O	6:H:54:SER:HA	2.11	0.50
6:H:118:PHE:HB2	6:H:121:LEU:HB2	1.92	0.50
8:J:25:LEU:O	8:J:29:GLU:HA	2.12	0.50
1:A:606:LEU:HD23	1:A:614:PHE:CE2	2.47	0.50
1:A:848:ILE:HG12	1:A:864:ILE:CD1	2.41	0.50
1:A:1187:GLN:CG	1:A:1188:GLN:H	2.24	0.50
1:A:1285:MET:HG3	1:A:1307:GLU:OE1	2.11	0.50
2:B:824:ILE:HG12	8:J:48:ARG:HH12	1.77	0.50
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.93	0.50
3:C:175:ALA:O	3:C:176:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:81:THR:CG2	5:F:82:THR:N	2.75	0.50
1:A:1096:SER:O	1:A:1099:PRO:HG2	2.11	0.50
2:B:18:PHE:N	2:B:18:PHE:CD2	2.80	0.50
2:B:733:HIS:O	2:B:735:ALA:N	2.38	0.50
2:B:900:ALA:HB2	10:L:58:LYS:NZ	2.26	0.50
2:B:1185:CYS:O	2:B:1186:ASP:HB2	2.12	0.50
3:C:7:GLN:HG2	9:K:104:ASN:ND2	2.26	0.50
3:C:57:VAL:HG11	8:J:60:PHE:CB	2.41	0.50
3:C:258:ILE:HD13	9:K:35:PHE:CE2	2.38	0.50
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.25	0.50
1:A:557:ASP:OD1	1:A:557:ASP:N	2.45	0.50
2:B:294:ASP:H	7:I:12:ASN:HD22	1.57	0.50
2:B:969:ARG:HB3	2:B:969:ARG:NH1	2.25	0.50
3:C:148:ARG:HH12	8:J:64:ASN:CA	2.20	0.50
6:H:105:GLU:H	6:H:105:GLU:CD	2.19	0.50
7:I:55:THR:O	7:I:58:VAL:HG23	2.11	0.50
1:A:128:ILE:HG22	1:A:130:ASP:H	1.77	0.50
1:A:1395:GLY:O	1:A:1397:LEU:N	2.45	0.50
2:B:357:GLN:OE1	2:B:358:LYS:HE3	2.11	0.50
2:B:957:ASN:CG	2:B:958:GLN:N	2.70	0.50
2:B:976:ILE:O	2:B:1099:VAL:HG21	2.11	0.50
3:C:179:GLU:CG	3:C:180:TYR:N	2.74	0.50
4:E:12:LEU:CD1	4:E:58:MET:HE1	2.42	0.50
5:F:109:VAL:HG13	5:F:127:GLU:OE1	2.11	0.50
8:J:24:LEU:O	8:J:30:LEU:HB2	2.11	0.50
8:J:57:ILE:HA	8:J:60:PHE:CD2	2.47	0.50
1:A:443:LEU:HG	1:A:455:MET:HE2	1.93	0.50
1:A:535:THR:O	1:A:575:LYS:HE3	2.12	0.50
2:B:46:GLN:OE1	2:B:47:GLN:HG2	2.12	0.50
2:B:680:THR:CG2	2:B:681:TRP:H	2.24	0.50
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.10	0.50
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.52	0.50
1:A:523:ILE:HD12	1:A:622:VAL:CG2	2.42	0.50
1:A:1394:THR:HG23	1:A:1398:MET:CE	2.41	0.50
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.31	0.50
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.42	0.50
1:A:705:LYS:O	1:A:708:MET:HB2	2.11	0.50
2:B:235:SER:OG	2:B:236:HIS:HD2	1.95	0.50
2:B:284:ILE:HD13	2:B:324:ILE:HD12	1.93	0.50
6:H:100:THR:HG23	6:H:138:GLU:CB	2.42	0.50
8:J:2:ILE:HG22	8:J:3:VAL:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:542:MET:HG3	2:B:747:MET:CE	2.29	0.49
2:B:621:GLU:O	2:B:623:GLU:HG3	2.12	0.49
2:B:969:ARG:HE	3:C:59:ALA:HB1	1.77	0.49
1:A:106:VAL:HG22	1:A:111:GLY:HA2	1.93	0.49
1:A:407:ARG:O	1:A:408:ASP:C	2.56	0.49
1:A:472:LEU:O	1:A:475:THR:HB	2.12	0.49
1:A:1101:LEU:O	1:A:1105:LEU:HG	2.11	0.49
2:B:126:SER:OG	2:B:172:ILE:HD12	2.12	0.49
3:C:203:GLN:HG2	3:C:207:CYS:SG	2.51	0.49
9:K:31:VAL:HG12	9:K:32:VAL:N	2.27	0.49
9:K:110:ASN:C	9:K:112:GLN:H	2.20	0.49
10:L:30:ILE:HG22	10:L:31:CYS:H	1.77	0.49
10:L:32:ALA:HB2	10:L:55:ILE:CB	2.42	0.49
1:A:185:TRP:O	1:A:186:LYS:HB2	2.12	0.49
2:B:134:LYS:HZ1	2:B:446:LEU:HD13	1.77	0.49
3:C:56:THR:HG23	3:C:57:VAL:N	2.26	0.49
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.47	0.49
1:A:92:HIS:CD2	1:A:92:HIS:C	2.91	0.49
1:A:329:LEU:C	1:A:331:GLY:N	2.70	0.49
1:A:1391:ARG:HH21	1:A:1417:GLU:CD	2.20	0.49
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.52	0.49
2:B:983:ARG:HD3	14:B:2018:HOH:O	2.12	0.49
3:C:128:ASN:O	3:C:129:ILE:HG13	2.12	0.49
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.94	0.49
3:C:231:ASN:C	3:C:231:ASN:OD1	2.54	0.49
1:A:1277:GLU:O	1:A:1278:ASN:CB	2.61	0.49
5:F:85:MET:HE2	5:F:93:ILE:CD1	2.42	0.49
8:J:11:GLY:O	8:J:12:LYS:C	2.55	0.49
1:A:328:ARG:HB3	1:A:332:LYS:HZ2	1.77	0.49
1:A:767:GLN:HG2	11:M:4:ILE:CD1	2.42	0.49
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.76	0.49
1:A:1402:PHE:C	1:A:1404:GLU:H	2.20	0.49
2:B:305:VAL:O	2:B:305:VAL:HG12	2.12	0.49
2:B:735:ALA:HB3	2:B:738:PHE:CZ	2.47	0.49
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.95	0.49
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.94	0.49
2:B:241:ARG:HG2	2:B:251:ILE:CG2	2.41	0.49
2:B:809:MET:HG2	2:B:814:PHE:HB3	1.93	0.49
2:B:979:LYS:CE	2:B:987:LYS:HD2	2.41	0.49
3:C:244:VAL:HG12	3:C:248:ILE:HD11	1.94	0.49
6:H:126:GLU:N	6:H:130:ARG:HH12	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:PRO:HB2	1:A:497:THR:CG2	2.39	0.49
1:A:606:LEU:HD11	1:A:608:ILE:CD1	2.43	0.49
1:A:871:ASP:CG	4:E:204:THR:HG23	2.38	0.49
1:A:964:ILE:HD13	1:A:1035:TYR:CE1	2.46	0.49
2:B:103:ASN:HB2	2:B:169:ARG:HH12	1.77	0.49
3:C:165:LYS:O	9:K:6:ARG:NH1	2.46	0.49
10:L:43:THR:HG22	10:L:43:THR:O	2.12	0.49
1:A:328:ARG:HD3	1:A:332:LYS:HZ2	1.77	0.49
1:A:329:LEU:HD23	1:A:332:LYS:HB2	1.94	0.49
1:A:786:HIS:CD2	1:A:786:HIS:N	2.81	0.49
1:A:849:MET:CE	1:A:1436:ILE:HA	2.31	0.49
2:B:876:LYS:HE2	2:B:893:LEU:C	2.37	0.49
3:C:183:TRP:O	3:C:185:LYS:N	2.41	0.49
6:H:103:LYS:NZ	6:H:114:VAL:CG2	2.76	0.49
11:M:4:ILE:H	11:M:4:ILE:HD12	1.78	0.49
1:A:5:GLN:OE1	2:B:1175:LEU:HD12	2.13	0.49
1:A:220:THR:O	1:A:222:LEU:O	2.31	0.49
1:A:541:ILE:HG21	1:A:549:MET:HE3	1.94	0.49
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.13	0.49
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.28	0.49
2:B:784:ASN:OD1	2:B:788:ARG:HD2	2.12	0.49
2:B:1020:ARG:O	2:B:1021:MET:HB2	2.12	0.49
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.48	0.49
5:F:140:ASP:C	5:F:140:ASP:OD1	2.56	0.49
1:A:332:LYS:O	1:A:336:ILE:HD12	2.13	0.48
1:A:829:VAL:O	1:A:830:LYS:C	2.54	0.48
1:A:982:THR:HG22	1:A:984:LYS:N	2.22	0.48
1:A:1030:ARG:HD3	1:A:1034:GLU:OE1	2.12	0.48
1:A:1190:PRO:HG3	7:I:18:GLU:OE2	2.13	0.48
2:B:241:ARG:HG2	2:B:251:ILE:HG23	1.93	0.48
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.95	0.48
2:B:787:VAL:O	2:B:787:VAL:HG12	2.12	0.48
5:F:109:VAL:CG1	5:F:110:ASP:N	2.64	0.48
6:H:81:PRO:CB	6:H:82:PRO:CD	2.91	0.48
7:I:95:THR:HG22	7:I:96:SER:O	2.13	0.48
9:K:82:ASP:OD1	9:K:84:LYS:N	2.44	0.48
1:A:1204:ASP:C	1:A:1206:ASP:H	2.20	0.48
1:A:1225:PHE:O	1:A:1240:CYS:HA	2.13	0.48
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.52	0.48
1:A:1384:VAL:O	1:A:1386:ARG:N	2.46	0.48
2:B:35:SER:HA	2:B:811:TYR:CE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLU:OE1	2:B:680:THR:CG2	2.60	0.48
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.13	0.48
2:B:234:ILE:CD1	2:B:257:LYS:HD3	2.43	0.48
2:B:542:MET:HE2	2:B:747:MET:HE2	1.94	0.48
2:B:1162:ILE:HD11	2:B:1216:LEU:HD12	1.94	0.48
3:C:227:THR:HG22	3:C:229:TYR:CE1	2.47	0.48
4:E:147:HIS:CD2	4:E:149:LEU:H	2.31	0.48
1:A:55:ASP:N	1:A:56:PRO:CD	2.74	0.48
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.48	0.48
1:A:697:ALA:HB2	1:A:702:LEU:CD1	2.43	0.48
1:A:756:ILE:HD13	1:A:756:ILE:C	2.37	0.48
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.23	0.48
2:B:181:LEU:HD22	2:B:189:LEU:CD2	2.43	0.48
2:B:756:ILE:HG12	2:B:770:GLN:HG2	1.96	0.48
3:C:209:TYR:N	3:C:209:TYR:CD1	2.80	0.48
4:E:98:ILE:O	4:E:102:GLU:HG3	2.13	0.48
1:A:535:THR:HG22	1:A:575:LYS:HE2	1.94	0.48
1:A:849:MET:CE	1:A:1437:GLY:H	2.27	0.48
1:A:982:THR:HG22	1:A:983:ILE:N	2.28	0.48
1:A:1127:ASP:C	1:A:1129:GLU:H	2.22	0.48
2:B:365:THR:HG22	2:B:367:LEU:N	2.16	0.48
2:B:1099:VAL:O	2:B:1101:ASP:N	2.45	0.48
3:C:31:ASN:O	3:C:34:ARG:HB3	2.13	0.48
3:C:258:ILE:HD12	9:K:42:LEU:HD21	1.93	0.48
10:L:60:ARG:HG2	10:L:61:THR:N	2.27	0.48
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.94	0.48
1:A:767:GLN:HG3	1:A:768:GLN:O	2.12	0.48
1:A:1016:THR:CG2	4:E:206:GLY:HA3	2.43	0.48
1:A:1129:GLU:O	1:A:1133:LEU:HG	2.14	0.48
1:A:1152:ILE:HA	1:A:1192:LEU:O	2.14	0.48
1:A:1217:LYS:C	1:A:1219:THR:H	2.21	0.48
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.48	0.48
3:C:8:VAL:HG12	3:C:9:LYS:H	1.78	0.48
3:C:148:ARG:HG2	3:C:149:LYS:N	2.29	0.48
7:I:69:PRO:HG2	7:I:85:PHE:O	2.14	0.48
1:A:884:ASP:OD2	1:A:1030:ARG:NH2	2.46	0.48
1:A:1398:MET:O	1:A:1399:ARG:C	2.56	0.48
5:F:111:LEU:C	5:F:113:GLY:H	2.21	0.48
5:F:127:GLU:O	5:F:129:LYS:HG3	2.13	0.48
7:I:84:VAL:HG12	7:I:102:VAL:HB	1.94	0.48
7:I:111:THR:CG2	7:I:112:SER:N	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:96:ASN:O	9:K:99:GLY:N	2.46	0.48
1:A:528:LEU:HD23	1:A:751:SER:N	2.29	0.48
1:A:903:ASN:HD22	1:A:903:ASN:C	2.22	0.48
1:A:1159:ARG:O	1:A:1170:ILE:HG21	2.12	0.48
2:B:514:LEU:HD12	2:B:518:HIS:CD2	2.49	0.48
2:B:552:MET:N	2:B:553:PRO:HD2	2.28	0.48
2:B:859:TYR:N	2:B:859:TYR:CD1	2.82	0.48
2:B:898:LEU:CD2	2:B:964:VAL:HG11	2.41	0.48
2:B:969:ARG:HH11	2:B:969:ARG:CB	2.26	0.48
3:C:145:CYS:SG	3:C:146:LYS:N	2.86	0.48
3:C:152:GLU:OE2	3:C:154:LYS:HE3	2.12	0.48
7:I:111:THR:HG1	7:I:121:PHE:HE2	1.61	0.48
9:K:70:ARG:O	9:K:70:ARG:HG3	2.12	0.48
1:A:384:ASN:ND2	1:A:388:LEU:HD11	2.29	0.48
2:B:339:THR:CG2	2:B:343:ILE:HB	2.44	0.48
2:B:566:LEU:HD13	2:B:588:GLY:HA2	1.96	0.48
2:B:731:VAL:CG1	2:B:732:SER:H	2.27	0.48
4:E:64:PRO:HG2	4:E:75:MET:O	2.14	0.48
1:A:179:LEU:HG	1:A:308:ILE:HG21	1.96	0.48
1:A:438:ASP:O	1:A:439:ASN:HB2	2.14	0.48
1:A:567:LYS:HD3	6:H:95:TYR:CG	2.49	0.48
1:A:871:ASP:CB	4:E:204:THR:CG2	2.90	0.48
1:A:1258:HIS:O	1:A:1259:MET:C	2.56	0.48
2:B:644:GLU:HG3	2:B:654:ARG:NH2	2.26	0.48
2:B:652:LYS:CE	2:B:688:GLY:O	2.61	0.48
2:B:842:ASN:OD1	2:B:844:SER:HB2	2.14	0.48
2:B:1160:VAL:HG12	2:B:1161:HIS:H	1.79	0.48
1:A:32:VAL:HB	1:A:57:ARG:HD2	1.96	0.48
1:A:122:MET:HE1	1:A:138:ILE:CG2	2.39	0.48
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.49	0.48
2:B:38:PHE:HZ	2:B:541:LEU:HB3	1.79	0.48
2:B:642:ASP:C	2:B:644:GLU:H	2.20	0.48
2:B:999:MET:HA	2:B:999:MET:CE	2.41	0.48
4:E:102:GLU:C	4:E:104:ASN:H	2.22	0.48
7:I:103:CYS:HB3	7:I:108:HIS:H	1.79	0.48
1:A:867:ILE:HD11	1:A:999:VAL:HG11	1.95	0.47
1:A:899:VAL:CG1	1:A:929:LEU:HD13	2.44	0.47
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.44	0.47
3:C:186:LEU:N	3:C:186:LEU:HD12	2.28	0.47
4:E:12:LEU:HD21	4:E:58:MET:SD	2.54	0.47
1:A:528:LEU:O	1:A:531:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:LEU:HD13	1:A:556:TRP:CZ2	2.48	0.47
1:A:968:GLN:NE2	1:A:1035:TYR:O	2.47	0.47
2:B:332:ASP:OD2	2:B:345:LYS:HG3	2.14	0.47
4:E:197:LYS:HG3	4:E:211:TYR:CE2	2.48	0.47
1:A:1111:MET:HE1	1:A:1114:PRO:HA	1.97	0.47
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	2.14	0.47
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.39	0.47
2:B:221:ASN:O	2:B:222:ILE:HG13	2.14	0.47
2:B:235:SER:HA	2:B:261:ARG:HH21	1.79	0.47
2:B:887:HIS:O	2:B:888:GLY:C	2.58	0.47
3:C:206:ASN:ND2	3:C:229:TYR:CB	2.78	0.47
4:E:202:SER:O	4:E:205:SER:O	2.33	0.47
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.44	0.47
