



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 07:12 PM EDT

PDB ID : 6CGV / pdb_00006cgv
Title : Revised crystal structure of human adenovirus
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Deposited on : 2018-02-21
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

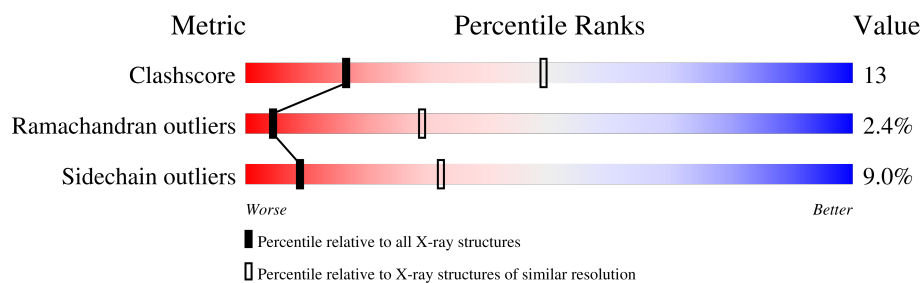
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 99723 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 Hexon protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	917	Total	C	N	O	S	0	0	0
			7345	4668	1243	1400	34			
1	B	911	Total	C	N	O	S	0	0	0
			7295	4636	1235	1390	34			
1	C	921	Total	C	N	O	S	0	0	0
			7374	4686	1247	1405	36			
1	D	917	Total	C	N	O	S	0	0	0
			7345	4668	1243	1400	34			
1	E	910	Total	C	N	O	S	0	0	0
			7302	4645	1235	1388	34			
1	F	914	Total	C	N	O	S	0	0	0
			7325	4658	1239	1393	35			
1	G	909	Total	C	N	O	S	0	0	0
			7291	4636	1234	1387	34			
1	H	913	Total	C	N	O	S	0	0	0
			7317	4653	1238	1392	34			
1	I	917	Total	C	N	O	S	0	0	0
			7345	4669	1243	1398	35			
1	J	915	Total	C	N	O	S	0	0	0
			7329	4658	1240	1397	34			
1	K	904	Total	C	N	O	S	0	0	0
			7247	4606	1227	1380	34			
1	L	918	Total	C	N	O	S	0	0	0
			7353	4673	1244	1401	35			

- Molecule 2 is a protein called Penton protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	447	Total	C	N	O	S	0	0	0
			3577	2264	621	680	12			

- Molecule 3 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	0
			2343	1447	430	460	6			

- Molecule 4 is a protein called Hexon-interlacing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	95	Total	C	N	O	S	0	0	0
			717	443	126	146	2			
4	Q	133	Total	C	N	O	S	0	0	0
			965	594	170	199	2			
4	R	98	Total	C	N	O	S	0	0	0
			734	450	132	150	2			
4	S	96	Total	C	N	O	S	0	0	0
			728	450	129	147	2			

- Molecule 5 is a protein called Pre-hexon-linking protein VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	U	171	Total	C	N	O	S	0	0	0
			1329	839	235	250	5			
5	V	174	Total	C	N	O	S	0	0	0
			1346	848	238	255	5			

- Molecule 6 is a protein called Pre-protein VI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	W	24	Total	C	N	O	0	0	0
			116	68	24	24			

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	854.25Å 855.32Å 865.91Å 60.38° 60.43° 61.98°	Depositor
Resolution (Å)	129.00 – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) (129.00-3.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.36	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 3.78Å)	Xtriage
Refinement program	REFMAC 5.8	Depositor
R, R_{free}	0.422 , 0.427	Depositor
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.080	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.10$	Xtriage
Estimated twinning fraction	0.226 for h-l,h,h-k 0.226 for k,k-l,-h+k 0.220 for h-k,h-l,h 0.220 for l,-h+l,-k+l 0.226 for -k+l,l,-h+l 0.226 for k-l,-h+k,k 0.220 for l,h,k 0.220 for k,l,h 0.226 for -l,k-l,h-l 0.226 for -h+l,-h+k,-h 0.220 for -k,h-k,-k+l 0.220 for -h+k,-h,-h+l 0.226 for h-k,-k+l,-k 0.226 for h-l,-l,k-l 0.226 for h,h-k,h-l 0.226 for -h+k,k,k-l 0.226 for -h,-l,-k 0.236 for -k,-h,-l 0.226 for k-l,h-l,-l 0.226 for -k+l,-k,h-k 0.226 for -h+l,-k+l,l 0.226 for -l,-k,-h 0.226 for -h,-h+l,-h+k	Xtriage

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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.

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Property	Value	Source
Total number of atoms	99723	wwPDB-VP
Average B, all atoms ($\text{\AA}^2$)	103.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.24% of the height of the origin peak. No significant pseudotranslation is detected.*

4 Model quality ⓘ

4.1 Standard geometry ⓘ

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	0.76	13/7543 (0.2%)	1.14	60/10258 (0.6%)
1	B	0.69	6/7490 (0.1%)	1.07	48/10185 (0.5%)
1	C	0.71	6/7573 (0.1%)	1.05	32/10298 (0.3%)
1	D	0.67	7/7543 (0.1%)	1.04	26/10258 (0.3%)
1	E	0.63	4/7500 (0.1%)	0.95	16/10200 (0.2%)
1	F	0.63	2/7523 (0.0%)	0.97	17/10231 (0.2%)
1	G	0.74	8/7488 (0.1%)	1.09	44/10184 (0.4%)
1	H	0.68	4/7515 (0.1%)	1.08	47/10220 (0.5%)
1	I	0.73	5/7543 (0.1%)	1.12	46/10259 (0.4%)
1	J	0.64	0/7526	1.03	36/10235 (0.4%)
1	K	0.71	7/7440 (0.1%)	1.06	40/10116 (0.4%)
1	L	0.71	6/7551 (0.1%)	1.08	39/10269 (0.4%)
2	N	0.86	12/3663 (0.3%)	1.27	47/4989 (0.9%)
3	M	0.68	1/2380 (0.0%)	1.06	12/3240 (0.4%)
4	P	1.28	10/726 (1.4%)	1.50	25/989 (2.5%)
4	Q	1.26	9/977 (0.9%)	1.45	11/1333 (0.8%)
4	R	1.12	7/741 (0.9%)	1.47	13/1006 (1.3%)
4	S	1.63	16/736 (2.2%)	1.86	32/1000 (3.2%)
5	U	0.62	0/1367	0.99	3/1868 (0.2%)
5	V	0.75	1/1384 (0.1%)	1.20	14/1891 (0.7%)
6	W	1.29	0/115	2.25	9/157 (5.7%)
All	All	0.73	124/102324 (0.1%)	1.09	617/139186 (0.4%)

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	H	0	1
3	M	0	1
All	All	0	2

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	56	PRO	C-N	14.90	1.54	1.33
4	Q	55	THR	CA-C	14.69	1.71	1.52
4	S	56	PRO	CA-C	13.97	1.72	1.52
4	S	57	LEU	N-CA	13.91	1.62	1.45
4	Q	55	THR	C-N	13.78	1.51	1.33
4	P	6	PHE	N-CA	13.57	1.62	1.46
4	P	5	SER	CA-C	12.23	1.68	1.52
1	G	21	SER	C-N	10.91	1.49	1.33
4	R	6	PHE	N-CA	10.22	1.58	1.46
4	R	5	SER	CA-C	9.74	1.65	1.52
4	R	5	SER	C-N	9.40	1.46	1.33
4	P	5	SER	C-N	8.99	1.45	1.33
1	A	581	TYR	CA-C	8.86	1.63	1.52
1	C	173	PRO	CA-C	8.65	1.61	1.52
4	Q	4	ASN	CA-C	8.61	1.61	1.52
4	R	5	SER	N-CA	8.42	1.55	1.45
4	P	4	ASN	N-CA	8.38	1.57	1.46
1	G	22	GLU	N-CA	8.21	1.55	1.45
2	N	291	ALA	C-N	7.74	1.44	1.33
4	P	3	THR	CA-C	7.72	1.61	1.52
4	S	57	LEU	CA-C	7.72	1.63	1.53
1	A	582	GLU	CA-C	7.43	1.61	1.52
1	D	54	HIS	CB-CG	7.42	1.60	1.50
1	K	654	TYR	C-N	7.37	1.43	1.33
2	N	201	VAL	N-CA	7.36	1.55	1.46
1	G	23	TYR	C-N	-7.23	1.23	1.33
4	Q	5	SER	CA-C	7.21	1.61	1.52
4	P	3	THR	C-N	7.15	1.43	1.33
1	E	735	ASP	C-N	-6.92	1.24	1.33
1	F	712	PHE	N-CA	6.85	1.57	1.47
4	S	19	MET	C-N	-6.85	1.25	1.33
1	C	749	VAL	CA-C	6.83	1.61	1.52
1	G	561	GLN	C-N	6.73	1.41	1.33
4	Q	5	SER	N-CA	6.63	1.54	1.46
1	A	61	SER	C-N	-6.62	1.27	1.33
1	A	928	VAL	N-CA	-6.54	1.38	1.46
4	Q	24	GLY	CA-C	6.49	1.58	1.51
1	D	79	SER	N-CA	-6.47	1.38	1.46
4	S	110	LEU	N-CA	-6.43	1.37	1.46
1	A	582	GLU	C-N	6.42	1.42	1.33
1	C	214	THR	N-CA	6.30	1.53	1.46
1	F	711	THR	CA-C	6.30	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	4	ASN	C-N	6.28	1.42	1.33
1	I	348	LEU	CA-CB	6.23	1.60	1.53
4	P	5	SER	N-CA	6.23	1.54	1.46
4	Q	4	ASN	C-N	6.21	1.41	1.33
2	N	292	TYR	N-CA	6.20	1.54	1.46
1	A	218	HIS	CB-CG	6.19	1.58	1.50
1	B	731	TRP	N-CA	6.18	1.54	1.46
2	N	290	ASP	CA-C	6.18	1.61	1.52
1	A	582	GLU	N-CA	6.12	1.53	1.45
5	V	37	GLY	C-N	6.11	1.40	1.34
4	S	22	TRP	CA-CB	6.08	1.63	1.53
1	A	581	TYR	C-N	5.96	1.41	1.33
1	B	602	ARG	C-N	-5.94	1.26	1.33
1	C	866	CYS	C-N	5.88	1.41	1.33
1	L	421	ILE	N-CA	5.84	1.53	1.46
1	G	562	VAL	N-CA	5.84	1.53	1.46
4	S	127	GLN	C-N	-5.84	1.26	1.33
4	P	41	PRO	CA-C	5.83	1.60	1.52
1	H	833	ALA	N-CA	5.82	1.50	1.46
4	P	3	THR	N-CA	5.82	1.54	1.46
1	G	938	THR	N-CA	5.81	1.52	1.46
1	D	226	LYS	N-CA	5.77	1.53	1.46
4	S	116	VAL	CA-C	5.75	1.60	1.52
1	I	808	ASP	CA-C	5.73	1.60	1.53
2	N	454	THR	CA-C	5.70	1.58	1.53
1	H	278	ASP	N-CA	5.69	1.52	1.45
1	H	272	ALA	N-CA	5.63	1.53	1.46
1	B	794	PHE	N-CA	5.62	1.53	1.46
1	E	729	VAL	N-CA	-5.62	1.39	1.46
4	S	127	GLN	CA-CB	5.62	1.62	1.53
1	B	189	GLU	N-CA	-5.59	1.39	1.46
1	I	808	ASP	N-CA	5.59	1.53	1.46
2	N	62	PRO	N-CA	5.56	1.53	1.47
1	A	927	ARG	C-N	-5.54	1.27	1.33
4	R	104	LEU	CA-C	5.54	1.57	1.52
4	S	28	ASN	N-CA	-5.49	1.42	1.47
1	E	10	TRP	CA-CB	5.48	1.62	1.53
2	N	291	ALA	N-CA	5.46	1.53	1.46
1	A	583	TRP	N-CA	5.41	1.53	1.46
2	N	277	ASP	N-CA	5.39	1.53	1.46
1	G	20	ALA	C-N	-5.36	1.27	1.33
4	S	117	VAL	N-CA	5.35	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	116	VAL	C-N	5.35	1.39	1.33
1	I	734	ASN	N-CA	-5.30	1.39	1.46
1	B	796	ARG	C-N	-5.30	1.26	1.33
1	E	736	ARG	N-CA	-5.27	1.39	1.46
2	N	475	PHE	CA-C	-5.27	1.46	1.52
1	H	60	ARG	CA-C	5.26	1.59	1.52
1	L	444	THR	C-N	-5.25	1.26	1.33
3	M	285	LEU	CA-C	5.25	1.58	1.52
1	D	228	THR	C-N	5.24	1.40	1.33
4	Q	21	PRO	C-N	-5.23	1.26	1.33
1	C	613	ILE	N-CA	-5.23	1.40	1.46
1	K	653	LEU	N-CA	5.23	1.51	1.45
4	Q	113	GLU	CA-C	5.23	1.59	1.52
1	K	699	TYR	CA-C	5.22	1.59	1.52
1	K	700	THR	N-CA	5.22	1.51	1.47
1	D	229	PRO	C-N	-5.21	1.25	1.33
1	A	838	GLU	CA-C	5.20	1.59	1.52
1	K	731	TRP	C-N	5.19	1.39	1.34
1	D	76	THR	CA-C	-5.18	1.46	1.52
1	A	62	GLN	N-CA	-5.18	1.40	1.46
1	L	725	PHE	N-CA	5.18	1.52	1.46
2	N	291	ALA	CA-C	5.18	1.59	1.52
4	S	22	TRP	N-CA	5.14	1.51	1.45
1	L	682	ARG	C-N	5.13	1.40	1.33
1	B	184	ILE	C-N	-5.12	1.26	1.33
1	K	276	ASN	CA-C	5.12	1.59	1.52
2	N	456	GLN	CA-CB	5.12	1.60	1.53
1	L	823	HIS	CB-CG	5.12	1.57	1.50
1	G	856	VAL	C-N	-5.11	1.26	1.33
1	C	823	HIS	CB-CG	5.10	1.57	1.50
1	L	35	THR	N-CA	5.10	1.52	1.46
1	I	730	SER	CA-C	5.09	1.58	1.52
1	A	663	VAL	C-N	5.08	1.39	1.33
1	K	386	MET	CA-C	5.06	1.59	1.52
4	S	109	SER	C-N	-5.05	1.25	1.33
4	S	131	LEU	CA-C	5.04	1.59	1.52
4	P	2	SER	C-N	5.03	1.42	1.33
1	D	54	HIS	CA-CB	5.03	1.61	1.53
4	R	4	ASN	CA-C	5.02	1.59	1.52
2	N	274	THR	N-CA	5.01	1.53	1.46

All (617) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	496	ASP	N-CA-C	17.29	131.59	111.71
1	B	725	PHE	CA-CB-CG	16.50	130.30	113.80
1	B	532	VAL	CB-CA-C	-16.49	92.98	111.45
1	J	571	ASN	CB-CA-C	-14.59	91.69	111.82
1	I	824	ASN	CA-CB-CG	-13.64	98.96	112.60
4	R	7	ASP	CA-CB-CG	12.62	125.22	112.60
1	L	856	VAL	CB-CA-C	11.99	127.62	111.19
1	H	276	ASN	CA-CB-CG	11.77	124.37	112.60
2	N	47	ARG	CA-C-N	11.63	131.60	119.85
2	N	47	ARG	C-N-CA	11.63	131.60	119.85
1	G	563	PRO	CB-CA-C	-11.48	92.62	111.56
1	C	242	ASN	CB-CA-C	-11.30	95.90	109.80
1	H	867	ASP	CA-CB-CG	-11.21	101.39	112.60
1	L	54	HIS	N-CA-C	11.15	124.75	111.82
1	A	431	PRO	N-CA-C	10.85	127.95	113.84
4	P	6	PHE	N-CA-C	10.81	127.00	109.59
2	N	48	PRO	CB-CA-C	-10.71	96.95	110.98
1	I	794	PHE	N-CA-C	10.67	124.42	111.40
1	H	272	ALA	N-CA-C	10.43	124.91	109.59
1	B	534	PRO	CB-CA-C	-10.27	94.62	111.56
5	V	185	THR	CA-C-N	-10.24	106.01	121.99
5	V	185	THR	C-N-CA	-10.24	106.01	121.99
1	I	783	ILE	N-CA-C	10.20	118.50	109.02
4	P	6	PHE	CA-CB-CG	10.15	123.95	113.80
1	D	229	PRO	N-CA-C	-9.96	95.38	111.21
1	H	611	ASP	CA-CB-CG	9.88	122.48	112.60
1	A	689	PRO	CB-CA-C	-9.86	94.59	110.96
1	D	35	THR	CB-CA-C	-9.86	95.80	111.18
1	A	664	PRO	CB-CA-C	-9.78	96.65	110.63
4	R	122	LEU	N-CA-C	-9.78	101.70	114.31
1	B	254	GLN	N-CA-C	9.68	121.83	111.28
1	K	273	THR	N-CA-C	-9.67	101.61	113.41
1	L	54	HIS	CA-CB-CG	-9.65	104.15	113.80
1	L	726	ASP	CA-CB-CG	9.61	122.21	112.60
1	D	52	PRO	CB-CA-C	-9.60	95.72	111.56
4	S	19	MET	O-C-N	9.47	129.82	121.39
1	J	657	PRO	CB-CA-C	-9.45	98.65	111.21
2	N	141	ASN	CA-CB-CG	-9.44	103.16	112.60
1	I	831	TYR	CA-CB-CG	-9.38	97.01	113.90
5	V	184	GLY	N-CA-C	-9.36	100.56	112.54
4	P	136	PRO	CB-CA-C	-9.35	99.51	110.92
1	F	712	PHE	N-CA-C	9.35	127.21	107.67
2	N	455	ARG	N-CA-C	9.21	123.61	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	21	PRO	N-CA-C	9.19	126.30	113.53
1	L	725	PHE	N-CA-C	9.18	121.28	111.28
1	C	179	ILE	CB-CA-C	-9.15	99.62	111.25
1	H	278	ASP	CA-CB-CG	9.14	121.74	112.60
1	G	21	SER	CA-C-N	-9.07	103.80	122.03
1	G	21	SER	C-N-CA	-9.07	103.80	122.03
1	L	823	HIS	CA-C-N	8.93	135.29	121.99
1	L	823	HIS	C-N-CA	8.93	135.29	121.99
1	I	738	LEU	N-CA-C	8.90	121.80	111.11
2	N	477	ASN	CA-CB-CG	8.88	121.48	112.60
1	C	825	ASN	CA-CB-CG	8.87	121.47	112.60
1	I	794	PHE	CA-CB-CG	-8.80	105.00	113.80
1	D	193	PRO	CB-CA-C	-8.69	100.95	111.46
4	S	20	PRO	CA-C-N	8.66	128.66	119.05
4	S	20	PRO	C-N-CA	8.66	128.66	119.05
1	G	563	PRO	N-CA-CB	8.60	112.28	103.25
5	V	185	THR	N-CA-C	8.57	123.00	112.54
3	M	195	GLY	N-CA-C	-8.54	96.09	110.95
4	Q	22	TRP	CB-CA-C	8.54	126.29	110.24
1	B	941	LEU	CB-CA-C	-8.52	100.03	110.94
1	J	19	ASP	CA-CB-CG	8.49	121.09	112.60
1	E	735	ASP	CA-CB-CG	-8.42	104.18	112.60
1	J	757	ALA	CA-C-N	8.41	134.44	122.08
1	J	757	ALA	C-N-CA	8.41	134.44	122.08
1	C	179	ILE	N-CA-C	8.38	120.80	107.73
4	S	19	MET	CA-C-N	8.38	129.01	120.38
4	S	19	MET	C-N-CA	8.38	129.01	120.38
1	A	928	VAL	CB-CA-C	8.28	121.76	111.25
1	H	571	ASN	CA-CB-CG	8.26	120.86	112.60
1	A	430	LYS	CA-C-N	8.21	127.94	119.56
1	A	430	LYS	C-N-CA	8.21	127.94	119.56
6	W	4	LEU	N-CA-C	8.21	122.26	111.75
4	S	22	TRP	CA-CB-CG	8.21	129.19	113.60
2	N	64	PHE	CA-CB-CG	-8.19	105.61	113.80
1	C	13	MET	CA-C-N	8.15	135.95	123.47
1	C	13	MET	C-N-CA	8.15	135.95	123.47
1	C	664	PRO	CB-CA-C	-8.09	97.53	110.96
1	I	654	TYR	CA-C-N	8.02	127.91	120.21
1	I	654	TYR	C-N-CA	8.02	127.91	120.21
1	A	794	PHE	CB-CA-C	-8.02	96.12	110.23
2	N	200	GLY	N-CA-C	8.01	124.64	111.27
1	B	15	ILE	CB-CA-C	-8.00	102.13	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	758	GLN	CB-CA-C	-7.98	97.99	110.04
1	H	725	PHE	CA-CB-CG	7.96	121.76	113.80
4	R	6	PHE	CA-CB-CG	7.85	121.65	113.80
1	B	533	ASN	CA-CB-CG	7.84	120.44	112.60
1	A	432	LYS	N-CA-C	7.80	120.68	111.71
1	L	21	SER	CA-C-N	-7.78	109.98	122.66
1	L	21	SER	C-N-CA	-7.78	109.98	122.66
1	A	677	GLY	N-CA-C	7.77	120.92	110.43
1	H	504	MET	CB-CA-C	7.74	126.17	110.38
3	M	196	LEU	N-CA-C	7.71	121.40	110.68
2	N	475	PHE	CA-C-N	-7.69	112.85	122.84
2	N	475	PHE	C-N-CA	-7.69	112.85	122.84
1	G	558	PHE	N-CA-C	7.68	119.69	108.86
1	L	16	SER	CA-C-N	7.67	128.44	120.00
1	L	16	SER	C-N-CA	7.67	128.44	120.00
6	W	6	PRO	N-CA-CB	7.66	111.29	103.25
1	A	657	PRO	CB-CA-C	7.65	121.02	111.23
1	I	793	SER	CA-C-N	7.65	133.49	120.71
1	I	793	SER	C-N-CA	7.65	133.49	120.71
1	E	15	ILE	CB-CA-C	-7.63	102.37	110.62
1	H	504	MET	CA-C-N	7.61	130.80	120.38
1	H	504	MET	C-N-CA	7.61	130.80	120.38
4	Q	56	PRO	N-CA-CB	7.61	110.41	103.34
1	A	471	ASN	CA-CB-CG	-7.60	105.00	112.60
1	B	185	GLN	N-CA-C	-7.59	96.14	108.52
4	R	46	THR	CB-CA-C	-7.59	99.51	110.06
1	K	331	ASP	CA-CB-CG	-7.57	105.03	112.60
2	N	61	ALA	CA-C-N	7.55	127.46	120.21
2	N	61	ALA	C-N-CA	7.55	127.46	120.21
1	A	478	ALA	CA-C-N	-7.54	108.74	122.38
1	A	478	ALA	C-N-CA	-7.54	108.74	122.38
1	A	217	ASN	N-CA-C	-7.53	97.62	109.07
1	G	689	PRO	CB-CA-C	-7.52	99.87	111.22
1	K	62	GLN	CA-C-N	7.51	132.78	122.19
1	K	62	GLN	C-N-CA	7.51	132.78	122.19
1	I	783	ILE	CB-CA-C	-7.43	103.72	111.00
1	I	347	VAL	CB-CA-C	-7.43	99.11	111.29
1	B	732	PRO	CB-CA-C	-7.39	99.36	111.56
1	L	858	SER	N-CA-C	7.39	121.42	110.48
4	R	6	PHE	CA-C-N	-7.39	112.71	123.05
4	R	6	PHE	C-N-CA	-7.39	112.71	123.05
4	S	130	ALA	CA-C-N	-7.38	110.09	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	130	ALA	C-N-CA	-7.38	110.09	122.64
1	A	654	TYR	CA-C-N	7.36	127.79	119.92
1	A	654	TYR	C-N-CA	7.36	127.79	119.92
1	C	173	PRO	CB-CA-C	-7.34	98.58	110.25
1	G	845	ASN	CA-CB-CG	-7.23	105.37	112.60
1	A	431	PRO	CB-CA-C	-7.23	101.59	111.85
1	I	734	ASN	CB-CA-C	7.23	122.39	109.38
1	L	445	GLU	CB-CA-C	7.20	122.39	109.64
1	A	19	ASP	CA-C-N	7.20	135.29	121.54
1	A	19	ASP	C-N-CA	7.20	135.29	121.54
1	J	273	THR	N-CA-C	-7.18	103.63	113.18
1	C	255	ASN	CA-CB-CG	7.18	119.78	112.60
1	H	732	PRO	CB-CA-C	-7.17	99.73	111.56
1	B	794	PHE	N-CA-C	7.15	126.02	110.80
1	H	612	SER	N-CA-C	7.15	119.75	108.67
1	K	415	PHE	CA-CB-CG	7.14	120.94	113.80
3	M	217	PRO	CB-CA-C	-7.13	99.80	111.56
4	Q	55	THR	CA-C-O	-7.12	110.41	120.16
1	I	656	ILE	N-CA-CB	7.11	121.17	111.21
4	R	46	THR	CA-C-N	7.10	132.52	122.08
4	R	46	THR	C-N-CA	7.10	132.52	122.08
1	G	923	PHE	CA-C-N	-7.09	113.13	123.05
1	G	923	PHE	C-N-CA	-7.09	113.13	123.05
1	H	505	ASN	N-CA-C	7.06	119.88	111.33
1	C	867	ASP	CA-C-N	7.05	135.01	121.54
1	C	867	ASP	C-N-CA	7.05	135.01	121.54
1	E	12	TYR	CA-C-N	-7.03	111.41	122.65
1	E	12	TYR	C-N-CA	-7.03	111.41	122.65
4	S	57	LEU	N-CA-C	7.02	120.84	110.46
1	H	708	LEU	N-CA-C	7.01	121.92	113.23
2	N	292	TYR	CA-C-N	7.01	132.98	122.68
2	N	292	TYR	C-N-CA	7.01	132.98	122.68
4	Q	55	THR	O-C-N	-7.00	113.27	121.32
5	V	38	PRO	CA-C-N	-6.97	110.36	122.36
5	V	38	PRO	C-N-CA	-6.97	110.36	122.36
1	C	52	PRO	CB-CA-C	-6.96	100.08	111.56
1	G	355	LEU	N-CA-C	6.95	120.49	109.65
1	L	444	THR	CB-CA-C	-6.94	99.65	111.31
1	G	191	GLN	CA-C-N	-6.94	111.88	122.42
1	G	191	GLN	C-N-CA	-6.94	111.88	122.42
5	V	39	HIS	N-CA-C	-6.91	105.38	113.88
1	C	56	VAL	N-CA-C	6.91	118.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	53	ASN	CA-CB-CG	6.91	119.50	112.60
4	P	4	ASN	CA-CB-CG	6.89	119.49	112.60
1	I	347	VAL	CA-C-N	6.88	132.38	121.66
1	I	347	VAL	C-N-CA	6.88	132.38	121.66
1	K	748	SER	CA-C-N	6.87	134.33	121.97
1	K	748	SER	C-N-CA	6.87	134.33	121.97
1	H	505	ASN	CA-CB-CG	-6.87	105.73	112.60
2	N	65	ASP	CA-CB-CG	6.87	119.47	112.60
1	L	420	VAL	N-CA-C	6.84	118.66	108.46
1	H	839	GLY	N-CA-C	6.84	119.81	110.58
1	I	725	PHE	CA-CB-CG	6.84	120.64	113.80
1	B	530	ASP	N-CA-C	6.83	121.20	113.01
2	N	441	LEU	CA-C-N	6.82	126.78	119.28
2	N	441	LEU	C-N-CA	6.82	126.78	119.28
4	S	110	LEU	N-CA-C	-6.82	104.95	113.20
1	D	794	PHE	N-CA-C	6.82	125.33	110.80
1	K	551	GLY	N-CA-C	6.81	119.07	110.96
4	S	35	ASP	CB-CA-C	-6.80	102.38	111.63
4	Q	23	ALA	CA-C-N	6.80	130.38	120.11
4	Q	23	ALA	C-N-CA	6.80	130.38	120.11
1	L	26	PRO	CB-CA-C	-6.79	100.35	111.56
1	A	253	GLN	N-CA-C	-6.79	95.89	107.23
1	J	925	VAL	N-CA-C	6.78	118.91	109.55
1	E	725	PHE	CA-CB-CG	6.77	120.57	113.80
4	P	5	SER	CA-C-O	-6.77	113.34	120.58
1	H	724	THR	CA-C-N	-6.75	110.79	123.27
1	H	724	THR	C-N-CA	-6.75	110.79	123.27
1	K	495	SER	CA-C-N	6.74	129.99	120.28
1	K	495	SER	C-N-CA	6.74	129.99	120.28
2	N	48	PRO	N-CA-CB	6.73	109.59	103.33
1	I	655	PRO	CB-CA-C	-6.73	101.06	111.22
1	H	59	ASP	CA-CB-CG	-6.68	105.92	112.60
1	H	517	TYR	CA-C-N	-6.67	109.97	121.97
1	H	517	TYR	C-N-CA	-6.67	109.97	121.97
4	R	19	MET	CA-C-N	6.66	127.24	120.38
4	R	19	MET	C-N-CA	6.66	127.24	120.38
1	K	63	ARG	N-CA-C	6.63	120.47	109.46
1	D	229	PRO	N-CA-CB	6.62	109.11	103.35
1	E	757	ALA	N-CA-C	6.62	118.93	108.67
1	B	250	LEU	CA-C-N	-6.61	113.46	122.91
1	B	250	LEU	C-N-CA	-6.61	113.46	122.91
1	B	533	ASN	CA-C-N	6.61	128.10	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	ASN	C-N-CA	6.61	128.10	119.84
4	P	41	PRO	CB-CA-C	-6.61	100.66	111.56
1	B	188	VAL	N-CA-CB	6.59	119.97	111.67
1	I	794	PHE	N-CA-CB	-6.58	100.39	110.13
1	K	705	ILE	CA-C-N	6.58	127.10	119.47
1	K	705	ILE	C-N-CA	6.58	127.10	119.47
1	D	794	PHE	CA-CB-CG	-6.57	107.23	113.80
1	J	654	TYR	CA-C-N	6.56	128.04	119.84
1	J	654	TYR	C-N-CA	6.56	128.04	119.84
1	D	18	GLN	N-CA-C	6.56	118.43	111.28
1	E	438	GLY	N-CA-C	-6.56	97.63	113.18
2	N	272	ARG	CA-C-N	6.56	133.78	121.97
2	N	272	ARG	C-N-CA	6.56	133.78	121.97
5	U	15	PRO	CB-CA-C	-6.55	100.74	111.56
4	S	48	THR	CB-CA-C	-6.55	101.81	112.03
1	F	865	LEU	CA-C-N	6.53	130.48	121.33
1	F	865	LEU	C-N-CA	6.53	130.48	121.33
1	J	266	PHE	N-CA-C	6.53	119.80	109.81
1	F	712	PHE	CB-CA-C	-6.52	102.77	112.09
1	A	220	ALA	N-CA-C	6.49	120.00	110.59
6	W	17	TRP	N-CA-C	6.49	119.73	109.81
1	G	897	SER	N-CA-C	6.47	118.92	111.02
2	N	47	ARG	CB-CA-C	6.47	118.60	108.63
1	E	575	LEU	CA-C-N	6.47	127.92	119.84
1	E	575	LEU	C-N-CA	6.47	127.92	119.84
1	B	842	TYR	CA-C-N	6.46	127.92	119.84
1	B	842	TYR	C-N-CA	6.46	127.92	119.84
1	L	810	LYS	N-CA-C	6.46	118.20	111.03
4	S	10	ILE	N-CA-C	6.46	117.46	108.23
1	A	52	PRO	CB-CA-C	-6.46	100.91	111.56
1	J	333	PHE	CB-CA-C	-6.44	101.33	111.51
1	H	732	PRO	N-CA-CB	6.44	110.01	103.25
1	A	202	PRO	CA-C-N	-6.42	111.47	120.39
1	A	202	PRO	C-N-CA	-6.42	111.47	120.39
1	K	276	ASN	CA-CB-CG	6.40	119.00	112.60
1	K	270	THR	CB-CA-C	-6.39	101.49	111.39
1	G	804	GLN	N-CA-C	6.38	118.85	108.26
1	H	503	TYR	CA-C-N	-6.37	109.85	120.68
1	H	503	TYR	C-N-CA	-6.37	109.85	120.68
1	G	193	PRO	CB-CA-C	-6.36	101.06	111.56
1	G	22	GLU	CA-CB-CG	-6.36	101.39	114.10
1	L	96	MET	N-CA-C	6.35	118.28	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	242	ASN	CA-CB-CG	-6.34	106.26	112.60
1	G	923	PHE	CB-CA-C	-6.33	100.59	111.23
2	N	455	ARG	CA-C-N	-6.33	110.05	122.02
2	N	455	ARG	C-N-CA	-6.33	110.05	122.02
1	I	482	PRO	CB-CA-C	6.33	119.28	111.12
2	N	454	THR	CA-C-N	6.32	130.71	120.60
2	N	454	THR	C-N-CA	6.32	130.71	120.60
4	S	19	MET	CA-C-O	6.32	126.14	119.69
1	E	734	ASN	CA-CB-CG	6.30	118.91	112.60
1	G	23	TYR	CB-CG-CD2	6.30	130.25	120.80
1	I	729	VAL	CB-CA-C	6.28	121.59	111.29
1	I	487	TYR	N-CA-C	6.27	119.57	110.42
1	G	696	ASP	CB-CA-C	6.26	118.44	109.92
2	N	200	GLY	CA-C-N	6.26	133.24	121.97
2	N	200	GLY	C-N-CA	6.26	133.24	121.97
4	P	40	LEU	CA-C-N	6.25	127.65	119.84
4	P	40	LEU	C-N-CA	6.25	127.65	119.84
1	G	21	SER	O-C-N	6.25	130.53	121.78
1	A	930	ARG	CA-C-N	6.25	125.81	119.19
1	A	930	ARG	C-N-CA	6.25	125.81	119.19
1	D	794	PHE	CB-CA-C	-6.24	98.00	110.42
5	V	203	GLY	CA-C-N	6.23	124.14	119.66
5	V	203	GLY	C-N-CA	6.23	124.14	119.66
1	J	924	ASP	CA-C-N	6.22	131.57	121.62
1	J	924	ASP	C-N-CA	6.22	131.57	121.62
1	H	795	PHE	N-CA-C	6.20	120.23	111.92
1	I	483	ASP	CA-CB-CG	6.20	118.80	112.60
1	G	923	PHE	N-CA-C	6.19	120.14	107.69
4	S	34	ILE	N-CA-C	6.19	122.22	109.34
4	S	16	THR	CB-CA-C	6.19	119.88	109.48
1	K	330	ARG	CB-CA-C	6.18	122.72	110.42
1	A	750	ASP	N-CA-C	6.15	118.06	111.36
5	U	83	SER	N-CA-C	6.15	117.14	109.57
2	N	453	SER	N-CA-C	6.15	118.97	109.07
1	A	19	ASP	N-CA-C	6.15	118.51	108.55
1	H	21	SER	N-CA-C	6.14	117.64	111.07
1	H	517	TYR	N-CA-C	6.14	123.88	110.80
1	K	732	PRO	CB-CA-C	-6.13	100.72	111.21
1	G	23	TYR	CB-CG-CD1	-6.13	111.61	120.80
2	N	199	ASN	CA-CB-CG	6.13	118.73	112.60
1	G	806	VAL	CB-CA-C	-6.13	102.07	111.08
3	M	216	ALA	CA-C-N	6.13	127.50	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	216	ALA	C-N-CA	6.13	127.50	119.84
4	P	39	VAL	CB-CA-C	6.13	120.04	111.34
1	H	60	ARG	CB-CA-C	6.11	119.75	109.48
3	M	251	ASP	CA-CB-CG	-6.11	106.50	112.60
6	W	12	PRO	N-CA-CB	6.10	109.66	103.25
4	P	107	LEU	N-CA-C	-6.08	104.00	112.45
1	B	530	ASP	CA-C-N	6.07	131.01	120.68
1	B	530	ASP	C-N-CA	6.07	131.01	120.68
1	B	908	ASP	CA-C-N	6.07	127.43	119.84
1	B	908	ASP	C-N-CA	6.07	127.43	119.84
1	G	22	GLU	N-CA-C	6.07	119.39	110.59
1	B	534	PRO	N-CA-CB	6.06	109.61	103.25
1	A	691	LEU	N-CA-C	6.05	120.53	111.81
1	C	867	ASP	CA-C-O	6.05	126.65	120.24
1	A	663	VAL	CA-C-N	6.05	126.55	120.14
1	A	663	VAL	C-N-CA	6.05	126.55	120.14
1	B	417	LEU	N-CA-C	6.05	123.68	110.80
2	N	476	TYR	CA-CB-CG	6.05	124.78	113.90
1	B	16	SER	N-CA-C	-6.04	104.01	113.02
1	J	269	THR	CA-C-N	6.03	133.06	121.54
1	J	269	THR	C-N-CA	6.03	133.06	121.54
1	D	731	TRP	CA-C-N	-6.02	115.57	121.65
1	D	731	TRP	C-N-CA	-6.02	115.57	121.65
1	B	794	PHE	CA-C-N	-6.02	111.16	120.31
1	B	794	PHE	C-N-CA	-6.02	111.16	120.31
1	A	928	VAL	N-CA-CB	-6.01	103.91	111.31
1	K	657	PRO	N-CA-C	6.01	119.93	111.33
1	A	663	VAL	CB-CA-C	-6.00	104.09	110.16
4	P	5	SER	O-C-N	-6.00	115.72	122.93
1	J	656	ILE	CA-C-N	6.00	125.76	119.76
1	J	656	ILE	C-N-CA	6.00	125.76	119.76
1	A	659	ASN	N-CA-C	5.99	122.20	113.40
1	A	252	LYS	N-CA-C	5.98	118.91	110.23
1	B	867	ASP	CA-CB-CG	-5.98	106.62	112.60
1	D	78	TYR	CB-CA-C	-5.98	102.98	111.95
2	N	139	PHE	N-CA-C	5.97	123.52	110.80
1	D	54	HIS	CA-CB-CG	5.97	119.77	113.80
1	J	657	PRO	N-CA-CB	5.96	108.88	103.34
1	J	332	ASN	CA-CB-CG	-5.95	106.65	112.60
1	F	508	VAL	N-CA-C	5.95	114.92	106.53
2	N	259	LEU	N-CA-C	5.95	117.57	111.14
1	A	253	GLN	CB-CG-CD	5.94	122.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	823	HIS	CB-CA-C	-5.94	98.23	111.77
1	G	868	ARG	N-CA-C	5.93	121.40	114.04
1	G	922	VAL	CB-CA-C	5.93	121.02	111.29
1	I	656	ILE	N-CA-C	-5.93	96.07	108.88
1	J	756	VAL	CB-CA-C	5.93	119.82	111.63
1	F	464	LEU	N-CA-C	5.93	117.42	111.07
4	P	104	LEU	N-CA-C	5.92	117.54	111.14
1	L	421	ILE	CB-CA-C	-5.92	101.58	111.29
1	C	19	ASP	CA-C-N	5.91	128.48	120.44
1	C	19	ASP	C-N-CA	5.91	128.48	120.44
1	E	632	ALA	N-CA-C	5.91	118.48	111.33
1	H	270	THR	N-CA-C	5.90	119.33	111.30
1	L	26	PRO	N-CA-CB	5.89	109.44	103.25
1	H	795	PHE	CA-CB-CG	5.89	119.69	113.80
1	H	879	PHE	O-C-N	5.88	128.17	121.88
4	P	4	ASN	CA-C-O	-5.86	114.74	121.07
1	I	173	PRO	N-CA-CB	5.86	108.22	103.36
1	L	756	VAL	CB-CA-C	-5.85	100.62	111.79
2	N	50	GLY	N-CA-C	-5.85	99.32	113.18
1	H	501	TYR	CA-C-N	5.84	132.69	121.54
1	H	501	TYR	C-N-CA	5.84	132.69	121.54
1	L	421	ILE	N-CA-C	5.84	121.48	109.34
1	A	56	VAL	CB-CA-C	-5.82	101.74	111.29
6	W	22	THR	N-CA-C	5.81	117.30	110.97
1	D	169	PHE	N-CA-C	5.81	118.52	109.52
1	A	660	ALA	N-CA-C	5.80	119.05	110.46
1	A	794	PHE	N-CA-C	5.80	120.90	113.18
1	J	331	ASP	CA-CB-CG	5.79	118.39	112.60
1	L	240	PRO	N-CA-CB	5.79	108.47	103.31
1	K	698	TYR	CA-C-N	-5.78	112.67	120.87
1	K	698	TYR	C-N-CA	-5.78	112.67	120.87
1	C	110	GLY	CA-C-N	5.77	125.63	119.28
1	C	110	GLY	C-N-CA	5.77	125.63	119.28
1	A	689	PRO	N-CA-CB	5.77	109.96	102.86
2	N	276	ASP	CA-CB-CG	5.76	118.36	112.60
2	N	139	PHE	CA-CB-CG	-5.76	108.04	113.80
1	I	758	GLN	CA-C-N	5.76	129.99	120.94
1	I	758	GLN	C-N-CA	5.76	129.99	120.94
1	H	796	ARG	N-CA-C	-5.75	98.56	110.80
1	F	397	ASP	CA-CB-CG	5.73	118.33	112.60
1	K	387	TRP	CB-CA-C	5.72	119.65	110.09
4	S	56	PRO	CA-C-N	5.72	132.57	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	56	PRO	C-N-CA	5.72	132.57	122.67
1	L	654	TYR	CA-C-N	5.71	126.98	119.84
1	L	654	TYR	C-N-CA	5.71	126.98	119.84
4	P	129	SER	N-CA-C	-5.71	106.27	113.18
1	L	867	ASP	CB-CA-C	-5.70	98.48	109.37
5	U	204	PRO	N-CA-C	5.70	117.65	110.70
1	J	122	ASN	CA-CB-CG	5.70	118.30	112.60
4	P	37	ARG	CA-C-N	5.69	126.00	119.92
4	P	37	ARG	C-N-CA	5.69	126.00	119.92
1	K	749	VAL	N-CA-C	5.68	121.16	109.34
1	J	22	GLU	N-CA-C	5.68	118.57	111.24
1	G	691	LEU	N-CA-C	5.68	118.47	110.23
1	G	869	THR	N-CA-C	5.68	117.55	108.41
4	P	136	PRO	N-CA-C	5.68	117.63	110.70
4	R	104	LEU	N-CA-C	5.68	120.48	112.93
4	S	126	GLN	CA-C-N	5.68	132.38	121.54
4	S	126	GLN	C-N-CA	5.68	132.38	121.54
2	N	62	PRO	CB-CA-C	-5.67	102.65	111.22
1	B	730	SER	CB-CA-C	-5.67	100.65	109.61
1	I	808	ASP	N-CA-C	5.67	120.20	112.04
1	K	656	ILE	CA-C-N	5.66	126.45	120.11
1	K	656	ILE	C-N-CA	5.66	126.45	120.11
5	V	183	ILE	CB-CA-C	-5.66	103.82	111.63
1	C	663	VAL	CA-C-N	5.66	127.03	120.98
1	C	663	VAL	C-N-CA	5.66	127.03	120.98
1	C	254	GLN	N-CA-C	5.66	122.85	110.80
1	G	851	ILE	N-CA-C	5.66	116.43	110.72
1	G	805	VAL	CA-C-N	5.65	128.21	120.35
1	G	805	VAL	C-N-CA	5.65	128.21	120.35
4	Q	108	ASP	N-CA-C	-5.65	105.41	112.93
1	D	760	ASN	N-CA-C	-5.64	106.24	113.23
1	B	794	PHE	CA-CB-CG	-5.63	108.17	113.80
1	L	22	GLU	N-CA-C	5.63	118.94	112.97
1	A	61	SER	CA-C-N	-5.62	114.74	122.16
1	A	61	SER	C-N-CA	-5.62	114.74	122.16
4	P	111	THR	N-CA-C	-5.62	104.78	111.69
1	A	794	PHE	CA-C-N	-5.62	113.42	122.24
1	A	794	PHE	C-N-CA	-5.62	113.42	122.24
4	S	131	LEU	CB-CA-C	5.61	118.99	109.50
1	F	713	TYR	N-CA-C	5.61	119.87	113.19
1	A	836	MET	N-CA-C	5.61	118.37	109.50
1	B	730	SER	CA-C-N	5.61	135.48	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	730	SER	C-N-CA	5.61	135.48	121.80
1	F	745	ILE	N-CA-C	-5.60	106.74	111.56
4	S	112	ARG	N-CA-C	-5.60	105.95	112.89
1	D	79	SER	CB-CA-C	5.60	119.94	109.86
1	H	879	PHE	CA-CB-CG	-5.60	108.20	113.80
1	E	441	LYS	CA-C-N	5.59	132.22	121.54
1	E	441	LYS	C-N-CA	5.59	132.22	121.54
1	D	273	THR	N-CA-C	-5.59	106.59	113.41
1	G	464	LEU	N-CA-C	5.59	118.30	111.82
1	G	266	PHE	N-CA-C	5.58	118.32	109.50
5	V	34	MET	CA-C-N	5.58	130.17	120.68
5	V	34	MET	C-N-CA	5.58	130.17	120.68
1	G	907	VAL	CB-CA-C	-5.58	101.97	110.95
1	B	731	TRP	N-CA-C	5.57	122.13	109.81
1	C	13	MET	O-C-N	5.57	130.15	122.46
1	I	483	ASP	CA-C-N	-5.57	112.15	121.39
1	I	483	ASP	C-N-CA	-5.57	112.15	121.39
4	P	36	GLY	N-CA-C	-5.56	103.24	111.03
1	B	798	PHE	N-CA-C	5.56	119.30	109.96
4	P	4	ASN	O-C-N	-5.55	116.46	123.12
1	B	12	TYR	CA-C-N	-5.54	113.78	122.65
1	B	12	TYR	C-N-CA	-5.54	113.78	122.65
1	K	417	LEU	N-CA-CB	5.54	118.37	109.28
1	L	855	ALA	CA-C-N	-5.54	115.07	122.77
1	L	855	ALA	C-N-CA	-5.54	115.07	122.77
1	H	739	THR	CA-C-N	5.54	126.76	119.84
1	H	739	THR	C-N-CA	5.54	126.76	119.84
1	K	850	LEU	N-CA-C	-5.52	105.99	114.16
1	A	655	PRO	CB-CA-C	-5.51	104.01	111.12
1	D	69	ILE	CA-C-N	5.51	126.73	119.84
1	D	69	ILE	C-N-CA	5.51	126.73	119.84
4	R	15	LEU	N-CA-C	5.51	118.03	109.60
1	D	231	LYS	CB-CA-C	5.51	116.31	108.76
2	N	141	ASN	N-CA-C	5.51	120.21	112.72
1	F	868	ARG	CB-CA-C	-5.50	102.82	111.51
1	F	77	ALA	N-CA-C	5.50	119.16	112.23
1	G	562	VAL	CA-C-N	5.50	126.71	119.84
1	G	562	VAL	C-N-CA	5.50	126.71	119.84
1	I	680	PHE	N-CA-C	5.49	118.14	108.75
3	M	284	ALA	CA-C-N	-5.48	112.29	122.60
3	M	284	ALA	C-N-CA	-5.48	112.29	122.60
1	C	826	SER	N-CA-C	-5.47	101.21	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	417	LEU	CA-C-N	5.47	132.13	121.41
1	K	417	LEU	C-N-CA	5.47	132.13	121.41
2	N	441	LEU	N-CA-C	-5.47	101.04	109.79
1	A	61	SER	N-CA-C	5.47	118.50	110.30
1	L	36	GLU	N-CA-C	5.46	117.23	111.28
2	N	68	ARG	N-CA-C	5.46	118.88	110.42
1	C	659	ASN	CA-CB-CG	-5.45	107.15	112.60
1	H	798	PHE	N-CA-C	5.44	117.66	109.23
1	I	728	SER	N-CA-C	5.44	121.77	113.61
4	S	37	ARG	N-CA-C	-5.44	97.79	109.81
1	L	943	THR	CA-C-N	-5.42	114.17	119.64
1	L	943	THR	C-N-CA	-5.42	114.17	119.64
4	S	49	TYR	N-CA-CB	5.42	119.65	110.49
4	P	132	LYS	N-CA-C	-5.41	106.53	113.02
1	B	182	GLU	CA-C-N	5.40	132.00	121.41
1	B	182	GLU	C-N-CA	5.40	132.00	121.41
1	D	527	ASP	N-CA-C	5.40	116.85	111.07
4	S	109	SER	O-C-N	5.40	128.54	122.22
2	N	291	ALA	N-CA-C	5.40	119.99	113.41
2	N	292	TYR	N-CA-CB	5.38	117.92	109.69
1	K	638	THR	N-CA-C	-5.37	108.50	114.62
1	K	751	GLY	N-CA-C	-5.37	100.45	113.18
1	F	239	LYS	CA-C-N	-5.36	113.14	119.84
1	F	239	LYS	C-N-CA	-5.36	113.14	119.84
1	H	272	ALA	CA-C-N	5.36	130.90	122.11
1	H	272	ALA	C-N-CA	5.36	130.90	122.11
1	G	651	ASN	N-CA-C	5.35	116.17	107.23
1	B	188	VAL	CA-C-O	5.35	126.92	120.66
1	B	756	VAL	N-CA-C	5.35	117.57	109.12
4	S	13	SER	N-CA-C	5.35	122.19	110.80
3	M	251	ASP	N-CA-C	5.34	119.92	113.41
1	K	846	PHE	CA-CB-CG	5.34	119.14	113.80
1	H	793	SER	N-CA-C	5.33	117.51	109.41
1	I	178	ASN	N-CA-C	5.33	117.07	109.14
4	R	5	SER	O-C-N	-5.32	117.02	123.03
1	I	172	ALA	N-CA-C	5.31	116.41	108.76
1	L	892	LEU	N-CA-C	5.30	116.86	111.14
3	M	13	ALA	N-CA-C	-5.30	105.17	111.69
1	A	266	PHE	N-CA-C	5.30	116.70	109.18
1	A	925	VAL	N-CA-C	5.29	115.57	108.17
1	G	553	GLY	N-CA-C	5.28	117.14	110.38
1	G	880	MET	CA-C-N	-5.28	113.33	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	880	MET	C-N-CA	-5.28	113.33	122.14
1	L	59	ASP	N-CA-C	-5.28	106.89	113.38
4	Q	78	ASP	N-CA-C	5.28	117.94	111.82
1	I	823	HIS	N-CA-C	5.28	116.77	110.44
1	F	395	ASP	N-CA-C	5.26	116.56	109.24
1	A	664	PRO	N-CA-CB	5.26	108.25	103.15
1	C	240	PRO	CB-CA-C	-5.26	104.50	111.23
4	S	56	PRO	N-CA-CB	-5.26	97.73	103.25
1	B	531	ASN	CA-CB-CG	-5.26	107.34	112.60
1	D	908	ASP	CA-C-N	5.25	126.41	119.84
1	D	908	ASP	C-N-CA	5.25	126.41	119.84
1	A	931	PRO	CB-CA-C	-5.25	104.44	112.11
1	C	658	ALA	N-CA-C	5.24	120.02	111.37
1	K	277	GLY	N-CA-C	5.24	120.40	113.37
1	C	213	GLU	CA-C-N	5.24	128.67	122.44
1	C	213	GLU	C-N-CA	5.24	128.67	122.44
1	F	806	VAL	N-CA-C	5.24	115.85	109.30
6	W	23	SER	CA-C-N	5.23	131.11	121.70
6	W	23	SER	C-N-CA	5.23	131.11	121.70
1	K	754	TYR	N-CA-C	-5.22	107.08	113.50
1	J	653	LEU	N-CA-C	5.22	116.82	107.80
1	C	611	ASP	CA-CB-CG	-5.21	107.39	112.60
1	G	22	GLU	CB-CA-C	-5.21	100.65	110.51
1	H	704	SER	CA-C-N	-5.21	112.49	122.13
1	H	704	SER	C-N-CA	-5.21	112.49	122.13
1	I	729	VAL	CA-C-N	5.20	130.33	122.99
1	I	729	VAL	C-N-CA	5.20	130.33	122.99
4	P	2	SER	CA-C-N	5.20	133.35	122.58
4	P	2	SER	C-N-CA	5.20	133.35	122.58
1	D	269	THR	CB-CA-C	-5.20	104.55	111.88
1	I	354	GLN	CB-CG-CD	5.20	121.44	112.60
1	H	677	GLY	N-CA-C	5.19	117.02	110.38
1	J	103	ILE	N-CA-C	5.19	114.22	106.85
1	D	421	ILE	N-CA-C	5.18	115.23	107.51
1	B	939	VAL	CA-C-N	5.18	131.51	122.81
1	B	939	VAL	C-N-CA	5.18	131.51	122.81
1	J	713	TYR	N-CA-C	5.18	117.67	111.71
5	V	42	SER	N-CA-C	-5.18	106.80	113.01
1	B	30	GLN	N-CA-C	5.17	116.61	111.07
1	C	829	VAL	CB-CA-C	-5.17	103.50	111.31
1	A	20	ALA	N-CA-C	5.17	121.81	110.80
4	S	29	VAL	N-CA-C	5.17	115.35	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	63	LEU	CB-CA-C	5.17	120.70	110.42
1	A	835	THR	CA-C-O	-5.17	116.59	122.01
2	N	451	PHE	N-CA-C	5.16	117.57	108.75
1	I	461	GLU	N-CA-C	5.15	116.94	110.24
4	Q	60	ALA	N-CA-C	5.15	116.90	111.28
1	B	42	ASN	N-CA-C	-5.15	104.26	110.44
1	C	96	MET	N-CA-C	5.15	118.34	111.75
1	E	867	ASP	CA-CB-CG	-5.15	107.45	112.60
1	K	907	VAL	N-CA-C	5.15	114.81	108.53
1	G	201	GLN	CB-CA-C	5.14	120.30	110.17
1	I	665	ILE	N-CA-C	5.14	117.13	108.81
5	V	183	ILE	N-CA-C	5.14	116.64	109.55
1	I	756	VAL	N-CA-C	5.13	117.50	111.09
1	K	464	LEU	N-CA-C	5.13	116.95	111.36
1	D	868	ARG	CB-CA-C	-5.13	102.87	111.23
1	K	332	ASN	CA-CB-CG	5.13	117.73	112.60
3	M	194	GLN	CA-C-N	5.12	127.06	122.20
3	M	194	GLN	C-N-CA	5.12	127.06	122.20
4	S	128	VAL	N-CA-C	5.12	117.49	111.09
1	A	255	ASN	N-CA-C	5.11	117.52	111.33
4	Q	132	LYS	N-CA-C	-5.11	105.40	111.69
1	A	58	THR	CA-C-N	-5.11	111.78	121.54
1	A	58	THR	C-N-CA	-5.11	111.78	121.54
2	N	274	THR	CB-CA-C	-5.11	103.78	112.00
1	A	553	GLY	N-CA-C	5.10	117.76	110.46
1	G	856	VAL	CB-CA-C	-5.10	102.92	111.29
1	H	278	ASP	N-CA-C	-5.10	101.79	109.85
1	K	465	ASN	N-CA-C	5.10	117.57	111.71
1	E	15	ILE	N-CA-C	5.10	118.62	113.47
1	K	749	VAL	CB-CA-C	-5.09	102.94	111.29
1	J	923	PHE	N-CA-C	5.08	117.53	109.96
1	F	592	VAL	N-CA-C	5.08	115.80	110.62
1	L	55	ASP	N-CA-C	-5.08	107.63	113.88
1	J	120	ALA	CA-C-N	5.08	130.21	122.65
1	J	120	ALA	C-N-CA	5.08	130.21	122.65
1	K	849	PRO	CB-CA-C	-5.08	103.56	111.22
2	N	64	PHE	N-CA-C	5.08	121.61	110.80
1	A	842	TYR	CA-C-N	5.07	125.35	119.92
1	A	842	TYR	C-N-CA	5.07	125.35	119.92
1	J	655	PRO	CB-CA-C	-5.07	103.19	111.56
1	J	739	THR	CA-C-N	5.07	124.24	118.97
1	J	739	THR	C-N-CA	5.07	124.24	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	949	ASN	N-CA-C	5.07	118.44	107.49
1	H	175	SER	N-CA-C	5.07	116.49	110.97
1	J	121	TYR	CA-C-N	5.07	131.22	121.54
1	J	121	TYR	C-N-CA	5.07	131.22	121.54
1	L	254	GLN	CB-CA-C	-5.07	100.22	109.54
1	L	100	TYR	N-CA-C	5.06	114.83	108.45
4	P	3	THR	CA-C-N	5.05	128.84	121.31
4	P	3	THR	C-N-CA	5.05	128.84	121.31
1	J	105	GLY	N-CA-C	5.05	118.06	110.18
1	J	514	VAL	N-CA-C	5.05	111.61	106.21
4	Q	23	ALA	N-CA-C	5.05	117.66	110.24
1	I	745	ILE	N-CA-C	-5.04	107.81	111.90
4	S	25	VAL	N-CA-C	-5.04	104.98	112.04
1	B	366	THR	N-CA-C	-5.04	108.88	114.62
1	B	531	ASN	N-CA-CB	-5.04	102.55	110.30
2	N	276	ASP	N-CA-C	-5.04	103.84	111.34
1	B	181	LYS	N-CA-C	-5.03	107.82	114.31
1	G	23	TYR	O-C-N	5.03	128.29	122.00
4	S	56	PRO	N-CA-C	5.03	122.84	112.47
6	W	11	ARG	CA-C-N	5.03	126.13	119.84
6	W	11	ARG	C-N-CA	5.03	126.13	119.84
1	C	180	THR	CB-CA-C	5.03	120.42	110.42
1	E	201	GLN	CB-CA-C	5.02	120.07	110.17
1	A	461	GLU	N-CA-C	5.01	117.57	110.50
1	H	280	LEU	CB-CA-C	5.01	120.06	111.68
1	I	828	PHE	N-CA-C	-5.01	106.76	112.92
1	I	179	ILE	N-CA-C	5.00	115.69	108.48
1	I	704	SER	N-CA-C	5.00	117.41	109.96

