



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:42 AM UTC

PDB ID : 4QIW / pdb_00004qiw
Title : Crystal structure of euryarchaeal RNA polymerase from *Thermococcus kodakarensis*
Authors : Jun, S.-H.; Murakami, K.S.
Deposited on : 2014-06-02
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

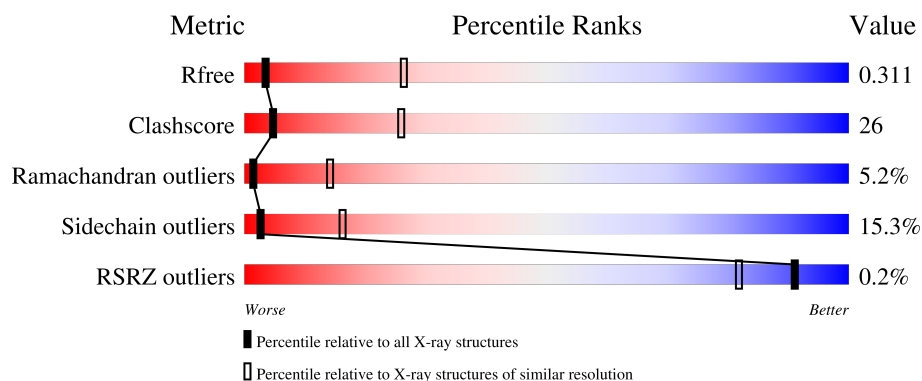
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	906	
1	I	906	
2	B	1123	
2	J	1123	
3	C	391	

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Mol	Chain	Length	Quality of chain
3	M	391	
4	D	259	
4	O	259	
5	E	190	
5	Q	190	
6	F	122	
6	R	122	
7	H	82	
7	S	82	
8	K	57	
8	T	57	
9	L	100	
9	U	100	
10	N	65	
10	V	65	
11	P	49	
11	W	49	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 51069 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	863	Total	C	N	O	S	0	0	0
			6891	4357	1221	1275	38			
1	I	862	Total	C	N	O	S	0	0	0
			6875	4347	1220	1270	38			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1069	Total	C	N	O	S	0	0	0
			8536	5396	1520	1584	36			
2	J	1069	Total	C	N	O	S	0	0	0
			8536	5396	1520	1584	36			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit A''.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	369	Total	C	N	O	S	0	0	0
			2882	1819	498	555	10			
3	M	369	Total	C	N	O	S	0	0	0
			2879	1816	498	555	10			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	258	Total	C	N	O	S	0	0	0
			2066	1330	341	390	5			
4	O	258	Total	C	N	O	S	0	0	0
			2066	1330	341	390	5			

- Molecule 5 is a protein called DNA-directed RNA polymerase, subunit E'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	181	Total	C	N	O	S	0	0	0
			1465	939	250	267	9			
5	Q	181	Total	C	N	O	S	0	0	0
			1465	939	250	267	9			

- Molecule 6 is a protein called DNA-directed RNA polymerase, subunit F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	122	Total	C	N	O	S	0	0	0
			1020	654	169	193	4			
6	R	122	Total	C	N	O	S	0	0	0
			1020	654	169	193	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	115	ILE	-	expression tag	UNP Q5JI52
F	116	ASP	-	expression tag	UNP Q5JI52
F	117	GLU	-	expression tag	UNP Q5JI52
F	118	TYR	-	expression tag	UNP Q5JI52
F	119	ARG	-	expression tag	UNP Q5JI52
F	120	PRO	-	expression tag	UNP Q5JI52
F	121	LEU	-	expression tag	UNP Q5JI52
F	122	GLU	-	expression tag	UNP Q5JI52
R	115	ILE	-	expression tag	UNP Q5JI52
R	116	ASP	-	expression tag	UNP Q5JI52
R	117	GLU	-	expression tag	UNP Q5JI52
R	118	TYR	-	expression tag	UNP Q5JI52
R	119	ARG	-	expression tag	UNP Q5JI52
R	120	PRO	-	expression tag	UNP Q5JI52
R	121	LEU	-	expression tag	UNP Q5JI52
R	122	GLU	-	expression tag	UNP Q5JI52

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit H.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	H	76	Total	C	N	O	0	0	0
			627	408	105	114			
7	S	76	Total	C	N	O	0	0	0
			627	408	105	114			

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	56	Total 433	C 284	N 75	O 73	S 1	0	0	0
8	T	56	Total 433	C 284	N 75	O 73	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	L	94	Total 775	C 493	N 134	O 146	S 2	0	0	0
9	U	94	Total 775	C 493	N 134	O 146	S 2	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	95	HIS	-	expression tag	UNP Q5JE88
L	96	HIS	-	expression tag	UNP Q5JE88
L	97	HIS	-	expression tag	UNP Q5JE88
L	98	HIS	-	expression tag	UNP Q5JE88
L	99	HIS	-	expression tag	UNP Q5JE88
L	100	HIS	-	expression tag	UNP Q5JE88
U	95	HIS	-	expression tag	UNP Q5JE88
U	96	HIS	-	expression tag	UNP Q5JE88
U	97	HIS	-	expression tag	UNP Q5JE88
U	98	HIS	-	expression tag	UNP Q5JE88
U	99	HIS	-	expression tag	UNP Q5JE88
U	100	HIS	-	expression tag	UNP Q5JE88

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	63	Total 510	C 326	N 87	O 91	S 6	0	0	0
10	V	63	Total 510	C 326	N 87	O 91	S 6	0	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	42	Total 329	C 206	N 65	O 54	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	W	42	Total	C	N	O	S	0	0	0
			329	206	65	54	4			

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	Mg	0	0
			2	2		
12	I	2	Total	Mg	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		
13	B	1	Total	Zn	0	0
			1	1		
13	N	1	Total	Zn	0	0
			1	1		
13	P	1	Total	Zn	0	0
			1	1		
13	I	2	Total	Zn	0	0
			2	2		
13	J	1	Total	Zn	0	0
			1	1		
13	V	1	Total	Zn	0	0
			1	1		
13	W	1	Total	Zn	0	0
			1	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	O	0	0
			1	1		
14	B	1	Total	O	0	0
			1	1		
14	C	1	Total	O	0	0
			1	1		
14	I	1	Total	O	0	0
			1	1		

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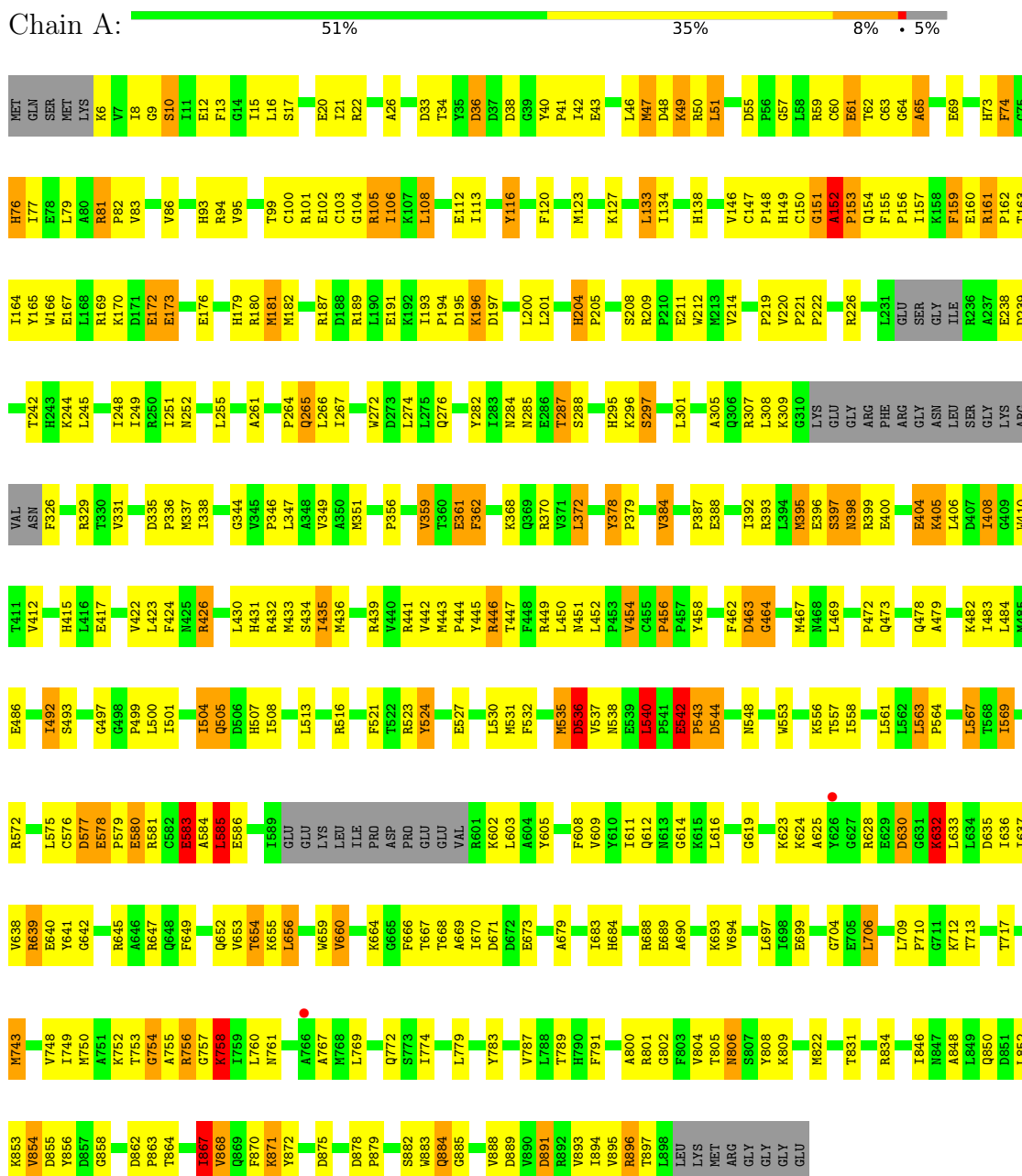
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total	O	0	0
			1	1		
14	M	1	Total	O	0	0
			1	1		

3 Residue-property plots

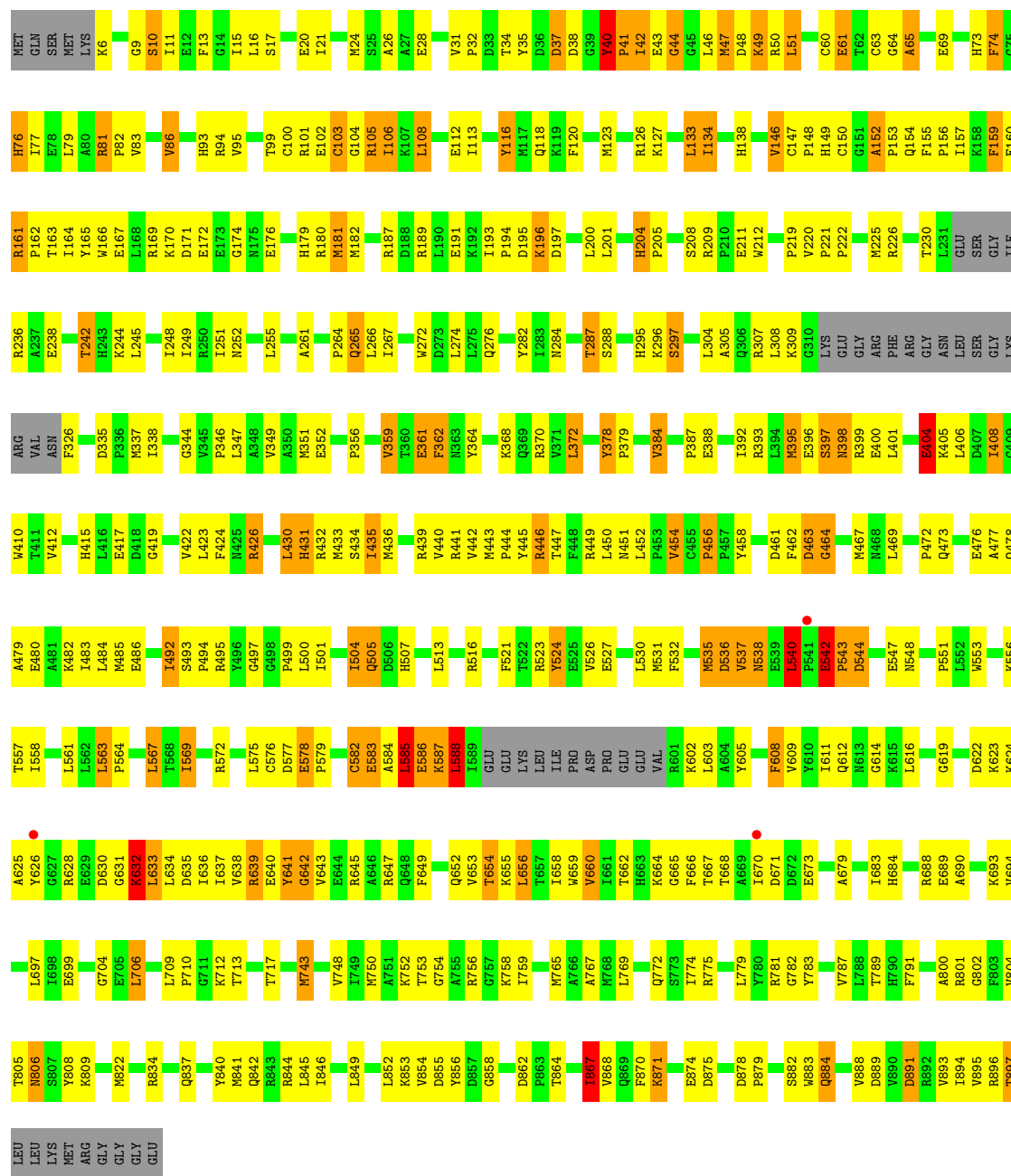
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNA-directed RNA polymerase



- Molecule 1: DNA-directed RNA polymerase

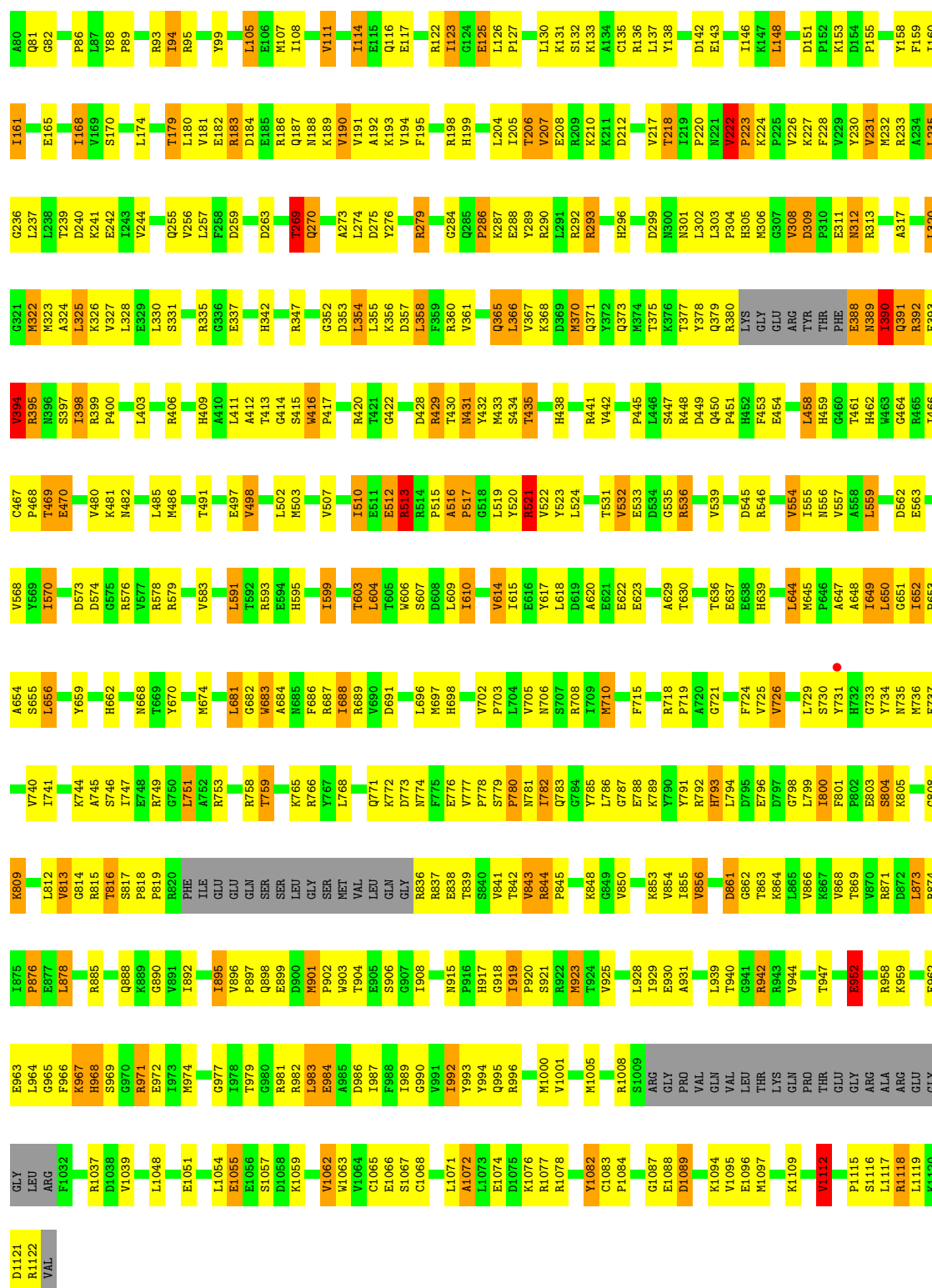
Chain I:



- Molecule 2: DNA-directed RNA polymerase

Chain B:



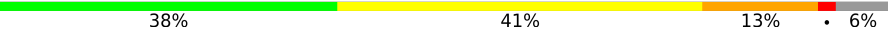


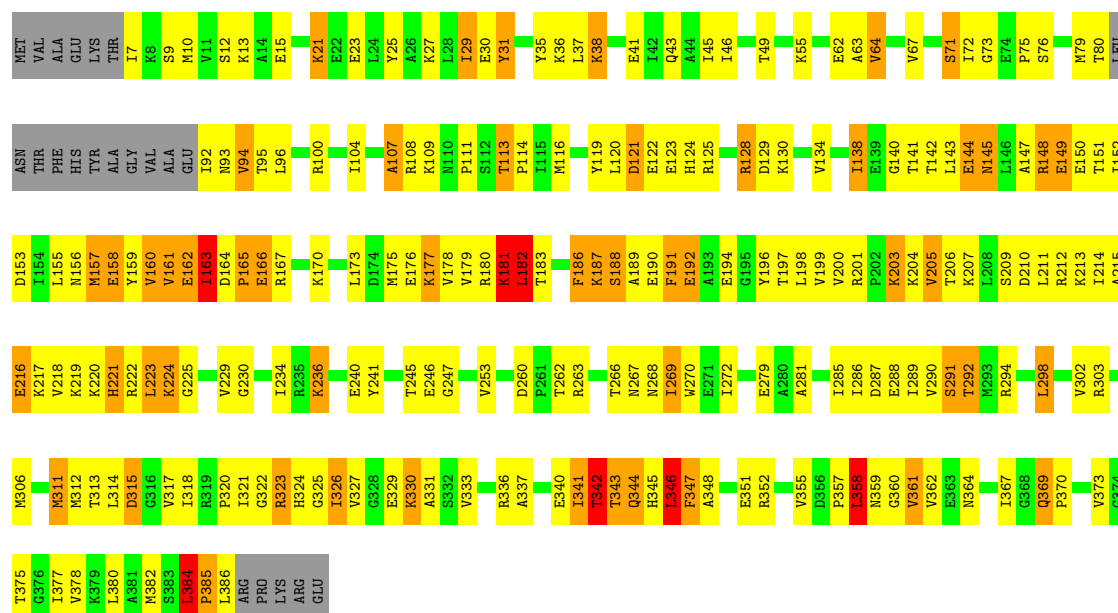
• Molecule 2: DNA-directed RNA polymerase

Chain J: 44% 40% 10% 5%

F1032	L964	P876	K809	M736	G851	E563	I466	R392	G321	L235	F159	E76
F1033	G965	L877	L812	E737	I652	V568	C467	F393	M322	G236	I160	F77
L1040	F966	L378	R813	V740	P653	G569	P468	V394	N323	I237	I161	G78
L1041	K967	R885	G814	I741	A654	I570	T469	R395	A324	L238	E79	E80
G1042	S969	R815	R815	I741	S655	I570	E470	N396	L325	T239	E165	Q81
G1043	G970	Q888	T816	K744	L656	D573	V480	S397	K326	D240	I168	G82
L1044	R971	S817	S817	A745	Y659	R576	K481	I398	V327	K241	V169	P86
A1045	E972	I892	P818	S746	H662	R576	N482	L328	E329	E242	S170	
L1046	L973	R819	R819	I747	H662	R577		L330	L243			
M1047	M974	I895	R820	E748	M674	R578	L485	L403	L330	V244	L174	Y88
L1048		V896	PHE	R749	N668	R579		L406	S331			P89
L1049	T979	P897	ILE	R750	T669	R579	T491	R406	R335	V256	T179	
L1050	G980	Q898	GLU	L751	Y670	V583	G492	L406	G336	L257	L180	R93
E1051	R981	E899	GLU	A752	Y670	V583		H409	E337	F258	V181	I94
R1052	R982	L1052	GLN	R753	M674	N586	E497	A410	K340	D259	E182	R95
L1053	L983	D901	SER	R753	M674	N586	Y498	L411	K340	D263	R183	V20
L1054	E984	P902	SER	R758	L681	L591	Y498	L411	D341	D263	D184	Y99
E1055	A985	W903	LEU	T759	G682	R592		A412	H342			
E1056	R986	T904	GLY	T759	W683	R593	L502	T413	D341			
S1057	R987	E905	SER	K765	A684	E594	M503	G414	H342			
D1058	F988	S906	MET	R766	N685	H595	V507	S415	R347	Y269	E106	L105
K1059	G990	G907	VAL	K766	N685	H595	V507	W416	R347	Q270	K187	M107
G990	G990	I908	VAL	R775	F686		V508	P417	G352	A273	K189	I108
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
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V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
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V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
V991	I908	I908	LEU	Q771	R687	L599	P509	P417	D353	L274	V190	P109
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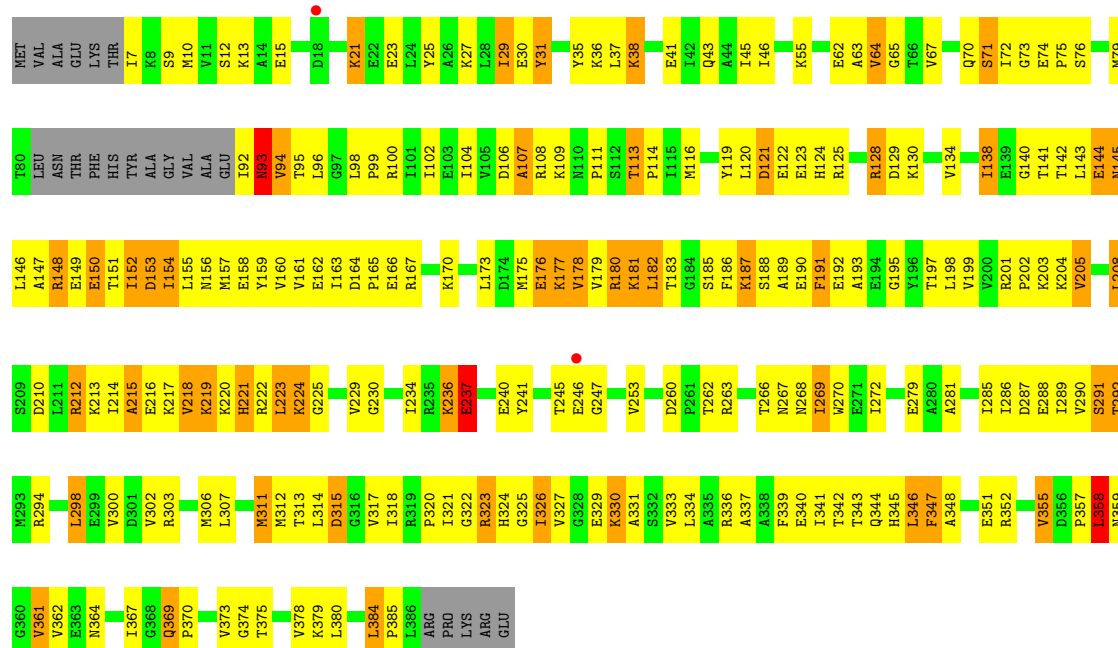
- Molecule 3: DNA-directed RNA polymerase subunit A''

Chain C:  38% 41% 13% 6%



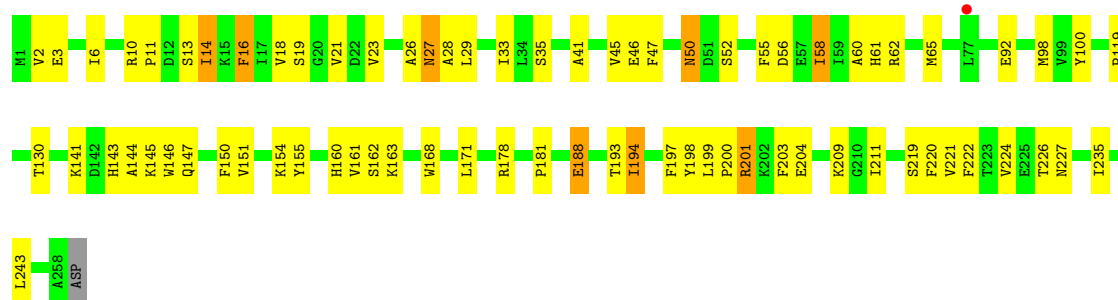
• Molecule 3: DNA-directed RNA polymerase subunit A''

Chain M:  36% 44% 13% 6%



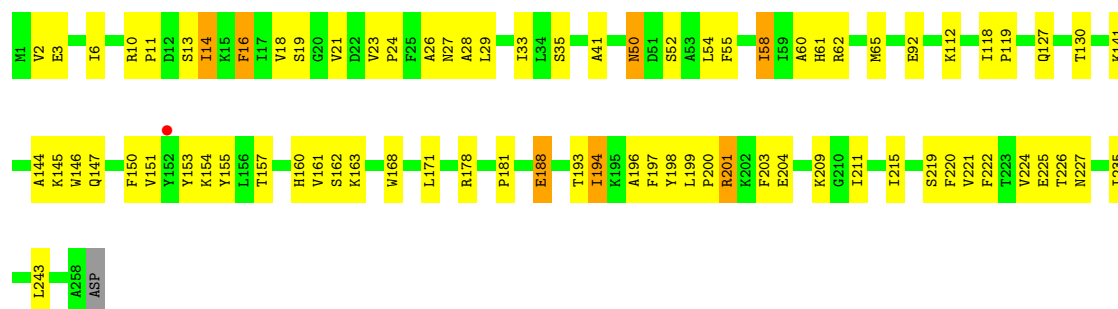
• Molecule 4: DNA-directed RNA polymerase subunit D

Chain D:  71% 26%



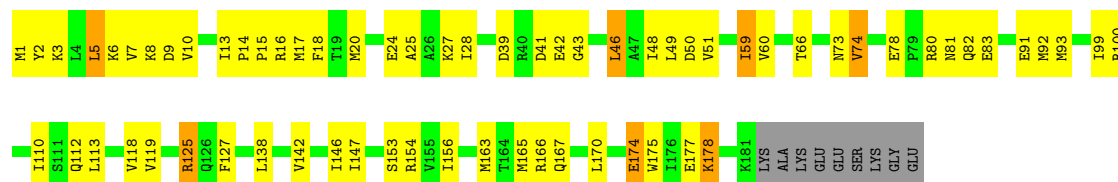
• Molecule 4: DNA-directed RNA polymerase subunit D

Chain O: 69% 27% .



• Molecule 5: DNA-directed RNA polymerase, subunit E'

Chain E: 60% 32% 5% .



• Molecule 5: DNA-directed RNA polymerase, subunit E'

Chain Q: 62% 30% 5% .



• Molecule 6: DNA-directed RNA polymerase, subunit F

Chain F: 71% 25% .



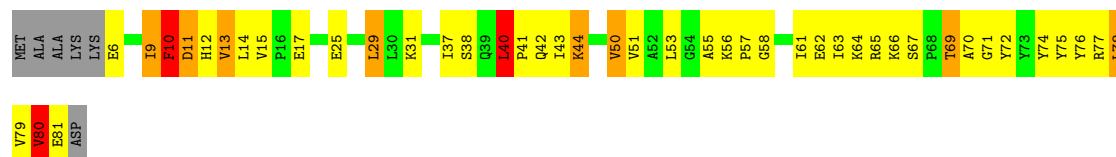
- Molecule 6: DNA-directed RNA polymerase, subunit F

Chain R: 

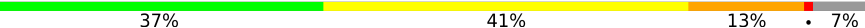


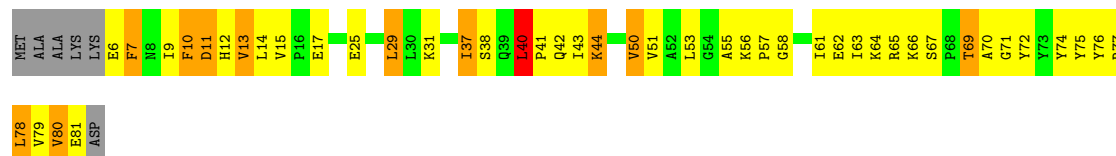
- Molecule 7: DNA-directed RNA polymerase subunit H

Chain H: 



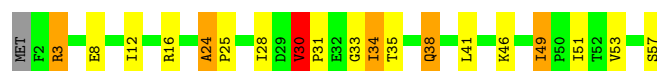
- Molecule 7: DNA-directed RNA polymerase subunit H

Chain S: 



- Molecule 8: DNA-directed RNA polymerase subunit K

Chain K: 



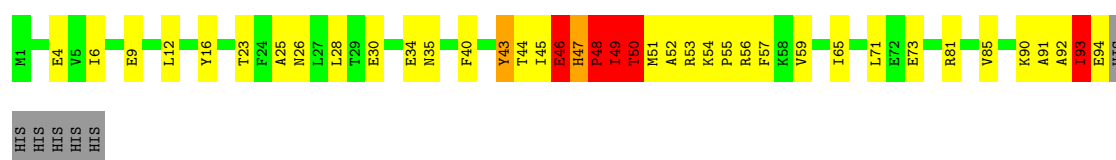
- Molecule 8: DNA-directed RNA polymerase subunit K

Chain T: 

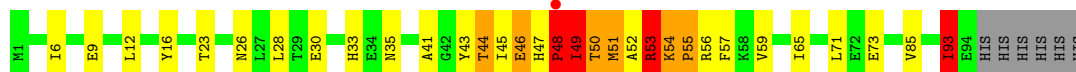


- Molecule 9: DNA-directed RNA polymerase subunit L

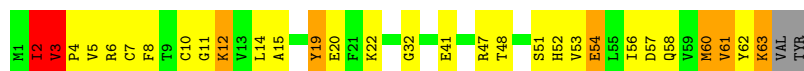
Chain L: 



- Molecule 9: DNA-directed RNA polymerase subunit L



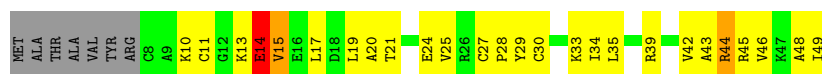
- Molecule 10: DNA-directed RNA polymerase subunit N



- Molecule 10: DNA-directed RNA polymerase subunit N



- Molecule 11: DNA-directed RNA polymerase subunit P



- Molecule 11: DNA-directed RNA polymerase subunit P



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.97Å 206.61Å 365.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.50 49.73 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (49.73-3.50) 95.1 (49.73-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.277 , 0.316 0.278 , 0.311	Depositor DCC
R_{free} test set	5658 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	88.2	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 178.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	51069	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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: ZN, MG

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	0.34	0/7028	0.83	7/9489 (0.1%)
1	I	0.37	0/7011	0.84	10/9465 (0.1%)
2	B	0.35	0/8706	0.85	17/11765 (0.1%)
2	J	0.35	0/8706	0.84	18/11765 (0.2%)
3	C	0.38	0/2917	0.82	2/3936 (0.1%)
3	M	0.35	0/2914	0.80	1/3932 (0.0%)
4	D	0.32	0/2111	0.76	0/2858
4	O	0.32	0/2111	0.77	0/2858
5	E	0.28	0/1491	0.78	2/2008 (0.1%)
5	Q	0.28	0/1491	0.78	2/2008 (0.1%)
6	F	0.30	0/1040	0.76	2/1399 (0.1%)
6	R	0.30	0/1040	0.76	2/1399 (0.1%)
7	H	0.48	0/641	0.90	4/866 (0.5%)
7	S	0.48	0/641	0.90	4/866 (0.5%)
8	K	0.36	0/441	0.89	3/598 (0.5%)
8	T	0.37	0/441	0.89	3/598 (0.5%)
9	L	0.42	1/790 (0.1%)	0.75	3/1066 (0.3%)
9	U	0.46	2/790 (0.3%)	0.82	5/1066 (0.5%)
10	N	0.34	0/518	0.89	0/695
10	V	0.34	0/518	0.89	0/695
11	P	0.38	0/333	0.96	1/445 (0.2%)
11	W	0.38	0/333	0.89	1/445 (0.2%)
All	All	0.35	3/52012 (0.0%)	0.83	87/70222 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	4
2	J	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	U	55	PRO	N-CD	5.06	1.54	1.47
9	U	48	PRO	N-CD	5.05	1.54	1.47
9	L	48	PRO	N-CD	5.03	1.54	1.47

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	642	GLY	N-CA-C	11.30	127.23	112.77
2	J	901	MET	CA-C-N	8.46	128.39	119.85
2	J	901	MET	C-N-CA	8.46	128.39	119.85
1	I	548	ASN	N-CA-C	8.26	115.56	108.78
1	I	404	GLU	N-CA-C	-8.24	102.24	111.14
1	A	152	ALA	CA-C-N	-8.03	109.80	119.84
1	A	152	ALA	C-N-CA	-8.03	109.80	119.84
2	B	901	MET	CA-C-N	7.95	128.57	120.14
2	B	901	MET	C-N-CA	7.95	128.57	120.14
2	B	125	GLU	CA-CB-CG	7.58	129.26	114.10
2	J	817	SER	CA-C-N	6.91	127.50	120.38
2	J	817	SER	C-N-CA	6.91	127.50	120.38
2	B	817	SER	CA-C-N	6.90	127.48	120.38
2	B	817	SER	C-N-CA	6.90	127.48	120.38
2	J	57	VAL	C-N-CD	-6.80	105.63	120.60
3	C	384	LEU	CA-C-N	-6.76	111.39	119.84
3	C	384	LEU	C-N-CA	-6.76	111.39	119.84
2	B	57	VAL	C-N-CD	-6.70	105.86	120.60
2	J	57	VAL	CA-C-N	6.61	142.87	127.00
2	J	57	VAL	C-N-CA	6.61	142.87	127.00
2	B	57	VAL	CA-C-N	6.50	142.60	127.00
2	B	57	VAL	C-N-CA	6.50	142.60	127.00
1	I	220	VAL	CA-C-N	6.38	124.32	119.66
1	I	220	VAL	C-N-CA	6.38	124.32	119.66
1	A	220	VAL	CA-C-N	6.29	124.25	119.66
1	A	220	VAL	C-N-CA	6.29	124.25	119.66
3	M	180	ARG	N-CA-C	-6.11	105.68	113.01
1	I	40	TYR	CA-C-N	-6.09	112.23	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	40	TYR	C-N-CA	-6.09	112.23	119.84
8	K	30	VAL	CA-C-N	-6.07	112.25	119.84
8	K	30	VAL	C-N-CA	-6.07	112.25	119.84
8	T	30	VAL	CA-C-N	-6.04	112.29	119.84
8	T	30	VAL	C-N-CA	-6.04	112.29	119.84
2	J	952	GLU	CA-CB-CG	6.03	126.16	114.10
2	B	125	GLU	CB-CA-C	5.95	119.91	109.80
2	B	513	ARG	N-CA-C	5.85	123.25	110.80
2	J	125	GLU	CA-CB-CG	5.85	125.80	114.10
2	B	844	ARG	CA-C-N	5.73	127.01	119.84
2	B	844	ARG	C-N-CA	5.73	127.01	119.84
1	I	446	ARG	CB-CG-CD	5.73	124.49	111.30
2	J	844	ARG	CA-C-N	5.68	126.94	119.84
2	J	844	ARG	C-N-CA	5.68	126.94	119.84
9	U	93	ILE	N-CA-C	5.53	120.85	109.34
2	B	123	ILE	N-CA-C	-5.46	108.18	113.53
2	J	123	ILE	N-CA-C	-5.42	108.22	113.53
5	E	13	ILE	CA-C-N	5.38	123.58	119.66
5	E	13	ILE	C-N-CA	5.38	123.58	119.66
2	J	1091	ARG	CA-C-N	-5.34	116.21	123.10
2	J	1091	ARG	C-N-CA	-5.34	116.21	123.10
5	Q	13	ILE	CA-C-N	5.33	123.55	119.66
5	Q	13	ILE	C-N-CA	5.33	123.55	119.66
2	J	187	GLN	N-CA-C	-5.30	107.47	114.04
1	A	446	ARG	CB-CG-CD	5.25	123.39	111.30
2	B	187	GLN	N-CA-C	-5.25	107.53	114.04
9	L	47	HIS	CA-C-N	-5.23	113.30	119.84
9	L	47	HIS	C-N-CA	-5.23	113.30	119.84
7	H	40	LEU	CA-C-N	5.22	125.27	119.32
7	H	40	LEU	C-N-CA	5.22	125.27	119.32
7	S	40	LEU	CA-C-N	5.20	125.25	119.32
7	S	40	LEU	C-N-CA	5.20	125.25	119.32
6	R	55	LYS	CA-C-N	5.19	126.33	119.84
6	R	55	LYS	C-N-CA	5.19	126.33	119.84
6	F	55	LYS	CA-C-N	5.19	126.32	119.84
6	F	55	LYS	C-N-CA	5.19	126.32	119.84
9	U	47	HIS	CA-C-N	-5.18	113.36	119.84
9	U	47	HIS	C-N-CA	-5.18	113.36	119.84
7	S	15	VAL	CA-C-N	5.18	125.65	120.52
7	S	15	VAL	C-N-CA	5.18	125.65	120.52
2	J	222	VAL	CA-C-N	5.17	126.31	119.84
2	J	222	VAL	C-N-CA	5.17	126.31	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	15	VAL	N-CA-C	5.16	117.03	108.99
7	H	15	VAL	CA-C-N	5.16	125.62	120.52
7	H	15	VAL	C-N-CA	5.16	125.62	120.52
9	U	54	LYS	CA-C-N	-5.15	113.40	119.84
9	U	54	LYS	C-N-CA	-5.15	113.40	119.84
1	I	456	PRO	N-CA-C	5.14	116.97	110.70
11	P	15	VAL	N-CA-C	5.13	117.00	108.99
1	A	456	PRO	N-CA-C	5.13	116.95	110.70
9	L	55	PRO	CA-N-CD	-5.12	104.83	112.00
2	B	222	VAL	CA-C-N	5.08	126.20	119.84
2	B	222	VAL	C-N-CA	5.08	126.20	119.84
8	K	30	VAL	N-CA-C	5.04	119.77	108.88
8	T	30	VAL	N-CA-C	5.04	119.76	108.88
1	I	548	ASN	CB-CA-C	-5.03	109.82	117.07
1	I	118	GLN	CA-CB-CG	-5.03	104.04	114.10
2	B	952	GLU	CA-CB-CG	5.03	124.15	114.10
2	J	586	ASN	CB-CA-C	-5.01	110.42	117.23