1:A:38:PRO:HA	1:A:270:LEU:CD1	2.40	0.47
1:A:95:PHE:CE2	1:A:1414:ALA:HB2	2.49	0.47
1:A:399:HIS:CB	1:A:400:PRO:CD	2.92	0.47
1:A:444:PHE:CE2	1:A:487:MET:HE3	2.49	0.47
1:A:1394:THR:CG2	1:A:1398:MET:HE3	2.43	0.47
2:B:64:CYS:HA	2:B:67:SER:HB3	1.95	0.47
2:B:89:GLU:O	2:B:90:ILE:HB	2.14	0.47
2:B:123:THR:OG1	2:B:458:LYS:HE3	2.14	0.47
2:B:824:ILE:CG1	8:J:48:ARG:NH1	2.77	0.47
4:E:96:PHE:CE1	4:E:100:ILE:HD11	2.48	0.47
1:A:523:ILE:CD1	1:A:649:ILE:HG21	2.43	0.47
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.14	0.47
2:B:46:GLN:H	2:B:46:GLN:HG3	1.30	0.47
2:B:557:PHE:HZ	2:B:599:THR:HG21	1.79	0.47
2:B:1065:GLN:HG3	2:B:1065:GLN:O	2.14	0.47
3:C:252:GLN:HE22	9:K:99:GLY:HA2	1.79	0.47
8:J:12:LYS:HZ1	8:J:17:LYS:NZ	2.11	0.47
2:B:1051:THR:CG2	2:B:1052:VAL:N	2.77	0.47
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.96	0.47
3:C:68:GLY:O	3:C:169:LYS:HB2	2.14	0.47
5:F:76:LYS:C	5:F:79:ARG:HD2	2.39	0.47
1:A:10:PRO:HG2	2:B:1192:TYR:CD2	2.49	0.47
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.97	0.47
1:A:69:THR:C	1:A:71:GLN:H	2.21	0.47
1:A:264:PHE:O	1:A:267:ALA:HB3	2.15	0.47
1:A:537:ARG:HH11	1:A:537:ARG:HG2	1.80	0.47
1:A:1169:ILE:O	1:A:1173:HIS:CD2	2.68	0.47
1:A:1295:THR:O	1:A:1295:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:THR:CG2	2:B:270:LYS:HE3	2.36	0.47
2:B:274:PRO:HG3	2:B:359:GLU:HB3	1.96	0.47
2:B:581:PHE:HA	2:B:585:VAL:O	2.15	0.47
2:B:863:GLU:O	2:B:864:LYS:O	2.33	0.47
2:B:915:THR:HG22	2:B:916:THR:N	2.29	0.47
2:B:997:GLU:H	2:B:997:GLU:HG3	1.52	0.47
3:C:8:VAL:HG21	9:K:105:PHE:HB2	1.97	0.47
8:J:48:ARG:HG2	8:J:48:ARG:NH1	2.26	0.47
9:K:7:PHE:HB2	9:K:11:LEU:CD2	2.44	0.47
10:L:63:ARG:O	10:L:64:LEU:C	2.57	0.47
10:L:68:GLU:C	10:L:70:ARG:H	2.22	0.47
1:A:946:VAL:HG22	4:E:201:LYS:HD2	1.96	0.47
1:A:1431:GLY:O	2:B:1148:LYS:HE3	2.15	0.47
2:B:169:ARG:N	2:B:454:THR:OG1	2.48	0.47
2:B:351:TYR:O	2:B:355:ILE:HG13	2.15	0.47
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.36	0.47
3:C:206:ASN:ND2	3:C:229:TYR:HB2	2.30	0.47
1:A:112:LYS:NZ	1:A:165:GLY:N	2.54	0.47
1:A:602:ASP:O	1:A:615:GLY:HA2	2.14	0.47
1:A:705:LYS:O	1:A:706:HIS:C	2.57	0.47
2:B:315:LYS:N	2:B:316:PRO:HD2	2.29	0.47
2:B:392:ARG:HH22	7:I:52:ILE:HD11	1.75	0.47
2:B:876:LYS:HE3	2:B:894:ASP:C	2.40	0.47
2:B:882:THR:HG21	2:B:935:ARG:HA	1.97	0.47
4:E:117:THR:C	4:E:119:SER:N	2.72	0.47
7:I:95:THR:CG2	7:I:96:SER:N	2.78	0.47
1:A:54:ASN:O	1:A:55:ASP:HB2	2.15	0.47
1:A:517:ASN:HD22	1:A:1364:ASN:HB2	1.80	0.47
1:A:740:LEU:HD21	3:C:193:TYR:CE2	2.51	0.47
1:A:1400:CYS:SG	1:A:1405:THR:HG21	2.55	0.47
2:B:114:PRO:HD3	2:B:124:TYR:CZ	2.49	0.47
2:B:579:ARG:HG3	2:B:581:PHE:HE1	1.80	0.47
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.14	0.47
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.50	0.47
6:H:31:THR:O	6:H:32:THR:CB	2.62	0.47
1:A:626:ASN:O	1:A:631:HIS:CD2	2.69	0.46
2:B:46:GLN:NE2	2:B:496:ARG:HD2	2.30	0.46
2:B:882:THR:HG22	2:B:884:ARG:H	1.80	0.46
3:C:18:VAL:HG23	3:C:240:VAL:HG12	1.96	0.46
5:F:79:ARG:NH2	5:F:150:GLU:OE2	2.44	0.46
5:F:111:LEU:O	5:F:113:GLY:N	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:26:LEU:HD23	7:I:37:GLU:HA	1.95	0.46
1:A:465:TYR:CE2	9:K:4:PRO:HD2	2.50	0.46
1:A:840:ARG:HG3	1:A:1385:THR:CG2	2.45	0.46
1:A:1206:ASP:HB2	1:A:1274:ARG:NH1	2.30	0.46
2:B:296:GLU:O	2:B:300:HIS:CD2	2.66	0.46
2:B:705:MET:HB3	2:B:706:GLN:HE21	1.81	0.46
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.97	0.46
4:E:177:ARG:HD3	4:E:215:MET:HE2	1.97	0.46
6:H:6:PHE:O	6:H:58:THR:HG23	2.14	0.46
6:H:27:GLU:HA	6:H:38:LEU:O	2.15	0.46
10:L:60:ARG:HG2	10:L:61:THR:H	1.80	0.46
1:A:65:LEU:HD22	1:A:72:GLU:O	2.16	0.46
1:A:108:MET:HE3	1:A:210:ILE:HD12	1.96	0.46
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.79	0.46
1:A:1434:ALA:C	1:A:1436:ILE:H	2.22	0.46
2:B:121:ASN:HA	2:B:207:GLY:CA	2.45	0.46
2:B:313:MET:CE	2:B:386:LEU:HD22	2.37	0.46
2:B:314:LEU:O	2:B:315:LYS:C	2.58	0.46
2:B:899:ILE:CG2	2:B:900:ALA:H	2.28	0.46
3:C:264:GLN:C	3:C:266:ASP:H	2.24	0.46
1:A:417:TYR:O	1:A:418:SER:HB2	2.15	0.46
1:A:418:SER:C	1:A:420:ARG:N	2.73	0.46
2:B:122:LEU:HD22	2:B:958:GLN:CG	2.45	0.46
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.96	0.46
2:B:324:ILE:HD11	2:B:333:PHE:CG	2.50	0.46
2:B:757:PRO:HG2	2:B:984:HIS:HE1	1.81	0.46
3:C:229:TYR:N	3:C:229:TYR:CD1	2.83	0.46
3:C:266:ASP:O	3:C:267:GLN:HB2	2.15	0.46
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.79	0.46
2:B:404:LYS:O	2:B:405:ARG:NH1	2.37	0.46
3:C:179:GLU:HG3	3:C:180:TYR:H	1.79	0.46
7:I:40:SER:HB2	7:I:41:PRO:HD2	1.97	0.46
7:I:74:GLU:HB2	7:I:81:ARG:NH1	2.30	0.46
9:K:49:GLU:HG3	9:K:94:ILE:HG13	1.97	0.46
1:A:416:ARG:HG3	1:A:417:TYR:CD1	2.51	0.46
1:A:567:LYS:NZ	6:H:95:TYR:CE1	2.72	0.46
1:A:854:ASN:ND2	1:A:999:VAL:O	2.48	0.46
1:A:939:ASP:OD1	1:A:1023:ARG:NH1	2.49	0.46
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.64	0.46
2:B:731:VAL:CG1	2:B:732:SER:N	2.77	0.46
3:C:259:LEU:HD21	9:K:91:CYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.96	0.46
6:H:99:GLY:N	6:H:118:PHE:CD2	2.84	0.46
6:H:127:GLY:O	6:H:128:ASN:HB2	2.15	0.46
7:I:59:VAL:HG12	7:I:61:ASP:H	1.81	0.46
10:L:27:LEU:HD13	10:L:37:LYS:CG	2.45	0.46
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.98	0.46
1:A:345:VAL:HG12	2:B:1150:ARG:HH22	1.80	0.46
2:B:571:PRO:C	2:B:573:GLN:N	2.73	0.46
2:B:642:ASP:C	2:B:644:GLU:N	2.74	0.46
2:B:651:LEU:HD23	2:B:710:LEU:HD11	1.96	0.46
3:C:248:ILE:H	3:C:248:ILE:HG13	1.40	0.46
6:H:100:THR:CB	6:H:138:GLU:HG3	2.46	0.46
1:A:265:LYS:O	1:A:269:ILE:HG13	2.15	0.46
1:A:345:VAL:HG13	2:B:1150:ARG:NH1	2.31	0.46
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.98	0.46
2:B:25:ILE:HG23	2:B:29:ASP:CB	2.46	0.46
2:B:310:MET:HE1	2:B:387:LEU:HD13	1.97	0.46
2:B:484:ASN:O	2:B:485:ARG:HD2	2.15	0.46
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.38	0.46
2:B:1008:PRO:HB3	2:B:1087:PHE:CE1	2.50	0.46
1:A:5:GLN:CG	1:A:6:TYR:H	2.21	0.46
1:A:53:LEU:HB3	1:A:54:ASN:OD1	2.16	0.46
1:A:79:GLY:HA3	1:A:245:PRO:CG	2.46	0.46
1:A:596:THR:C	1:A:598:LEU:H	2.24	0.46
1:A:786:HIS:CD2	1:A:786:HIS:H	2.34	0.46
1:A:834:THR:HG22	1:A:1077:THR:OG1	2.16	0.46
2:B:101:MET:SD	2:B:109:THR:HG21	2.55	0.46
2:B:564:GLU:HB2	2:B:589:VAL:HG12	1.96	0.46
2:B:979:LYS:HB3	2:B:979:LYS:HE2	1.81	0.46
2:B:1082:MET:HA	3:C:189:THR:HA	1.98	0.46
3:C:20:PHE:HE1	3:C:22:LEU:HG	1.80	0.46
6:H:113:ALA:CB	6:H:124:ARG:HH21	2.29	0.46
1:A:35:ILE:HB	1:A:83:HIS:O	2.16	0.46
1:A:834:THR:HG21	1:A:1077:THR:OG1	2.16	0.46
1:A:849:MET:HE1	1:A:1436:ILE:CA	2.31	0.46
1:A:1277:GLU:CD	1:A:1277:GLU:N	2.73	0.46
2:B:47:GLN:OE1	2:B:47:GLN:HA	2.15	0.46
2:B:120:ARG:NH2	10:L:54:ARG:HH11	2.14	0.46
2:B:821:GLN:OE1	2:B:850:LEU:HD12	2.15	0.46
2:B:996:ARG:HD3	14:B:2017:HOH:O	2.16	0.46
3:C:60:ASP:OD2	10:L:60:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:HG22	1:A:239:LEU:O	2.15	0.45
1:A:368:LYS:HB2	1:A:368:LYS:HE3	1.68	0.45
1:A:714:PHE:CG	7:I:97:MET:HE1	2.51	0.45
1:A:870:GLU:HG2	4:E:208:TYR:CD2	2.51	0.45
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.46	0.45
1:A:973:ILE:HD11	1:A:1041:ALA:CB	2.47	0.45
1:A:1148:ILE:HD12	1:A:1196:GLU:HG2	1.99	0.45
1:A:1391:ARG:O	1:A:1392:SER:HB3	2.16	0.45
2:B:295:GLY:HA3	7:I:11:ASN:ND2	2.32	0.45
2:B:484:ASN:ND2	2:B:486:TYR:CE1	2.83	0.45
2:B:904:ARG:HH21	2:B:948:ILE:HD11	1.81	0.45
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.98	0.45
7:I:15:TYR:N	7:I:15:TYR:CD1	2.85	0.45
1:A:69:THR:HB	2:B:1174:LYS:HE2	1.98	0.45
1:A:148:CYS:O	1:A:167:CYS:O	2.35	0.45
1:A:261:ASP:O	1:A:264:PHE:HB2	2.17	0.45
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.51	0.45
1:A:738:LYS:NZ	3:C:194:GLU:O	2.42	0.45
1:A:857:ARG:CZ	5:F:139:PRO:HG3	2.46	0.45
2:B:25:ILE:HD12	2:B:653:VAL:CB	2.46	0.45
2:B:118:ARG:NH2	2:B:194:GLU:CD	2.74	0.45
2:B:339:THR:HG23	2:B:343:ILE:HB	1.98	0.45
2:B:351:TYR:CE2	2:B:355:ILE:HD11	2.51	0.45
2:B:416:LEU:HD11	2:B:466:TRP:CE2	2.52	0.45
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.51	0.45
7:I:59:VAL:HG12	7:I:60:GLN:N	2.31	0.45
8:J:7:CYS:HA	8:J:49:MET:HG2	1.98	0.45
9:K:108:GLU:O	9:K:112:GLN:HG2	2.17	0.45
1:A:265:LYS:NZ	1:A:302:THR:HB	2.30	0.45
1:A:505:CYS:O	1:A:506:ALA:C	2.59	0.45
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.51	0.45
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.97	0.45
3:C:186:LEU:N	3:C:186:LEU:CD1	2.79	0.45
4:E:75:MET:O	4:E:76:GLY:O	2.34	0.45
6:H:4:THR:HA	6:H:60:ALA:HA	1.98	0.45
6:H:103:LYS:HA	6:H:115:TYR:HB2	1.98	0.45
1:A:381:THR:HG21	1:A:383:TYR:HD1	1.82	0.45
2:B:1162:ILE:HG22	2:B:1163:CYS:O	2.16	0.45
3:C:179:GLU:HG3	3:C:180:TYR:N	2.32	0.45
6:H:95:TYR:HE2	6:H:97:MET:CG	2.29	0.45
10:L:46:VAL:CG1	10:L:56:LEU:HD12	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:O	1:A:79:GLY:O	2.35	0.45
1:A:90:VAL:HG12	1:A:91:PHE:O	2.17	0.45
1:A:130:ASP:OD2	1:A:133:LYS:HG3	2.16	0.45
1:A:156:ASP:HB2	1:A:157:ASP:H	1.55	0.45
1:A:541:ILE:HG12	1:A:549:MET:HE1	1.98	0.45
1:A:577:ILE:H	1:A:577:ILE:HG12	1.57	0.45
1:A:1111:MET:CE	1:A:1114:PRO:HA	2.46	0.45
4:E:43:LYS:O	4:E:47:CYS:HB2	2.16	0.45
6:H:81:PRO:HD2	6:H:82:PRO:HD2	1.98	0.45
1:A:142:CYS:C	1:A:144:THR:N	2.73	0.45
1:A:982:THR:O	1:A:985:ASP:HB2	2.16	0.45
2:B:341:LEU:O	2:B:341:LEU:CG	2.64	0.45
2:B:1072:MET:HE3	2:B:1085:ILE:CB	2.26	0.45
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.98	0.45
3:C:100:THR:HG22	3:C:101:LEU:N	2.30	0.45
4:E:28:TYR:CE2	4:E:78:LEU:HG	2.51	0.45
6:H:96:VAL:HG22	6:H:143:LEU:HD22	1.97	0.45
1:A:236:LEU:HD11	1:A:304:MET:HE1	1.99	0.45
1:A:1392:SER:O	1:A:1393:ASN:CB	2.65	0.45
2:B:863:GLU:OE1	2:B:962:LYS:HD2	2.17	0.45
8:J:48:ARG:HH11	8:J:48:ARG:CG	2.24	0.45
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.52	0.45
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.99	0.45
3:C:14:SER:O	3:C:240:VAL:HG21	2.16	0.45
5:F:72:LYS:N	5:F:142:SER:HA	2.31	0.45
5:F:75:PRO:C	5:F:77:ASP:N	2.74	0.45
5:F:90:ARG:HD3	5:F:155:LEU:HD12	1.98	0.45
6:H:100:THR:HG23	6:H:138:GLU:HB2	1.99	0.45
8:J:23:ASN:C	8:J:25:LEU:N	2.74	0.45
9:K:63:VAL:O	9:K:63:VAL:HG22	2.17	0.45
1:A:444:PHE:HE2	1:A:487:MET:HE3	1.82	0.45
2:B:99:LYS:HB3	2:B:180:TYR:CZ	2.52	0.45
2:B:315:LYS:HB2	2:B:315:LYS:HE3	1.72	0.45
2:B:766:ARG:NH1	2:B:985:GLY:O	2.44	0.45
2:B:771:SER:O	2:B:775:LYS:HE3	2.17	0.45
2:B:950:ASP:O	2:B:951:GLN:HG3	2.17	0.45
3:C:22:LEU:O	3:C:227:THR:HA	2.17	0.45
1:A:327:ALA:O	1:A:330:LYS:N	2.50	0.45
2:B:169:ARG:HB2	2:B:454:THR:CG2	2.43	0.45
2:B:977:GLY:HA3	2:B:1099:VAL:CG2	2.47	0.45