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	501	TYR	Sidechain
3	M	106	ASN	Peptide

4.2 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	7345	0	7042	234	0
1	B	7295	0	6999	228	0
1	C	7374	0	7074	196	0
1	D	7345	0	7045	172	0
1	E	7302	0	7006	157	0
1	F	7325	0	7027	142	0
1	G	7291	0	6997	260	0
1	H	7317	0	7019	241	0
1	I	7345	0	7045	267	0
1	J	7329	0	7028	205	0
1	K	7247	0	6957	213	0
1	L	7353	0	7052	199	0
2	N	3577	0	3508	148	0
3	M	2343	0	2313	51	0
4	P	717	0	724	39	0
4	Q	965	0	971	57	0
4	R	734	0	741	28	0
4	S	728	0	739	62	0
5	U	1329	0	1290	17	0
5	V	1346	0	1302	19	0
6	W	116	0	54	21	0
All	All	99723	0	95933	2529	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (2529) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:698:TYR:CE1	4:Q:24:GLY:HA2	1.10	1.58
1:H:698:TYR:HE1	4:Q:24:GLY:CA	1.19	1.54
4:P:40:LEU:HB2	4:P:41:PRO:CD	1.44	1.46
1:A:18:GLN:HB2	6:W:10:SER:CB	1.30	1.46
6:W:7:ARG:CB	6:W:11:ARG:O	1.65	1.42
1:G:758:GLN:OE1	1:I:549:LEU:CD1	1.69	1.39
1:J:656:ILE:HD11	1:J:910:MET:CG	1.51	1.39
1:G:847:PRO:HG2	1:I:121:TYR:CD1	1.57	1.38
1:I:831:TYR:CG	1:I:831:TYR:O	1.75	1.37
1:L:55:ASP:O	1:L:623:ALA:HB3	1.24	1.32
4:S:37:ARG:HB3	4:S:38:PRO:CD	1.60	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:41:PRO:HG2	4:P:44:SER:CB	1.58	1.31
1:G:332:ASN:O	1:G:565:LYS:NZ	1.65	1.30
1:I:356:ASN:ND2	1:I:940:TYR:CE2	1.99	1.29
1:L:824:ASN:HB3	1:L:844:ALA:CB	1.60	1.29
1:H:698:TYR:CE1	4:Q:24:GLY:CA	2.00	1.29
1:I:728:SER:O	1:I:729:VAL:HG23	1.19	1.28
1:C:182:GLU:O	1:C:264:MET:SD	1.92	1.27
1:H:748:SER:HB2	4:R:50:GLU:CD	1.58	1.26
1:I:728:SER:O	1:I:729:VAL:CG2	1.81	1.26
1:J:720:LYS:NZ	4:Q:22:TRP:HZ3	1.35	1.25
1:J:757:ALA:CB	1:L:386:MET:HB3	1.65	1.25
1:G:758:GLN:OE1	1:I:549:LEU:HD11	1.10	1.24
1:C:104:ARG:HD3	1:C:612:SER:OG	1.20	1.24
1:I:831:TYR:O	1:I:831:TYR:CD2	1.91	1.23
1:G:121:TYR:O	1:H:824:ASN:OD1	1.56	1.21
1:H:748:SER:HB2	4:R:50:GLU:OE1	1.39	1.21
1:A:559:HIS:NE2	1:B:755:ASN:O	1.71	1.21
1:E:13:MET:O	1:E:14:HIS:ND1	1.73	1.21
4:P:40:LEU:CB	4:P:41:PRO:CD	2.18	1.21
2:N:67:THR:O	2:N:563:PRO:HD2	1.34	1.20
1:A:62:GLN:O	1:B:735:ASP:O	1.60	1.19
4:P:41:PRO:CG	4:P:44:SER:HB3	1.73	1.18
1:B:81:LYS:HZ2	2:N:457:ILE:HG21	1.08	1.18
1:G:929:HIS:HB2	1:G:937:GLU:HG3	1.24	1.17
1:J:720:LYS:CE	4:Q:22:TRP:CZ3	2.26	1.17
1:I:654:TYR:OH	1:I:665:ILE:HD12	1.43	1.17
1:L:32:ALA:O	1:L:36:GLU:HB3	1.41	1.17
5:V:183:ILE:HG22	5:V:184:GLY:O	1.43	1.16
1:J:757:ALA:HB2	1:L:386:MET:HB3	1.26	1.15
1:J:18:GLN:HG3	1:J:19:ASP:H	1.05	1.15
1:K:755:ASN:ND2	1:K:759:CYS:O	1.79	1.15
6:W:7:ARG:CB	6:W:12:PRO:O	1.94	1.15
4:P:41:PRO:CG	4:P:44:SER:CB	2.23	1.14
1:B:941:LEU:HA	1:B:948:GLY:HA2	1.24	1.13
2:N:287:LEU:O	2:N:381:PRO:HA	1.45	1.13
1:D:868:ARG:HG3	1:D:868:ARG:O	1.43	1.13
1:L:824:ASN:HB3	1:L:844:ALA:HB2	1.30	1.13
2:N:55:ILE:HG21	2:N:67:THR:OG1	1.46	1.12
1:G:759:CYS:SG	1:G:800:PRO:HB3	1.89	1.11
1:G:121:TYR:O	1:H:824:ASN:CG	1.92	1.11
1:J:720:LYS:NZ	4:Q:22:TRP:CZ3	2.17	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLN:HG2	1:A:202:PRO:HD2	1.32	1.11
1:I:831:TYR:O	1:I:831:TYR:CD1	2.02	1.10
2:N:448:PRO:HB3	2:N:529:LEU:CD2	1.80	1.10
1:I:654:TYR:OH	1:I:665:ILE:CD1	1.98	1.10
1:G:757:ALA:HA	1:I:386:MET:HB3	1.34	1.10
1:L:824:ASN:HB3	1:L:844:ALA:HB1	1.33	1.10
3:M:196:LEU:O	5:U:197:TYR:CE1	2.03	1.10
1:H:748:SER:CB	4:R:50:GLU:OE2	1.98	1.10
1:I:356:ASN:ND2	1:I:940:TYR:HE2	1.36	1.10
1:A:201:GLN:CG	1:A:202:PRO:HD2	1.81	1.09
1:H:517:TYR:HA	1:H:520:LEU:HD11	1.33	1.09
1:A:793:SER:O	1:A:869:THR:CG2	2.00	1.09
1:G:648:SER:O	1:G:922:VAL:O	1.69	1.09
1:G:758:GLN:CD	1:I:549:LEU:HD11	1.77	1.09
1:G:850:LEU:CD1	1:G:856:VAL:O	2.00	1.08
1:J:426:LEU:HA	1:K:268:SER:O	1.48	1.08
1:L:824:ASN:CB	1:L:844:ALA:HB2	1.84	1.08
1:A:176:GLY:H	1:A:219:ALA:HB2	0.96	1.07
1:A:269:THR:HA	1:C:426:LEU:HD23	1.29	1.07
1:G:847:PRO:CG	1:I:121:TYR:HD1	1.67	1.07
1:C:747:ARG:HG3	1:C:762:THR:HB	1.29	1.07
1:D:53:THR:O	1:D:56:VAL:HG12	1.55	1.07
2:N:446:GLN:HB2	2:N:532:ARG:NE	1.70	1.07
4:S:48:THR:HG23	4:S:48:THR:O	1.28	1.06
1:A:201:GLN:HG3	1:A:202:PRO:HD3	1.38	1.06
1:C:536:ASN:O	1:C:596:SER:O	1.73	1.06
1:C:318:GLN:HE22	1:C:836:MET:HG3	1.16	1.06
1:J:720:LYS:HD2	4:Q:22:TRP:CZ3	1.90	1.06
1:K:204:PRO:O	1:L:826:SER:O	1.70	1.05
1:G:757:ALA:O	1:G:758:GLN:HG3	1.54	1.05
4:S:37:ARG:HB3	4:S:38:PRO:HD3	1.09	1.05
1:K:489:PRO:HB3	1:K:494:ILE:HG13	1.39	1.04
1:D:135:TRP:NE1	1:D:230:MET:SD	2.29	1.04
1:C:747:ARG:CG	1:C:762:THR:HB	1.88	1.04
1:F:481:LEU:HB3	1:F:482:PRO:HD2	1.37	1.04
1:G:771:LEU:O	1:G:880:MET:O	1.73	1.04
1:A:201:GLN:CG	1:A:202:PRO:CD	2.36	1.04
1:H:874:PRO:CB	1:H:879:PHE:O	2.05	1.04
1:I:652:MET:CE	1:I:654:TYR:OH	2.06	1.04
1:I:654:TYR:CZ	1:I:665:ILE:HD12	1.92	1.04
1:J:648:SER:CB	1:J:922:VAL:O	2.06	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:850:LEU:HD13	1:G:856:VAL:O	1.57	1.03
1:H:793:SER:O	1:H:797:ASN:ND2	1.91	1.03
1:D:135:TRP:CE2	1:D:230:MET:SD	2.51	1.03
1:J:656:ILE:HD11	1:J:910:MET:HG3	1.08	1.03
2:N:448:PRO:CB	2:N:529:LEU:HD22	1.88	1.03
1:D:78:TYR:CD1	1:D:78:TYR:O	2.11	1.02
1:F:76:THR:O	1:F:587:LYS:NZ	1.92	1.02
4:P:28:ASN:HA	4:P:42:ALA:CB	1.89	1.02
1:C:34:ALA:HB1	6:W:13:PHE:CB	1.89	1.02
1:B:726:ASP:CB	1:B:900:ALA:H	1.71	1.02
1:D:78:TYR:O	1:D:78:TYR:HD1	1.42	1.02
1:E:439:TRP:O	1:F:280:LEU:HD21	1.60	1.02
1:L:535:PHE:HD2	1:L:704:SER:HB3	1.17	1.02
2:N:448:PRO:HB3	2:N:529:LEU:HD22	1.04	1.02
1:A:793:SER:O	1:A:869:THR:HG21	1.57	1.02
1:K:333:PHE:HE1	1:K:386:MET:O	1.40	1.02
4:P:28:ASN:HA	4:P:42:ALA:HB2	1.41	1.02
4:S:19:MET:HE2	4:S:19:MET:HA	1.40	1.02
4:P:40:LEU:CB	4:P:41:PRO:HD3	1.86	1.01
4:S:48:THR:O	4:S:48:THR:CG2	2.04	1.01
1:A:18:GLN:CB	6:W:10:SER:CB	2.26	1.01
1:D:561:GLN:HB2	1:E:757:ALA:HB2	1.42	1.01
1:E:437:ASN:OD1	1:E:437:ASN:O	1.77	1.01
2:N:141:ASN:ND2	2:N:141:ASN:O	1.94	1.01
1:B:64:LEU:CD1	1:B:619:PHE:O	2.09	1.01
4:P:40:LEU:HB2	4:P:41:PRO:HD2	1.04	1.01
1:K:759:CYS:SG	1:K:864:PHE:HB3	1.99	1.00
1:G:847:PRO:CG	1:I:121:TYR:CD1	2.40	1.00
1:L:757:ALA:HB2	1:L:766:PHE:CZ	1.96	1.00
1:A:176:GLY:H	1:A:219:ALA:CB	1.75	1.00
1:H:874:PRO:CG	1:H:879:PHE:O	2.08	1.00
2:N:457:ILE:O	2:N:457:ILE:HG12	1.59	1.00
1:L:55:ASP:O	1:L:623:ALA:CB	2.08	1.00
1:J:656:ILE:CD1	1:J:910:MET:CG	2.39	0.99
1:G:804:GLN:CG	1:G:850:LEU:HD21	1.90	0.99
1:J:720:LYS:CD	4:Q:22:TRP:CZ3	2.45	0.99
1:A:58:THR:O	1:A:58:THR:HG23	1.61	0.98
1:B:941:LEU:O	1:B:941:LEU:HG	1.62	0.98
1:G:929:HIS:O	1:G:937:GLU:HG2	1.61	0.98
1:J:648:SER:HB3	1:J:922:VAL:O	1.63	0.98
4:P:40:LEU:HB2	4:P:41:PRO:HD3	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:804:GLN:HG3	1:G:850:LEU:CD2	1.95	0.97
1:J:821:HIS:CG	1:L:244:ASN:O	2.17	0.97
1:G:927:ARG:HB3	1:G:939:VAL:HG23	1.45	0.97
2:N:446:GLN:O	2:N:447:ASP:OD1	1.83	0.97
1:B:347:VAL:HG21	2:N:455:ARG:HG2	1.44	0.96
1:G:712:PHE:O	1:G:867:ASP:O	1.82	0.96
2:N:52:ARG:O	2:N:52:ARG:HG2	1.64	0.96
1:C:747:ARG:HB2	1:C:760:ASN:O	1.65	0.96
1:G:847:PRO:HB2	1:I:121:TYR:HE1	1.28	0.96
1:G:758:GLN:OE1	1:I:549:LEU:HD12	1.66	0.96
1:A:176:GLY:N	1:A:219:ALA:HB2	1.81	0.95
1:G:201:GLN:HB3	1:G:202:PRO:CD	1.95	0.95
1:L:106:VAL:HG21	4:Q:56:PRO:HD2	1.48	0.95
6:W:7:ARG:CB	6:W:12:PRO:C	2.39	0.95
1:G:804:GLN:HG2	1:G:850:LEU:HD21	1.47	0.95
1:B:81:LYS:NZ	2:N:457:ILE:HG21	1.81	0.95
1:D:135:TRP:CZ2	1:D:230:MET:SD	2.59	0.95
1:J:720:LYS:HZ1	4:Q:22:TRP:HZ3	1.08	0.95
2:N:446:GLN:CB	2:N:532:ARG:NE	2.28	0.95
1:G:689:PRO:HD3	1:G:699:TYR:HD1	1.29	0.95
1:G:713:TYR:HA	1:G:867:ASP:O	1.65	0.95
1:G:804:GLN:CG	1:G:850:LEU:CD2	2.43	0.95
1:C:104:ARG:HD3	1:C:612:SER:HG	1.13	0.94
1:J:18:GLN:HG3	1:J:19:ASP:N	1.75	0.94
1:J:720:LYS:HD2	4:Q:22:TRP:CE3	2.02	0.94
1:A:269:THR:O	1:C:426:LEU:HA	1.67	0.94
1:E:13:MET:O	1:E:14:HIS:CG	2.21	0.94
1:A:269:THR:O	1:C:425:THR:O	1.86	0.94
1:J:757:ALA:HB2	1:L:386:MET:CB	1.98	0.94
1:L:824:ASN:CB	1:L:844:ALA:CB	2.43	0.94
1:F:108:ASP:O	1:F:606:ALA:HB1	1.68	0.93
1:C:104:ARG:CD	1:C:612:SER:OG	2.14	0.93
1:H:867:ASP:O	1:H:868:ARG:HB2	1.68	0.93
1:I:728:SER:C	1:I:729:VAL:HG23	1.94	0.93
1:J:720:LYS:CE	4:Q:22:TRP:HZ3	1.72	0.93
1:H:748:SER:HB2	4:R:50:GLU:OE2	1.62	0.93
1:K:333:PHE:CE1	1:K:386:MET:O	2.21	0.93
1:B:941:LEU:CA	1:B:948:GLY:HA2	2.00	0.92
1:C:536:ASN:C	1:C:596:SER:O	2.12	0.92
1:C:656:ILE:HG23	1:C:660:ALA:CB	1.99	0.92
1:H:330:ARG:HD2	1:H:708:LEU:CD2	1.97	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:653:LEU:HD23	1:I:653:LEU:H	1.32	0.92
1:G:844:ALA:O	1:I:237:TYR:HB2	1.68	0.92
1:H:874:PRO:HB2	1:H:879:PHE:O	1.68	0.92
2:N:225:LEU:HD22	2:N:285:ALA:HB3	1.49	0.92
1:E:488:SER:HB2	1:E:489:PRO:HD3	1.52	0.92
1:A:174:TYR:HB2	1:A:202:PRO:HB3	1.50	0.92
1:K:201:GLN:HB3	1:K:202:PRO:CD	2.00	0.92
1:G:712:PHE:C	1:G:867:ASP:O	2.13	0.91
1:A:201:GLN:HG3	1:A:202:PRO:CD	1.97	0.91
1:D:789:ASP:OD2	1:F:382:ARG:NH1	2.03	0.91
1:A:56:VAL:HG23	1:A:56:VAL:O	1.67	0.91
1:A:58:THR:O	1:A:58:THR:CG2	2.18	0.91
1:A:179:ILE:HG12	1:A:218:HIS:HB3	1.52	0.91
1:G:847:PRO:HB2	1:I:121:TYR:CE1	2.04	0.90
1:C:179:ILE:HG22	1:C:180:THR:O	1.70	0.90
1:G:757:ALA:HB2	1:I:386:MET:HG2	1.53	0.90
1:K:759:CYS:HB2	1:K:800:PRO:HB3	1.51	0.90
1:H:570:LYS:O	1:H:643:PHE:CE1	2.24	0.90
1:G:548:MET:HB3	1:H:523:ARG:HB2	1.51	0.90
1:B:532:VAL:O	1:B:534:PRO:HD3	1.71	0.90
1:J:18:GLN:CG	1:J:19:ASP:H	1.85	0.90
1:A:460:MET:HG2	1:B:416:PRO:HA	1.55	0.89
1:G:201:GLN:HB3	1:G:202:PRO:HD3	1.55	0.89
1:K:748:SER:CA	1:K:760:ASN:HD21	1.84	0.89
2:N:446:GLN:HB2	2:N:532:ARG:CZ	2.02	0.89
1:K:201:GLN:HB3	1:K:202:PRO:HD3	1.56	0.88
1:C:656:ILE:CG2	1:C:660:ALA:HB3	2.03	0.88
2:N:52:ARG:NH2	2:N:62:PRO:C	2.31	0.88
1:G:847:PRO:HG2	1:I:121:TYR:HD1	0.75	0.88
1:G:201:GLN:O	1:G:203:GLU:HG2	1.72	0.88
1:I:652:MET:HE2	1:I:654:TYR:OH	1.70	0.88
1:D:269:THR:O	1:D:270:THR:HG22	1.72	0.88
1:G:775:ASN:HD22	1:G:881:SER:HB2	1.39	0.88
4:P:41:PRO:CG	4:P:44:SER:HB2	2.02	0.88
1:H:748:SER:CB	4:R:50:GLU:CD	2.42	0.88
1:I:724:THR:HG23	1:I:729:VAL:O	1.73	0.88
1:B:14:HIS:O	1:B:14:HIS:CD2	2.26	0.87
1:A:476:ASN:O	1:A:537:HIS:NE2	2.07	0.87
1:A:581:TYR:HE2	1:A:583:TRP:HD1	1.21	0.87
1:F:533:ASN:CB	1:F:713:TYR:CE2	2.58	0.87
4:S:106:GLN:O	4:S:110:LEU:HG	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:ILE:HG22	1:A:903:MET:HB2	1.56	0.87
1:H:492:VAL:HG11	1:H:506:LYS:HD3	1.54	0.87
2:N:287:LEU:O	2:N:381:PRO:CA	2.22	0.87
1:A:431:PRO:HA	1:A:439:TRP:HD1	1.40	0.87
1:C:824:ASN:HB3	1:C:844:ALA:HB1	1.57	0.87
1:J:757:ALA:CB	1:L:386:MET:CB	2.53	0.86
1:H:698:TYR:CD1	4:Q:24:GLY:HA2	2.05	0.86
1:K:755:ASN:CG	1:K:759:CYS:O	2.17	0.86
1:B:715:ASN:HB3	1:B:866:CYS:O	1.74	0.86
1:H:724:THR:O	1:H:902:ASP:O	1.93	0.86
2:N:52:ARG:NH2	2:N:62:PRO:HB2	1.91	0.86
1:J:656:ILE:HD11	1:J:910:MET:HG2	1.54	0.86
1:D:14:HIS:CE1	1:D:24:LEU:HD21	2.09	0.86
2:N:52:ARG:HH21	2:N:63:LEU:C	1.84	0.86
2:N:52:ARG:HH21	2:N:63:LEU:N	1.74	0.86
1:A:55:ASP:O	1:A:56:VAL:HG22	1.75	0.86
1:B:726:ASP:O	1:B:726:ASP:OD1	1.93	0.86
1:B:726:ASP:HB3	1:B:900:ALA:H	1.41	0.86
1:H:97:ALA:HB2	1:H:571:ASN:H	1.38	0.86
1:B:13:MET:O	1:B:14:HIS:ND1	2.08	0.86
1:B:922:VAL:HA	1:B:944:PRO:HG2	1.56	0.86
1:A:793:SER:O	1:A:869:THR:HG23	1.74	0.85
1:D:868:ARG:O	1:D:868:ARG:CG	2.24	0.85
1:H:748:SER:HB3	4:R:50:GLU:OE2	1.77	0.85
1:B:184:ILE:O	1:B:195:TYR:HD2	1.59	0.85
1:I:662:ASN:OD1	1:I:906:GLU:HA	1.76	0.85
1:B:252:LYS:CG	1:B:253:GLN:H	1.89	0.85
2:N:52:ARG:HH21	2:N:63:LEU:CA	1.90	0.85
2:N:55:ILE:CG2	2:N:67:THR:OG1	2.24	0.85
1:E:15:ILE:CG2	1:E:15:ILE:O	2.24	0.85
1:J:656:ILE:CD1	1:J:910:MET:HG3	2.00	0.85
1:L:757:ALA:O	1:L:758:GLN:HB2	1.74	0.84
1:L:797:ASN:CB	1:L:867:ASP:O	2.24	0.84
4:S:37:ARG:CB	4:S:38:PRO:HD3	2.02	0.84
1:G:929:HIS:CB	1:G:937:GLU:HG3	2.08	0.84
1:B:726:ASP:HB2	1:B:900:ALA:H	1.42	0.84
1:E:724:THR:CG2	1:E:728:SER:O	2.25	0.84
3:M:251:ASP:OD1	3:M:251:ASP:O	1.96	0.84
1:I:724:THR:CG2	1:I:729:VAL:O	2.25	0.84
1:A:927:ARG:O	1:A:938:THR:HG23	1.78	0.84
4:S:37:ARG:CB	4:S:38:PRO:CD	2.48	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:758:GLN:HA	1:I:559:HIS:CE1	2.13	0.83
1:A:789:ASP:HB3	1:A:796:ARG:HG3	1.59	0.83
1:C:536:ASN:CA	1:C:596:SER:O	2.26	0.83
1:J:201:GLN:HB3	1:J:202:PRO:HD3	1.59	0.83
1:G:856:VAL:O	1:G:856:VAL:HG12	1.76	0.83
1:B:941:LEU:O	1:B:941:LEU:CG	2.26	0.83
1:G:824:ASN:HA	1:G:844:ALA:HB2	1.58	0.83
1:B:602:ARG:HH22	1:B:695:TYR:HE1	1.25	0.83
1:H:732:PRO:HG2	1:H:740:PRO:O	1.78	0.83
4:S:116:VAL:O	4:S:120:GLN:CG	2.27	0.83
1:I:356:ASN:HD21	1:I:940:TYR:HE2	0.85	0.83
1:J:922:VAL:HG12	1:J:944:PRO:HG2	1.60	0.83
4:P:30:MET:HG2	4:P:40:LEU:O	1.79	0.83
4:P:40:LEU:HB3	4:P:41:PRO:HD3	1.60	0.83
1:H:492:VAL:CG2	1:H:506:LYS:HZ3	1.92	0.82
1:I:737:LEU:HD13	1:I:764:ASP:HB2	1.60	0.82
1:J:757:ALA:HB3	1:L:386:MET:HB3	1.60	0.82
1:L:20:ALA:O	1:L:45:PHE:HE2	1.61	0.82
2:N:45:TYR:O	2:N:46:LEU:HG	1.79	0.82
1:F:533:ASN:CG	1:F:713:TYR:CE2	2.57	0.82
1:J:648:SER:HB2	1:J:922:VAL:O	1.79	0.82
4:S:15:LEU:HD12	4:S:15:LEU:H	1.42	0.82
1:D:478:ALA:HB2	1:D:514:VAL:HG21	1.61	0.82
1:I:652:MET:CE	1:I:654:TYR:CZ	2.62	0.82
1:K:331:ASP:O	1:K:388:ASN:HB3	1.78	0.82
1:F:533:ASN:CG	1:F:713:TYR:HE2	1.87	0.82
1:J:720:LYS:HE3	4:Q:22:TRP:CZ3	2.13	0.82
1:J:656:ILE:HB	1:J:660:ALA:HB3	1.62	0.82
1:A:581:TYR:OH	1:A:583:TRP:NE1	2.11	0.82
1:C:597:LEU:HG	1:C:597:LEU:O	1.78	0.81
1:K:204:PRO:C	1:L:826:SER:O	2.22	0.81
1:G:204:PRO:HB3	1:H:840:GLN:HB3	1.61	0.81
1:H:513:LEU:O	1:H:518:ILE:HD13	1.80	0.81
1:J:126:PRO:HB3	1:K:461:GLU:HB3	1.62	0.81
1:K:331:ASP:O	1:K:388:ASN:CB	2.27	0.81
1:K:469:TRP:NE1	1:K:516:CYS:SG	2.53	0.81
2:N:448:PRO:CA	2:N:529:LEU:HD13	2.11	0.81
1:J:656:ILE:HG13	1:J:656:ILE:O	1.80	0.81
1:B:201:GLN:HB3	1:B:202:PRO:HD3	1.62	0.81
1:G:804:GLN:HG2	1:G:850:LEU:CD2	2.10	0.81
2:N:52:ARG:NE	2:N:63:LEU:O	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:TYR:CE2	1:A:583:TRP:CD1	2.69	0.81
1:I:831:TYR:O	1:I:831:TYR:CE2	2.33	0.81
1:G:804:GLN:NE2	1:G:858:SER:OG	2.14	0.81
1:I:589:VAL:HG22	1:I:602:ARG:HD2	1.63	0.80
1:I:720:LYS:H	1:I:906:GLU:HB2	1.46	0.80
1:J:656:ILE:CD1	1:J:910:MET:HG2	2.10	0.80
1:K:755:ASN:HD21	1:K:759:CYS:C	1.89	0.80
3:M:251:ASP:OD1	3:M:251:ASP:C	2.24	0.80
1:A:472:PHE:O	1:A:476:ASN:CG	2.25	0.80
1:A:479:LEU:HD21	1:A:505:ASN:HA	1.62	0.80
1:F:242:ASN:O	1:F:242:ASN:OD1	1.98	0.80
1:G:621:PRO:HG2	1:H:878:ASN:OD1	1.82	0.80
1:K:497:ASN:OD1	1:K:498:PRO:HD2	1.82	0.80
1:K:842:TYR:CD2	1:K:843:PRO:HD2	2.17	0.80
1:L:757:ALA:HB2	1:L:766:PHE:HZ	1.47	0.80
2:N:52:ARG:HH22	2:N:62:PRO:C	1.87	0.80
1:K:493:LYS:O	1:K:494:ILE:CD1	2.30	0.79
1:E:15:ILE:O	1:E:15:ILE:HG22	1.80	0.79
1:J:179:ILE:HG12	1:J:218:HIS:HB3	1.64	0.79
1:G:679:ALA:HB1	1:G:870:LEU:HD22	1.64	0.79
2:N:275:TYR:O	2:N:275:TYR:CD1	2.35	0.79
1:A:833:ALA:O	1:A:835:THR:HG22	1.83	0.79
1:I:349:ALA:CB	1:I:353:SER:O	2.30	0.79
1:C:656:ILE:HG23	1:C:660:ALA:HB3	1.62	0.79
1:H:514:VAL:HA	1:H:518:ILE:HD11	1.62	0.79
1:H:517:TYR:HA	1:H:520:LEU:CD1	2.10	0.79
1:G:928:VAL:HA	1:G:938:THR:HA	1.64	0.79
2:N:247:GLY:HA3	2:N:274:THR:HG23	1.64	0.78
1:D:797:ASN:CB	1:D:867:ASP:O	2.30	0.78
1:G:201:GLN:O	1:G:203:GLU:N	2.16	0.78
1:G:689:PRO:HD3	1:G:699:TYR:CD1	2.18	0.78
1:A:797:ASN:ND2	1:A:869:THR:OG1	2.15	0.78
1:G:929:HIS:O	1:G:937:GLU:CG	2.31	0.78
4:S:37:ARG:HB3	4:S:38:PRO:HD2	1.66	0.78
1:H:698:TYR:CD1	4:Q:24:GLY:CA	2.64	0.78
1:K:493:LYS:O	1:K:494:ILE:HD13	1.83	0.78
2:N:123:LEU:HD22	2:N:441:LEU:HD12	1.66	0.78
4:Q:115:ASN:O	4:Q:118:SER:HB3	1.83	0.78
1:C:823:HIS:O	1:C:844:ALA:HA	1.83	0.78
1:G:23:TYR:O	1:G:23:TYR:CD2	2.36	0.78
1:H:698:TYR:CE1	4:Q:24:GLY:N	2.50	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:535:PHE:CD2	1:L:704:SER:HB3	2.10	0.78
1:H:698:TYR:OH	4:Q:26:ARG:HG3	1.84	0.78
4:P:41:PRO:HG2	4:P:44:SER:HB3	0.82	0.78
4:S:19:MET:HE2	4:S:20:PRO:HD3	1.65	0.77
1:C:215:GLU:O	1:C:216:ILE:HG13	1.85	0.77
1:H:492:VAL:HG22	1:H:506:LYS:HZ3	1.48	0.77
1:J:663:VAL:O	1:J:663:VAL:HG12	1.84	0.77
1:I:728:SER:O	1:I:729:VAL:HG22	1.80	0.77
1:J:119:THR:HG23	1:J:297:ASP:HB2	1.66	0.77
4:S:116:VAL:O	4:S:120:GLN:HG3	1.83	0.77
1:K:561:GLN:HB2	1:L:756:VAL:HG13	1.67	0.77
1:A:200:PHE:O	1:A:200:PHE:CD1	2.37	0.77
1:H:726:ASP:HB3	1:H:900:ALA:HB3	1.66	0.77
1:E:756:VAL:HG22	1:E:757:ALA:H	1.49	0.77
2:N:52:ARG:NH2	2:N:63:LEU:O	2.17	0.77
1:C:33:ARG:HG2	6:W:17:TRP:H	1.49	0.77
1:G:682:ARG:HH21	1:G:907:VAL:HG12	1.49	0.77
1:H:367:GLU:OE2	1:H:708:LEU:HD11	1.84	0.77
1:D:25:SER:O	1:D:29:VAL:HG23	1.84	0.77
1:H:519:ASN:ND2	1:H:803:ARG:HH11	1.82	0.77
1:A:431:PRO:O	1:A:434:GLY:O	2.03	0.76
1:D:76:THR:OG1	1:D:77:ALA:N	2.18	0.76
1:G:722:ALA:HB2	1:G:742:GLU:HB3	1.68	0.76
1:H:332:ASN:H	1:H:388:ASN:HB2	1.50	0.76
1:H:698:TYR:CD1	4:Q:24:GLY:N	2.53	0.76
1:I:356:ASN:O	1:I:356:ASN:OD1	2.03	0.76
1:B:64:LEU:HD12	1:B:619:PHE:O	1.83	0.76
1:J:655:PRO:HG3	1:J:915:LEU:HD23	1.65	0.76
1:K:63:ARG:HG3	1:K:63:ARG:O	1.84	0.76
1:D:201:GLN:HB3	1:D:202:PRO:HD3	1.67	0.76
1:H:790:ARG:HB2	1:H:793:SER:OG	1.86	0.76
1:A:824:ASN:HA	1:A:844:ALA:HB2	1.68	0.76
1:C:84:PHE:HB2	1:C:581:TYR:HB3	1.67	0.76
1:C:533:ASN:HB3	1:C:704:SER:HB2	1.67	0.76
1:H:797:ASN:HB3	1:H:867:ASP:O	1.86	0.76
1:I:661:THR:C	1:I:662:ASN:HD22	1.94	0.76
1:A:411:PRO:HB3	1:C:127:LYS:HG3	1.67	0.76
1:I:722:ALA:HB3	1:I:904:THR:HB	1.66	0.75
1:D:523:ARG:HB2	1:F:548:MET:HB3	1.68	0.75
1:H:272:ALA:O	1:H:280:LEU:CD2	2.34	0.75
1:B:756:VAL:HG12	1:B:763:LYS:HG2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:84:PHE:HB2	1:L:581:TYR:HB3	1.69	0.75
2:N:52:ARG:NH2	2:N:63:LEU:N	2.33	0.75
1:G:757:ALA:CA	1:I:386:MET:HB3	2.15	0.75
1:J:640:ASP:H	1:L:24:LEU:HD22	1.51	0.75
2:N:445:MET:HB3	2:N:529:LEU:CD1	2.17	0.75
1:I:349:ALA:HB3	1:I:353:SER:O	1.86	0.75
1:D:330:ARG:HG2	1:D:594:GLN:HB2	1.68	0.75
1:H:705:ILE:HG22	1:H:707:TYR:H	1.50	0.75
1:J:546:ARG:HH22	1:J:560:ILE:HG21	1.52	0.75
2:N:445:MET:HB3	2:N:529:LEU:HD11	1.67	0.75
1:F:533:ASN:HB2	1:F:713:TYR:CE2	2.22	0.75
1:G:929:HIS:HB2	1:G:937:GLU:CG	2.12	0.75
1:I:653:LEU:H	1:I:653:LEU:CD2	1.98	0.74
2:N:45:TYR:O	2:N:46:LEU:CG	2.35	0.74
2:N:287:LEU:O	2:N:381:PRO:C	2.29	0.74
1:A:860:THR:HG21	1:C:551:GLY:HA2	1.69	0.74
1:C:10:TRP:HB3	1:C:15:ILE:HB	1.68	0.74
1:C:179:ILE:HG12	1:C:184:ILE:HG23	1.69	0.74
1:C:536:ASN:HA	1:C:596:SER:O	1.86	0.74
1:A:665:ILE:CG2	1:A:903:MET:HB2	2.18	0.74
3:M:200:ASN:HD21	3:M:235:LEU:HB2	1.50	0.74
1:G:691:LEU:HD13	1:G:692:GLY:N	2.03	0.74
1:H:665:ILE:HG23	1:H:903:MET:HB3	1.70	0.74
1:C:333:PHE:O	1:C:333:PHE:HD1	1.70	0.74
1:H:874:PRO:HG3	1:H:879:PHE:O	1.88	0.74
1:F:481:LEU:HB3	1:F:482:PRO:CD	2.18	0.74
2:N:446:GLN:CB	2:N:532:ARG:HE	1.97	0.74
1:G:929:HIS:C	1:G:937:GLU:CG	2.61	0.74
1:H:59:ASP:O	1:I:734:ASN:CG	2.30	0.74
1:J:656:ILE:HD11	1:J:910:MET:CB	2.18	0.74