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	536	ASP	Peptide
1	I	582	CYS	Peptide
1	I	632	LYS	Peptide
1	I	641	TYR	Peptide
1	I	642	GLY	Peptide
2	J	513	ARG	Peptide

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	6891	0	6945	323	0
1	I	6875	0	6927	401	1
2	B	8536	0	8585	487	10
2	J	8536	0	8583	601	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2882	0	2982	315	0
3	M	2879	0	2973	258	0
4	D	2066	0	2080	60	0
4	O	2066	0	2080	70	0
5	E	1465	0	1503	73	2
5	Q	1465	0	1503	71	3
6	F	1020	0	1024	40	12
6	R	1020	0	1024	49	7
7	H	627	0	642	33	0
7	S	627	0	642	37	0
8	K	433	0	466	16	0
8	T	433	0	466	19	0
9	L	775	0	770	55	0
9	U	775	0	770	72	0
10	N	510	0	523	44	0
10	V	510	0	523	31	0
11	P	329	0	356	27	5
11	W	329	0	355	15	0
12	A	2	0	0	0	0
12	I	2	0	0	0	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	N	1	0	0	0	0
13	P	1	0	0	1	0
13	V	1	0	0	0	0
13	W	1	0	0	0	0
14	A	1	0	0	0	0
14	B	1	0	0	1	0
14	C	1	0	0	0	0
14	I	1	0	0	2	0
14	J	1	0	0	0	0
14	M	1	0	0	3	0
All	All	51069	0	51722	2636	20