2:B:1154:ALA:O	2:B:1155:SER:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:260:LEU:HD12	3:C:260:LEU:O	2.16	0.45
4:E:50:MET:HE3	4:E:50:MET:O	2.17	0.45
10:L:51:CYS:C	10:L:53:HIS:N	2.75	0.45
1:A:78:PRO:O	1:A:78:PRO:HG2	2.17	0.44
1:A:164:ARG:HB2	1:A:165:GLY:H	1.60	0.44
1:A:329:LEU:O	1:A:333:GLU:HG2	2.18	0.44
1:A:774:ARG:CB	1:A:797:LYS:HG2	2.47	0.44
2:B:25:ILE:HD12	2:B:653:VAL:CG2	2.47	0.44
2:B:69:LEU:HD21	2:B:425:THR:CG2	2.47	0.44
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.99	0.44
2:B:913:GLY:HA2	2:B:938:SER:HB3	2.00	0.44
1:A:63:ARG:N	1:A:74:MET:HE2	2.31	0.44
1:A:476:SER:N	1:A:477:PRO:HD2	2.33	0.44
2:B:313:MET:HE3	2:B:386:LEU:CD2	2.39	0.44
2:B:805:THR:HB	2:B:809:MET:SD	2.57	0.44
3:C:175:ALA:O	3:C:176:ILE:CG1	2.65	0.44
4:E:114:ASN:OD1	4:E:115:ASN:N	2.50	0.44
6:H:18:GLY:C	6:H:20:TYR:H	2.24	0.44
1:A:32:VAL:HG23	1:A:33:ALA:N	2.32	0.44
1:A:740:LEU:N	1:A:740:LEU:CD1	2.80	0.44
1:A:1111:MET:HE3	1:A:1114:PRO:HG3	1.98	0.44
1:A:1166:ASP:CG	1:A:1194:ARG:HH21	2.25	0.44
2:B:188:ASP:O	2:B:192:LEU:HD12	2.17	0.44
2:B:590:HIS:HD2	2:B:593:PRO:HA	1.83	0.44
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.52	0.44
2:B:1159:ARG:HD2	2:B:1159:ARG:C	2.42	0.44
3:C:71:PRO:O	3:C:72:LEU:HD23	2.18	0.44
4:E:136:ASN:O	4:E:137:GLU:C	2.59	0.44
1:A:31:SER:OG	1:A:83:HIS:HB2	2.18	0.44
1:A:1001:ARG:O	1:A:1002:GLY:C	2.59	0.44
2:B:276:ILE:HG21	2:B:280:ILE:HD11	2.00	0.44
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.47	0.44
3:C:226:ASP:O	3:C:227:THR:HB	2.18	0.44
1:A:38:PRO:HB3	1:A:270:LEU:CB	2.48	0.44
1:A:49:LYS:HD3	1:A:55:ASP:CG	2.42	0.44
1:A:278:THR:O	1:A:278:THR:HG22	2.18	0.44
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.51	0.44
2:B:1100:ASP:HA	2:B:1103:ILE:CD1	2.48	0.44
3:C:66:ARG:NH1	3:C:144:ILE:O	2.47	0.44
3:C:221:TYR:HE1	3:C:222:LYS:HE3	1.82	0.44
6:H:31:THR:O	6:H:32:THR:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.18	0.44
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.48	0.44
1:A:499:ALA:O	1:A:503:GLN:HB2	2.18	0.44
1:A:741:ASN:ND2	1:A:743:VAL:HB	2.33	0.44
2:B:692:TYR:O	2:B:693:ILE:HG13	2.18	0.44
6:H:42:ILE:HG23	6:H:95:TYR:CZ	2.53	0.44
6:H:103:LYS:HZ1	6:H:114:VAL:HG21	1.81	0.44
6:H:130:ARG:HA	6:H:133:ASN:CG	2.42	0.44
7:I:50:THR:HG22	7:I:51:ASN:H	1.82	0.44
1:A:70:CYS:O	1:A:71:GLN:C	2.60	0.44
1:A:445:ASN:HB3	1:A:455:MET:HE3	1.99	0.44
1:A:642:CYS:O	1:A:645:LEU:HB3	2.18	0.44
1:A:973:ILE:HD11	1:A:1041:ALA:HB2	1.99	0.44
1:A:1102:LYS:HG2	1:A:1106:ASN:ND2	2.31	0.44
1:A:1295:THR:O	1:A:1295:THR:CG2	2.66	0.44
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.36	0.44
2:B:311:LEU:HB3	7:I:4:PHE:CZ	2.53	0.44
2:B:826:ALA:HB2	2:B:1087:PHE:CE1	2.53	0.44
2:B:860:MET:O	2:B:861:ASP:HB2	2.18	0.44
4:E:26:ARG:NH1	4:E:189:GLY:HA3	2.33	0.44
7:I:2:THR:O	7:I:2:THR:HG22	2.17	0.44
1:A:605:MET:HE2	1:A:607:ILE:HD11	2.00	0.44
1:A:666:ILE:CD1	2:B:1030:LEU:HB2	2.47	0.44
2:B:650:GLU:HG3	2:B:651:LEU:N	2.33	0.44
3:C:114:TYR:HB3	3:C:140:ASN:O	2.18	0.44
6:H:123:MET:HE1	6:H:142:LEU:CD1	2.47	0.44
7:I:68:LEU:HB3	7:I:84:VAL:HG22	1.99	0.44
9:K:7:PHE:CD1	9:K:7:PHE:C	2.96	0.44
10:L:33:GLU:O	10:L:35:SER:N	2.51	0.44
1:A:1438:THR:HG22	2:B:1144:ALA:H	1.83	0.44
2:B:653:VAL:HG13	2:B:689:LEU:HB3	1.99	0.44
2:B:778:MET:SD	2:B:1094:ARG:HD3	2.57	0.44
4:E:54:GLN:HB3	4:E:57:MET:HE3	1.99	0.44
9:K:61:TYR:HA	9:K:72:LYS:O	2.18	0.44
1:A:67:CYS:O	1:A:68:GLN:CB	2.66	0.43
1:A:360:GLU:OE2	1:A:651:LYS:NZ	2.51	0.43
1:A:672:ASP:CG	1:A:736:ASN:HD21	2.25	0.43
1:A:752:LYS:HD2	2:B:1015:HIS:O	2.18	0.43
1:A:1402:PHE:C	1:A:1404:GLU:N	2.76	0.43
2:B:104:GLU:CG	10:L:54:ARG:NH1	2.80	0.43
2:B:571:PRO:C	2:B:573:GLN:H	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:LYS:HD3	2:B:871:THR:OG1	2.17	0.43
2:B:912:ILE:O	2:B:938:SER:HB2	2.18	0.43
6:H:138:GLU:O	6:H:139:ASN:C	2.60	0.43
7:I:55:THR:HG23	7:I:58:VAL:HG21	2.00	0.43
1:A:230:ARG:HB3	1:A:232:GLU:HG2	1.99	0.43
1:A:464:PRO:O	1:A:465:TYR:C	2.60	0.43
1:A:511:ILE:HA	1:A:521:MET:HE3	2.00	0.43
1:A:709:THR:HB	1:A:712:GLU:HG3	1.99	0.43
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.00	0.43
2:B:513:GLN:HG3	14:B:2008:HOH:O	2.17	0.43
3:C:17:ASN:HD22	3:C:17:ASN:N	2.16	0.43
3:C:137:LYS:HD2	3:C:137:LYS:N	2.27	0.43
4:E:106:GLN:O	4:E:106:GLN:HG2	2.17	0.43
4:E:124:VAL:HB	4:E:125:PRO:HD3	2.00	0.43
8:J:44:TYR:HA	8:J:47:ARG:CG	2.35	0.43
10:L:49:LYS:HA	10:L:49:LYS:HD3	1.67	0.43
1:A:7:SER:C	1:A:9:ALA:N	2.76	0.43
1:A:367:PRO:CG	1:A:370:ILE:HD12	2.48	0.43
1:A:492:PRO:CB	1:A:497:THR:CG2	2.96	0.43
1:A:622:VAL:HG13	1:A:622:VAL:O	2.17	0.43
1:A:709:THR:HG22	1:A:710:LEU:N	2.33	0.43
1:A:1035:TYR:O	1:A:1036:ARG:HB2	2.19	0.43
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	2.00	0.43
1:A:1422:ARG:HA	1:A:1435:PRO:CG	2.48	0.43
2:B:108:VAL:HG12	2:B:109:THR:N	2.34	0.43
2:B:872:GLU:HA	2:B:915:THR:O	2.18	0.43
2:B:953:LEU:HD23	2:B:953:LEU:C	2.44	0.43
2:B:1034:VAL:HG22	2:B:1059:LEU:HB2	2.00	0.43
2:B:1065:GLN:HE21	2:B:1067:ARG:N	2.09	0.43
2:B:1200:ALA:O	2:B:1201:LYS:C	2.60	0.43
3:C:244:VAL:O	3:C:245:VAL:C	2.61	0.43
6:H:12:VAL:HA	6:H:28:ALA:HB2	2.00	0.43
1:A:666:ILE:HD11	2:B:1026:LEU:O	2.17	0.43
1:A:699:ALA:O	1:A:700:ASN:HB3	2.19	0.43
1:A:1111:MET:HE2	1:A:1331:SER:CB	2.47	0.43
1:A:1187:GLN:HG3	1:A:1188:GLN:N	2.33	0.43
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.53	0.43
2:B:485:ARG:HH11	2:B:485:ARG:HG3	1.84	0.43
3:C:214:ASN:HB2	3:C:217:ASP:CG	2.43	0.43
3:C:241:ASP:O	3:C:245:VAL:HG23	2.19	0.43
1:A:367:PRO:HB3	1:A:466:SER:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1279:ILE:HD12	1:A:1279:ILE:N	2.32	0.43
4:E:94:LYS:O	4:E:98:ILE:HG13	2.18	0.43
8:J:36:LEU:HD11	8:J:51:LEU:HB2	2.00	0.43
9:K:68:PHE:CD1	9:K:68:PHE:N	2.87	0.43
10:L:26:THR:C	10:L:27:LEU:HD23	2.43	0.43
11:M:1:ILX:HB	11:M:7:ASN:OD1	2.17	0.43
1:A:682:THR:CG2	1:A:728:LYS:HE3	2.48	0.43
2:B:172:ILE:CD1	2:B:178:ASN:ND2	2.82	0.43
2:B:397:ASP:OD2	2:B:515:HIS:HE1	2.02	0.43
2:B:792:MET:SD	2:B:857:ARG:NH2	2.91	0.43
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.67	0.43
5:F:89:GLU:HB3	5:F:134:ILE:CD1	2.49	0.43
1:A:324:SER:O	1:A:327:ALA:HB3	2.19	0.43
2:B:66:ASP:C	2:B:68:THR:H	2.27	0.43
2:B:119:LEU:HD22	2:B:953:LEU:HD13	2.01	0.43
2:B:120:ARG:HG3	2:B:955:THR:CG2	2.47	0.43
2:B:205:ILE:HD11	2:B:461:LEU:HB3	1.97	0.43
2:B:221:ASN:OD1	2:B:242:SER:HA	2.19	0.43
2:B:322:PHE:O	2:B:323:VAL:C	2.61	0.43
2:B:324:ILE:HG21	2:B:330:ALA:HA	2.00	0.43
2:B:397:ASP:OD2	2:B:515:HIS:CE1	2.72	0.43
2:B:1002:THR:HG21	14:B:2021:HOH:O	2.18	0.43
5:F:107:VAL:HG12	5:F:108:PHE:N	2.34	0.43
7:I:50:THR:HG22	7:I:51:ASN:N	2.34	0.43
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	2.00	0.43
1:A:73:GLY:O	1:A:75:ASN:N	2.51	0.43
1:A:310:GLY:C	1:A:311:GLN:HG3	2.44	0.43
1:A:423:ASP:O	1:A:423:ASP:CG	2.62	0.43
1:A:987:VAL:O	1:A:991:LYS:HB2	2.19	0.43
1:A:1336:MET:CE	1:A:1381:LEU:H	2.31	0.43
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.52	0.43
2:B:175:ARG:HB3	2:B:175:ARG:HH11	1.84	0.43
2:B:1160:VAL:CG1	2:B:1161:HIS:N	2.78	0.43
3:C:75:MET:CE	3:C:239:PRO:HG2	2.48	0.43
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.53	0.43
3:C:239:PRO:O	3:C:240:VAL:C	2.62	0.43
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.53	0.43
6:H:103:LYS:HD3	6:H:114:VAL:CG1	2.48	0.43
1:A:115:LEU:HD22	1:A:119:ASN:HD22	1.84	0.43
1:A:673:GLY:N	1:A:674:PRO:CD	2.82	0.43
8:J:6:ARG:HD3	8:J:11:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:113:THR:O	9:K:114:LEU:CB	2.55	0.43
1:A:329:LEU:HD21	2:B:1203:LEU:CD1	2.48	0.43
1:A:535:THR:HG23	1:A:575:LYS:CG	2.40	0.43
1:A:915:SER:O	1:A:919:ILE:HB	2.18	0.43
1:A:1015:VAL:HG13	1:A:1015:VAL:O	2.18	0.43
1:A:1059:HIS:CD2	1:A:1059:HIS:N	2.87	0.43
1:A:1161:THR:CG2	1:A:1162:VAL:N	2.81	0.43
1:A:1341:ILE:HD12	1:A:1379:GLY:C	2.43	0.43
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.53	0.43
2:B:544:CYS:HB2	2:B:634:TYR:CZ	2.54	0.43
2:B:889:THR:HG22	2:B:890:TYR:N	2.34	0.43
2:B:1191:ILE:CG2	2:B:1192:TYR:N	2.82	0.43
3:C:169:LYS:NZ	10:L:69:ALA:HB3	2.34	0.43
8:J:12:LYS:NZ	8:J:17:LYS:HZ2	2.17	0.43
10:L:32:ALA:CB	10:L:55:ILE:HB	2.44	0.43
1:A:16:GLU:HG3	2:B:1220:ARG:HA	2.01	0.42
1:A:239:LEU:HD23	1:A:239:LEU:C	2.44	0.42
1:A:447:GLN:HA	1:A:448:PRO:C	2.44	0.42
1:A:879:GLU:CD	1:A:962:ARG:HH22	2.26	0.42
1:A:1204:ASP:C	1:A:1204:ASP:OD1	2.62	0.42
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.19	0.42
4:E:58:MET:O	4:E:59:SER:C	2.60	0.42
6:H:40:LEU:HD12	6:H:41:ASP:N	2.33	0.42
1:A:13:THR:CA	1:A:1432:GLN:HE22	2.32	0.42
1:A:179:LEU:CG	1:A:308:ILE:HG21	2.48	0.42
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.54	0.42
1:A:618:GLU:HB2	1:A:619:LYS:H	1.72	0.42
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.54	0.42
1:A:1059:HIS:HB3	5:F:86:THR:HB	2.00	0.42
2:B:122:LEU:CD2	2:B:958:GLN:HG3	2.49	0.42
2:B:841:MET:O	2:B:993:THR:HA	2.19	0.42
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.54	0.42
7:I:90:GLN:O	7:I:91:ARG:HD3	2.18	0.42
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.84	0.42
1:A:500:GLU:OE2	2:B:1145:SER:OG	2.36	0.42
1:A:878:ILE:HG21	1:A:955:PRO:HB2	2.01	0.42
2:B:34:ILE:O	2:B:37:PHE:HB3	2.18	0.42
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.19	0.42
2:B:1165:ILE:CD1	2:B:1187:ASN:HD21	2.32	0.42
3:C:125:MET:HE2	3:C:127:ARG:HH22	1.84	0.42
7:I:19:ASP:OD1	7:I:22:ASN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ARG:NH2	1:A:433:GLU:OE2	2.52	0.42
1:A:1061:GLY:O	1:A:1437:GLY:HA2	2.19	0.42
1:A:1260:LEU:HD12	1:A:1260:LEU:HA	1.89	0.42
2:B:900:ALA:HA	10:L:58:LYS:HD2	2.02	0.42
1:A:464:PRO:HB2	1:A:465:TYR:H	1.67	0.42
1:A:677:ARG:HE	1:A:677:ARG:HB2	1.67	0.42
1:A:980:ASP:OD2	1:A:1039:LYS:HB3	2.19	0.42
1:A:1015:VAL:CG1	1:A:1015:VAL:O	2.67	0.42
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.41	0.42
4:E:31:THR:O	4:E:33:GLU:N	2.52	0.42
7:I:15:TYR:CE1	7:I:30:ARG:HG3	2.55	0.42
7:I:115:LYS:O	7:I:116:ASN:C	2.62	0.42
1:A:523:ILE:HG23	1:A:527:THR:HB	2.02	0.42
1:A:1201:ALA:O	1:A:1205:LYS:HG3	2.20	0.42
2:B:176:SER:O	2:B:177:LYS:C	2.61	0.42
3:C:64:ALA:HA	3:C:67:LEU:HD12	2.01	0.42
3:C:146:LYS:HB2	8:J:57:ILE:CD1	2.49	0.42
7:I:45:ARG:NH1	7:I:47:GLU:OE2	2.52	0.42
8:J:48:ARG:HG3	8:J:49:MET:N	2.34	0.42
1:A:325:ILE:O	1:A:326:ARG:C	2.62	0.42
1:A:537:ARG:HD2	6:H:20:TYR:CZ	2.55	0.42
1:A:613:ILE:HG23	6:H:117:SER:HB2	2.01	0.42
1:A:633:VAL:HG21	1:A:645:LEU:HD22	2.02	0.42
1:A:994:GLN:HG2	1:A:1019:CYS:SG	2.60	0.42
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.34	0.42