1:J:126:PRO:HB3	1:K:461:GLU:CB	2.17	0.74
2:N:446:GLN:HB2	2:N:532:ARG:HE	1.46	0.73
4:S:30:MET:CE	4:S:41:PRO:HB3	2.18	0.73
1:A:748:SER:O	1:A:749:VAL:HG23	1.88	0.73
1:G:929:HIS:C	1:G:937:GLU:HG2	2.13	0.73
1:K:776:ILE:HG21	1:K:782:TYR:H	1.53	0.73
3:M:196:LEU:O	5:U:197:TYR:CD1	2.41	0.73
1:C:922:VAL:HG13	1:C:944:PRO:HD2	1.69	0.73
1:K:748:SER:HA	1:K:760:ASN:HD21	1.51	0.73
4:P:28:ASN:CA	4:P:42:ALA:HB2	2.18	0.73
1:A:837:ARG:O	1:A:837:ARG:HG2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:TYR:HE2	1:A:583:TRP:CD1	2.04	0.73
1:B:726:ASP:OD1	1:B:726:ASP:C	2.32	0.73
1:B:798:PHE:HB2	1:B:866:CYS:HA	1.69	0.73
1:D:731:TRP:HB3	1:D:732:PRO:HD3	1.71	0.73
2:N:446:GLN:C	2:N:447:ASP:OD1	2.32	0.73
1:I:831:TYR:O	1:I:831:TYR:CE1	2.42	0.73
1:K:493:LYS:O	1:K:494:ILE:HG12	1.88	0.73
4:Q:112:ARG:O	4:Q:116:VAL:HG23	1.88	0.73
4:S:113:GLU:O	4:S:117:VAL:HG23	1.89	0.73
1:G:931:PRO:HD3	1:G:937:GLU:CD	2.14	0.73
1:J:676:ARG:HB2	1:J:921:GLU:HB3	1.71	0.73
1:D:794:PHE:CD2	1:D:794:PHE:O	2.42	0.72
2:N:444:MET:HE1	2:N:561:VAL:HG21	1.71	0.72
1:B:13:MET:O	1:B:14:HIS:CG	2.41	0.72
1:C:35:THR:HG23	6:W:5:ALA:HB2	1.71	0.72
1:G:713:TYR:CA	1:G:867:ASP:O	2.36	0.72
4:S:116:VAL:O	4:S:120:GLN:HG2	1.89	0.72
1:G:775:ASN:ND2	1:G:881:SER:HB2	2.03	0.72
1:J:460:MET:HB3	1:K:416:PRO:HA	1.72	0.72
4:R:42:ALA:O	4:R:46:THR:HG22	1.89	0.72
1:A:267:PHE:HE1	1:A:284:VAL:HB	1.54	0.72
1:I:441:LYS:HG3	1:I:442:ASP:H	1.53	0.72
4:S:18:ARG:HG2	4:S:19:MET:H	1.54	0.72
4:S:19:MET:HE2	4:S:19:MET:CA	2.15	0.72
1:I:730:SER:OG	1:I:740:PRO:HB2	1.90	0.72
1:I:922:VAL:HG13	1:I:944:PRO:HD2	1.71	0.72
2:N:448:PRO:HA	2:N:529:LEU:HD13	1.71	0.72
1:L:10:TRP:HB2	1:L:16:SER:OG	1.89	0.72
1:L:656:ILE:HG23	1:L:660:ALA:HB3	1.70	0.72
2:N:287:LEU:O	2:N:381:PRO:O	2.07	0.72
1:B:941:LEU:HA	1:B:948:GLY:CA	2.13	0.72
1:A:581:TYR:CE2	1:A:583:TRP:HD1	2.02	0.72
1:K:823:HIS:HD2	1:K:843:PRO:O	1.72	0.72
1:B:184:ILE:O	1:B:195:TYR:CD2	2.43	0.71
1:E:716:HIS:HB3	1:E:866:CYS:H	1.55	0.71
2:N:448:PRO:HB3	2:N:529:LEU:CG	2.19	0.71
1:H:492:VAL:HG22	1:H:506:LYS:NZ	2.05	0.71
1:I:654:TYR:OH	1:I:665:ILE:HD11	1.90	0.71
4:Q:27:GLN:O	4:Q:29:VAL:HG23	1.91	0.71
4:S:125:ARG:O	4:S:129:SER:OG	2.02	0.71
1:D:98:SER:HB3	1:E:780:GLY:HA2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:794:PHE:O	1:D:794:PHE:CG	2.43	0.71
2:N:52:ARG:NH2	2:N:63:LEU:CA	2.54	0.71
1:A:13:MET:HE1	1:B:941:LEU:HB3	1.73	0.71
1:B:794:PHE:O	1:B:798:PHE:HD2	1.71	0.71
1:D:269:THR:O	1:D:270:THR:CG2	2.38	0.71
1:I:664:PRO:HB3	1:I:905:PHE:H	1.56	0.71
4:P:28:ASN:HA	4:P:42:ALA:HB3	1.72	0.71
1:A:201:GLN:HG2	1:A:202:PRO:CD	2.11	0.71
1:C:18:GLN:O	1:C:19:ASP:OD1	2.08	0.71
1:C:656:ILE:CG2	1:C:660:ALA:CB	2.67	0.71
1:G:508:VAL:HG11	1:G:834:PRO:HD3	1.73	0.71
1:I:793:SER:O	1:I:797:ASN:ND2	2.23	0.71
1:A:837:ARG:O	1:B:456:ASN:ND2	2.24	0.70
1:B:252:LYS:HG2	1:B:253:GLN:H	1.56	0.70
1:B:529:MET:O	1:B:532:VAL:HG22	1.92	0.70
1:C:333:PHE:O	1:C:333:PHE:CD1	2.44	0.70
1:G:943:THR:HB	1:G:944:PRO:HD3	1.72	0.70
1:A:833:ALA:C	1:A:835:THR:H	2.00	0.70
1:G:201:GLN:HB2	1:G:287:TYR:CZ	2.26	0.70
1:K:493:LYS:O	1:K:494:ILE:CG1	2.38	0.70
4:P:29:VAL:H	4:P:42:ALA:HB2	1.57	0.70
2:N:450:THR:O	2:N:450:THR:OG1	2.09	0.70
1:D:797:ASN:HB3	1:D:867:ASP:O	1.91	0.70
1:I:652:MET:HE3	1:I:654:TYR:CZ	2.26	0.70
1:J:922:VAL:CG1	1:J:944:PRO:HG2	2.22	0.70
3:M:196:LEU:CB	3:M:199:VAL:HG21	2.22	0.70
3:M:200:ASN:HD21	3:M:235:LEU:CA	2.04	0.70
1:G:682:ARG:NH2	1:G:907:VAL:HG12	2.07	0.70
1:E:797:ASN:ND2	1:E:868:ARG:O	2.25	0.69
1:G:927:ARG:HB3	1:G:939:VAL:CG2	2.19	0.69
1:D:757:ALA:O	1:D:758:GLN:HB2	1.92	0.69
1:C:797:ASN:HB2	1:C:867:ASP:O	1.92	0.69
1:E:560:ILE:HG12	1:F:758:GLN:HB3	1.74	0.69
1:L:535:PHE:HD2	1:L:704:SER:CB	2.01	0.69
1:L:756:VAL:O	1:L:756:VAL:HG12	1.92	0.69
2:N:67:THR:O	2:N:563:PRO:CD	2.28	0.69
2:N:243:LEU:HB3	2:N:244:PRO:CD	2.22	0.69
1:A:11:SER:OG	1:A:16:SER:HB2	1.93	0.69
1:G:775:ASN:HD22	1:G:881:SER:CB	2.04	0.69
1:H:46:ARG:HG3	1:I:644:ASN:H	1.57	0.69
1:K:508:VAL:HG11	1:K:834:PRO:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:446:PHE:O	1:L:447:SER:O	2.11	0.69
3:M:200:ASN:ND2	3:M:235:LEU:N	2.39	0.69
1:A:431:PRO:HA	1:A:439:TRP:CD1	2.25	0.69
1:B:724:THR:O	1:B:902:ASP:N	2.26	0.69
1:D:758:GLN:HE22	1:F:560:ILE:HA	1.57	0.69
1:G:850:LEU:O	1:G:850:LEU:HG	1.89	0.69
4:S:30:MET:HE2	4:S:41:PRO:HA	1.74	0.69
1:B:679:ALA:HB1	1:B:870:LEU:HB3	1.75	0.69
1:K:332:ASN:CG	1:K:387:TRP:O	2.36	0.69
1:L:757:ALA:O	1:L:758:GLN:CB	2.40	0.69
1:C:318:GLN:HE22	1:C:836:MET:CG	1.99	0.69
1:C:318:GLN:NE2	1:C:836:MET:HG3	2.00	0.69
1:I:720:LYS:HG3	1:I:906:GLU:HG3	1.73	0.69
1:C:824:ASN:HB3	1:C:844:ALA:CB	2.22	0.69
1:F:330:ARG:HG2	1:F:594:GLN:HB2	1.75	0.69
1:K:332:ASN:O	1:K:333:PHE:HB2	1.92	0.69
1:K:332:ASN:HA	1:K:387:TRP:O	1.92	0.69
2:N:446:GLN:HB3	2:N:532:ARG:HG2	1.75	0.69
4:P:41:PRO:HG3	4:P:44:SER:CB	2.20	0.69
1:E:429:VAL:HG22	1:F:267:PHE:HA	1.73	0.68
1:A:582:GLU:O	1:A:583:TRP:CD1	2.46	0.68
1:E:69:ILE:HG21	1:J:73:ARG:O	1.92	0.68
1:H:514:VAL:HA	1:H:518:ILE:CD1	2.23	0.68
1:F:922:VAL:HG13	1:F:944:PRO:HD2	1.74	0.68
4:Q:19:MET:O	4:Q:21:PRO:HD3	1.93	0.68
1:H:748:SER:CB	4:R:50:GLU:OE1	2.31	0.68
1:K:759:CYS:CB	1:K:800:PRO:HB3	2.23	0.68
1:F:713:TYR:CE1	1:F:714:LEU:HG	2.29	0.68
1:B:837:ARG:HH12	1:C:416:PRO:HD2	1.59	0.68
1:E:184:ILE:HG21	1:E:220:ALA:HB2	1.74	0.68
1:G:135:TRP:HD1	1:G:310:ASN:HB2	1.59	0.68
1:I:831:TYR:CD2	1:I:831:TYR:C	2.63	0.68
1:L:256:GLY:O	1:L:257:LYS:C	2.36	0.68
2:N:449:VAL:HG12	2:N:450:THR:HG22	1.75	0.68
1:A:833:ALA:O	1:A:835:THR:N	2.25	0.68
1:E:798:PHE:HB2	1:E:865:LEU:O	1.93	0.68
1:H:367:GLU:OE2	1:H:708:LEU:CD1	2.41	0.68
1:K:700:THR:O	1:K:700:THR:OG1	2.08	0.68
1:C:573:LEU:H	1:C:641:GLN:HE22	1.42	0.68
1:G:119:THR:HG23	1:G:297:ASP:HB2	1.76	0.68
1:G:850:LEU:HD12	1:G:856:VAL:O	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:513:LEU:HA	1:L:518:ILE:HD11	1.76	0.68
1:G:847:PRO:CB	1:I:121:TYR:CE1	2.77	0.68
1:H:330:ARG:HD2	1:H:708:LEU:HD21	1.75	0.68
1:K:493:LYS:C	1:K:494:ILE:HG12	2.19	0.68
4:R:41:PRO:HA	4:R:46:THR:HB	1.75	0.68
1:K:837:ARG:HB2	1:L:459:ALA:HB2	1.75	0.67
1:L:797:ASN:HB3	1:L:867:ASP:O	1.92	0.67
2:N:243:LEU:HB3	2:N:244:PRO:HD2	1.74	0.67
1:L:106:VAL:CG2	4:Q:56:PRO:HD2	2.24	0.67
1:F:602:ARG:HG2	4:R:34:ILE:HA	1.75	0.67
1:G:757:ALA:C	1:G:758:GLN:HG3	2.18	0.67
1:B:759:CYS:SG	1:B:761:MET:HG3	2.35	0.67
1:D:382:ARG:HH22	1:E:796:ARG:HG3	1.60	0.67
1:K:561:GLN:CB	1:L:756:VAL:HG13	2.24	0.67
1:C:822:GLN:O	1:C:823:HIS:ND1	2.27	0.67
1:L:758:GLN:O	1:L:862:LYS:HD3	1.94	0.67
1:B:184:ILE:HG22	1:B:185:GLN:O	1.94	0.67
1:C:747:ARG:HG2	1:C:762:THR:HB	1.77	0.67
1:H:670:ARG:HB2	1:H:672:TRP:HD1	1.59	0.67
1:I:485:LEU:O	1:I:509:VAL:HG23	1.95	0.67
1:K:748:SER:HA	1:K:760:ASN:ND2	2.10	0.67
1:A:79:SER:HB2	1:A:584:ASN:HD22	1.59	0.67
1:G:568:ALA:HA	1:G:926:VAL:HG11	1.76	0.67
1:I:65:THR:C	1:I:66:LEU:HG	2.20	0.67
1:A:78:TYR:HB3	1:A:695:TYR:HB2	1.77	0.67
1:B:252:LYS:CG	1:B:253:GLN:N	2.56	0.67
1:B:724:THR:HG22	1:B:725:PHE:N	2.10	0.67
1:B:756:VAL:CG1	1:B:763:LYS:HG2	2.24	0.67
1:D:14:HIS:CE1	1:D:24:LEU:CD2	2.77	0.67
1:E:731:TRP:HB3	1:E:732:PRO:HD3	1.76	0.67
1:I:654:TYR:CE2	1:I:665:ILE:HD12	2.30	0.67
1:J:522:ALA:HB2	1:L:552:ASN:HB2	1.76	0.67
1:C:109:ARG:HH22	1:C:550:LEU:HB2	1.58	0.67
1:J:272:ALA:HB3	1:J:280:LEU:HD21	1.77	0.67
1:K:755:ASN:ND2	1:K:760:ASN:C	2.53	0.67
1:A:176:GLY:N	1:A:219:ALA:CB	2.50	0.67
1:A:656:ILE:HG13	1:A:914:THR:O	1.95	0.67
1:G:663:VAL:O	1:G:905:PHE:O	2.13	0.67
1:G:867:ASP:N	1:G:867:ASP:OD1	2.27	0.67
1:I:661:THR:O	1:I:662:ASN:ND2	2.28	0.67
1:I:763:LYS:HA	1:I:766:PHE:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:LEU:CG	1:A:691:LEU:O	2.41	0.66
1:D:135:TRP:HD1	1:D:310:ASN:HB2	1.60	0.66
1:G:434:GLY:HA2	1:G:438:GLY:O	1.95	0.66
1:H:794:PHE:O	1:H:795:PHE:CD2	2.48	0.66
1:I:797:ASN:CG	1:I:867:ASP:O	2.38	0.66
1:H:330:ARG:HD2	1:H:708:LEU:HD23	1.76	0.66
1:J:840:GLN:HG2	1:L:173:PRO:HD2	1.78	0.66
1:D:269:THR:O	1:D:269:THR:OG1	2.04	0.66
1:A:748:SER:C	1:A:749:VAL:CG2	2.68	0.66
1:A:52:PRO:HD3	6:W:6:PRO:CB	2.26	0.66
1:A:477:ILE:HA	1:A:537:HIS:CE1	2.31	0.66
1:B:681:THR:HG23	1:B:715:ASN:OD1	1.96	0.66
1:C:13:MET:HB3	1:C:15:ILE:HG13	1.77	0.66
1:D:757:ALA:HB2	1:F:386:MET:HE2	1.77	0.66
1:I:177:ILE:HG23	1:I:178:ASN:N	2.10	0.66
1:A:267:PHE:CE1	1:A:284:VAL:HB	2.30	0.66
1:B:726:ASP:HB2	1:B:900:ALA:N	2.10	0.66
1:H:772:ALA:O	1:H:881:SER:OG	2.14	0.66
1:I:822:GLN:HA	1:I:845:ASN:HD21	1.61	0.66
1:I:825:ASN:CG	1:I:825:ASN:O	2.37	0.66
1:B:327:ILE:HG21	1:B:601:LEU:HD21	1.78	0.66
1:A:885:LEU:HB2	1:C:51:ALA:HB3	1.77	0.66
1:C:649:ALA:HA	1:C:922:VAL:H	1.59	0.66
1:G:96:MET:HG2	1:G:569:ILE:HG22	1.77	0.66
1:H:272:ALA:O	1:H:280:LEU:HD21	1.95	0.66
1:I:729:VAL:HG12	1:I:730:SER:H	1.60	0.66
1:J:904:THR:HG21	4:Q:20:PRO:HD3	1.77	0.66
1:D:561:GLN:HB2	1:E:757:ALA:CB	2.24	0.66
1:G:121:TYR:O	1:H:824:ASN:ND2	2.29	0.66
1:H:342:THR:HB	1:J:740:PRO:HD2	1.78	0.66
1:J:104:ARG:HG2	1:K:752:GLU:HB2	1.78	0.66
1:A:691:LEU:O	1:A:691:LEU:HG	1.94	0.65
1:I:661:THR:C	1:I:662:ASN:ND2	2.54	0.65
1:J:561:GLN:H	1:K:757:ALA:HB2	1.61	0.65
3:M:200:ASN:HD21	3:M:235:LEU:CB	2.09	0.65
4:S:57:LEU:HD23	4:S:58:GLU:H	1.59	0.65
1:A:269:THR:CA	1:C:426:LEU:HD23	2.16	0.65
1:G:756:VAL:HG11	1:G:763:LYS:HB3	1.79	0.65
4:S:57:LEU:HD23	4:S:58:GLU:N	2.12	0.65
1:D:222:ARG:H	1:E:840:GLN:HE22	1.43	0.65
1:E:429:VAL:HA	1:E:442:ASP:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:104:ARG:HD3	1:I:612:SER:HB3	1.77	0.65
1:D:350:GLY:HA2	1:D:580:THR:H	1.61	0.65
1:J:821:HIS:CB	1:L:244:ASN:O	2.45	0.65
3:M:200:ASN:HD21	3:M:235:LEU:N	1.94	0.65
3:M:220:ASP:O	3:M:221:ARG:C	2.39	0.65
1:I:909:PRO:HG3	4:S:45:THR:HA	1.79	0.65
1:K:331:ASP:O	1:K:388:ASN:HB2	1.97	0.65
1:K:548:MET:HB3	1:L:523:ARG:H	1.60	0.65
1:D:110:GLY:HA2	1:D:554:ARG:HE	1.62	0.65
1:E:434:GLY:HA3	1:E:438:GLY:O	1.97	0.65
2:N:225:LEU:HD12	2:N:287:LEU:HD23	1.79	0.65
4:P:41:PRO:CB	4:P:44:SER:HB2	2.27	0.65
1:A:323:ARG:HG3	1:A:479:LEU:HD13	1.78	0.65
1:A:679:ALA:HB3	1:A:919:LEU:HD12	1.79	0.65
1:A:837:ARG:O	1:A:837:ARG:CG	2.45	0.65
1:H:877:SER:H	1:H:887:ASP:HB2	1.61	0.65
2:N:256:SER:O	2:N:261:ILE:O	2.14	0.65
1:E:548:MET:HB3	1:F:523:ARG:HB2	1.78	0.64
1:H:300:ILE:HG23	1:H:318:GLN:O	1.97	0.64
1:L:922:VAL:HG13	1:L:944:PRO:HD2	1.79	0.64
4:S:108:ASP:O	4:S:111:THR:N	2.29	0.64
1:A:658:ALA:O	1:A:659:ASN:HB2	1.97	0.64
1:C:716:HIS:HB3	1:C:866:CYS:H	1.62	0.64
1:H:272:ALA:O	1:H:280:LEU:HD22	1.95	0.64
1:H:837:ARG:HH22	1:I:415:PHE:HA	1.62	0.64
1:J:184:ILE:HG21	1:J:220:ALA:HB2	1.79	0.64
1:L:109:ARG:HH22	1:L:550:LEU:HB3	1.63	0.64
2:N:52:ARG:NH2	2:N:63:LEU:C	2.54	0.64
3:M:80:LEU:HB3	3:M:86:ILE:HG12	1.78	0.64
3:M:196:LEU:O	3:M:199:VAL:HG23	1.98	0.64
3:M:197:GLN:O	3:M:198:THR:HG23	1.96	0.64
1:I:718:PHE:HA	1:I:907:VAL:HA	1.80	0.64
1:L:256:GLY:O	1:L:258:LEU:N	2.31	0.64
2:N:45:TYR:O	2:N:46:LEU:CD2	2.45	0.64
2:N:45:TYR:O	2:N:46:LEU:HD23	1.98	0.64
2:N:445:MET:SD	2:N:529:LEU:HD11	2.38	0.64
1:A:748:SER:O	1:A:749:VAL:CG2	2.45	0.64
1:C:339:TYR:HB2	1:C:367:GLU:HG2	1.79	0.64
1:D:755:ASN:HB3	1:D:759:CYS:O	1.97	0.64
1:G:757:ALA:HB2	1:I:386:MET:CG	2.27	0.64
1:K:92:ARG:H	1:K:576:PRO:HG3	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:183:ILE:CG2	5:V:184:GLY:O	2.34	0.64
1:A:472:PHE:O	1:A:476:ASN:OD1	2.16	0.64
1:E:722:ALA:HB3	1:E:904:THR:HB	1.78	0.64
1:F:805:VAL:HG12	1:F:806:VAL:H	1.62	0.64
1:H:795:PHE:O	1:H:795:PHE:CD1	2.51	0.64
1:I:202:PRO:HG2	1:I:222:ARG:HH11	1.63	0.64
1:B:342:THR:HB	2:N:92:LEU:HD22	1.80	0.63
1:C:514:VAL:HA	1:C:518:ILE:HD11	1.79	0.63
1:G:23:TYR:O	1:G:23:TYR:CG	2.50	0.63
1:G:771:LEU:O	1:G:880:MET:HA	1.97	0.63
1:H:792:TYR:HD2	1:H:868:ARG:O	1.81	0.63
1:I:127:LYS:HE2	1:I:834:PRO:HB2	1.80	0.63
1:J:216:ILE:HG12	1:L:454:VAL:HB	1.80	0.63
1:L:756:VAL:O	1:L:756:VAL:CG1	2.47	0.63
4:S:30:MET:HE1	4:S:41:PRO:HB3	1.81	0.63
1:A:35:THR:HG23	1:A:38:TYR:HB2	1.80	0.63
1:C:104:ARG:CD	1:C:612:SER:HG	2.01	0.63
1:F:110:GLY:HA3	1:F:606:ALA:HB2	1.81	0.63
1:I:252:LYS:HG3	1:I:253:GLN:H	1.64	0.63
3:M:111:GLN:HA	3:M:114:LEU:HB2	1.81	0.63
1:D:106:VAL:HG12	1:D:557:PRO:HB3	1.81	0.63
1:G:759:CYS:SG	1:G:800:PRO:CB	2.78	0.63
1:I:682:ARG:HH21	1:I:717:THR:HB	1.63	0.63
1:B:13:MET:HE3	1:C:925:VAL:HB	1.81	0.63
2:N:188:ILE:HD11	2:N:208:VAL:HB	1.79	0.63
2:N:448:PRO:CB	2:N:529:LEU:HD13	2.29	0.63
1:A:748:SER:C	1:A:749:VAL:HG22	2.23	0.63
1:E:583:TRP:HE3	1:E:584:ASN:H	1.45	0.63
1:J:559:HIS:CE1	1:K:756:VAL:O	2.51	0.63
1:J:720:LYS:HE3	4:Q:22:TRP:CH2	2.33	0.63
2:N:462:VAL:HG12	2:N:464:GLY:H	1.64	0.63
1:D:850:LEU:HG	1:F:554:ARG:H	1.64	0.63
1:F:533:ASN:HA	1:F:713:TYR:CD2	2.34	0.63
1:G:44:LYS:HG2	1:H:571:ASN:O	1.99	0.63
1:G:191:GLN:HG2	1:G:191:GLN:O	1.97	0.63
1:G:201:GLN:HB3	1:G:202:PRO:HD2	1.80	0.63
1:I:330:ARG:HD2	1:I:334:ILE:HG22	1.80	0.62
1:B:252:LYS:HG3	1:B:253:GLN:H	1.64	0.62
1:H:59:ASP:O	1:I:734:ASN:ND2	2.32	0.62
1:K:300:ILE:HG21	1:K:303:MET:HB2	1.81	0.62
1:K:416:PRO:HD2	1:K:458:PHE:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:200:ASN:ND2	3:M:235:LEU:HB2	2.14	0.62
1:A:324:PRO:HG2	1:A:538:HIS:HB2	1.80	0.62
1:K:929:HIS:HB2	1:K:937:GLU:HB2	1.82	0.62
1:L:930:ARG:N	1:L:931:PRO:HD2	2.14	0.62
1:E:420:VAL:HG22	1:E:457:ASN:HB3	1.80	0.62
1:H:719:LYS:NZ	4:R:47:LEU:O	2.26	0.62
1:C:182:GLU:C	1:C:264:MET:SD	2.80	0.62
1:C:598:GLY:HA2	1:C:703:GLY:HA3	1.81	0.62
1:D:566:PHE:HB2	1:D:569:ILE:HG22	1.82	0.62
1:J:96:MET:HE3	1:J:574:LEU:HD11	1.80	0.62
2:N:52:ARG:CZ	2:N:63:LEU:O	2.47	0.62
1:A:429:VAL:HG13	1:B:266:PHE:HD1	1.64	0.62
1:G:324:PRO:HG2	1:G:538:HIS:HB2	1.82	0.62
1:I:429:VAL:HB	1:I:439:TRP:CD1	2.35	0.62
1:K:755:ASN:OD1	1:K:759:CYS:O	2.17	0.62
2:N:275:TYR:O	2:N:275:TYR:CG	2.53	0.62
1:H:790:ARG:O	1:H:793:SER:HB2	1.99	0.62
2:N:446:GLN:HB3	2:N:532:ARG:NE	2.11	0.62
4:P:40:LEU:CB	4:P:41:PRO:HD2	1.99	0.62
1:H:475:SER:O	1:H:479:LEU:HG	2.00	0.62
1:L:683:LEU:HB3	1:L:706:PRO:HG2	1.81	0.62
4:P:40:LEU:HD12	4:P:46:THR:OG1	2.00	0.62
4:R:40:LEU:O	4:R:46:THR:HA	2.00	0.62
1:C:661:THR:HG23	1:C:662:ASN:ND2	2.15	0.61
1:I:221:GLY:HA3	1:I:286:LEU:HD23	1.81	0.61
1:J:252:LYS:HG3	1:J:253:GLN:H	1.65	0.61
1:B:354:GLN:HG3	2:N:446:GLN:HA	1.83	0.61
1:B:602:ARG:NH2	1:B:695:TYR:HE1	1.98	0.61
1:H:867:ASP:O	1:H:867:ASP:CG	2.43	0.61
3:M:193:ARG:HB2	3:M:195:GLY:O	1.99	0.61
4:S:30:MET:HE2	4:S:41:PRO:CA	2.29	0.61
1:G:923:PHE:O	1:G:941:LEU:HD23	2.01	0.61
4:S:106:GLN:O	4:S:110:LEU:CG	2.48	0.61
1:A:670:ARG:HH12	1:A:947:ALA:HB2	1.65	0.61
1:J:922:VAL:HG11	1:J:944:PRO:HB2	1.81	0.61
1:L:685:THR:HG23	1:L:915:LEU:HD21	1.83	0.61
3:M:196:LEU:HB2	3:M:199:VAL:HG21	1.81	0.61
1:D:119:THR:HG23	1:D:297:ASP:HB2	1.83	0.61
1:I:652:MET:HE1	1:I:654:TYR:OH	1.98	0.61
1:J:413:TYR:HB2	1:J:415:PHE:CE2	2.36	0.61
4:S:19:MET:HA	4:S:19:MET:CE	2.23	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:ASN:ND2	1:B:602:ARG:HB3	2.16	0.61
1:G:844:ALA:O	1:I:237:TYR:CB	2.47	0.61
1:H:32:ALA:O	1:H:36:GLU:HB3	2.01	0.61
1:H:455:GLY:O	1:I:173:PRO:HB3	2.01	0.61
1:I:652:MET:HE2	1:I:654:TYR:CZ	2.31	0.61
1:J:426:LEU:CA	1:K:268:SER:O	2.39	0.61
1:J:650:ALA:HB3	1:J:920:PHE:HB2	1.83	0.61
1:E:575:LEU:HG	1:E:930:ARG:HG3	1.82	0.61
1:H:328:ALA:HB1	1:H:546:ARG:HB2	1.82	0.61
1:I:661:THR:HB	1:I:909:PRO:HA	1.82	0.61
1:D:840:GLN:HG2	1:F:173:PRO:HD2	1.82	0.61
1:H:519:ASN:HD21	1:H:803:ARG:HH11	1.44	0.61
4:Q:111:THR:HA	4:Q:114:LEU:HD22	1.83	0.61
1:A:439:TRP:HZ2	1:B:180:THR:O	1.83	0.61
1:B:681:THR:OG1	1:B:870:LEU:HD23	2.00	0.61
1:E:331:ASP:HA	1:E:388:ASN:HB2	1.81	0.61
1:F:793:SER:O	1:F:869:THR:OG1	2.19	0.61
1:C:33:ARG:HB3	6:W:16:ASN:CA	2.31	0.61
1:C:836:MET:O	1:C:838:GLU:HG3	2.01	0.61
1:F:772:ALA:HB3	1:F:872:ARG:HB3	1.83	0.61
2:N:141:ASN:O	2:N:141:ASN:CG	2.42	0.61
1:D:133:CYS:HB2	1:D:224:LEU:HD12	1.82	0.60
1:I:909:PRO:CG	4:S:45:THR:HA	2.31	0.60
1:A:350:GLY:HA2	1:A:579:TYR:HA	1.82	0.60
1:B:922:VAL:HG12	1:B:923:PHE:H	1.66	0.60
1:E:797:ASN:HB3	1:E:867:ASP:O	2.01	0.60
1:J:124:LEU:HD21	1:K:467:ASN:HB2	1.83	0.60
1:A:384:PHE:HB3	1:A:387:TRP:O	2.01	0.60
1:B:562:VAL:HB	1:B:563:PRO:HD2	1.82	0.60
1:D:94:LEU:HD13	1:D:574:LEU:HD12	1.84	0.60
1:G:924:ASP:HA	1:G:941:LEU:HB3	1.83	0.60
1:K:748:SER:CB	1:K:760:ASN:HD21	2.13	0.60
3:M:196:LEU:HB3	3:M:199:VAL:HG21	1.82	0.60
1:C:756:VAL:HG12	1:C:757:ALA:H	1.66	0.60
1:G:677:GLY:HA2	1:G:874:PRO:HA	1.83	0.60
2:N:283:ILE:HG21	2:N:403:TYR:HB2	1.82	0.60
3:M:196:LEU:HD11	5:U:207:HIS:O	2.00	0.60
1:B:14:HIS:O	1:B:14:HIS:HD2	1.80	0.60
1:E:101:PHE:HB2	1:E:562:VAL:HG22	1.83	0.60
1:E:724:THR:HG23	1:E:728:SER:O	2.00	0.60
1:J:233:CYS:SG	1:K:841:ALA:HB1	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:415:PHE:HA	1:K:459:ALA:HA	1.83	0.60
1:B:354:GLN:HG3	2:N:446:GLN:O	2.01	0.60
1:E:837:ARG:HH22	1:F:415:PHE:HA	1.66	0.60
1:G:464:LEU:HD12	1:I:467:ASN:HD21	1.67	0.60
1:A:439:TRP:CZ2	1:B:180:THR:O	2.54	0.60
1:F:225:LYS:HG3	1:F:226:LYS:H	1.66	0.60
4:Q:113:GLU:O	4:Q:117:VAL:HG23	2.02	0.60
4:S:108:ASP:O	4:S:111:THR:HB	2.02	0.60
1:C:333:PHE:CD1	1:C:333:PHE:C	2.79	0.60
1:L:15:ILE:O	1:L:48:PRO:HB3	2.01	0.60
1:A:572:LEU:HD13	1:A:928:VAL:HG11	1.84	0.60
1:E:715:ASN:HD22	1:E:866:CYS:HB3	1.67	0.60
1:I:908:ASP:OD1	4:S:48:THR:HG21	2.02	0.60
1:J:817:VAL:HG22	1:J:818:GLY:N	2.16	0.60
1:H:850:LEU:H	1:H:851:ILE:HD12	1.67	0.60
2:N:242:LEU:HD21	2:N:248:VAL:HG22	1.84	0.60
2:N:445:MET:CB	2:N:529:LEU:HD11	2.32	0.60
4:S:40:LEU:HD13	4:S:46:THR:OG1	2.01	0.60
1:A:201:GLN:CB	1:A:202:PRO:HD2	2.32	0.59
1:E:634:LEU:HD12	1:E:639:ASN:HB3	1.84	0.59
1:I:724:THR:HG22	1:I:729:VAL:O	2.00	0.59
1:C:132:PRO:HB3	1:C:170:GLY:HA2	1.84	0.59
1:D:568:ALA:HA	1:D:926:VAL:HG11	1.85	0.59
1:G:869:THR:O	1:G:869:THR:HG23	2.02	0.59
1:B:354:GLN:CG	2:N:446:GLN:O	2.51	0.59
1:F:431:PRO:HA	1:F:439:TRP:HD1	1.67	0.59
1:H:134:GLU:HB3	1:H:167:HIS:HD2	1.67	0.59
1:K:748:SER:HA	1:K:760:ASN:OD1	2.02	0.59
1:K:245:GLY:HA3	1:L:821:HIS:HB3	1.83	0.59
1:F:132:PRO:HB3	1:F:170:GLY:HA2	1.84	0.59
1:I:719:LYS:HB2	1:I:906:GLU:HB3	1.83	0.59
1:I:806:VAL:HG11	1:I:811:TYR:HE1	1.67	0.59
1:L:17:GLY:O	1:L:18:GLN:HG2	2.02	0.59
1:H:492:VAL:CG1	1:H:506:LYS:HZ3	2.15	0.59
1:J:301:SER:HB3	1:J:320:MET:HB2	1.85	0.59
1:K:824:ASN:HB3	1:K:844:ALA:CB	2.32	0.59
1:B:947:ALA:HA	2:N:109:GLN:HB2	1.85	0.59
1:F:242:ASN:O	1:F:242:ASN:CG	2.46	0.59
1:H:469:TRP:CD1	1:H:516:CYS:HG	2.19	0.59
1:I:380:ARG:HE	1:I:391:VAL:HG11	1.66	0.59
1:K:759:CYS:HB2	1:K:800:PRO:CB	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:SER:OG	1:E:734:ASN:O	2.13	0.59
1:I:831:TYR:O	1:I:831:TYR:CZ	2.55	0.59
1:A:269:THR:HA	1:C:426:LEU:CD2	2.20	0.59
1:B:354:GLN:NE2	2:N:446:GLN:O	2.34	0.59
1:E:249:ILE:HG12	1:E:260:SER:HA	1.85	0.59