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 26.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:TYR:CE1	2:B:388:GLU:CA	1.79	1.63
1:I:444:PRO:CG	9:U:50:THR:HG23	1.32	1.58
1:I:444:PRO:HG3	9:U:50:THR:CG2	1.09	1.56
2:J:378:TYR:CE1	2:J:388:GLU:HG3	1.38	1.56
3:C:194:GLU:HB2	3:C:196:TYR:CE2	1.41	1.55
2:J:394:VAL:HB	2:J:395:ARG:CG	1.08	1.54
3:C:161:VAL:CG2	3:C:199:VAL:HG23	1.06	1.53
3:M:148:ARG:CZ	3:M:162:GLU:HB2	1.39	1.51
2:B:378:TYR:CE1	2:B:388:GLU:N	1.69	1.48
2:J:107:MET:HB3	2:J:395:ARG:NH2	1.17	1.47
3:C:161:VAL:CG2	3:C:199:VAL:CG2	1.89	1.46
3:C:161:VAL:HG21	3:C:199:VAL:CG2	1.44	1.45
3:C:162:GLU:CA	3:C:196:TYR:HB2	1.45	1.44
1:I:6:LYS:HE3	2:J:1122:ARG:NH2	1.30	1.44
2:J:378:TYR:HH	2:J:388:GLU:N	0.95	1.43
2:B:378:TYR:CE1	2:B:388:GLU:HA	1.35	1.43
2:J:63:PHE:HZ	2:J:388:GLU:CD	1.28	1.40
2:B:389:ASN:ND2	2:B:392:ARG:HD3	1.37	1.40
1:I:6:LYS:CE	2:J:1122:ARG:HH22	1.35	1.38
2:J:394:VAL:CB	2:J:395:ARG:HG3	1.54	1.38
1:I:666:PHE:H	2:J:729:LEU:CD1	1.37	1.37
2:J:63:PHE:CZ	2:J:388:GLU:CD	2.03	1.35
3:M:148:ARG:NH2	3:M:162:GLU:CB	1.86	1.35
3:M:148:ARG:NH2	3:M:162:GLU:HB2	1.05	1.34
2:J:394:VAL:CB	2:J:395:ARG:CG	2.05	1.33
2:J:107:MET:CB	2:J:395:ARG:NH2	1.95	1.28
1:I:445:TYR:CE2	9:U:49:ILE:CG2	2.17	1.28
2:J:39:ASN:O	2:J:43:ASP:OD1	1.53	1.27
1:I:147:CYS:SG	1:I:152:ALA:HB2	1.73	1.27
2:J:1086:CYS:SG	2:J:1090:GLU:OE1	1.92	1.26
2:B:389:ASN:HD21	2:B:392:ARG:CD	1.48	1.26
3:C:162:GLU:C	3:C:196:TYR:HB2	1.61	1.24
2:B:378:TYR:CZ	2:B:388:GLU:HA	1.71	1.24
2:B:378:TYR:CD1	2:B:388:GLU:N	2.05	1.23
1:I:461:ASP:OD2	14:I:1201:HOH:O	1.55	1.23
2:J:107:MET:CB	2:J:395:ARG:CZ	2.08	1.21
2:J:378:TYR:OH	2:J:388:GLU:N	1.67	1.21
3:C:148:ARG:NE	3:C:163:ILE:HG12	1.56	1.20
3:M:165:PRO:HB3	3:M:195:GLY:CA	1.71	1.20
5:E:92:MET:HE3	5:E:127:PHE:CE2	1.76	1.20
3:C:161:VAL:HG23	3:C:199:VAL:N	1.56	1.19
5:Q:9:ASP:OD2	6:R:3:GLY:HA2	1.40	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:63:PHE:HZ	2:J:388:GLU:CG	1.56	1.18
2:J:378:TYR:HE1	2:J:388:GLU:CA	1.56	1.18
3:C:148:ARG:HD2	3:C:163:ILE:CG1	1.70	1.18
1:I:100:CYS:SG	1:I:155:PHE:HZ	1.64	1.18
2:J:378:TYR:CE1	2:J:388:GLU:CG	2.26	1.18
2:J:378:TYR:CZ	2:J:388:GLU:N	2.11	1.18
5:E:92:MET:CE	5:E:127:PHE:CD2	2.28	1.17
1:A:100:CYS:SG	1:A:155:PHE:HZ	1.68	1.16
1:I:445:TYR:CE2	9:U:49:ILE:HG21	1.78	1.15
1:I:666:PHE:H	2:J:729:LEU:HD11	1.11	1.15
2:J:389:ASN:HA	2:J:390:ILE:HG23	1.16	1.14
1:I:445:TYR:CD2	9:U:49:ILE:HG21	1.83	1.13
3:C:162:GLU:HA	3:C:196:TYR:HB2	1.21	1.11
1:I:666:PHE:N	2:J:729:LEU:CD1	2.11	1.11
2:B:389:ASN:ND2	2:B:392:ARG:CD	2.11	1.11
9:L:49:ILE:HD12	9:L:50:THR:H	1.11	1.11
1:A:666:PHE:O	2:B:729:LEU:HD13	1.51	1.10
5:E:9:ASP:OD2	6:F:3:GLY:HA2	1.51	1.10
1:A:666:PHE:O	2:B:729:LEU:CD1	1.98	1.10
1:I:445:TYR:CE2	9:U:49:ILE:HG23	1.86	1.09
2:J:378:TYR:CE1	2:J:388:GLU:CA	2.35	1.09
1:I:100:CYS:SG	1:I:155:PHE:CZ	2.45	1.09
1:I:444:PRO:HG3	9:U:50:THR:HG22	1.29	1.09
2:J:378:TYR:HE1	2:J:388:GLU:HA	1.16	1.08
2:J:107:MET:CB	2:J:395:ARG:HH22	1.58	1.08
2:J:1122:ARG:HG3	6:R:4:ARG:HH21	1.15	1.08
3:C:148:ARG:CD	3:C:163:ILE:CG1	2.31	1.07
3:C:194:GLU:CB	3:C:196:TYR:CE2	2.36	1.07
11:P:14:GLU:HG2	11:P:30:CYS:SG	1.94	1.07
1:A:150:CYS:O	1:A:152:ALA:N	1.86	1.07
2:B:378:TYR:CZ	2:B:388:GLU:CA	2.32	1.07
1:I:444:PRO:HG2	9:U:49:ILE:HB	1.31	1.07
2:J:1122:ARG:CD	5:Q:10:VAL:HG11	1.85	1.07
3:C:152:ILE:HG12	3:C:153:ASP:H	1.19	1.06
2:J:107:MET:HB3	2:J:395:ARG:CZ	1.61	1.06
1:I:666:PHE:N	2:J:729:LEU:HD11	1.67	1.06
2:J:391:GLN:O	2:J:392:ARG:HG3	1.55	1.06
2:B:393:PHE:O	2:B:394:VAL:HB	1.49	1.06
1:I:665:GLY:HA2	2:J:729:LEU:HD11	1.32	1.06
3:M:148:ARG:CZ	3:M:162:GLU:CB	2.24	1.05
2:J:1083:CYS:SG	2:J:1086:CYS:HB2	1.96	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:107:MET:HB2	2:J:395:ARG:CZ	1.86	1.05
1:I:6:LYS:HE3	2:J:1122:ARG:CZ	1.86	1.04
2:J:1122:ARG:CG	6:R:4:ARG:HH21	1.70	1.04
3:M:165:PRO:HB3	3:M:195:GLY:HA3	1.06	1.04
3:C:162:GLU:HA	3:C:196:TYR:CB	1.85	1.04
5:E:92:MET:CE	5:E:127:PHE:CE2	2.40	1.04
2:J:378:TYR:CE1	2:J:388:GLU:N	2.25	1.04
2:B:390:ILE:HD12	2:B:391:GLN:H	1.18	1.04
3:C:162:GLU:C	3:C:196:TYR:CB	2.30	1.04
1:I:444:PRO:CG	9:U:50:THR:CG2	2.04	1.04
3:C:162:GLU:CA	3:C:196:TYR:CB	2.36	1.03
5:E:1:MET:HE1	6:F:11:TYR:HE1	1.19	1.03
1:A:100:CYS:SG	1:A:155:PHE:CZ	2.51	1.03
1:A:758:LYS:O	1:A:761:ASN:OD1	1.76	1.03
2:J:38:TYR:O	2:J:41:PHE:HB3	1.59	1.03
2:J:394:VAL:HB	2:J:395:ARG:HG2	1.08	1.02
5:E:1:MET:HE3	6:F:11:TYR:CD1	1.95	1.02
1:I:103:CYS:SG	1:I:105:ARG:N	2.32	1.02
2:B:744:LYS:HZ3	9:L:53:ARG:NH2	1.57	1.01
3:C:161:VAL:HG12	3:C:162:GLU:H	1.22	1.01
2:B:378:TYR:HE1	2:B:388:GLU:CA	1.35	1.01
10:N:57:ASP:HA	10:N:60:MET:HE3	1.40	1.01
1:A:531:MET:HB2	9:L:44:THR:CG2	1.91	1.01
11:P:14:GLU:CD	11:P:30:CYS:SG	2.44	1.01
11:P:14:GLU:CG	11:P:30:CYS:SG	2.49	1.01
5:E:1:MET:HE1	6:F:11:TYR:CE1	1.95	1.01
3:M:151:THR:HG22	3:M:152:ILE:H	1.26	1.01
1:I:100:CYS:HB3	1:I:103:CYS:HB3	1.42	1.00
1:I:445:TYR:CZ	9:U:49:ILE:CG2	2.43	1.00
3:C:152:ILE:HG13	3:C:159:TYR:CE2	1.95	1.00
2:J:389:ASN:HA	2:J:390:ILE:CG2	1.92	1.00
2:J:393:PHE:O	2:J:394:VAL:HG22	1.60	0.99
2:B:729:LEU:HD23	2:B:731:TYR:HE1	1.21	0.99
2:B:744:LYS:NZ	9:L:53:ARG:NH2	2.09	0.99
1:I:665:GLY:HA2	2:J:729:LEU:CD1	1.92	0.99
1:I:461:ASP:CG	14:I:1201:HOH:O	1.97	0.99
3:C:148:ARG:HD2	3:C:163:ILE:CB	1.91	0.99
1:I:6:LYS:HE2	2:J:1122:ARG:HH12	1.28	0.99
2:B:389:ASN:HD21	2:B:392:ARG:HD3	0.84	0.98
3:C:194:GLU:HB2	3:C:196:TYR:CD2	1.98	0.98
3:C:148:ARG:HG2	3:C:149:GLU:HG3	1.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:VAL:HG22	3:C:199:VAL:CG2	1.92	0.98
5:E:92:MET:HE1	5:E:127:PHE:CD2	1.97	0.98
11:W:27:CYS:HB3	11:W:30:CYS:SG	2.04	0.97
5:Q:1:MET:HE1	6:R:11:TYR:CE1	2.00	0.97
2:B:391:GLN:O	2:B:393:PHE:N	1.96	0.97
9:U:51:MET:HG2	9:U:53:ARG:HB2	1.46	0.97
2:J:1122:ARG:HD3	5:Q:10:VAL:HG11	1.43	0.97
1:A:749:ILE:O	1:A:753:THR:HG22	1.65	0.97
2:J:394:VAL:CB	2:J:395:ARG:HG2	1.79	0.97
3:C:162:GLU:HG2	3:C:196:TYR:CD1	1.99	0.96
1:I:147:CYS:SG	1:I:152:ALA:CB	2.53	0.96
1:A:10:SER:HA	3:C:358:LEU:HD21	1.46	0.96
5:E:3:LYS:NZ	6:F:9:GLU:OE1	1.98	0.96
1:A:753:THR:HG23	1:A:754:GLY:H	1.26	0.96
2:J:378:TYR:CE1	2:J:388:GLU:HA	1.99	0.96
2:J:42:ILE:CG2	2:J:72:ILE:HD13	1.96	0.95
2:J:979:THR:HA	9:U:26:ASN:HD21	1.31	0.95
3:C:148:ARG:NH2	3:C:149:GLU:O	2.00	0.95
3:C:148:ARG:CD	3:C:163:ILE:HG12	1.94	0.95
9:U:51:MET:HG2	9:U:53:ARG:CB	1.96	0.95
2:J:42:ILE:CG2	2:J:72:ILE:CD1	2.44	0.94
3:M:165:PRO:CB	3:M:195:GLY:HA3	1.96	0.94
5:Q:3:LYS:NZ	6:R:9:GLU:OE1	2.00	0.94
2:B:183:ARG:HB2	2:B:186:ARG:HH22	1.33	0.94
2:B:744:LYS:HZ3	9:L:53:ARG:HH22	0.96	0.94
1:I:665:GLY:CA	2:J:729:LEU:HD11	1.95	0.94
2:J:116:GLN:CD	2:J:393:PHE:HD1	1.76	0.94
5:Q:1:MET:HE3	6:R:11:TYR:CD1	2.03	0.94
3:M:148:ARG:HH22	3:M:162:GLU:HB2	1.15	0.93
2:J:183:ARG:HB3	2:J:186:ARG:HH22	1.31	0.93
5:Q:1:MET:CE	6:R:11:TYR:CD1	2.50	0.93
2:J:63:PHE:CZ	2:J:388:GLU:CG	2.46	0.93
2:B:510:ILE:HG22	2:B:513:ARG:HE	1.33	0.93
2:B:1063:TRP:NE1	2:B:1094:LYS:HE3	1.84	0.93
5:Q:1:MET:HE3	6:R:11:TYR:HD1	1.32	0.93
3:M:148:ARG:NH2	3:M:162:GLU:CG	2.31	0.92
2:B:378:TYR:CZ	2:B:388:GLU:N	2.37	0.92
5:Q:9:ASP:OD2	6:R:3:GLY:CA	2.17	0.92
2:B:389:ASN:ND2	2:B:392:ARG:HB2	1.83	0.92
3:C:148:ARG:NE	3:C:163:ILE:CG1	2.30	0.92
2:J:378:TYR:CZ	2:J:388:GLU:HG3	2.04	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1063:TRP:CZ3	2:B:1074:GLU:CG	2.53	0.92
5:E:1:MET:CE	6:F:11:TYR:CE1	2.53	0.92
2:J:57:VAL:HG21	2:J:371:GLN:HA	1.52	0.92
3:C:161:VAL:HG23	3:C:199:VAL:HG23	1.47	0.91
2:B:389:ASN:CG	2:B:392:ARG:HD3	1.95	0.91
5:E:1:MET:CE	6:F:11:TYR:CD1	2.52	0.91
3:C:194:GLU:CB	3:C:196:TYR:HE2	1.80	0.91
3:M:152:ILE:CG2	3:M:159:TYR:HA	2.01	0.91
2:B:57:VAL:HG21	2:B:371:GLN:HA	1.52	0.91
2:J:391:GLN:O	2:J:392:ARG:CG	2.19	0.91
1:I:6:LYS:CE	2:J:1122:ARG:HH12	1.84	0.91
1:A:531:MET:CB	9:L:44:THR:CG2	2.47	0.90
2:B:729:LEU:HD23	2:B:731:TYR:CE1	2.06	0.90
3:C:163:ILE:N	3:C:196:TYR:CB	2.35	0.90
3:C:161:VAL:CG2	3:C:199:VAL:CB	2.48	0.90
2:B:1063:TRP:CE2	2:B:1094:LYS:HE3	2.07	0.90
3:C:163:ILE:HD13	3:C:163:ILE:H	1.34	0.90
2:J:1086:CYS:SG	2:J:1090:GLU:CG	2.60	0.90
5:Q:1:MET:HE1	6:R:11:TYR:HE1	1.34	0.90
1:I:13:PHE:HE2	3:M:333:VAL:HG21	1.36	0.89
3:C:211:LEU:HA	3:C:214:ILE:CD1	2.02	0.89
1:I:40:TYR:H	1:I:41:PRO:HD3	1.37	0.89
1:I:6:LYS:HE3	2:J:1122:ARG:HH22	0.75	0.89
2:B:394:VAL:HG22	2:B:395:ARG:HG3	1.54	0.89
1:I:443:MET:HB3	9:U:49:ILE:HD12	1.55	0.89
2:J:393:PHE:O	2:J:394:VAL:CG2	2.20	0.89
3:C:148:ARG:HD2	3:C:163:ILE:HB	1.54	0.88
2:J:206:THR:HG1	2:J:218:THR:HG1	1.22	0.88
2:B:1063:TRP:CD1	2:B:1094:LYS:HG3	2.09	0.88
1:I:103:CYS:N	1:I:150:CYS:SG	2.47	0.88
2:J:1086:CYS:SG	2:J:1090:GLU:CD	2.57	0.88
3:M:21:LYS:HD3	7:S:71:GLY:HA3	1.54	0.88
3:C:216:GLU:O	3:C:220:LYS:HB3	1.72	0.88
11:P:30:CYS:SG	13:P:1501:ZN:ZN	1.62	0.88
2:J:1086:CYS:SG	2:J:1090:GLU:HG3	2.13	0.88
9:U:49:ILE:O	9:U:50:THR:OG1	1.92	0.88
2:J:63:PHE:CZ	2:J:388:GLU:OE1	2.27	0.88
2:J:41:PHE:O	2:J:45:GLY:O	1.92	0.87
2:B:391:GLN:OE1	2:B:393:PHE:CD2	2.27	0.87
3:C:163:ILE:N	3:C:196:TYR:HB2	1.89	0.87
1:I:126:ARG:NH2	7:S:40:LEU:O	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:1:MET:CE	6:R:11:TYR:HD1	1.87	0.87
1:I:444:PRO:O	9:U:49:ILE:HD13	1.74	0.87
9:L:49:ILE:HD12	9:L:50:THR:N	1.90	0.87
9:L:92:ALA:O	9:L:94:GLU:N	2.06	0.87
3:M:182:LEU:HD23	3:M:185:SER:CB	2.05	0.87
3:C:148:ARG:CD	3:C:163:ILE:HG13	2.05	0.87
3:C:163:ILE:HB	3:C:164:ASP:HA	1.56	0.86
10:N:62:TYR:O	10:N:63:LYS:NZ	2.09	0.86
2:B:1063:TRP:CZ3	2:B:1074:GLU:HG3	2.09	0.86
1:I:531:MET:HB2	9:U:44:THR:HG23	1.56	0.86
5:Q:7:VAL:HG13	6:R:5:LYS:O	1.75	0.86
2:J:398:ILE:O	2:J:398:ILE:HG22	1.75	0.85
3:C:21:LYS:HD3	7:H:71:GLY:HA3	1.58	0.85
2:B:1063:TRP:NE1	2:B:1094:LYS:HG3	1.90	0.85
2:J:1122:ARG:HD2	5:Q:10:VAL:HG11	1.55	0.85
2:B:286:PRO:HB2	2:B:289:TYR:HB2	1.58	0.85
3:C:194:GLU:HB2	3:C:196:TYR:HE2	1.09	0.85
1:I:444:PRO:CD	9:U:50:THR:HG23	2.06	0.85
1:I:666:PHE:H	2:J:729:LEU:HD12	1.41	0.85
2:J:286:PRO:HB2	2:J:289:TYR:HB2	1.58	0.85
5:E:1:MET:HE3	6:F:11:TYR:HD1	1.33	0.85
1:I:666:PHE:N	2:J:729:LEU:HD12	1.92	0.84
3:M:187:LYS:HD2	3:M:202:PRO:HD2	1.58	0.84
3:M:163:ILE:O	3:M:195:GLY:O	1.96	0.84
2:B:393:PHE:O	2:B:394:VAL:CB	2.25	0.84
3:C:216:GLU:O	3:C:220:LYS:CB	2.25	0.84
5:E:81:ASN:O	5:E:82:GLN:HG2	1.77	0.84
3:C:148:ARG:CZ	3:C:163:ILE:HG12	2.06	0.84
3:C:148:ARG:NH1	3:C:163:ILE:O	2.11	0.84
3:C:191:PHE:HB3	3:C:198:LEU:HB2	1.60	0.84
3:C:162:GLU:HA	3:C:196:TYR:CD1	2.13	0.83
3:C:148:ARG:CZ	3:C:149:GLU:O	2.26	0.83
2:J:46:LEU:HD12	2:J:46:LEU:O	1.78	0.83
1:A:666:PHE:O	2:B:729:LEU:HD12	1.76	0.83
2:J:63:PHE:CZ	2:J:388:GLU:HG2	2.12	0.83
9:U:49:ILE:HG22	9:U:50:THR:H	1.42	0.83
3:C:148:ARG:HD2	3:C:163:ILE:HG13	1.59	0.83
3:C:162:GLU:C	3:C:196:TYR:CA	2.52	0.83
2:J:45:GLY:O	2:J:46:LEU:HB3	1.77	0.82
3:C:151:THR:HG22	3:C:152:ILE:H	1.44	0.82
3:C:163:ILE:CB	3:C:164:ASP:HA	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:6:LYS:NZ	2:J:1122:ARG:HH22	1.76	0.82
1:A:750:MET:HA	1:A:753:THR:CG2	2.09	0.82
3:C:153:ASP:OD2	3:C:157:MET:HB3	1.78	0.82
3:C:161:VAL:HG23	3:C:198:LEU:C	2.04	0.82
3:C:212:ARG:HG3	3:C:213:LYS:N	1.91	0.82
1:I:100:CYS:SG	1:I:103:CYS:HB2	2.20	0.82
3:M:148:ARG:NH1	3:M:162:GLU:HB2	1.94	0.82
4:D:2:VAL:HG11	9:L:85:VAL:HA	1.59	0.82
1:I:103:CYS:HB2	1:I:150:CYS:SG	2.20	0.82
1:I:531:MET:HB3	9:U:44:THR:OG1	1.79	0.82
2:B:1063:TRP:CZ2	2:B:1094:LYS:HE3	2.13	0.81
11:W:30:CYS:SG	11:W:32:SER:HB3	2.20	0.81
1:I:445:TYR:CZ	9:U:49:ILE:HG21	2.12	0.81
1:I:563:LEU:HB2	1:I:614:GLY:HA2	1.62	0.81
3:M:160:VAL:HG12	3:M:161:VAL:H	1.43	0.81
1:A:531:MET:CB	9:L:44:THR:HG21	2.10	0.81
2:J:394:VAL:CG2	2:J:395:ARG:HG3	2.11	0.81
1:A:563:LEU:HB2	1:A:614:GLY:HA2	1.63	0.81
2:B:390:ILE:CD1	2:B:391:GLN:H	1.93	0.81
5:E:7:VAL:HG13	6:F:5:LYS:O	1.80	0.81
2:J:395:ARG:O	2:J:397:SER:N	2.14	0.81
2:B:146:ILE:HG21	10:N:61:VAL:HG21	1.61	0.81
5:Q:3:LYS:NZ	6:R:9:GLU:CD	2.39	0.81
1:A:79:LEU:HA	1:A:252:ASN:HD21	1.46	0.80
1:I:100:CYS:HB3	1:I:103:CYS:CB	2.10	0.80
1:I:432:ARG:O	2:J:1043:HIS:ND1	2.15	0.80
3:C:162:GLU:HG2	3:C:196:TYR:CG	2.16	0.80
2:J:183:ARG:HG3	2:J:337:GLU:OE2	1.82	0.80
1:A:508:ILE:HG13	1:A:754:GLY:O	1.81	0.80
2:J:952:GLU:OE2	2:J:952:GLU:N	2.15	0.80
3:M:182:LEU:O	3:M:185:SER:HB2	1.82	0.80
2:B:378:TYR:OH	2:B:388:GLU:HA	1.80	0.80
2:J:1122:ARG:HG2	2:J:1122:ARG:HH11	1.47	0.80
3:M:148:ARG:HG2	3:M:149:GLU:HG3	1.63	0.80
1:A:531:MET:CB	9:L:44:THR:HG23	2.12	0.80
2:J:1122:ARG:NH2	5:Q:67:TYR:CE2	2.49	0.80
3:M:204:LYS:HG3	3:M:205:VAL:HG23	1.62	0.80
1:I:452:LEU:HB3	1:I:504:ILE:HD11	1.64	0.80
1:I:384:VAL:HG12	1:I:392:ILE:HB	1.65	0.79
7:S:41:PRO:HB2	7:S:77:ARG:HG2	1.63	0.79
3:C:152:ILE:HG12	3:C:153:ASP:N	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:34:ILE:HB	8:K:38:GLN:HG3	1.64	0.79
8:T:34:ILE:HB	8:T:38:GLN:HG3	1.64	0.79
2:J:1122:ARG:HG3	6:R:4:ARG:NH2	1.96	0.79
5:E:92:MET:HE1	5:E:127:PHE:HD2	1.43	0.79
3:C:162:GLU:CB	3:C:196:TYR:HB2	2.13	0.79
1:I:6:LYS:CE	2:J:1122:ARG:NH1	2.45	0.79
1:I:531:MET:HB2	9:U:44:THR:CG2	2.12	0.79
5:E:9:ASP:OD2	6:F:3:GLY:CA	2.29	0.79
2:J:391:GLN:O	2:J:392:ARG:CB	2.31	0.79
4:O:2:VAL:HG11	9:U:85:VAL:HA	1.63	0.79
5:Q:1:MET:CE	6:R:11:TYR:CE1	2.66	0.79
1:I:6:LYS:CE	2:J:1122:ARG:NH2	2.11	0.78
1:I:103:CYS:SG	1:I:105:ARG:HB2	2.23	0.78
2:J:107:MET:HB3	2:J:395:ARG:HH22	0.76	0.78
1:A:834:ARG:HG3	3:C:80:THR:HG22	1.66	0.78
7:H:41:PRO:HB2	7:H:77:ARG:HG2	1.63	0.78
1:I:79:LEU:HA	1:I:252:ASN:HD21	1.47	0.78
2:J:1122:ARG:CG	6:R:4:ARG:NH2	2.47	0.78
3:M:173:LEU:HB3	3:M:177:LYS:HZ3	1.47	0.78
2:B:389:ASN:ND2	2:B:392:ARG:CB	2.45	0.78
5:E:8:LYS:HE3	6:F:5:LYS:HD2	1.64	0.78
2:J:979:THR:HA	9:U:26:ASN:ND2	1.99	0.78
3:C:153:ASP:HB2	3:C:158:GLU:O	1.84	0.78
2:B:996:ARG:HH22	2:B:1000:MET:HE3	1.49	0.78
2:J:996:ARG:HH22	2:J:1000:MET:HE3	1.49	0.78
3:M:187:LYS:O	3:M:188:SER:OG	2.02	0.78
10:N:58:GLN:O	10:N:61:VAL:HG12	1.84	0.78
2:J:1122:ARG:HD2	5:Q:10:VAL:CG1	2.13	0.78
1:A:452:LEU:HB3	1:A:504:ILE:HD11	1.64	0.77
2:B:391:GLN:OE1	2:B:393:PHE:CE2	2.37	0.77
3:C:164:ASP:CG	3:C:165:PRO:HD2	2.09	0.77
1:A:384:VAL:HG12	1:A:392:ILE:HB	1.65	0.77
1:I:665:GLY:C	2:J:729:LEU:HD11	2.09	0.77
2:J:63:PHE:HZ	2:J:388:GLU:HG2	1.43	0.77
3:M:182:LEU:CD2	3:M:185:SER:HB2	2.14	0.77
3:C:196:TYR:CE1	3:C:198:LEU:HD11	2.20	0.77
1:A:666:PHE:C	2:B:729:LEU:HD13	2.10	0.77
3:C:161:VAL:HG23	3:C:199:VAL:CG2	2.10	0.77
2:B:390:ILE:C	2:B:392:ARG:H	1.93	0.76
11:P:14:GLU:CD	11:P:30:CYS:HG	1.92	0.76
2:J:370:MET:SD	2:J:398:ILE:HG12	2.24	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:57:VAL:HB	2:J:58:PRO:HA	1.67	0.76
2:B:1063:TRP:HE1	2:B:1094:LYS:HE3	1.48	0.76
3:C:186:PHE:C	3:C:187:LYS:HG2	2.10	0.76
2:J:394:VAL:HB	2:J:395:ARG:HG3	0.77	0.76
3:M:152:ILE:HG23	3:M:159:TYR:HA	1.66	0.76
1:I:147:CYS:SG	1:I:152:ALA:CA	2.74	0.76
2:B:390:ILE:O	2:B:392:ARG:N	2.19	0.76
2:J:361:VAL:HG11	2:J:417:PRO:HG3	1.67	0.76
2:B:952:GLU:OE2	2:B:952:GLU:N	2.17	0.76
1:I:632:LYS:HZ2	1:I:634:LEU:H	1.30	0.76
2:B:390:ILE:HD12	2:B:391:GLN:N	1.99	0.76
1:A:531:MET:HB2	9:L:44:THR:HG21	1.66	0.75
2:B:232:MET:HE1	2:B:317:ALA:HA	1.69	0.75
3:C:161:VAL:HG23	3:C:199:VAL:CB	2.16	0.75
3:C:173:LEU:HB3	3:C:177:LYS:HZ3	1.49	0.75
1:I:9:GLY:CA	2:J:1120:LYS:HB2	2.15	0.75
4:O:35:SER:HB2	4:O:141:LYS:HB3	1.68	0.75
9:L:46:GLU:OE2	9:L:56:ARG:HD2	1.85	0.75
2:B:361:VAL:HG11	2:B:417:PRO:HG3	1.67	0.75
2:J:1122:ARG:HG2	2:J:1122:ARG:NH1	2.01	0.75
2:B:378:TYR:HE1	2:B:388:GLU:C	1.93	0.75
2:B:749:ARG:NH2	4:D:147:GLN:OE1	2.20	0.75
1:I:480:GLU:HA	8:T:10:ALA:HB1	1.68	0.75
1:I:585:LEU:O	1:I:586:GLU:HB3	1.86	0.75
1:I:9:GLY:HA3	2:J:1120:LYS:HB2	1.67	0.75
3:C:194:GLU:OE1	3:C:196:TYR:HE2	1.69	0.75
4:D:35:SER:HB2	4:D:141:LYS:HB3	1.68	0.75
2:J:39:ASN:C	2:J:41:PHE:H	1.94	0.75
3:C:343:THR:O	3:C:347:PHE:HB3	1.87	0.75
2:J:735:ASN:HB3	2:J:741:ILE:HG13	1.69	0.75
3:M:67:VAL:O	3:M:71:SER:OG	2.05	0.75
2:J:683:TRP:CD1	2:J:686:PHE:HB3	2.22	0.74
2:B:683:TRP:CD1	2:B:686:PHE:HB3	2.22	0.74
2:B:183:ARG:HG2	2:B:337:GLU:OE1	1.87	0.74
2:B:735:ASN:HB3	2:B:741:ILE:HG13	1.69	0.74
2:J:394:VAL:CG1	2:J:395:ARG:HG2	2.17	0.74
1:A:16:LEU:HD11	2:B:1109:LYS:HG3	1.68	0.74
2:B:57:VAL:HB	2:B:58:PRO:HA	1.67	0.74
2:B:123:ILE:HG22	2:B:403:LEU:HD22	1.69	0.74
1:A:625:ALA:O	1:A:632:LYS:NZ	2.18	0.74
7:H:13:VAL:HG22	7:H:14:LEU:HG	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3:LYS:NZ	6:F:9:GLU:CD	2.46	0.74
2:J:771:GLN:HB3	2:J:818:PRO:HG3	1.69	0.74
1:I:6:LYS:HE3	2:J:1122:ARG:NH1	2.02	0.74
2:B:286:PRO:HD2	2:B:290:ARG:HE	1.53	0.73
3:C:160:VAL:CG2	3:C:198:LEU:HG	2.18	0.73
3:C:67:VAL:O	3:C:71:SER:OG	2.05	0.73
2:B:239:THR:HB	2:B:242:GLU:HG2	1.70	0.73
2:B:389:ASN:HD22	2:B:392:ARG:HB2	1.52	0.73
2:B:771:GLN:HB3	2:B:818:PRO:HG3	1.69	0.73
3:C:212:ARG:HG3	3:C:213:LYS:H	1.49	0.73
3:C:345:HIS:O	3:C:348:ALA:N	2.20	0.73
2:J:123:ILE:HG22	2:J:403:LEU:HD22	1.69	0.73
2:J:286:PRO:HD2	2:J:290:ARG:HE	1.53	0.73
2:J:239:THR:HB	2:J:242:GLU:HG2	1.70	0.73
3:M:148:ARG:HH12	3:M:162:GLU:C	1.96	0.73
3:C:134:VAL:HG12	3:C:138:ILE:HD11	1.70	0.73
3:M:134:VAL:HG12	3:M:138:ILE:HD11	1.70	0.73
3:C:162:GLU:C	3:C:196:TYR:HA	2.13	0.73
1:A:444:PRO:CD	9:L:50:THR:HG22	2.19	0.72
2:B:21:MET:HE2	2:B:25:TRP:HE1	1.54	0.72
1:I:63:CYS:HG	1:I:73:HIS:HE2	1.35	0.72
2:J:392:ARG:C	2:J:394:VAL:H	1.96	0.72
2:J:393:PHE:C	2:J:394:VAL:HG22	2.14	0.72
2:J:395:ARG:HB3	2:J:398:ILE:CD1	2.19	0.72
5:E:1:MET:CE	6:F:11:TYR:HD1	1.98	0.72
1:I:445:TYR:CG	9:U:49:ILE:HG21	2.24	0.72
2:J:232:MET:HE1	2:J:317:ALA:HA	1.71	0.72
2:J:42:ILE:HG21	2:J:72:ILE:HD13	1.71	0.72
3:M:148:ARG:NH1	3:M:162:GLU:C	2.47	0.72
1:A:671:ASP:OD1	2:B:969:SER:OG	2.07	0.72
2:J:21:MET:HE2	2:J:25:TRP:HE1	1.54	0.72
2:J:939:LEU:HD11	2:J:966:PHE:HD2	1.54	0.72
11:W:27:CYS:CB	11:W:30:CYS:SG	2.77	0.72
2:B:939:LEU:HD11	2:B:966:PHE:HD2	1.54	0.72
1:I:74:PHE:HE1	1:I:222:PRO:HD3	1.54	0.72
7:S:13:VAL:HG22	7:S:14:LEU:HG	1.71	0.72
2:J:309:ASP:OD1	2:J:309:ASP:N	2.23	0.72
2:J:378:TYR:HE1	2:J:388:GLU:CB	2.01	0.72
2:J:904:THR:HG22	2:J:906:SER:H	1.55	0.72
1:I:666:PHE:H	2:J:729:LEU:CG	2.03	0.72
2:J:378:TYR:CZ	2:J:388:GLU:CG	2.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1101:PHE:CG	3:M:367:ILE:HG13	2.25	0.72
3:M:153:ASP:CB	3:M:157:MET:HB2	2.20	0.72
2:J:395:ARG:HD3	2:J:398:ILE:HD11	1.72	0.72
2:B:309:ASP:OD1	2:B:309:ASP:N	2.23	0.71
2:J:42:ILE:HG23	2:J:72:ILE:HD11	1.72	0.71
2:J:433:MET:HE1	2:J:652:ILE:HG12	1.71	0.71
2:B:904:THR:HG22	2:B:906:SER:H	1.56	0.71
2:B:63:PHE:CD1	2:B:392:ARG:NH2	2.58	0.71
9:L:48:PRO:O	9:L:49:ILE:HG23	1.89	0.71
1:I:13:PHE:CE2	3:M:333:VAL:HG21	2.25	0.71
2:J:392:ARG:O	2:J:394:VAL:N	2.22	0.71
3:M:152:ILE:HG23	3:M:160:VAL:H	1.54	0.71
3:C:163:ILE:HB	3:C:164:ASP:CA	2.20	0.71
2:B:433:MET:HE1	2:B:652:ILE:HG12	1.71	0.71
2:B:981:ARG:NH2	9:L:30:GLU:OE2	2.22	0.71
2:B:432:TYR:HB2	2:B:682:GLY:HA2	1.73	0.71
3:C:151:THR:HG22	3:C:152:ILE:N	2.04	0.71
2:J:749:ARG:NH2	4:O:147:GLN:OE1	2.24	0.71
2:B:146:ILE:CG2	10:N:61:VAL:HG21	2.20	0.71
1:I:670:ILE:HD11	2:J:929:ILE:HG12	1.71	0.71
1:A:181:MET:SD	1:A:189:ARG:NH1	2.64	0.71
3:C:223:LEU:O	3:C:225:GLY:N	2.23	0.71
1:A:564:PRO:HD2	1:A:567:LEU:HD11	1.72	0.71
1:A:749:ILE:O	1:A:753:THR:CG2	2.39	0.71
9:L:25:ALA:HB1	9:L:43:TYR:CE2	2.26	0.71
2:J:1068:CYS:SG	2:J:1070:HIS:CD2	2.84	0.71
3:M:165:PRO:HB3	3:M:195:GLY:HA2	1.72	0.71
9:U:51:MET:HA	9:U:52:ALA:C	2.15	0.71
3:C:162:GLU:HA	3:C:196:TYR:CG	2.25	0.71
9:L:25:ALA:HB1	9:L:43:TYR:CD2	2.26	0.71
9:L:49:ILE:CD1	9:L:50:THR:H	1.98	0.71
1:I:449:ARG:CZ	9:U:49:ILE:HD11	2.21	0.71
3:M:145:ASN:OD1	3:M:145:ASN:N	2.24	0.71
5:Q:9:ASP:OD1	6:R:4:ARG:HG2	1.90	0.71
5:E:9:ASP:OD1	5:E:10:VAL:N	2.23	0.70
2:J:729:LEU:HD23	2:J:730:SER:C	2.15	0.70
1:A:531:MET:HB3	9:L:44:THR:CG2	2.20	0.70
1:I:822:MET:HG2	2:J:458:LEU:HB3	1.72	0.70
2:B:47:GLN:HE22	2:B:69:LYS:HA	1.56	0.70
2:B:275:ASP:O	2:B:279:ARG:HB2	1.91	0.70
2:J:432:TYR:HB2	2:J:682:GLY:HA2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:CYS:SG	1:A:61:GLU:N	2.64	0.70
2:B:744:LYS:NZ	9:L:53:ARG:HH22	1.74	0.70
2:J:116:GLN:OE1	2:J:393:PHE:HD1	1.73	0.70
3:M:153:ASP:HB3	3:M:157:MET:HB2	1.73	0.70
1:A:74:PHE:HE1	1:A:222:PRO:HD3	1.57	0.70
1:I:181:MET:SD	1:I:189:ARG:NH1	2.64	0.70
1:I:840:TYR:OH	3:M:323:ARG:NH2	2.25	0.70
3:M:223:LEU:O	3:M:225:GLY:N	2.23	0.70
3:C:196:TYR:CD1	3:C:196:TYR:O	2.45	0.70
1:A:712:LYS:HD2	3:C:92:ILE:HB	1.74	0.70
1:I:476:GLU:OE1	8:T:11:ARG:NH1	2.23	0.70
2:J:41:PHE:CD1	2:J:42:ILE:HD13	2.27	0.70
1:A:863:PRO:HB3	3:C:360:GLY:HA2	1.75	0.69
3:M:120:LEU:O	3:M:125:ARG:NH1	2.26	0.69
3:M:152:ILE:O	3:M:160:VAL:HB	1.92	0.69
3:C:148:ARG:HG2	3:C:149:GLU:CG	2.18	0.69
1:I:564:PRO:HD2	1:I:567:LEU:HD11	1.72	0.69
2:J:378:TYR:CD1	2:J:388:GLU:HG3	2.22	0.69
3:C:342:THR:HB	3:C:345:HIS:HB2	1.73	0.69
1:I:60:CYS:SG	1:I:61:GLU:N	2.65	0.69
3:C:145:ASN:N	3:C:145:ASN:OD1	2.25	0.69
2:J:42:ILE:HG23	2:J:72:ILE:CD1	2.21	0.69
2:J:63:PHE:CE1	2:J:388:GLU:OE1	2.45	0.69
1:A:13:PHE:HE1	2:B:1115:PRO:HB3	1.57	0.69
1:A:894:ILE:HG13	3:C:29:ILE:HD12	1.75	0.69
2:B:730:SER:HA	2:B:735:ASN:HD21	1.58	0.69
2:B:874:ARG:HB3	2:B:1000:MET:HE1	1.74	0.69
3:C:120:LEU:O	3:C:125:ARG:NH1	2.26	0.69
1:A:758:LYS:HG2	1:A:760:LEU:HD21	1.74	0.69
2:B:389:ASN:HD21	2:B:392:ARG:NE	1.88	0.69
3:C:211:LEU:HA	3:C:214:ILE:HD12	1.73	0.69
10:N:60:MET:O	10:N:62:TYR:N	2.23	0.69
1:I:447:THR:O	1:I:449:ARG:NH1	2.26	0.69
1:I:640:GLU:HG2	1:I:896:ARG:NH1	2.07	0.69
1:I:834:ARG:HH12	3:M:99:PRO:HD3	1.58	0.69
2:J:874:ARG:HB3	2:J:1000:MET:HE1	1.74	0.69
1:A:531:MET:HB3	9:L:44:THR:HG23	1.72	0.69
5:Q:8:LYS:HE3	6:R:5:LYS:HD2	1.73	0.69
2:J:275:ASP:O	2:J:279:ARG:HB2	1.91	0.69
3:M:182:LEU:CD2	3:M:185:SER:CB	2.71	0.69
1:I:103:CYS:CA	1:I:150:CYS:SG	2.81	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:378:TYR:CE1	2:J:388:GLU:CB	2.74	0.68
2:J:730:SER:HA	2:J:735:ASN:HD21	1.57	0.68
3:M:153:ASP:OD2	3:M:160:VAL:HG21	1.93	0.68
1:A:872:TYR:CZ	3:C:64:VAL:HG11	2.28	0.68
2:B:719:PRO:HG3	10:N:53:VAL:HG11	1.76	0.68
2:J:395:ARG:HB3	2:J:398:ILE:HD11	1.76	0.68
3:M:64:VAL:HA	3:M:67:VAL:HG22	1.75	0.68
5:Q:9:ASP:OD1	5:Q:10:VAL:N	2.23	0.68
3:C:161:VAL:HG23	3:C:199:VAL:CA	2.23	0.68
1:A:447:THR:O	1:A:449:ARG:NH1	2.25	0.68
1:A:894:ILE:O	1:A:897:THR:HG23	1.93	0.68
3:C:161:VAL:CG2	3:C:198:LEU:C	2.67	0.68
1:A:445:TYR:HB2	1:A:449:ARG:HH22	1.59	0.68
3:C:286:ILE:HD13	3:C:306:MET:HG2	1.76	0.68
1:I:671:ASP:OD1	2:J:969:SER:OG	2.11	0.68
3:M:160:VAL:HG12	3:M:161:VAL:N	2.09	0.68
1:I:100:CYS:CB	1:I:103:CYS:HB3	2.20	0.68
3:C:358:LEU:HD12	3:C:359:ASN:H	1.59	0.67
3:C:64:VAL:HA	3:C:67:VAL:HG22	1.75	0.67
2:B:731:TYR:CE2	2:B:902:PRO:HG3	2.29	0.67
3:C:55:LYS:HE2	8:K:3:ARG:HH22	1.60	0.67
3:C:161:VAL:HG12	3:C:162:GLU:N	2.03	0.67
1:I:103:CYS:SG	1:I:105:ARG:CB	2.82	0.67
1:A:753:THR:HG23	1:A:754:GLY:N	2.05	0.67
4:D:6:ILE:HG13	4:D:14:ILE:HD11	1.77	0.67
1:I:775:ARG:HD3	2:J:453:PHE:HD2	1.60	0.67
2:J:42:ILE:CG2	2:J:72:ILE:HD11	2.22	0.67
2:J:56:VAL:HG12	2:J:367:VAL:HG13	1.77	0.67
1:I:94:ARG:HG3	1:I:138:HIS:CD2	2.30	0.67
2:J:211:LYS:HA	3:M:212:ARG:NH2	2.09	0.67
1:A:868:VAL:HG11	3:C:311:MET:HG2	1.77	0.67
1:I:445:TYR:HB2	1:I:449:ARG:HH22	1.60	0.67
1:A:150:CYS:C	1:A:152:ALA:N	2.52	0.67
2:B:365:GLN:OE1	2:B:406:ARG:NH1	2.28	0.67
5:E:81:ASN:O	5:E:82:GLN:CG	2.43	0.67
3:M:286:ILE:HD13	3:M:306:MET:HG2	1.77	0.67
5:Q:41:ASP:OD2	6:R:1:MET:SD	2.53	0.67
1:A:94:ARG:HG3	1:A:138:HIS:CD2	2.30	0.67
2:B:389:ASN:ND2	2:B:389:ASN:O	2.27	0.67
4:D:56:ASP:HB3	11:P:46:VAL:HG21	1.75	0.67
2:J:41:PHE:CE1	2:J:42:ILE:HD13	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:6:ILE:HG13	4:O:14:ILE:HD11	1.77	0.67
2:J:378:TYR:HE1	2:J:388:GLU:HG3	1.34	0.67
9:U:51:MET:CG	9:U:53:ARG:HB2	2.24	0.67
1:A:556:LYS:HD2	1:A:616:LEU:HD22	1.77	0.66
3:C:287:ASP:O	3:C:291:SER:OG	2.13	0.66
1:I:147:CYS:SG	1:I:152:ALA:N	2.68	0.66
9:U:44:THR:C	9:U:45:ILE:HG13	2.21	0.66
1:A:850:GLN:OE1	2:B:1037:ARG:NH1	2.29	0.66
2:B:433:MET:HG3	2:B:656:LEU:HD11	1.78	0.66
2:B:856:VAL:HG12	11:P:35:LEU:HB2	1.77	0.66
3:M:287:ASP:O	3:M:291:SER:OG	2.13	0.66
1:I:16:LEU:HG	2:J:1114:ARG:HB3	1.77	0.66
2:J:365:GLN:OE1	2:J:406:ARG:NH1	2.28	0.66
2:J:1109:LYS:HD3	2:J:1115:PRO:HD2	1.78	0.66
1:A:508:ILE:HG21	1:A:754:GLY:CA	2.25	0.66
2:J:433:MET:HG3	2:J:656:LEU:HD11	1.78	0.66
1:A:750:MET:HA	1:A:753:THR:HG22	1.76	0.66
1:I:775:ARG:HD3	2:J:453:PHE:CD2	2.31	0.66
2:J:1065:CYS:HB3	2:J:1068:CYS:HB3	1.75	0.66
2:B:56:VAL:HG12	2:B:367:VAL:HG13	1.77	0.66
1:I:894:ILE:HG13	3:M:29:ILE:HD12	1.78	0.66
2:J:43:ASP:OD1	2:J:43:ASP:N	2.28	0.66
2:J:546:ARG:NH1	2:J:555:ILE:O	2.29	0.66
2:J:800:ILE:HD11	2:J:812:LEU:HA	1.77	0.66
1:A:508:ILE:HG21	1:A:754:GLY:C	2.20	0.66
9:L:25:ALA:CB	9:L:43:TYR:CE2	2.78	0.66
2:J:174:LEU:HD21	2:J:180:LEU:HD11	1.77	0.66
1:A:505:GLN:HB2	2:B:917:HIS:CD2	2.30	0.65
2:J:556:ASN:OD1	2:J:576:ARG:NH1	2.29	0.65
3:M:321:ILE:HA	3:M:326:ILE:HG13	1.78	0.65
5:Q:17:MET:HE3	5:Q:25:ALA:HB1	1.78	0.65
1:A:63:CYS:HG	1:A:73:HIS:HE2	1.44	0.65
2:B:959:LYS:HA	4:D:201:ARG:HH21	1.61	0.65
2:J:389:ASN:CA	2:J:390:ILE:HG23	2.11	0.65
2:J:820:ARG:O	2:J:837:ARG:NH1	2.28	0.65
3:C:96:LEU:HB2	3:C:100:ARG:HB2	1.78	0.65
1:I:6:LYS:HE2	2:J:1122:ARG:NH1	2.04	0.65
1:I:304:LEU:HB3	2:J:1111:MET:HE2	1.78	0.65
3:M:96:LEU:HB2	3:M:100:ARG:HB2	1.78	0.65
4:O:162:SER:HA	4:O:188:GLU:HB3	1.78	0.65
3:C:162:GLU:CG	3:C:196:TYR:CD1	2.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:546:ARG:NH1	2:B:555:ILE:O	2.29	0.65
2:B:556:ASN:OD1	2:B:576:ARG:NH1	2.30	0.65
2:B:744:LYS:HZ1	9:L:53:ARG:NH2	1.93	0.65
3:C:203:LYS:HB2	3:C:203:LYS:HZ2	1.59	0.65
5:Q:100:ARG:CZ	6:R:43:VAL:HG13	2.26	0.65
2:B:174:LEU:HD21	2:B:180:LEU:HD11	1.78	0.65
2:B:759:THR:HB	2:B:869:THR:HG22	1.79	0.65
5:E:17:MET:HE3	5:E:25:ALA:HB1	1.78	0.65
1:A:309:LYS:HB3	3:C:341:ILE:HG23	1.77	0.65
3:C:386:LEU:HD11	5:E:20:MET:C	2.21	0.65
2:J:614:VAL:HG13	2:J:615:ILE:HG12	1.79	0.65
1:A:863:PRO:CB	3:C:360:GLY:HA2	2.27	0.65
2:B:800:ILE:HD11	2:B:812:LEU:HA	1.77	0.65
2:J:389:ASN:O	2:J:389:ASN:ND2	2.29	0.65
2:J:759:THR:HB	2:J:869:THR:HG22	1.79	0.65
2:J:793:HIS:HB3	2:J:800:ILE:HG23	1.79	0.65
4:D:162:SER:HA	4:D:188:GLU:HB3	1.78	0.65
2:J:198:ARG:HD3	2:J:304:PRO:HB2	1.78	0.65
1:A:248:ILE:HD11	1:A:282:TYR:HB2	1.79	0.65
2:B:45:GLY:O	2:B:47:GLN:N	2.30	0.65
3:C:194:GLU:OE1	3:C:196:TYR:CE2	2.48	0.65
1:I:40:TYR:H	1:I:41:PRO:CD	2.10	0.65
1:I:445:TYR:CD2	9:U:49:ILE:CG2	2.61	0.65
1:I:480:GLU:CD	2:J:1047:MET:HB2	2.22	0.64
1:I:556:LYS:HD2	1:I:616:LEU:HD22	1.77	0.64
5:Q:14:PRO:HB3	5:Q:16:ARG:HH11	1.63	0.64
4:D:200:PRO:HB2	4:D:203:PHE:HD1	1.61	0.64
1:I:147:CYS:H	1:I:152:ALA:HB2	1.62	0.64
2:J:46:LEU:HD12	2:J:46:LEU:C	2.21	0.64
2:B:614:VAL:HG13	2:B:615:ILE:HG12	1.79	0.64
1:A:712:LYS:HZ2	3:C:92:ILE:N	1.96	0.64
2:B:793:HIS:HB3	2:B:800:ILE:HG23	1.79	0.64
1:A:750:MET:CA	1:A:753:THR:HG22	2.26	0.64
3:C:113:THR:O	3:C:113:THR:OG1	2.15	0.64
3:C:157:MET:HE2	3:C:157:MET:HA	1.77	0.64
3:M:148:ARG:NH2	3:M:162:GLU:HG2	2.11	0.64
4:O:154:LYS:NZ	4:O:155:TYR:O	2.31	0.64
2:B:198:ARG:HD3	2:B:304:PRO:HB2	1.78	0.64
5:E:14:PRO:HB3	5:E:16:ARG:HH11	1.63	0.64
3:C:164:ASP:OD1	3:C:165:PRO:HD2	1.97	0.64
2:J:1122:ARG:CD	6:R:4:ARG:HH21	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:52:ALA:O	9:U:53:ARG:HB3	1.96	0.64
2:B:183:ARG:NH2	2:B:454:GLU:OE2	2.30	0.64
3:C:162:GLU:HA	3:C:196:TYR:HD1	1.59	0.64
9:L:93:ILE:O	9:L:94:GLU:HG3	1.97	0.64
1:I:248:ILE:HD11	1:I:282:TYR:HB2	1.79	0.64
2:J:25:TRP:CZ2	2:J:485:LEU:HB3	2.33	0.64
3:C:186:PHE:O	3:C:187:LYS:HG2	1.96	0.63
2:J:39:ASN:C	2:J:41:PHE:N	2.55	0.63
2:J:746:SER:HB3	2:J:751:LEU:HD12	1.80	0.63
2:J:969:SER:HB3	2:J:971:ARG:HG3	1.80	0.63
1:A:623:LYS:HB2	1:A:754:GLY:HA3	1.80	0.63
2:B:25:TRP:CZ2	2:B:485:LEU:HB3	2.33	0.63
3:C:157:MET:O	3:C:158:GLU:HB2	1.96	0.63
2:J:981:ARG:NH2	9:U:30:GLU:OE2	2.29	0.63
1:A:150:CYS:C	1:A:152:ALA:H	2.06	0.63
2:B:57:VAL:HG11	2:B:371:GLN:HG3	1.80	0.63
1:I:100:CYS:SG	1:I:103:CYS:CB	2.86	0.63
1:I:492:ILE:HA	1:I:499:PRO:HA	1.79	0.63
5:E:5:LEU:CD1	6:F:6:LYS:HD3	2.29	0.63
1:I:895:VAL:O	1:I:897:THR:N	2.31	0.63
3:M:229:VAL:HG21	3:M:245:THR:HG22	1.81	0.63
4:O:194:ILE:HA	4:O:221:VAL:HG21	1.79	0.63
3:C:321:ILE:HA	3:C:326:ILE:HG13	1.79	0.63
1:I:436:MET:HE1	1:I:501:ILE:HD11	1.80	0.63
3:M:358:LEU:HD12	3:M:359:ASN:H	1.62	0.63
2:B:532:VAL:HG12	2:B:533:GLU:H	1.64	0.63
3:C:160:VAL:CG2	3:C:198:LEU:CG	2.77	0.63
5:E:41:ASP:OD2	6:F:1:MET:SD	2.56	0.63
2:J:57:VAL:HG11	2:J:371:GLN:HG3	1.79	0.63
3:M:182:LEU:HD22	3:M:185:SER:HB2	1.80	0.63
4:O:62:ARG:NH2	10:V:2:ILE:O	2.32	0.63
4:O:200:PRO:HB2	4:O:203:PHE:HD1	1.63	0.63
4:D:145:LYS:NZ	11:P:48:ALA:O	2.31	0.63
4:D:194:ILE:HA	4:D:221:VAL:HG21	1.79	0.63
2:J:42:ILE:HG22	2:J:72:ILE:HD13	1.80	0.63
4:D:154:LYS:NZ	4:D:155:TYR:O	2.32	0.63
1:A:656:LEU:HD13	1:A:659:TRP:HE1	1.64	0.62
2:B:161:ILE:HG21	2:B:412:ALA:HB2	1.81	0.62
3:C:55:LYS:HG2	8:K:3:ARG:HH21	1.65	0.62
2:J:1063:TRP:HE3	2:J:1092:ILE:HG22	1.64	0.62
1:A:897:THR:HG21	3:C:45:ILE:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:979:THR:HA	9:L:26:ASN:HD21	1.64	0.62
1:I:47:MET:O	1:I:49:LYS:N	2.32	0.62
7:S:17:GLU:HB2	7:S:64:LYS:HB2	1.81	0.62
2:B:969:SER:HB3	2:B:971:ARG:HG3	1.81	0.62
3:C:180:ARG:O	3:C:182:LEU:N	2.32	0.62
3:C:229:VAL:HG21	3:C:245:THR:HG22	1.81	0.62
2:J:11:THR:O	2:J:593:ARG:NH2	2.31	0.62
2:J:38:TYR:C	2:J:41:PHE:HB3	2.23	0.62
2:J:65:VAL:HG13	2:J:395:ARG:NH2	2.14	0.62
2:J:398:ILE:O	2:J:398:ILE:CG2	2.46	0.62
2:B:1109:LYS:HD3	2:B:1115:PRO:HD2	1.81	0.62
3:C:93:ASN:O	3:C:95:THR:N	2.33	0.62
1:A:806:ASN:N	1:A:806:ASN:OD1	2.32	0.62
2:B:522:VAL:HG22	2:B:568:VAL:HB	1.82	0.62
1:I:449:ARG:NH2	9:U:49:ILE:HD11	2.13	0.62
3:M:113:THR:O	3:M:113:THR:OG1	2.15	0.62
1:A:436:MET:HE1	1:A:501:ILE:HD11	1.80	0.62
9:U:51:MET:HG2	9:U:53:ARG:HB3	1.77	0.62
9:U:51:MET:HA	9:U:52:ALA:HB3	1.81	0.62
3:C:211:LEU:HA	3:C:214:ILE:HD11	1.80	0.62
2:J:532:VAL:HG12	2:J:533:GLU:H	1.64	0.62
5:Q:125:ARG:HE	5:Q:125:ARG:H	1.48	0.62
3:C:187:LYS:NZ	3:C:206:THR:HB	2.15	0.62
3:M:191:PHE:HB2	3:M:198:LEU:HB2	1.82	0.62
1:A:492:ILE:HA	1:A:499:PRO:HA	1.80	0.62
2:J:37:SER:O	2:J:41:PHE:HB2	1.99	0.62
2:B:11:THR:O	2:B:593:ARG:NH2	2.32	0.62
2:B:190:VAL:HG21	2:B:331:SER:HB3	1.82	0.62
2:B:746:SER:HB3	2:B:751:LEU:HD12	1.81	0.61
3:C:163:ILE:N	3:C:196:TYR:HB3	2.15	0.61
7:H:50:VAL:HG13	7:H:55:ALA:HB3	1.81	0.61
1:I:665:GLY:CA	2:J:729:LEU:CD1	2.65	0.61
2:J:161:ILE:HG21	2:J:412:ALA:HB2	1.81	0.61
2:J:207:VAL:HG12	2:J:217:VAL:HG22	1.81	0.61
2:J:330:LEU:HD21	2:J:337:GLU:HG2	1.82	0.61
3:M:339:PHE:O	3:M:341:ILE:N	2.33	0.61
1:A:463:ASP:HA	2:B:890:GLY:HA2	1.81	0.61
2:B:330:LEU:HD21	2:B:337:GLU:HG2	1.82	0.61
2:B:931:ALA:HB1	2:B:990:GLY:HA3	1.81	0.61
3:C:331:ALA:H	3:C:336:ARG:HH12	1.46	0.61
6:F:116:ASP:HA	6:F:119:ARG:HE	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:93:ARG:HG3	2:J:160:ILE:HD13	1.82	0.61
5:Q:5:LEU:CD1	6:R:6:LYS:HD3	2.30	0.61
5:Q:99:ILE:HD13	5:Q:142:VAL:HG21	1.82	0.61
6:R:116:ASP:HA	6:R:119:ARG:HE	1.65	0.61
7:S:50:VAL:HG13	7:S:55:ALA:HB3	1.81	0.61
1:A:47:MET:O	1:A:49:LYS:N	2.33	0.61
2:B:979:THR:HA	9:L:26:ASN:ND2	2.16	0.61
7:H:17:GLU:HB2	7:H:64:LYS:HB2	1.81	0.61
2:J:183:ARG:HG2	2:J:184:ASP:N	2.15	0.61
3:M:182:LEU:O	3:M:185:SER:CB	2.48	0.61
2:B:276:TYR:O	2:B:279:ARG:HB3	2.01	0.61
3:C:143:LEU:HB2	3:C:222:ARG:HG3	1.81	0.61
2:J:165:GLU:OE1	2:J:429:ARG:NH1	2.33	0.61
2:J:818:PRO:HA	2:J:836:ARG:HB3	1.83	0.61
3:M:279:GLU:OE1	7:S:65:ARG:NH1	2.34	0.61
5:E:39:ASP:HA	5:E:154:ARG:HH11	1.66	0.61
5:E:125:ARG:HE	5:E:125:ARG:H	1.48	0.61
1:I:656:LEU:HD13	1:I:659:TRP:HE1	1.64	0.61
2:J:116:GLN:OE1	2:J:393:PHE:CD1	2.53	0.61
2:J:190:VAL:HG21	2:J:331:SER:HB3	1.82	0.61
2:J:931:ALA:HB1	2:J:990:GLY:HA3	1.81	0.61
3:M:214:ILE:C	3:M:216:GLU:H	2.08	0.61
7:S:55:ALA:HB1	7:S:79:VAL:HG21	1.82	0.61
10:V:57:ASP:HA	10:V:60:MET:HE3	1.83	0.61
2:J:971:ARG:HB2	2:J:986:ASP:HB3	1.82	0.61
1:I:103:CYS:HB2	1:I:150:CYS:HG	1.64	0.61
2:J:522:VAL:HG22	2:J:568:VAL:HB	1.81	0.61
1:A:150:CYS:O	1:A:151:GLY:C	2.44	0.61
2:B:411:LEU:HD12	2:B:416:TRP:HH2	1.66	0.60
5:E:49:LEU:N	5:E:73:ASN:O	2.33	0.60
2:J:803:GLU:O	11:W:44:ARG:NE	2.34	0.60
2:B:971:ARG:HB2	2:B:986:ASP:HB3	1.82	0.60
3:C:153:ASP:HB2	3:C:158:GLU:C	2.26	0.60
4:D:50:ASN:HD22	4:D:52:SER:H	1.48	0.60
2:J:233:ARG:NH2	2:J:240:ASP:OD1	2.35	0.60
2:J:986:ASP:C	2:J:987:ILE:HD13	2.26	0.60
5:Q:39:ASP:HA	5:Q:154:ARG:HH11	1.66	0.60
3:C:279:GLU:OE1	7:H:65:ARG:NH1	2.34	0.60
3:M:378:VAL:HG21	8:T:8:GLU:HG2	1.83	0.60
4:O:50:ASN:HD22	4:O:52:SER:H	1.49	0.60
2:B:233:ARG:NH2	2:B:240:ASP:OD1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:470:GLU:OE2	2:B:482:ASN:ND2	2.35	0.60
3:C:160:VAL:HG21	3:C:198:LEU:CG	2.32	0.60
3:C:160:VAL:HG23	3:C:198:LEU:HB3	1.82	0.60
2:J:411:LEU:HD12	2:J:416:TRP:HH2	1.66	0.60
1:A:6:LYS:HG2	2:B:1094:LYS:O	2.02	0.60
1:A:630:ASP:N	1:A:630:ASP:OD1	2.34	0.60
2:B:207:VAL:HG12	2:B:217:VAL:HG22	1.82	0.60
2:B:758:ARG:HH11	2:B:844:ARG:HG3	1.66	0.60
2:B:818:PRO:HA	2:B:836:ARG:HB3	1.82	0.60
3:C:217:LYS:HA	3:C:221:HIS:HB2	1.83	0.60
7:H:55:ALA:HB1	7:H:79:VAL:HG21	1.82	0.60
1:I:806:ASN:N	1:I:806:ASN:OD1	2.32	0.60
4:O:62:ARG:HH12	10:V:2:ILE:HB	1.66	0.60
1:A:444:PRO:HD2	9:L:50:THR:HG23	1.82	0.60
2:B:165:GLU:OE1	2:B:429:ARG:NH1	2.34	0.60
1:I:11:ILE:HD12	3:M:358:LEU:CD2	2.32	0.60
1:A:62:THR:HG21	2:B:1078:ARG:HH11	1.66	0.60
1:A:666:PHE:H	2:B:729:LEU:HD13	1.66	0.60
5:E:5:LEU:HD11	6:F:6:LYS:HD3	1.83	0.60
7:H:43:ILE:N	7:H:78:LEU:O	2.29	0.60
2:J:276:TYR:O	2:J:279:ARG:HB3	2.01	0.60
2:J:378:TYR:CZ	2:J:388:GLU:OE2	2.55	0.60
5:Q:80:ARG:HG3	5:Q:83:GLU:HB2	1.84	0.60
1:A:95:VAL:HG22	1:A:201:LEU:HD23	1.84	0.60
2:B:1065:CYS:HB3	2:B:1068:CYS:HB2	1.83	0.60
2:J:391:GLN:O	2:J:392:ARG:HB2	2.02	0.60
1:A:444:PRO:HD2	9:L:50:THR:CG2	2.32	0.60
4:D:60:ALA:HB1	11:P:48:ALA:HB2	1.82	0.60
9:U:59:VAL:HG21	9:U:71:LEU:HD21	1.83	0.60
2:B:146:ILE:CG2	10:N:61:VAL:CG2	2.80	0.60
3:M:134:VAL:O	3:M:138:ILE:HG13	2.02	0.60
3:M:189:ALA:HB3	3:M:199:VAL:HA	1.83	0.60
10:V:7:CYS:SG	10:V:8:PHE:N	2.75	0.60
11:W:30:CYS:SG	11:W:32:SER:CB	2.90	0.60
1:A:535:MET:HE1	1:A:652:GLN:HE22	1.66	0.59
3:C:134:VAL:O	3:C:138:ILE:HG13	2.02	0.59
9:L:59:VAL:HG21	9:L:71:LEU:HD21	1.82	0.59
1:I:756:ARG:HG3	2:J:917:HIS:HB3	1.83	0.59
2:J:41:PHE:O	2:J:45:GLY:C	2.44	0.59
2:J:758:ARG:HH11	2:J:844:ARG:HG3	1.66	0.59
1:A:63:CYS:O	2:B:1076:LYS:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:PHE:H	2:B:729:LEU:CD1	2.15	0.59
2:B:394:VAL:CG2	2:B:395:ARG:HG3	2.30	0.59
5:E:100:ARG:CZ	6:F:43:VAL:HG13	2.31	0.59
10:N:61:VAL:HG13	10:N:61:VAL:O	2.02	0.59
1:I:449:ARG:NE	9:U:49:ILE:HD11	2.17	0.59
2:J:205:ILE:HD11	2:J:303:LEU:H	1.67	0.59
2:J:1091:ARG:H	2:J:1091:ARG:HD3	1.67	0.59
3:M:151:THR:C	3:M:152:ILE:HG12	2.27	0.59
5:Q:2:TYR:OH	6:R:44:SER:OG	2.17	0.59
1:A:758:LYS:HG2	1:A:760:LEU:CD2	2.33	0.59
2:B:93:ARG:HG3	2:B:160:ILE:HD13	1.83	0.59
2:B:789:LYS:HB3	2:B:792:ARG:HB2	1.84	0.59
3:C:161:VAL:O	3:C:162:GLU:HG3	2.01	0.59
1:I:535:MET:HE1	1:I:652:GLN:HE22	1.66	0.59
1:I:666:PHE:O	2:J:729:LEU:HG	2.03	0.59
2:J:1122:ARG:CG	2:J:1122:ARG:HH11	2.15	0.59
5:Q:5:LEU:HD11	6:R:6:LYS:HD3	1.83	0.59
2:B:20:VAL:O	2:B:23:SER:OG	2.18	0.59
5:E:99:ILE:HD13	5:E:142:VAL:HG21	1.83	0.59
10:N:57:ASP:HA	10:N:60:MET:CE	2.23	0.59
1:I:690:ALA:HA	1:I:693:LYS:HD2	1.83	0.59
2:J:789:LYS:HB3	2:J:792:ARG:HB2	1.83	0.59
1:A:583:GLU:CG	1:A:584:ALA:H	2.15	0.59
2:B:49:VAL:HG11	2:B:360:ARG:HA	1.84	0.59
2:B:702:VAL:HG23	10:N:53:VAL:HG12	1.84	0.59
2:B:986:ASP:C	2:B:987:ILE:HD13	2.28	0.59
3:M:313:THR:HG22	3:M:318:ILE:HG22	1.85	0.59
4:O:145:LYS:NZ	11:W:48:ALA:O	2.35	0.59
3:C:216:GLU:O	3:C:220:LYS:N	2.35	0.59
5:E:80:ARG:HG3	5:E:83:GLU:HB2	1.84	0.59
2:J:183:ARG:HG3	2:J:337:GLU:CD	2.26	0.59
2:J:599:ILE:HD11	2:J:609:LEU:HD11	1.84	0.59
3:C:181:LYS:C	3:C:183:THR:H	2.09	0.59
3:C:216:GLU:O	3:C:220:LYS:CA	2.51	0.59
4:D:151:VAL:HG22	4:D:224:VAL:HG22	1.84	0.59
5:E:46:LEU:HD22	6:F:21:LEU:HD21	1.84	0.59
1:A:444:PRO:CD	9:L:50:THR:CG2	2.80	0.59
2:B:599:ILE:HD11	2:B:609:LEU:HD11	1.84	0.59
3:C:148:ARG:H	3:C:148:ARG:HD3	1.68	0.59
9:U:43:TYR:HB2	9:U:56:ARG:O	2.03	0.59
2:B:389:ASN:ND2	2:B:392:ARG:CG	2.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:2:ILE:HD11	10:N:56:ILE:HD12	1.85	0.59
1:I:497:GLY:O	1:I:884:GLN:NE2	2.35	0.59
1:I:583:GLU:CG	1:I:584:ALA:H	2.16	0.59
2:J:20:VAL:O	2:J:23:SER:OG	2.18	0.59
3:C:160:VAL:HG21	3:C:198:LEU:HG	1.83	0.59
3:C:189:ALA:HB3	3:C:199:VAL:HA	1.84	0.59
1:I:444:PRO:HG3	9:U:50:THR:HG23	0.59	0.59
3:M:148:ARG:HH22	3:M:162:GLU:CB	1.82	0.59
1:A:690:ALA:HA	1:A:693:LYS:HD2	1.84	0.58
2:B:79:GLU:HG2	2:B:95:ARG:HH22	1.68	0.58
2:B:205:ILE:HD11	2:B:303:LEU:H	1.67	0.58
3:C:229:VAL:HG22	3:C:230:GLY:H	1.68	0.58
3:C:298:LEU:HD13	3:C:298:LEU:H	1.68	0.58
3:C:313:THR:HG22	3:C:318:ILE:HG22	1.85	0.58
10:N:7:CYS:SG	10:N:8:PHE:N	2.76	0.58
1:I:147:CYS:H	1:I:152:ALA:CB	2.16	0.58
2:J:395:ARG:CD	2:J:398:ILE:HD11	2.32	0.58
2:J:470:GLU:OE2	2:J:482:ASN:ND2	2.35	0.58
3:M:119:TYR:HD2	3:M:263:ARG:HD2	1.68	0.58
3:M:128:ARG:HG3	3:M:241:TYR:CE2	2.38	0.58
3:M:331:ALA:H	3:M:336:ARG:HH12	1.51	0.58
1:A:444:PRO:HD3	9:L:50:THR:HG22	1.83	0.58
2:B:1122:ARG:HG3	5:E:60:VAL:HG21	1.84	0.58
4:D:160:HIS:ND1	4:D:188:GLU:OE1	2.27	0.58
1:I:779:LEU:HD13	1:I:822:MET:HE3	1.85	0.58
2:J:391:GLN:C	2:J:392:ARG:HG3	2.26	0.58
4:O:16:PHE:CE1	4:O:222:PHE:HB2	2.38	0.58
3:C:194:GLU:C	3:C:196:TYR:H	2.11	0.58
1:I:95:VAL:HG22	1:I:201:LEU:HD23	1.83	0.58
1:I:783:TYR:CE1	2:J:461:THR:HG22	2.38	0.58
2:J:801:PHE:HB2	11:W:40:PRO:HD3	1.84	0.58
3:C:191:PHE:HD2	3:C:198:LEU:HD13	1.68	0.58
1:I:100:CYS:CB	1:I:103:CYS:CB	2.80	0.58
1:I:163:THR:HB	1:I:276:GLN:HE21	1.69	0.58
1:I:870:PHE:CE2	7:S:76:TYR:HD2	2.21	0.58
3:M:143:LEU:HB2	3:M:222:ARG:HG3	1.84	0.58
3:M:151:THR:HG22	3:M:152:ILE:N	2.06	0.58
3:M:153:ASP:CG	3:M:157:MET:HB2	2.28	0.58
3:M:175:MET:HE3	3:M:193:ALA:O	2.04	0.58
3:M:358:LEU:CD1	14:M:401:HOH:O	2.51	0.58
1:A:875:ASP:HB3	7:H:70:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:338:ILE:HG21	1:I:443:MET:HE1	1.85	0.58
2:J:45:GLY:O	2:J:46:LEU:CB	2.50	0.58
2:J:508:VAL:O	2:J:513:ARG:NH1	2.36	0.58
3:M:148:ARG:H	3:M:148:ARG:HD3	1.68	0.58
1:A:105:ARG:HH21	1:A:148:PRO:HB2	1.69	0.58
2:B:766:ARG:HG2	2:B:772:LYS:HG2	1.86	0.58
3:C:343:THR:OG1	3:C:344:GLN:N	2.35	0.58
3:M:55:LYS:HE2	8:T:3:ARG:HH22	1.67	0.58
1:A:497:GLY:O	1:A:884:GLN:NE2	2.36	0.58
2:B:151:ASP:HB3	2:B:684:ALA:HB3	1.85	0.58
1:I:103:CYS:CB	1:I:150:CYS:SG	2.91	0.58
1:I:449:ARG:NH2	9:U:49:ILE:CD1	2.66	0.58
2:J:513:ARG:HG2	2:J:514:ARG:N	2.17	0.58
3:M:154:ILE:HD12	3:M:154:ILE:H	1.69	0.58
3:M:229:VAL:HG22	3:M:230:GLY:H	1.69	0.58
1:A:163:THR:HB	1:A:276:GLN:HE21	1.68	0.58
1:A:338:ILE:HG21	1:A:443:MET:HE1	1.85	0.58
2:B:789:LYS:HD2	1:I:37:ASP:OD1	2.03	0.58
10:N:19:TYR:HD1	10:N:20:GLU:H	1.52	0.58
3:M:312:MET:HA	3:M:326:ILE:HD11	1.86	0.58
2:J:79:GLU:HG2	2:J:95:ARG:HH22	1.68	0.58
3:M:358:LEU:HD11	14:M:401:HOH:O	2.04	0.58
2:B:378:TYR:HE1	2:B:389:ASN:N	2.00	0.58
4:D:65:MET:HE3	10:N:6:ARG:HD2	1.86	0.58
9:L:46:GLU:OE2	9:L:56:ARG:CD	2.51	0.58
3:C:157:MET:HA	3:C:157:MET:CE	2.33	0.57
3:M:147:ALA:O	3:M:167:ARG:NH2	2.37	0.57
4:O:151:VAL:HG22	4:O:224:VAL:HG22	1.84	0.57
10:V:19:TYR:HD1	10:V:20:GLU:H	1.52	0.57
1:A:13:PHE:CE1	2:B:1115:PRO:HB3	2.39	0.57
3:C:128:ARG:HG3	3:C:241:TYR:CE2	2.39	0.57
3:C:161:VAL:HB	3:C:198:LEU:CA	2.33	0.57
4:D:47:PHE:N	11:P:44:ARG:O	2.34	0.57
1:I:665:GLY:C	2:J:729:LEU:CD1	2.75	0.57
10:V:2:ILE:HD11	10:V:56:ILE:HD12	1.85	0.57
2:B:803:GLU:OE2	2:B:871:ARG:NH2	2.36	0.57
3:C:177:LYS:HA	3:C:180:ARG:HB2	1.85	0.57
9:L:52:ALA:C	9:L:54:LYS:H	2.13	0.57
1:I:74:PHE:CE1	1:I:222:PRO:HD3	2.38	0.57
1:I:284:ASN:HB3	1:I:287:THR:HG23	1.86	0.57
2:J:968:HIS:CD2	2:J:968:HIS:C	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:182:LEU:HD23	3:M:185:SER:HB2	1.75	0.57
5:Q:48:ILE:HD13	5:Q:74:VAL:HG13	1.86	0.57
2:B:237:LEU:HD22	2:B:242:GLU:HB3	1.85	0.57
2:B:749:ARG:HE	4:D:144:ALA:HB1	1.68	0.57
3:C:147:ALA:O	3:C:167:ARG:NH2	2.37	0.57
3:C:216:GLU:HA	3:C:220:LYS:CB	2.33	0.57
4:D:226:THR:OG1	4:D:227:ASN:N	2.29	0.57
2:J:237:LEU:HD22	2:J:242:GLU:HB3	1.85	0.57
3:M:298:LEU:HD13	3:M:298:LEU:H	1.68	0.57
5:Q:49:LEU:N	5:Q:73:ASN:O	2.36	0.57
1:I:159:PHE:HB3	1:I:166:TRP:HE3	1.69	0.57
3:M:262:THR:HG22	7:S:12:HIS:CG	2.38	0.57
2:B:731:TYR:HE2	2:B:902:PRO:HG3	1.69	0.57
8:K:12:ILE:HD11	8:K:53:VAL:HG23	1.87	0.57
1:I:146:VAL:HA	1:I:152:ALA:HB3	1.86	0.57
1:I:156:PRO:HB3	1:I:169:ARG:HA	1.87	0.57
1:I:858:GLY:O	1:I:871:LYS:HA	2.05	0.57
2:J:151:ASP:HB3	2:J:684:ALA:HB3	1.86	0.57
3:M:217:LYS:HD2	3:M:217:LYS:N	2.19	0.57
2:B:378:TYR:OH	2:B:388:GLU:CA	2.48	0.57
3:C:161:VAL:HB	3:C:198:LEU:HA	1.87	0.57
1:I:105:ARG:HH21	1:I:148:PRO:HB2	1.69	0.57
1:I:326:PHE:N	2:J:1052:ARG:HH12	2.03	0.57
1:I:527:GLU:OE2	9:U:41:ALA:N	2.37	0.57
2:J:395:ARG:CB	2:J:398:ILE:CD1	2.83	0.57
2:J:803:GLU:OE2	2:J:871:ARG:NH2	2.36	0.57
2:J:816:THR:HB	2:J:836:ARG:HH21	1.70	0.57
8:T:12:ILE:HD11	8:T:53:VAL:HG23	1.87	0.57
10:N:56:ILE:O	10:N:60:MET:HG3	2.05	0.57
1:A:284:ASN:HB3	1:A:287:THR:HG23	1.86	0.57
1:A:640:GLU:HG2	1:A:896:ARG:HH12	1.68	0.57
1:A:709:LEU:HB2	1:A:717:THR:HG22	1.87	0.57
2:B:816:THR:HB	2:B:836:ARG:HH21	1.70	0.57
3:C:114:PRO:HG2	3:C:247:GLY:HA2	1.86	0.57
4:D:50:ASN:H	11:P:39:ARG:HD3	1.70	0.57
1:A:750:MET:HA	1:A:753:THR:HG21	1.87	0.56
1:A:885:GLY:HA2	3:C:303:ARG:HH12	1.70	0.56
1:I:445:TYR:CZ	9:U:49:ILE:HG22	2.40	0.56
1:I:635:ASP:O	1:I:639:ARG:HG3	2.05	0.56
1:I:709:LEU:HB2	1:I:717:THR:HG22	1.87	0.56
2:J:211:LYS:HA	3:M:212:ARG:HH21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:GLY:O	1:A:871:LYS:HA	2.05	0.56
3:C:153:ASP:OD1	3:C:159:TYR:HA	2.05	0.56
1:I:105:ARG:NH2	1:I:148:PRO:HB2	2.20	0.56
1:I:356:PRO:HG3	1:I:473:GLN:HB3	1.87	0.56
1:I:624:LYS:O	1:I:632:LYS:HB3	2.05	0.56
2:J:688:ILE:HD11	10:V:62:TYR:CD1	2.40	0.56
2:J:747:ILE:HG23	2:J:876:PRO:HG2	1.88	0.56
4:O:119:PRO:HD2	10:V:15:ALA:HB1	1.86	0.56
4:O:226:THR:OG1	4:O:227:ASN:N	2.29	0.56
2:B:864:LYS:HG3	11:P:25:VAL:HG11	1.88	0.56
2:B:968:HIS:CD2	2:B:968:HIS:C	2.82	0.56
3:C:92:ILE:HG13	3:C:93:ASN:H	1.70	0.56
4:D:28:ALA:HB1	4:D:243:LEU:HD21	1.87	0.56
2:J:58:PRO:HG2	2:J:60:ILE:O	2.05	0.56
2:J:645:MET:HE3	2:J:647:ALA:HB3	1.87	0.56
2:J:766:ARG:HG2	2:J:772:LYS:HG2	1.87	0.56
2:J:1088:GLU:OE2	5:Q:40:ARG:HB2	2.05	0.56
10:V:22:LYS:NZ	10:V:54:GLU:HG2	2.21	0.56
1:A:74:PHE:CE1	1:A:222:PRO:HD3	2.40	0.56
1:A:769:LEU:HB2	1:A:804:VAL:HG21	1.87	0.56
2:B:58:PRO:HG2	2:B:60:ILE:O	2.05	0.56
2:B:899:GLU:OE1	2:B:899:GLU:N	2.32	0.56
3:C:119:TYR:CD2	3:C:263:ARG:HB3	2.41	0.56
3:C:119:TYR:HD2	3:C:263:ARG:HB3	1.70	0.56
3:C:162:GLU:O	3:C:196:TYR:HA	2.05	0.56
3:C:312:MET:HA	3:C:326:ILE:HD11	1.86	0.56
2:J:116:GLN:CD	2:J:393:PHE:CD1	2.69	0.56
2:J:708:ARG:H	2:J:947:THR:HG1	1.53	0.56
2:J:1063:TRP:NE1	2:J:1074:GLU:OE1	2.39	0.56
2:J:1122:ARG:HD2	6:R:4:ARG:NH2	2.21	0.56
1:A:150:CYS:SG	1:A:153:PRO:HD3	2.45	0.56
2:B:65:VAL:HG11	2:B:395:ARG:HH12	1.71	0.56
2:B:645:MET:HE3	2:B:647:ALA:HB3	1.87	0.56
3:C:160:VAL:HG21	3:C:198:LEU:HD23	1.86	0.56
4:O:28:ALA:HB1	4:O:243:LEU:HD21	1.87	0.56
2:B:854:VAL:HG13	2:B:868:VAL:HG22	1.87	0.56
1:A:779:LEU:HD13	1:A:822:MET:HE3	1.86	0.56
3:C:216:GLU:C	3:C:220:LYS:HB3	2.31	0.56
1:A:584:ALA:O	1:A:605:TYR:OH	2.23	0.56
2:B:76:GLU:HG2	2:B:86:PRO:HA	1.88	0.56
2:B:747:ILE:HG23	2:B:876:PRO:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:81:ASN:C	5:E:82:GLN:HG2	2.31	0.56
1:I:112:GLU:O	1:I:116:TYR:HB2	2.06	0.56
1:I:309:LYS:HE3	3:M:347:PHE:HB2	1.88	0.56
1:I:513:LEU:HD13	1:I:664:LYS:HZ2	1.71	0.56
1:I:632:LYS:HD3	1:I:633:LEU:H	1.71	0.56
2:J:1042:GLY:O	3:M:70:GLN:NE2	2.35	0.56
3:M:55:LYS:HG2	8:T:3:ARG:HH21	1.70	0.56
1:A:112:GLU:O	1:A:116:TYR:HB2	2.05	0.56
1:A:387:PRO:HD3	1:A:410:TRP:CD1	2.41	0.56
2:B:959:LYS:HA	4:D:201:ARG:NH2	2.21	0.56
3:M:111:PRO:HG3	3:M:268:ASN:HA	1.88	0.56
1:A:159:PHE:HB3	1:A:166:TRP:HE3	1.69	0.56
2:B:206:THR:OG1	2:B:218:THR:OG1	2.19	0.56
2:B:683:TRP:HD1	2:B:683:TRP:O	1.89	0.56
10:N:22:LYS:NZ	10:N:54:GLU:HG2	2.21	0.56
2:J:521:ARG:H	2:J:531:THR:HG22	1.71	0.56
2:B:815:ARG:HD2	2:B:839:THR:HB	1.88	0.55
5:E:48:ILE:HD13	5:E:74:VAL:HG13	1.88	0.55
1:I:10:SER:HA	3:M:358:LEU:HD21	1.87	0.55
2:J:719:PRO:HG3	10:V:53:VAL:HG11	1.88	0.55
3:M:114:PRO:HG2	3:M:247:GLY:HA2	1.87	0.55
1:A:452:LEU:HD13	2:B:736:MET:SD	2.46	0.55
1:A:640:GLU:HG2	1:A:896:ARG:NH1	2.22	0.55
2:B:606:TRP:CZ2	2:B:615:ILE:HG21	2.41	0.55
3:C:181:LYS:HE3	3:C:188:SER:HB3	1.87	0.55
1:I:625:ALA:O	1:I:632:LYS:NZ	2.21	0.55
2:J:39:ASN:O	2:J:41:PHE:N	2.39	0.55
2:J:394:VAL:HG11	2:J:395:ARG:HE	1.72	0.55
2:B:227:LYS:HB2	2:B:230:TYR:CD2	2.42	0.55
2:B:967:LYS:HG3	2:B:969:SER:H	1.71	0.55
4:D:16:PHE:CE1	4:D:222:PHE:HB2	2.41	0.55
2:J:854:VAL:HG13	2:J:868:VAL:HG22	1.87	0.55
5:Q:46:LEU:HD22	6:R:21:LEU:HD21	1.87	0.55
3:C:27:LYS:O	3:C:31:TYR:HB2	2.06	0.55
2:B:59:ASP:H	2:B:375:THR:HG22	1.72	0.55
2:B:449:ASP:OD1	2:B:449:ASP:N	2.39	0.55
3:C:119:TYR:HD2	3:C:263:ARG:HD2	1.70	0.55
1:I:769:LEU:HB2	1:I:804:VAL:HG21	1.87	0.55
1:I:844:ARG:NH2	3:M:106:ASP:OD2	2.39	0.55
2:J:227:LYS:HB2	2:J:230:TYR:CD2	2.42	0.55
2:J:967:LYS:HG3	2:J:969:SER:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:160:HIS:ND1	4:O:188:GLU:OE1	2.27	0.55
1:A:105:ARG:NH2	1:A:148:PRO:HB2	2.22	0.55
1:I:584:ALA:O	1:I:605:TYR:OH	2.24	0.55
2:J:968:HIS:ND1	4:O:201:ARG:HG2	2.21	0.55
2:J:1042:GLY:C	3:M:70:GLN:HE22	2.13	0.55
2:J:1063:TRP:CE2	2:J:1094:LYS:HG3	2.41	0.55
4:O:65:MET:HE3	10:V:6:ARG:HD2	1.89	0.55
1:I:387:PRO:HD3	1:I:410:TRP:CD1	2.42	0.55
2:J:286:PRO:O	2:J:288:GLU:N	2.40	0.55
2:J:606:TRP:CZ2	2:J:615:ILE:HG21	2.42	0.55
2:J:1066:GLU:HG2	2:J:1119:LEU:HD13	1.89	0.55
1:A:106:ILE:HG23	1:A:108:LEU:HB2	1.89	0.55
2:B:466:ILE:HG21	2:B:481:LYS:HD2	1.88	0.55
3:C:160:VAL:HG21	3:C:198:LEU:CD2	2.37	0.55
1:I:450:LEU:HD11	1:I:454:VAL:HB	1.89	0.55
1:I:640:GLU:HG2	1:I:896:ARG:HH12	1.72	0.55
2:J:449:ASP:OD1	2:J:449:ASP:N	2.39	0.55
2:J:513:ARG:HG2	2:J:514:ARG:H	1.70	0.55
2:J:815:ARG:HD2	2:J:839:THR:HB	1.89	0.55
1:A:450:LEU:HD11	1:A:454:VAL:HB	1.89	0.55
1:A:635:ASP:O	1:A:639:ARG:HG3	2.05	0.55
2:B:878:LEU:HD23	2:B:892:ILE:HG22	1.89	0.55
1:I:856:TYR:CE1	8:T:55:ARG:HD3	2.41	0.55
2:B:95:ARG:CZ	11:P:33:LYS:HD3	2.36	0.55
2:B:708:ARG:H	2:B:947:THR:HG1	1.54	0.55
2:J:76:GLU:HG2	2:J:86:PRO:HA	1.89	0.55
2:J:211:LYS:HG3	3:M:212:ARG:CZ	2.37	0.55
2:J:899:GLU:HG2	4:O:35:SER:HB3	1.89	0.55
3:M:75:PRO:HB3	3:M:298:LEU:HG	1.88	0.55
3:C:151:THR:CG2	3:C:152:ILE:H	2.18	0.54
1:I:783:TYR:HE1	2:J:461:THR:HG22	1.71	0.54
2:J:466:ILE:HG21	2:J:481:LYS:HD2	1.88	0.54
2:B:1063:TRP:NE1	2:B:1094:LYS:CG	2.69	0.54
1:I:585:LEU:O	1:I:586:GLU:CB	2.54	0.54
2:J:683:TRP:HD1	2:J:683:TRP:O	1.89	0.54
5:Q:8:LYS:HG3	6:R:7:LEU:HD22	1.89	0.54
7:S:43:ILE:N	7:S:78:LEU:O	2.28	0.54
2:B:183:ARG:NH1	2:B:337:GLU:OE1	2.40	0.54
2:J:59:ASP:H	2:J:375:THR:HG22	1.72	0.54
2:J:559:LEU:HD22	2:J:568:VAL:HG22	1.90	0.54
1:A:513:LEU:HD13	1:A:664:LYS:HZ2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:380:LEU:HB2	5:E:59:ILE:HB	1.88	0.54
2:J:183:ARG:HB3	2:J:186:ARG:NH2	2.13	0.54
9:U:9:GLU:HB2	9:U:12:LEU:HD22	1.90	0.54
3:C:158:GLU:C	3:C:159:TYR:CD1	2.86	0.54
7:H:67:SER:N	7:H:71:GLY:O	2.28	0.54
1:I:426:ARG:HB2	1:I:467:MET:HE3	1.90	0.54
2:J:42:ILE:HG22	2:J:72:ILE:CD1	2.36	0.54
2:J:1063:TRP:NE1	2:J:1094:LYS:HE3	2.23	0.54
9:U:45:ILE:HG12	9:U:55:PRO:HA	1.88	0.54
1:A:13:PHE:CE2	3:C:333:VAL:HG21	2.43	0.54
3:C:161:VAL:CG2	3:C:199:VAL:HB	2.36	0.54
1:I:106:ILE:HG23	1:I:108:LEU:HB2	1.89	0.54
1:I:578:GLU:HB3	1:I:579:PRO:HD2	1.88	0.54
2:J:962:GLU:O	2:J:965:GLY:N	2.37	0.54
3:M:27:LYS:O	3:M:31:TYR:HB2	2.06	0.54
1:A:10:SER:HA	3:C:358:LEU:CD2	2.28	0.54
3:C:75:PRO:HB3	3:C:298:LEU:HG	1.88	0.54
4:D:50:ASN:N	11:P:39:ARG:HH11	2.05	0.54
1:I:630:ASP:CG	1:I:631:GLY:H	2.16	0.54
2:J:959:LYS:HA	4:O:201:ARG:HH21	1.73	0.54
1:A:531:MET:C	9:L:44:THR:HG21	2.33	0.54
2:B:521:ARG:H	2:B:531:THR:HG22	1.72	0.54
2:B:939:LEU:HD11	2:B:966:PHE:CD2	2.39	0.54
2:B:1063:TRP:HE1	2:B:1094:LYS:CE	2.19	0.54
1:I:61:GLU:O	1:I:63:CYS:N	2.36	0.54
2:J:182:GLU:N	2:J:191:VAL:O	2.39	0.54
1:A:361:GLU:HG2	1:A:408:ILE:HD11	1.90	0.54
1:A:867:ILE:HD13	1:A:870:PHE:HE1	1.73	0.54
3:C:111:PRO:HG3	3:C:268:ASN:HA	1.89	0.54
1:I:609:VAL:HG13	1:I:619:GLY:HA3	1.90	0.54
1:I:842:GLN:NE2	3:M:70:GLN:HA	2.23	0.54
9:U:50:THR:O	9:U:51:MET:HB2	2.08	0.54
1:A:308:LEU:HD12	1:A:309:LYS:HG3	1.89	0.54
2:B:227:LYS:HB2	2:B:230:TYR:HD2	1.73	0.54
2:B:793:HIS:NE2	2:B:805:LYS:O	2.41	0.54
1:I:397:SER:OG	1:I:398:ASN:N	2.40	0.54
1:I:837:GLN:HB3	3:M:102:ILE:HD11	1.90	0.54
2:J:793:HIS:NE2	2:J:805:LYS:O	2.40	0.54
3:M:279:GLU:HG3	7:S:63:ILE:HG21	1.90	0.54
1:A:396:GLU:HB3	1:I:40:TYR:OH	2.08	0.53
9:L:9:GLU:HB2	9:L:12:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:326:PHE:HB2	2:J:1052:ARG:HH22	1.73	0.53
2:J:438:HIS:HD2	2:J:441:ARG:HE	1.55	0.53
3:M:10:MET:HE3	3:M:46:ILE:HD12	1.90	0.53
3:M:262:THR:HG22	7:S:12:HIS:CD2	2.43	0.53
1:A:8:ILE:HD13	3:C:367:ILE:HD11	1.90	0.53
1:A:326:PHE:HA	2:B:1008:ARG:O	2.09	0.53
2:B:183:ARG:HB2	2:B:186:ARG:NH2	2.14	0.53
2:B:286:PRO:O	2:B:288:GLU:N	2.40	0.53
3:C:191:PHE:CD2	3:C:198:LEU:HD22	2.43	0.53
2:J:63:PHE:CZ	2:J:388:GLU:OE2	2.55	0.53
1:A:397:SER:OG	1:A:398:ASN:N	2.41	0.53
1:A:426:ARG:HB2	1:A:467:MET:HE3	1.90	0.53
2:B:1066:GLU:HG2	2:B:1119:LEU:HD13	1.91	0.53
2:J:878:LEU:HD23	2:J:892:ILE:HG22	1.90	0.53
2:J:1076:LYS:O	2:J:1078:ARG:N	2.41	0.53
3:M:266:THR:HG22	3:M:268:ASN:H	1.73	0.53
1:A:49:LYS:HG3	1:A:50:ARG:HH21	1.74	0.53
2:B:182:GLU:N	2:B:191:VAL:O	2.40	0.53
3:C:266:THR:HG22	3:C:268:ASN:H	1.73	0.53
3:C:369:GLN:HG3	3:C:370:PRO:HD2	1.90	0.53
11:P:11:CYS:SG	11:P:30:CYS:SG	3.05	0.53
1:I:10:SER:C	2:J:1118:ARG:HB3	2.34	0.53
2:J:800:ILE:HD11	2:J:812:LEU:HD23	1.90	0.53
1:A:667:THR:HG23	2:B:971:ARG:HH21	1.73	0.53
3:C:192:GLU:OE1	3:C:197:THR:HG23	2.09	0.53
11:W:47:LYS:HB3	11:W:49:ILE:HG13	1.90	0.53
1:A:8:ILE:HG13	2:B:1095:VAL:HG11	1.91	0.53
1:A:127:LYS:HB2	3:C:330:LYS:HB3	1.91	0.53
2:B:299:ASP:HB3	2:B:308:VAL:O	2.09	0.53
2:B:392:ARG:HG2	2:B:392:ARG:O	2.07	0.53
3:C:161:VAL:CG1	3:C:162:GLU:H	2.05	0.53
4:D:3:GLU:HG3	4:D:19:SER:HB2	1.91	0.53
4:D:143:HIS:NE2	11:P:49:ILE:O	2.41	0.53
1:I:462:PHE:O	1:I:464:GLY:N	2.42	0.53
2:J:227:LYS:HB2	2:J:230:TYR:HD2	1.73	0.53
2:J:939:LEU:HD11	2:J:966:PHE:CD2	2.39	0.53
2:J:1122:ARG:HH11	6:R:4:ARG:NH2	2.07	0.53
1:A:156:PRO:HG3	1:A:169:ARG:HG3	1.90	0.53
1:A:194:PRO:HB2	1:A:196:LYS:HD2	1.91	0.53
1:A:329:ARG:O	2:B:1005:MET:HA	2.08	0.53
1:A:609:VAL:HG13	1:A:619:GLY:HA3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:VAL:HG21	2:B:395:ARG:HH12	1.74	0.53
1:I:531:MET:C	9:U:44:THR:HG21	2.33	0.53
3:M:375:THR:O	3:M:378:VAL:HG12	2.09	0.53
1:A:462:PHE:O	1:A:464:GLY:N	2.40	0.53
2:B:273:ALA:HA	2:B:276:TYR:CD2	2.44	0.53
2:B:438:HIS:HD2	2:B:441:ARG:HE	1.55	0.53
2:B:800:ILE:HD11	2:B:812:LEU:HD23	1.90	0.53
2:B:962:GLU:O	2:B:965:GLY:N	2.38	0.53
2:B:1054:LEU:HD22	2:B:1059:LYS:HE3	1.91	0.53
4:D:62:ARG:HH12	10:N:2:ILE:HD12	1.74	0.53
2:J:299:ASP:HB3	2:J:308:VAL:O	2.09	0.53
1:A:404:GLU:O	1:A:406:LEU:N	2.41	0.53
3:C:10:MET:HE3	3:C:46:ILE:HD12	1.91	0.53
1:I:194:PRO:HB2	1:I:196:LYS:HD2	1.91	0.53
1:I:344:GLY:HA3	1:I:449:ARG:HB2	1.91	0.53
1:I:444:PRO:CD	9:U:50:THR:CG2	2.78	0.53
2:J:959:LYS:HA	4:O:201:ARG:NH2	2.24	0.53
2:J:1054:LEU:HD22	2:J:1059:LYS:HE3	1.91	0.53
3:C:348:ALA:O	3:C:351:GLU:HG2	2.08	0.53
10:N:60:MET:C	10:N:62:TYR:H	2.15	0.53
2:J:273:ALA:HA	2:J:276:TYR:CD2	2.44	0.53
3:M:153:ASP:CB	3:M:157:MET:CB	2.87	0.53
3:M:216:GLU:O	3:M:221:HIS:N	2.42	0.53
3:C:262:THR:HG22	7:H:12:HIS:CG	2.44	0.52
5:E:92:MET:HE2	5:E:127:PHE:CD2	2.39	0.52
1:I:361:GLU:HG2	1:I:408:ILE:HD11	1.90	0.52
4:O:3:GLU:HG3	4:O:19:SER:HB2	1.91	0.52
1:A:264:PRO:HB2	1:A:267:ILE:HD13	1.91	0.52
1:A:753:THR:CG2	1:A:754:GLY:H	2.09	0.52
1:A:808:TYR:HE2	2:B:923:MET:SD	2.32	0.52
2:B:559:LEU:HD22	2:B:568:VAL:HG22	1.90	0.52
2:B:1063:TRP:CE3	2:B:1074:GLU:HG2	2.44	0.52
1:I:633:LEU:O	1:I:636:ILE:HG12	2.10	0.52
1:I:867:ILE:HD11	7:S:40:LEU:HD22	1.91	0.52
2:J:729:LEU:HD23	2:J:730:SER:N	2.24	0.52
2:J:749:ARG:HE	4:O:144:ALA:HB1	1.74	0.52
3:M:153:ASP:OD2	3:M:157:MET:HG3	2.09	0.52
3:M:156:ASN:O	3:M:158:GLU:HG2	2.09	0.52
3:M:178:VAL:O	3:M:181:LYS:NZ	2.38	0.52
5:Q:3:LYS:HZ2	6:R:9:GLU:CD	2.16	0.52
1:A:156:PRO:HB3	1:A:169:ARG:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:ASP:HB2	1:A:632:LYS:HE2	1.92	0.52
3:C:178:VAL:O	3:C:181:LYS:HB3	2.09	0.52
4:D:62:ARG:HH22	10:N:2:ILE:HB	1.73	0.52
1:A:344:GLY:HA3	1:A:449:ARG:HB2	1.91	0.52
1:I:264:PRO:HB2	1:I:267:ILE:HD13	1.91	0.52
3:M:369:GLN:HG3	3:M:370:PRO:HD2	1.92	0.52
4:O:163:LYS:HG2	4:O:168:TRP:CE2	2.44	0.52
5:Q:82:GLN:HB3	6:R:98:LYS:HG3	1.90	0.52
2:B:94:ILE:HG21	11:P:34:ILE:HG12	1.90	0.52
2:B:373:GLN:HG2	2:B:397:SER:HB2	1.91	0.52
3:C:73:GLY:O	3:C:76:SER:OG	2.27	0.52
3:C:192:GLU:HG3	3:C:197:THR:OG1	2.10	0.52
4:D:163:LYS:HG2	4:D:168:TRP:CE2	2.44	0.52
3:M:197:THR:HG22	3:M:198:LEU:N	2.24	0.52
3:M:322:GLY:O	3:M:324:HIS:N	2.42	0.52
4:O:62:ARG:HH22	10:V:2:ILE:HB	1.72	0.52
2:B:467:CYS:SG	2:B:470:GLU:HB2	2.49	0.52
2:B:579:ARG:HH21	2:B:623:GLU:CD	2.18	0.52
2:B:702:VAL:HG23	10:N:53:VAL:CG1	2.40	0.52
2:B:1063:TRP:CE3	2:B:1074:GLU:CG	2.93	0.52
1:I:852:LEU:HD11	3:M:311:MET:HG3	1.91	0.52
2:J:373:GLN:CG	2:J:397:SER:HB2	2.40	0.52
2:J:392:ARG:C	2:J:394:VAL:N	2.63	0.52
2:J:462:HIS:HB3	2:J:466:ILE:HB	1.92	0.52
3:M:348:ALA:O	3:M:351:GLU:HG2	2.10	0.52
9:U:49:ILE:C	9:U:50:THR:HG1	2.03	0.52
1:A:187:ARG:NE	1:A:211:GLU:O	2.42	0.52
1:A:872:TYR:CE1	3:C:64:VAL:HG11	2.45	0.52
3:C:148:ARG:HD3	3:C:148:ARG:N	2.25	0.52
3:C:160:VAL:HG22	3:C:198:LEU:HG	1.91	0.52
1:I:156:PRO:HG3	1:I:169:ARG:HG3	1.92	0.52
1:I:842:GLN:HE21	3:M:70:GLN:HA	1.75	0.52
2:J:467:CYS:SG	2:J:470:GLU:HB2	2.50	0.52
2:J:962:GLU:HA	2:J:966:PHE:O	2.09	0.52
3:M:220:LYS:C	3:M:222:ARG:H	2.17	0.52
1:A:295:HIS:O	1:A:297:SER:N	2.43	0.52
2:B:557:VAL:HG22	2:B:570:ILE:HG23	1.92	0.52
2:B:782:ILE:HG22	2:B:783:GLN:H	1.74	0.52
2:B:888:GLN:NE2	2:B:918:GLY:O	2.43	0.52
3:C:104:ILE:HD13	3:C:289:ILE:HG12	1.92	0.52
3:C:161:VAL:H	3:C:199:VAL:H	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:431:HIS:HA	3:M:70:GLN:HB3	1.91	0.52
2:J:731:TYR:CE2	2:J:902:PRO:HG3	2.44	0.52
3:M:152:ILE:HG23	3:M:160:VAL:N	2.23	0.52
2:B:395:ARG:O	2:B:397:SER:N	2.41	0.52
3:C:155:LEU:CD2	3:C:156:ASN:ND2	2.73	0.52
2:J:41:PHE:CE2	2:J:356:LYS:HG2	2.45	0.52
2:J:730:SER:HB3	2:J:915:ASN:ND2	2.25	0.52
2:B:808:GLY:O	2:B:843:VAL:HG12	2.10	0.52
3:C:196:TYR:O	3:C:198:LEU:HD12	2.10	0.52
3:C:322:GLY:O	3:C:324:HIS:N	2.42	0.52
1:I:527:GLU:CD	9:U:33:HIS:HE2	2.18	0.52
1:I:834:ARG:HD2	3:M:98:LEU:HD13	1.92	0.52
2:J:469:THR:HG21	2:J:668:ASN:HB3	1.92	0.52
2:J:1122:ARG:CD	6:R:4:ARG:NH2	2.72	0.52
1:A:195:ASP:HB3	1:A:205:PRO:HB3	1.92	0.51
2:B:462:HIS:HB3	2:B:466:ILE:HB	1.91	0.51
2:B:467:CYS:SG	2:B:651:GLY:N	2.78	0.51
11:P:11:CYS:SG	11:P:14:GLU:OE2	2.68	0.51
1:I:150:CYS:HB3	1:I:153:PRO:HD3	1.92	0.51
1:I:445:TYR:HB2	1:I:449:ARG:NH2	2.25	0.51
2:J:107:MET:CA	2:J:395:ARG:HH22	2.20	0.51
2:J:557:VAL:HG22	2:J:570:ILE:HG23	1.92	0.51
2:J:888:GLN:NE2	2:J:918:GLY:O	2.43	0.51
1:A:508:ILE:HG21	1:A:754:GLY:O	2.10	0.51
2:B:1048:LEU:O	2:B:1051:GLU:HB3	2.10	0.51
3:C:160:VAL:CG2	3:C:198:LEU:CB	2.88	0.51
3:C:203:LYS:HB2	3:C:203:LYS:NZ	2.23	0.51
3:C:358:LEU:CD1	3:C:359:ASN:H	2.23	0.51
1:I:309:LYS:CE	3:M:347:PHE:HB2	2.40	0.51
1:I:849:LEU:O	3:M:65:GLY:HA3	2.09	0.51
2:J:361:VAL:O	2:J:365:GLN:HG2	2.10	0.51
3:M:104:ILE:HD13	3:M:289:ILE:HG12	1.92	0.51
7:S:67:SER:N	7:S:71:GLY:O	2.26	0.51
1:A:356:PRO:HG3	1:A:473:GLN:HB3	1.90	0.51
2:B:1063:TRP:O	2:B:1072:ALA:N	2.35	0.51
3:C:124:HIS:ND1	3:C:130:LYS:HB3	2.25	0.51
3:C:187:LYS:HD3	3:C:203:LYS:HZ2	1.74	0.51
2:J:789:LYS:HE2	2:J:792:ARG:HB2	1.93	0.51
2:J:982:ARG:HD3	4:O:155:TYR:CD2	2.45	0.51
3:M:119:TYR:CD2	3:M:263:ARG:HB3	2.45	0.51
7:S:61:ILE:HG22	7:S:63:ILE:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:VAL:O	2:B:365:GLN:HG2	2.11	0.51
2:B:390:ILE:HD12	2:B:391:GLN:HB2	1.92	0.51
2:B:791:TYR:OH	2:B:838:GLU:OE2	2.25	0.51
2:B:962:GLU:HA	2:B:966:PHE:O	2.09	0.51
2:B:996:ARG:NH2	2:B:1000:MET:HE3	2.23	0.51
3:C:217:LYS:O	3:C:218:VAL:HB	2.10	0.51
5:E:9:ASP:OD1	6:F:4:ARG:HG2	2.09	0.51
2:J:414:GLY:O	2:J:422:GLY:N	2.44	0.51
2:J:782:ILE:HG22	2:J:783:GLN:H	1.74	0.51
3:M:124:HIS:ND1	3:M:130:LYS:HB3	2.25	0.51
1:A:99:THR:HG21	1:A:193:ILE:HD11	1.93	0.51
1:A:783:TYR:HE2	1:A:789:THR:HB	1.74	0.51
2:B:389:ASN:HD22	2:B:392:ARG:CB	2.19	0.51
3:C:216:GLU:HA	3:C:220:LYS:HB2	1.93	0.51
3:C:375:THR:O	3:C:378:VAL:HG12	2.10	0.51
7:H:61:ILE:HG22	7:H:63:ILE:HG13	1.93	0.51
3:M:187:LYS:NZ	3:M:201:ARG:HB3	2.26	0.51
9:U:51:MET:CA	9:U:52:ALA:HB3	2.41	0.51
3:C:220:LYS:C	3:C:222:ARG:H	2.18	0.51
1:I:49:LYS:HG3	1:I:50:ARG:HH21	1.75	0.51
1:I:445:TYR:CE1	9:U:49:ILE:HG21	2.46	0.51
1:A:113:ILE:HG23	1:A:200:LEU:HD11	1.93	0.51
2:B:812:LEU:HD11	2:B:843:VAL:HG23	1.93	0.51
2:B:1087:GLY:C	2:B:1089:ASP:H	2.18	0.51
5:E:2:TYR:OH	6:F:44:SER:OG	2.27	0.51
5:E:39:ASP:O	5:E:43:GLY:N	2.43	0.51
1:I:113:ILE:HG23	1:I:200:LEU:HD11	1.92	0.51
1:I:867:ILE:HD13	1:I:870:PHE:HE1	1.76	0.51
1:A:101:ARG:O	1:A:102:GLU:HB2	2.10	0.51
2:B:885:ARG:HD2	2:B:993:TYR:HB3	1.92	0.51
3:C:161:VAL:HG21	3:C:199:VAL:HG23	0.51	0.51
10:N:10:CYS:O	10:N:12:LYS:HG2	2.10	0.51
1:I:351:MET:HG2	1:I:415:HIS:HD1	1.75	0.51
2:J:885:ARG:HD2	2:J:993:TYR:HB3	1.92	0.51
3:M:119:TYR:HD2	3:M:263:ARG:HB3	1.76	0.51
2:B:899:GLU:HG2	4:D:35:SER:HB3	1.92	0.51
4:D:26:ALA:HB1	4:D:222:PHE:HZ	1.76	0.51
1:I:308:LEU:HD12	1:I:309:LYS:HG3	1.93	0.51
1:I:544:ASP:OD2	1:I:551:PRO:HB2	2.11	0.51
2:J:459:HIS:ND1	2:J:461:THR:HG23	2.26	0.51
3:M:186:PHE:O	3:M:187:LYS:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:26:ALA:HB1	4:O:222:PHE:HZ	1.74	0.51