2:B:763:GLN:HB2	2:B:1021:MET:CB	2.50	0.42
2:B:906:SER:CB	2:B:946:ASN:HB2	2.50	0.42
3:C:39:ALA:O	3:C:164:ALA:HB3	2.20	0.42
3:C:209:TYR:HD1	3:C:209:TYR:H	1.68	0.42
3:C:258:ILE:HD11	9:K:42:LEU:CD2	2.49	0.42
5:F:118:LEU:O	5:F:122:MET:HG3	2.19	0.42
9:K:65:HIS:HD2	9:K:67:PHE:N	1.89	0.42
1:A:265:LYS:HZ1	1:A:302:THR:HB	1.84	0.42
1:A:324:SER:O	1:A:328:ARG:HG3	2.20	0.42
1:A:351:THR:O	1:A:486:GLU:HA	2.20	0.42
1:A:463:ILE:HD12	1:A:469:ARG:HD2	2.02	0.42
1:A:1143:LEU:HD13	1:A:1273:LEU:HD11	2.00	0.42
2:B:287:ARG:HG2	2:B:292:ILE:HA	2.01	0.42
2:B:550:ASP:OD1	2:B:552:MET:HG3	2.20	0.42
2:B:824:ILE:HD13	2:B:1089:PRO:HB3	2.01	0.42
3:C:180:TYR:CD1	3:C:180:TYR:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:61:GLN:HB2	4:E:79:TRP:CZ3	2.54	0.42
6:H:96:VAL:HG13	6:H:143:LEU:CD2	2.50	0.42
6:H:105:GLU:CD	6:H:105:GLU:N	2.78	0.42
7:I:14:LEU:HB3	7:I:27:PHE:HB3	2.02	0.42
10:L:46:VAL:O	10:L:46:VAL:HG12	2.19	0.42
1:A:93:VAL:HB	1:A:305:ASP:OD2	2.19	0.42
1:A:452:LYS:HG2	14:A:2026:HOH:O	2.18	0.42
1:A:606:LEU:HD12	1:A:607:ILE:N	2.35	0.42
1:A:1157:ASP:O	1:A:1159:ARG:N	2.53	0.42
1:A:1438:THR:HG22	2:B:1144:ALA:CB	2.48	0.42
2:B:864:LYS:HD3	2:B:871:THR:HA	2.01	0.42
2:B:1165:ILE:CD1	2:B:1187:ASN:ND2	2.83	0.42
4:E:191:LYS:N	4:E:194:GLU:OE1	2.43	0.42
6:H:17:PRO:HA	6:H:24:CYS:SG	2.59	0.42
7:I:72:ASP:C	7:I:73:ARG:O	2.62	0.42
10:L:38:LEU:HD13	10:L:48:CYS:HA	2.01	0.42
10:L:49:LYS:O	10:L:50:ASP:HB2	2.19	0.42
1:A:106:VAL:CG2	1:A:111:GLY:HA2	2.50	0.42
1:A:142:CYS:C	1:A:144:THR:H	2.27	0.42
1:A:903:ASN:O	1:A:907:THR:OG1	2.37	0.42
1:A:977:LYS:HA	1:A:978:PRO:HD3	1.95	0.42
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.83	0.42
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.50	0.42
2:B:120:ARG:CZ	10:L:54:ARG:HD2	2.49	0.42
2:B:175:ARG:HB3	2:B:175:ARG:NH1	2.35	0.42
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.01	0.42
2:B:1022:THR:O	2:B:1022:THR:CG2	2.67	0.42
3:C:17:ASN:HA	3:C:232:VAL:O	2.20	0.42
3:C:125:MET:HE2	3:C:127:ARG:NH2	2.35	0.42
3:C:175:ALA:C	3:C:176:ILE:CG1	2.93	0.42
4:E:124:VAL:CB	4:E:125:PRO:CD	2.98	0.42
6:H:62:SER:O	6:H:63:LEU:O	2.37	0.42
7:I:98:VAL:CG2	7:I:113:ASP:HB2	2.45	0.42
8:J:23:ASN:C	8:J:25:LEU:H	2.28	0.42
10:L:61:THR:HG21	10:L:63:ARG:HD3	2.02	0.42
1:A:23:SER:CB	1:A:233:TRP:CE2	3.03	0.41
1:A:34:LYS:HA	1:A:83:HIS:CD2	2.55	0.41
1:A:878:ILE:HG22	1:A:955:PRO:HB2	2.00	0.41
1:A:1155:ASP:HA	1:A:1156:PRO:HD2	1.87	0.41
1:A:1171:GLN:C	1:A:1173:HIS:H	2.27	0.41
1:A:31:SER:CB	1:A:83:HIS:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:VAL:O	1:A:832:ALA:N	2.53	0.41
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.28	0.41
2:B:335:GLY:O	2:B:339:THR:HB	2.19	0.41
2:B:566:LEU:HD11	2:B:586:TRP:CE2	2.55	0.41
2:B:872:GLU:OE1	2:B:914:LYS:HE2	2.19	0.41
3:C:22:LEU:HA	3:C:22:LEU:HD23	1.87	0.41
1:A:140:THR:O	1:A:140:THR:HG22	2.20	0.41
1:A:353:ILE:HG21	1:A:487:MET:HE2	1.99	0.41
1:A:849:MET:HE2	1:A:1061:GLY:HA2	2.02	0.41
1:A:1191:TRP:CZ3	7:I:43:VAL:HG21	2.48	0.41
1:A:1391:ARG:NH2	1:A:1417:GLU:HG3	2.34	0.41
2:B:778:MET:HE2	2:B:794:ASN:OD1	2.21	0.41
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.83	0.41
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.02	0.41
6:H:103:LYS:NZ	6:H:114:VAL:CB	2.79	0.41
10:L:34:CYS:C	10:L:36:SER:N	2.77	0.41
1:A:440:ASP:OD1	1:A:498:ARG:NH2	2.48	0.41
1:A:529:CYS:HB2	2:B:1015:HIS:CE1	2.56	0.41
1:A:883:LEU:O	1:A:886:ILE:HG22	2.21	0.41
1:A:1317:MET:HE1	1:A:1338:VAL:CG1	2.50	0.41
2:B:344:LYS:H	2:B:347:LYS:NZ	2.18	0.41
2:B:461:LEU:HD12	2:B:466:TRP:HH2	1.85	0.41
2:B:519:TRP:CD1	2:B:519:TRP:C	2.98	0.41
9:K:7:PHE:HA	9:K:10:PHE:CZ	2.56	0.41
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.55	0.41
1:A:778:GLY:HA3	2:B:516:ASN:ND2	2.36	0.41
1:A:858:ASN:ND2	1:A:862:ASN:H	2.18	0.41
1:A:1125:ALA:HB1	1:A:1303:GLU:HB2	2.03	0.41
1:A:1223:ASP:O	1:A:1224:LEU:HB2	2.21	0.41
1:A:1319:VAL:HG12	1:A:1320:PRO:O	2.20	0.41
2:B:60:GLN:HA	2:B:95:ILE:HD12	2.02	0.41
2:B:65:GLU:O	2:B:66:ASP:HB2	2.20	0.41
2:B:322:PHE:CZ	7:I:30:ARG:HB2	2.55	0.41
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.92	0.41
3:C:76:ASP:OD2	3:C:128:ASN:N	2.49	0.41
3:C:167:HIS:CD2	3:C:169:LYS:H	2.36	0.41
7:I:4:PHE:H	7:I:4:PHE:HD2	1.68	0.41
7:I:32:CYS:SG	7:I:33:SER:N	2.92	0.41
1:A:68:GLN:C	1:A:70:CYS:N	2.77	0.41
1:A:351:THR:CG2	2:B:1103:ILE:HG12	2.50	0.41
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:PRO:O	1:A:586:ILE:HG12	2.20	0.41
2:B:1158:PHE:CE2	2:B:1160:VAL:HG22	2.55	0.41
2:B:1163:CYS:SG	2:B:1165:ILE:N	2.90	0.41
3:C:7:GLN:HG2	9:K:104:ASN:HD22	1.85	0.41
3:C:78:GLU:C	3:C:80:LEU:H	2.28	0.41
4:E:14:ARG:O	4:E:17:ARG:HB3	2.20	0.41
6:H:41:ASP:C	6:H:42:ILE:HG13	2.46	0.41
7:I:59:VAL:CG1	7:I:60:GLN:N	2.83	0.41
7:I:111:THR:OG1	7:I:121:PHE:HE2	2.04	0.41
10:L:33:GLU:C	10:L:35:SER:N	2.78	0.41
1:A:211:PHE:HA	1:A:214:ILE:CD1	2.50	0.41
1:A:571:LEU:HD22	6:H:46:LEU:HD11	2.02	0.41
1:A:1336:MET:CE	1:A:1381:LEU:N	2.83	0.41
2:B:549:THR:HG22	2:B:628:THR:CG2	2.50	0.41
2:B:616:ILE:O	2:B:624:LEU:HD12	2.21	0.41
9:K:31:VAL:CG1	9:K:32:VAL:N	2.83	0.41
1:A:130:ASP:OD1	1:A:132:LYS:HB2	2.21	0.41
1:A:592:ASP:HB2	1:A:603:ASN:OD1	2.21	0.41
1:A:599:SER:O	1:A:600:PRO:C	2.63	0.41
1:A:719:VAL:HG22	11:M:4:ILE:HD13	2.03	0.41
1:A:1438:THR:CG2	2:B:1144:ALA:HB3	2.49	0.41
2:B:591:ARG:O	2:B:592:ASN:C	2.63	0.41
2:B:737:THR:CG2	2:B:737:THR:O	2.69	0.41
2:B:813:LYS:HA	2:B:816:GLU:OE1	2.21	0.41
2:B:853:SER:OG	2:B:1094:ARG:NH1	2.53	0.41
3:C:206:ASN:OD1	3:C:206:ASN:N	2.54	0.41
6:H:100:THR:HG23	6:H:138:GLU:HA	2.03	0.41
6:H:145:ARG:O	6:H:146:ARG:OXT	2.39	0.41
9:K:24:ASP:OD1	9:K:26:LYS:N	2.54	0.41
1:A:13:THR:HB	1:A:1432:GLN:NE2	2.36	0.41
1:A:70:CYS:O	1:A:70:CYS:SG	2.79	0.41
1:A:381:THR:CG2	1:A:383:TYR:CD1	3.04	0.41
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.03	0.41
1:A:846:GLU:HA	1:A:1066:VAL:HG23	2.03	0.41
1:A:1111:MET:HB2	1:A:1114:PRO:HG3	2.02	0.41
1:A:1166:ASP:O	1:A:1169:ILE:HG22	2.21	0.41
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.21	0.41
1:A:1214:GLU:OE1	1:A:1214:GLU:HA	2.21	0.41
1:A:1254:ALA:HB3	1:A:1256:GLU:HG2	2.02	0.41
1:A:1438:THR:O	5:F:92:ARG:HD2	2.20	0.41
2:B:243:ALA:CB	2:B:251:ILE:HG12	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:883:LEU:O	2:B:885:MET:HG3	2.21	0.41
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	2.03	0.41
2:B:1221:SER:O	2:B:1222:ARG:O	2.39	0.41
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.03	0.41
3:C:214:ASN:O	3:C:215:GLU:C	2.64	0.41
3:C:240:VAL:O	3:C:241:ASP:C	2.64	0.41
4:E:198:ILE:CD1	4:E:212:ARG:HG3	2.51	0.41
6:H:126:GLU:N	6:H:130:ARG:HH22	2.18	0.41
10:L:31:CYS:SG	10:L:34:CYS:SG	3.19	0.41
1:A:84:ILE:CG2	1:A:239:LEU:O	2.69	0.41
1:A:825:ILE:O	1:A:828:ALA:HB3	2.21	0.41
1:A:1401:SER:O	1:A:1402:PHE:HB2	2.21	0.41
2:B:387:LEU:HA	2:B:387:LEU:HD12	1.76	0.41
2:B:915:THR:CG2	2:B:916:THR:N	2.84	0.41
3:C:33:LEU:HD12	3:C:33:LEU:O	2.21	0.41
3:C:181:ASP:CG	3:C:183:TRP:O	2.64	0.41
4:E:41:ASP:O	4:E:42:PHE:C	2.64	0.41
4:E:200:ARG:HD2	14:E:2004:HOH:O	2.20	0.41
5:F:97:ARG:NE	5:F:124:GLU:OE1	2.38	0.41
7:I:2:THR:HG21	7:I:43:VAL:O	2.21	0.41
7:I:120:GLN:O	7:I:121:PHE:HB2	2.21	0.41
1:A:260:ASP:OD1	1:A:261:ASP:N	2.53	0.40
1:A:584:ASN:O	1:A:637:LYS:HE3	2.21	0.40
1:A:596:THR:HG22	1:A:597:LEU:HD12	2.03	0.40
1:A:596:THR:CG2	1:A:597:LEU:H	2.28	0.40
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.21	0.40
1:A:1438:THR:HA	5:F:88:TYR:HB3	2.02	0.40
2:B:25:ILE:HD13	2:B:658:ILE:CD1	2.50	0.40
2:B:281:PRO:HB3	2:B:320:ASP:OD2	2.21	0.40
2:B:360:PHE:O	2:B:361:LEU:C	2.64	0.40
2:B:737:THR:HG21	7:I:66:PRO:C	2.46	0.40
2:B:882:THR:HB	2:B:934:LYS:O	2.21	0.40
3:C:242:GLN:O	3:C:243:VAL:C	2.64	0.40
4:E:84:ASP:O	4:E:86:PRO:HD3	2.21	0.40
4:E:169:ARG:NE	5:F:140:ASP:OD2	2.54	0.40
5:F:111:LEU:H	5:F:111:LEU:CD1	2.06	0.40
8:J:2:ILE:O	8:J:3:VAL:C	2.64	0.40
8:J:52:THR:HG22	8:J:52:THR:O	2.20	0.40
1:A:36:ARG:O	1:A:37:PHE:C	2.64	0.40
1:A:587:HIS:HE2	1:A:969:GLN:HG2	1.76	0.40
1:A:738:LYS:NZ	3:C:194:GLU:C	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:GLY:O	1:A:839:ARG:HG3	2.21	0.40
1:A:867:ILE:HG22	4:E:208:TYR:HE1	1.86	0.40
1:A:1341:ILE:HD11	1:A:1376:THR:O	2.21	0.40
2:B:874:PHE:HA	2:B:913:GLY:O	2.21	0.40
2:B:1065:GLN:HE22	2:B:1067:ARG:CB	2.35	0.40
3:C:108:GLU:HG2	3:C:149:LYS:HD2	2.01	0.40
3:C:209:TYR:N	3:C:209:TYR:HD1	2.19	0.40
4:E:116:ILE:HG22	4:E:117:THR:H	1.85	0.40
4:E:198:ILE:HD12	4:E:212:ARG:HG3	2.03	0.40
6:H:12:VAL:HG13	6:H:26:ILE:HG23	2.04	0.40
6:H:51:ALA:O	6:H:53:ASP:N	2.54	0.40
6:H:106:GLU:C	6:H:108:SER:N	2.78	0.40
1:A:7:SER:C	1:A:9:ALA:H	2.29	0.40
1:A:112:LYS:HD2	1:A:165:GLY:HA3	2.03	0.40
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	2.03	0.40
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.52	0.40
1:A:466:SER:C	1:A:467:THR:HG23	2.46	0.40
1:A:535:THR:O	1:A:535:THR:CG2	2.66	0.40
1:A:1079:MET:HG2	1:A:1359:ASP:OD2	2.21	0.40
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.51	0.40
2:B:590:HIS:CD2	2:B:591:ARG:O	2.74	0.40
2:B:610:ASN:OD1	2:B:611:PRO:HD2	2.22	0.40
2:B:788:ARG:CB	2:B:788:ARG:HH11	2.34	0.40
2:B:997:GLU:CD	3:C:39:ALA:HB2	2.46	0.40
2:B:1102:LYS:C	2:B:1104:HIS:H	2.30	0.40
3:C:63:ILE:HD13	3:C:153:LEU:HD11	2.04	0.40
6:H:10:PHE:HB3	6:H:28:ALA:HB1	2.04	0.40
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.56	0.40
2:B:51:PHE:O	2:B:54:PHE:HB3	2.22	0.40
2:B:1035:ALA:HB1	2:B:1040:ASN:O	2.21	0.40
2:B:1222:ARG:C	2:B:1224:PHE:H	2.30	0.40
3:C:39:ALA:HA	3:C:164:ALA:CB	2.41	0.40
3:C:73:GLN:NE2	3:C:75:MET:CB	2.84	0.40
3:C:104:PHE:HD1	3:C:152:GLU:HG3	1.87	0.40
4:E:136:ASN:O	4:E:139:ALA:N	2.53	0.40
4:E:178:ILE:O	4:E:178:ILE:HG23	2.22	0.40
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.56	0.40
7:I:75:CYS:C	7:I:77:LYS:H	2.29	0.40
1:A:84:ILE:HG23	1:A:84:ILE:O	2.22	0.40
1:A:388:LEU:O	1:A:389:THR:C	2.64	0.40
1:A:767:GLN:HG2	11:M:4:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:PHE:CZ	1:A:796:SER:HA	2.56	0.40
1:A:1394:THR:HG23	1:A:1398:MET:SD	2.62	0.40
1:A:1431:GLY:HA2	2:B:1152:MET:CE	2.48	0.40
2:B:167:ILE:HG22	2:B:453:ILE:CD1	2.49	0.40
2:B:242:SER:OG	2:B:362:PRO:HD2	2.22	0.40
2:B:864:LYS:HB3	2:B:871:THR:CA	2.50	0.40
2:B:1099:VAL:C	2:B:1101:ASP:N	2.77	0.40
3:C:99:LEU:N	3:C:99:LEU:HD12	2.36	0.40
4:E:31:THR:O	4:E:32:GLN:C	2.65	0.40
5:F:119:ARG:HA	5:F:122:MET:HE3	2.02	0.40
5:F:143:PHE:CD1	5:F:143:PHE:C	2.99	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:28:LYS:NZ	10:L:28:LYS:NZ[3_655]	2.05	0.15