1:H:173:PRO:HD2	1:H:220:ALA:O	2.03	0.59
1:K:678:TRP:HB2	1:K:873:ILE:HD12	1.83	0.59
1:A:280:LEU:HB3	1:C:429:VAL:HG11	1.84	0.58
1:B:772:ALA:HA	1:B:874:PRO:HG3	1.85	0.58
1:D:800:PRO:HG2	1:F:385:SER:HB2	1.82	0.58
1:J:266:PHE:HB3	1:J:285:VAL:HG23	1.85	0.58
2:N:446:GLN:HB2	2:N:532:ARG:NH2	2.18	0.58
1:G:691:LEU:HD13	1:G:692:GLY:H	1.67	0.58
1:I:349:ALA:HB1	1:I:353:SER:O	2.02	0.58
1:L:632:ALA:HA	1:L:635:ARG:HG2	1.85	0.58
4:S:30:MET:CE	4:S:41:PRO:CB	2.81	0.58
1:F:241:THR:HG22	1:F:242:ASN:H	1.68	0.58
1:B:184:ILE:HG22	1:B:185:GLN:N	2.18	0.58
1:D:794:PHE:CD2	1:D:794:PHE:C	2.74	0.58
1:H:689:PRO:HB3	1:H:699:TYR:HB2	1.85	0.58
1:K:755:ASN:ND2	1:K:756:VAL:H	2.01	0.58
1:D:300:ILE:HG21	1:D:317:GLN:HG2	1.85	0.58
1:D:798:PHE:HD1	1:D:866:CYS:HB2	1.67	0.58
1:H:428:LYS:HG2	1:I:267:PHE:HB3	1.85	0.58
1:L:716:HIS:HB3	1:L:866:CYS:H	1.68	0.58
1:A:58:THR:O	1:A:60:ARG:N	2.36	0.58
1:C:728:SER:O	1:C:729:VAL:C	2.46	0.58
1:D:101:PHE:HB2	1:D:562:VAL:HG23	1.86	0.58
1:D:269:THR:C	1:D:270:THR:HG22	2.28	0.58
1:F:399:ARG:CZ	1:F:534:PRO:HG2	2.34	0.58
1:G:388:ASN:HB3	1:G:546:ARG:HH11	1.68	0.58
1:J:794:PHE:HA	1:J:869:THR:HG21	1.84	0.58
1:J:821:HIS:HB3	1:L:244:ASN:O	2.03	0.58
1:K:754:TYR:HB3	1:K:762:THR:HG23	1.85	0.58
1:E:200:PHE:CG	1:E:200:PHE:O	2.55	0.58
1:G:323:ARG:HD3	1:G:479:LEU:HB3	1.85	0.58
1:G:771:LEU:O	1:G:880:MET:C	2.44	0.58
1:A:844:ALA:HB3	1:C:121:TYR:HD2	1.67	0.58
1:B:373:LEU:HD22	1:B:646:TYR:H	1.67	0.58
1:B:756:VAL:HB	1:B:763:LYS:HE2	1.85	0.58
1:G:757:ALA:CB	1:I:386:MET:HG2	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLY:H	1:A:554:ARG:HG3	1.68	0.58
1:A:338:TYR:HB3	1:A:341:SER:HB3	1.85	0.58
1:B:594:GLN:HE22	1:B:704:SER:HA	1.68	0.58
1:B:924:ASP:HA	1:B:941:LEU:O	2.04	0.58
1:D:833:ALA:HB3	1:D:835:THR:HG23	1.85	0.58
1:H:25:SER:H	1:I:639:ASN:HD22	1.52	0.58
1:H:708:LEU:HG	1:H:708:LEU:O	2.04	0.58
4:Q:107:LEU:HD23	4:Q:110:LEU:HD22	1.86	0.58
1:K:823:HIS:HB3	1:K:845:ASN:N	2.19	0.57
1:L:757:ALA:CB	1:L:766:PHE:HZ	2.16	0.57
4:S:109:SER:O	4:S:113:GLU:HG2	2.04	0.57
1:A:837:ARG:HE	1:B:458:PHE:HA	1.69	0.57
1:E:681:THR:HG21	1:E:712:PHE:HB3	1.86	0.57
1:G:412:ASN:HD21	1:I:462:ILE:HD11	1.69	0.57
1:G:562:VAL:HB	1:G:585:PHE:HE2	1.69	0.57
4:S:10:ILE:HG23	4:S:11:VAL:N	2.19	0.57
2:N:278:LEU:HD22	2:N:406:TRP:HA	1.86	0.57
1:B:794:PHE:O	1:B:798:PHE:CD2	2.55	0.57
1:H:20:ALA:HB2	1:H:48:PRO:HD2	1.86	0.57
1:A:323:ARG:HG3	1:A:479:LEU:HD22	1.86	0.57
1:C:173:PRO:HB2	1:C:207:GLY:HA2	1.87	0.57
1:G:201:GLN:CB	1:G:202:PRO:CD	2.75	0.57
1:H:84:PHE:HB2	1:H:581:TYR:HB3	1.87	0.57
1:I:730:SER:C	1:I:732:PRO:HD2	2.29	0.57
2:N:230:VAL:HG12	2:N:231:TYR:H	1.70	0.57
1:D:78:TYR:CD1	1:D:78:TYR:C	2.81	0.57
1:D:94:LEU:HB3	1:D:574:LEU:HB2	1.87	0.57
1:G:794:PHE:HA	1:G:869:THR:HG21	1.86	0.57
1:H:590:ASN:HD21	1:H:602:ARG:HD2	1.70	0.57
1:J:664:PRO:HG2	4:P:15:LEU:HA	1.87	0.57
1:E:90:ASP:HA	1:E:576:PRO:HB3	1.87	0.57
1:J:572:LEU:HG	1:J:573:LEU:O	2.04	0.57
1:J:624:HIS:HA	1:J:627:ALA:HB2	1.85	0.57
1:L:329:PHE:HB2	1:L:546:ARG:HG2	1.86	0.57
2:N:70:TYR:H	2:N:111:ILE:HD12	1.70	0.57
1:A:204:PRO:HD2	1:B:823:HIS:CE1	2.40	0.57
1:G:621:PRO:CG	1:H:878:ASN:OD1	2.51	0.57
1:G:689:PRO:HG3	1:G:699:TYR:HB2	1.86	0.57
1:G:757:ALA:HA	1:I:386:MET:CB	2.24	0.57
1:I:47:ASN:H	1:I:48:PRO:HD3	1.68	0.57
1:B:179:ILE:CG2	1:B:182:GLU:O	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:ILE:HD12	1:E:186:ILE:HD11	1.87	0.57
1:E:850:LEU:HD21	1:E:858:SER:HB3	1.86	0.57
1:K:102:ASP:HB2	1:K:616:TYR:HE1	1.70	0.57
2:N:227:MET:HB2	2:N:228:PRO:HD3	1.86	0.57
1:A:26:PRO:HD3	3:M:19:SER:HB2	1.87	0.57
1:A:201:GLN:CB	1:A:202:PRO:CD	2.83	0.57
1:A:211:TRP:HZ3	1:A:417:LEU:HB3	1.69	0.57
1:H:792:TYR:CD2	1:H:868:ARG:O	2.58	0.57
1:I:179:ILE:HG23	1:I:218:HIS:CG	2.40	0.57
1:J:113:PHE:HE2	1:J:552:ASN:HA	1.70	0.57
1:J:127:LYS:HD2	1:K:411:PRO:HG3	1.86	0.57
1:G:553:GLY:HA3	1:H:850:LEU:HG	1.87	0.56
1:I:797:ASN:HB3	1:I:867:ASP:O	2.05	0.56
1:L:731:TRP:HB3	1:L:732:PRO:HD3	1.87	0.56
1:G:171:GLN:HA	1:I:452:ILE:HG21	1.86	0.56
1:I:723:ILE:HG23	1:I:903:MET:HG2	1.87	0.56
2:N:231:TYR:OH	2:N:284:PRO:O	2.23	0.56
1:A:840:GLN:HE21	1:C:204:PRO:HA	1.70	0.56
1:G:713:TYR:N	1:G:867:ASP:O	2.37	0.56
1:H:252:LYS:HG3	1:H:253:GLN:H	1.70	0.56
1:I:589:VAL:HB	1:I:593:LEU:HD12	1.86	0.56
1:J:106:VAL:HG12	1:J:557:PRO:HB3	1.87	0.56
1:L:184:ILE:HG12	1:L:220:ALA:HB2	1.87	0.56
1:L:824:ASN:HB2	1:L:844:ALA:HB2	1.84	0.56
2:N:446:GLN:HB3	2:N:532:ARG:CD	2.36	0.56
4:Q:110:LEU:O	4:Q:114:LEU:HD13	2.05	0.56
1:A:752:GLU:HA	1:A:755:ASN:HD22	1.70	0.56
1:B:15:ILE:O	1:B:15:ILE:HG22	2.06	0.56
1:B:182:GLU:HB2	1:B:195:TYR:CD2	2.40	0.56
1:G:849:PRO:O	1:G:851:ILE:N	2.38	0.56
1:H:876:SER:OG	1:H:880:MET:O	2.12	0.56
1:J:648:SER:O	1:J:922:VAL:O	2.23	0.56
1:K:732:PRO:O	1:K:733:GLY:C	2.49	0.56
1:C:88:VAL:HG23	1:C:577:GLY:H	1.70	0.56
1:G:758:GLN:HG3	1:I:385:SER:HG	1.71	0.56
1:G:774:TYR:HB3	1:G:788:LYS:HD3	1.88	0.56
1:H:691:LEU:O	4:Q:21:PRO:HB2	2.06	0.56
1:A:17:GLY:C	1:A:48:PRO:HG2	2.31	0.56
1:B:81:LYS:NZ	2:N:457:ILE:CG2	2.65	0.56
1:B:795:PHE:O	1:B:796:ARG:O	2.22	0.56
1:H:685:THR:HG23	4:Q:26:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:509:VAL:HG13	1:L:510:ALA:H	1.71	0.56
2:N:134:VAL:HG12	2:N:172:GLU:HG2	1.88	0.56
1:A:316:GLY:HA3	1:C:210:GLN:HB2	1.88	0.56
1:B:726:ASP:CB	1:B:900:ALA:N	2.56	0.56
1:D:681:THR:HG21	1:D:712:PHE:HB3	1.88	0.56
1:H:519:ASN:HD21	1:H:803:ARG:NH1	2.03	0.56
1:H:828:PHE:O	1:H:836:MET:O	2.24	0.56
1:A:56:VAL:CG1	6:W:4:LEU:O	2.54	0.56
1:B:447:SER:HB2	1:C:167:HIS:HB3	1.88	0.56
1:F:110:GLY:H	1:F:554:ARG:HG3	1.70	0.56
1:L:224:LEU:HD23	1:L:289:GLU:HB3	1.88	0.56
3:M:158:GLN:HB2	3:M:213:GLY:HA3	1.87	0.56
1:D:723:ILE:HB	1:D:731:TRP:HB2	1.87	0.56
1:G:759:CYS:HG	1:G:800:PRO:HB3	1.69	0.56
1:H:323:ARG:CZ	1:H:504:MET:O	2.53	0.56
1:K:447:SER:HB2	1:L:167:HIS:HB3	1.86	0.56
1:K:549:LEU:HD12	1:L:800:PRO:HB2	1.88	0.56
1:B:249:ILE:HG22	1:B:260:SER:HA	1.86	0.56
1:B:797:ASN:HB3	1:B:867:ASP:O	2.06	0.56
1:C:35:THR:HG23	6:W:5:ALA:CB	2.36	0.56
1:L:763:LYS:HA	1:L:766:PHE:HB2	1.88	0.56
1:E:731:TRP:HE1	1:E:879:PHE:HZ	1.52	0.55
1:G:559:HIS:CE1	1:H:756:VAL:HA	2.41	0.55
1:H:341:SER:HA	1:H:362:GLN:HG2	1.88	0.55
1:K:97:ALA:HB2	1:K:570:LYS:O	2.06	0.55
2:N:231:TYR:CZ	2:N:284:PRO:O	2.59	0.55
4:P:10:ILE:HG12	4:Q:26:ARG:O	2.06	0.55
1:C:332:ASN:O	1:C:333:PHE:CD2	2.59	0.55
1:H:97:ALA:CB	1:H:571:ASN:H	2.14	0.55
1:H:323:ARG:NE	1:H:504:MET:O	2.40	0.55
1:I:831:TYR:CD1	1:I:831:TYR:C	2.71	0.55
4:S:50:GLU:HG3	4:S:52:VAL:HG13	1.88	0.55
1:J:329:PHE:H	1:J:546:ARG:HG2	1.71	0.55
1:K:756:VAL:HG21	1:K:766:PHE:CD1	2.42	0.55
1:C:34:ALA:CB	6:W:13:PHE:CB	2.77	0.55
1:F:533:ASN:CA	1:F:713:TYR:CE2	2.89	0.55
1:L:19:ASP:O	1:L:48:PRO:HG2	2.07	0.55
1:B:590:ASN:HB3	1:B:699:TYR:CD2	2.42	0.55
1:G:18:GLN:CD	1:G:22:GLU:HB3	2.31	0.55
1:H:887:ASP:O	1:H:891:ASN:HB2	2.06	0.55
1:J:204:PRO:HB3	1:K:840:GLN:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:225:LEU:HD22	2:N:285:ALA:CB	2.31	0.55
1:G:847:PRO:HG2	1:I:121:TYR:CE1	2.31	0.55
1:H:245:GLY:HA3	1:I:821:HIS:HB3	1.89	0.55
1:J:340:ASN:HB3	1:J:366:THR:H	1.72	0.55
1:L:930:ARG:N	1:L:931:PRO:CD	2.69	0.55
2:N:455:ARG:HH21	2:N:540:ARG:HB2	1.71	0.55
1:A:431:PRO:CA	1:A:439:TRP:CD1	2.90	0.55
1:B:14:HIS:O	1:B:14:HIS:CG	2.57	0.55
1:G:929:HIS:C	1:G:937:GLU:HG3	2.31	0.55
1:H:364:ARG:HH22	1:H:940:TYR:HE2	1.53	0.55
1:H:705:ILE:HG22	1:H:707:TYR:N	2.20	0.55
1:L:20:ALA:HA	1:L:48:PRO:HD2	1.88	0.55
1:I:130:PRO:HG2	1:I:315:MET:HA	1.88	0.55
1:K:388:ASN:O	1:K:389:GLN:C	2.50	0.55
1:B:252:LYS:HG2	1:B:253:GLN:N	2.18	0.55
1:C:669:SER:HB2	1:K:664:PRO:HG2	1.88	0.55
1:G:716:HIS:HB3	1:G:866:CYS:H	1.70	0.55
1:J:323:ARG:HG3	1:J:479:LEU:HD13	1.88	0.55
1:K:350:GLY:H	1:K:353:SER:HB3	1.72	0.55
1:K:384:PHE:HB2	1:K:389:GLN:HB2	1.87	0.55
1:L:53:THR:O	1:L:57:THR:OG1	2.16	0.55
1:B:327:ILE:HD13	1:B:601:LEU:HD21	1.89	0.55
1:D:23:TYR:O	1:D:23:TYR:CD2	2.60	0.55
1:J:171:GLN:HB3	1:K:840:GLN:HG2	1.88	0.55
1:L:18:GLN:O	1:L:19:ASP:C	2.49	0.55
1:B:748:SER:HB3	1:B:760:ASN:HD21	1.72	0.54
1:E:829:VAL:HG22	1:E:830:GLY:H	1.71	0.54
1:I:334:ILE:HA	1:I:565:LYS:HZ1	1.72	0.54
1:J:121:TYR:OH	1:K:849:PRO:HG3	2.07	0.54
1:G:655:PRO:HB3	1:G:915:LEU:HD23	1.89	0.54
1:G:937:GLU:HG3	1:G:937:GLU:O	2.07	0.54
1:I:730:SER:O	1:I:732:PRO:HD2	2.07	0.54
1:J:850:LEU:HG	1:L:554:ARG:H	1.72	0.54
1:L:824:ASN:HD22	1:L:824:ASN:H	1.54	0.54
1:E:724:THR:HB	1:E:902:ASP:HB3	1.89	0.54
1:G:757:ALA:C	1:G:758:GLN:CG	2.80	0.54
1:I:797:ASN:CB	1:I:867:ASP:O	2.55	0.54
1:J:41:LEU:HD13	1:J:44:LYS:HD2	1.89	0.54
1:J:112:THR:HG21	1:J:599:ASN:HD21	1.73	0.54
4:Q:115:ASN:O	4:Q:118:SER:CB	2.54	0.54
1:B:942:ARG:HB3	1:B:947:ALA:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:807:ASP:HB2	1:C:858:SER:HA	1.89	0.54
1:E:943:THR:HB	1:E:944:PRO:HD3	1.87	0.54
1:H:716:HIS:HB3	1:H:866:CYS:SG	2.47	0.54
1:K:705:ILE:HB	1:K:708:LEU:HD12	1.88	0.54
4:Q:28:ASN:HA	4:Q:42:ALA:HB3	1.88	0.54
4:R:119:GLN:HA	4:R:122:LEU:HG	1.88	0.54
1:G:79:SER:HB2	1:G:584:ASN:HD22	1.73	0.54
1:H:492:VAL:HG11	1:H:506:LYS:CD	2.32	0.54
1:J:415:PHE:HA	1:L:837:ARG:HH22	1.72	0.54
1:A:678:TRP:HB2	1:A:873:ILE:HD12	1.90	0.54
1:B:649:ALA:HA	1:B:922:VAL:H	1.72	0.54
1:C:332:ASN:O	1:C:333:PHE:CG	2.60	0.54
1:D:656:ILE:HB	1:D:910:MET:HE1	1.89	0.54
1:H:524:TRP:HD1	1:H:801:MET:HB3	1.71	0.54
1:I:656:ILE:HD13	1:I:907:VAL:HG21	1.90	0.54
1:J:756:VAL:HG21	1:J:766:PHE:CB	2.37	0.54
2:N:138:MET:HE3	2:N:432:CYS:SG	2.47	0.54
3:M:155:PRO:HG2	3:M:159:GLU:HG3	1.90	0.54
1:A:723:ILE:HG12	1:A:903:MET:HE3	1.90	0.54
1:A:775:ASN:HD22	1:A:779:GLN:HE22	1.56	0.54
1:B:325:ASN:HA	1:B:596:SER:HB3	1.89	0.54
1:C:198:LYS:HB3	1:C:262:VAL:HB	1.89	0.54
1:D:824:ASN:HA	1:D:844:ALA:HB2	1.89	0.54
1:H:724:THR:HB	1:H:902:ASP:HB3	1.89	0.54
1:J:201:GLN:HB3	1:J:202:PRO:CD	2.35	0.54
1:K:478:ALA:HB2	1:K:514:VAL:HG21	1.90	0.54
1:L:252:LYS:HG2	1:L:253:GLN:H	1.72	0.54
2:N:283:ILE:CG2	2:N:283:ILE:O	2.55	0.54
1:A:548:MET:HB3	1:B:523:ARG:H	1.72	0.54
1:B:188:VAL:HG23	1:B:188:VAL:O	2.06	0.54
1:D:96:MET:HG3	1:D:572:LEU:HB3	1.89	0.54
1:D:368:LEU:HD21	1:D:917:TYR:OH	2.08	0.54
1:F:323:ARG:HG2	1:F:479:LEU:HD13	1.89	0.54
1:L:649:ALA:HA	1:L:922:VAL:H	1.73	0.54
5:V:47:ILE:HA	5:V:50:HIS:HB2	1.90	0.54
1:C:113:PHE:HD1	1:C:327:ILE:HB	1.72	0.54
1:I:474:TYR:HA	1:I:478:ALA:HB3	1.90	0.54
1:I:728:SER:O	1:I:728:SER:OG	2.25	0.54
2:N:94:THR:C	2:N:96:ILE:H	2.13	0.54
1:A:720:LYS:HG2	1:A:744:GLU:HG2	1.90	0.54
1:E:422:ASN:HB3	1:E:453:ARG:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:847:PRO:CG	1:I:121:TYR:CE1	2.90	0.54
1:I:132:PRO:HG3	1:I:171:GLN:HB2	1.90	0.54
2:N:139:PHE:HB3	2:N:253:SER:O	2.08	0.54
1:B:725:PHE:C	1:B:900:ALA:O	2.51	0.53
1:E:332:ASN:H	1:E:388:ASN:HB2	1.73	0.53
1:L:797:ASN:HB2	1:L:867:ASP:O	2.06	0.53
4:P:30:MET:HA	4:P:40:LEU:O	2.08	0.53
1:F:365:ASN:HB3	1:F:368:LEU:HB2	1.89	0.53
1:F:533:ASN:HA	1:F:713:TYR:CE2	2.44	0.53
1:H:350:GLY:HA2	1:H:579:TYR:HA	1.90	0.53
1:I:339:TYR:HB2	1:I:367:GLU:HG3	1.91	0.53
1:J:233:CYS:CB	1:K:841:ALA:HB1	2.39	0.53
1:J:821:HIS:ND1	1:L:244:ASN:O	2.41	0.53
4:S:19:MET:HE2	4:S:20:PRO:CD	2.37	0.53
1:A:119:THR:HG21	1:A:235:GLY:HA2	1.91	0.53
1:A:328:ALA:HB2	1:A:547:SER:HB2	1.90	0.53
1:J:425:THR:O	1:K:269:THR:HA	2.09	0.53
4:P:16:THR:HA	4:R:13:SER:HB2	1.89	0.53
4:S:108:ASP:O	4:S:111:THR:CB	2.57	0.53
1:B:340:ASN:HA	1:B:360:ASP:HB3	1.89	0.53
1:G:202:PRO:HG3	1:G:220:ALA:HB1	1.91	0.53
1:J:281:THR:HA	1:L:439:TRP:HZ3	1.73	0.53
4:P:29:VAL:N	4:P:42:ALA:HB2	2.20	0.53
1:G:102:ASP:HB3	1:G:614:CYS:H	1.72	0.53
1:G:204:PRO:HB3	1:H:840:GLN:CB	2.36	0.53
1:H:324:PRO:HD3	1:H:479:LEU:HD22	1.89	0.53
1:H:722:ALA:HB3	1:H:904:THR:HB	1.90	0.53
1:J:906:GLU:OE2	4:Q:22:TRP:CD1	2.62	0.53
1:K:828:PHE:HA	1:K:837:ARG:HG2	1.88	0.53
1:A:772:ALA:HB1	1:A:872:ARG:HB2	1.90	0.53
1:B:64:LEU:HD11	1:B:619:PHE:O	2.01	0.53
1:C:659:ASN:O	1:C:659:ASN:ND2	2.42	0.53
1:D:113:PHE:HB2	1:D:327:ILE:HD12	1.91	0.53
1:F:572:LEU:HD22	1:F:641:GLN:HB3	1.91	0.53
1:H:719:LYS:HZ3	1:H:746:LYS:HD3	1.74	0.53
1:I:177:ILE:CG2	1:I:178:ASN:N	2.71	0.53
1:I:205:GLN:HG3	1:I:206:ILE:HG13	1.91	0.53
1:J:461:GLU:HB2	1:L:126:PRO:HB3	1.91	0.53
1:B:724:THR:CG2	1:B:725:PHE:N	2.71	0.53
1:C:430:LYS:HB2	1:C:442:ASP:HA	1.91	0.53
1:D:184:ILE:HD12	1:D:186:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:780:GLY:H	1:F:98:SER:HB2	1.74	0.53
1:H:126:PRO:HB2	1:H:129:ALA:HB2	1.89	0.53
1:J:132:PRO:HB2	1:J:223:VAL:HG23	1.90	0.53
1:L:54:HIS:O	1:L:54:HIS:CG	2.61	0.53
1:E:672:TRP:HE1	1:E:899:HIS:HB2	1.73	0.53
1:G:758:GLN:HG3	1:I:385:SER:OG	2.08	0.53
1:I:333:PHE:HZ	1:I:563:PRO:HD2	1.74	0.53
1:I:752:GLU:HG2	1:I:755:ASN:HB2	1.89	0.53
1:L:594:GLN:NE2	1:L:705:ILE:H	2.07	0.53
1:A:559:HIS:CE1	1:B:755:ASN:O	2.58	0.53
1:A:848:TYR:HB3	1:A:856:VAL:HG21	1.91	0.53
1:B:941:LEU:HD11	1:B:943:THR:OG1	2.09	0.53
1:D:365:ASN:H	1:D:651:ASN:HD21	1.55	0.53
1:F:334:ILE:HG12	1:F:565:LYS:HZ3	1.73	0.53
1:K:748:SER:HA	1:K:760:ASN:CG	2.34	0.53
2:N:446:GLN:HB3	2:N:532:ARG:CG	2.39	0.53
1:A:383:TYR:HA	1:A:389:GLN:HB3	1.89	0.53
1:A:745:ILE:HG23	1:A:765:TRP:CE2	2.44	0.53
1:B:722:ALA:HB3	1:B:904:THR:HB	1.91	0.53
1:D:166:THR:N	1:F:447:SER:HG	2.06	0.53
1:E:384:PHE:HB2	1:E:389:GLN:HB3	1.90	0.53
1:E:757:ALA:O	1:E:758:GLN:HB2	2.09	0.53
1:F:320:MET:HE1	1:F:506:LYS:HA	1.90	0.53
1:J:173:PRO:HG3	1:K:840:GLN:HG3	1.91	0.53
1:J:749:VAL:HG21	4:Q:50:GLU:HA	1.91	0.53
1:L:723:ILE:HG12	1:L:903:MET:HE3	1.91	0.53
3:M:291:GLY:HA2	3:M:294:GLU:HB2	1.91	0.53
4:S:30:MET:HE1	4:S:41:PRO:CB	2.39	0.53
1:E:238:ALA:HB2	1:F:843:PRO:HB2	1.90	0.52
1:G:621:PRO:HD2	1:H:878:ASN:OD1	2.09	0.52
1:G:678:TRP:HD1	1:G:920:PHE:HA	1.74	0.52
1:J:112:THR:HG21	1:J:599:ASN:ND2	2.24	0.52
1:J:906:GLU:CD	4:Q:22:TRP:HE1	2.17	0.52
1:K:430:LYS:HB2	1:K:442:ASP:HA	1.92	0.52
1:A:840:GLN:HE22	1:C:221:GLY:HA2	1.74	0.52
1:G:201:GLN:O	1:G:202:PRO:C	2.51	0.52
1:H:514:VAL:CA	1:H:518:ILE:HD11	2.34	0.52
1:H:671:ASN:HD21	1:H:946:SER:HB2	1.74	0.52
1:H:732:PRO:CG	1:H:740:PRO:O	2.56	0.52
1:E:333:PHE:HB2	1:E:563:PRO:HD2	1.91	0.52
1:G:760:ASN:HD22	1:G:863:LYS:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:594:GLN:HE21	1:L:705:ILE:HG13	1.74	0.52
3:M:252:THR:HG23	3:M:254:LEU:H	1.74	0.52
6:W:2:ALA:O	6:W:12:PRO:CB	2.58	0.52
1:C:536:ASN:HA	1:C:596:SER:C	2.34	0.52
1:G:104:ARG:HD3	1:G:612:SER:HB3	1.91	0.52
1:G:336:LEU:HB2	1:G:562:VAL:HG11	1.92	0.52
1:I:223:VAL:HB	1:I:286:LEU:HD22	1.90	0.52
2:N:455:ARG:O	2:N:455:ARG:HG3	2.07	0.52
1:A:735:ASP:HB2	1:C:61:SER:HB2	1.92	0.52
1:B:888:LEU:HA	1:B:891:ASN:HB2	1.91	0.52
1:C:850:LEU:H	1:C:851:ILE:HD12	1.73	0.52
1:D:231:LYS:HE2	1:D:236:SER:HA	1.91	0.52
1:G:201:GLN:HB2	1:G:287:TYR:CE2	2.45	0.52
1:I:63:ARG:HB2	1:I:66:LEU:HD21	1.92	0.52
1:J:906:GLU:HG3	4:Q:20:PRO:HG2	1.91	0.52
1:K:133:CYS:HB3	1:K:230:MET:HG2	1.89	0.52
1:L:132:PRO:HB2	1:L:223:VAL:HA	1.92	0.52
1:B:867:ASP:O	1:B:868:ARG:HB3	2.09	0.52
1:C:174:TYR:HB2	1:C:220:ALA:H	1.73	0.52
1:C:481:LEU:H	1:C:486:LYS:HZ1	1.57	0.52
1:D:797:ASN:CG	1:D:867:ASP:O	2.52	0.52
1:J:252:LYS:HB3	1:J:257:LYS:HA	1.91	0.52
1:L:747:ARG:HB2	1:L:755:ASN:HD21	1.75	0.52
1:L:824:ASN:CB	1:L:844:ALA:HB1	2.24	0.52
5:V:183:ILE:HG22	5:V:184:GLY:N	2.24	0.52
1:B:765:TRP:HZ2	1:B:871:TRP:HB3	1.74	0.52
1:C:747:ARG:HG3	1:C:762:THR:CB	2.21	0.52
1:E:524:TRP:CD1	1:E:803:ARG:HB3	2.45	0.52
1:F:104:ARG:HB3	1:F:612:SER:HB3	1.91	0.52
1:G:440:GLU:O	1:G:441:LYS:HG3	2.10	0.52
1:G:719:LYS:HB3	1:G:906:GLU:HG3	1.92	0.52
1:I:117:SER:HB3	1:I:324:PRO:HG3	1.90	0.52
1:J:405:GLY:HA2	1:J:520:LEU:HD21	1.92	0.52
4:S:20:PRO:HB2	4:S:25:VAL:HG21	1.90	0.52
1:A:107:LEU:HB3	1:A:556:VAL:HG23	1.91	0.52
1:B:338:TYR:HB2	1:B:341:SER:HB3	1.92	0.52
1:B:925:VAL:H	1:B:941:LEU:HD23	1.75	0.52
1:F:84:PHE:HB2	1:F:581:TYR:HB3	1.91	0.52
1:H:121:TYR:CD2	1:H:237:TYR:HA	2.45	0.52
1:J:756:VAL:HG21	1:J:766:PHE:HB2	1.91	0.52
1:K:687:GLU:HA	1:K:701:TYR:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:348:LEU:HD21	1:L:569:ILE:HD13	1.91	0.52
1:C:112:THR:HG22	1:C:501:TYR:HB2	1.91	0.52
1:H:225:LYS:HE3	1:H:290:ASP:HB2	1.91	0.52
1:I:718:PHE:HD1	1:I:907:VAL:HG12	1.75	0.52
3:M:80:LEU:HG	3:M:85:ALA:HB3	1.92	0.52
1:A:200:PHE:O	1:A:200:PHE:HD1	1.91	0.52
1:A:830:GLY:HA3	1:A:835:THR:HG23	1.91	0.52
1:D:328:ALA:HB1	1:D:546:ARG:HG3	1.91	0.52
1:G:121:TYR:HA	1:H:824:ASN:ND2	2.24	0.52
1:H:517:TYR:CB	1:H:847:PRO:HG3	2.40	0.52
1:H:660:ALA:HB1	4:Q:11:VAL:HG11	1.92	0.52
1:J:119:THR:HG22	1:J:120:ALA:H	1.75	0.52
1:K:24:LEU:HD22	1:L:639:ASN:HD22	1.75	0.52
1:B:403:ASN:HB3	1:B:520:LEU:HD23	1.90	0.51
1:B:590:ASN:HB3	1:B:699:TYR:HD2	1.74	0.51
1:B:933:ARG:HH12	3:M:93:LEU:HD23	1.74	0.51
1:D:173:PRO:HG3	1:E:840:GLN:HG3	1.91	0.51
1:H:324:PRO:HG3	1:H:479:LEU:HD13	1.92	0.51
1:H:655:PRO:HA	1:H:915:LEU:HA	1.93	0.51
1:J:655:PRO:HG3	1:J:915:LEU:CD2	2.39	0.51
1:A:58:THR:C	1:A:60:ARG:H	2.18	0.51
1:B:119:THR:HG22	1:B:121:TYR:H	1.75	0.51
1:B:940:TYR:HB3	2:N:108:THR:HB	1.92	0.51
1:C:113:PHE:CD1	1:C:327:ILE:HB	2.45	0.51
1:D:52:PRO:HG2	1:D:55:ASP:HB2	1.91	0.51
1:G:738:LEU:HD11	1:G:763:LYS:HE3	1.92	0.51
1:J:575:LEU:HD21	1:J:635:ARG:HE	1.74	0.51
1:B:725:PHE:O	1:B:900:ALA:O	2.28	0.51
1:E:429:VAL:HG12	1:E:441:LYS:HA	1.91	0.51
1:J:428:LYS:HD2	1:J:446:PHE:CD1	2.44	0.51
1:L:328:ALA:HB2	1:L:547:SER:HB2	1.92	0.51
1:L:755:ASN:HA	1:L:762:THR:HA	1.92	0.51
2:N:440:SER:C	2:N:442:PRO:HD3	2.35	0.51
1:A:356:ASN:HD22	1:A:356:ASN:H	1.59	0.51
1:C:249:ILE:HG12	1:C:290:ASP:HB2	1.93	0.51
1:D:61:SER:CB	1:E:734:ASN:O	2.59	0.51
1:I:823:HIS:HB2	1:I:844:ALA:HA	1.91	0.51
2:N:196:GLY:O	2:N:200:GLY:O	2.28	0.51
1:C:80:TYR:HB3	1:C:585:PHE:HB2	1.92	0.51
1:C:428:LYS:HB2	1:C:446:PHE:H	1.75	0.51
1:F:501:TYR:O	1:F:505:ASN:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:664:PRO:HA	1:F:904:THR:HA	1.91	0.51
1:I:732:PRO:HB2	1:I:734:ASN:O	2.09	0.51
1:J:904:THR:HG21	4:Q:20:PRO:CD	2.40	0.51
1:L:20:ALA:O	1:L:45:PHE:CE2	2.51	0.51
2:N:449:VAL:C	2:N:450:THR:HG22	2.36	0.51
1:A:202:PRO:HG3	1:A:220:ALA:HB3	1.93	0.51
1:B:776:ILE:HG12	1:B:782:TYR:HB2	1.93	0.51
1:J:639:ASN:HD21	1:L:25:SER:HB2	1.75	0.51
1:K:429:VAL:HG12	1:K:441:LYS:HA	1.92	0.51
1:L:656:ILE:O	1:L:913:PRO:HA	2.11	0.51
1:L:768:VAL:HG13	1:L:873:ILE:HB	1.93	0.51
4:Q:85:LEU:HB3	4:Q:92:ARG:HH12	1.76	0.51
1:H:798:PHE:HB3	1:H:866:CYS:HA	1.91	0.51
1:H:823:HIS:HB2	1:H:845:ASN:HB2	1.93	0.51
1:I:272:ALA:HB3	1:I:280:LEU:HB3	1.92	0.51
1:I:349:ALA:O	1:I:350:GLY:O	2.29	0.51
1:K:755:ASN:HD21	1:K:760:ASN:CA	2.24	0.51
1:L:446:PHE:O	1:L:447:SER:C	2.54	0.51
1:A:855:ALA:HB2	1:C:554:ARG:HD3	1.92	0.51