5:E:42:GLU:HG3	6:F:2:ILE:HG12	1.92	0.51
1:I:531:MET:CB	9:U:44:THR:CG2	2.85	0.51
2:J:378:TYR:HE1	2:J:388:GLU:CG	1.93	0.51
2:J:899:GLU:OE1	2:J:899:GLU:N	2.32	0.51
7:S:25:GLU:O	7:S:29:LEU:HB2	2.11	0.51
10:V:2:ILE:HG12	10:V:56:ILE:HG21	1.93	0.51
1:A:21:ILE:HD11	2:B:1112:VAL:HG23	1.92	0.50
1:A:61:GLU:O	1:A:63:CYS:N	2.36	0.50
2:B:326:LYS:HD2	2:B:335:ARG:HE	1.76	0.50
2:B:554:VAL:HA	2:B:578:ARG:HH12	1.76	0.50
2:B:607:SER:O	2:B:610:ILE:HG13	2.12	0.50
2:B:789:LYS:HE2	2:B:792:ARG:HB2	1.92	0.50
3:C:279:GLU:HG3	7:H:63:ILE:HG21	1.93	0.50
4:D:171:LEU:HD21	4:D:200:PRO:HD2	1.93	0.50
5:E:6:LYS:O	6:F:7:LEU:HD23	2.10	0.50
5:E:8:LYS:HG3	6:F:7:LEU:HD22	1.93	0.50
1:I:101:ARG:O	1:I:102:GLU:HB2	2.11	0.50
2:J:352:GLY:O	2:J:356:LYS:HG3	2.12	0.50
3:M:148:ARG:HD3	3:M:148:ARG:N	2.26	0.50
2:B:70:ILE:HG12	2:B:105:LEU:HG	1.94	0.50
2:B:458:LEU:HD11	2:B:468:PRO:HA	1.93	0.50
2:B:1063:TRP:CZ2	2:B:1094:LYS:CE	2.89	0.50
9:L:45:ILE:C	9:L:47:HIS:H	2.19	0.50
1:I:83:VAL:HG13	1:I:276:GLN:OE1	2.10	0.50
2:J:70:ILE:HG12	2:J:105:LEU:HG	1.94	0.50
2:J:458:LEU:HD11	2:J:468:PRO:HA	1.92	0.50
3:M:337:ALA:HA	3:M:346:LEU:HB2	1.93	0.50
6:R:18:LYS:HD2	6:R:49:GLU:HA	1.94	0.50
1:A:578:GLU:HB3	1:A:579:PRO:HD2	1.92	0.50
1:A:755:ALA:HB1	2:B:917:HIS:CD2	2.46	0.50
2:B:429:ARG:HB3	2:B:683:TRP:HZ3	1.76	0.50
2:J:429:ARG:HB3	2:J:683:TRP:HZ3	1.76	0.50
3:M:38:LYS:HG2	3:M:41:GLU:HG3	1.92	0.50
3:M:178:VAL:HB	3:M:190:GLU:OE2	2.10	0.50
2:B:63:PHE:CG	2:B:392:ARG:NH2	2.80	0.50
2:B:312:ASN:HD22	2:B:312:ASN:H	1.59	0.50
2:B:1087:GLY:O	2:B:1089:ASP:N	2.32	0.50
3:C:38:LYS:HG2	3:C:41:GLU:HG3	1.92	0.50
5:E:15:PRO:HB2	8:K:24:ALA:HB2	1.92	0.50
1:I:9:GLY:HA3	2:J:1120:LYS:CB	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:24:TYR:HB2	2:J:606:TRP:NE1	2.27	0.50
1:A:633:LEU:O	1:A:636:ILE:HG12	2.11	0.50
2:B:50:VAL:HG11	2:B:70:ILE:HG13	1.93	0.50
2:B:390:ILE:CG1	2:B:391:GLN:H	2.24	0.50
1:I:308:LEU:HD13	3:M:346:LEU:HD11	1.93	0.50
1:I:359:VAL:HG22	1:I:408:ILE:HA	1.94	0.50
2:J:192:ALA:HB3	2:J:207:VAL:HG23	1.94	0.50
2:J:373:GLN:HG2	2:J:397:SER:HB2	1.93	0.50
2:J:779:SER:O	2:J:781:ASN:N	2.44	0.50
4:O:171:LEU:HD21	4:O:200:PRO:HD2	1.94	0.50
1:A:63:CYS:O	1:A:65:ALA:N	2.45	0.50
1:A:81:ARG:HG3	1:A:82:PRO:HD2	1.94	0.50
2:B:464:GLY:HA3	2:B:579:ARG:HD3	1.94	0.50
10:N:62:TYR:C	10:N:63:LYS:HZ2	2.10	0.50
1:I:187:ARG:NE	1:I:211:GLU:O	2.42	0.50
1:I:505:GLN:OE1	2:J:737:GLU:N	2.40	0.50
2:J:393:PHE:C	2:J:394:VAL:CG2	2.80	0.50
2:J:579:ARG:HH21	2:J:623:GLU:CD	2.19	0.50
2:J:724:PHE:CD1	2:J:994:TYR:HB2	2.47	0.50
2:J:808:GLY:O	2:J:843:VAL:HG12	2.10	0.50
3:M:177:LYS:C	3:M:179:VAL:H	2.19	0.50
2:B:378:TYR:OH	2:B:388:GLU:CB	2.60	0.50
2:B:803:GLU:O	11:P:44:ARG:NE	2.45	0.50
2:B:1062:VAL:HG11	2:B:1071:LEU:HD13	1.94	0.50
1:I:204:HIS:ND1	1:I:205:PRO:HD2	2.27	0.50
2:J:312:ASN:HD22	2:J:312:ASN:H	1.60	0.50
2:B:469:THR:HG21	2:B:668:ASN:HB3	1.93	0.50
7:H:25:GLU:O	7:H:29:LEU:HB2	2.11	0.50
1:I:99:THR:HG21	1:I:193:ILE:HD11	1.93	0.50
1:I:195:ASP:HB3	1:I:205:PRO:HB3	1.92	0.50
1:I:238:GLU:HG2	1:I:242:THR:HB	1.94	0.50
2:J:368:LYS:O	2:J:371:GLN:HB3	2.12	0.50
2:J:464:GLY:HA3	2:J:579:ARG:HD3	1.94	0.50
2:J:856:VAL:HG22	2:J:866:VAL:HG22	1.94	0.50
2:J:1062:VAL:HG11	2:J:1071:LEU:HD13	1.93	0.50
5:Q:3:LYS:HD2	6:R:11:TYR:CE1	2.47	0.50
5:Q:146:ILE:HA	5:Q:163:MET:HG2	1.94	0.50
9:U:51:MET:HA	9:U:52:ALA:CB	2.41	0.50
2:B:24:TYR:HB2	2:B:606:TRP:NE1	2.27	0.50
2:B:111:VAL:O	2:B:114:ILE:HG12	2.11	0.50
3:C:121:ASP:OD1	3:C:123:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:GLU:HB3	3:C:163:ILE:HD13	1.94	0.50
9:L:46:GLU:C	9:L:47:HIS:CG	2.89	0.50
1:I:891:ASP:OD1	1:I:891:ASP:N	2.42	0.50
2:J:326:LYS:HD2	2:J:335:ARG:HE	1.76	0.50
2:J:659:TYR:HB3	2:J:662:HIS:CD2	2.47	0.50
2:J:812:LEU:HD11	2:J:843:VAL:HG23	1.92	0.50
3:M:153:ASP:CG	3:M:157:MET:HG3	2.37	0.50
4:O:178:ARG:NH2	4:O:196:ALA:O	2.28	0.50
7:S:66:LYS:HG2	7:S:72:TYR:CE1	2.47	0.50
1:A:204:HIS:ND1	1:A:205:PRO:HD2	2.27	0.49
1:A:449:ARG:NH2	2:B:878:LEU:HD12	2.27	0.49
2:B:579:ARG:NH2	2:B:623:GLU:OE2	2.44	0.49
2:B:606:TRP:O	2:B:609:LEU:HB2	2.12	0.49
2:B:779:SER:O	2:B:781:ASN:N	2.44	0.49
2:B:856:VAL:HG22	2:B:866:VAL:HG22	1.94	0.49
1:I:9:GLY:N	2:J:1120:LYS:HB2	2.27	0.49
1:I:44:GLY:HA2	1:I:49:LYS:HG2	1.94	0.49
1:I:493:SER:HB3	1:I:500:LEU:HB2	1.94	0.49
1:I:867:ILE:HD13	1:I:870:PHE:CE1	2.47	0.49
2:J:1091:ARG:HD3	2:J:1091:ARG:N	2.27	0.49
1:A:891:ASP:O	1:A:895:VAL:HG23	2.12	0.49
2:B:370:MET:HE1	2:B:395:ARG:HH11	1.76	0.49
2:B:659:TYR:HB3	2:B:662:HIS:CD2	2.48	0.49
1:I:694:VAL:HA	1:I:697:LEU:HD12	1.94	0.49
2:J:395:ARG:CB	2:J:398:ILE:HD11	2.40	0.49
2:J:554:VAL:HA	2:J:578:ARG:HH12	1.76	0.49
2:J:729:LEU:HD22	2:J:731:TYR:CD1	2.47	0.49
1:A:83:VAL:HG13	1:A:276:GLN:OE1	2.13	0.49
1:A:105:ARG:HA	1:A:197:ASP:OD2	2.13	0.49
1:A:161:ARG:HA	1:A:162:PRO:C	2.38	0.49
2:B:57:VAL:HB	2:B:58:PRO:CA	2.35	0.49
1:I:524:TYR:HD1	1:I:524:TYR:H	1.59	0.49
2:J:41:PHE:CE2	2:J:356:LYS:CG	2.95	0.49
3:M:121:ASP:OD1	3:M:123:GLU:HG2	2.12	0.49
1:A:694:VAL:HA	1:A:697:LEU:HD12	1.94	0.49
1:A:867:ILE:HD13	1:A:870:PHE:CE1	2.47	0.49
3:C:159:TYR:O	3:C:160:VAL:HB	2.12	0.49
1:I:161:ARG:HA	1:I:162:PRO:C	2.38	0.49
2:J:652:ILE:HG23	2:J:653:PRO:HD3	1.94	0.49
2:J:706:ASN:HB2	2:J:710:MET:SD	2.53	0.49
1:A:245:LEU:O	1:A:249:ILE:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1082:TYR:HD1	2:B:1088:GLU:H	1.59	0.49
1:I:26:ALA:HB3	1:I:51:LEU:HD23	1.95	0.49
1:A:783:TYR:CE2	1:A:789:THR:HB	2.48	0.49
3:C:262:THR:HG22	7:H:12:HIS:CD2	2.48	0.49
7:H:63:ILE:O	7:H:74:TYR:HA	2.12	0.49
1:I:245:LEU:O	1:I:249:ILE:HG13	2.12	0.49
1:I:401:LEU:HA	1:I:404:GLU:CG	2.43	0.49
1:I:666:PHE:O	2:J:729:LEU:HA	2.12	0.49
2:J:413:THR:HG23	2:J:415:SER:H	1.77	0.49
2:J:573:ASP:OD1	2:J:573:ASP:N	2.41	0.49
2:J:1078:ARG:HG3	2:J:1080:LYS:HG2	1.94	0.49
3:M:119:TYR:CD2	3:M:263:ARG:HD2	2.48	0.49
7:S:63:ILE:O	7:S:74:TYR:HA	2.12	0.49
2:B:65:VAL:HG11	2:B:395:ARG:NH1	2.28	0.49
2:B:192:ALA:HB3	2:B:207:VAL:HG23	1.94	0.49
2:B:459:HIS:ND1	2:B:461:THR:HG23	2.28	0.49
2:B:618:LEU:HD22	2:B:622:GLU:HG2	1.95	0.49
10:N:56:ILE:HG12	10:N:60:MET:HE2	1.95	0.49
1:I:713:THR:O	1:I:717:THR:HG23	2.12	0.49
1:I:769:LEU:HB2	1:I:804:VAL:CG2	2.43	0.49
2:J:41:PHE:CD1	2:J:42:ILE:CD1	2.96	0.49
2:J:111:VAL:O	2:J:114:ILE:HG12	2.11	0.49
2:J:467:CYS:SG	2:J:651:GLY:N	2.78	0.49
2:J:812:LEU:HD21	2:J:843:VAL:HG23	1.94	0.49
2:J:996:ARG:NH2	2:J:1000:MET:HE3	2.23	0.49
1:A:508:ILE:HG21	1:A:754:GLY:HA3	1.93	0.49
1:A:536:ASP:HA	1:A:540:LEU:HB2	1.93	0.49
1:A:669:ALA:HB2	2:B:971:ARG:NE	2.28	0.49
1:A:713:THR:O	1:A:717:THR:HG23	2.12	0.49
2:B:520:TYR:CZ	2:B:532:VAL:HB	2.48	0.49
2:B:885:ARG:HD2	2:B:993:TYR:HD2	1.78	0.49
2:B:982:ARG:HD3	4:D:155:TYR:CD2	2.48	0.49
2:B:1063:TRP:CZ3	2:B:1074:GLU:HG2	2.46	0.49
3:C:149:GLU:O	3:C:150:GLU:HG2	2.13	0.49
8:K:12:ILE:HG23	8:K:51:ILE:HB	1.95	0.49
10:N:56:ILE:HG23	10:N:60:MET:HE2	1.94	0.49
1:I:105:ARG:HA	1:I:197:ASP:OD2	2.13	0.49
1:I:588:LEU:C	1:I:588:LEU:CD2	2.86	0.49
2:J:107:MET:C	2:J:395:ARG:NH2	2.71	0.49
2:J:591:LEU:HG	2:J:614:VAL:HB	1.95	0.49
2:J:618:LEU:HD22	2:J:622:GLU:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:73:GLY:O	3:M:76:SER:OG	2.26	0.49
1:A:21:ILE:HD13	1:A:219:PRO:HD3	1.95	0.49
1:A:445:TYR:HB2	1:A:449:ARG:NH2	2.25	0.49
2:B:88:TYR:CD2	2:B:148:LEU:HD11	2.48	0.49
2:B:428:ASP:OD2	2:B:434:SER:OG	2.31	0.49
3:C:378:VAL:HG21	8:K:8:GLU:HG2	1.95	0.49
1:I:463:ASP:OD1	1:I:464:GLY:N	2.46	0.49
2:J:324:ALA:O	2:J:328:LEU:HG	2.13	0.49
1:A:33:ASP:HB3	1:A:43:GLU:OE1	2.12	0.49
2:B:429:ARG:HE	2:B:435:THR:HG21	1.78	0.49
2:B:606:TRP:HZ3	2:B:617:TYR:HH	1.57	0.49
2:B:730:SER:HB3	2:B:915:ASN:ND2	2.27	0.49
2:B:753:ARG:HA	2:B:876:PRO:HD3	1.95	0.49
3:C:175:MET:O	3:C:178:VAL:HB	2.13	0.49
4:D:10:ARG:HB2	4:D:13:SER:OG	2.13	0.49
1:I:446:ARG:HH21	2:J:1002:ALA:HA	1.77	0.49
2:J:607:SER:O	2:J:610:ILE:HG13	2.12	0.49
2:J:730:SER:HA	2:J:735:ASN:ND2	2.26	0.49
3:M:21:LYS:HE3	3:M:21:LYS:HB3	1.48	0.49
8:T:12:ILE:HG23	8:T:51:ILE:HB	1.95	0.49
1:A:439:ARG:NH2	1:A:482:LYS:HE3	2.28	0.48
2:B:24:TYR:HB2	2:B:606:TRP:CE2	2.48	0.48
2:B:414:GLY:O	2:B:422:GLY:N	2.43	0.48
3:C:183:THR:O	3:C:183:THR:HG22	2.12	0.48
1:I:94:ARG:HG3	1:I:138:HIS:HD2	1.74	0.48
1:I:346:PRO:HB2	1:I:349:VAL:HG23	1.95	0.48
2:J:244:VAL:HG13	2:J:257:LEU:HD12	1.96	0.48
2:J:354:LEU:HD12	2:J:416:TRP:NE1	2.28	0.48
2:J:429:ARG:HE	2:J:435:THR:HG21	1.78	0.48
1:A:338:ILE:O	1:A:451:ASN:ND2	2.47	0.48
2:B:591:LEU:HG	2:B:614:VAL:HB	1.95	0.48
2:B:629:ALA:HB2	2:B:639:HIS:CG	2.49	0.48
2:B:652:ILE:HG23	2:B:653:PRO:HD3	1.95	0.48
3:C:196:TYR:CG	3:C:196:TYR:O	2.66	0.48
3:C:331:ALA:H	3:C:336:ARG:NH1	2.09	0.48
1:I:572:ARG:HD2	1:I:576:CYS:HB3	1.95	0.48
1:I:875:ASP:HB3	7:S:70:ALA:HB2	1.95	0.48
2:J:428:ASP:OD2	2:J:434:SER:OG	2.31	0.48
1:A:435:ILE:HB	2:B:1039:VAL:HG21	1.94	0.48
1:A:493:SER:HB3	1:A:500:LEU:HB2	1.94	0.48
1:A:572:ARG:HD2	1:A:576:CYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:VAL:HG21	2:B:323:MET:HB3	1.95	0.48
2:B:368:LYS:O	2:B:371:GLN:HB3	2.12	0.48
2:B:378:TYR:OH	2:B:388:GLU:HB2	2.13	0.48
2:B:812:LEU:HD21	2:B:843:VAL:HG23	1.94	0.48
6:F:18:LYS:HD2	6:F:49:GLU:HA	1.94	0.48
1:I:779:LEU:HD12	1:I:802:GLY:HA3	1.95	0.48
2:J:159:PHE:HE1	2:J:168:ILE:HG13	1.78	0.48
2:J:606:TRP:O	2:J:609:LEU:HB2	2.12	0.48
2:J:731:TYR:CZ	2:J:902:PRO:HG3	2.48	0.48
2:J:799:LEU:HG	2:J:813:VAL:HG22	1.95	0.48
3:M:122:GLU:HG2	3:M:125:ARG:NH2	2.29	0.48
1:A:463:ASP:OD1	1:A:464:GLY:N	2.46	0.48
2:B:724:PHE:CD1	2:B:994:TYR:HB2	2.47	0.48
10:N:2:ILE:HG12	10:N:56:ILE:HG21	1.94	0.48
1:I:6:LYS:NZ	2:J:1122:ARG:NH2	2.48	0.48
3:M:270:TRP:HA	3:M:318:ILE:HD11	1.95	0.48
4:O:201:ARG:HA	4:O:204:GLU:HG2	1.96	0.48
10:V:10:CYS:O	10:V:12:LYS:HG2	2.12	0.48
1:A:221:PRO:HG2	1:A:226:ARG:HE	1.78	0.48
1:A:769:LEU:HB2	1:A:804:VAL:CG2	2.43	0.48
2:B:191:VAL:HG13	2:B:208:GLU:HB3	1.96	0.48
2:B:536:ARG:HA	2:B:539:VAL:HG22	1.95	0.48
2:B:799:LEU:HG	2:B:813:VAL:HG22	1.95	0.48
1:I:42:ILE:HG22	1:I:47:MET:HB3	1.96	0.48
2:J:88:TYR:CD2	2:J:148:LEU:HD11	2.48	0.48
2:J:1122:ARG:CD	5:Q:10:VAL:CG1	2.69	0.48
3:M:191:PHE:N	3:M:197:THR:HG23	2.29	0.48
3:M:290:VAL:O	3:M:294:ARG:HG3	2.13	0.48
5:Q:6:LYS:O	6:R:7:LEU:HD23	2.13	0.48
5:Q:16:ARG:H	5:Q:16:ARG:HD2	1.79	0.48
1:A:346:PRO:HB2	1:A:349:VAL:HG23	1.96	0.48
2:B:785:TYR:CE2	2:B:787:GLY:HA2	2.49	0.48
3:C:270:TRP:HA	3:C:318:ILE:HD11	1.95	0.48
1:I:15:ILE:HD12	1:I:208:SER:HB2	1.96	0.48
1:I:21:ILE:HD13	1:I:219:PRO:HD3	1.96	0.48
2:J:24:TYR:HB2	2:J:606:TRP:CE2	2.48	0.48
2:J:191:VAL:HG13	2:J:208:GLU:HB3	1.96	0.48
2:J:289:TYR:O	2:J:293:ARG:HB2	2.14	0.48
2:J:579:ARG:NH2	2:J:623:GLU:OE2	2.46	0.48
2:B:159:PHE:HE1	2:B:168:ILE:HG13	1.78	0.48
2:B:413:THR:HG23	2:B:415:SER:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:794:LEU:HB3	2:B:798:GLY:HA2	1.95	0.48
1:I:11:ILE:HD12	3:M:358:LEU:HD22	1.96	0.48
1:I:63:CYS:O	1:I:65:ALA:N	2.46	0.48
1:I:81:ARG:HG3	1:I:82:PRO:HD2	1.95	0.48
1:I:378:TYR:HB2	1:I:379:PRO:HD3	1.95	0.48
1:I:783:TYR:HE2	1:I:789:THR:HB	1.79	0.48
2:J:885:ARG:HD2	2:J:993:TYR:HD2	1.79	0.48
3:M:321:ILE:O	3:M:327:VAL:HG23	2.14	0.48
1:A:163:THR:CB	1:A:276:GLN:HE21	2.27	0.48
1:A:443:MET:SD	1:A:449:ARG:HD3	2.53	0.48
1:A:535:MET:HB3	1:A:540:LEU:HD12	1.95	0.48
1:A:779:LEU:HD12	1:A:802:GLY:HA3	1.95	0.48
2:B:706:ASN:HB2	2:B:710:MET:SD	2.53	0.48
5:E:146:ILE:HA	5:E:163:MET:HG2	1.94	0.48
9:L:91:ALA:C	9:L:94:GLU:OE1	2.57	0.48
1:I:444:PRO:CG	9:U:50:THR:HG22	2.10	0.48
1:I:874:GLU:HG3	7:S:67:SER:OG	2.13	0.48
3:M:176:GLU:O	3:M:179:VAL:N	2.47	0.48
4:O:10:ARG:HB2	4:O:13:SER:OG	2.13	0.48
1:A:10:SER:HB2	2:B:1118:ARG:HB3	1.94	0.48
2:B:759:THR:HA	2:B:869:THR:HA	1.95	0.48
3:C:122:GLU:HG2	3:C:125:ARG:NH2	2.29	0.48
3:C:160:VAL:HG23	3:C:198:LEU:CB	2.44	0.48
3:C:196:TYR:CE1	3:C:198:LEU:CD1	2.94	0.48
1:I:535:MET:HB3	1:I:540:LEU:HD12	1.95	0.48
1:I:750:MET:HE3	2:J:920:PRO:HG3	1.96	0.48
2:J:49:VAL:HG13	2:J:199:HIS:HE1	1.79	0.48
2:J:729:LEU:HD23	2:J:730:SER:O	2.13	0.48
1:A:81:ARG:HG2	1:A:272:TRP:CD2	2.49	0.48
1:A:654:THR:OG1	1:A:655:LYS:N	2.46	0.48
2:B:354:LEU:HD12	2:B:416:TRP:NE1	2.28	0.48
3:C:173:LEU:HD12	3:C:177:LYS:HZ2	1.78	0.48
3:C:290:VAL:O	3:C:294:ARG:HG3	2.13	0.48
1:I:163:THR:CB	1:I:276:GLN:HE21	2.27	0.48
1:I:439:ARG:NH2	1:I:482:LYS:HE3	2.28	0.48
1:I:837:GLN:HB3	3:M:102:ILE:CD1	2.44	0.48
2:J:1122:ARG:NH2	5:Q:67:TYR:HE2	2.08	0.48
3:M:152:ILE:CG2	3:M:159:TYR:CA	2.86	0.48
3:M:314:LEU:HD13	3:M:315:ASP:N	2.29	0.48
1:A:26:ALA:HB3	1:A:51:LEU:HD23	1.95	0.47
1:A:359:VAL:HG22	1:A:408:ILE:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:VAL:HG13	2:B:257:LEU:HD12	1.96	0.47
2:B:697:MET:HE1	2:B:721:GLY:HA2	1.95	0.47
3:C:155:LEU:CD2	3:C:156:ASN:HD22	2.27	0.47
3:C:187:LYS:HB3	3:C:201:ARG:HG2	1.96	0.47
3:M:148:ARG:HH21	3:M:162:GLU:CG	2.21	0.47
2:B:352:GLY:O	2:B:356:LYS:HG3	2.13	0.47
2:B:766:ARG:NH1	2:B:862:GLY:O	2.47	0.47
3:C:119:TYR:CD2	3:C:263:ARG:HD2	2.48	0.47
3:C:314:LEU:HD13	3:C:315:ASP:N	2.29	0.47
1:I:221:PRO:HG2	1:I:226:ARG:HE	1.79	0.47
1:I:623:LYS:HB2	1:I:754:GLY:HA3	1.96	0.47
2:J:207:VAL:HG21	2:J:323:MET:HB3	1.95	0.47
2:J:378:TYR:C	2:J:380:ARG:H	2.22	0.47
2:J:451:PRO:HB2	2:J:453:PHE:CE1	2.49	0.47
2:J:591:LEU:HD13	2:J:595:HIS:CE1	2.49	0.47
2:J:606:TRP:HZ3	2:J:617:TYR:HH	1.60	0.47
2:J:766:ARG:NH1	2:J:862:GLY:O	2.47	0.47
2:J:794:LEU:HB3	2:J:798:GLY:HA2	1.96	0.47
3:M:325:GLY:O	3:M:329:GLU:HG2	2.15	0.47
8:T:30:VAL:HB	8:T:31:PRO:HD3	1.96	0.47
1:A:704:GLY:C	1:A:706:LEU:H	2.21	0.47
3:C:155:LEU:HD21	3:C:156:ASN:ND2	2.29	0.47
3:C:236:LYS:HE3	3:C:241:TYR:CE2	2.49	0.47
2:J:395:ARG:CB	2:J:398:ILE:HD12	2.44	0.47
2:J:536:ARG:HA	2:J:539:VAL:HG22	1.94	0.47
2:J:1122:ARG:NE	5:Q:67:TYR:CD2	2.81	0.47
3:M:151:THR:O	3:M:152:ILE:HD13	2.13	0.47
3:M:163:ILE:HD12	3:M:197:THR:HB	1.95	0.47
3:M:236:LYS:HE3	3:M:241:TYR:CE2	2.49	0.47
3:M:380:LEU:HB2	5:Q:59:ILE:HB	1.95	0.47
4:O:55:PHE:HB2	4:O:58:ILE:HD12	1.95	0.47
1:A:378:TYR:HB2	1:A:379:PRO:HD3	1.95	0.47
1:A:524:TYR:H	1:A:524:TYR:HD1	1.58	0.47
1:A:893:VAL:HG11	3:C:49:THR:HA	1.96	0.47
3:C:207:LYS:HE3	3:C:210:ASP:OD1	2.14	0.47
3:C:337:ALA:HA	3:C:346:LEU:HB2	1.97	0.47
5:E:16:ARG:H	5:E:16:ARG:HD2	1.79	0.47
9:L:25:ALA:HB3	9:L:43:TYR:CE2	2.49	0.47
1:I:338:ILE:O	1:I:451:ASN:ND2	2.47	0.47
1:I:499:PRO:HD2	1:I:630:ASP:HB2	1.96	0.47
2:J:520:TYR:CZ	2:J:532:VAL:HB	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1081:VAL:HG22	2:J:1092:ILE:HD13	1.95	0.47
3:M:76:SER:HA	3:M:79:MET:HE3	1.96	0.47
3:M:93:ASN:HB3	3:M:94:VAL:HG22	1.94	0.47
3:M:177:LYS:C	3:M:179:VAL:N	2.72	0.47
2:B:17:LEU:HD22	2:B:644:LEU:HA	1.97	0.47
2:B:591:LEU:HD13	2:B:595:HIS:CE1	2.49	0.47
2:B:768:LEU:O	2:J:380:ARG:NH2	2.47	0.47
3:C:161:VAL:HG22	3:C:199:VAL:CB	2.33	0.47
3:C:204:LYS:C	3:C:206:THR:N	2.71	0.47
3:C:321:ILE:O	3:C:327:VAL:HG23	2.15	0.47
1:I:165:TYR:HB2	1:I:181:MET:HB3	1.97	0.47
1:I:352:GLU:OE2	2:J:1009:SER:HB3	2.14	0.47
2:J:591:LEU:HB3	2:J:595:HIS:CD2	2.50	0.47
2:J:629:ALA:HB2	2:J:639:HIS:CG	2.49	0.47
2:J:753:ARG:HA	2:J:876:PRO:HD3	1.95	0.47
2:J:759:THR:HA	2:J:869:THR:HA	1.96	0.47
2:J:785:TYR:CE2	2:J:787:GLY:HA2	2.49	0.47
2:J:962:GLU:OE1	4:O:201:ARG:NH1	2.48	0.47
3:M:180:ARG:O	3:M:180:ARG:HD3	2.15	0.47
4:O:50:ASN:HD22	4:O:50:ASN:C	2.22	0.47
1:A:15:ILE:HD12	1:A:208:SER:HB2	1.96	0.47
1:A:569:ILE:HG13	1:A:636:ILE:HD13	1.97	0.47
2:B:591:LEU:HB3	2:B:595:HIS:CD2	2.50	0.47
5:E:6:LYS:O	6:F:7:LEU:CD2	2.62	0.47
7:H:40:LEU:HB2	7:H:78:LEU:HD12	1.97	0.47
2:J:429:ARG:O	2:J:431:ASN:N	2.48	0.47
2:J:729:LEU:HD22	2:J:731:TYR:CE1	2.49	0.47
1:A:165:TYR:HB2	1:A:181:MET:HB3	1.96	0.47
1:A:209:ARG:HB2	1:A:212:TRP:CD2	2.50	0.47
1:A:645:ARG:HB3	1:A:649:PHE:CE2	2.50	0.47
1:A:750:MET:C	1:A:753:THR:HG22	2.40	0.47
2:B:289:TYR:O	2:B:293:ARG:HB2	2.13	0.47
2:B:324:ALA:O	2:B:328:LEU:HG	2.15	0.47
2:B:429:ARG:O	2:B:431:ASN:N	2.48	0.47
2:B:744:LYS:HB3	2:B:897:PRO:HA	1.97	0.47
2:B:919:ILE:H	2:B:920:PRO:HD2	1.80	0.47
2:B:940:THR:O	10:N:32:GLY:HA3	2.14	0.47
3:C:76:SER:HA	3:C:79:MET:HE3	1.96	0.47
7:H:29:LEU:HD11	7:H:76:TYR:CZ	2.49	0.47
8:K:30:VAL:HB	8:K:31:PRO:HD3	1.96	0.47
10:N:56:ILE:C	10:N:58:GLN:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:160:GLU:HA	1:I:164:ILE:O	2.15	0.47
2:J:57:VAL:HB	2:J:58:PRO:CA	2.35	0.47
2:J:681:LEU:HD13	2:J:696:LEU:HD23	1.97	0.47
3:M:187:LYS:HE3	3:M:201:ARG:HB3	1.96	0.47
9:U:6:ILE:HD11	9:U:16:TYR:CE2	2.50	0.47
10:V:5:VAL:O	10:V:6:ARG:HB2	2.14	0.47
10:V:8:PHE:HB2	10:V:47:ARG:HH22	1.80	0.47
1:A:758:LYS:HA	1:A:758:LYS:HE3	1.96	0.47
1:A:848:ALA:HB2	3:C:327:VAL:HG22	1.97	0.47
2:B:681:LEU:HD13	2:B:696:LEU:HD23	1.97	0.47
4:D:55:PHE:HB2	4:D:58:ILE:HD12	1.95	0.47
1:I:209:ARG:HB2	1:I:212:TRP:CD2	2.49	0.47
1:I:370:ARG:HH21	1:I:417:GLU:CD	2.22	0.47
1:I:704:GLY:C	1:I:706:LEU:H	2.21	0.47
2:J:323:MET:O	2:J:327:VAL:HG23	2.14	0.47
2:J:856:VAL:HG12	11:W:35:LEU:HB2	1.95	0.47
3:M:358:LEU:CD1	3:M:359:ASN:H	2.25	0.47
7:S:29:LEU:HD11	7:S:76:TYR:CZ	2.49	0.47
9:U:50:THR:OG1	9:U:51:MET:N	2.46	0.47
11:W:17:LEU:HD22	11:W:28:PRO:HD2	1.97	0.47
1:A:632:LYS:N	1:A:632:LYS:HE3	2.30	0.47
2:B:378:TYR:C	2:B:380:ARG:H	2.22	0.47
2:B:395:ARG:HD3	2:B:398:ILE:HD11	1.96	0.47
3:C:161:VAL:HG22	3:C:199:VAL:HB	1.95	0.47
5:E:125:ARG:H	5:E:125:ARG:NE	2.12	0.47
10:N:8:PHE:HB2	10:N:47:ARG:HH22	1.80	0.47
1:I:225:MET:HE1	2:J:1106:ASP:O	2.15	0.47
1:I:443:MET:SD	1:I:449:ARG:HD3	2.55	0.47
1:I:476:GLU:HA	8:T:14:GLY:HA3	1.96	0.47
1:I:480:GLU:OE2	2:J:1047:MET:HB2	2.14	0.47
2:J:325:LEU:HD23	2:J:326:LYS:HG2	1.97	0.47
3:M:148:ARG:NH1	3:M:162:GLU:CB	2.66	0.47
5:Q:39:ASP:O	5:Q:43:GLY:N	2.43	0.47
6:R:117:GLU:O	6:R:119:ARG:N	2.48	0.47
1:A:585:LEU:O	1:A:586:GLU:HB3	2.15	0.47
2:B:31:VAL:CG2	2:B:155:PRO:HB2	2.45	0.47
2:B:323:MET:O	2:B:327:VAL:HG23	2.15	0.47
2:B:325:LEU:HD23	2:B:326:LYS:HG2	1.97	0.47
2:B:636:THR:H	2:B:639:HIS:HD2	1.63	0.47
3:C:181:LYS:O	3:C:183:THR:N	2.48	0.47
9:L:6:ILE:HD11	9:L:16:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:305:ALA:O	1:I:309:LYS:HD2	2.14	0.47
1:I:783:TYR:CE2	1:I:789:THR:HB	2.50	0.47
2:J:697:MET:HE1	2:J:721:GLY:HA2	1.95	0.47
2:J:1122:ARG:HD2	6:R:4:ARG:HH21	1.77	0.47
3:M:120:LEU:C	3:M:260:ASP:HB2	2.40	0.47
3:M:160:VAL:HG11	3:M:198:LEU:HD12	1.96	0.47
3:M:266:THR:HB	3:M:272:ILE:HD11	1.97	0.47
10:V:56:ILE:C	10:V:58:GLN:H	2.23	0.47
2:B:373:GLN:CG	2:B:397:SER:HB2	2.45	0.46
2:B:925:VAL:HA	2:B:928:LEU:HD12	1.97	0.46
1:I:430:LEU:HD23	3:M:74:GLU:HG3	1.96	0.46
2:J:151:ASP:HB2	2:J:718:ARG:HH22	1.80	0.46
3:M:187:LYS:CE	3:M:201:ARG:HB3	2.45	0.46
3:M:323:ARG:H	3:M:327:VAL:HB	1.80	0.46
5:Q:6:LYS:O	6:R:7:LEU:CD2	2.63	0.46
9:U:28:LEU:HD23	9:U:57:PHE:HE2	1.79	0.46
1:A:370:ARG:HH21	1:A:417:GLU:CD	2.22	0.46
2:B:342:HIS:HE1	2:B:620:ALA:HB1	1.81	0.46
2:B:574:ASP:OD1	14:B:1301:HOH:O	2.20	0.46
3:C:120:LEU:C	3:C:260:ASP:HB2	2.40	0.46
3:C:189:ALA:HB3	3:C:199:VAL:HG13	1.97	0.46
3:C:323:ARG:H	3:C:327:VAL:HB	1.79	0.46
3:C:325:GLY:O	3:C:329:GLU:HG2	2.14	0.46
3:C:330:LYS:H	3:C:330:LYS:HD3	1.80	0.46
4:D:201:ARG:HA	4:D:204:GLU:HG2	1.96	0.46
10:N:56:ILE:HG12	10:N:60:MET:CG	2.45	0.46
1:I:81:ARG:HG2	1:I:272:TRP:CD2	2.50	0.46
1:I:435:ILE:O	2:J:1043:HIS:CE1	2.68	0.46
3:M:128:ARG:HG3	3:M:241:TYR:HE2	1.77	0.46
4:O:178:ARG:HH12	4:O:197:PHE:HA	1.80	0.46
3:C:194:GLU:CG	3:C:196:TYR:HE2	2.29	0.46
4:D:50:ASN:HD22	4:D:50:ASN:C	2.23	0.46
1:I:645:ARG:HB3	1:I:649:PHE:CE2	2.50	0.46
2:J:513:ARG:HA	2:J:514:ARG:HH11	1.81	0.46
2:J:861:ASP:HB3	2:J:863:THR:HG23	1.98	0.46
5:Q:8:LYS:CG	6:R:7:LEU:HD22	2.45	0.46
9:U:44:THR:C	9:U:45:ILE:CG1	2.88	0.46
1:A:12:GLU:N	2:B:1116:SER:O	2.29	0.46
1:A:462:PHE:HB2	2:B:737:GLU:O	2.15	0.46
2:B:603:THR:HB	2:B:604:LEU:HD23	1.98	0.46
2:B:683:TRP:CD1	2:B:683:TRP:O	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:477:ALA:HA	2:J:1047:MET:HB3	1.97	0.46
2:J:342:HIS:HE1	2:J:620:ALA:HB1	1.81	0.46
2:J:744:LYS:HB3	2:J:897:PRO:HA	1.97	0.46
2:J:1083:CYS:HG	2:J:1086:CYS:HB2	1.76	0.46
3:M:153:ASP:CG	3:M:157:MET:CB	2.87	0.46
1:A:160:GLU:HA	1:A:164:ILE:O	2.15	0.46
2:B:205:ILE:CD1	2:B:303:LEU:H	2.29	0.46
2:B:269:THR:HB	2:B:270:GLN:H	1.55	0.46
2:B:904:THR:HG21	2:B:972:GLU:OE1	2.15	0.46
3:C:194:GLU:CD	3:C:196:TYR:HE2	2.22	0.46
8:K:49:ILE:H	8:K:49:ILE:HG13	1.46	0.46
11:P:43:ALA:O	11:P:44:ARG:HD3	2.16	0.46
1:I:536:ASP:O	1:I:537:VAL:C	2.59	0.46
2:J:21:MET:SD	2:J:645:MET:HB3	2.55	0.46
2:J:636:THR:H	2:J:639:HIS:HD2	1.63	0.46
2:J:650:LEU:HB2	2:J:654:ALA:HB3	1.97	0.46
2:J:683:TRP:CD1	2:J:683:TRP:O	2.66	0.46
2:J:726:VAL:HG11	2:J:992:ILE:HG12	1.98	0.46
3:M:216:GLU:O	3:M:221:HIS:HB2	2.15	0.46
5:Q:27:LYS:HD3	5:Q:51:VAL:HG23	1.97	0.46
1:A:347:LEU:HD22	1:A:444:PRO:HA	1.97	0.46
1:A:405:LYS:HB2	1:A:405:LYS:HE3	1.72	0.46
2:B:861:ASP:HB3	2:B:863:THR:HG23	1.97	0.46
3:C:128:ARG:HG3	3:C:241:TYR:HE2	1.78	0.46
3:C:342:THR:CB	3:C:345:HIS:HB2	2.43	0.46
4:D:200:PRO:HB2	4:D:203:PHE:CD1	2.48	0.46
1:I:569:ILE:HG13	1:I:636:ILE:HD13	1.97	0.46
2:J:17:LEU:HD22	2:J:644:LEU:HA	1.97	0.46
2:J:235:LEU:HD13	2:J:313:ARG:HB3	1.97	0.46
3:M:215:ALA:HA	3:M:219:LYS:HG3	1.98	0.46
9:U:28:LEU:HD23	9:U:57:PHE:CE2	2.51	0.46
2:B:766:ARG:HD3	2:B:772:LYS:HE2	1.98	0.46
3:C:187:LYS:HD3	3:C:203:LYS:NZ	2.30	0.46
10:N:5:VAL:O	10:N:6:ARG:HB2	2.15	0.46
1:I:61:GLU:C	1:I:63:CYS:H	2.23	0.46
1:I:654:THR:OG1	1:I:655:LYS:N	2.47	0.46
1:I:756:ARG:HH12	2:J:922:ARG:HH12	1.64	0.46
2:J:31:VAL:CG2	2:J:155:PRO:HB2	2.45	0.46
2:J:189:LYS:HZ2	3:M:212:ARG:NH1	2.14	0.46
3:M:160:VAL:C	3:M:161:VAL:HG23	2.40	0.46
7:S:40:LEU:HB2	7:S:78:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:75:TYR:HD1	7:S:76:TYR:H	1.64	0.46
1:A:59:ARG:HH12	11:W:21:THR:HG21	1.81	0.46
1:A:94:ARG:HG3	1:A:138:HIS:HD2	1.75	0.46
1:A:580:GLU:H	1:A:580:GLU:HG3	1.63	0.46
1:A:624:LYS:O	1:A:632:LYS:HD3	2.14	0.46
1:A:666:PHE:N	2:B:729:LEU:HD13	2.30	0.46
2:B:432:TYR:O	2:B:435:THR:HG23	2.16	0.46
2:B:447:SER:HB2	2:B:450:GLN:HG2	1.98	0.46
2:B:451:PRO:HB2	2:B:453:PHE:CE1	2.50	0.46
2:B:730:SER:HA	2:B:735:ASN:ND2	2.27	0.46
2:B:731:TYR:OH	2:B:902:PRO:HG3	2.16	0.46
4:D:29:LEU:O	4:D:33:ILE:HG13	2.16	0.46
1:I:103:CYS:SG	1:I:105:ARG:CA	3.03	0.46
1:I:670:ILE:HG21	2:J:932:ILE:HD11	1.97	0.46
2:J:902:PRO:HB2	2:J:974:MET:CG	2.46	0.46
2:J:986:ASP:O	2:J:987:ILE:HD13	2.16	0.46
3:M:152:ILE:HG21	3:M:158:GLU:O	2.16	0.46
3:M:374:GLY:HA2	8:T:7:PHE:CE2	2.51	0.46
5:Q:125:ARG:H	5:Q:125:ARG:NE	2.12	0.46
1:A:307:ARG:C	1:A:309:LYS:H	2.23	0.46
1:A:336:PRO:HD2	2:B:734:TYR:CE1	2.51	0.46
1:A:757:GLY:O	1:A:758:LYS:HD2	2.16	0.46
1:A:805:THR:OG1	1:A:806:ASN:OD1	2.28	0.46
2:B:161:ILE:HD12	2:B:411:LEU:HB3	1.97	0.46
2:B:416:TRP:HB2	2:B:420:ARG:HG3	1.98	0.46
2:B:731:TYR:C	2:B:733:GLY:H	2.23	0.46
2:B:749:ARG:HE	4:D:144:ALA:CB	2.27	0.46
4:D:46:GLU:HA	11:P:45:ARG:HA	1.97	0.46
6:F:117:GLU:O	6:F:119:ARG:N	2.48	0.46
11:P:17:LEU:HD22	11:P:28:PRO:HD2	1.97	0.46
1:I:347:LEU:HD22	1:I:444:PRO:HA	1.97	0.46
1:I:446:ARG:HB3	2:J:1005:MET:SD	2.56	0.46
1:I:639:ARG:NH2	1:I:882:SER:O	2.48	0.46
2:J:429:ARG:HA	2:J:429:ARG:HD2	1.78	0.46
2:J:513:ARG:NH1	2:J:531:THR:OG1	2.48	0.46
2:J:968:HIS:HD2	2:J:969:SER:CA	2.29	0.46
1:A:670:ILE:HG21	2:B:958:ARG:HD3	1.97	0.46
2:B:21:MET:SD	2:B:645:MET:HB3	2.55	0.46
3:C:269:ILE:HG22	3:C:270:TRP:H	1.80	0.46
4:D:178:ARG:HH12	4:D:197:PHE:HA	1.80	0.46
9:L:92:ALA:C	9:L:94:GLU:CD	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:542:GLU:H	1:I:542:GLU:HG2	1.49	0.46
2:J:228:PHE:CE1	2:J:320:LEU:HD22	2.51	0.46
3:M:100:ARG:HH21	3:M:288:GLU:HG2	1.81	0.46
3:M:286:ILE:O	3:M:290:VAL:HG23	2.16	0.46
4:O:127:GLN:HE21	10:V:63:LYS:HG2	1.81	0.46
4:O:219:SER:C	4:O:220:PHE:HD1	2.24	0.46
10:V:56:ILE:HG12	10:V:60:MET:HG2	1.97	0.46
1:A:305:ALA:O	1:A:309:LYS:HD2	2.16	0.45
2:B:56:VAL:CG2	2:B:65:VAL:HB	2.46	0.45
2:B:744:LYS:HG3	2:B:895:ILE:HD11	1.98	0.45
3:C:155:LEU:HD23	3:C:156:ASN:HD22	1.81	0.45
3:C:266:THR:HB	3:C:272:ILE:HD11	1.97	0.45
1:I:443:MET:CB	9:U:49:ILE:HD12	2.38	0.45
1:I:665:GLY:HA2	2:J:729:LEU:HD13	1.91	0.45
1:I:787:VAL:HG23	1:I:801:ARG:HH11	1.81	0.45
1:I:805:THR:OG1	1:I:806:ASN:OD1	2.29	0.45
2:J:901:MET:HE2	2:J:901:MET:HA	1.98	0.45
2:J:925:VAL:HA	2:J:928:LEU:HD12	1.97	0.45
2:J:1059:LYS:HE2	2:J:1096:GLU:HG2	1.98	0.45
2:J:1101:PHE:CD2	3:M:367:ILE:HG13	2.52	0.45
3:M:62:GLU:HG3	3:M:63:ALA:H	1.81	0.45
3:M:157:MET:C	3:M:159:TYR:H	2.24	0.45
5:Q:100:ARG:NE	6:R:43:VAL:HG13	2.31	0.45
11:W:43:ALA:O	11:W:44:ARG:HD3	2.15	0.45
1:A:167:GLU:HG3	1:A:179:HIS:HB3	1.98	0.45
3:C:333:VAL:O	3:C:337:ALA:N	2.50	0.45
1:I:6:LYS:CE	2:J:1122:ARG:CZ	2.63	0.45
1:I:134:ILE:HD13	1:I:134:ILE:HA	1.82	0.45
1:I:507:HIS:NE2	1:I:654:THR:HB	2.32	0.45
2:J:205:ILE:CD1	2:J:303:LEU:H	2.29	0.45
2:J:211:LYS:HG3	3:M:212:ARG:NH2	2.31	0.45
2:J:358:LEU:HD23	2:J:416:TRP:CE2	2.51	0.45
2:J:603:THR:HB	2:J:604:LEU:HD23	1.99	0.45
2:J:904:THR:HG21	2:J:972:GLU:OE1	2.15	0.45
3:M:160:VAL:HG11	3:M:198:LEU:CD1	2.46	0.45
3:M:187:LYS:O	3:M:187:LYS:HG3	2.15	0.45
1:A:264:PRO:O	1:A:266:LEU:N	2.50	0.45
1:A:577:ASP:HA	1:A:581:ARG:HG3	1.97	0.45
2:B:126:LEU:HD12	2:B:127:PRO:HD2	1.99	0.45
2:B:378:TYR:HE1	2:B:388:GLU:HA	0.95	0.45
2:B:636:THR:N	2:B:639:HIS:HD2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:986:ASP:O	2:B:987:ILE:HD13	2.15	0.45
2:B:1059:LYS:HE2	2:B:1096:GLU:HG2	1.98	0.45
3:C:181:LYS:C	3:C:183:THR:N	2.74	0.45
5:E:5:LEU:HD13	6:F:6:LYS:CD	2.46	0.45
1:I:750:MET:HA	1:I:753:THR:HG22	1.97	0.45
2:J:232:MET:HE2	2:J:232:MET:HA	1.99	0.45
2:J:269:THR:HB	2:J:270:GLN:H	1.55	0.45
2:J:432:TYR:O	2:J:435:THR:HG23	2.16	0.45
2:J:637:GLU:H	2:J:637:GLU:HG2	1.42	0.45
2:J:968:HIS:HD2	2:J:969:SER:N	2.15	0.45
2:J:1122:ARG:NE	2:J:1122:ARG:C	2.75	0.45
3:M:104:ILE:HD12	3:M:288:GLU:HB3	1.98	0.45
3:M:217:LYS:C	3:M:218:VAL:HG23	2.41	0.45
4:O:226:THR:HB	4:O:235:ILE:HD11	1.99	0.45
1:A:150:CYS:O	1:A:153:PRO:HD3	2.16	0.45
1:A:639:ARG:NH2	1:A:882:SER:O	2.49	0.45
2:B:122:ARG:HE	2:B:400:PRO:HG3	1.82	0.45
2:B:389:ASN:OD1	2:B:392:ARG:HD3	2.15	0.45
2:B:902:PRO:HB2	2:B:974:MET:CG	2.46	0.45
2:B:942:ARG:CZ	2:B:942:ARG:HB2	2.47	0.45
3:C:62:GLU:HG3	3:C:63:ALA:H	1.81	0.45
3:C:194:GLU:CB	3:C:196:TYR:CD2	2.84	0.45
4:D:50:ASN:ND2	4:D:52:SER:H	2.13	0.45
5:E:3:LYS:CE	6:F:9:GLU:CD	2.90	0.45
6:F:112:ILE:O	6:F:116:ASP:N	2.49	0.45
10:N:60:MET:C	10:N:62:TYR:N	2.73	0.45
1:I:307:ARG:C	1:I:309:LYS:H	2.24	0.45
2:J:25:TRP:HZ2	2:J:485:LEU:HB3	1.80	0.45
2:J:189:LYS:NZ	3:M:212:ARG:NH1	2.64	0.45
2:J:731:TYR:OH	2:J:902:PRO:HG3	2.17	0.45
2:J:919:ILE:H	2:J:920:PRO:HD2	1.80	0.45
3:M:331:ALA:H	3:M:336:ARG:NH1	2.15	0.45
2:B:228:PHE:CE1	2:B:320:LEU:HD22	2.51	0.45
2:B:778:PRO:HD3	2:B:814:GLY:HA3	1.99	0.45
1:I:666:PHE:O	2:J:916:PRO:HG3	2.16	0.45
2:J:56:VAL:CG2	2:J:65:VAL:HB	2.46	0.45
2:J:485:LEU:HD12	2:J:648:ALA:HA	1.98	0.45
2:J:636:THR:N	2:J:639:HIS:HD2	2.14	0.45
2:J:766:ARG:HD3	2:J:772:LYS:HE2	1.99	0.45
3:M:330:LYS:H	3:M:330:LYS:HD3	1.82	0.45
1:A:632:LYS:HE3	1:A:632:LYS:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:TYR:OH	2:B:623:GLU:OE2	2.31	0.45
2:B:131:LYS:N	2:B:135:CYS:SG	2.90	0.45
2:B:231:VAL:O	2:B:235:LEU:HB2	2.17	0.45
2:B:235:LEU:HD13	2:B:313:ARG:HB3	1.98	0.45
2:B:609:LEU:HD22	2:B:614:VAL:HG11	1.97	0.45
2:B:726:VAL:HG11	2:B:992:ILE:HG12	1.98	0.45
3:C:286:ILE:O	3:C:290:VAL:HG23	2.17	0.45
3:C:386:LEU:HD12	3:C:386:LEU:HA	1.66	0.45
6:F:117:GLU:C	6:F:119:ARG:H	2.24	0.45
1:I:445:TYR:CD1	9:U:49:ILE:HG21	2.51	0.45
1:I:791:PHE:CE2	1:I:800:ALA:HA	2.52	0.45
2:J:67:PHE:CD1	2:J:107:MET:HG2	2.52	0.45
2:J:89:PRO:HG3	2:J:99:TYR:CE2	2.51	0.45
2:J:416:TRP:HB2	2:J:420:ARG:HG3	1.98	0.45
2:J:744:LYS:HG3	2:J:895:ILE:HD11	1.98	0.45
2:J:942:ARG:CZ	2:J:942:ARG:HB2	2.47	0.45
2:B:151:ASP:HB2	2:B:718:ARG:HH22	1.81	0.45
2:B:232:MET:HE2	2:B:232:MET:HA	1.99	0.45
2:B:878:LEU:HD23	2:B:878:LEU:HA	1.74	0.45
2:B:939:LEU:HB2	2:B:964:LEU:HD13	1.99	0.45
5:E:5:LEU:HD13	6:F:6:LYS:HD3	1.98	0.45
5:E:42:GLU:O	5:E:78:GLU:HB2	2.17	0.45
1:I:167:GLU:HG3	1:I:179:HIS:HB3	1.99	0.45
2:J:1121:ASP:OD2	3:M:379:LYS:HE3	2.17	0.45
3:M:269:ILE:HG22	3:M:270:TRP:H	1.80	0.45
5:Q:5:LEU:HD13	6:R:6:LYS:CD	2.47	0.45
6:R:112:ILE:O	6:R:116:ASP:N	2.49	0.45
6:R:117:GLU:C	6:R:119:ARG:H	2.24	0.45
1:A:507:HIS:NE2	1:A:654:THR:HB	2.32	0.45
1:A:749:ILE:C	1:A:753:THR:HG22	2.39	0.45
4:D:226:THR:HB	4:D:235:ILE:HD11	1.98	0.45
8:K:24:ALA:HA	8:K:25:PRO:HD2	1.84	0.45
1:I:870:PHE:HE2	7:S:75:TYR:HD1	1.64	0.45
2:J:161:ILE:HD12	2:J:411:LEU:HB3	1.97	0.45
2:J:231:VAL:O	2:J:235:LEU:HB2	2.16	0.45
2:J:239:THR:HG22	2:J:241:LYS:H	1.82	0.45
2:J:447:SER:HB2	2:J:450:GLN:HG2	1.98	0.45
4:O:29:LEU:O	4:O:33:ILE:HG13	2.16	0.45
1:A:147:CYS:HA	1:A:148:PRO:HD3	1.81	0.45
1:A:187:ARG:O	1:A:191:GLU:HG3	2.17	0.45
1:A:543:PRO:O	1:A:544:ASP:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:PHE:CD1	2:B:107:MET:HG2	2.51	0.45
2:B:650:LEU:HB2	2:B:654:ALA:HB3	1.97	0.45
2:B:901:MET:HE2	2:B:901:MET:HA	1.99	0.45
9:L:43:TYR:C	9:L:44:THR:CG2	2.89	0.45
11:P:10:LYS:O	11:P:35:LEU:HA	2.17	0.45
1:I:180:ARG:NH1	1:I:182:MET:SD	2.89	0.45
2:J:63:PHE:HD1	2:J:111:VAL:HG13	1.82	0.45
3:M:157:MET:O	3:M:158:GLU:HB2	2.17	0.45
4:O:50:ASN:ND2	4:O:52:SER:H	2.13	0.45
1:A:791:PHE:CE2	1:A:800:ALA:HA	2.52	0.45
1:A:895:VAL:O	1:A:897:THR:N	2.50	0.45
2:B:63:PHE:HD1	2:B:111:VAL:HG13	1.82	0.45
2:B:89:PRO:HG3	2:B:99:TYR:CE2	2.51	0.45
2:B:815:ARG:HG2	2:B:816:THR:H	1.82	0.45
5:E:27:LYS:HD3	5:E:51:VAL:HG23	1.98	0.45
1:I:103:CYS:SG	1:I:104:GLY:N	2.89	0.45
1:I:639:ARG:HH22	1:I:882:SER:C	2.24	0.45
2:J:41:PHE:HD1	2:J:42:ILE:HD13	1.79	0.45
2:J:503:MET:HA	2:J:507:VAL:HB	1.99	0.45
2:J:731:TYR:C	2:J:733:GLY:H	2.24	0.45
2:J:791:TYR:OH	2:J:838:GLU:OE2	2.25	0.45
3:M:281:ALA:O	3:M:285:ILE:HG12	2.17	0.45
1:A:639:ARG:HH22	1:A:882:SER:C	2.24	0.44
2:B:773:ASP:OD2	2:B:815:ARG:NH1	2.44	0.44
2:B:1062:VAL:HG21	2:B:1097:MET:HE2	1.98	0.44
3:C:104:ILE:HD12	3:C:288:GLU:HB3	1.98	0.44
3:C:288:GLU:O	3:C:292:THR:OG1	2.35	0.44
4:D:27:ASN:HD22	4:D:27:ASN:HA	1.51	0.44
7:H:75:TYR:HD1	7:H:76:TYR:H	1.64	0.44
1:I:485:MET:HE3	2:J:1043:HIS:CD2	2.53	0.44
1:I:750:MET:HE1	2:J:917:HIS:HA	1.98	0.44
1:I:867:ILE:H	1:I:867:ILE:HG13	1.27	0.44
2:J:609:LEU:HD22	2:J:614:VAL:HG11	1.98	0.44
2:J:1080:LYS:HB3	5:Q:154:ARG:HD3	1.99	0.44
3:M:153:ASP:HB2	3:M:160:VAL:HG23	1.98	0.44
5:Q:42:GLU:O	5:Q:78:GLU:HB2	2.17	0.44
7:S:62:GLU:CD	7:S:64:LYS:HZ2	2.25	0.44
9:U:56:ARG:C	9:U:57:PHE:HD1	2.25	0.44
11:W:10:LYS:O	11:W:35:LEU:HA	2.17	0.44
1:A:666:PHE:C	2:B:729:LEU:CD1	2.79	0.44
2:B:968:HIS:HD2	2:B:969:SER:CA	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:ALA:HB1	3:C:270:TRP:CZ2	2.52	0.44
3:C:385:PRO:HA	3:C:386:LEU:CD1	2.48	0.44
4:D:201:ARG:H	4:D:201:ARG:HG3	1.18	0.44
2:B:10:PRO:O	2:B:11:THR:OG1	2.24	0.44
2:B:357:ASP:HA	2:B:360:ARG:NH1	2.32	0.44
2:B:358:LEU:HD23	2:B:416:TRP:CE2	2.51	0.44
3:C:210:ASP:O	3:C:214:ILE:HG13	2.17	0.44
9:L:46:GLU:O	9:L:47:HIS:CG	2.71	0.44
1:I:187:ARG:O	1:I:191:GLU:HG3	2.17	0.44
1:I:404:GLU:O	1:I:406:LEU:HG	2.17	0.44
1:I:758:LYS:HB3	1:I:759:ILE:H	1.53	0.44
2:J:179:THR:HA	2:J:194:VAL:HG22	1.99	0.44
2:J:305:HIS:CE1	2:J:306:MET:HG2	2.53	0.44
9:U:45:ILE:HD13	9:U:53:ARG:NH1	2.32	0.44
1:A:787:VAL:HG23	1:A:801:ARG:HH11	1.82	0.44
2:B:222:VAL:HA	2:B:223:PRO:HD2	1.79	0.44
2:B:286:PRO:HD2	2:B:290:ARG:NE	2.29	0.44
2:B:398:ILE:O	2:B:399:ARG:C	2.61	0.44
2:B:503:MET:HA	2:B:507:VAL:HB	2.00	0.44
2:B:510:ILE:C	2:B:512:GLU:H	2.25	0.44
2:B:853:LYS:HE2	2:B:869:THR:HG21	2.00	0.44
3:C:348:ALA:O	3:C:352:ARG:HG2	2.16	0.44
4:D:181:PRO:HD3	4:D:194:ILE:HD13	1.99	0.44
3:M:154:ILE:HD12	3:M:154:ILE:N	2.32	0.44
5:Q:113:LEU:HD12	5:Q:118:VAL:HG11	2.00	0.44
7:S:42:GLN:HA	7:S:78:LEU:H	1.82	0.44
1:A:50:ARG:C	1:A:61:GLU:HB2	2.43	0.44
1:A:251:ILE:HD13	1:A:274:LEU:HD22	2.00	0.44
1:A:542:GLU:H	1:A:542:GLU:HG2	1.49	0.44
2:B:182:GLU:HG3	2:B:183:ARG:H	1.82	0.44
2:B:239:THR:HG22	2:B:241:LYS:H	1.82	0.44
2:B:485:LEU:HD12	2:B:648:ALA:HA	1.99	0.44
2:B:562:ASP:CG	2:B:563:GLU:H	2.25	0.44
2:B:649:ILE:HD13	2:B:649:ILE:HA	1.80	0.44
5:E:8:LYS:CG	6:F:7:LEU:HD22	2.47	0.44
1:I:41:PRO:HB2	1:I:42:ILE:HD13	2.00	0.44
2:J:25:TRP:CH2	2:J:485:LEU:HD22	2.52	0.44
2:J:131:LYS:N	2:J:135:CYS:SG	2.89	0.44
2:J:509:PRO:C	2:J:511:GLU:H	2.24	0.44
2:J:729:LEU:HB3	2:J:731:TYR:HE1	1.82	0.44
2:J:809:LYS:H	2:J:809:LYS:HG2	1.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1068:CYS:SG	2:J:1070:HIS:CG	3.11	0.44
4:O:50:ASN:ND2	4:O:52:SER:OG	2.42	0.44
9:U:51:MET:CA	9:U:52:ALA:C	2.86	0.44
1:A:180:ARG:NH1	1:A:182:MET:SD	2.90	0.44
1:A:632:LYS:HZ2	1:A:633:LEU:H	1.66	0.44
1:A:743:MET:HA	1:A:748:VAL:HG11	2.00	0.44
2:B:25:TRP:CH2	2:B:485:LEU:HD22	2.53	0.44
2:B:703:PRO:HG3	2:B:715:PHE:HE2	1.83	0.44
2:B:745:ALA:HB1	2:B:749:ARG:CZ	2.48	0.44
2:B:781:ASN:CG	2:B:782:ILE:H	2.25	0.44
2:B:902:PRO:HB2	2:B:974:MET:HG2	1.99	0.44
3:C:177:LYS:H	3:C:177:LYS:HG3	1.64	0.44
4:D:50:ASN:ND2	4:D:52:SER:OG	2.41	0.44
5:E:3:LYS:CE	6:F:9:GLU:OE1	2.64	0.44
1:I:152:ALA:HA	1:I:153:PRO:HD2	1.79	0.44
1:I:445:TYR:HD2	2:J:878:LEU:HD12	1.83	0.44
1:I:667:THR:HA	2:J:916:PRO:HB3	1.99	0.44
2:J:322:MET:HE1	2:J:523:TYR:HE2	1.83	0.44
5:Q:112:GLN:HA	5:Q:166:ARG:HG3	2.00	0.44
7:S:37:ILE:H	7:S:37:ILE:HG12	1.31	0.44
10:V:6:ARG:HB3	10:V:7:CYS:H	1.44	0.44
1:A:891:ASP:OD1	1:A:891:ASP:N	2.42	0.44
2:B:322:MET:HE1	2:B:523:TYR:HE2	1.83	0.44
3:C:216:GLU:HA	3:C:220:LYS:HB3	2.00	0.44
4:D:199:LEU:HD21	4:D:211:ILE:HG21	1.99	0.44
5:E:112:GLN:HA	5:E:166:ARG:HG3	2.00	0.44
1:I:244:LYS:HE3	1:I:244:LYS:HB2	1.66	0.44
1:I:295:HIS:O	1:I:297:SER:N	2.49	0.44
2:J:35:LEU:CD2	2:J:132:SER:HA	2.48	0.44
2:J:122:ARG:HE	2:J:400:PRO:HG3	1.82	0.44
3:M:107:ALA:HB1	3:M:270:TRP:CZ2	2.52	0.44
3:M:159:TYR:C	3:M:160:VAL:CG2	2.91	0.44
3:M:364:ASN:O	3:M:367:ILE:HG22	2.18	0.44
1:A:93:HIS:CE1	1:A:160:GLU:HB2	2.53	0.44
2:B:573:ASP:OD1	2:B:576:ARG:NE	2.40	0.44
3:C:144:GLU:H	3:C:144:GLU:HG2	1.54	0.44
5:E:113:LEU:HD12	5:E:118:VAL:HG11	2.00	0.44
11:P:14:GLU:OE2	11:P:30:CYS:SG	2.75	0.44
1:I:74:PHE:CE1	1:I:221:PRO:HA	2.53	0.44
1:I:93:HIS:NE2	1:I:160:GLU:HB2	2.33	0.44
1:I:673:GLU:CB	1:I:809:LYS:HD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:756:ARG:NH2	2:J:922:ARG:HH22	2.16	0.44
2:J:41:PHE:HE2	2:J:356:LYS:CG	2.31	0.44
2:J:126:LEU:HD12	2:J:127:PRO:HD2	1.99	0.44
2:J:393:PHE:O	2:J:394:VAL:HG23	2.13	0.44
2:J:902:PRO:HB2	2:J:974:MET:HG2	2.00	0.44
3:M:384:LEU:O	5:Q:22:PRO:HG3	2.18	0.44
11:W:14:GLU:HB2	11:W:15:VAL:H	1.59	0.44
1:A:100:CYS:O	1:A:103:CYS:SG	2.75	0.44
1:A:104:GLY:O	1:A:194:PRO:HD2	2.17	0.44
1:A:852:LEU:HD11	3:C:311:MET:HG3	1.99	0.44
2:B:539:VAL:HG12	2:B:557:VAL:HG12	1.99	0.44
3:C:100:ARG:HH21	3:C:288:GLU:HG2	1.81	0.44
3:C:281:ALA:O	3:C:285:ILE:HG12	2.18	0.44
4:D:219:SER:C	4:D:220:PHE:HD1	2.26	0.44
9:L:43:TYR:C	9:L:44:THR:HG23	2.41	0.44
9:L:52:ALA:O	9:L:53:ARG:HB2	2.17	0.44
1:I:104:GLY:O	1:I:194:PRO:HD2	2.18	0.44
1:I:106:ILE:HD13	1:I:201:LEU:HD11	2.00	0.44
1:I:351:MET:HG2	1:I:415:HIS:ND1	2.33	0.44
2:J:357:ASP:HA	2:J:360:ARG:NH1	2.32	0.44
2:J:778:PRO:HD3	2:J:814:GLY:HA3	1.99	0.44
2:J:905:GLU:CD	4:O:154:LYS:HE2	2.43	0.44
2:J:1062:VAL:HG21	2:J:1097:MET:HE2	1.98	0.44
2:J:1063:TRP:HE1	2:J:1094:LYS:HE3	1.82	0.44
3:M:160:VAL:CG1	3:M:161:VAL:H	2.21	0.44
4:O:54:LEU:HD11	10:V:2:ILE:HD12	1.98	0.44
5:Q:61:PRO:HA	8:T:11:ARG:NH2	2.33	0.44
7:S:41:PRO:HG2	7:S:75:TYR:CE1	2.53	0.44
9:U:35:ASN:ND2	9:U:73:GLU:OE1	2.51	0.44
1:A:93:HIS:NE2	1:A:160:GLU:HB2	2.33	0.43
1:A:172:GLU:OE1	1:A:173:GLU:N	2.51	0.43
1:A:867:ILE:H	1:A:867:ILE:HG13	1.28	0.43
2:B:365:GLN:HE21	2:B:365:GLN:HB3	1.56	0.43
2:B:688:ILE:HD11	10:N:62:TYR:CD1	2.52	0.43
2:B:968:HIS:HD2	2:B:969:SER:N	2.16	0.43
3:C:163:ILE:H	3:C:163:ILE:CD1	2.08	0.43
3:C:303:ARG:HA	3:C:306:MET:HE2	1.99	0.43
3:C:384:LEU:HD21	5:E:18:PHE:HA	2.00	0.43
7:H:42:GLN:HA	7:H:78:LEU:H	1.82	0.43
9:L:35:ASN:ND2	9:L:73:GLU:OE1	2.52	0.43
1:I:50:ARG:C	1:I:61:GLU:HB2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:536:ASP:HA	1:I:540:LEU:HB2	2.00	0.43
1:I:852:LEU:HD13	3:M:307:LEU:HD21	1.99	0.43
2:J:182:GLU:HG3	2:J:183:ARG:H	1.82	0.43
2:J:222:VAL:HA	2:J:223:PRO:HD2	1.79	0.43
2:J:491:THR:HB	2:J:492:GLY:H	1.58	0.43
2:J:992:ILE:HD11	2:J:994:TYR:CE1	2.53	0.43
3:M:269:ILE:H	3:M:269:ILE:HG13	1.57	0.43
3:M:288:GLU:O	3:M:292:THR:OG1	2.35	0.43
3:M:303:ARG:HA	3:M:306:MET:HE2	1.99	0.43
4:O:62:ARG:HH12	10:V:2:ILE:HD12	1.83	0.43
4:O:181:PRO:HD3	4:O:194:ILE:HD13	1.99	0.43
5:Q:14:PRO:HD2	5:Q:17:MET:HE2	2.01	0.43
5:Q:167:GLN:HB2	5:Q:170:LEU:HD12	1.99	0.43
6:R:120:PRO:O	6:R:122:GLU:N	2.44	0.43
1:A:664:LYS:HG2	2:B:984:GLU:OE2	2.18	0.43
2:B:179:THR:HA	2:B:194:VAL:HG22	2.00	0.43
5:E:167:GLN:HB2	5:E:170:LEU:HD12	1.99	0.43
8:K:8:GLU:HB3	8:K:53:VAL:HG21	2.00	0.43
1:I:264:PRO:O	1:I:266:LEU:N	2.49	0.43
1:I:894:ILE:HD13	3:M:45:ILE:HD13	2.00	0.43
2:J:280:LEU:HD23	2:J:280:LEU:HA	1.89	0.43
2:J:562:ASP:CG	2:J:563:GLU:H	2.24	0.43
2:J:745:ALA:HB1	2:J:749:ARG:CZ	2.48	0.43
2:J:925:VAL:O	2:J:929:ILE:HG13	2.18	0.43
4:O:199:LEU:HD21	4:O:211:ILE:HG21	1.99	0.43
1:A:155:PHE:HA	1:A:156:PRO:HD2	1.75	0.43
1:A:163:THR:HB	1:A:276:GLN:NE2	2.33	0.43
1:A:673:GLU:CB	1:A:809:LYS:HD2	2.48	0.43
2:B:148:LEU:HA	2:B:148:LEU:HD13	1.63	0.43
2:B:391:GLN:HE22	2:B:393:PHE:HE2	1.65	0.43
2:B:391:GLN:C	2:B:393:PHE:N	2.68	0.43
2:B:510:ILE:C	2:B:512:GLU:N	2.76	0.43
2:B:574:ASP:OD1	2:B:574:ASP:N	2.51	0.43
3:C:149:GLU:C	3:C:150:GLU:HG2	2.43	0.43
4:D:119:PRO:HD2	10:N:15:ALA:HB1	2.00	0.43
5:E:174:GLU:HG3	5:E:175:TRP:N	2.33	0.43
1:I:150:CYS:C	1:I:152:ALA:N	2.77	0.43
1:I:309:LYS:HZ1	3:M:346:LEU:HG	1.83	0.43
1:I:765:MET:HG3	2:J:923:MET:HG2	1.99	0.43
2:J:391:GLN:HB3	2:J:392:ARG:H	1.67	0.43
2:J:539:VAL:HG12	2:J:557:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:853:LYS:HE2	2:J:869:THR:HG21	2.00	0.43
3:M:336:ARG:HB3	3:M:345:HIS:HB3	2.00	0.43
3:M:385:PRO:HA	5:Q:22:PRO:HD3	1.99	0.43
9:U:48:PRO:O	9:U:51:MET:HE3	2.17	0.43
1:A:10:SER:CB	2:B:1118:ARG:HB3	2.48	0.43
1:A:527:GLU:HG3	9:L:40:PHE:CD1	2.53	0.43
4:D:92:GLU:HB2	4:D:130:THR:HG23	2.00	0.43
1:I:127:LYS:HB2	3:M:330:LYS:HB3	2.01	0.43
2:J:31:VAL:C	2:J:33:GLN:H	2.27	0.43
2:J:1040:LEU:O	2:J:1042:GLY:N	2.49	0.43
3:M:236:LYS:O	3:M:237:GLU:HB3	2.18	0.43
3:M:359:ASN:OD1	14:M:401:HOH:O	2.21	0.43
1:A:8:ILE:HB	3:C:369:GLN:OE1	2.19	0.43
1:A:757:GLY:O	1:A:758:LYS:HB2	2.17	0.43
2:B:25:TRP:HZ2	2:B:485:LEU:HB3	1.80	0.43
2:B:485:LEU:HD11	2:B:655:SER:OG	2.19	0.43
2:B:702:VAL:O	10:N:51:SER:HB2	2.19	0.43
2:B:992:ILE:HD11	2:B:994:TYR:CE1	2.53	0.43
3:C:152:ILE:HG13	3:C:159:TYR:CD2	2.48	0.43
10:N:62:TYR:C	10:N:63:LYS:HD2	2.42	0.43
1:I:444:PRO:O	9:U:49:ILE:CD1	2.58	0.43
2:J:378:TYR:CZ	2:J:388:GLU:CD	2.96	0.43
2:J:749:ARG:HE	4:O:144:ALA:CB	2.30	0.43
1:A:351:MET:HG2	1:A:415:HIS:ND1	2.33	0.43
1:A:635:ASP:O	1:A:638:VAL:HG22	2.18	0.43
1:A:885:GLY:O	3:C:303:ARG:NH2	2.46	0.43
2:B:35:LEU:CD2	2:B:132:SER:HA	2.48	0.43
3:C:187:LYS:CE	3:C:206:THR:HB	2.48	0.43
1:I:76:HIS:C	1:I:76:HIS:CD2	2.97	0.43
1:I:93:HIS:CE1	1:I:160:GLU:HB2	2.53	0.43
2:J:46:LEU:O	2:J:50:VAL:HG12	2.19	0.43
3:M:162:GLU:C	3:M:163:ILE:HG13	2.44	0.43
4:O:24:PRO:HG3	9:U:30:GLU:CD	2.44	0.43
5:Q:5:LEU:CD1	6:R:6:LYS:CD	2.96	0.43
7:S:43:ILE:HG22	7:S:44:LYS:N	2.34	0.43
1:A:106:ILE:HD13	1:A:201:LEU:HD11	2.01	0.43
2:B:99:TYR:HB2	2:B:160:ILE:HB	2.01	0.43
2:B:305:HIS:CE1	2:B:306:MET:HG2	2.53	0.43
2:B:1066:GLU:HA	2:B:1119:LEU:HD22	2.00	0.43
7:H:10:PHE:O	7:H:11:ASP:C	2.61	0.43
7:H:41:PRO:HG2	7:H:75:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:436:MET:HB2	1:I:458:TYR:OH	2.19	0.43
1:I:834:ARG:NH1	3:M:99:PRO:HD3	2.30	0.43
2:J:749:ARG:HG2	4:O:65:MET:HE1	2.00	0.43
3:M:177:LYS:HZ2	3:M:224:LYS:HD3	1.83	0.43
3:M:333:VAL:O	3:M:337:ALA:N	2.51	0.43
4:O:225:GLU:OE2	10:V:42:ARG:NH2	2.51	0.43
6:R:93:ARG:HG2	6:R:102:MET:HE1	2.00	0.43
7:S:67:SER:C	7:S:69:THR:H	2.27	0.43
1:A:684:HIS:O	1:A:688:ARG:HG3	2.19	0.43
2:B:516:ALA:HA	2:B:517:PRO:HA	1.72	0.43
2:B:698:HIS:HE1	2:B:873:LEU:HD21	1.84	0.43
2:B:749:ARG:NH1	4:D:150:PHE:HZ	2.17	0.43
1:I:150:CYS:CB	1:I:153:PRO:HD3	2.48	0.43
1:I:251:ILE:HD13	1:I:274:LEU:HD22	2.00	0.43
1:I:582:CYS:HB2	1:I:608:PHE:CE1	2.54	0.43
2:J:780:PRO:HA	2:J:785:TYR:CZ	2.54	0.43
3:M:100:ARG:O	3:M:104:ILE:HG22	2.19	0.43
3:M:182:LEU:O	3:M:183:THR:C	2.61	0.43
8:T:38:GLN:H	8:T:38:GLN:HG2	1.37	0.43
1:A:103:CYS:SG	1:A:104:GLY:N	2.91	0.43
3:C:13:LYS:HE2	3:C:13:LYS:HB2	1.82	0.43
1:I:370:ARG:HD3	1:I:379:PRO:O	2.19	0.43
1:I:432:ARG:C	1:I:434:SER:H	2.27	0.43
1:I:447:THR:HG22	2:J:1001:VAL:HG21	2.00	0.43
1:I:543:PRO:O	1:I:544:ASP:HB2	2.18	0.43
1:I:632:LYS:NZ	1:I:634:LEU:H	2.08	0.43
1:I:808:TYR:HE2	2:J:923:MET:SD	2.42	0.43
2:J:429:ARG:HG3	2:J:683:TRP:CZ3	2.54	0.43
3:M:100:ARG:NH2	3:M:267:ASN:O	2.52	0.43
4:O:92:GLU:HB2	4:O:130:THR:HG23	1.99	0.43
2:B:780:PRO:HA	2:B:785:TYR:CZ	2.54	0.43
5:E:100:ARG:NE	6:F:43:VAL:HG13	2.34	0.43
1:I:564:PRO:HB2	1:I:567:LEU:HD21	2.01	0.43
1:I:743:MET:HA	1:I:748:VAL:HG11	2.00	0.43
2:J:41:PHE:HD1	2:J:42:ILE:CD1	2.32	0.43
3:M:205:VAL:O	3:M:205:VAL:HG12	2.19	0.43
7:S:43:ILE:HG22	7:S:44:LYS:H	1.84	0.43
7:S:56:LYS:O	7:S:58:GLY:N	2.51	0.43
1:A:150:CYS:SG	1:A:153:PRO:CD	3.07	0.42
1:A:370:ARG:HD3	1:A:379:PRO:O	2.19	0.42
2:B:17:LEU:HB3	2:B:644:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:PHE:O	2:B:394:VAL:CG1	2.67	0.42
2:B:591:LEU:HD22	2:B:595:HIS:NE2	2.34	0.42
3:C:164:ASP:CG	3:C:165:PRO:CD	2.86	0.42
3:C:179:VAL:HG22	3:C:190:GLU:OE2	2.19	0.42
3:C:385:PRO:HA	3:C:386:LEU:HD13	2.01	0.42
4:D:45:VAL:O	11:P:46:VAL:N	2.47	0.42
4:D:98:MET:HG2	4:D:100:TYR:HE1	1.84	0.42
5:E:92:MET:HE1	5:E:127:PHE:CE2	2.29	0.42
7:H:13:VAL:HG13	7:H:14:LEU:H	1.84	0.42
7:H:56:LYS:O	7:H:58:GLY:N	2.51	0.42
10:N:62:TYR:O	10:N:63:LYS:HG3	2.20	0.42
1:I:17:SER:HB3	1:I:20:GLU:HG3	2.00	0.42
1:I:159:PHE:HD1	1:I:159:PHE:HA	1.78	0.42
1:I:626:TYR:HA	1:I:632:LYS:NZ	2.34	0.42
2:J:165:GLU:OE2	2:J:689:ARG:NH2	2.52	0.42
2:J:220:PRO:HD2	2:J:301:ASN:HB3	2.01	0.42
2:J:591:LEU:HD22	2:J:595:HIS:NE2	2.34	0.42
2:J:703:PRO:HG3	2:J:715:PHE:HE2	1.83	0.42
2:J:781:ASN:CG	2:J:782:ILE:H	2.25	0.42
2:J:939:LEU:HB2	2:J:964:LEU:HD13	1.99	0.42
2:J:1066:GLU:HA	2:J:1119:LEU:HD22	2.00	0.42
2:J:1101:PHE:CD1	3:M:367:ILE:HG13	2.54	0.42
3:M:178:VAL:O	3:M:190:GLU:OE1	2.37	0.42
3:M:347:PHE:CD1	3:M:347:PHE:C	2.96	0.42
8:T:8:GLU:HB3	8:T:53:VAL:HG21	2.00	0.42
1:A:120:PHE:CD2	1:A:133:LEU:HD11	2.54	0.42
1:A:221:PRO:O	1:A:226:ARG:NH2	2.49	0.42
2:B:41:PHE:HD1	2:B:356:LYS:HG2	1.83	0.42
2:B:389:ASN:CG	2:B:392:ARG:HB2	2.44	0.42
2:B:429:ARG:HG3	2:B:683:TRP:CZ3	2.54	0.42
3:C:100:ARG:O	3:C:104:ILE:HG22	2.19	0.42
3:C:116:MET:HE1	3:C:253:VAL:HG21	2.01	0.42
3:C:214:ILE:HG22	3:C:218:VAL:HB	2.01	0.42
3:C:347:PHE:CD1	3:C:347:PHE:C	2.96	0.42
3:C:364:ASN:O	3:C:367:ILE:HG22	2.19	0.42
7:H:67:SER:C	7:H:69:THR:H	2.27	0.42
9:L:28:LEU:HD23	9:L:57:PHE:HE2	1.84	0.42
1:I:444:PRO:CB	9:U:50:THR:HG22	2.48	0.42
2:J:573:ASP:OD1	2:J:576:ARG:NE	2.40	0.42
2:J:649:ILE:HD13	2:J:649:ILE:HA	1.79	0.42
2:J:815:ARG:HG2	2:J:816:THR:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:262:THR:HA	7:S:12:HIS:HB3	2.01	0.42
5:Q:174:GLU:HG3	5:Q:175:TRP:N	2.33	0.42
6:R:38:PHE:CD2	6:R:40:GLU:HG2	2.54	0.42
2:B:573:ASP:HB2	2:B:574:ASP:H	1.63	0.42
3:C:160:VAL:CG2	3:C:198:LEU:HB3	2.47	0.42
5:E:14:PRO:HD2	5:E:17:MET:HE2	2.01	0.42
6:F:93:ARG:HG2	6:F:102:MET:HE1	2.00	0.42
7:H:65:ARG:NH1	7:H:75:TYR:HD2	2.18	0.42
1:I:495:ARG:HG2	3:M:300:VAL:HG23	2.02	0.42
1:I:684:HIS:O	1:I:688:ARG:HG3	2.19	0.42
1:I:889:ASP:O	1:I:893:VAL:HG23	2.20	0.42
2:J:99:TYR:HB2	2:J:160:ILE:HB	2.01	0.42
2:J:498:VAL:O	2:J:502:LEU:HG	2.19	0.42
2:J:749:ARG:HH21	4:O:144:ALA:HB1	1.83	0.42
2:J:903:TRP:HE1	4:O:153:TYR:H	1.67	0.42
3:M:116:MET:HE1	3:M:253:VAL:HG21	2.01	0.42
3:M:159:TYR:C	3:M:160:VAL:HG23	2.45	0.42
1:A:9:GLY:O	3:C:358:LEU:HD11	2.19	0.42
1:A:17:SER:HB3	1:A:20:GLU:HG3	2.01	0.42
1:A:445:TYR:C	1:A:446:ARG:HG3	2.44	0.42
2:B:31:VAL:C	2:B:33:GLN:H	2.26	0.42
2:B:220:PRO:HD2	2:B:301:ASN:HB3	2.01	0.42
2:B:1063:TRP:CZ3	2:B:1074:GLU:CD	2.77	0.42
7:H:43:ILE:HG22	7:H:44:LYS:H	1.84	0.42
10:N:52:HIS:CE1	10:N:54:GLU:H	2.38	0.42
1:I:31:VAL:HA	1:I:32:PRO:HD3	1.86	0.42
1:I:364:TYR:OH	1:I:406:LEU:HB3	2.19	0.42
1:I:878:ASP:HA	1:I:879:PRO:HD2	1.85	0.42
2:J:365:GLN:HG2	2:J:365:GLN:H	1.66	0.42
2:J:510:ILE:HA	2:J:513:ARG:NH2	2.34	0.42
3:M:182:LEU:HA	3:M:185:SER:OG	2.19	0.42
4:O:60:ALA:HB1	11:W:48:ALA:HB2	2.00	0.42
5:Q:145:ARG:NH2	6:R:94:VAL:HG23	2.35	0.42
5:Q:174:GLU:O	5:Q:178:LYS:HB2	2.19	0.42
8:T:49:ILE:H	8:T:49:ILE:HG13	1.46	0.42
1:A:55:ASP:C	1:A:57:GLY:H	2.26	0.42
2:B:378:TYR:CE1	2:B:389:ASN:N	2.83	0.42
2:B:925:VAL:O	2:B:929:ILE:HG13	2.20	0.42
3:C:187:LYS:O	3:C:188:SER:HB2	2.20	0.42
6:F:38:PHE:CD2	6:F:40:GLU:HG2	2.54	0.42
9:L:28:LEU:HD23	9:L:57:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:456:PRO:HB3	1:I:628:ARG:NH1	2.35	0.42
1:I:712:LYS:HD2	3:M:93:ASN:OD1	2.20	0.42
3:M:130:LYS:O	3:M:134:VAL:HG23	2.19	0.42
3:M:148:ARG:HB3	3:M:164:ASP:CG	2.44	0.42
3:M:160:VAL:CG1	3:M:161:VAL:N	2.79	0.42
3:M:183:THR:C	3:M:185:SER:N	2.75	0.42
3:M:213:LYS:O	3:M:216:GLU:HG3	2.18	0.42
2:B:58:PRO:HG3	2:B:63:PHE:HB2	2.02	0.42
2:B:498:VAL:O	2:B:502:LEU:HG	2.19	0.42
3:C:153:ASP:CG	3:C:159:TYR:HA	2.45	0.42
4:D:161:VAL:HG11	4:D:171:LEU:HD12	2.01	0.42
5:E:3:LYS:HZ2	6:F:9:GLU:CD	2.27	0.42
5:E:174:GLU:O	5:E:178:LYS:HB2	2.19	0.42
1:I:404:GLU:H	1:I:404:GLU:HG2	1.69	0.42
2:J:517:PRO:C	2:J:519:LEU:H	2.27	0.42
3:M:109:LYS:HA	3:M:270:TRP:CD1	2.55	0.42
3:M:343:THR:OG1	3:M:344:GLN:OE1	2.34	0.42
9:U:49:ILE:HG22	9:U:50:THR:N	2.21	0.42
1:A:456:PRO:HB3	1:A:628:ARG:NH1	2.35	0.42
1:A:462:PHE:CD2	2:B:737:GLU:HB2	2.55	0.42
2:B:554:VAL:HA	2:B:578:ARG:NH1	2.35	0.42
1:I:9:GLY:HA3	2:J:1120:LYS:CG	2.50	0.42
1:I:44:GLY:HA2	1:I:49:LYS:HD3	2.01	0.42
1:I:120:PHE:CD2	1:I:133:LEU:HD11	2.54	0.42
1:I:439:ARG:NH1	1:I:486:GLU:OE2	2.52	0.42
1:I:635:ASP:O	1:I:638:VAL:HG22	2.18	0.42
1:I:658:ILE:HD13	2:J:733:GLY:HA3	2.02	0.42
1:I:756:ARG:NH1	2:J:922:ARG:HH12	2.17	0.42
7:S:65:ARG:NH1	7:S:75:TYR:HD2	2.17	0.42
1:A:852:LEU:HD21	3:C:311:MET:HE2	2.02	0.42
1:A:863:PRO:HB2	3:C:360:GLY:HA2	2.02	0.42
2:B:31:VAL:HG21	2:B:155:PRO:HB2	2.02	0.42
2:B:77:PHE:HD1	2:B:77:PHE:HA	1.67	0.42
2:B:189:LYS:HB3	2:B:190:VAL:H	1.60	0.42
2:B:681:LEU:O	2:B:718:ARG:HB3	2.20	0.42
3:C:72:ILE:HD12	3:C:72:ILE:HA	1.89	0.42
7:H:62:GLU:CD	7:H:64:LYS:HZ2	2.27	0.42
1:I:368:LYS:O	1:I:372:LEU:HB2	2.20	0.42
1:I:781:ARG:HH22	2:J:341:ASP:HB2	1.84	0.42
2:J:645:MET:HA	2:J:646:PRO:HD2	1.95	0.42
2:J:1054:LEU:C	2:J:1056:GLU:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:150:GLU:CD	3:M:219:LYS:HE2	2.44	0.42
3:M:348:ALA:O	3:M:352:ARG:HG2	2.18	0.42
4:O:24:PRO:HB3	9:U:30:GLU:OE1	2.19	0.42
5:Q:48:ILE:HA	5:Q:74:VAL:HG13	2.01	0.42
2:B:63:PHE:HB3	2:B:392:ARG:NH2	2.34	0.42
2:B:365:GLN:HG2	2:B:365:GLN:H	1.67	0.42
3:C:163:ILE:HG22	3:C:165:PRO:HD3	2.02	0.42
1:I:147:CYS:SG	1:I:152:ALA:HA	2.58	0.42
1:I:587:LYS:HB2	1:I:588:LEU:H	1.72	0.42
1:I:656:LEU:O	1:I:660:VAL:HG23	2.20	0.42
2:J:17:LEU:HB3	2:J:644:LEU:O	2.19	0.42
2:J:485:LEU:HD11	2:J:655:SER:OG	2.19	0.42
2:J:898:GLN:O	2:J:901:MET:HB2	2.20	0.42
8:T:16:ARG:HG2	8:T:49:ILE:HG22	2.02	0.42
1:A:61:GLU:C	1:A:63:CYS:H	2.23	0.42
1:A:150:CYS:O	1:A:152:ALA:CA	2.65	0.42
1:A:439:ARG:NH1	1:A:486:GLU:OE2	2.52	0.42
1:A:521:PHE:N	1:A:521:PHE:CD1	2.88	0.42
1:A:772:GLN:HB2	1:A:779:LEU:HD11	2.02	0.42
2:B:366:LEU:HD21	2:B:398:ILE:O	2.20	0.42
3:C:109:LYS:HA	3:C:270:TRP:CD1	2.55	0.42
3:C:177:LYS:HE2	3:C:178:VAL:N	2.34	0.42
7:H:43:ILE:HG22	7:H:44:LYS:N	2.34	0.42
9:L:93:ILE:C	9:L:94:GLU:CD	2.87	0.42
1:I:432:ARG:O	1:I:434:SER:N	2.53	0.42
1:I:553:TRP:HB3	1:I:558:ILE:HD11	2.01	0.42
2:J:31:VAL:HG21	2:J:155:PRO:HB2	2.02	0.42
2:J:758:ARG:NH1	2:J:844:ARG:HG3	2.34	0.42
3:M:160:VAL:C	3:M:161:VAL:CG2	2.93	0.42
1:A:76:HIS:C	1:A:76:HIS:CD2	2.97	0.41
1:A:463:ASP:HA	2:B:890:GLY:CA	2.49	0.41
1:A:656:LEU:O	1:A:660:VAL:HG23	2.20	0.41
2:B:486:MET:HE3	2:B:486:MET:HB3	1.84	0.41
2:B:510:ILE:HA	2:B:513:ARG:HG3	2.01	0.41
2:B:801:PHE:O	2:B:804:SER:OG	2.36	0.41
3:C:165:PRO:HG2	3:C:166:GLU:OE2	2.20	0.41
3:C:194:GLU:C	3:C:196:TYR:N	2.76	0.41
3:C:262:THR:C	7:H:13:VAL:HB	2.45	0.41
4:D:23:VAL:HA	4:D:220:PHE:HE2	1.85	0.41
1:I:782:GLY:O	2:J:459:HIS:HE1	2.03	0.41
2:J:681:LEU:O	2:J:718:ARG:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:61:HIS:O	4:O:65:MET:HG2	2.20	0.41
1:A:756:ARG:HB3	2:B:921:SER:HB3	2.01	0.41
2:B:130:LEU:HD22	2:B:158:TYR:CZ	2.55	0.41
2:B:165:GLU:OE2	2:B:689:ARG:NH2	2.52	0.41
2:B:183:ARG:HH21	2:B:454:GLU:CD	2.29	0.41
2:B:731:TYR:HE2	2:B:902:PRO:CG	2.31	0.41
2:B:809:LYS:H	2:B:809:LYS:HG2	1.52	0.41
7:H:66:LYS:HG2	7:H:72:TYR:CE1	2.55	0.41
2:J:148:LEU:HA	2:J:148:LEU:HD13	1.63	0.41
2:J:286:PRO:HD2	2:J:290:ARG:NE	2.28	0.41
2:J:498:VAL:HG12	2:J:502:LEU:HD11	2.02	0.41
2:J:554:VAL:HA	2:J:578:ARG:NH1	2.35	0.41
2:J:749:ARG:NH1	4:O:150:PHE:HZ	2.18	0.41
2:J:968:HIS:C	2:J:968:HIS:HD2	2.27	0.41
4:O:112:LYS:HE2	4:O:112:LYS:HB3	1.89	0.41
1:A:432:ARG:C	1:A:434:SER:H	2.27	0.41
1:A:441:ARG:O	1:A:443:MET:HG3	2.20	0.41
1:A:553:TRP:HB3	1:A:558:ILE:HD11	2.02	0.41
1:A:854:VAL:CG2	3:C:62:GLU:HB3	2.50	0.41
2:B:940:THR:OG1	2:B:964:LEU:HD11	2.20	0.41
3:C:21:LYS:HE3	3:C:21:LYS:HB3	1.41	0.41
3:C:100:ARG:NH2	3:C:267:ASN:O	2.52	0.41
5:E:3:LYS:HD2	6:F:11:TYR:CE1	2.55	0.41
5:E:48:ILE:HA	5:E:74:VAL:HG13	2.03	0.41
9:L:93:ILE:C	9:L:94:GLU:CG	2.93	0.41
1:I:31:VAL:HG11	1:I:43:GLU:OE1	2.20	0.41
1:I:222:PRO:CD	1:I:225:MET:HE2	2.50	0.41
1:I:521:PHE:N	1:I:521:PHE:CD1	2.88	0.41
2:J:940:THR:OG1	2:J:964:LEU:HD11	2.20	0.41
4:O:161:VAL:HG11	4:O:171:LEU:HD12	2.01	0.41
1:A:244:LYS:O	1:A:248:ILE:HG13	2.21	0.41
1:A:331:VAL:HG23	2:B:1001:VAL:HG23	2.01	0.41
1:A:368:LYS:O	1:A:372:LEU:HB2	2.20	0.41
1:A:635:ASP:OD1	1:A:639:ARG:NE	2.50	0.41
1:A:878:ASP:HA	1:A:879:PRO:HD2	1.85	0.41
1:A:889:ASP:O	1:A:893:VAL:HG23	2.20	0.41
2:B:517:PRO:C	2:B:519:LEU:H	2.27	0.41
3:C:215:ALA:O	3:C:220:LYS:HB2	2.19	0.41
4:D:61:HIS:O	4:D:65:MET:HG2	2.20	0.41
4:D:201:ARG:HA	4:D:204:GLU:CG	2.50	0.41
1:I:709:LEU:H	1:I:717:THR:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:508:VAL:HA	2:J:509:PRO:HD2	1.88	0.41
2:J:592:THR:HB	2:J:593:ARG:H	1.64	0.41
2:J:801:PHE:O	2:J:804:SER:OG	2.37	0.41
3:M:55:LYS:HG2	8:T:3:ARG:NH2	2.35	0.41
3:M:143:LEU:HA	3:M:146:LEU:HB2	2.03	0.41
1:A:238:GLU:HG2	1:A:239:ASP:N	2.35	0.41
1:A:679:ALA:O	1:A:683:ILE:HG12	2.21	0.41
1:A:854:VAL:HG22	3:C:64:VAL:HG23	2.03	0.41
2:B:274:LEU:HD12	2:B:274:LEU:HA	1.89	0.41
2:B:670:TYR:O	2:B:674:MET:HB2	2.20	0.41
2:B:983:LEU:H	2:B:983:LEU:HG	1.65	0.41
2:B:1083:CYS:HB2	2:B:1084:PRO:HD2	2.02	0.41
3:C:55:LYS:HG2	8:K:3:ARG:NH2	2.33	0.41
3:C:130:LYS:O	3:C:134:VAL:HG23	2.19	0.41
3:C:345:HIS:O	3:C:346:LEU:C	2.64	0.41
1:I:13:PHE:HB2	3:M:355:VAL:O	2.20	0.41
1:I:171:ASP:CG	1:I:172:GLU:H	2.28	0.41
1:I:209:ARG:HB2	1:I:212:TRP:CE2	2.56	0.41
1:I:635:ASP:OD1	1:I:639:ARG:NE	2.50	0.41
3:M:385:PRO:HA	5:Q:22:PRO:CD	2.50	0.41
4:O:41:ALA:HB3	4:O:146:TRP:CD1	2.56	0.41
4:O:201:ARG:HA	4:O:204:GLU:CG	2.50	0.41
5:Q:5:LEU:HD13	6:R:6:LYS:HD3	2.02	0.41
5:Q:27:LYS:HD2	5:Q:50:ASP:HA	2.03	0.41
7:S:13:VAL:HG13	7:S:14:LEU:H	1.84	0.41
10:V:2:ILE:O	10:V:3:VAL:C	2.63	0.41
10:V:52:HIS:CE1	10:V:54:GLU:H	2.38	0.41
1:A:456:PRO:HB3	1:A:628:ARG:HH11	1.85	0.41
1:A:472:PRO:HG2	1:A:478:GLN:HG2	2.03	0.41
1:A:709:LEU:H	1:A:717:THR:HG21	1.85	0.41
2:B:193:LYS:HE3	2:B:204:LEU:HD11	2.03	0.41
3:C:189:ALA:HB2	3:C:200:VAL:O	2.21	0.41
3:C:382:MET:HE2	5:E:66:THR:HG21	2.02	0.41
1:I:244:LYS:O	1:I:248:ILE:HG13	2.21	0.41
1:I:456:PRO:HB3	1:I:628:ARG:HH11	1.86	0.41
2:J:107:MET:C	2:J:395:ARG:HH22	2.28	0.41
2:J:912:LEU:HD23	2:J:912:LEU:HA	1.89	0.41
3:M:191:PHE:HD1	3:M:191:PHE:HA	1.69	0.41
1:A:74:PHE:CE1	1:A:221:PRO:HA	2.55	0.41
1:A:867:ILE:HD12	7:H:40:LEU:HA	2.03	0.41
2:B:116:GLN:HE21	2:B:117:GLU:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:LEU:HD13	2:B:595:HIS:ND1	2.35	0.41
6:F:121:LEU:HD23	6:F:121:LEU:HA	1.91	0.41
9:L:43:TYR:O	9:L:44:THR:HG22	2.21	0.41
10:N:2:ILE:O	10:N:3:VAL:C	2.63	0.41
10:N:7:CYS:HB2	10:N:14:LEU:HD12	2.03	0.41
1:I:507:HIS:CE1	2:J:736:MET:HE1	2.56	0.41
2:J:16:GLU:HA	2:J:19:LEU:HD12	2.03	0.41
2:J:174:LEU:HD11	2:J:340:LYS:HB2	2.02	0.41
2:J:373:GLN:HE21	2:J:397:SER:HA	1.84	0.41
1:A:62:THR:HA	2:B:1077:ARG:HH11	1.85	0.41
1:A:244:LYS:HB2	1:A:244:LYS:HE3	1.66	0.41
1:A:848:ALA:HB2	3:C:327:VAL:CG2	2.51	0.41
2:B:691:ASP:O	2:B:759:THR:HG23	2.21	0.41
2:B:898:GLN:O	2:B:901:MET:HB2	2.20	0.41
2:B:1082:TYR:HD1	2:B:1088:GLU:N	2.18	0.41
9:L:4:GLU:HB2	9:L:16:TYR:HB2	2.03	0.41
1:I:472:PRO:HG2	1:I:478:GLN:HG2	2.02	0.41
1:I:772:GLN:HB2	1:I:779:LEU:HD11	2.01	0.41
2:J:135:CYS:O	2:J:137:LEU:N	2.54	0.41
2:J:773:ASP:OD2	2:J:815:ARG:NH1	2.44	0.41
3:M:72:ILE:HD12	3:M:72:ILE:HA	1.88	0.41
3:M:144:GLU:H	3:M:144:GLU:HG2	1.56	0.41
3:M:157:MET:HB3	3:M:160:VAL:CG2	2.51	0.41
10:V:53:VAL:C	10:V:54:GLU:HG3	2.46	0.41
1:A:22:ARG:HA	1:A:76:HIS:ND1	2.36	0.41
1:A:159:PHE:HD1	1:A:159:PHE:HA	1.78	0.41
1:A:285:ASN:ND2	1:A:301:LEU:O	2.43	0.41
1:A:479:ALA:O	1:A:483:ILE:HG12	2.21	0.41
1:A:542:GLU:HA	1:A:543:PRO:HA	1.90	0.41
1:A:564:PRO:HB2	1:A:567:LEU:HD21	2.02	0.41
1:A:583:GLU:HG3	1:A:584:ALA:H	1.86	0.41
2:B:16:GLU:HA	2:B:19:LEU:HD12	2.03	0.41
2:B:135:CYS:O	2:B:137:LEU:N	2.54	0.41
2:B:498:VAL:HG12	2:B:502:LEU:HD11	2.02	0.41
2:B:731:TYR:CZ	2:B:902:PRO:HG3	2.55	0.41
2:B:903:TRP:HZ3	2:B:977:GLY:HA2	1.86	0.41
2:B:1082:TYR:HB2	2:B:1088:GLU:CD	2.46	0.41
3:C:187:LYS:HB2	3:C:188:SER:H	1.73	0.41
8:K:38:GLN:H	8:K:38:GLN:HG2	1.37	0.41
10:N:61:VAL:O	10:N:61:VAL:HG22	2.21	0.41
1:I:24:MET:HA	2:J:1084:PRO:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:230:THR:HG22	1:I:236:ARG:HD3	2.03	0.41
1:I:441:ARG:O	1:I:443:MET:HG3	2.20	0.41
1:I:479:ALA:O	1:I:483:ILE:HG12	2.21	0.41
1:I:480:GLU:CD	3:M:375:THR:HG21	2.45	0.41
1:I:679:ALA:O	1:I:683:ILE:HG12	2.21	0.41
2:J:116:GLN:HE21	2:J:117:GLU:HB3	1.86	0.41
2:J:520:TYR:OH	2:J:535:GLY:HA2	2.21	0.41
2:J:691:ASP:O	2:J:759:THR:HG23	2.21	0.41
2:J:698:HIS:HE1	2:J:873:LEU:HD21	1.84	0.41
2:J:980:GLY:HA3	4:O:23:VAL:HG13	2.03	0.41
2:J:1054:LEU:O	2:J:1056:GLU:N	2.54	0.41
4:O:23:VAL:HA	4:O:220:PHE:HE2	1.85	0.41
4:O:225:GLU:HG3	10:V:12:LYS:NZ	2.36	0.41
10:V:25:VAL:C	10:V:27:ALA:H	2.29	0.41
1:A:209:ARG:HB2	1:A:212:TRP:CE2	2.56	0.41
1:A:856:TYR:HE2	3:C:377:ILE:O	2.04	0.41
2:B:47:GLN:HE21	2:B:51:ASN:ND2	2.19	0.41
2:B:204:LEU:HD23	2:B:205:ILE:N	2.36	0.41
2:B:520:TYR:OH	2:B:535:GLY:HA2	2.21	0.41
2:B:968:HIS:CD2	2:B:969:SER:N	2.89	0.41
8:K:16:ARG:HG2	8:K:49:ILE:HG22	2.02	0.41
11:P:17:LEU:HD11	11:P:27:CYS:HA	2.03	0.41
1:I:86:VAL:HG11	1:I:287:THR:HG21	2.03	0.41
1:I:493:SER:HA	1:I:494:PRO:HD3	1.92	0.41
1:I:789:THR:HG21	2:J:623:GLU:OE2	2.21	0.41
2:J:109:PRO:HG2	2:J:116:GLN:OE1	2.21	0.41
2:J:189:LYS:NZ	3:M:212:ARG:HH12	2.19	0.41
2:J:1050:ILE:HD11	3:M:370:PRO:CA	2.50	0.41
3:M:148:ARG:CZ	3:M:162:GLU:HB3	2.38	0.41
1:A:362:PHE:HD2	8:K:34:ILE:O	2.03	0.40
3:C:96:LEU:CB	3:C:100:ARG:HB2	2.49	0.40
3:C:107:ALA:HB1	3:C:270:TRP:HZ2	1.86	0.40
5:E:27:LYS:HD2	5:E:50:ASP:HA	2.03	0.40
10:N:53:VAL:C	10:N:54:GLU:HG3	2.46	0.40
1:I:147:CYS:HA	1:I:148:PRO:HD3	1.83	0.40
1:I:622:ASP:OD1	1:I:624:LYS:HB2	2.21	0.40
1:I:662:THR:HG23	2:J:731:TYR:HA	2.03	0.40
2:J:130:LEU:HD22	2:J:158:TYR:CZ	2.55	0.40
2:J:520:TYR:CZ	2:J:535:GLY:HA2	2.56	0.40
2:J:521:ARG:N	2:J:531:THR:HG22	2.36	0.40
2:J:968:HIS:CD2	2:J:969:SER:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:183:THR:O	3:M:185:SER:N	2.53	0.40
10:V:7:CYS:HB2	10:V:14:LEU:HD12	2.03	0.40
1:A:55:ASP:O	1:A:57:GLY:N	2.52	0.40
1:A:628:ARG:O	1:A:630:ASP:N	2.46	0.40
1:A:831:THR:HA	3:C:80:THR:HG21	2.03	0.40
5:E:156:ILE:H	5:E:156:ILE:HG13	1.68	0.40
7:H:43:ILE:O	7:H:80:VAL:N	2.53	0.40
1:I:841:MET:O	1:I:845:LEU:HG	2.22	0.40
2:J:58:PRO:HG3	2:J:63:PHE:HB2	2.02	0.40
2:J:309:ASP:HB2	2:J:312:ASN:ND2	2.37	0.40
2:J:670:TYR:O	2:J:674:MET:HB2	2.20	0.40
3:M:214:ILE:C	3:M:216:GLU:N	2.73	0.40
4:O:157:THR:HG22	4:O:215:ILE:HA	2.03	0.40
5:Q:92:MET:HE2	5:Q:126:GLN:HA	2.03	0.40
1:A:187:ARG:HD2	1:A:214:VAL:HB	2.03	0.40
1:A:436:MET:HB2	1:A:458:TYR:OH	2.21	0.40
2:B:95:ARG:NH2	11:P:33:LYS:HD3	2.37	0.40
2:B:114:ILE:HG12	2:B:114:ILE:H	1.79	0.40
2:B:153:LYS:HD2	2:B:153:LYS:HA	1.86	0.40
2:B:429:ARG:HA	2:B:429:ARG:HD2	1.78	0.40
3:C:177:LYS:HZ2	3:C:224:LYS:HD3	1.85	0.40
3:C:320:PRO:O	3:C:325:GLY:HA3	2.22	0.40
4:D:41:ALA:HB3	4:D:146:TRP:CD1	2.56	0.40
5:E:24:GLU:O	5:E:28:ILE:HG13	2.22	0.40
9:L:34:GLU:CD	9:L:81:ARG:HH22	2.29	0.40
1:I:362:PHE:CZ	8:T:26:VAL:HG21	2.57	0.40
3:M:107:ALA:HB1	3:M:270:TRP:HZ2	1.87	0.40
3:M:320:PRO:O	3:M:325:GLY:HA3	2.21	0.40
3:M:334:LEU:HA	3:M:337:ALA:HB3	2.03	0.40
4:O:219:SER:O	4:O:220:PHE:HD1	2.05	0.40
10:V:22:LYS:HZ3	10:V:54:GLU:HG2	1.84	0.40
3:C:55:LYS:HE2	8:K:3:ARG:NH2	2.32	0.40
10:N:12:LYS:HE3	10:N:12:LYS:HB3	1.65	0.40
10:N:22:LYS:HZ3	10:N:54:GLU:HG2	1.85	0.40
1:I:419:GLY:N	1:I:440:VAL:O	2.52	0.40
1:I:526:VAL:HG21	1:I:553:TRP:CD1	2.57	0.40
1:I:709:LEU:HD12	1:I:717:THR:HA	2.04	0.40
2:J:121:VAL:HG12	2:J:122:ARG:O	2.21	0.40
2:J:193:LYS:HE2	2:J:195:PHE:CE2	2.56	0.40
2:J:591:LEU:HD13	2:J:595:HIS:ND1	2.35	0.40
3:M:13:LYS:HE2	3:M:13:LYS:HB2	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:160:VAL:HG13	3:M:199:VAL:H	1.86	0.40
4:O:118:ILE:HG23	10:V:15:ALA:HB3	2.04	0.40
4:O:141:LYS:HE3	4:O:141:LYS:HB2	1.96	0.40
9:U:45:ILE:C	9:U:46:GLU:HG3	2.45	0.40
2:B:193:LYS:HE2	2:B:195:PHE:CE2	2.56	0.40
2:B:968:HIS:C	2:B:968:HIS:HD2	2.27	0.40
3:C:204:LYS:HG3	3:C:205:VAL:N	2.36	0.40
1:I:28:GLU:HB2	1:I:76:HIS:HE2	1.87	0.40
2:J:459:HIS:CE1	2:J:461:THR:HG23	2.57	0.40
2:J:516:ALA:HA	2:J:517:PRO:HA	1.72	0.40
7:S:10:PHE:O	7:S:11:ASP:C	2.64	0.40