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1348/1733 (78%)	1160 (86%)	134 (10%)	54 (4%)	2	8
2	B	1062/1224 (87%)	931 (88%)	107 (10%)	24 (2%)	5	18
3	C	264/318 (83%)	223 (84%)	30 (11%)	11 (4%)	2	7
4	E	211/215 (98%)	180 (85%)	23 (11%)	8 (4%)	2	9
5	F	82/155 (53%)	71 (87%)	10 (12%)	1 (1%)	10	34
6	H	129/146 (88%)	88 (68%)	23 (18%)	18 (14%)	0	0
7	I	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	7	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	63/70 (90%)	58 (92%)	5 (8%)	0	100	100
9	K	112/120 (93%)	98 (88%)	13 (12%)	1 (1%)	14	41
10	L	43/70 (61%)	23 (54%)	13 (30%)	7 (16%)	0	0
11	M	4/8 (50%)	4 (100%)	0	0	100	100
All	All	3438/4181 (82%)	2938 (86%)	374 (11%)	126 (4%)	2	9

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	56	PRO
1	A	399	HIS
1	A	464	PRO
1	A	465	TYR
1	A	466	SER
1	A	567	LYS
1	A	752	LYS
1	A	1385	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1392	SER
1	A	1393	ASN
2	B	864	LYS
2	B	879	ARG
2	B	1100	ASP
2	B	1222	ARG
3	C	4	GLU
3	C	206	ASN
4	E	4	GLU
4	E	5	ASN
4	E	59	SER
6	H	19	ARG
6	H	52	GLN
6	H	81	PRO
6	H	88	SER
6	H	105	GLU
6	H	128	ASN
6	H	138	GLU
10	L	39	SER
10	L	64	LEU
1	A	35	ILE