1:B:66:LEU:HD12	1:B:92:ARG:HH22	1.76	0.51
1:D:752:GLU:HB3	1:F:559:HIS:HE1	1.76	0.51
1:E:705:ILE:HB	1:E:708:LEU:HB2	1.93	0.51
1:I:172:ALA:CB	1:I:284:VAL:HG11	2.40	0.51
1:J:720:LYS:CE	4:Q:22:TRP:CH2	2.90	0.51
1:K:329:PHE:O	1:K:330:ARG:O	2.28	0.51
1:L:369:SER:HA	1:L:647:LEU:HB3	1.93	0.51
1:F:713:TYR:CD1	1:F:714:LEU:HG	2.45	0.51
1:J:929:HIS:HB2	1:J:937:GLU:HB2	1.93	0.51
1:A:238:ALA:HB2	1:B:843:PRO:HB2	1.93	0.51
1:A:833:ALA:C	1:A:835:THR:N	2.66	0.51
1:D:135:TRP:HE1	1:D:230:MET:CG	2.24	0.51
1:F:525:SER:H	1:F:801:MET:HE3	1.76	0.51
1:H:200:PHE:HA	1:H:246:GLY:HA3	1.93	0.51
1:I:676:ARG:HB3	1:I:921:GLU:HB3	1.93	0.51
1:J:205:GLN:HG3	1:J:206:ILE:HG13	1.93	0.51
4:R:110:LEU:O	4:R:110:LEU:HD22	2.11	0.51
1:A:476:ASN:C	1:A:537:HIS:NE2	2.68	0.50
1:B:225:LYS:HG3	1:B:288:SER:HB3	1.93	0.50
1:B:636:ASN:ND2	3:M:16:SER:HB2	2.26	0.50
1:E:179:ILE:O	1:E:179:ILE:HG22	2.12	0.50
1:E:245:GLY:H	1:F:821:HIS:HB3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:552:ASN:H	1:H:804:GLN:HB2	1.75	0.50
1:K:386:MET:SD	1:L:756:VAL:O	2.69	0.50
4:S:41:PRO:HG2	4:S:44:SER:HB2	1.93	0.50
1:D:522:ALA:HB2	1:F:552:ASN:HB2	1.93	0.50
1:E:121:TYR:HD2	1:F:844:ALA:HB3	1.75	0.50
1:F:683:LEU:HD13	1:F:707:TYR:HB2	1.92	0.50
1:G:849:PRO:C	1:G:851:ILE:H	2.20	0.50
1:K:798:PHE:HB3	1:K:866:CYS:HA	1.93	0.50
3:M:214:VAL:O	3:M:251:ASP:O	2.29	0.50
1:C:652:MET:HE3	1:C:667:ILE:HD12	1.94	0.50
1:G:706:PRO:HA	1:G:711:THR:HG23	1.93	0.50
1:H:723:ILE:HA	1:H:903:MET:HG3	1.93	0.50
1:H:748:SER:OG	4:R:47:LEU:HD23	2.10	0.50
1:K:493:LYS:C	1:K:494:ILE:CG1	2.81	0.50
1:A:19:ASP:OD1	6:W:8:HIS:O	2.28	0.50
1:A:179:ILE:HG22	1:A:184:ILE:HA	1.93	0.50
1:A:225:LYS:HD2	1:A:290:ASP:HB2	1.93	0.50
1:A:683:LEU:O	1:A:914:THR:HA	2.12	0.50
1:B:28:LEU:HD12	1:C:633:MET:HB3	1.94	0.50
1:F:600:ASP:HA	1:F:702:SER:HB2	1.94	0.50
1:H:455:GLY:C	1:I:173:PRO:HB3	2.36	0.50
1:I:219:ALA:HB3	1:I:284:VAL:HG22	1.94	0.50
1:I:680:PHE:HB3	1:I:918:VAL:HG22	1.94	0.50
1:K:549:LEU:HD21	1:L:758:GLN:HE22	1.77	0.50
1:K:824:ASN:HB3	1:K:844:ALA:HB2	1.92	0.50
2:N:149:VAL:O	2:N:200:GLY:HA3	2.10	0.50
3:M:134:GLN:C	3:M:136:ASN:H	2.19	0.50
1:C:14:HIS:CD2	1:C:14:HIS:O	2.64	0.50
1:E:334:ILE:HG21	1:E:708:LEU:HG	1.94	0.50
1:F:301:SER:HB3	1:F:320:MET:HB2	1.94	0.50
1:F:566:PHE:HB2	1:F:569:ILE:HG22	1.93	0.50
1:G:798:PHE:HE1	1:G:864:PHE:HB2	1.75	0.50
1:G:824:ASN:HA	1:G:844:ALA:CB	2.35	0.50
1:G:926:VAL:HA	1:G:939:VAL:O	2.12	0.50
1:H:648:SER:HB2	1:H:924:ASP:HB3	1.94	0.50
1:A:582:GLU:O	1:A:583:TRP:CG	2.65	0.50
1:B:240:PRO:HD3	1:C:845:ASN:HB2	1.93	0.50
1:B:470:ARG:O	1:B:474:TYR:HB3	2.11	0.50
1:C:479:LEU:HD21	1:C:508:VAL:HG12	1.94	0.50
1:D:53:THR:O	1:D:56:VAL:CG1	2.45	0.50
1:F:431:PRO:HA	1:F:439:TRP:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:650:ALA:HB2	1:G:922:VAL:HG21	1.93	0.50
1:J:96:MET:HB2	1:J:572:LEU:H	1.75	0.50
1:J:265:GLN:HE22	1:L:431:PRO:HD2	1.76	0.50
1:K:755:ASN:ND2	1:K:760:ASN:CA	2.75	0.50
2:N:149:VAL:HG22	2:N:191:HIS:HE1	1.75	0.50
1:A:24:LEU:HD21	1:A:45:PHE:CZ	2.47	0.50
1:A:784:PRO:HB3	1:A:788:LYS:HD2	1.92	0.50
1:B:188:VAL:O	1:B:188:VAL:CG2	2.59	0.50
1:B:795:PHE:O	1:B:796:ARG:C	2.55	0.50
1:B:798:PHE:CB	1:B:866:CYS:HA	2.40	0.50
1:C:310:ASN:HA	1:C:314:LEU:HD12	1.93	0.50
1:D:25:SER:H	1:E:639:ASN:HD21	1.60	0.50
1:E:201:GLN:HB3	1:E:202:PRO:HD2	1.93	0.50
1:H:134:GLU:HB3	1:H:167:HIS:CD2	2.47	0.50
1:H:492:VAL:HG13	1:H:506:LYS:HZ3	1.77	0.50
1:I:96:MET:HG3	1:I:569:ILE:HG13	1.92	0.50
1:I:475:SER:HA	1:I:479:LEU:HD13	1.93	0.50
1:I:661:THR:HB	1:I:909:PRO:CA	2.40	0.50
1:J:561:GLN:N	1:K:757:ALA:HB2	2.26	0.50
1:C:797:ASN:CB	1:C:867:ASP:O	2.60	0.50
1:G:757:ALA:HB1	1:I:385:SER:HB3	1.94	0.50
1:G:804:GLN:CG	1:G:850:LEU:HD23	2.37	0.50
1:J:675:PHE:HB3	1:J:875:PHE:HB2	1.94	0.50
1:L:499:ASN:HB3	1:L:599:ASN:HA	1.93	0.50
1:L:600:ASP:HA	1:L:702:SER:OG	2.11	0.50
3:M:196:LEU:CB	3:M:199:VAL:CG2	2.89	0.50
4:S:108:ASP:O	4:S:111:THR:CA	2.60	0.50
1:A:386:MET:HB3	1:B:757:ALA:HB1	1.93	0.50
1:A:737:LEU:HD22	1:A:764:ASP:HA	1.94	0.50
1:A:804:GLN:HB2	1:C:552:ASN:HB3	1.94	0.50
1:D:227:THR:OG1	1:D:290:ASP:OD1	2.28	0.50
1:E:837:ARG:HH21	1:F:413:TYR:HB3	1.76	0.50
1:G:113:PHE:HB2	1:G:327:ILE:HD12	1.94	0.50
1:H:609:LYS:HG2	4:S:58:GLU:HB3	1.92	0.50
1:K:648:SER:HB2	1:K:924:ASP:HB3	1.94	0.50
4:P:39:VAL:O	4:P:40:LEU:O	2.30	0.50
5:V:208:TYR:HB2	5:V:209:PRO:HD2	1.93	0.50
1:A:330:ARG:HH22	1:A:705:ILE:H	1.59	0.49
1:A:691:LEU:O	1:A:691:LEU:HD23	2.12	0.49
1:B:941:LEU:CD1	1:B:943:THR:OG1	2.60	0.49
1:B:943:THR:HB	1:B:944:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:926:VAL:O	1:G:926:VAL:HG13	2.12	0.49
1:K:824:ASN:HB3	1:K:844:ALA:HB1	1.94	0.49
2:N:250:PHE:CE1	2:N:261:ILE:HD12	2.46	0.49
1:A:28:LEU:HD11	1:B:630:LEU:HG	1.94	0.49
1:A:98:SER:HB3	1:B:780:GLY:HA2	1.94	0.49
1:B:339:TYR:HB3	1:B:366:THR:HB	1.93	0.49
1:G:26:PRO:HB2	1:G:30:GLN:HE21	1.77	0.49
1:G:384:PHE:H	1:G:389:GLN:HB3	1.78	0.49
1:H:778:TYR:CZ	1:H:878:ASN:ND2	2.80	0.49
1:I:655:PRO:O	1:I:656:ILE:HG13	2.11	0.49
1:K:65:THR:HA	1:K:618:THR:HG22	1.94	0.49
1:K:127:LYS:HG3	1:L:411:PRO:HB3	1.94	0.49
2:N:52:ARG:HG3	2:N:64:PHE:HA	1.93	0.49
2:N:217:LEU:HB3	2:N:232:THR:HG21	1.93	0.49
1:A:119:THR:HG23	1:A:297:ASP:HB2	1.95	0.49
1:A:321:PRO:HG2	1:B:409:GLU:HG3	1.93	0.49
1:B:704:SER:HB2	1:B:711:THR:HG21	1.93	0.49
1:C:108:ASP:HB2	1:C:607:SER:H	1.77	0.49
1:C:765:TRP:C	1:C:767:LEU:H	2.20	0.49
1:E:204:PRO:HG3	1:F:842:TYR:HB2	1.94	0.49
1:E:672:TRP:HA	1:E:944:PRO:HB3	1.94	0.49
1:H:663:VAL:HB	1:H:905:PHE:HB3	1.93	0.49
1:I:747:ARG:HB2	1:I:755:ASN:HD21	1.77	0.49
1:L:324:PRO:HG3	1:L:538:HIS:ND1	2.28	0.49
2:N:286:LEU:O	2:N:382:LEU:HD22	2.12	0.49
5:U:90:VAL:HG13	5:U:168:ILE:HG12	1.94	0.49
1:A:100:TYR:CE1	1:A:616:TYR:HB2	2.47	0.49
1:A:649:ALA:HB1	1:A:919:LEU:HB3	1.93	0.49
1:A:885:LEU:CB	1:C:51:ALA:HB3	2.41	0.49
1:E:83:ARG:HD2	1:E:582:GLU:HB3	1.94	0.49
1:E:323:ARG:HD2	1:E:479:LEU:HD21	1.93	0.49
1:E:684:LYS:HB3	1:E:687:GLU:HB2	1.95	0.49
1:F:10:TRP:HB3	1:F:16:SER:HB2	1.94	0.49
1:G:804:GLN:NE2	1:G:858:SER:O	2.38	0.49
1:H:361:LEU:HD11	1:J:729:VAL:HG23	1.94	0.49
1:H:535:PHE:HZ	1:H:868:ARG:HG3	1.77	0.49
1:K:425:THR:HG23	1:K:448:ASP:HB3	1.94	0.49
1:K:755:ASN:HD21	1:K:760:ASN:C	2.21	0.49
3:M:74:LEU:HA	3:M:77:VAL:HG12	1.94	0.49
1:A:27:GLY:HA3	3:M:15:GLN:HA	1.94	0.49
1:A:646:TYR:CE1	6:W:22:THR:O	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:756:VAL:HG12	1:C:757:ALA:N	2.27	0.49
1:D:384:PHE:HB2	1:D:389:GLN:HB2	1.94	0.49
1:D:459:ALA:HB3	1:F:836:MET:HE2	1.94	0.49
1:E:455:GLY:H	1:F:173:PRO:HA	1.78	0.49
1:G:633:MET:HG3	1:I:28:LEU:HD13	1.94	0.49
1:I:662:ASN:OD1	1:I:906:GLU:CA	2.55	0.49
1:J:365:ASN:H	1:J:651:ASN:HD21	1.60	0.49
1:J:804:GLN:HB3	1:L:552:ASN:HB3	1.93	0.49
1:L:685:THR:OG1	1:L:913:PRO:HB2	2.13	0.49
2:N:227:MET:HA	2:N:287:LEU:HD11	1.94	0.49
1:A:171:GLN:HA	1:C:452:ILE:HG23	1.93	0.49
1:A:722:ALA:HB2	1:A:742:GLU:HG2	1.95	0.49
1:D:941:LEU:HD13	1:D:949:ASN:HD22	1.78	0.49
1:E:342:THR:HG23	1:E:360:ASP:H	1.78	0.49
1:L:238:ALA:HB1	1:L:291:VAL:HG11	1.94	0.49
1:A:523:ARG:H	1:C:548:MET:HB2	1.78	0.49
1:C:383:TYR:CD2	1:C:390:ALA:HA	2.48	0.49
1:D:325:ASN:HB3	1:D:597:LEU:HD13	1.93	0.49
1:E:678:TRP:HB2	1:E:873:ILE:HD12	1.95	0.49
1:E:683:LEU:HD12	1:E:706:PRO:HB2	1.95	0.49
1:F:96:MET:HG2	1:F:569:ILE:HG12	1.95	0.49
1:G:823:HIS:HA	1:G:826:SER:HB3	1.95	0.49
1:J:655:PRO:CG	1:J:915:LEU:HD23	2.38	0.49
2:N:194:LYS:HG3	2:N:195:VAL:HG23	1.95	0.49
1:B:549:LEU:HD22	1:C:801:MET:HA	1.95	0.49
1:F:76:THR:HG23	1:F:79:SER:O	2.12	0.49
1:G:25:SER:H	1:H:639:ASN:HD21	1.60	0.49
1:H:611:ASP:CG	4:S:57:LEU:HD22	2.38	0.49
1:J:654:TYR:O	1:J:654:TYR:HD1	1.96	0.49
1:K:674:ALA:HB1	1:K:923:PHE:CD1	2.48	0.49
1:K:738:LEU:HD11	1:K:763:LYS:HG3	1.94	0.49
1:L:709:ASP:HB2	1:L:711:THR:HG22	1.95	0.49
2:N:176:SER:HB2	2:N:179:MET:HB2	1.95	0.49
3:M:203:GLN:HE21	3:M:206:LYS:HD2	1.78	0.49
1:B:868:ARG:O	1:B:868:ARG:HG2	2.12	0.49
1:D:650:ALA:HB3	1:D:920:PHE:HB2	1.95	0.49
1:E:41:LEU:HD22	1:E:44:LYS:HB2	1.93	0.49
1:E:474:TYR:HA	1:E:478:ALA:HB3	1.94	0.49
1:E:579:TYR:CE2	1:E:936:ILE:HG12	2.48	0.49
1:E:724:THR:HG22	1:E:728:SER:O	2.11	0.49
1:G:211:TRP:CE3	1:G:417:LEU:HD22	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:198:LYS:HB3	1:H:262:VAL:HB	1.94	0.49
1:H:202:PRO:HD2	1:H:222:ARG:HE	1.76	0.49
1:J:57:THR:HG21	1:K:878:ASN:HB3	1.95	0.49
1:J:571:ASN:O	1:L:44:LYS:HD3	2.12	0.49
1:A:316:GLY:HA2	1:C:211:TRP:CD1	2.48	0.49
1:B:182:GLU:OE1	1:B:182:GLU:HA	2.13	0.49
1:F:592:VAL:HG13	1:F:593:LEU:HG	1.94	0.49
1:I:130:PRO:HA	1:I:232:PRO:HA	1.93	0.49
1:I:665:ILE:HG23	1:I:903:MET:HB2	1.95	0.49
1:J:299:HIS:HB2	1:J:322:ASN:HD21	1.78	0.49
1:J:682:ARG:HH12	1:J:907:VAL:HB	1.78	0.49
1:L:179:ILE:HG23	1:L:218:HIS:HB3	1.94	0.49
1:A:114:LYS:HB3	1:A:324:PRO:HA	1.95	0.48
1:C:892:LEU:HD23	5:U:217:ASP:HB2	1.95	0.48
1:F:679:ALA:HB3	1:F:919:LEU:HD23	1.95	0.48
1:H:380:ARG:HD3	1:H:391:VAL:HG13	1.95	0.48
1:I:47:ASN:N	1:I:48:PRO:HD3	2.28	0.48
1:J:385:SER:HB3	1:K:758:GLN:HB3	1.95	0.48
1:K:876:SER:HA	1:K:888:LEU:H	1.78	0.48
1:A:204:PRO:HD2	1:B:823:HIS:NE2	2.28	0.48
1:A:280:LEU:HB2	1:C:439:TRP:HB2	1.94	0.48
1:H:235:GLY:O	1:H:298:THR:HG21	2.13	0.48
1:L:545:TYR:O	1:L:549:LEU:HB3	2.13	0.48
1:A:204:PRO:O	1:B:839:GLY:HA3	2.12	0.48
1:B:532:VAL:O	1:B:532:VAL:HG23	2.10	0.48
1:C:41:LEU:HB3	1:C:44:LYS:HG3	1.94	0.48
1:F:110:GLY:CA	1:F:606:ALA:HB2	2.42	0.48
1:G:804:GLN:HG3	1:G:850:LEU:HD22	1.91	0.48
1:H:430:LYS:HB2	1:H:442:ASP:HA	1.96	0.48
1:K:748:SER:N	1:K:760:ASN:HD21	2.11	0.48
1:A:400:ILE:HG12	1:A:801:MET:HE1	1.95	0.48
1:A:476:ASN:O	1:A:537:HIS:CD2	2.66	0.48
1:B:726:ASP:HB3	1:B:900:ALA:N	2.20	0.48
1:F:589:VAL:HA	1:F:592:VAL:HG12	1.96	0.48
1:H:779:GLN:HE21	1:I:39:PHE:HA	1.78	0.48
1:I:133:CYS:HB2	1:I:230:MET:HG3	1.94	0.48
1:J:338:TYR:HB3	1:J:341:SER:HB3	1.95	0.48
1:K:132:PRO:HB3	1:K:170:GLY:HA2	1.95	0.48
1:K:332:ASN:OD1	1:K:387:TRP:O	2.31	0.48
1:K:896:ASN:HB2	5:U:194:PRO:HG2	1.95	0.48
2:N:231:TYR:CE2	2:N:284:PRO:O	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:452:ARG:HG2	2:N:453:SER:N	2.27	0.48
1:B:326:TYR:HE1	1:B:543:LEU:HB3	1.78	0.48
1:F:349:ALA:HA	1:F:936:ILE:HD12	1.95	0.48
1:G:632:ALA:HA	1:G:635:ARG:HB2	1.96	0.48
1:J:226:LYS:HB3	1:J:310:ASN:HD21	1.78	0.48
1:K:797:ASN:HD22	1:K:869:THR:HB	1.77	0.48
1:L:24:LEU:O	1:L:26:PRO:HD3	2.14	0.48
2:N:52:ARG:HB2	2:N:64:PHE:HD2	1.77	0.48
4:S:28:ASN:O	4:S:28:ASN:ND2	2.46	0.48
1:A:338:TYR:CZ	1:A:586:ARG:HG2	2.49	0.48
1:B:336:LEU:HD22	1:B:563:PRO:HD2	1.95	0.48
1:D:268:SER:C	1:F:426:LEU:HD23	2.38	0.48
1:G:353:SER:HB3	1:G:355:LEU:HB2	1.95	0.48
1:G:412:ASN:ND2	1:I:462:ILE:HD11	2.28	0.48
1:G:837:ARG:HH11	1:H:459:ALA:HB2	1.77	0.48
1:I:833:ALA:O	1:I:835:THR:N	2.47	0.48
1:J:535:PHE:CE1	1:J:711:THR:HG21	2.48	0.48
1:J:570:LYS:HG3	1:J:571:ASN:HD22	1.79	0.48
1:J:922:VAL:HG11	1:J:944:PRO:CB	2.44	0.48
4:S:28:ASN:O	4:S:28:ASN:CG	2.57	0.48
1:A:416:PRO:HG3	1:A:458:PHE:HB2	1.96	0.48
1:A:843:PRO:HB2	1:C:238:ALA:HB2	1.96	0.48
1:B:64:LEU:HD13	1:B:621:PRO:HD3	1.96	0.48
1:F:824:ASN:HD21	1:F:847:PRO:HD3	1.79	0.48
1:G:414:CYS:HB2	1:G:460:MET:HB2	1.95	0.48
1:I:663:VAL:HA	1:I:664:PRO:HD3	1.61	0.48
1:J:483:ASP:HA	1:J:486:LYS:HD3	1.95	0.48
1:K:201:GLN:CB	1:K:202:PRO:CD	2.85	0.48
1:K:495:SER:O	1:K:503:TYR:HD1	1.97	0.48
2:N:467:LEU:HB2	2:N:524:THR:HG21	1.96	0.48
1:A:63:ARG:HA	1:B:736:ARG:HA	1.95	0.48
1:A:113:PHE:HB2	1:A:327:ILE:HD12	1.95	0.48
1:A:365:ASN:HB3	1:A:368:LEU:HB3	1.95	0.48
1:B:922:VAL:HG12	1:B:923:PHE:N	2.28	0.48
1:C:477:ILE:HG12	1:C:529:MET:HE1	1.95	0.48
1:D:23:TYR:O	1:D:23:TYR:CG	2.65	0.48
1:E:798:PHE:CB	1:E:865:LEU:O	2.61	0.48
1:H:863:LYS:NZ	4:R:48:THR:HG22	2.29	0.48
1:I:757:ALA:CB	1:I:766:PHE:HZ	2.26	0.48
1:L:478:ALA:HB2	1:L:514:VAL:HG21	1.95	0.48
4:Q:55:THR:O	4:Q:55:THR:OG1	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:183:ILE:HG23	5:V:187:GLN:HE21	1.79	0.48
1:A:58:THR:C	1:A:60:ARG:N	2.72	0.48
1:H:234:TYR:HE2	1:H:321:PRO:HD3	1.79	0.48
1:I:652:MET:HE2	1:I:654:TYR:HH	1.74	0.48
1:I:825:ASN:O	1:I:825:ASN:OD1	2.32	0.48
1:L:757:ALA:CB	1:L:766:PHE:CZ	2.83	0.48
1:A:370:TYR:HA	1:A:373:LEU:HD12	1.96	0.48
1:A:754:TYR:HE1	1:E:76:THR:HG21	1.79	0.48
1:B:22:GLU:HA	5:U:176:SER:HB2	1.94	0.48
1:B:548:MET:HB3	1:C:523:ARG:H	1.79	0.48
1:C:949:ASN:HA	1:K:904:THR:HB	1.95	0.48
1:D:212:TYR:CE1	1:E:315:MET:HB3	2.49	0.48
1:G:379:ASP:HB3	1:G:381:THR:HG22	1.95	0.48
1:G:641:GLN:O	1:G:927:ARG:HA	2.14	0.48
1:G:851:ILE:HD11	1:I:115:PRO:HD2	1.95	0.48
1:I:648:SER:HB3	1:I:923:PHE:HA	1.95	0.48
1:I:654:TYR:O	1:I:915:LEU:HA	2.14	0.48
1:J:682:ARG:HH22	1:J:907:VAL:HG21	1.78	0.48
4:R:19:MET:HA	4:R:20:PRO:HD2	1.70	0.48
1:D:135:TRP:HZ2	1:D:230:MET:SD	2.33	0.47
1:E:572:LEU:HD21	1:E:928:VAL:HG21	1.95	0.47
1:G:550:LEU:HD13	1:H:758:GLN:HE21	1.78	0.47
1:I:386:MET:HG3	1:I:387:TRP:H	1.79	0.47
1:K:386:MET:O	1:K:386:MET:HG2	2.13	0.47
1:K:494:ILE:HG22	1:K:495:SER:N	2.27	0.47
1:K:583:TRP:HE3	1:K:584:ASN:H	1.62	0.47
1:L:225:LYS:HG3	1:L:288:SER:HB2	1.95	0.47
2:N:283:ILE:HG22	2:N:401:THR:HB	1.96	0.47
1:A:429:VAL:HG22	1:A:430:LYS:N	2.28	0.47
1:D:430:LYS:HB3	1:D:442:ASP:HA	1.96	0.47
1:D:917:TYR:CE2	1:D:919:LEU:HD11	2.49	0.47
1:E:249:ILE:HG21	1:E:261:GLN:HB2	1.96	0.47
1:E:553:GLY:HA3	1:F:850:LEU:HB3	1.95	0.47
1:E:797:ASN:HD22	1:E:869:THR:HB	1.78	0.47
1:G:88:VAL:HB	1:G:576:PRO:HA	1.96	0.47
1:G:299:HIS:HD2	1:G:322:ASN:HD21	1.61	0.47
1:G:848:TYR:C	1:G:850:LEU:H	2.21	0.47
1:I:469:TRP:CD1	1:I:516:CYS:HB3	2.49	0.47
2:N:88:HIS:HB2	2:N:554:VAL:HB	1.96	0.47
1:A:591:MET:HA	1:A:699:TYR:HE2	1.79	0.47
1:A:712:PHE:HB2	1:A:715:ASN:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:928:VAL:HA	1:D:938:THR:HG23	1.95	0.47
1:H:492:VAL:CG1	1:H:506:LYS:HD3	2.37	0.47
1:I:574:LEU:HD23	1:I:930:ARG:HH12	1.79	0.47
1:L:682:ARG:HH21	1:L:916:LEU:HD22	1.80	0.47
4:S:18:ARG:HG2	4:S:19:MET:N	2.26	0.47
1:A:216:ILE:HG21	1:C:454:VAL:HB	1.95	0.47
1:B:241:THR:HA	1:C:813:ASP:HB2	1.95	0.47
1:B:356:ASN:HB3	2:N:455:ARG:HH12	1.79	0.47
1:G:478:ALA:HB2	1:G:514:VAL:HG21	1.95	0.47
1:H:201:GLN:HB3	1:H:202:PRO:HD3	1.97	0.47
1:I:712:PHE:HB2	1:I:868:ARG:HA	1.96	0.47
1:K:842:TYR:CG	1:K:843:PRO:HD2	2.50	0.47
4:Q:14:TYR:HA	4:R:15:LEU:O	2.14	0.47
1:A:94:LEU:HD11	1:A:617:ALA:HB1	1.96	0.47
1:A:665:ILE:HG21	1:A:903:MET:SD	2.55	0.47
1:B:676:ARG:HB3	1:B:921:GLU:HB3	1.97	0.47
1:F:533:ASN:CB	1:F:713:TYR:HE2	2.15	0.47
1:I:471:ASN:HA	1:I:474:TYR:HB3	1.95	0.47
1:J:654:TYR:HB2	4:P:16:THR:HG22	1.97	0.47
1:K:202:PRO:HD2	1:K:222:ARG:HG3	1.95	0.47
1:C:328:ALA:HB2	1:C:547:SER:HB3	1.96	0.47
1:D:798:PHE:CD1	1:D:866:CYS:HB2	2.49	0.47
1:E:656:ILE:HD13	1:E:910:MET:HE2	1.97	0.47
1:F:682:ARG:HB3	1:F:714:LEU:HB3	1.97	0.47
1:H:519:ASN:OD1	1:H:805:VAL:HG13	2.14	0.47
1:I:91:ASN:HB3	1:I:624:HIS:HA	1.95	0.47
1:I:361:LEU:HB3	1:I:362:GLN:H	1.61	0.47
1:I:734:ASN:O	1:I:736:ARG:HG2	2.15	0.47
1:K:469:TRP:CD1	1:K:516:CYS:SG	3.08	0.47
1:K:504:MET:O	1:K:507:ARG:HG2	2.14	0.47
1:L:19:ASP:O	1:L:48:PRO:HD2	2.14	0.47
1:L:444:THR:O	1:L:445:GLU:C	2.56	0.47
1:A:201:GLN:CG	1:A:202:PRO:HD3	2.12	0.47
1:A:414:CYS:HB3	1:C:414:CYS:HB2	1.79	0.47
1:C:35:THR:CG2	6:W:5:ALA:HB2	2.41	0.47
1:D:268:SER:O	1:F:426:LEU:HD23	2.13	0.47
1:E:13:MET:O	1:E:14:HIS:CE1	2.58	0.47
1:F:247:GLN:HB2	1:F:291:VAL:HG21	1.97	0.47
1:G:747:ARG:HE	1:G:750:ASP:HB3	1.78	0.47
1:G:759:CYS:C	1:G:761:MET:N	2.71	0.47
1:G:823:HIS:CE1	1:I:204:PRO:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:925:VAL:H	1:G:941:LEU:HB2	1.80	0.47
1:H:127:LYS:HG3	1:I:411:PRO:HB3	1.96	0.47
1:H:517:TYR:CG	1:H:847:PRO:HG3	2.50	0.47
1:H:662:ASN:HB2	4:Q:11:VAL:HB	1.95	0.47
1:I:544:ARG:O	1:I:548:MET:HG2	2.14	0.47
1:I:653:LEU:CD2	1:I:653:LEU:N	2.71	0.47
1:I:831:TYR:HD2	1:I:838:GLU:OE2	1.97	0.47
1:J:330:ARG:HE	1:J:594:GLN:HG3	1.79	0.47
1:J:817:VAL:HG22	1:J:818:GLY:H	1.77	0.47
1:K:504:MET:O	1:K:507:ARG:CG	2.63	0.47
1:L:19:ASP:O	1:L:48:PRO:CG	2.62	0.47
1:L:112:THR:HG22	1:L:501:TYR:HB2	1.95	0.47
1:L:683:LEU:HD12	1:L:915:LEU:HD12	1.96	0.47
1:L:765:TRP:HE1	1:L:871:TRP:CD1	2.33	0.47
2:N:79:VAL:HG12	2:N:81:SER:H	1.79	0.47
2:N:90:ASN:HD21	2:N:457:ILE:HD12	1.80	0.47
2:N:185:ASN:HD21	2:N:499:PHE:HE1	1.63	0.47
4:P:28:ASN:CA	4:P:42:ALA:CB	2.77	0.47
4:P:135:SER:OG	4:P:136:PRO:HD3	2.14	0.47
1:A:46:ARG:HH21	1:B:923:PHE:HZ	1.63	0.47
1:C:179:ILE:HG23	1:C:183:GLY:O	2.15	0.47
1:D:323:ARG:HD2	1:D:479:LEU:HB3	1.96	0.47
1:F:180:THR:HG23	1:F:182:GLU:H	1.80	0.47
1:H:517:TYR:CD2	1:H:517:TYR:N	2.82	0.47
1:H:775:ASN:HB3	1:H:880:MET:SD	2.54	0.47
1:J:602:ARG:HB3	4:P:34:ILE:HA	1.96	0.47
1:B:420:VAL:HG11	1:B:453:ARG:HB2	1.96	0.47
1:D:223:VAL:HB	1:D:286:LEU:HD22	1.96	0.47
1:E:756:VAL:HG22	1:E:757:ALA:N	2.25	0.47
1:G:681:THR:HG21	1:G:712:PHE:HB3	1.97	0.47
1:G:735:ASP:HB3	1:I:63:ARG:HE	1.80	0.47
1:H:388:ASN:HB3	1:H:546:ARG:HG2	1.97	0.47
1:J:758:GLN:HE21	1:J:862:LYS:HE3	1.79	0.47
1:K:824:ASN:HA	1:K:844:ALA:HA	1.96	0.47
2:N:250:PHE:CZ	2:N:261:ILE:HD12	2.50	0.47
1:A:676:ARG:HB2	1:A:921:GLU:HB3	1.97	0.47
1:A:840:GLN:HA	1:B:457:ASN:HD21	1.79	0.47
1:D:30:GLN:O	1:D:31:PHE:C	2.56	0.47
1:F:931:PRO:HD2	1:F:932:HIS:CD2	2.50	0.47
1:G:135:TRP:CD1	1:G:310:ASN:HB2	2.46	0.47
1:G:486:LYS:HB3	1:G:507:ARG:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:266:PHE:HB2	1:J:282:PRO:HB3	1.97	0.47
1:J:824:ASN:HA	1:J:844:ALA:HB2	1.95	0.47
1:K:110:GLY:HA2	1:K:554:ARG:HE	1.78	0.47
1:K:755:ASN:CG	1:K:760:ASN:HA	2.40	0.47
1:K:824:ASN:CB	1:K:844:ALA:HB2	2.45	0.47
1:B:687:GLU:O	1:B:699:TYR:HE1	1.98	0.46
1:D:486:LYS:HB3	1:D:507:ARG:HG2	1.96	0.46
1:D:536:ASN:HA	1:D:596:SER:O	2.14	0.46
1:E:15:ILE:O	1:E:15:ILE:HG23	2.11	0.46
1:G:848:TYR:O	1:G:850:LEU:N	2.48	0.46
1:H:602:ARG:HH21	4:Q:34:ILE:HG13	1.80	0.46
1:I:429:VAL:HB	1:I:439:TRP:HD1	1.80	0.46
1:J:663:VAL:HG13	4:P:16:THR:HB	1.95	0.46
1:K:426:LEU:HD23	1:L:269:THR:HA	1.98	0.46
1:K:575:LEU:HG	1:K:930:ARG:HH11	1.80	0.46
1:L:595:SER:H	1:L:703:GLY:HA2	1.80	0.46
2:N:445:MET:HB3	2:N:529:LEU:HD12	1.97	0.46
3:M:86:ILE:HG21	3:M:94:VAL:HG21	1.96	0.46
5:V:183:ILE:CG2	5:V:184:GLY:N	2.78	0.46
1:D:620:PHE:HB3	1:D:622:MET:HG3	1.97	0.46
1:J:428:LYS:HD2	1:J:446:PHE:HD1	1.79	0.46
1:J:573:LEU:HD13	1:J:573:LEU:HA	1.72	0.46
4:P:10:ILE:CG1	4:Q:26:ARG:O	2.63	0.46
5:V:59:ALA:HA	5:V:193:VAL:HB	1.97	0.46
1:A:800:PRO:HG2	1:C:549:LEU:HD21	1.97	0.46
1:B:124:LEU:HG	1:C:828:PHE:CD2	2.51	0.46
1:C:215:GLU:C	1:C:216:ILE:HG13	2.40	0.46
1:C:822:GLN:HB3	1:C:824:ASN:OD1	2.15	0.46
1:D:269:THR:HG23	1:D:271:GLU:HG3	1.96	0.46
1:D:413:TYR:HB2	1:F:837:ARG:HD2	1.97	0.46
1:G:18:GLN:OE1	1:G:22:GLU:HB3	2.15	0.46