All (20) 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)
6:F:98:LYS:NZ	5:Q:82:GLN:NE2[3_445]	1.00	1.20
2:B:61:PRO:C	6:F:31:GLU:OE1[1_655]	1.06	1.14
2:B:61:PRO:O	6:F:31:GLU:OE1[1_655]	1.11	1.09
2:B:61:PRO:CB	6:F:31:GLU:CD[1_655]	1.35	0.85
2:B:61:PRO:CA	6:F:31:GLU:OE1[1_655]	1.41	0.79
2:B:61:PRO:CA	6:F:31:GLU:CD[1_655]	1.59	0.61
2:B:61:PRO:CB	6:F:31:GLU:OE2[1_655]	1.66	0.54
11:P:29:TYR:CD2	6:R:122:GLU:CD[1_655]	1.66	0.54
2:B:61:PRO:CA	6:F:31:GLU:OE2[1_655]	1.70	0.50
11:P:29:TYR:CD2	6:R:122:GLU:OE1[1_655]	1.73	0.47
11:P:29:TYR:CD2	6:R:122:GLU:OE2[1_655]	1.75	0.45
11:P:29:TYR:CG	6:R:122:GLU:OE1[1_655]	1.77	0.43
6:F:98:LYS:NZ	5:Q:82:GLN:CD[3_445]	1.86	0.34
2:B:61:PRO:CB	6:F:31:GLU:OE1[1_655]	1.97	0.23
6:F:97:ALA:O	5:Q:81:ASN:ND2[3_445]	2.05	0.15
2:B:61:PRO:CB	6:F:31:GLU:CG[1_655]	2.08	0.12
5:E:81:ASN:ND2	6:R:97:ALA:O[3_445]	2.08	0.12
5:E:82:GLN:OE1	6:R:98:LYS:CD[3_445]	2.08	0.12
11:P:29:TYR:CB	6:R:122:GLU:OE1[1_655]	2.08	0.12
2:B:284:GLY:N	1:I:150:CYS:O[3_545]	2.17	0.03