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Mol	Chain	Res	Type
1	A	57	ARG
1	A	58	LEU
1	A	67	CYS
1	A	71	GLN
1	A	74	MET
1	A	79	GLY
1	A	84	ILE
1	A	400	PRO
1	A	419	LYS
1	A	626	ASN
1	A	628	GLY
1	A	846	GLU
1	A	885	THR
1	A	1202	MET
1	A	1221	LYS
1	A	1396	ALA
1	A	1399	ARG
1	A	1400	CYS
2	B	165	VAL
2	B	266	ALA
2	B	367	LEU
2	B	646	LEU
2	B	648	HIS
2	B	1066	SER
3	C	137	LYS
3	C	184	ASN
3	C	215	GLU
3	C	231	ASN
3	C	245	VAL
4	E	50	MET
4	E	76	GLY
6	H	18	GLY
6	H	90	ALA
10	L	34	CYS
10	L	35	SER
10	L	52	GLY
10	L	59	ALA
1	A	68	GLN
1	A	72	GLU
1	A	308	ILE
1	A	408	ASP
1	A	409	SER

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Mol	Chain	Res	Type
1	A	418	SER
1	A	467	THR
1	A	1278	ASN
2	B	666	TYR
2	B	734	HIS
2	B	906	SER
2	B	907	GLY
2	B	1099	VAL
3	C	90	ASP
4	E	115	ASN
5	F	73	ALA
6	H	32	THR
6	H	77	ARG
6	H	82	PRO
6	H	83	GLN
6	H	139	ASN
7	I	3	THR
9	K	111	LEU
1	A	599	SER
1	A	829	VAL
2	B	124	TYR
2	B	323	VAL
2	B	369	GLY
2	B	883	LEU
3	C	9	LYS
3	C	10	ILE
3	C	267	GLN
6	H	3	ASN
6	H	8	ASP
1	A	307	ASP
1	A	538	ASP
1	A	904	THR
1	A	958	VAL
1	A	1200	ALA
2	B	90	ILE
2	B	909	ASP
4	E	103	LYS
4	E	124	VAL
6	H	14	GLU
10	L	56	LEU
1	A	283	GLY
1	A	737	LEU