1:H:64:LEU:HD13	1:H:621:PRO:HD3	1.97	0.46
1:I:654:TYR:HH	1:I:665:ILE:CD1	2.24	0.46
1:J:393:SER:HB3	1:J:541:ALA:HB3	1.97	0.46
1:K:837:ARG:HH12	1:L:419:GLY:HA2	1.79	0.46
2:N:52:ARG:O	2:N:52:ARG:CG	2.46	0.46
1:A:350:GLY:H	1:A:353:SER:HB3	1.80	0.46
1:C:591:MET:HA	1:C:699:TYR:CE2	2.50	0.46
1:K:428:LYS:HG3	1:K:446:PHE:HB2	1.97	0.46
1:K:723:ILE:HA	1:K:903:MET:HB3	1.97	0.46
2:N:488:GLN:HE21	2:N:507:ARG:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:TYR:HB2	1:B:587:LYS:HE3	1.96	0.46
1:B:761:MET:HB2	1:B:766:PHE:HD1	1.80	0.46
1:B:941:LEU:CB	1:B:948:GLY:HA2	2.44	0.46
1:D:20:ALA:HA	1:D:47:ASN:HB3	1.98	0.46
1:D:722:ALA:HB3	1:D:904:THR:HB	1.98	0.46
1:G:927:ARG:CB	1:G:939:VAL:HG23	2.31	0.46
1:H:116:TYR:HE2	1:I:851:ILE:HD13	1.80	0.46
1:J:426:LEU:HB3	1:K:267:PHE:HB3	1.96	0.46
1:L:429:VAL:HB	1:L:439:TRP:HB2	1.96	0.46
5:U:9:TYR:HB3	5:U:23:ALA:HB1	1.97	0.46
1:D:130:PRO:HD2	1:F:418:GLY:HA2	1.98	0.46
1:D:204:PRO:HB3	1:E:840:GLN:HB2	1.97	0.46
1:D:757:ALA:HA	1:F:386:MET:HB3	1.95	0.46
1:G:13:MET:HB2	1:G:15:ILE:HG23	1.98	0.46
1:G:682:ARG:HH22	1:G:718:PHE:HA	1.80	0.46
1:I:654:TYR:HD1	1:I:916:LEU:O	1.98	0.46
1:A:646:TYR:CD1	6:W:22:THR:O	2.69	0.46
1:A:677:GLY:HA3	1:A:873:ILE:O	2.15	0.46
1:I:659:ASN:O	1:I:659:ASN:OD1	2.34	0.46
1:K:422:ASN:HB2	1:K:453:ARG:HB2	1.98	0.46
1:L:96:MET:HB2	1:L:572:LEU:H	1.80	0.46
1:L:353:SER:HB2	1:L:935:VAL:HG22	1.96	0.46
1:L:930:ARG:H	1:L:931:PRO:CD	2.28	0.46
3:M:96:ASP:HA	3:M:99:LEU:HB2	1.98	0.46
1:A:121:TYR:HB3	1:B:844:ALA:HB3	1.97	0.46
1:A:555:TYR:H	1:B:850:LEU:HD23	1.80	0.46
1:B:554:ARG:H	1:C:850:LEU:HG	1.81	0.46
1:C:179:ILE:CG2	1:C:180:THR:O	2.54	0.46
1:D:428:LYS:HG3	1:D:446:PHE:HB2	1.98	0.46
1:D:672:TRP:CZ2	1:D:901:LEU:HB2	2.51	0.46
1:E:179:ILE:HG13	1:E:184:ILE:HA	1.98	0.46
1:F:135:TRP:HA	1:F:135:TRP:CE3	2.51	0.46
1:F:657:PRO:HB2	1:F:660:ALA:HB3	1.97	0.46
1:G:333:PHE:CD2	1:G:562:VAL:HG22	2.51	0.46
1:G:592:VAL:HG13	1:G:593:LEU:HD13	1.96	0.46
1:I:180:THR:OG1	1:I:181:LYS:N	2.48	0.46
1:J:328:ALA:HB3	1:J:543:LEU:HD22	1.98	0.46
5:V:194:PRO:HB2	5:V:196:VAL:HG13	1.97	0.46
1:A:269:THR:OG1	1:A:283:LYS:HD2	2.15	0.46
1:B:796:ARG:O	1:B:797:ASN:C	2.59	0.46
1:E:535:PHE:CG	1:E:711:THR:HG23	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:833:ALA:HB1	1:H:834:PRO:HD2	1.97	0.46
1:J:592:VAL:HG13	1:J:593:LEU:HD12	1.98	0.46
1:K:249:ILE:HG22	1:K:260:SER:HA	1.96	0.46
1:K:266:PHE:HB3	1:K:282:PRO:HG2	1.98	0.46
1:L:679:ALA:HB3	1:L:919:LEU:HB3	1.98	0.46
3:M:196:LEU:HB3	3:M:199:VAL:CG2	2.45	0.46
1:B:726:ASP:HA	1:B:900:ALA:O	2.16	0.46
1:D:104:ARG:HA	1:E:752:GLU:HB2	1.98	0.46
1:D:923:PHE:HD2	1:D:942:ARG:HA	1.81	0.46
1:G:824:ASN:CA	1:G:844:ALA:HB2	2.39	0.46
1:I:832:LEU:HD23	1:I:832:LEU:O	2.16	0.46
1:K:683:LEU:HD11	1:K:688:THR:HG22	1.96	0.46
1:L:636:ASN:HB2	1:L:639:ASN:HB3	1.98	0.46
4:S:18:ARG:CG	4:S:19:MET:H	2.26	0.46
5:V:37:GLY:O	5:V:41:ILE:N	2.49	0.46
1:A:21:SER:O	1:A:29:VAL:HG22	2.16	0.45
1:A:56:VAL:HG13	6:W:4:LEU:O	2.15	0.45
1:A:561:GLN:HE22	1:B:756:VAL:HB	1.80	0.45
1:B:332:ASN:H	1:B:388:ASN:HB2	1.80	0.45
1:D:197:ASP:C	1:D:199:THR:H	2.24	0.45
1:E:732:PRO:HG3	1:E:743:PHE:CE1	2.51	0.45
1:F:513:LEU:HD21	1:F:819:ILE:HG12	1.97	0.45
1:G:114:LYS:HB2	1:G:325:ASN:H	1.80	0.45
1:G:461:GLU:HB2	1:I:126:PRO:HB3	1.98	0.45
1:I:589:VAL:HG22	1:I:602:ARG:CD	2.42	0.45
1:K:267:PHE:O	1:K:282:PRO:HB3	2.16	0.45
1:L:797:ASN:CG	1:L:867:ASP:O	2.59	0.45
2:N:448:PRO:HB3	2:N:529:LEU:CD1	2.45	0.45
3:M:230:PRO:HA	3:M:233:ARG:HB3	1.98	0.45
1:A:205:GLN:HG3	1:A:206:ILE:HG13	1.98	0.45
1:B:711:THR:HG22	1:B:713:TYR:HD2	1.81	0.45
1:C:178:ASN:O	1:C:185:GLN:HB2	2.17	0.45
1:D:19:ASP:HB2	1:D:22:GLU:HB2	1.98	0.45
1:D:922:VAL:HB	1:D:944:PRO:HG2	1.97	0.45
1:F:577:GLY:HA3	1:F:934:GLY:HA2	1.97	0.45
1:H:403:ASN:HA	1:H:469:TRP:HZ2	1.81	0.45
1:K:90:ASP:HA	1:K:576:PRO:HB3	1.98	0.45
1:L:924:ASP:HB3	1:L:942:ARG:HG2	1.98	0.45
1:B:14:HIS:O	1:B:48:PRO:HG3	2.16	0.45
1:C:249:ILE:HD12	1:C:261:GLN:H	1.82	0.45
1:D:311:SER:H	1:D:314:LEU:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:673:ALA:HB3	1:E:943:THR:HG22	1.99	0.45
1:E:689:PRO:HB3	1:E:698:TYR:HB2	1.98	0.45
1:F:135:TRP:HE1	1:F:315:MET:HE2	1.82	0.45
1:G:650:ALA:N	1:G:922:VAL:HG22	2.31	0.45
1:G:746:LYS:HG3	1:G:760:ASN:OD1	2.15	0.45
1:H:349:ALA:HA	1:H:355:LEU:HB2	1.98	0.45
1:H:437:ASN:OD1	1:I:179:ILE:HD11	2.16	0.45
1:H:644:ASN:HB3	1:H:925:VAL:HA	1.98	0.45
1:I:572:LEU:HD22	1:I:641:GLN:HB3	1.98	0.45
1:J:136:ASP:HA	1:J:166:THR:HA	1.98	0.45
1:J:654:TYR:O	1:J:654:TYR:CD1	2.69	0.45
1:L:10:TRP:HB2	1:L:16:SER:CB	2.46	0.45
1:A:653:LEU:HD22	1:A:915:LEU:HD13	1.99	0.45
1:A:677:GLY:HA2	1:A:875:PHE:HD1	1.81	0.45
1:C:722:ALA:HB3	1:C:904:THR:HB	1.99	0.45
1:D:67:ARG:HH21	1:E:763:LYS:HB2	1.82	0.45
1:E:428:LYS:HG3	1:E:446:PHE:HB2	1.98	0.45
1:E:828:PHE:CZ	1:E:841:ALA:HA	2.52	0.45
1:I:179:ILE:HG23	1:I:218:HIS:HB3	1.98	0.45
1:I:732:PRO:HD3	1:I:743:PHE:CZ	2.51	0.45
1:K:716:HIS:HB3	1:K:866:CYS:H	1.82	0.45
1:L:32:ALA:O	1:L:36:GLU:CB	2.36	0.45
1:L:722:ALA:HB3	1:L:904:THR:HB	1.99	0.45
3:M:154:VAL:N	3:M:155:PRO:HD3	2.31	0.45
4:S:48:THR:O	4:S:49:TYR:CD2	2.70	0.45
1:A:109:ARG:HB2	1:A:554:ARG:HA	1.98	0.45
1:A:581:TYR:CZ	1:A:583:TRP:NE1	2.84	0.45
1:A:691:LEU:O	1:A:691:LEU:CD2	2.65	0.45
1:B:103:ILE:HG13	1:B:562:VAL:HG21	1.99	0.45
1:D:70:PRO:HA	1:D:84:PHE:HB3	1.99	0.45
1:D:77:ALA:O	1:D:78:TYR:CG	2.69	0.45
1:D:878:ASN:C	1:D:880:MET:H	2.25	0.45
1:E:174:TYR:HB2	1:E:220:ALA:H	1.82	0.45
1:F:714:LEU:HD23	1:F:714:LEU:HA	1.71	0.45
1:G:172:ALA:HA	1:G:221:GLY:HA2	1.99	0.45
1:G:678:TRP:CD1	1:G:920:PHE:HA	2.51	0.45
1:G:719:LYS:HG2	1:G:720:LYS:HD3	1.98	0.45
1:I:10:TRP:HB3	1:I:15:ILE:HB	1.98	0.45
1:I:93:VAL:HB	1:I:573:LEU:HD22	1.98	0.45
1:I:732:PRO:C	1:I:734:ASN:H	2.25	0.45
1:J:656:ILE:HD11	1:J:910:MET:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:122:ASN:HA	1:L:825:ASN:HB3	1.98	0.45
4:R:2:SER:HA	4:R:3:THR:HA	1.66	0.45
1:A:56:VAL:HG11	6:W:4:LEU:O	2.17	0.45
1:A:167:HIS:HE1	1:A:223:VAL:HG21	1.82	0.45
1:C:804:GLN:HE21	1:C:858:SER:HB2	1.81	0.45
1:E:201:GLN:HB3	1:E:202:PRO:CD	2.46	0.45
1:F:732:PRO:C	1:F:734:ASN:H	2.25	0.45
1:G:804:GLN:HE22	1:G:858:SER:C	2.25	0.45
1:H:74:GLU:HG2	1:L:69:ILE:HD12	1.99	0.45
1:H:670:ARG:HB2	1:H:672:TRP:CD1	2.47	0.45
1:I:720:LYS:N	1:I:906:GLU:HB2	2.25	0.45
1:L:71:VAL:HG13	1:L:72:ASP:H	1.82	0.45
1:L:184:ILE:H	1:L:184:ILE:HG13	1.59	0.45
1:L:804:GLN:HG2	1:L:860:THR:HA	1.99	0.45
2:N:450:THR:O	2:N:451:PHE:CG	2.69	0.45
1:A:323:ARG:NH2	1:A:474:TYR:O	2.43	0.45
1:C:323:ARG:HG2	1:C:479:LEU:HD13	1.98	0.45
1:E:420:VAL:HG12	1:E:453:ARG:HB3	1.99	0.45
1:F:517:TYR:HB2	1:F:847:PRO:HG3	1.98	0.45
1:F:533:ASN:HB2	1:F:713:TYR:CZ	2.52	0.45
1:G:631:GLU:HB2	1:G:635:ARG:CZ	2.46	0.45
1:I:732:PRO:HD3	1:I:743:PHE:HZ	1.82	0.45
1:J:566:PHE:HB3	1:J:569:ILE:HG22	1.98	0.45
1:K:83:ARG:HA	1:K:582:GLU:HG3	1.99	0.45
1:K:674:ALA:HB1	1:K:923:PHE:HD1	1.81	0.45
2:N:271:PHE:HE2	2:N:273:ILE:HG12	1.81	0.45
2:N:283:ILE:CG2	2:N:403:TYR:HB2	2.47	0.45
3:M:208:LEU:HD21	3:M:236:LEU:HD11	1.98	0.45
1:D:731:TRP:HB3	1:D:732:PRO:CD	2.45	0.45
1:E:437:ASN:O	1:E:437:ASN:CG	2.46	0.45
1:E:626:THR:HG22	1:E:630:LEU:HB2	1.99	0.45
1:E:706:PRO:HA	1:E:711:THR:HB	1.99	0.45
1:F:721:VAL:HG23	1:F:745:ILE:HD11	1.99	0.45
1:G:18:GLN:CG	1:G:22:GLU:HB3	2.47	0.45
1:G:561:GLN:HE22	1:H:757:ALA:H	1.65	0.45
1:G:896:ASN:HD22	1:G:896:ASN:N	2.15	0.45
1:H:69:ILE:HA	1:H:70:PRO:HD3	1.84	0.45
1:H:561:GLN:HB2	1:I:756:VAL:HG22	1.98	0.45
1:J:25:SER:HA	1:J:26:PRO:HD3	1.84	0.45
1:K:550:LEU:HG	1:K:556:VAL:HG11	1.99	0.45
1:L:594:GLN:HA	1:L:702:SER:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:171:PRO:HG2	2:N:183:LEU:HD13	1.98	0.45
3:M:197:GLN:HG2	5:U:66:ARG:NH1	2.32	0.45
1:C:524:TRP:CG	1:C:803:ARG:HB3	2.52	0.45
1:D:33:ARG:O	1:D:36:GLU:HG3	2.15	0.45
1:D:481:LEU:HD12	1:D:509:VAL:HG11	1.98	0.45
1:D:590:ASN:HB3	1:D:699:TYR:CD2	2.52	0.45
1:F:426:LEU:HB2	1:F:450:ASN:HD21	1.82	0.45
1:G:679:ALA:HB3	1:G:919:LEU:HB2	1.98	0.45
1:I:719:LYS:HA	1:I:746:LYS:HB2	1.98	0.45
1:J:374:LEU:HA	1:J:377:ILE:HG22	1.98	0.45
1:J:696:ASP:C	1:J:698:TYR:H	2.24	0.45
1:J:772:ALA:HA	1:J:879:PHE:O	2.17	0.45
1:K:63:ARG:HA	1:L:735:ASP:O	2.16	0.45
1:L:628:SER:HB3	5:V:92:PRO:HG3	1.99	0.45
1:A:58:THR:O	1:A:59:ASP:C	2.57	0.45
1:A:716:HIS:HB3	1:A:866:CYS:H	1.82	0.45
1:B:104:ARG:HA	1:B:559:HIS:HD2	1.82	0.45
1:D:230:MET:HE2	1:D:314:LEU:HB3	0.74	0.45
1:D:403:ASN:HD21	1:D:516:CYS:HA	1.81	0.45
1:G:267:PHE:HA	1:I:428:LYS:HA	1.99	0.45
1:G:682:ARG:NH2	1:G:718:PHE:HA	2.32	0.45
1:H:104:ARG:HG3	1:H:559:HIS:CD2	2.52	0.45
1:H:611:ASP:OD2	4:S:57:LEU:HD22	2.17	0.45
1:H:719:LYS:H	1:H:907:VAL:HA	1.81	0.45
1:I:394:TYR:OH	1:I:867:ASP:HB3	2.17	0.45
1:I:867:ASP:O	1:I:869:THR:N	2.50	0.45
1:J:723:ILE:HG12	1:J:903:MET:HE3	1.99	0.45
1:K:656:ILE:HD12	1:K:914:THR:O	2.16	0.45
1:K:718:PHE:HB3	1:K:745:ILE:HD13	1.99	0.45
1:L:241:THR:OG1	1:L:248:GLY:HA3	2.17	0.45
2:N:89:SER:HA	2:N:543:ILE:HD12	1.98	0.45
2:N:196:GLY:O	2:N:200:GLY:C	2.60	0.45
3:M:197:GLN:HA	5:U:197:TYR:CD1	2.52	0.45
1:A:500:THR:HA	1:A:599:ASN:HB2	2.00	0.44
1:B:171:GLN:HB3	1:C:840:GLN:HG3	1.98	0.44
1:D:533:ASN:HD21	1:D:706:PRO:HG3	1.82	0.44
1:G:711:THR:HA	1:G:868:ARG:HG3	1.99	0.44
1:H:49:THR:HB	1:I:883:GLY:HA2	1.99	0.44
1:H:95:ASP:H	1:H:619:PHE:HB3	1.82	0.44
1:I:422:ASN:HB3	1:I:453:ARG:HB2	1.99	0.44
1:K:401:ILE:HD12	1:K:525:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:44:VAL:O	5:V:48:ARG:HB3	2.16	0.44
1:B:333:PHE:HB3	1:B:563:PRO:HG3	1.98	0.44
1:D:84:PHE:CE1	1:D:581:TYR:HB3	2.52	0.44
1:D:330:ARG:HB2	1:D:334:ILE:HG22	1.98	0.44
1:F:668:PRO:HD2	1:H:726:ASP:O	2.17	0.44
1:G:537:HIS:HB3	1:G:540:ASN:HD21	1.82	0.44
1:J:115:PRO:HD3	1:K:851:ILE:HG21	1.99	0.44
1:J:264:MET:HE2	1:J:285:VAL:HG22	2.00	0.44
1:J:566:PHE:CE2	1:J:568:ALA:HB3	2.53	0.44
1:J:720:LYS:HE2	1:J:747:ARG:HD2	1.98	0.44
1:L:59:ASP:HB3	5:V:102:THR:HB	2.00	0.44
1:L:575:LEU:HD22	1:L:631:GLU:HB2	1.99	0.44
1:L:783:ILE:H	1:L:783:ILE:HG13	1.62	0.44
1:L:865:LEU:HD23	1:L:865:LEU:HA	1.71	0.44
1:E:524:TRP:HH2	1:E:863:LYS:HD3	1.82	0.44
1:F:655:PRO:HA	1:F:915:LEU:HA	1.99	0.44
1:F:867:ASP:O	1:F:868:ARG:HB2	2.17	0.44
1:G:771:LEU:O	1:G:880:MET:CA	2.66	0.44
1:H:867:ASP:O	1:H:868:ARG:CB	2.47	0.44
1:J:347:VAL:HG13	1:J:356:ASN:HB3	2.00	0.44
1:J:922:VAL:HG12	1:J:944:PRO:CG	2.39	0.44
1:K:486:LYS:HB3	1:K:507:ARG:HB2	1.98	0.44
1:K:649:ALA:HB1	1:K:920:PHE:O	2.17	0.44
2:N:271:PHE:CE2	2:N:273:ILE:HG12	2.52	0.44
2:N:285:ALA:CB	2:N:393:LEU:HD22	2.46	0.44
2:N:443:ASP:HB2	2:N:539:GLN:HG2	2.00	0.44
3:M:212:TRP:HD1	3:M:254:LEU:HD11	1.83	0.44
4:S:19:MET:CA	4:S:19:MET:CE	2.88	0.44
1:B:524:TRP:CD1	1:B:803:ARG:HB3	2.53	0.44
1:C:325:ASN:HB3	1:C:597:LEU:HB3	1.98	0.44
1:D:799:GLN:HA	1:D:800:PRO:HD3	1.83	0.44
1:E:266:PHE:HB3	1:E:282:PRO:HG3	1.99	0.44
1:G:325:ASN:HB3	1:G:597:LEU:HB2	1.99	0.44
1:G:513:LEU:HG	1:G:518:ILE:HD12	1.98	0.44
1:G:682:ARG:HD2	1:G:714:LEU:HB3	1.99	0.44
1:K:132:PRO:HB2	1:K:223:VAL:HA	2.00	0.44
1:K:426:LEU:HB2	1:K:450:ASN:HD21	1.82	0.44
1:K:823:HIS:HB3	1:K:844:ALA:C	2.42	0.44
1:L:676:ARG:HB3	1:L:921:GLU:HB3	2.00	0.44
1:L:723:ILE:HA	1:L:903:MET:HG2	1.99	0.44
1:A:216:ILE:HD12	1:A:283:LYS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:TYR:HA	6:W:22:THR:CB	2.48	0.44
1:B:647:LEU:C	1:B:649:ALA:H	2.26	0.44
1:C:824:ASN:HA	1:C:844:ALA:HB2	2.00	0.44
1:D:798:PHE:HD1	1:D:866:CYS:CB	2.29	0.44
1:F:430:LYS:HD2	1:F:442:ASP:HA	1.98	0.44
1:G:245:GLY:HA3	1:H:821:HIS:HB3	2.00	0.44
1:G:931:PRO:HD3	1:G:937:GLU:OE2	2.16	0.44
1:G:938:THR:OG1	1:G:939:VAL:N	2.49	0.44
1:H:487:TYR:HB2	1:H:508:VAL:O	2.16	0.44
1:H:552:ASN:HD22	1:I:851:ILE:HD11	1.82	0.44
1:H:571:ASN:O	1:H:643:PHE:HZ	2.00	0.44
1:J:690:SER:HA	4:P:26:ARG:HH21	1.81	0.44
1:K:253:GLN:H	1:K:253:GLN:HG3	1.63	0.44
1:K:876:SER:HB3	1:K:887:ASP:H	1.83	0.44
1:L:823:HIS:HB3	1:L:843:PRO:O	2.17	0.44
1:A:251:VAL:HG13	1:A:252:LYS:N	2.33	0.44
1:B:602:ARG:NH2	1:B:695:TYR:CE1	2.66	0.44
1:C:35:THR:HG22	1:C:38:TYR:HB3	1.99	0.44
1:G:676:ARG:HG3	1:G:921:GLU:HG2	2.00	0.44
1:H:70:PRO:HG2	1:H:82:ALA:HB1	1.98	0.44
1:J:720:LYS:CD	4:Q:22:TRP:CH2	2.99	0.44
1:K:755:ASN:OD1	1:K:862:LYS:HE2	2.17	0.44
2:N:83:ASN:HB3	2:N:91:PHE:HB2	2.00	0.44
2:N:480:ALA:HB1	2:N:510:ALA:HB3	1.99	0.44
1:A:330:ARG:HH12	1:A:705:ILE:H	1.66	0.44
1:A:513:LEU:HD13	1:A:819:ILE:HG12	2.00	0.44
1:D:211:TRP:CD1	1:E:836:MET:HG3	2.53	0.44
1:D:380:ARG:HE	1:D:391:VAL:HG22	1.83	0.44
1:D:476:ASN:HA	1:D:538:HIS:HD2	1.82	0.44
1:D:644:ASN:CG	1:D:645:ASP:H	2.26	0.44
1:E:513:LEU:O	1:E:518:ILE:HD12	2.17	0.44
1:F:478:ALA:HA	1:F:481:LEU:HG	1.98	0.44
1:G:13:MET:HA	1:H:927:ARG:HD2	2.00	0.44
1:H:428:LYS:HA	1:I:267:PHE:HB3	2.00	0.44
1:J:179:ILE:HG21	1:J:184:ILE:HG22	1.99	0.44
1:L:252:LYS:HB3	1:L:257:LYS:HA	1.98	0.44
1:L:336:LEU:O	1:L:337:MET:HB2	2.18	0.44
1:L:824:ASN:CA	1:L:844:ALA:HB2	2.46	0.44
2:N:45:TYR:C	2:N:46:LEU:HG	2.42	0.44
2:N:139:PHE:HZ	2:N:547:ARG:HE	1.66	0.44
4:Q:114:LEU:N	4:Q:114:LEU:CD1	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LEU:HD21	1:B:44:LYS:HD2	2.00	0.44
1:B:269:THR:HB	1:B:271:GLU:HG2	2.00	0.44
1:B:943:THR:C	1:B:945:PHE:H	2.26	0.44
1:D:848:TYR:HA	1:D:849:PRO:HD3	1.80	0.44
1:E:332:ASN:HA	1:E:387:TRP:HB3	1.99	0.44
1:F:487:TYR:HB2	1:F:508:VAL:O	2.18	0.44
1:H:414:CYS:HB2	1:I:414:CYS:HB3	1.84	0.44
1:I:387:TRP:CE2	1:I:563:PRO:HG3	2.53	0.44
1:I:659:ASN:O	1:I:659:ASN:CG	2.59	0.44
4:S:15:LEU:HD12	4:S:15:LEU:N	2.22	0.44
1:C:69:ILE:HG23	1:C:70:PRO:HD2	2.00	0.44
1:F:198:LYS:HB3	1:F:262:VAL:HG23	1.99	0.44
1:F:648:SER:O	1:F:921:GLU:HA	2.18	0.44
1:G:45:PHE:HD2	1:G:46:ARG:H	1.64	0.44
1:H:837:ARG:HG3	1:I:459:ALA:HB2	1.98	0.44
1:I:661:THR:C	1:I:907:VAL:HG22	2.43	0.44
1:I:880:MET:HB3	1:I:882:MET:HE3	2.00	0.44
1:K:186:ILE:HD11	1:K:196:ALA:HB2	2.00	0.44
1:K:748:SER:CA	1:K:760:ASN:ND2	2.64	0.44
1:K:755:ASN:OD1	1:K:760:ASN:HA	2.18	0.44
1:L:299:HIS:HB2	1:L:322:ASN:HD21	1.83	0.44
1:C:635:ARG:HE	1:C:932:HIS:HA	1.83	0.43
1:D:798:PHE:HD1	1:D:866:CYS:SG	2.41	0.43
1:G:757:ALA:O	1:G:758:GLN:CG	2.44	0.43
1:H:926:VAL:HG22	1:H:940:TYR:HA	2.00	0.43
1:I:356:ASN:O	1:I:356:ASN:CG	2.61	0.43
1:I:739:THR:O	1:I:740:PRO:C	2.60	0.43
1:J:415:PHE:HZ	1:K:124:LEU:HD23	1.82	0.43
1:K:348:LEU:HD13	1:K:357:ALA:HB3	1.99	0.43
1:K:383:TYR:HB3	1:K:390:ALA:HB2	2.00	0.43
2:N:53:ASN:O	2:N:119:TRP:CZ2	2.70	0.43
2:N:283:ILE:HD12	2:N:408:LEU:HD11	1.99	0.43
5:U:86:PRO:HG3	5:U:172:GLN:HA	2.00	0.43
1:B:205:GLN:NE2	1:C:826:SER:OG	2.51	0.43
1:F:533:ASN:OD1	1:F:713:TYR:CD2	2.71	0.43
1:G:91:ASN:HB3	1:G:624:HIS:ND1	2.34	0.43
1:H:121:TYR:CD2	1:I:844:ALA:HB3	2.53	0.43
1:H:696:ASP:OD1	4:Q:23:ALA:HB2	2.18	0.43
1:I:96:MET:HG2	1:I:572:LEU:O	2.19	0.43
1:K:537:HIS:H	1:K:540:ASN:HD21	1.65	0.43
1:B:701:TYR:HD2	1:B:703:GLY:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:878:ASN:HD21	1:B:880:MET:HE2	1.83	0.43
1:E:486:LYS:HB2	1:E:507:ARG:HH11	1.82	0.43
1:F:328:ALA:HB2	1:F:547:SER:HB2	2.00	0.43
1:F:400:ILE:HA	1:F:525:SER:HB2	1.98	0.43
1:G:745:ILE:HG12	1:G:765:TRP:CD1	2.53	0.43
1:K:412:ASN:HB2	1:K:462:ILE:HG23	2.00	0.43
1:L:10:TRP:CG	1:L:16:SER:HB3	2.54	0.43
1:L:252:LYS:H	1:L:257:LYS:HG2	1.83	0.43
2:N:113:LEU:HD22	2:N:119:TRP:HE3	1.83	0.43
5:U:84:PRO:HB3	5:U:174:SER:HB3	2.01	0.43
1:A:414:CYS:HB2	1:B:414:CYS:HB3	1.82	0.43
1:F:224:LEU:HB3	1:F:228:THR:HG23	2.00	0.43
1:G:174:TYR:HB3	1:G:220:ALA:HB3	2.00	0.43
1:I:331:ASP:HB2	1:I:391:VAL:HA	2.01	0.43
1:J:183:GLY:HA3	1:J:201:GLN:HE22	1.83	0.43
1:J:653:LEU:HB2	1:J:915:LEU:HD22	1.99	0.43
4:S:109:SER:C	4:S:111:THR:H	2.26	0.43
1:B:489:PRO:HD3	1:B:494:ILE:HD13	1.99	0.43
1:C:237:TYR:HE1	1:C:239:LYS:HG3	1.83	0.43
1:D:14:HIS:HB2	1:D:45:PHE:HZ	1.84	0.43
1:D:523:ARG:CB	1:F:548:MET:HB3	2.41	0.43
1:G:475:SER:HA	1:G:479:LEU:HD12	2.00	0.43
1:G:849:PRO:C	1:G:851:ILE:N	2.75	0.43
1:I:850:LEU:HD13	1:I:856:VAL:O	2.18	0.43
1:J:829:VAL:HG22	1:J:830:GLY:H	1.82	0.43
1:K:863:LYS:HB3	1:K:864:PHE:H	1.62	0.43
2:N:444:MET:HG2	2:N:531:LEU:HD22	1.99	0.43
3:M:99:LEU:HA	3:M:102:VAL:HG22	1.99	0.43
4:R:50:GLU:OE1	4:R:50:GLU:HA	2.18	0.43
1:A:57:THR:HB	1:B:877:SER:HB2	2.00	0.43
1:B:211:TRP:CD1	1:C:316:GLY:HA2	2.53	0.43
1:E:113:PHE:HB3	1:E:327:ILE:HD12	1.99	0.43
1:E:871:TRP:HA	1:E:871:TRP:CE3	2.53	0.43
1:G:640:ASP:CG	1:G:929:HIS:HA	2.44	0.43
1:I:350:GLY:HA2	1:I:579:TYR:HA	2.00	0.43
1:I:661:THR:HB	1:I:909:PRO:N	2.34	0.43
1:I:730:SER:HB2	1:I:741:ASN:HA	2.00	0.43
1:J:817:VAL:CG2	1:J:818:GLY:N	2.81	0.43
1:K:65:THR:HG23	1:L:763:LYS:HD3	2.01	0.43
1:K:428:LYS:HA	1:L:267:PHE:HB3	2.01	0.43
1:L:825:ASN:O	1:L:825:ASN:OD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:128:VAL:HA	4:P:131:LEU:HD12	2.01	0.43
1:A:82:ALA:HB2	1:A:613:ILE:HD13	2.01	0.43
1:A:429:VAL:O	1:A:442:ASP:OD2	2.36	0.43
1:C:348:LEU:HD23	1:C:569:ILE:HD13	2.01	0.43
1:E:429:VAL:HA	1:E:442:ASP:N	2.33	0.43
1:G:395:ASP:HA	1:G:396:PRO:HD3	1.91	0.43
1:G:517:TYR:CD1	1:G:846:PHE:HD2	2.37	0.43
1:I:353:SER:O	1:I:353:SER:OG	2.36	0.43
1:K:223:VAL:HB	1:K:286:LEU:HD22	2.01	0.43
3:M:13:ALA:HB1	3:M:17:GLN:HE21	1.82	0.43
1:B:184:ILE:HG22	1:B:185:GLN:H	1.82	0.43
1:B:601:LEU:HB3	1:B:606:ALA:HB3	2.00	0.43
1:B:648:SER:HB2	1:B:924:ASP:H	1.83	0.43
1:D:689:PRO:HB3	1:D:699:TYR:HD1	1.84	0.43
1:E:429:VAL:HA	1:E:441:LYS:HA	2.01	0.43
1:E:656:ILE:HD11	1:E:916:LEU:HG	1.99	0.43
1:F:240:PRO:HB3	1:F:245:GLY:HA2	1.99	0.43
1:G:264:MET:HE2	1:G:264:MET:HA	2.01	0.43
1:K:351:GLN:HB3	1:K:578:SER:HB2	2.00	0.43
1:B:22:GLU:HG2	5:U:177:GLU:HB2	2.01	0.43
1:B:74:GLU:HB2	1:B:81:LYS:HB2	2.00	0.43
1:B:115:PRO:HA	1:B:326:TYR:HD2	1.83	0.43
1:B:184:ILE:HG22	1:B:185:GLN:C	2.44	0.43
1:B:413:TYR:HB3	1:B:459:ALA:HB1	2.01	0.43
1:B:426:LEU:HB3	1:C:267:PHE:HD1	1.83	0.43
1:B:725:PHE:HA	1:B:901:LEU:HA	2.00	0.43
1:C:817:VAL:HG11	1:C:846:PHE:HA	2.00	0.43
1:D:64:LEU:HD13	1:D:621:PRO:HD3	2.00	0.43
1:D:126:PRO:HB2	1:D:129:ALA:HB2	2.01	0.43
1:F:635:ARG:HA	1:F:931:PRO:HA	2.01	0.43
1:F:793:SER:HA	1:F:869:THR:HG23	2.01	0.43
1:G:101:PHE:O	1:G:561:GLN:HA	2.18	0.43
1:G:428:LYS:HG2	1:G:446:PHE:HD1	1.84	0.43
1:G:822:GLN:HA	1:G:845:ASN:HD21	1.84	0.43
1:H:492:VAL:HG13	1:H:506:LYS:NZ	2.33	0.43
1:J:114:LYS:HA	1:J:115:PRO:HD3	1.83	0.43
1:J:720:LYS:CD	4:Q:22:TRP:CE3	2.86	0.43
1:K:64:LEU:HB3	1:L:736:ARG:O	2.19	0.43
1:K:705:ILE:HG22	1:K:707:TYR:H	1.84	0.43
1:L:930:ARG:H	1:L:931:PRO:HD2	1.80	0.43
5:U:49:ALA:HA	5:U:52:ASN:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:ILE:HD12	1:B:916:LEU:HB2	2.01	0.43
1:C:333:PHE:HE2	1:C:387:TRP:HA	1.82	0.43
1:C:676:ARG:HB3	1:C:921:GLU:HB3	2.01	0.43