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	855/906 (94%)	689 (81%)	116 (14%)	50 (6%)	1	13
1	I	853/906 (94%)	692 (81%)	110 (13%)	51 (6%)	1	12
2	B	1061/1123 (94%)	872 (82%)	141 (13%)	48 (4%)	2	17
2	J	1061/1123 (94%)	864 (81%)	143 (14%)	54 (5%)	1	15
3	C	365/391 (93%)	258 (71%)	73 (20%)	34 (9%)	0	6
3	M	365/391 (93%)	266 (73%)	75 (20%)	24 (7%)	1	11
4	D	256/259 (99%)	241 (94%)	12 (5%)	3 (1%)	10	41
4	O	256/259 (99%)	242 (94%)	11 (4%)	3 (1%)	10	41
5	E	179/190 (94%)	161 (90%)	18 (10%)	0	100	100
5	Q	179/190 (94%)	161 (90%)	18 (10%)	0	100	100
6	F	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	3	23
6	R	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	3	23
7	H	74/82 (90%)	59 (80%)	10 (14%)	5 (7%)	1	10
7	S	74/82 (90%)	60 (81%)	10 (14%)	4 (5%)	1	14
8	K	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	9
8	T	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	9
9	L	92/100 (92%)	74 (80%)	12 (13%)	6 (6%)	1	11
9	U	92/100 (92%)	75 (82%)	10 (11%)	7 (8%)	1	8
10	N	61/65 (94%)	44 (72%)	11 (18%)	6 (10%)	0	6
10	V	61/65 (94%)	44 (72%)	11 (18%)	6 (10%)	0	6
11	P	40/49 (82%)	24 (60%)	10 (25%)	6 (15%)	0	2
11	W	40/49 (82%)	22 (55%)	11 (28%)	7 (18%)	0	2
All	All	6312/6688 (94%)	5150 (82%)	832 (13%)	330 (5%)	1	14