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Mol	Chain	Res	Type
1	A	1172	LEU
1	A	1257	ASP
2	B	464	GLY
2	B	1103	ILE
7	I	76	PRO
1	A	166	GLY
1	A	1002	GLY
1	A	246	VAL
2	B	647	GLY
6	H	59	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1196/1520 (79%)	1100 (92%)	96 (8%)	11	34
2	B	940/1061 (89%)	885 (94%)	55 (6%)	18	48
3	C	234/274 (85%)	220 (94%)	14 (6%)	17	47
4	E	195/197 (99%)	190 (97%)	5 (3%)	40	75
5	F	74/137 (54%)	68 (92%)	6 (8%)	11	33
6	H	117/128 (91%)	114 (97%)	3 (3%)	40	75
7	I	116/116 (100%)	110 (95%)	6 (5%)	21	53
8	J	60/65 (92%)	57 (95%)	3 (5%)	22	54
9	K	99/102 (97%)	86 (87%)	13 (13%)	4	14
10	L	40/57 (70%)	35 (88%)	5 (12%)	4	15
11	M	2/2 (100%)	2 (100%)	0	100	100
All	All	3073/3659 (84%)	2867 (93%)	206 (7%)	15	42

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE

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Mol	Chain	Res	Type
1	A	70	CYS
1	A	71	GLN
1	A	93	VAL
1	A	116	ASP
1	A	117	GLU
1	A	156	ASP
1	A	159	THR
1	A	164	ARG
1	A	208	LEU
1	A	226	GLU
1	A	237	THR
1	A	291	GLU
1	A	351	THR
1	A	373	THR
1	A	381	THR
1	A	385	ILE
1	A	389	THR
1	A	434	ARG
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	452	LYS
1	A	455	MET
1	A	466	SER
1	A	467	THR
1	A	469	ARG
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	493	GLN
1	A	497	THR
1	A	503	GLN
1	A	504	LEU
1	A	515	GLN
1	A	541	ILE
1	A	544	ASP
1	A	557	ASP
1	A	577	ILE
1	A	597	LEU
1	A	612	ILE
1	A	618	GLU

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Mol	Chain	Res	Type
1	A	622	VAL
1	A	636	GLU
1	A	650	GLN
1	A	666	ILE
1	A	672	ASP
1	A	703	THR
1	A	710	LEU
1	A	756	ILE
1	A	765	VAL
1	A	795	GLU
1	A	821	ARG
1	A	822	GLU
1	A	827	THR
1	A	831	THR
1	A	855	THR
1	A	858	ASN
1	A	867	ILE
1	A	873	MET
1	A	882	SER
1	A	885	THR
1	A	903	ASN
1	A	919	ILE
1	A	920	LEU
1	A	948	VAL
1	A	969	GLN
1	A	1006	ILE
1	A	1015	VAL
1	A	1030	ARG
1	A	1048	ASN
1	A	1060	PRO
1	A	1064	VAL
1	A	1118	VAL
1	A	1122	PRO
1	A	1128	GLN
1	A	1141	THR
1	A	1146	VAL
1	A	1240	CYS
1	A	1255	GLU
1	A	1257	ASP
1	A	1264	GLU
1	A	1280	GLU
1	A	1297	GLU

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Mol	Chain	Res	Type
1	A	1308	THR
1	A	1318	THR
1	A	1325	THR
1	A	1336	MET
1	A	1341	ILE
1	A	1376	THR
1	A	1385	THR
1	A	1387	HIS
1	A	1419	ASP
1	A	1426	GLU
1	A	1438	THR
2	B	18	PHE
2	B	20	ASP
2	B	46	GLN
2	B	63	ILE
2	B	128	LEU
2	B	178	ASN
2	B	183	GLU
2	B	194	GLU
2	B	211	VAL
2	B	217	ARG
2	B	241	ARG
2	B	261	ARG
2	B	268	THR
2	B	272	THR
2	B	276	ILE
2	B	277	LYS
2	B	337	ARG
2	B	339	THR
2	B	387	LEU
2	B	408	LEU
2	B	424	LEU
2	B	461	LEU
2	B	485	ARG
2	B	487	THR
2	B	490	SER
2	B	513	GLN
2	B	531	GLN
2	B	540	SER
2	B	541	LEU
2	B	547	VAL
2	B	549	THR

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Mol	Chain	Res	Type
2	B	567	GLU
2	B	589	VAL
2	B	644	GLU
2	B	648	HIS
2	B	653	VAL
2	B	693	ILE
2	B	736	THR
2	B	886	LYS
2	B	939	THR
2	B	951	GLN
2	B	954	VAL
2	B	955	THR
2	B	969	ARG
2	B	974	PRO
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1060	ARG
2	B	1065	GLN
2	B	1150	ARG
2	B	1159	ARG
2	B	1189	ILE
2	B	1211	ASN
2	B	1222	ARG
3	C	17	ASN
3	C	26	ASP
3	C	43	THR
3	C	50	GLU
3	C	52	GLU
3	C	57	VAL
3	C	77	ILE
3	C	129	ILE
3	C	138	GLU
3	C	163	ILE
3	C	206	ASN
3	C	209	TYR
3	C	233	GLU
3	C	240	VAL
4	E	104	ASN
4	E	123	LEU
4	E	149	LEU
4	E	196	VAL

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Mol	Chain	Res	Type
4	E	204	THR
5	F	79	ARG
5	F	81	THR
5	F	82	THR
5	F	110	ASP
5	F	111	LEU
5	F	115	THR
6	H	82	PRO
6	H	91	ASP
6	H	93	TYR
7	I	4	PHE
7	I	30	ARG
7	I	45	ARG
7	I	50	THR
7	I	52	ILE
7	I	98	VAL
8	J	3	VAL
8	J	22	LEU
8	J	48	ARG
9	K	6	ARG
9	K	11	LEU
9	K	29	ASN
9	K	47	ARG
9	K	50	LEU
9	K	51	LEU
9	K	63	VAL
9	K	73	LEU
9	K	76	GLN
9	K	101	LEU
9	K	103	THR
9	K	111	LEU
9	K	114	LEU
10	L	42	ARG
10	L	50	ASP
10	L	61	THR
10	L	65	VAL
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN

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Mol	Chain	Res	Type
1	A	68	GLN
1	A	92	HIS
1	A	118	HIS
1	A	169	ASN
1	A	299	HIS
1	A	358	ASN
1	A	390	GLN
1	A	394	ASN
1	A	397	ASN
1	A	479	ASN
1	A	493	GLN
1	A	503	GLN
1	A	517	ASN
1	A	631	HIS
1	A	659	HIS
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	854	ASN
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	935	GLN
1	A	994	GLN
1	A	1070	GLN
1	A	1124	HIS
1	A	1173	HIS
1	A	1218	GLN
1	A	1265	ASN
1	A	1364	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	178	ASN
2	B	236	HIS
2	B	255	GLN
2	B	300	HIS
2	B	366	GLN
2	B	465	ASN
2	B	484	ASN