1:D:398:VAL:HG21	1:D:539:ARG:HD2	2.01	0.43
1:D:405:GLY:HA2	1:D:520:LEU:HD11	2.01	0.43
1:E:47:ASN:HA	1:E:48:PRO:HD3	1.86	0.43
1:G:881:SER:O	1:G:882:MET:C	2.62	0.43
1:I:654:TYR:CD1	1:I:916:LEU:O	2.72	0.43
1:J:644:ASN:H	1:L:46:ARG:HD3	1.83	0.43
1:K:748:SER:HB3	1:K:760:ASN:HD21	1.82	0.43
1:L:126:PRO:HG2	1:L:129:ALA:HB2	2.00	0.43
1:L:575:LEU:H	1:L:930:ARG:HH21	1.67	0.43
4:S:30:MET:O	4:S:32:SER:N	2.52	0.43
1:A:55:ASP:O	1:A:56:VAL:CG2	2.58	0.42
1:A:836:MET:O	1:A:836:MET:SD	2.77	0.42
1:B:755:ASN:HD21	1:B:862:LYS:HE3	1.84	0.42
1:C:829:VAL:HG12	1:C:830:GLY:N	2.33	0.42
1:F:131:ASN:HA	1:F:132:PRO:HD3	1.92	0.42
1:G:775:ASN:ND2	1:G:881:SER:CB	2.73	0.42
1:H:834:PRO:HB3	1:I:410:LEU:HD23	2.01	0.42
1:I:656:ILE:O	1:I:657:PRO:O	2.37	0.42
1:J:430:LYS:HB2	1:J:442:ASP:CG	2.44	0.42
1:J:552:ASN:HB2	1:K:522:ALA:HB2	1.99	0.42
1:K:386:MET:HG3	1:L:758:GLN:HG3	2.00	0.42
1:K:449:LYS:HD3	1:L:312:ARG:HH22	1.84	0.42
1:K:494:ILE:CG2	1:K:495:SER:N	2.82	0.42
1:K:564:GLN:HE22	1:K:583:TRP:HE1	1.66	0.42
1:K:720:LYS:HG3	1:K:906:GLU:HB3	2.00	0.42
1:L:374:LEU:HD21	1:L:389:GLN:HG2	2.01	0.42
1:A:325:ASN:HA	1:A:596:SER:HB2	2.02	0.42
1:C:47:ASN:HA	1:C:48:PRO:HD3	1.89	0.42
1:C:237:TYR:HE2	1:C:294:GLU:HB2	1.83	0.42
1:C:368:LEU:HD22	1:C:708:LEU:HA	2.02	0.42
1:C:632:ALA:HB2	1:C:933:ARG:HH21	1.83	0.42
1:C:648:SER:HB3	1:C:923:PHE:HA	2.01	0.42
1:D:374:LEU:HD21	1:D:389:GLN:HE22	1.84	0.42
1:D:779:GLN:HA	1:F:95:ASP:HB3	2.02	0.42
1:D:840:GLN:HB2	1:F:204:PRO:HB3	2.02	0.42
1:E:420:VAL:HG13	1:E:457:ASN:HA	2.00	0.42
1:G:428:LYS:HE2	1:H:265:GLN:HB3	2.01	0.42
1:H:570:LYS:O	1:H:643:PHE:HE1	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:863:LYS:HZ3	4:R:48:THR:HG22	1.84	0.42
1:I:369:SER:HA	1:I:647:LEU:HB3	2.02	0.42
1:I:822:GLN:HB2	1:I:824:ASN:OD1	2.19	0.42
1:J:656:ILE:HG12	1:J:914:THR:OG1	2.19	0.42
3:M:134:GLN:HA	3:M:176:PRO:HB2	2.01	0.42
4:P:15:LEU:HD13	4:R:15:LEU:HD12	2.02	0.42
1:A:771:LEU:HB3	1:A:879:PHE:HB2	2.01	0.42
1:B:128:GLY:HA2	1:B:318:GLN:HA	2.01	0.42
1:E:357:ALA:HA	1:E:938:THR:HG21	2.01	0.42
1:E:464:LEU:HD22	1:F:464:LEU:HD21	2.01	0.42
1:J:923:PHE:HB3	1:J:944:PRO:HD3	2.02	0.42
1:K:328:ALA:HB1	1:K:546:ARG:HB2	2.00	0.42
1:K:941:LEU:HB3	5:U:31:ILE:HG23	2.01	0.42
2:N:137:PHE:CD2	2:N:137:PHE:O	2.73	0.42
1:B:760:ASN:HB3	1:B:864:PHE:HD2	1.83	0.42
1:C:388:ASN:HB2	1:C:546:ARG:HH11	1.84	0.42
1:C:661:THR:HG23	1:C:662:ASN:CG	2.44	0.42
1:D:657:PRO:HG2	1:D:660:ALA:HB2	2.01	0.42
1:E:589:VAL:HG12	1:E:601:LEU:HB3	2.01	0.42
1:F:118:GLY:HA2	1:F:321:PRO:HB3	2.00	0.42
1:H:415:PHE:HA	1:H:416:PRO:HD3	1.90	0.42
1:I:709:ASP:HB2	1:I:711:THR:HG22	2.02	0.42
1:J:349:ALA:HB1	1:J:354:GLN:HA	2.00	0.42
1:J:862:LYS:H	4:Q:50:GLU:HB2	1.83	0.42
1:K:230:MET:HB2	1:K:314:LEU:HB2	2.01	0.42
1:K:940:TYR:HB2	5:U:32:ASN:HD22	1.84	0.42
1:L:113:PHE:HD1	1:L:327:ILE:HB	1.83	0.42
1:L:850:LEU:HD13	1:L:856:VAL:O	2.19	0.42
2:N:382:LEU:HB2	2:N:393:LEU:HD23	2.01	0.42
2:N:449:VAL:C	2:N:450:THR:CG2	2.90	0.42
5:V:37:GLY:O	5:V:41:ILE:HB	2.20	0.42
5:V:183:ILE:HD13	5:V:191:GLU:OE1	2.18	0.42
1:A:132:PRO:HB2	1:A:223:VAL:HA	2.01	0.42
1:A:705:ILE:HG22	1:A:708:LEU:H	1.84	0.42
1:B:327:ILE:HG22	1:B:593:LEU:HD23	2.01	0.42
1:B:414:CYS:HB2	1:C:414:CYS:HB3	2.00	0.42
1:C:223:VAL:HB	1:C:286:LEU:HD22	2.01	0.42
1:F:51:ALA:HA	1:F:52:PRO:HD3	1.92	0.42
1:H:222:ARG:HA	1:H:287:TYR:H	1.85	0.42
1:I:730:SER:O	1:I:732:PRO:CD	2.68	0.42
1:A:97:ALA:HB3	1:B:780:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:ILE:HA	1:G:70:PRO:HD2	1.82	0.42
1:G:299:HIS:HB3	1:G:300:ILE:H	1.70	0.42
1:G:523:ARG:H	1:I:548:MET:HB2	1.84	0.42
1:I:63:ARG:H	1:I:63:ARG:HG2	1.71	0.42
1:I:102:ASP:HB2	1:I:616:TYR:HE1	1.84	0.42
1:I:113:PHE:HD1	1:I:327:ILE:HB	1.84	0.42
1:I:681:THR:HG21	1:I:712:PHE:HB3	2.02	0.42
1:K:108:ASP:HB3	1:K:607:SER:HB2	2.02	0.42
1:B:51:ALA:HA	1:B:52:PRO:HD3	1.94	0.42
1:B:681:THR:HB	1:B:712:PHE:CD2	2.55	0.42
1:C:654:TYR:HA	1:C:655:PRO:HD3	1.94	0.42
1:C:799:GLN:HA	1:C:800:PRO:HD3	1.92	0.42
1:D:270:THR:HG23	1:D:270:THR:O	2.20	0.42
1:E:726:ASP:C	1:E:728:SER:N	2.78	0.42
1:H:79:SER:HB2	1:H:584:ASN:HD21	1.85	0.42
1:I:326:TYR:H	1:I:596:SER:HB2	1.84	0.42
1:I:589:VAL:HG12	1:I:608:ILE:HD11	2.02	0.42
1:J:323:ARG:H	1:J:505:ASN:HB2	1.83	0.42
1:J:497:ASN:HA	1:J:498:PRO:HD3	1.88	0.42
1:K:750:ASP:O	1:K:750:ASP:OD1	2.38	0.42
1:L:600:ASP:HB3	1:L:700:THR:O	2.20	0.42
2:N:240:ILE:HD12	2:N:250:PHE:HZ	1.84	0.42
4:S:34:ILE:O	4:S:35:ASP:CB	2.68	0.42
1:A:581:TYR:CZ	1:A:583:TRP:CD1	3.07	0.42
1:D:337:MET:HB2	1:D:339:TYR:CE1	2.55	0.42
1:D:663:VAL:HB	1:D:905:PHE:HB3	2.02	0.42
1:E:589:VAL:HG13	1:E:608:ILE:HD12	2.01	0.42
1:E:732:PRO:C	1:E:734:ASN:H	2.27	0.42
1:F:653:LEU:O	4:R:19:MET:HB2	2.19	0.42
1:H:90:ASP:HA	1:H:576:PRO:HG2	2.01	0.42
1:H:518:ILE:HG23	1:H:846:PHE:HE2	1.83	0.42
1:I:810:LYS:HE2	1:I:859:ILE:HD12	2.02	0.42
1:L:179:ILE:HG12	1:L:218:HIS:CE1	2.55	0.42
2:N:441:LEU:N	2:N:442:PRO:HD3	2.35	0.42
4:R:41:PRO:CA	4:R:46:THR:HB	2.48	0.42
1:A:635:ARG:HB3	1:A:931:PRO:O	2.19	0.42
1:B:64:LEU:HD13	1:B:619:PHE:O	2.13	0.42
1:B:684:LYS:HG2	1:B:914:THR:HG22	2.00	0.42
1:C:365:ASN:HB3	1:C:368:LEU:HB2	2.01	0.42
1:C:534:PRO:HA	1:C:537:HIS:CD2	2.54	0.42
1:D:111:PRO:HD3	1:D:554:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:574:LEU:HA	1:D:930:ARG:HH12	1.85	0.42
1:E:131:ASN:C	1:E:133:CYS:H	2.27	0.42
1:E:374:LEU:HA	1:E:377:ILE:HD12	2.02	0.42
1:E:403:ASN:HB3	1:E:520:LEU:HD12	2.01	0.42
1:E:713:TYR:HD1	1:E:714:LEU:HG	1.84	0.42
1:H:90:ASP:HA	1:H:576:PRO:HB2	2.02	0.42
1:H:135:TRP:HA	1:H:310:ASN:HB3	2.02	0.42
1:J:41:LEU:HD22	1:J:44:LYS:HE3	2.02	0.42
1:J:742:GLU:OE2	4:Q:22:TRP:HB3	2.20	0.42
1:K:797:ASN:CG	1:K:868:ARG:HB3	2.45	0.42
1:L:421:ILE:O	1:L:421:ILE:HG12	2.18	0.42
1:L:684:LYS:HE2	1:L:912:GLU:HB2	2.01	0.42
4:S:55:THR:O	4:S:55:THR:HG23	2.19	0.42
5:V:51:ARG:HA	5:V:54:ILE:HG12	2.02	0.42
5:V:85:ALA:HA	5:V:86:PRO:HD2	1.88	0.42
1:A:414:CYS:HA	1:C:462:ILE:HB	2.02	0.42
1:A:715:ASN:HD22	1:A:869:THR:H	1.67	0.42
1:B:124:LEU:HD13	1:C:466:ALA:HB3	2.02	0.42
1:B:173:PRO:HB3	1:C:839:GLY:HA2	2.02	0.42
1:B:238:ALA:HA	1:B:293:ILE:HG22	2.02	0.42
1:B:350:GLY:HA2	1:B:579:TYR:HA	2.01	0.42
1:D:557:PRO:HD2	1:E:860:THR:HG22	2.00	0.42
1:E:651:ASN:HD22	1:E:917:TYR:HE1	1.67	0.42
1:F:769:GLN:HE21	1:F:871:TRP:HD1	1.67	0.42
1:G:925:VAL:H	1:G:941:LEU:CB	2.32	0.42
1:J:792:TYR:HA	1:J:796:ARG:HB2	2.02	0.42
1:K:101:PHE:O	1:K:561:GLN:HG2	2.20	0.42
1:L:365:ASN:HB3	1:L:368:LEU:HG	2.02	0.42
1:L:922:VAL:HG12	1:L:923:PHE:N	2.34	0.42
1:B:799:GLN:HA	1:B:800:PRO:HD3	1.95	0.41
1:B:922:VAL:CG1	1:B:942:ARG:O	2.67	0.41
1:E:488:SER:HB2	1:E:489:PRO:CD	2.35	0.41
1:F:240:PRO:HB3	1:F:245:GLY:C	2.45	0.41
1:G:552:ASN:ND2	1:H:520:LEU:O	2.53	0.41
1:G:712:PHE:O	1:G:867:ASP:C	2.59	0.41
1:G:763:LYS:HA	1:G:766:PHE:HB3	2.01	0.41
1:H:380:ARG:HB3	1:H:391:VAL:HG22	2.01	0.41
2:N:230:VAL:HG13	2:N:286:LEU:HD21	2.02	0.41
4:P:27:GLN:O	4:P:42:ALA:HB3	2.20	0.41
1:A:235:GLY:HA3	1:A:298:THR:HB	2.02	0.41
1:A:566:PHE:HD2	1:A:568:ALA:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:TYR:HB3	1:A:814:TYR:H	1.85	0.41
1:B:684:LYS:HB2	1:B:687:GLU:HG2	2.02	0.41
1:B:693:SER:HB3	2:N:84:TYR:HB3	2.02	0.41
1:C:228:THR:HA	1:C:229:PRO:HD3	1.86	0.41
1:D:336:LEU:HD23	1:D:562:VAL:HG11	2.02	0.41
1:D:833:ALA:C	1:D:835:THR:H	2.28	0.41
1:D:850:LEU:HG	1:F:554:ARG:N	2.34	0.41
1:E:179:ILE:HG23	1:E:183:GLY:O	2.20	0.41
1:G:650:ALA:CB	1:G:922:VAL:HG21	2.50	0.41
1:H:172:ALA:HB1	1:H:219:ALA:HB1	2.02	0.41
1:H:412:ASN:HB2	1:H:462:ILE:O	2.19	0.41
1:I:179:ILE:HG23	1:I:218:HIS:CB	2.50	0.41
1:I:682:ARG:HA	1:I:915:LEU:O	2.20	0.41
1:J:303:MET:HA	1:J:304:PRO:HD3	1.89	0.41
1:J:939:VAL:HG13	1:J:951:THR:HG21	2.01	0.41
1:K:375:ASP:HB3	1:K:790:ARG:HH11	1.84	0.41
1:K:684:LYS:HB2	1:K:687:GLU:HG2	2.02	0.41
1:L:85:THR:HG23	1:L:580:THR:HG22	2.02	0.41
4:P:124:LEU:O	4:P:128:VAL:HG13	2.19	0.41
4:Q:27:GLN:C	4:Q:29:VAL:H	2.27	0.41
1:A:783:ILE:HA	1:A:784:PRO:HD3	1.84	0.41
1:B:679:ALA:HA	1:B:871:TRP:O	2.21	0.41
1:C:17:GLY:O	1:C:48:PRO:HB2	2.20	0.41
1:C:672:TRP:HA	1:C:944:PRO:HA	2.02	0.41
1:C:771:LEU:HD22	1:C:778:TYR:CE1	2.54	0.41
1:D:720:LYS:HG2	1:D:744:GLU:HG2	2.01	0.41
1:E:907:VAL:HG11	1:E:916:LEU:HD21	2.01	0.41
1:F:536:ASN:HA	1:F:596:SER:O	2.20	0.41
1:G:336:LEU:HD12	1:G:562:VAL:HG21	2.02	0.41
1:G:414:CYS:HB2	1:H:414:CYS:HB3	1.98	0.41
1:G:517:TYR:CE1	1:G:846:PHE:CD2	3.08	0.41
1:H:789:ASP:OD2	1:H:796:ARG:HG2	2.20	0.41
1:J:94:LEU:HD22	1:J:574:LEU:HD12	2.03	0.41
1:K:706:PRO:HA	1:K:711:THR:HB	2.03	0.41
1:K:841:ALA:O	1:K:842:TYR:HD1	2.02	0.41
4:Q:54:GLY:C	4:Q:55:THR:HG22	2.45	0.41
5:U:189:ILE:H	5:U:189:ILE:HG13	1.57	0.41
1:C:678:TRP:H	1:C:873:ILE:HG23	1.84	0.41
1:C:867:ASP:O	1:C:868:ARG:HG3	2.19	0.41
1:D:338:TYR:HE2	1:D:694:GLY:HA2	1.86	0.41
1:E:222:ARG:HB2	1:F:842:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:LYS:HG3	1:H:411:PRO:HB3	2.01	0.41
1:G:573:LEU:H	1:G:641:GLN:HE22	1.68	0.41
1:H:517:TYR:CA	1:H:520:LEU:CD1	2.93	0.41
1:H:778:TYR:OH	1:H:878:ASN:ND2	2.53	0.41
1:I:186:ILE:HD12	1:I:194:LYS:HB3	2.01	0.41
1:K:179:ILE:HG13	1:K:218:HIS:HB3	2.03	0.41
1:L:134:GLU:HB3	1:L:168:VAL:HG12	2.01	0.41
1:L:386:MET:HB2	1:L:561:GLN:HB3	2.01	0.41
1:L:486:LYS:HG2	1:L:509:VAL:HB	2.01	0.41
1:L:707:TYR:HA	1:L:712:PHE:HE2	1.86	0.41
4:S:18:ARG:CG	4:S:19:MET:N	2.83	0.41
1:B:338:TYR:CE2	1:B:584:ASN:HB3	2.56	0.41
1:D:799:GLN:O	1:D:801:MET:HE3	2.21	0.41
1:E:110:GLY:H	1:E:554:ARG:HD3	1.86	0.41
1:E:391:VAL:C	1:E:393:SER:H	2.29	0.41
1:E:553:GLY:HA3	1:F:850:LEU:HD23	2.01	0.41
1:F:80:TYR:HB2	1:F:587:LYS:HE3	2.02	0.41
1:G:173:PRO:HB3	1:H:840:GLN:HB2	2.03	0.41
1:G:353:SER:HB3	1:G:355:LEU:HD12	2.03	0.41
1:H:715:ASN:HB2	1:H:866:CYS:O	2.20	0.41
1:I:811:TYR:HB2	1:I:814:TYR:HB2	2.02	0.41
1:J:415:PHE:HA	1:L:837:ARG:NH2	2.34	0.41
1:J:549:LEU:HG	1:K:801:MET:HG3	2.02	0.41
1:J:783:ILE:HD11	1:L:377:ILE:HG23	2.02	0.41
1:K:104:ARG:HD2	1:K:612:SER:HB3	2.03	0.41
1:L:350:GLY:HA2	1:L:579:TYR:HA	2.01	0.41
1:L:677:GLY:H	1:L:921:GLU:HB2	1.84	0.41
4:Q:114:LEU:HD13	4:Q:114:LEU:N	2.34	0.41
1:A:266:PHE:HB3	1:A:285:VAL:HG23	2.02	0.41
1:A:323:ARG:NH1	1:A:475:SER:O	2.54	0.41
1:A:736:ARG:HB2	1:C:64:LEU:HB3	2.03	0.41
1:D:168:VAL:HG21	1:D:312:ARG:HG3	2.03	0.41
1:D:205:GLN:HG3	1:D:206:ILE:HG13	2.02	0.41
1:D:460:MET:HB2	1:E:415:PHE:O	2.21	0.41
1:D:669:SER:HA	1:D:900:ALA:HA	2.01	0.41
1:E:188:VAL:HG12	1:E:193:PRO:HA	2.03	0.41
1:E:684:LYS:HG3	1:E:914:THR:HG22	2.02	0.41
1:E:687:GLU:O	1:E:699:TYR:HE1	2.04	0.41
1:F:15:ILE:HG23	1:F:48:PRO:HA	2.02	0.41
1:F:93:VAL:HB	1:F:573:LEU:HD11	2.01	0.41
1:F:113:PHE:HD1	1:F:327:ILE:HG22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:797:ASN:CG	1:F:867:ASP:O	2.64	0.41
1:G:44:LYS:CG	1:H:571:ASN:O	2.67	0.41
1:G:189:GLU:HB3	1:G:190:GLY:H	1.74	0.41
1:G:523:ARG:N	1:I:548:MET:HB2	2.35	0.41
1:G:621:PRO:CD	1:H:878:ASN:OD1	2.67	0.41
1:I:795:PHE:O	1:I:795:PHE:CG	2.73	0.41
1:K:121:TYR:OH	1:L:849:PRO:HG3	2.21	0.41
1:K:330:ARG:HD3	1:K:708:LEU:HD13	2.01	0.41
3:M:217:PRO:HB2	3:M:218:THR:H	1.05	0.41
4:Q:8:GLY:HA2	4:R:28:ASN:HB2	2.02	0.41
4:S:131:LEU:HD23	4:S:131:LEU:HA	1.82	0.41
1:A:757:ALA:HB1	1:C:560:ILE:HA	2.01	0.41
1:B:347:VAL:HG13	1:B:582:GLU:HB2	2.02	0.41
1:B:680:PHE:HB3	1:B:918:VAL:HG13	2.02	0.41
1:C:218:HIS:ND1	1:C:282:PRO:O	2.54	0.41
1:C:224:LEU:HD23	1:C:289:GLU:HB2	2.02	0.41
1:C:320:MET:HA	1:C:321:PRO:HD3	1.97	0.41
1:C:529:MET:HE3	1:C:537:HIS:CE1	2.55	0.41
1:E:824:ASN:HD22	1:E:847:PRO:HG2	1.86	0.41
1:F:574:LEU:HD23	1:F:930:ARG:HH22	1.86	0.41
1:G:39:PHE:HB3	1:G:44:LYS:NZ	2.36	0.41
1:H:113:PHE:HE2	1:H:554:ARG:HG3	1.86	0.41
1:H:492:VAL:CG1	1:H:506:LYS:CD	2.96	0.41
1:I:13:MET:HB3	1:I:15:ILE:HG13	2.01	0.41
1:I:672:TRP:HE1	1:I:899:HIS:H	1.68	0.41
1:J:477:ILE:HA	1:J:480:TYR:HB3	2.02	0.41
1:J:625:ASN:HB3	3:M:287:GLN:HG3	2.02	0.41
1:J:655:PRO:HB3	1:J:914:THR:O	2.20	0.41
1:A:200:PHE:O	1:A:200:PHE:CG	2.71	0.41
1:A:251:VAL:CG1	1:A:252:LYS:N	2.82	0.41
1:B:943:THR:O	1:B:945:PHE:N	2.53	0.41
1:C:180:THR:OG1	1:C:181:LYS:N	2.54	0.41
1:D:837:ARG:HH11	1:E:459:ALA:H	1.69	0.41
1:E:696:ASP:HA	1:E:697:PRO:HD3	1.92	0.41
1:E:731:TRP:HB3	1:E:732:PRO:CD	2.46	0.41
1:I:680:PHE:CB	1:I:918:VAL:HG22	2.50	0.41
1:I:757:ALA:HB2	1:I:766:PHE:HZ	1.86	0.41
1:I:885:LEU:HB3	1:I:890:GLN:HG3	2.03	0.41
1:J:184:ILE:CG2	1:J:220:ALA:HB2	2.49	0.41
1:J:211:TRP:CH2	1:K:318:GLN:HG3	2.55	0.41
1:J:267:PHE:HB3	1:L:426:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:362:GLN:HB3	4:P:21:PRO:HG2	2.03	0.41
1:K:679:ALA:HB3	1:K:919:LEU:HB2	2.02	0.41
1:L:311:SER:H	1:L:314:LEU:HD12	1.85	0.41
1:L:524:TRP:HA	1:L:801:MET:HB2	2.02	0.41
3:M:67:ASN:HA	3:M:68:PRO:HD3	1.92	0.41
4:S:109:SER:C	4:S:111:THR:N	2.79	0.41
1:B:101:PHE:HB2	1:B:562:VAL:HG23	2.03	0.41
1:B:113:PHE:HB3	1:B:327:ILE:HD12	2.02	0.41
1:B:173:PRO:HD2	1:B:220:ALA:O	2.21	0.41
1:B:247:GLN:HB2	1:B:291:VAL:HG11	2.03	0.41
1:C:174:TYR:CB	1:C:220:ALA:H	2.34	0.41
1:C:563:PRO:HG2	1:C:565:LYS:HE3	2.03	0.41
1:C:597:LEU:O	1:C:597:LEU:CG	2.58	0.41
1:D:543:LEU:HD11	1:D:594:GLN:HE21	1.86	0.41
1:D:559:HIS:O	1:E:757:ALA:HA	2.21	0.41
1:D:792:TYR:HB3	1:D:868:ARG:HG2	2.03	0.41
1:E:221:GLY:O	1:E:286:LEU:HA	2.20	0.41
1:E:340:ASN:O	1:E:341:SER:CB	2.68	0.41
1:E:561:GLN:HB2	1:F:756:VAL:CG1	2.51	0.41
1:F:223:VAL:HB	1:F:286:LEU:HD13	2.02	0.41
1:G:96:MET:HE1	1:G:574:LEU:HB3	2.02	0.41
1:G:826:SER:HB2	1:I:205:GLN:HA	2.03	0.41
1:G:839:GLY:O	1:I:173:PRO:HG2	2.21	0.41
1:H:307:LYS:HD2	1:H:311:SER:HB3	2.03	0.41
1:H:554:ARG:H	1:I:850:LEU:HG	1.86	0.41
1:H:724:THR:HG22	1:H:725:PHE:N	2.36	0.41
1:H:827:GLY:HA3	1:H:839:GLY:HA3	2.03	0.41
1:H:836:MET:HE3	1:H:836:MET:HB3	1.92	0.41
1:H:867:ASP:OD1	1:H:867:ASP:N	2.54	0.41
1:I:473:LEU:HG	1:I:477:ILE:HD12	2.03	0.41
1:I:775:ASN:HA	1:I:880:MET:HE1	2.03	0.41
1:J:756:VAL:HG11	1:J:766:PHE:CD1	2.55	0.41
1:K:110:GLY:H	1:K:554:ARG:HG3	1.86	0.41
1:K:329:PHE:C	1:K:330:ARG:O	2.64	0.41
1:L:53:THR:O	1:L:57:THR:CG2	2.68	0.41
5:V:27:TYR:C	5:V:29:THR:H	2.28	0.41
1:C:922:VAL:CG1	1:C:942:ARG:HB3	2.51	0.41
1:C:942:ARG:HB2	1:C:945:PHE:HB3	2.03	0.41
1:D:922:VAL:HG23	1:D:923:PHE:H	1.86	0.41
1:E:84:PHE:HB2	1:E:581:TYR:HB3	2.02	0.41
1:E:905:PHE:HE2	1:E:916:LEU:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:570:LYS:O	1:H:643:PHE:CZ	2.73	0.41
1:H:665:ILE:HD13	1:H:903:MET:HE2	2.03	0.41
1:H:748:SER:CA	4:R:50:GLU:OE2	2.63	0.41
1:I:267:PHE:CZ	1:I:284:VAL:HB	2.56	0.41
1:I:486:LYS:HG2	1:I:507:ARG:HB3	2.03	0.41
1:I:730:SER:O	1:I:733:GLY:N	2.44	0.41
1:K:373:LEU:HD11	1:K:645:ASP:HA	2.03	0.41
1:K:519:ASN:HB3	1:K:522:ALA:HB3	2.02	0.41
2:N:62:PRO:O	2:N:63:LEU:HD23	2.21	0.41
2:N:456:GLN:HG3	2:N:540:ARG:HH12	1.85	0.41
4:S:26:ARG:HA	4:S:26:ARG:HD2	1.53	0.41
1:A:96:MET:HE3	1:A:569:ILE:HD11	2.03	0.40
1:C:172:ALA:HB3	1:C:284:VAL:HG12	2.01	0.40
1:C:208:GLU:HB3	1:C:209:SER:H	1.77	0.40
1:D:844:ALA:HB3	1:F:121:TYR:HB3	2.02	0.40
1:E:428:LYS:HA	1:F:267:PHE:HB3	2.03	0.40
1:E:794:PHE:HB3	1:E:798:PHE:HE2	1.85	0.40
1:F:494:ILE:HD11	1:F:503:TYR:HA	2.02	0.40
1:G:130:PRO:HA	1:G:232:PRO:HA	2.02	0.40
1:H:300:ILE:CG2	1:H:318:GLN:O	2.67	0.40
1:H:338:TYR:HB3	1:H:583:TRP:HZ3	1.86	0.40
1:J:267:PHE:HE1	1:J:286:LEU:HD12	1.86	0.40
1:J:850:LEU:HD13	1:J:856:VAL:H	1.86	0.40
1:K:767:LEU:O	1:K:771:LEU:HB2	2.21	0.40
4:S:20:PRO:HA	4:S:21:PRO:HD3	1.56	0.40
5:V:90:VAL:HA	5:V:168:ILE:HG23	2.03	0.40
1:B:203:GLU:HA	1:B:204:PRO:HD2	1.93	0.40
1:B:941:LEU:HB2	1:B:948:GLY:HA2	2.02	0.40
1:B:945:PHE:HA	2:N:101:TYR:CZ	2.56	0.40
1:D:373:LEU:HD11	1:D:646:TYR:H	1.84	0.40
1:E:735:ASP:OD1	1:E:735:ASP:C	2.64	0.40
1:F:477:ILE:HG23	1:F:529:MET:HE2	2.03	0.40
1:G:414:CYS:HB3	1:I:414:CYS:HB2	1.92	0.40
1:H:211:TRP:HB2	1:I:836:MET:SD	2.61	0.40
1:H:325:ASN:HD22	1:H:599:ASN:HB3	1.85	0.40
1:H:577:GLY:HA3	1:H:934:GLY:HA2	2.03	0.40
1:I:486:LYS:HG3	1:I:509:VAL:HB	2.03	0.40
1:I:497:ASN:HA	1:I:498:PRO:HD3	1.89	0.40
1:K:837:ARG:HE	1:L:415:PHE:HD2	1.69	0.40
3:M:196:LEU:H	3:M:196:LEU:HG	1.54	0.40
4:R:108:ASP:HA	4:R:111:THR:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:GLY:C	1:C:111:PRO:HA	2.46	0.40
1:C:100:TYR:CD1	1:C:561:GLN:HB2	2.56	0.40
1:D:745:ILE:HG12	1:D:765:TRP:NE1	2.37	0.40
1:E:179:ILE:HG12	1:E:184:ILE:HG22	2.04	0.40
1:F:414:CYS:HB2	1:F:460:MET:HB2	2.04	0.40
1:F:731:TRP:HB3	1:F:732:PRO:HD3	2.04	0.40
1:G:524:TRP:CB	1:G:803:ARG:HB3	2.52	0.40
1:H:517:TYR:HB2	1:H:847:PRO:HG3	2.02	0.40
1:H:575:LEU:HD12	1:H:930:ARG:HB2	2.02	0.40
1:I:172:ALA:HB1	1:I:284:VAL:HG11	2.03	0.40
1:I:932:HIS:HB3	1:I:935:VAL:H	1.87	0.40
1:J:179:ILE:HG22	1:J:185:GLN:H	1.87	0.40
1:J:654:TYR:CZ	1:J:665:ILE:HG12	2.57	0.40
1:J:684:LYS:HA	1:J:914:THR:HA	2.02	0.40
1:K:656:ILE:HD11	1:K:916:LEU:HB2	2.03	0.40
1:K:842:TYR:HA	1:K:843:PRO:HD3	1.95	0.40
1:L:824:ASN:O	1:L:825:ASN:C	2.65	0.40
1:A:339:TYR:HD1	1:A:367:GLU:HG2	1.86	0.40
1:B:121:TYR:HD2	1:C:844:ALA:HB3	1.86	0.40
1:C:174:TYR:HD2	1:C:176:GLY:H	1.69	0.40
1:C:922:VAL:HG12	1:C:942:ARG:HB3	2.03	0.40
1:D:365:ASN:H	1:D:651:ASN:ND2	2.20	0.40
1:D:517:TYR:HA	1:D:520:LEU:HD22	2.03	0.40
1:F:41:LEU:HD13	1:F:44:LYS:HD2	2.04	0.40
1:G:13:MET:HG2	1:H:927:ARG:HB2	2.04	0.40
1:G:334:ILE:HD11	1:G:367:GLU:HB3	2.02	0.40
1:G:758:GLN:NE2	1:I:549:LEU:HD11	2.29	0.40
1:H:103:ILE:HG12	1:H:613:ILE:HG12	2.04	0.40
1:H:696:ASP:HA	1:H:697:PRO:HD2	2.00	0.40
1:I:238:ALA:HA	1:I:293:ILE:HG22	2.02	0.40
1:I:441:LYS:HG3	1:I:442:ASP:N	2.29	0.40
1:I:678:TRP:HB2	1:I:873:ILE:HG23	2.02	0.40
1:I:696:ASP:C	1:I:698:TYR:H	2.30	0.40
1:I:922:VAL:CG1	1:I:942:ARG:HB3	2.52	0.40
1:J:696:ASP:HB3	1:J:698:TYR:HD1	1.86	0.40
1:K:564:GLN:HE21	1:K:569:ILE:HD13	1.86	0.40
1:L:53:THR:O	1:L:57:THR:HG23	2.22	0.40
1:L:372:LEU:HD12	1:L:647:LEU:HB2	2.03	0.40
1:L:747:ARG:C	1:L:749:VAL:H	2.30	0.40
2:N:448:PRO:HA	2:N:529:LEU:HB2	2.04	0.40
1:A:429:VAL:CG1	1:B:266:PHE:HD1	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ALA:HB2	1:B:48:PRO:HD2	2.03	0.40
1:B:245:GLY:H	1:C:821:HIS:HB3	1.86	0.40
1:B:331:ASP:HA	1:B:388:ASN:HB2	2.03	0.40
1:B:440:GLU:HG3	1:B:441:LYS:H	1.87	0.40
1:B:575:LEU:HB2	1:B:930:ARG:HD3	2.03	0.40
1:C:732:PRO:HB3	1:C:736:ARG:HB2	2.03	0.40
1:E:486:LYS:HB3	1:E:507:ARG:HB3	2.02	0.40
1:F:655:PRO:HB3	1:F:915:LEU:HD23	2.03	0.40
1:G:325:ASN:HA	1:G:596:SER:HB3	2.04	0.40
1:I:10:TRP:HB2	1:I:16:SER:HB3	2.04	0.40
1:I:867:ASP:C	1:I:869:THR:N	2.79	0.40
1:K:416:PRO:HD2	1:K:458:PHE:C	2.47	0.40
1:K:908:ASP:HB3	1:K:909:PRO:HD2	2.02	0.40
1:L:656:ILE:O	1:L:656:ILE:HG22	2.20	0.40
2:N:120:GLY:HA2	2:N:531:LEU:HG	2.04	0.40
3:M:54:LEU:HA	3:M:57:ILE:HD12	2.04	0.40
4:S:34:ILE:N	4:S:34:ILE:HD12	2.36	0.40