All (330) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	151	GLY
1	A	153	PRO
1	A	154	GLN
1	A	398	ASN
1	A	400	GLU
1	A	430	LEU
1	A	463	ASP
1	A	537	VAL
1	A	583	GLU
1	A	630	ASP
2	B	57	VAL
2	B	183	ARG
2	B	286	PRO
2	B	287	LYS
2	B	391	GLN
2	B	392	ARG
2	B	394	VAL
2	B	430	THR
2	B	513	ARG
2	B	515	PRO
2	B	521	ARG
2	B	845	PRO
3	C	161	VAL
3	C	162	GLU
3	C	165	PRO
3	C	181	LYS
3	C	224	LYS
4	D	209	LYS
7	H	9	ILE
7	H	11	ASP
8	K	28	ILE
8	K	30	VAL
9	L	49	ILE
9	L	93	ILE
10	N	2	ILE
10	N	61	VAL
11	P	19	LEU
11	P	20	ALA
1	I	40	TYR
1	I	41	PRO
1	I	48	ASP
1	I	154	GLN

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Mol	Chain	Res	Type
1	I	395	MET
1	I	397	SER
1	I	398	ASN
1	I	400	GLU
1	I	430	LEU
1	I	463	ASP
1	I	537	VAL
1	I	583	GLU
1	I	587	LYS
1	I	642	GLY
1	I	643	VAL
2	J	43	ASP
2	J	57	VAL
2	J	183	ARG
2	J	286	PRO
2	J	287	LYS
2	J	392	ARG
2	J	393	PHE
2	J	394	VAL
2	J	396	ASN
2	J	430	THR
2	J	515	PRO
2	J	521	ARG
2	J	845	PRO
3	M	152	ILE
3	M	205	VAL
3	M	224	LYS
3	M	237	GLU
3	M	340	GLU
4	O	209	LYS
7	S	11	ASP
8	T	28	ILE
8	T	30	VAL
9	U	93	ILE
10	V	2	ILE
1	A	64	GLY
1	A	65	ALA
1	A	296	LYS
1	A	297	SER
1	A	405	LYS
1	A	578	GLU
1	A	585	LEU