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Mol	Chain	Res	Type
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	587	HIS
2	B	648	HIS
2	B	657	HIS
2	B	706	GLN
2	B	734	HIS
2	B	744	HIS
2	B	763	GLN
2	B	767	ASN
2	B	1015	HIS
2	B	1025	HIS
2	B	1062	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1176	ASN
2	B	1177	HIS
2	B	1187	ASN
2	B	1193	GLN
2	B	1211	ASN
3	C	24	ASN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	131	HIS
3	C	140	ASN
3	C	167	HIS
3	C	203	GLN
3	C	242	GLN
3	C	252	GLN
3	C	267	GLN
4	E	101	GLN
4	E	104	ASN
4	E	106	GLN
4	E	113	GLN
4	E	147	HIS
6	H	3	ASN

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Mol	Chain	Res	Type
6	H	11	GLN
6	H	83	GLN
6	H	128	ASN
7	I	12	ASN
7	I	51	ASN
7	I	89	GLN
7	I	108	HIS
7	I	114	GLN
8	J	64	ASN
9	K	29	ASN
9	K	65	HIS
9	K	76	GLN
9	K	110	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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	$\# Z > 2$
11	CSX	M	6	11	3,6,7	2.95	2 (66%)	1,6,8	0.39	0
11	ILX	M	1	11	8,9,10	2.47	3 (37%)	8,11,13	2.10	3 (37%)
11	TRX	M	2	11	15,16,17	3.22	10 (66%)	17,22,24	1.41	4 (23%)
11	HYP	M	8	11	7,8,9	2.73	1 (14%)	5,10,12	1.63	1 (20%)

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
11	CSX	M	6	11	-	2/2/5/7	-
11	ILX	M	1	11	-	1/11/12/14	-
11	TRX	M	2	11	-	2/5/6/8	0/2/2/2
11	HYP	M	8	11	-	0/0/11/13	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	8	HYP	CA-N	6.82	1.60	1.48
11	M	2	TRX	CZ2-CE2	6.13	1.49	1.39
11	M	2	TRX	CZ2-CH2	5.65	1.47	1.39
11	M	1	ILX	CB-CA	5.08	1.60	1.54
11	M	2	TRX	CD1-CG	4.36	1.43	1.36
11	M	2	TRX	CD2-CE2	4.35	1.46	1.41
11	M	6	CSX	CB-CA	4.09	1.63	1.53
11	M	2	TRX	CD1-NE1	3.38	1.42	1.37
11	M	2	TRX	CE3-CD2	3.19	1.44	1.39
11	M	1	ILX	OG1-CG1	3.14	1.49	1.43
11	M	2	TRX	CZ3-CH2	3.02	1.44	1.39
11	M	1	ILX	CA-N	2.85	1.56	1.47
11	M	6	CSX	O-C	2.82	1.30	1.20
11	M	2	TRX	OH2-CH2	2.17	1.41	1.37
11	M	2	TRX	CD2-CG	2.13	1.47	1.44
11	M	2	TRX	CB-CA	2.01	1.57	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	1	ILX	CB-CA-C	-3.55	108.02	112.87
11	M	1	ILX	CG2-CB-CG1	-3.37	105.72	111.09
11	M	2	TRX	OH2-CH2-CZ3	-2.94	111.82	120.00
11	M	8	HYP	CG-CB-CA	2.82	107.01	103.75
11	M	2	TRX	OH2-CH2-CZ2	2.79	127.15	119.85
11	M	1	ILX	OD1-CD1-CG1	2.46	116.32	111.16
11	M	2	TRX	CB-CG-CD1	2.03	130.92	126.97
11	M	2	TRX	CZ2-CE2-CD2	-2.02	120.91	122.52

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	M	6	CSX	N-CA-CB-SG

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Mol	Chain	Res	Type	Atoms
11	M	6	CSX	C-CA-CB-SG
11	M	2	TRX	CA-CB-CG-CD2
11	M	1	ILX	C-CA-CB-CG2
11	M	2	TRX	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	1	ILX	2	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1366/1733 (78%)	0.04	59 (4%) 40 31	18, 48, 107, 137	0
2	B	1082/1224 (88%)	0.03	54 (4%) 34 26	20, 46, 105, 128	0
3	C	266/318 (83%)	0.11	3 (1%) 78 70	30, 53, 83, 124	0
4	E	213/215 (99%)	0.15	5 (2%) 61 51	22, 59, 99, 109	0
5	F	84/155 (54%)	-0.25	1 (1%) 76 68	24, 44, 67, 82	0
6	H	133/146 (91%)	1.29	26 (19%) 3 2	64, 94, 122, 125	0
7	I	122/122 (100%)	0.15	6 (4%) 35 27	30, 51, 89, 106	0
8	J	65/70 (92%)	-0.19	1 (1%) 72 63	26, 47, 76, 85	0
9	K	114/120 (95%)	0.08	1 (0%) 81 74	31, 60, 79, 97	0
10	L	45/70 (64%)	1.21	12 (26%) 1 1	49, 86, 108, 110	0
11	M	4/8 (50%)	1.58	2 (50%) 0 0	73, 80, 83, 84	0
All	All	3494/4181 (83%)	0.11	170 (4%) 35 27	18, 50, 105, 137	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	H	104	PHE	6.0
1	A	69	THR	5.8
1	A	61	ILE	5.6
1	A	68	GLN	5.3
2	B	882	THR	5.1
1	A	305	ASP	4.9
2	B	247	GLY	4.6
1	A	1392	SER	4.6
1	A	1390	ASN	4.4
1	A	1403	GLU	4.3
1	A	166	GLY	4.3
2	B	137	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1081	LEU	4.1
2	B	1105	ALA	4.1
2	B	106	ASP	4.1
2	B	883	LEU	4.1
2	B	1155	SER	4.0
2	B	248	SER	4.0
1	A	1402	PHE	4.0
1	A	1391	ARG	3.8
6	H	132	LEU	3.8
8	J	65	PRO	3.7
1	A	60	SER	3.6
6	H	90	ALA	3.6
2	B	1102	LYS	3.6
6	H	131	ASN	3.6
1	A	1389	PHE	3.6
1	A	1254	ALA	3.6
2	B	1184	GLY	3.6
2	B	866	TYR	3.6
2	B	1221	SER	3.6
6	H	139	ASN	3.5
2	B	868	MET	3.5
2	B	249	ARG	3.5
6	H	130	ARG	3.5
1	A	826	ASP	3.5
2	B	869	SER	3.4
2	B	1189	ILE	3.4
11	M	4	ILE	3.4
2	B	1099	VAL	3.3
6	H	129	TYR	3.3
1	A	65	LEU	3.3
2	B	18	PHE	3.3
1	A	1175	SER	3.3
2	B	643	ASP	3.2
1	A	1092	LYS	3.2
2	B	1100	ASP	3.2
1	A	59	GLY	3.2
1	A	336	ILE	3.2
2	B	1103	ILE	3.2
2	B	1224	PHE	3.2
6	H	136	LYS	3.2
1	A	53	LEU	3.2
6	H	84	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	108	VAL	3.1
2	B	1156	ASP	3.1
1	A	72	GLU	3.0
1	A	330	LYS	3.0
10	L	49	LYS	3.0
1	A	1126	ALA	3.0
10	L	54	ARG	2.9
1	A	1386	ARG	2.9
2	B	104	GLU	2.9
9	K	114	LEU	2.9
1	A	1404	GLU	2.9
1	A	64	ASN	2.9
1	A	66	LYS	2.9
2	B	1172	ILE	2.9
1	A	62	ASP	2.9
1	A	309	ALA	2.9
1	A	58	LEU	2.9
6	H	127	GLY	2.8
2	B	103	ASN	2.8
1	A	308	ILE	2.8
1	A	280	GLU	2.8
2	B	509	ALA	2.8
10	L	46	VAL	2.8
7	I	121	PHE	2.7
6	H	63	LEU	2.7
6	H	133	ASN	2.7
1	A	73	GLY	2.7
2	B	70	ILE	2.7
1	A	157	ASP	2.7
1	A	1388	GLY	2.7
1	A	1401	SER	2.7
2	B	870	ILE	2.7
6	H	86	ASP	2.7
6	H	103	LYS	2.7
1	A	1393	ASN	2.7
2	B	1219	ASP	2.6
6	H	107	VAL	2.6
2	B	266	ALA	2.6
4	E	49	SER	2.6
2	B	734	HIS	2.6
2	B	1104	HIS	2.6
2	B	1183	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
7	I	1	MET	2.6
4	E	51	GLY	2.6
3	C	268	ASP	2.6
6	H	82	PRO	2.5
2	B	1222	ARG	2.5
4	E	53	PRO	2.5
10	L	27	LEU	2.5
2	B	1223	ASP	2.5
2	B	246	LYS	2.5
7	I	83	ASN	2.5
6	H	91	ASP	2.5
2	B	641	GLU	2.5
10	L	38	LEU	2.4
1	A	50	ILE	2.4
2	B	265	SER	2.4
2	B	250	PHE	2.4
2	B	1180	PHE	2.4
6	H	112	ILE	2.4
1	A	247	ARG	2.4
6	H	88	SER	2.4
2	B	963	PHE	2.4
6	H	31	THR	2.4
1	A	1172	LEU	2.4
6	H	134	ASN	2.4
1	A	326	ARG	2.4
1	A	327	ALA	2.4
6	H	113	ALA	2.4
4	E	88	VAL	2.4
1	A	1397	LEU	2.3
6	H	135	LEU	2.3
2	B	1110	PRO	2.3
1	A	1080	THR	2.3
2	B	1175	LEU	2.3
7	I	116	ASN	2.3
10	L	53	HIS	2.3
2	B	264	SER	2.3
10	L	45	ALA	2.2
1	A	702	LEU	2.2
5	F	72	LYS	2.2
10	L	50	ASP	2.2
1	A	56	PRO	2.2
2	B	867	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1109	GLY	2.2
1	A	331	GLY	2.2
2	B	429	PHE	2.2
1	A	1450	LEU	2.2
2	B	167	ILE	2.2
1	A	49	LYS	2.2
1	A	165	GLY	2.2
1	A	37	PHE	2.2
6	H	2	SER	2.2
10	L	33	GLU	2.2
1	A	74	MET	2.1
1	A	1127	ASP	2.1
7	I	119	THR	2.1
1	A	329	LEU	2.1
10	L	40	LEU	2.1
2	B	876	LYS	2.1
2	B	880	THR	2.1
1	A	1173	HIS	2.1
2	B	934	LYS	2.1
1	A	262	LEU	2.1
6	H	111	LEU	2.1
6	H	143	LEU	2.1
2	B	879	ARG	2.1
7	I	122	SER	2.1
4	E	50	MET	2.1
11	M	5	GLY	2.1
10	L	43	THR	2.1
3	C	3	GLU	2.1
1	A	334	GLY	2.0
10	L	52	GLY	2.0
1	A	332	LYS	2.0
3	C	209	TYR	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
11	CSX	M	6	7/8	0.71	0.15	80,82,84,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	ILX	M	1	10/11	0.82	0.23	72,74,79,80	0
11	TRX	M	2	15/16	0.90	0.15	75,77,79,80	0
11	HYP	M	8	8/9	0.91	0.12	70,72,72,73	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($\text{\AA}^2$)	Q<0.9
13	MN	A	3009	1/1	0.87	0.14	149,149,149,149	0
12	ZN	L	3005	1/1	0.96	0.04	86,86,86,86	0
12	ZN	A	3008	1/1	0.97	0.04	81,81,81,81	0
12	ZN	I	3004	1/1	0.97	0.04	62,62,62,62	0
12	ZN	B	3007	1/1	0.98	0.04	64,64,64,64	0
12	ZN	J	3001	1/1	0.99	0.03	46,46,46,46	0
12	ZN	C	3002	1/1	0.99	0.02	49,49,49,49	0
12	ZN	A	3006	1/1	0.99	0.04	64,64,64,64	0
12	ZN	I	3003	1/1	1.00	0.03	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.