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Mol	Chain	Res	Type
1	A	608	PHE
1	A	758	LYS
2	B	56	VAL
2	B	79	GLU
2	B	138	TYR
2	B	390	ILE
2	B	944	VAL
2	B	1055	GLU
2	B	1057	SER
2	B	1082	TYR
3	C	94	VAL
3	C	160	VAL
3	C	209	SER
3	C	323	ARG
3	C	342	THR
3	C	343	THR
3	C	346	LEU
3	C	357	PRO
3	C	358	LEU
3	C	361	VAL
3	C	385	PRO
10	N	11	GLY
11	P	13	LYS
11	P	14	GLU
1	I	35	TYR
1	I	64	GLY
1	I	65	ALA
1	I	103	CYS
1	I	174	GLY
1	I	297	SER
1	I	585	LEU
1	I	586	GLU
1	I	608	PHE
2	J	40	ALA
2	J	56	VAL
2	J	79	GLU
2	J	138	TYR
2	J	944	VAL
2	J	1055	GLU
2	J	1057	SER
2	J	1077	ARG
3	M	93	ASN

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Mol	Chain	Res	Type
3	M	323	ARG
3	M	357	PRO
3	M	358	LEU
3	M	361	VAL
7	S	7	PHE
9	U	48	PRO
10	V	11	GLY
11	W	13	LYS
11	W	14	GLU
1	A	172	GLU
1	A	173	GLU
1	A	261	ALA
1	A	378	TYR
1	A	395	MET
1	A	397	SER
1	A	404	GLU
1	A	548	ASN
1	A	710	PRO
1	A	754	GLY
1	A	896	ARG
2	B	136	ARG
2	B	212	ASP
2	B	222	VAL
2	B	591	LEU
2	B	780	PRO
2	B	819	PRO
3	C	35	TYR
3	C	36	LYS
3	C	108	ARG
3	C	140	GLY
3	C	158	GLU
3	C	182	LEU
3	C	188	SER
3	C	191	PHE
3	C	221	HIS
9	L	23	THR
9	L	50	THR
1	I	261	ALA
1	I	378	TYR
1	I	396	GLU
1	I	433	MET
1	I	578	GLU

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Mol	Chain	Res	Type
1	I	710	PRO
2	J	136	ARG
2	J	212	ASP
2	J	222	VAL
2	J	397	SER
2	J	591	LEU
2	J	780	PRO
2	J	1042	GLY
2	J	1076	LYS
3	M	35	TYR
3	M	36	LYS
3	M	108	ARG
3	M	140	GLY
3	M	208	LEU
3	M	215	ALA
3	M	218	VAL
3	M	221	HIS
9	U	23	THR
9	U	50	THR
1	A	69	GLU
1	A	152	ALA
1	A	161	ARG
1	A	265	GLN
1	A	433	MET
1	A	544	ASP
1	A	767	ALA
1	A	871	LYS
2	B	82	GLY
2	B	188	ASN
2	B	223	PRO
2	B	236	GLY
2	B	269	THR
2	B	379	GLN
2	B	774	ASN
2	B	919	ILE
2	B	923	MET
3	C	107	ALA
3	C	121	ASP
3	C	142	THR
3	C	163	ILE
3	C	344	GLN
6	F	28	GLY

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Mol	Chain	Res	Type
6	F	31	GLU
6	F	118	TYR
7	H	57	PRO
11	P	24	GLU
1	I	69	GLU
1	I	161	ARG
1	I	265	GLN
1	I	405	LYS
1	I	538	ASN
1	I	588	LEU
1	I	632	LYS
1	I	767	ALA
2	J	46	LEU
2	J	82	GLY
2	J	188	ASN
2	J	223	PRO
2	J	236	GLY
2	J	269	THR
2	J	379	GLN
2	J	774	ASN
2	J	919	ILE
3	M	107	ALA
3	M	121	ASP
3	M	142	THR
3	M	187	LYS
6	R	28	GLY
6	R	31	GLU
6	R	118	TYR
7	S	57	PRO
11	W	21	THR
11	W	24	GLU
1	A	535	MET
1	A	540	LEU
1	A	542	GLU
1	A	632	LYS
1	A	756	ARG
1	A	867	ILE
1	A	888	VAL
2	B	11	THR
2	B	32	ARG
2	B	224	LYS
2	B	445	PRO

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Mol	Chain	Res	Type
2	B	498	VAL
2	B	516	ALA
2	B	837	ARG
2	B	876	PRO
2	B	1072	ALA
3	C	187	LYS
3	C	341	ILE
3	C	384	LEU
4	D	11	PRO
7	H	10	PHE
9	L	48	PRO
10	N	41	GLU
11	P	42	VAL
1	I	44	GLY
1	I	152	ALA
1	I	296	LYS
1	I	540	LEU
1	I	542	GLU
1	I	544	ASP
1	I	867	ILE
1	I	871	LYS
1	I	888	VAL
2	J	11	THR
2	J	32	ARG
2	J	224	LYS
2	J	399	ARG
2	J	498	VAL
2	J	516	ALA
2	J	837	ARG
2	J	876	PRO
2	J	1046	ALA
2	J	1072	ALA
3	M	203	LYS
4	O	11	PRO
10	V	41	GLU
11	W	19	LEU
11	W	42	VAL
1	A	36	ASP
1	A	464	GLY
2	B	46	LEU
2	B	1112	VAL
7	H	80	VAL

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Mol	Chain	Res	Type
8	K	24	ALA
9	L	46	GLU
10	N	3	VAL
10	N	4	PRO
1	I	464	GLY
1	I	535	MET
1	I	633	LEU
2	J	445	PRO
2	J	1041	ILE
2	J	1112	VAL
3	M	95	THR
7	S	80	VAL
8	T	24	ALA
9	U	51	MET
9	U	53	ARG
10	V	3	VAL
10	V	4	PRO
11	W	20	ALA
2	B	705	VAL
4	D	21	VAL
2	J	705	VAL
4	O	21	VAL
9	U	49	ILE
10	V	61	VAL
1	A	543	PRO
2	B	517	PRO
3	C	205	VAL
6	F	33	PRO
1	I	543	PRO
2	J	517	PRO
6	R	33	PRO
1	A	41	PRO
8	K	33	GLY
2	J	390	ILE
8	T	33	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	743/779 (95%)	628 (84%)	115 (16%)	2	15
1	I	740/779 (95%)	625 (84%)	115 (16%)	2	15
2	B	923/969 (95%)	764 (83%)	159 (17%)	2	12
2	J	923/969 (95%)	761 (82%)	162 (18%)	2	11
3	C	314/334 (94%)	250 (80%)	64 (20%)	1	7
3	M	313/334 (94%)	244 (78%)	69 (22%)	1	5
4	D	227/228 (100%)	216 (95%)	11 (5%)	23	49
4	O	227/228 (100%)	216 (95%)	11 (5%)	23	49
5	E	160/167 (96%)	144 (90%)	16 (10%)	7	28
5	Q	160/167 (96%)	144 (90%)	16 (10%)	7	28
6	F	107/107 (100%)	98 (92%)	9 (8%)	10	34
6	R	107/107 (100%)	98 (92%)	9 (8%)	10	34
7	H	68/72 (94%)	51 (75%)	17 (25%)	0	4
7	S	68/72 (94%)	50 (74%)	18 (26%)	0	3
8	K	45/46 (98%)	37 (82%)	8 (18%)	2	10
8	T	45/46 (98%)	37 (82%)	8 (18%)	2	10
9	L	81/87 (93%)	73 (90%)	8 (10%)	7	29
9	U	81/87 (93%)	74 (91%)	7 (9%)	10	33
10	N	57/59 (97%)	49 (86%)	8 (14%)	3	19
10	V	57/59 (97%)	50 (88%)	7 (12%)	4	22
11	P	35/40 (88%)	31 (89%)	4 (11%)	5	24
11	W	35/40 (88%)	31 (89%)	4 (11%)	5	24
All	All	5516/5776 (96%)	4671 (85%)	845 (15%)	3	16

All (845) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	34	THR
1	A	36	ASP
1	A	38	ASP
1	A	40	TYR
1	A	42	ILE

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Mol	Chain	Res	Type
1	A	46	LEU
1	A	47	MET
1	A	49	LYS
1	A	51	LEU
1	A	61	GLU
1	A	74	PHE
1	A	76	HIS
1	A	77	ILE
1	A	81	ARG
1	A	86	VAL
1	A	105	ARG
1	A	106	ILE
1	A	108	LEU
1	A	116	TYR
1	A	123	MET
1	A	133	LEU
1	A	134	ILE
1	A	146	VAL
1	A	149	HIS
1	A	157	ILE
1	A	159	PHE
1	A	170	LYS
1	A	176	GLU
1	A	181	MET
1	A	196	LYS
1	A	204	HIS
1	A	242	THR
1	A	255	LEU
1	A	265	GLN
1	A	287	THR
1	A	288	SER
1	A	335	ASP
1	A	337	MET
1	A	359	VAL
1	A	361	GLU
1	A	362	PHE
1	A	372	LEU
1	A	384	VAL
1	A	388	GLU
1	A	393	ARG
1	A	395	MET
1	A	399	ARG

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Mol	Chain	Res	Type
1	A	408	ILE
1	A	412	VAL
1	A	422	VAL
1	A	423	LEU
1	A	424	PHE
1	A	426	ARG
1	A	431	HIS
1	A	435	ILE
1	A	442	VAL
1	A	454	VAL
1	A	469	LEU
1	A	484	LEU
1	A	492	ILE
1	A	504	ILE
1	A	505	GLN
1	A	516	ARG
1	A	523	ARG
1	A	524	TYR
1	A	530	LEU
1	A	532	PHE
1	A	536	ASP
1	A	538	ASN
1	A	540	LEU
1	A	542	GLU
1	A	557	THR
1	A	561	LEU
1	A	563	LEU
1	A	567	LEU
1	A	569	ILE
1	A	575	LEU
1	A	577	ASP
1	A	580	GLU
1	A	583	GLU
1	A	585	LEU
1	A	602	LYS
1	A	603	LEU
1	A	611	ILE
1	A	612	GLN
1	A	632	LYS
1	A	637	ILE
1	A	639	ARG
1	A	641	TYR

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Mol	Chain	Res	Type
1	A	647	ARG
1	A	653	VAL
1	A	654	THR
1	A	656	LEU
1	A	660	VAL
1	A	668	THR
1	A	689	GLU
1	A	699	GLU
1	A	706	LEU
1	A	743	MET
1	A	752	LYS
1	A	758	LYS
1	A	774	ILE
1	A	806	ASN
1	A	846	ILE
1	A	853	LYS
1	A	854	VAL
1	A	855	ASP
1	A	862	ASP
1	A	864	THR
1	A	867	ILE
1	A	868	VAL
1	A	883	TRP
1	A	884	GLN
1	A	891	ASP
2	B	46	LEU
2	B	50	VAL
2	B	55	GLU
2	B	56	VAL
2	B	57	VAL
2	B	59	ASP
2	B	66	LYS
2	B	77	PHE
2	B	81	GLN
2	B	94	ILE
2	B	105	LEU
2	B	108	ILE
2	B	111	VAL
2	B	114	ILE
2	B	125	GLU
2	B	133	LYS
2	B	142	ASP

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Mol	Chain	Res	Type
2	B	143	GLU
2	B	148	LEU
2	B	161	ILE
2	B	168	ILE
2	B	170	SER
2	B	179	THR
2	B	181	VAL
2	B	184	ASP
2	B	190	VAL
2	B	199	HIS
2	B	206	THR
2	B	207	VAL
2	B	210	LYS
2	B	218	THR
2	B	226	VAL
2	B	231	VAL
2	B	235	LEU
2	B	255	GLN
2	B	256	VAL
2	B	259	ASP
2	B	263	ASP
2	B	269	THR
2	B	270	GLN
2	B	279	ARG
2	B	292	ARG
2	B	293	ARG
2	B	296	HIS
2	B	302	LEU
2	B	308	VAL
2	B	309	ASP
2	B	311	GLU
2	B	312	ASN
2	B	320	LEU
2	B	322	MET
2	B	325	LEU
2	B	347	ARG
2	B	353	ASP
2	B	354	LEU
2	B	355	LEU
2	B	358	LEU
2	B	365	GLN
2	B	366	LEU

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Mol	Chain	Res	Type
2	B	370	MET
2	B	377	THR
2	B	388	GLU
2	B	389	ASN
2	B	390	ILE
2	B	394	VAL
2	B	395	ARG
2	B	398	ILE
2	B	409	HIS
2	B	416	TRP
2	B	429	ARG
2	B	431	ASN
2	B	435	THR
2	B	442	VAL
2	B	448	ARG
2	B	458	LEU
2	B	469	THR
2	B	470	GLU
2	B	480	VAL
2	B	491	THR
2	B	497	GLU
2	B	510	ILE
2	B	512	GLU
2	B	521	ARG
2	B	524	LEU
2	B	532	VAL
2	B	536	ARG
2	B	545	ASP
2	B	554	VAL
2	B	559	LEU
2	B	570	ILE
2	B	583	VAL
2	B	599	ILE
2	B	603	THR
2	B	604	LEU
2	B	610	ILE
2	B	614	VAL
2	B	630	THR
2	B	637	GLU
2	B	644	LEU
2	B	649	ILE
2	B	650	LEU

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Mol	Chain	Res	Type
2	B	652	ILE
2	B	656	LEU
2	B	681	LEU
2	B	683	TRP
2	B	687	ARG
2	B	688	ILE
2	B	710	MET
2	B	725	VAL
2	B	726	VAL
2	B	740	VAL
2	B	751	LEU
2	B	759	THR
2	B	765	LYS
2	B	776	GLU
2	B	777	VAL
2	B	782	ILE
2	B	786	LEU
2	B	788	GLU
2	B	793	HIS
2	B	796	GLU
2	B	800	ILE
2	B	804	SER
2	B	809	LYS
2	B	813	VAL
2	B	816	THR
2	B	841	VAL
2	B	842	THR
2	B	843	VAL
2	B	848	LYS
2	B	850	VAL
2	B	855	ILE
2	B	856	VAL
2	B	861	ASP
2	B	873	LEU
2	B	878	LEU
2	B	895	ILE
2	B	896	VAL
2	B	908	ILE
2	B	930	GLU
2	B	942	ARG
2	B	952	GLU
2	B	963	GLU

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Mol	Chain	Res	Type
2	B	967	LYS
2	B	968	HIS
2	B	971	ARG
2	B	983	LEU
2	B	984	GLU
2	B	989	ILE
2	B	992	ILE
2	B	995	GLN
2	B	1055	GLU
2	B	1062	VAL
2	B	1067	SER
2	B	1089	ASP
2	B	1112	VAL
2	B	1117	LEU
2	B	1118	ARG
2	B	1121	ASP
3	C	7	ILE
3	C	9	SER
3	C	12	SER
3	C	15	GLU
3	C	21	LYS
3	C	23	GLU
3	C	25	TYR
3	C	29	ILE
3	C	30	GLU
3	C	31	TYR
3	C	37	LEU
3	C	38	LYS
3	C	43	GLN
3	C	64	VAL
3	C	71	SER
3	C	94	VAL
3	C	113	THR
3	C	128	ARG
3	C	129	ASP
3	C	138	ILE
3	C	141	THR
3	C	144	GLU
3	C	145	ASN
3	C	148	ARG
3	C	149	GLU
3	C	157	MET

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Mol	Chain	Res	Type
3	C	163	ILE
3	C	166	GLU
3	C	170	LYS
3	C	176	GLU
3	C	177	LYS
3	C	181	LYS
3	C	182	LEU
3	C	186	PHE
3	C	192	GLU
3	C	203	LYS
3	C	216	GLU
3	C	219	LYS
3	C	223	LEU
3	C	234	ILE
3	C	236	LYS
3	C	240	GLU
3	C	246	GLU
3	C	269	ILE
3	C	291	SER
3	C	292	THR
3	C	298	LEU
3	C	302	VAL
3	C	311	MET
3	C	315	ASP
3	C	317	VAL
3	C	326	ILE
3	C	330	LYS
3	C	340	GLU
3	C	342	THR
3	C	346	LEU
3	C	347	PHE
3	C	355	VAL
3	C	358	LEU
3	C	361	VAL
3	C	362	VAL
3	C	369	GLN
3	C	373	VAL
3	C	384	LEU
4	D	14	ILE
4	D	16	PHE
4	D	18	VAL
4	D	27	ASN

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Mol	Chain	Res	Type
4	D	50	ASN
4	D	58	ILE
4	D	188	GLU
4	D	193	THR
4	D	194	ILE
4	D	198	TYR
4	D	201	ARG
5	E	5	LEU
5	E	46	LEU
5	E	59	ILE
5	E	74	VAL
5	E	91	GLU
5	E	93	MET
5	E	110	ILE
5	E	119	VAL
5	E	125	ARG
5	E	138	LEU
5	E	147	ILE
5	E	153	SER
5	E	165	MET
5	E	174	GLU
5	E	177	GLU
5	E	178	LYS
6	F	7	LEU
6	F	40	GLU
6	F	50	ARG
6	F	55	LYS
6	F	71	ASP
6	F	85	LEU
6	F	90	LEU
6	F	100	GLU
6	F	121	LEU
7	H	6	GLU
7	H	9	ILE
7	H	10	PHE
7	H	13	VAL
7	H	29	LEU
7	H	31	LYS
7	H	37	ILE
7	H	38	SER
7	H	40	LEU
7	H	44	LYS

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Mol	Chain	Res	Type
7	H	50	VAL
7	H	51	VAL
7	H	53	LEU
7	H	69	THR
7	H	78	LEU
7	H	80	VAL
7	H	81	GLU
8	K	3	ARG
8	K	34	ILE
8	K	35	THR
8	K	38	GLN
8	K	41	LEU
8	K	46	LYS
8	K	49	ILE
8	K	57	SER
9	L	43	TYR
9	L	46	GLU
9	L	49	ILE
9	L	50	THR
9	L	51	MET
9	L	65	ILE
9	L	90	LYS
9	L	93	ILE
10	N	2	ILE
10	N	3	VAL
10	N	12	LYS
10	N	19	TYR
10	N	48	THR
10	N	54	GLU
10	N	60	MET
10	N	63	LYS
11	P	14	GLU
11	P	15	VAL
11	P	21	THR
11	P	44	ARG
1	I	10	SER
1	I	34	THR
1	I	37	ASP
1	I	38	ASP
1	I	42	ILE
1	I	46	LEU
1	I	47	MET

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Mol	Chain	Res	Type
1	I	49	LYS
1	I	51	LEU
1	I	61	GLU
1	I	74	PHE
1	I	76	HIS
1	I	77	ILE
1	I	81	ARG
1	I	86	VAL
1	I	105	ARG
1	I	106	ILE
1	I	108	LEU
1	I	116	TYR
1	I	123	MET
1	I	133	LEU
1	I	134	ILE
1	I	146	VAL
1	I	149	HIS
1	I	157	ILE
1	I	159	PHE
1	I	170	LYS
1	I	176	GLU
1	I	181	MET
1	I	196	LYS
1	I	204	HIS
1	I	242	THR
1	I	255	LEU
1	I	265	GLN
1	I	287	THR
1	I	288	SER
1	I	335	ASP
1	I	337	MET
1	I	359	VAL
1	I	361	GLU
1	I	362	PHE
1	I	372	LEU
1	I	384	VAL
1	I	388	GLU
1	I	393	ARG
1	I	395	MET
1	I	399	ARG
1	I	404	GLU
1	I	408	ILE

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Mol	Chain	Res	Type
1	I	412	VAL
1	I	422	VAL
1	I	423	LEU
1	I	424	PHE
1	I	426	ARG
1	I	431	HIS
1	I	435	ILE
1	I	442	VAL
1	I	454	VAL
1	I	469	LEU
1	I	484	LEU
1	I	492	ILE
1	I	504	ILE
1	I	505	GLN
1	I	516	ARG
1	I	523	ARG
1	I	524	TYR
1	I	530	LEU
1	I	532	PHE
1	I	536	ASP
1	I	538	ASN
1	I	540	LEU
1	I	542	GLU
1	I	547	GLU
1	I	557	THR
1	I	561	LEU
1	I	563	LEU
1	I	567	LEU
1	I	569	ILE
1	I	575	LEU
1	I	577	ASP
1	I	585	LEU
1	I	588	LEU
1	I	602	LYS
1	I	603	LEU
1	I	611	ILE
1	I	612	GLN
1	I	632	LYS
1	I	637	ILE
1	I	639	ARG
1	I	641	TYR
1	I	647	ARG

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Mol	Chain	Res	Type
1	I	653	VAL
1	I	654	THR
1	I	656	LEU
1	I	660	VAL
1	I	668	THR
1	I	689	GLU
1	I	699	GLU
1	I	706	LEU
1	I	743	MET
1	I	752	LYS
1	I	774	ILE
1	I	806	ASN
1	I	846	ILE
1	I	853	LYS
1	I	854	VAL
1	I	855	ASP
1	I	862	ASP
1	I	864	THR
1	I	867	ILE
1	I	868	VAL
1	I	883	TRP
1	I	884	GLN
1	I	891	ASP
1	I	897	THR
2	J	43	ASP
2	J	46	LEU
2	J	55	GLU
2	J	56	VAL
2	J	57	VAL
2	J	59	ASP
2	J	66	LYS
2	J	77	PHE
2	J	81	GLN
2	J	94	ILE
2	J	105	LEU
2	J	108	ILE
2	J	111	VAL
2	J	114	ILE
2	J	125	GLU
2	J	133	LYS
2	J	142	ASP
2	J	143	GLU

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Mol	Chain	Res	Type
2	J	148	LEU
2	J	161	ILE
2	J	168	ILE
2	J	170	SER
2	J	179	THR
2	J	181	VAL
2	J	184	ASP
2	J	190	VAL
2	J	199	HIS
2	J	206	THR
2	J	207	VAL
2	J	210	LYS
2	J	218	THR
2	J	226	VAL
2	J	231	VAL
2	J	235	LEU
2	J	255	GLN
2	J	256	VAL
2	J	259	ASP
2	J	263	ASP
2	J	269	THR
2	J	270	GLN
2	J	279	ARG
2	J	292	ARG
2	J	293	ARG
2	J	296	HIS
2	J	302	LEU
2	J	308	VAL
2	J	309	ASP
2	J	311	GLU
2	J	312	ASN
2	J	320	LEU
2	J	322	MET
2	J	325	LEU
2	J	347	ARG
2	J	353	ASP
2	J	354	LEU
2	J	355	LEU
2	J	358	LEU
2	J	365	GLN
2	J	366	LEU
2	J	370	MET

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Mol	Chain	Res	Type
2	J	377	THR
2	J	388	GLU
2	J	389	ASN
2	J	390	ILE
2	J	409	HIS
2	J	416	TRP
2	J	429	ARG
2	J	431	ASN
2	J	435	THR
2	J	442	VAL
2	J	448	ARG
2	J	458	LEU
2	J	469	THR
2	J	470	GLU
2	J	480	VAL
2	J	491	THR
2	J	497	GLU
2	J	503	MET
2	J	510	ILE
2	J	513	ARG
2	J	521	ARG
2	J	524	LEU
2	J	532	VAL
2	J	536	ARG
2	J	545	ASP
2	J	554	VAL
2	J	559	LEU
2	J	570	ILE
2	J	583	VAL
2	J	599	ILE
2	J	603	THR
2	J	604	LEU
2	J	610	ILE
2	J	614	VAL
2	J	630	THR
2	J	637	GLU
2	J	644	LEU
2	J	649	ILE
2	J	650	LEU
2	J	652	ILE
2	J	656	LEU
2	J	681	LEU

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Mol	Chain	Res	Type
2	J	683	TRP
2	J	687	ARG
2	J	688	ILE
2	J	710	MET
2	J	725	VAL
2	J	726	VAL
2	J	740	VAL
2	J	751	LEU
2	J	759	THR
2	J	765	LYS
2	J	776	GLU
2	J	777	VAL
2	J	782	ILE
2	J	786	LEU
2	J	788	GLU
2	J	793	HIS
2	J	796	GLU
2	J	800	ILE
2	J	804	SER
2	J	809	LYS
2	J	813	VAL
2	J	816	THR
2	J	841	VAL
2	J	842	THR
2	J	843	VAL
2	J	848	LYS
2	J	850	VAL
2	J	855	ILE
2	J	856	VAL
2	J	861	ASP
2	J	873	LEU
2	J	878	LEU
2	J	895	ILE
2	J	896	VAL
2	J	908	ILE
2	J	930	GLU
2	J	942	ARG
2	J	952	GLU
2	J	963	GLU
2	J	967	LYS
2	J	968	HIS
2	J	971	ARG

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Mol	Chain	Res	Type
2	J	983	LEU
2	J	984	GLU
2	J	989	ILE
2	J	992	ILE
2	J	995	GLN
2	J	1032	PHE
2	J	1039	VAL
2	J	1055	GLU
2	J	1062	VAL
2	J	1067	SER
2	J	1080	LYS
2	J	1090	GLU
2	J	1091	ARG
2	J	1112	VAL
2	J	1117	LEU
2	J	1118	ARG
2	J	1120	LYS
2	J	1122	ARG
3	M	7	ILE
3	M	9	SER
3	M	12	SER
3	M	15	GLU
3	M	21	LYS
3	M	23	GLU
3	M	25	TYR
3	M	29	ILE
3	M	30	GLU
3	M	31	TYR
3	M	37	LEU
3	M	38	LYS
3	M	43	GLN
3	M	64	VAL
3	M	71	SER
3	M	92	ILE
3	M	93	ASN
3	M	94	VAL
3	M	113	THR
3	M	128	ARG
3	M	129	ASP
3	M	138	ILE
3	M	141	THR
3	M	144	GLU

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Mol	Chain	Res	Type
3	M	145	ASN
3	M	148	ARG
3	M	150	GLU
3	M	153	ASP
3	M	154	ILE
3	M	155	LEU
3	M	166	GLU
3	M	170	LYS
3	M	176	GLU
3	M	177	LYS
3	M	178	VAL
3	M	181	LYS
3	M	182	LEU
3	M	191	PHE
3	M	192	GLU
3	M	208	LEU
3	M	210	ASP
3	M	212	ARG
3	M	219	LYS
3	M	223	LEU
3	M	234	ILE
3	M	236	LYS
3	M	237	GLU
3	M	240	GLU
3	M	246	GLU
3	M	269	ILE
3	M	291	SER
3	M	292	THR
3	M	298	LEU
3	M	302	VAL
3	M	311	MET
3	M	315	ASP
3	M	317	VAL
3	M	326	ILE
3	M	330	LYS
3	M	342	THR
3	M	346	LEU
3	M	347	PHE
3	M	355	VAL
3	M	358	LEU
3	M	361	VAL
3	M	362	VAL

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Mol	Chain	Res	Type
3	M	369	GLN
3	M	373	VAL
3	M	384	LEU
4	O	14	ILE
4	O	16	PHE
4	O	18	VAL
4	O	27	ASN
4	O	50	ASN
4	O	58	ILE
4	O	188	GLU
4	O	193	THR
4	O	194	ILE
4	O	198	TYR
4	O	201	ARG
5	Q	5	LEU
5	Q	46	LEU
5	Q	59	ILE
5	Q	74	VAL
5	Q	91	GLU
5	Q	93	MET
5	Q	110	ILE
5	Q	119	VAL
5	Q	125	ARG
5	Q	138	LEU
5	Q	147	ILE
5	Q	153	SER
5	Q	165	MET
5	Q	174	GLU
5	Q	177	GLU
5	Q	178	LYS
6	R	7	LEU
6	R	40	GLU
6	R	50	ARG
6	R	55	LYS
6	R	71	ASP
6	R	85	LEU
6	R	90	LEU
6	R	100	GLU
6	R	121	LEU
7	S	6	GLU
7	S	7	PHE
7	S	9	ILE

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Mol	Chain	Res	Type
7	S	10	PHE
7	S	13	VAL
7	S	29	LEU
7	S	31	LYS
7	S	37	ILE
7	S	38	SER
7	S	40	LEU
7	S	44	LYS
7	S	50	VAL
7	S	51	VAL
7	S	53	LEU
7	S	69	THR
7	S	78	LEU
7	S	80	VAL
7	S	81	GLU
8	T	3	ARG
8	T	34	ILE
8	T	35	THR
8	T	38	GLN
8	T	41	LEU
8	T	46	LYS
8	T	49	ILE
8	T	57	SER
9	U	44	THR
9	U	46	GLU
9	U	49	ILE
9	U	53	ARG
9	U	54	LYS
9	U	65	ILE
9	U	93	ILE
10	V	2	ILE
10	V	3	VAL
10	V	12	LYS
10	V	19	TYR
10	V	48	THR
10	V	54	GLU
10	V	60	MET
11	W	14	GLU
11	W	15	VAL
11	W	23	ARG
11	W	44	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	252	ASN
1	A	258	ASN
1	A	265	GLN
1	A	451	ASN
1	A	478	GLN
1	A	528	GLN
1	A	573	ASN
1	A	648	GLN
1	A	847	ASN
1	A	869	GLN
1	A	884	GLN
2	B	47	GLN
2	B	116	GLN
2	B	162	ASN
2	B	260	ASN
2	B	312	ASN
2	B	389	ASN
2	B	391	GLN
2	B	595	HIS
2	B	639	HIS
2	B	774	ASN
2	B	898	GLN
2	B	968	HIS
3	C	43	GLN
3	C	156	ASN
4	D	27	ASN
4	D	50	ASN
5	E	162	ASN
5	E	167	GLN
9	L	26	ASN
10	N	52	HIS
1	I	138	HIS
1	I	252	ASN
1	I	258	ASN
1	I	265	GLN
1	I	451	ASN
1	I	478	GLN
1	I	573	ASN
1	I	648	GLN
1	I	772	GLN
1	I	842	GLN

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Mol	Chain	Res	Type
1	I	847	ASN
1	I	869	GLN
1	I	884	GLN
2	J	51	ASN
2	J	162	ASN
2	J	260	ASN
2	J	312	ASN
2	J	595	HIS
2	J	639	HIS
2	J	774	ASN
2	J	898	GLN
2	J	1070	HIS
3	M	43	GLN
4	O	27	ASN
4	O	50	ASN
5	Q	162	ASN
5	Q	167	GLN
9	U	47	HIS
10	V	52	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 14 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	896:ARG	C	897:THR	N	3.01

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	863/906 (95%)	-0.44	2 (0%) 91 82	41, 157, 264, 370	0
1	I	862/906 (95%)	-0.39	3 (0%) 90 76	54, 163, 263, 381	0
2	B	1069/1123 (95%)	-0.44	1 (0%) 92 86	46, 149, 253, 402	0
2	J	1069/1123 (95%)	-0.43	3 (0%) 90 76	39, 139, 248, 360	0
3	C	369/391 (94%)	-0.41	0 100 100	68, 192, 319, 372	0
3	M	369/391 (94%)	-0.41	2 (0%) 87 68	71, 193, 327, 419	0
4	D	258/259 (99%)	-0.52	1 (0%) 88 72	71, 143, 235, 295	0
4	O	258/259 (99%)	-0.53	1 (0%) 88 72	63, 136, 226, 319	0
5	E	181/190 (95%)	-0.52	0 100 100	69, 158, 250, 398	0
5	Q	181/190 (95%)	-0.60	0 100 100	90, 163, 244, 317	0
6	F	122/122 (100%)	-0.47	0 100 100	133, 164, 244, 447	0
6	R	122/122 (100%)	-0.49	0 100 100	142, 184, 257, 324	0
7	H	76/82 (92%)	-0.52	0 100 100	105, 157, 228, 268	0
7	S	76/82 (92%)	-0.54	0 100 100	114, 166, 248, 293	0
8	K	56/57 (98%)	-0.55	0 100 100	88, 131, 196, 288	0
8	T	56/57 (98%)	-0.53	0 100 100	62, 119, 227, 330	0
9	L	94/100 (94%)	-0.44	0 100 100	78, 142, 221, 331	0
9	U	94/100 (94%)	-0.48	1 (1%) 78 54	83, 149, 223, 474	0
10	N	63/65 (96%)	-0.49	0 100 100	81, 141, 218, 281	0
10	V	63/65 (96%)	-0.41	0 100 100	69, 131, 196, 232	0
11	P	42/49 (85%)	-0.43	0 100 100	125, 173, 254, 294	0
11	W	42/49 (85%)	-0.50	0 100 100	90, 147, 201, 253	0
All	All	6385/6688 (95%)	-0.45	14 (0%) 91 82	39, 156, 270, 474	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	626	TYR	2.9
1	I	626	TYR	2.9
2	B	731	TYR	2.6
2	J	1044	GLY	2.6
1	I	541	PRO	2.5
4	O	152	TYR	2.4
9	U	48	PRO	2.3
3	M	18	ASP	2.3
1	I	670	ILE	2.2
3	M	246	GLU	2.1
2	J	1048	LEU	2.1
2	J	731	TYR	2.1
4	D	77	LEU	2.1
1	A	766	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	ZN	P	1501	1/1	0.66	0.09	354,354,354,354	0
12	MG	I	1101	1/1	0.83	0.08	175,175,175,175	0
12	MG	I	1104	1/1	0.88	0.13	54,54,54,54	0
13	ZN	B	1201	1/1	0.91	0.08	364,364,364,364	0
13	ZN	A	1003	1/1	0.92	0.11	488,488,488,488	0
13	ZN	I	1103	1/1	0.93	0.10	527,527,527,527	0
13	ZN	J	1301	1/1	0.93	0.09	521,521,521,521	0
13	ZN	V	1601	1/1	0.94	0.06	210,210,210,210	0
13	ZN	N	1401	1/1	0.95	0.06	127,127,127,127	0
13	ZN	A	1002	1/1	0.95	0.05	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	ZN	I	1102	1/1	0.95	0.04	147,147,147,147	0
12	MG	A	1004	1/1	0.96	0.08	58,58,58,58	0
12	MG	A	1001	1/1	0.97	0.09	52,52,52,52	0
13	ZN	W	1701	1/1	0.99	0.02	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.