There are no symmetry-related clashes.

4.3 Torsion angles ⓘ

4.3.1 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	913/949 (96%)	749 (82%)	143 (16%)	21 (2%)	5	30
1	B	907/949 (96%)	748 (82%)	130 (14%)	29 (3%)	3	24
1	C	917/949 (97%)	745 (81%)	149 (16%)	23 (2%)	4	28
1	D	913/949 (96%)	766 (84%)	124 (14%)	23 (2%)	4	28
1	E	906/949 (96%)	752 (83%)	138 (15%)	16 (2%)	6	33
1	F	910/949 (96%)	748 (82%)	144 (16%)	18 (2%)	6	32
1	G	905/949 (95%)	738 (82%)	144 (16%)	23 (2%)	4	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	909/949 (96%)	747 (82%)	140 (15%)	22 (2%)	4	29
1	I	913/949 (96%)	756 (83%)	125 (14%)	32 (4%)	3	23
1	J	911/949 (96%)	751 (82%)	149 (16%)	11 (1%)	10	40
1	K	900/949 (95%)	735 (82%)	145 (16%)	20 (2%)	5	30
1	L	914/949 (96%)	759 (83%)	131 (14%)	24 (3%)	4	27
2	N	443/571 (78%)	352 (80%)	77 (17%)	14 (3%)	3	24
3	M	301/585 (52%)	263 (87%)	32 (11%)	6 (2%)	6	32
4	P	91/140 (65%)	74 (81%)	15 (16%)	2 (2%)	5	30
4	Q	131/140 (94%)	113 (86%)	15 (12%)	3 (2%)	5	30
4	R	94/140 (67%)	81 (86%)	11 (12%)	2 (2%)	5	31
4	S	92/140 (66%)	73 (79%)	15 (16%)	4 (4%)	2	19
5	U	167/227 (74%)	141 (84%)	22 (13%)	4 (2%)	4	29
5	V	170/227 (75%)	138 (81%)	26 (15%)	6 (4%)	3	23
6	W	22/24 (92%)	19 (86%)	2 (9%)	1 (4%)	2	18
All	All	12429/13582 (92%)	10248 (82%)	1877 (15%)	304 (2%)	4	29

All (304) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	271	GLU
1	A	388	ASN
1	B	417	LEU
1	B	570	LYS
1	B	791	MET
1	B	796	ARG
1	B	943	THR
1	C	8	PRO
1	C	732	PRO
1	D	173	PRO
1	D	296	PRO
1	D	501	TYR
1	D	731	TRP
1	E	518	ILE
1	E	824	ASN
1	E	829	VAL
1	F	296	PRO

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Mol	Chain	Res	Type
1	F	879	PHE
1	G	77	ALA
1	G	173	PRO
1	G	189	GLU
1	G	296	PRO
1	G	932	HIS
1	H	173	PRO
1	H	296	PRO
1	H	726	ASP
1	H	824	ASN
1	I	624	HIS
1	I	729	VAL
1	J	173	PRO
1	J	180	THR
1	J	270	THR
1	K	201	GLN
1	K	330	ARG
1	L	447	SER
1	L	668	PRO
1	L	704	SER
1	L	732	PRO
2	N	139	PHE
2	N	201	VAL
2	N	381	PRO
3	M	217	PRO
4	P	40	LEU
4	S	37	ARG
1	A	99	THR
1	A	234	TYR
1	A	269	THR
1	A	296	PRO
1	A	694	GLY
1	A	752	GLU
1	B	234	TYR
1	B	296	PRO
1	B	512	GLY
1	B	641	GLN
1	B	735	ASP
1	C	312	ARG
1	C	405	GLY
1	C	605	GLY
1	C	668	PRO

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Mol	Chain	Res	Type
1	C	837	ARG
1	C	871	TRP
1	D	879	PHE
1	D	933	ARG
1	E	668	PRO
1	F	234	TYR
1	F	333	PHE
1	F	343	GLY
1	F	794	PHE
1	G	279	ASN
1	G	850	LEU
1	G	940	TYR
1	H	61	SER
1	H	515	ASP
1	H	532	VAL
1	I	350	GLY
1	I	671	ASN
1	I	731	TRP
1	I	837	ARG
1	J	213	GLU
1	J	816	GLN
1	J	837	ARG
1	K	24	LEU
1	K	392	ASP
1	K	490	SER
1	K	735	ASP
1	K	795	PHE
1	L	257	LYS
1	L	438	GLY
1	L	509	VAL
1	L	603	VAL
2	N	273	ILE
2	N	457	ILE
4	Q	28	ASN
4	Q	35	ASP
4	Q	68	ALA
4	S	49	TYR
5	V	32	ASN
5	V	90	VAL
1	A	501	TYR
1	A	846	PHE
1	B	173	PRO

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Mol	Chain	Res	Type
1	B	201	GLN
1	B	253	GLN
1	B	440	GLU
1	B	772	ALA
1	B	797	ASN
1	C	296	PRO
1	C	417	LEU
1	D	824	ASN
1	D	837	ARG
1	D	948	GLY
1	F	825	ASN
1	G	390	ALA
1	G	554	ARG
1	G	882	MET
1	G	939	VAL
1	H	596	SER
1	I	52	PRO
1	I	89	GLY
1	I	181	LYS
1	I	296	PRO
1	I	316	GLY
1	I	760	ASN
1	I	786	SER
1	I	791	MET
1	I	868	ARG
1	K	173	PRO
1	K	331	ASP
1	K	343	GLY
1	K	378	GLY
1	K	891	ASN
1	L	19	ASP
1	L	269	THR
1	L	296	PRO
1	L	337	MET
1	L	943	THR
3	M	176	PRO
3	M	177	GLN
4	R	111	THR
4	S	127	GLN
1	A	20	ALA
1	A	173	PRO
1	A	853	LYS

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Mol	Chain	Res	Type
1	B	202	PRO
1	B	386	MET
1	B	909	PRO
1	C	254	GLN
1	C	576	PRO
1	D	132	PRO
1	D	198	LYS
1	D	563	PRO
1	E	181	LYS
1	E	234	TYR
1	E	442	ASP
1	E	488	SER
1	F	513	LEU
1	F	697	PRO
1	G	202	PRO
1	G	824	ASN
1	G	849	PRO
1	H	727	SER
1	H	785	GLU
1	H	896	ASN
1	I	132	PRO
1	I	340	ASN
1	I	780	GLY
1	I	943	THR
1	J	388	ASN
1	J	791	MET
1	K	668	PRO
1	K	805	VAL
1	L	195	TYR
1	L	462	ILE
1	L	536	ASN
2	N	270	GLY
2	N	500	PRO
5	U	84	PRO
1	A	59	ASP
1	B	418	GLY
1	B	436	GLU
1	C	251	VAL
1	C	302	TYR
1	C	450	ASN
1	C	729	VAL
1	D	48	PRO

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Mol	Chain	Res	Type
1	D	122	ASN
1	D	748	SER
1	E	198	LYS
1	F	89	GLY
1	F	749	VAL
1	G	115	PRO
1	G	201	GLN
1	G	852	GLY
1	H	42	ASN
1	H	304	PRO
1	H	605	GLY
1	H	619	PHE
1	I	234	TYR
1	I	356	ASN
1	I	664	PRO
1	I	916	LEU
1	K	807	ASP
1	K	843	PRO
1	L	312	ARG
2	N	275	TYR
2	N	509	PRO
2	N	545	ASP
4	P	34	ILE
4	R	15	LEU
5	U	185	THR
5	V	28	SER
5	V	209	PRO
1	A	834	PRO
1	B	489	PRO
1	B	557	PRO
1	B	605	GLY
1	C	335	GLY
1	E	576	PRO
1	E	756	VAL
1	E	944	PRO
1	F	324	PRO
1	F	664	PRO
1	F	834	PRO
1	G	19	ASP
1	G	358	VAL
1	G	443	ALA
1	G	664	PRO

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Mol	Chain	Res	Type
1	H	190	GLY
1	H	377	ILE
1	H	698	TYR
1	H	740	PRO
1	H	777	GLY
1	I	253	GLN
1	I	563	PRO
1	I	697	PRO
1	I	703	GLY
1	J	749	VAL
1	J	824	ASN
1	L	418	GLY
1	L	825	ASN
6	W	12	PRO
1	A	304	PRO
1	B	843	PRO
1	D	777	GLY
1	D	829	VAL
1	D	849	PRO
1	E	512	GLY
1	H	438	GLY
1	I	47	ASN
1	J	56	VAL
1	K	697	PRO
1	K	909	PRO
2	N	415	PRO
2	N	418	GLY
2	N	559	GLY
3	M	155	PRO
4	S	31	GLY
5	U	204	PRO
1	A	115	PRO
1	C	26	PRO
1	C	692	GLY
1	C	777	GLY
1	D	70	PRO
1	D	694	GLY
1	E	202	PRO
1	F	563	PRO
1	I	438	GLY
1	I	657	PRO
5	V	64	THR

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Mol	Chain	Res	Type
1	B	753	GLY
1	C	183	GLY
1	C	657	PRO
1	F	934	GLY
1	K	207	GLY
2	N	228	PRO
1	A	56	VAL
1	A	207	GLY
1	B	533	ASN
1	B	731	TRP
1	C	805	VAL
1	D	177	ILE
1	D	482	PRO
1	D	494	ILE
1	E	418	GLY
1	E	732	PRO
1	F	316	GLY
1	F	481	LEU
1	G	692	GLY
1	H	256	GLY
1	L	71	VAL
1	L	256	GLY
1	L	749	VAL
1	L	777	GLY
1	L	930	ARG
3	M	213	GLY
5	U	184	GLY
5	V	208	TYR
1	A	240	PRO
1	B	692	GLY
1	I	418	GLY
1	I	849	PRO
1	K	689	PRO
3	M	68	PRO

4.3.2 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	799/827 (97%)	739 (92%)	60 (8%)	12	38
1	B	794/827 (96%)	742 (94%)	52 (6%)	15	42
1	C	803/827 (97%)	737 (92%)	66 (8%)	10	35
1	D	799/827 (97%)	732 (92%)	67 (8%)	10	34
1	E	795/827 (96%)	726 (91%)	69 (9%)	9	33
1	F	797/827 (96%)	722 (91%)	75 (9%)	8	30
1	G	794/827 (96%)	724 (91%)	70 (9%)	9	33
1	H	796/827 (96%)	730 (92%)	66 (8%)	10	34
1	I	799/827 (97%)	711 (89%)	88 (11%)	6	24
1	J	797/827 (96%)	718 (90%)	79 (10%)	7	28
1	K	789/827 (95%)	709 (90%)	80 (10%)	7	27
1	L	800/827 (97%)	737 (92%)	63 (8%)	11	36
2	N	404/489 (83%)	361 (89%)	43 (11%)	6	26
3	M	253/500 (51%)	233 (92%)	20 (8%)	11	36
4	P	84/112 (75%)	73 (87%)	11 (13%)	4	20
4	Q	106/112 (95%)	97 (92%)	9 (8%)	10	33
4	R	84/112 (75%)	66 (79%)	18 (21%)	1	6
4	S	84/112 (75%)	66 (79%)	18 (21%)	1	6
5	U	144/186 (77%)	132 (92%)	12 (8%)	10	34
5	V	145/186 (78%)	132 (91%)	13 (9%)	9	32
All	All	10866/11733 (93%)	9887 (91%)	979 (9%)	9	32

All (979) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	49	THR
1	A	50	VAL
1	A	53	THR
1	A	55	ASP
1	A	56	VAL
1	A	57	THR
1	A	58	THR
1	A	94	LEU
1	A	103	ILE
1	A	116	TYR

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Mol	Chain	Res	Type
1	A	121	TYR
1	A	184	ILE
1	A	230	MET
1	A	249	ILE
1	A	251	VAL
1	A	270	THR
1	A	284	VAL
1	A	299	HIS
1	A	356	ASN
1	A	360	ASP
1	A	366	THR
1	A	375	ASP
1	A	413	TYR
1	A	420	VAL
1	A	425	THR
1	A	427	THR
1	A	476	ASN
1	A	477	ILE
1	A	479	LEU
1	A	508	VAL
1	A	514	VAL
1	A	549	LEU
1	A	556	VAL
1	A	562	VAL
1	A	566	PHE
1	A	622	MET
1	A	626	THR
1	A	683	LEU
1	A	691	LEU
1	A	700	THR
1	A	717	THR
1	A	749	VAL
1	A	762	THR
1	A	764	ASP
1	A	778	TYR
1	A	805	VAL
1	A	817	VAL
1	A	819	ILE
1	A	850	LEU
1	A	851	ILE
1	A	860	THR
1	A	873	ILE

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Mol	Chain	Res	Type
1	A	875	PHE
1	A	888	LEU
1	A	892	LEU
1	A	910	MET
1	A	927	ARG
1	A	941	LEU
1	A	952	THR
1	B	15	ILE
1	B	24	LEU
1	B	36	GLU
1	B	56	VAL
1	B	76	THR
1	B	85	THR
1	B	124	LEU
1	B	184	ILE
1	B	206	ILE
1	B	247	GLN
1	B	266	PHE
1	B	269	THR
1	B	280	LEU
1	B	281	THR
1	B	305	THR
1	B	344	ASN
1	B	345	MET
1	B	359	VAL
1	B	361	LEU
1	B	373	LEU
1	B	381	THR
1	B	391	VAL
1	B	442	ASP
1	B	508	VAL
1	B	531	ASN
1	B	550	LEU
1	B	556	VAL
1	B	560	ILE
1	B	575	LEU
1	B	624	HIS
1	B	681	THR
1	B	709	ASP
1	B	717	THR
1	B	723	ILE
1	B	726	ASP

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Mol	Chain	Res	Type
1	B	737	LEU
1	B	756	VAL
1	B	759	CYS
1	B	768	VAL
1	B	798	PHE
1	B	835	THR
1	B	850	LEU
1	B	851	ILE
1	B	873	ILE
1	B	886	THR
1	B	926	VAL
1	B	930	ARG
1	B	933	ARG
1	B	939	VAL
1	B	941	LEU
1	B	943	THR
1	B	945	PHE
1	C	15	ILE
1	C	35	THR
1	C	46	ARG
1	C	64	LEU
1	C	103	ILE
1	C	107	LEU
1	C	177	ILE
1	C	180	THR
1	C	184	ILE
1	C	195	TYR
1	C	241	THR
1	C	242	ASN
1	C	243	GLU
1	C	249	ILE
1	C	250	LEU
1	C	253	GLN
1	C	254	GLN
1	C	280	LEU
1	C	284	VAL
1	C	285	VAL
1	C	295	THR
1	C	305	THR
1	C	306	ILE
1	C	332	ASN
1	C	359	VAL

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Mol	Chain	Res	Type
1	C	381	THR
1	C	391	VAL
1	C	400	ILE
1	C	401	ILE
1	C	440	GLU
1	C	464	LEU
1	C	508	VAL
1	C	518	ILE
1	C	549	LEU
1	C	564	GLN
1	C	569	ILE
1	C	597	LEU
1	C	613	ILE
1	C	624	HIS
1	C	626	THR
1	C	630	LEU
1	C	633	MET
1	C	634	LEU
1	C	636	ASN
1	C	663	VAL
1	C	672	TRP
1	C	675	PHE
1	C	682	ARG
1	C	723	ILE
1	C	724	THR
1	C	735	ASP
1	C	747	ARG
1	C	750	ASP
1	C	766	PHE
1	C	767	LEU
1	C	770	MET
1	C	805	VAL
1	C	806	VAL
1	C	824	ASN
1	C	825	ASN
1	C	867	ASP
1	C	868	ARG
1	C	869	THR
1	C	885	LEU
1	C	886	THR
1	C	943	THR
1	D	28	LEU

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Mol	Chain	Res	Type
1	D	35	THR
1	D	41	LEU
1	D	53	THR
1	D	64	LEU
1	D	73	ARG
1	D	79	SER
1	D	95	ASP
1	D	96	MET
1	D	107	LEU
1	D	119	THR
1	D	121	TYR
1	D	169	PHE
1	D	177	ILE
1	D	180	THR
1	D	184	ILE
1	D	186	ILE
1	D	223	VAL
1	D	227	THR
1	D	231	LYS
1	D	268	SER
1	D	269	THR
1	D	280	LEU
1	D	299	HIS
1	D	300	ILE
1	D	306	ILE
1	D	342	THR
1	D	366	THR
1	D	368	LEU
1	D	414	CYS
1	D	420	VAL
1	D	439	TRP
1	D	442	ASP
1	D	469	TRP
1	D	473	LEU
1	D	494	ILE
1	D	514	VAL
1	D	527	ASP
1	D	562	VAL
1	D	589	VAL
1	D	597	LEU
1	D	613	ILE
1	D	626	THR

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Mol	Chain	Res	Type
1	D	645	ASP
1	D	651	ASN
1	D	656	ILE
1	D	678	TRP
1	D	681	THR
1	D	683	LEU
1	D	700	THR
1	D	717	THR
1	D	723	ILE
1	D	724	THR
1	D	737	LEU
1	D	739	THR
1	D	749	VAL
1	D	758	GLN
1	D	762	THR
1	D	765	TRP
1	D	804	GLN
1	D	805	VAL
1	D	815	GLN
1	D	819	ILE
1	D	837	ARG
1	D	851	ILE
1	D	901	LEU
1	D	916	LEU
1	E	31	PHE
1	E	44	LYS
1	E	71	VAL
1	E	76	THR
1	E	112	THR
1	E	133	CYS
1	E	179	ILE
1	E	186	ILE
1	E	201	GLN
1	E	241	THR
1	E	264	MET
1	E	269	THR
1	E	280	LEU
1	E	291	VAL
1	E	305	THR
1	E	306	ILE
1	E	320	MET
1	E	334	ILE

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Mol	Chain	Res	Type
1	E	336	LEU
1	E	337	MET
1	E	341	SER
1	E	342	THR
1	E	348	LEU
1	E	359	VAL
1	E	372	LEU
1	E	375	ASP
1	E	430	LYS
1	E	439	TRP
1	E	441	LYS
1	E	457	ASN
1	E	460	MET
1	E	480	TYR
1	E	481	LEU
1	E	500	THR
1	E	508	VAL
1	E	509	VAL
1	E	514	VAL
1	E	526	LEU
1	E	538	HIS
1	E	549	LEU
1	E	559	HIS
1	E	560	ILE
1	E	562	VAL
1	E	569	ILE
1	E	572	LEU
1	E	574	LEU
1	E	575	LEU
1	E	582	GLU
1	E	589	VAL
1	E	624	HIS
1	E	634	LEU
1	E	656	ILE
1	E	675	PHE
1	E	681	THR
1	E	708	LEU
1	E	724	THR
1	E	727	SER
1	E	728	SER
1	E	730	SER
1	E	742	GLU

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Mol	Chain	Res	Type
1	E	755	ASN
1	E	760	ASN
1	E	770	MET
1	E	778	TYR
1	E	835	THR
1	E	908	ASP
1	E	930	ARG
1	E	941	LEU
1	E	943	THR
1	F	9	GLN
1	F	11	SER
1	F	35	THR
1	F	36	GLU
1	F	37	THR
1	F	66	LEU
1	F	76	THR
1	F	88	VAL
1	F	107	LEU
1	F	121	TYR
1	F	179	ILE
1	F	181	LYS
1	F	184	ILE
1	F	228	THR
1	F	273	THR
1	F	280	LEU
1	F	291	VAL
1	F	295	THR
1	F	299	HIS
1	F	300	ILE
1	F	305	THR
1	F	306	ILE
1	F	327	ILE
1	F	334	ILE
1	F	337	MET
1	F	360	ASP
1	F	362	GLN
1	F	366	THR
1	F	368	LEU
1	F	383	TYR
1	F	391	VAL
1	F	399	ARG
1	F	425	THR

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Mol	Chain	Res	Type
1	F	429	VAL
1	F	450	ASN
1	F	454	VAL
1	F	457	ASN
1	F	464	LEU
1	F	471	ASN
1	F	476	ASN
1	F	509	VAL
1	F	569	ILE
1	F	613	ILE
1	F	626	THR
1	F	634	LEU
1	F	647	LEU
1	F	653	LEU
1	F	663	VAL
1	F	667	ILE
1	F	681	THR
1	F	683	LEU
1	F	684	LYS
1	F	688	THR
1	F	690	SER
1	F	711	THR
1	F	714	LEU
1	F	719	LYS
1	F	724	THR
1	F	729	VAL
1	F	741	ASN
1	F	756	VAL
1	F	767	LEU
1	F	797	ASN
1	F	801	MET
1	F	829	VAL
1	F	835	THR
1	F	866	CYS
1	F	867	ASP
1	F	899	HIS
1	F	908	ASP
1	F	923	PHE
1	F	925	VAL
1	F	929	HIS
1	F	941	LEU
1	F	943	THR

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Mol	Chain	Res	Type
1	G	56	VAL
1	G	78	TYR
1	G	116	TYR
1	G	119	THR
1	G	122	ASN
1	G	124	LEU
1	G	166	THR
1	G	178	ASN
1	G	184	ILE
1	G	188	VAL
1	G	212	TYR
1	G	241	THR
1	G	249	ILE
1	G	269	THR
1	G	284	VAL
1	G	366	THR
1	G	373	LEU
1	G	375	ASP
1	G	417	LEU
1	G	422	ASN
1	G	444	THR
1	G	477	ILE
1	G	485	LEU
1	G	494	ILE
1	G	500	THR
1	G	549	LEU
1	G	556	VAL
1	G	560	ILE
1	G	561	GLN
1	G	589	VAL
1	G	614	CYS
1	G	637	ASP
1	G	639	ASN
1	G	651	ASN
1	G	681	THR
1	G	685	THR
1	G	691	LEU
1	G	693	SER
1	G	696	ASP
1	G	711	THR
1	G	717	THR
1	G	720	LYS

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Mol	Chain	Res	Type
1	G	726	ASP
1	G	737	LEU
1	G	756	VAL
1	G	758	GLN
1	G	762	THR
1	G	763	LYS
1	G	765	TRP
1	G	774	TYR
1	G	776	ILE
1	G	783	ILE
1	G	790	ARG
1	G	805	VAL
1	G	806	VAL
1	G	808	ASP
1	G	809	THR
1	G	812	LYS
1	G	813	ASP
1	G	814	TYR
1	G	829	VAL
1	G	832	LEU
1	G	835	THR
1	G	848	TYR
1	G	867	ASP
1	G	886	THR
1	G	891	ASN
1	G	896	ASN
1	G	939	VAL
1	G	943	THR
1	H	10	TRP
1	H	13	MET
1	H	35	THR
1	H	59	ASP
1	H	76	THR
1	H	96	MET
1	H	184	ILE
1	H	199	THR
1	H	216	ILE
1	H	236	SER
1	H	270	THR
1	H	276	ASN
1	H	291	VAL
1	H	295	THR

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Mol	Chain	Res	Type
1	H	298	THR
1	H	300	ILE
1	H	302	TYR
1	H	336	LEU
1	H	348	LEU
1	H	356	ASN
1	H	368	LEU
1	H	381	THR
1	H	391	VAL
1	H	406	THR
1	H	410	LEU
1	H	487	TYR
1	H	492	VAL
1	H	505	ASN
1	H	509	VAL
1	H	516	CYS
1	H	517	TYR
1	H	518	ILE
1	H	520	LEU
1	H	533	ASN
1	H	559	HIS
1	H	560	ILE
1	H	569	ILE
1	H	570	LYS
1	H	574	LEU
1	H	587	LYS
1	H	589	VAL
1	H	592	VAL
1	H	600	ASP
1	H	602	ARG
1	H	638	THR
1	H	651	ASN
1	H	656	ILE
1	H	665	ILE
1	H	675	PHE
1	H	682	ARG
1	H	683	LEU
1	H	725	PHE
1	H	738	LEU
1	H	745	ILE
1	H	766	PHE
1	H	778	TYR

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Mol	Chain	Res	Type
1	H	835	THR
1	H	836	MET
1	H	840	GLN
1	H	851	ILE
1	H	871	TRP
1	H	886	THR
1	H	890	GLN
1	H	916	LEU
1	H	922	VAL
1	H	929	HIS
1	I	25	SER
1	I	46	ARG
1	I	50	VAL
1	I	54	HIS
1	I	63	ARG
1	I	66	LEU
1	I	69	ILE
1	I	75	ASP
1	I	121	TYR
1	I	179	ILE
1	I	180	THR
1	I	184	ILE
1	I	216	ILE
1	I	224	LEU
1	I	226	LYS
1	I	280	LEU
1	I	313	GLU
1	I	334	ILE
1	I	336	LEU
1	I	340	ASN
1	I	351	GLN
1	I	353	SER
1	I	354	GLN
1	I	381	THR
1	I	413	TYR
1	I	415	PHE
1	I	444	THR
1	I	452	ILE
1	I	462	ILE
1	I	471	ASN
1	I	479	LEU
1	I	485	LEU

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Mol	Chain	Res	Type
1	I	487	TYR
1	I	508	VAL
1	I	514	VAL
1	I	549	LEU
1	I	565	LYS
1	I	572	LEU
1	I	584	ASN
1	I	589	VAL
1	I	597	LEU
1	I	602	ARG
1	I	618	THR
1	I	624	HIS
1	I	626	THR
1	I	651	ASN
1	I	653	LEU
1	I	661	THR
1	I	662	ASN
1	I	663	VAL
1	I	685	THR
1	I	691	LEU
1	I	701	TYR
1	I	724	THR
1	I	728	SER
1	I	737	LEU
1	I	739	THR
1	I	749	VAL
1	I	756	VAL
1	I	766	PHE
1	I	774	TYR
1	I	776	ILE
1	I	789	ASP
1	I	808	ASP
1	I	809	THR
1	I	820	LEU
1	I	822	GLN
1	I	824	ASN
1	I	825	ASN
1	I	828	PHE
1	I	829	VAL
1	I	831	TYR
1	I	832	LEU
1	I	836	MET

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Mol	Chain	Res	Type
1	I	856	VAL
1	I	869	THR
1	I	893	LEU
1	I	907	VAL
1	I	908	ASP
1	I	910	MET
1	I	912	GLU
1	I	920	PHE
1	I	925	VAL
1	I	935	VAL
1	I	936	ILE
1	I	941	LEU
1	I	942	ARG
1	I	943	THR
1	J	11	SER
1	J	35	THR
1	J	37	THR
1	J	41	LEU
1	J	46	ARG
1	J	58	THR
1	J	84	PHE
1	J	94	LEU
1	J	112	THR
1	J	119	THR
1	J	121	TYR
1	J	131	ASN
1	J	188	VAL
1	J	227	THR
1	J	230	MET
1	J	241	THR
1	J	250	LEU
1	J	264	MET
1	J	297	ASP
1	J	299	HIS
1	J	305	THR
1	J	306	ILE
1	J	336	LEU
1	J	360	ASP
1	J	372	LEU
1	J	384	PHE
1	J	392	ASP
1	J	413	TYR

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Mol	Chain	Res	Type
1	J	414	CYS
1	J	415	PHE
1	J	430	LYS
1	J	442	ASP
1	J	479	LEU
1	J	481	LEU
1	J	485	LEU
1	J	494	ILE
1	J	505	ASN
1	J	508	VAL
1	J	532	VAL
1	J	547	SER
1	J	554	ARG
1	J	560	ILE
1	J	570	LYS
1	J	571	ASN
1	J	573	LEU
1	J	589	VAL
1	J	594	GLN
1	J	618	THR
1	J	626	THR
1	J	653	LEU
1	J	665	ILE
1	J	675	PHE
1	J	681	THR
1	J	695	TYR
1	J	700	THR
1	J	724	THR
1	J	738	LEU
1	J	758	GLN
1	J	773	ASN
1	J	801	MET
1	J	809	THR
1	J	816	GLN
1	J	819	ILE
1	J	828	PHE
1	J	832	LEU
1	J	837	ARG
1	J	848	TYR
1	J	890	GLN
1	J	893	LEU
1	J	896	ASN

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Mol	Chain	Res	Type
1	J	904	THR
1	J	907	VAL
1	J	918	VAL
1	J	919	LEU
1	J	922	VAL
1	J	926	VAL
1	J	932	HIS
1	J	935	VAL
1	J	941	LEU
1	K	76	THR
1	K	85	THR
1	K	94	LEU
1	K	119	THR
1	K	167	HIS
1	K	178	ASN
1	K	184	ILE
1	K	253	GLN
1	K	257	LYS
1	K	268	SER
1	K	280	LEU
1	K	281	THR
1	K	305	THR
1	K	329	PHE
1	K	339	TYR
1	K	342	THR
1	K	348	LEU
1	K	351	GLN
1	K	361	LEU
1	K	364	ARG
1	K	368	LEU
1	K	372	LEU
1	K	374	LEU
1	K	375	ASP
1	K	383	TYR
1	K	386	MET
1	K	391	VAL
1	K	399	ARG
1	K	402	GLU
1	K	417	LEU
1	K	420	VAL
1	K	422	ASN
1	K	450	ASN

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Mol	Chain	Res	Type
1	K	461	GLU
1	K	472	PHE
1	K	473	LEU
1	K	488	SER
1	K	490	SER
1	K	495	SER
1	K	496	ASP
1	K	504	MET
1	K	509	VAL
1	K	520	LEU
1	K	529	MET
1	K	546	ARG
1	K	549	LEU
1	K	561	GLN
1	K	569	ILE
1	K	570	LYS
1	K	624	HIS
1	K	656	ILE
1	K	667	ILE
1	K	681	THR
1	K	688	THR
1	K	700	THR
1	K	734	ASN
1	K	738	LEU
1	K	748	SER
1	K	749	VAL
1	K	750	ASP
1	K	762	THR
1	K	771	LEU
1	K	776	ILE
1	K	801	MET
1	K	805	VAL
1	K	819	ILE
1	K	835	THR
1	K	837	ARG
1	K	842	TYR
1	K	848	TYR
1	K	850	LEU
1	K	851	ILE
1	K	866	CYS
1	K	877	SER
1	K	893	LEU

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Mol	Chain	Res	Type
1	K	907	VAL
1	K	910	MET
1	K	916	LEU
1	K	922	VAL
1	K	939	VAL
1	L	35	THR
1	L	37	THR
1	L	60	ARG
1	L	96	MET
1	L	121	TYR
1	L	184	ILE
1	L	188	VAL
1	L	228	THR
1	L	291	VAL
1	L	292	ASP
1	L	295	THR
1	L	300	ILE
1	L	306	ILE
1	L	355	LEU
1	L	360	ASP
1	L	368	LEU
1	L	373	LEU
1	L	381	THR
1	L	382	ARG
1	L	391	VAL
1	L	429	VAL
1	L	444	THR
1	L	445	GLU
1	L	454	VAL
1	L	546	ARG
1	L	549	LEU
1	L	550	LEU
1	L	569	ILE
1	L	584	ASN
1	L	626	THR
1	L	634	LEU
1	L	656	ILE
1	L	663	VAL
1	L	671	ASN
1	L	672	TRP
1	L	681	THR
1	L	683	LEU

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Mol	Chain	Res	Type
1	L	684	LYS
1	L	685	THR
1	L	707	TYR
1	L	708	LEU
1	L	761	MET
1	L	762	THR
1	L	769	GLN
1	L	774	TYR
1	L	783	ILE
1	L	805	VAL
1	L	806	VAL
1	L	823	HIS
1	L	824	ASN
1	L	825	ASN
1	L	865	LEU
1	L	866	CYS
1	L	867	ASP
1	L	869	THR
1	L	885	LEU
1	L	893	LEU
1	L	910	MET
1	L	929	HIS
1	L	936	ILE
1	L	943	THR
1	L	951	THR
1	L	952	THR
2	N	49	THR
2	N	52	ARG
2	N	69	VAL
2	N	77	THR
2	N	84	TYR
2	N	91	PHE
2	N	135	ASN
2	N	140	THR
2	N	147	VAL
2	N	161	LEU
2	N	170	LEU
2	N	178	THR
2	N	201	VAL
2	N	211	ASP
2	N	217	LEU
2	N	230	VAL

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Mol	Chain	Res	Type
2	N	241	ILE
2	N	251	THR
2	N	283	ILE
2	N	287	LEU
2	N	394	ILE
2	N	397	ASP
2	N	417	THR
2	N	430	VAL
2	N	439	TRP
2	N	445	MET
2	N	447	ASP
2	N	450	THR
2	N	454	THR
2	N	457	ILE
2	N	468	LEU
2	N	474	SER
2	N	477	ASN
2	N	481	VAL
2	N	482	TYR
2	N	495	VAL
2	N	499	PHE
2	N	504	ILE
2	N	505	LEU
2	N	529	LEU
2	N	545	ASP
2	N	553	TYR
2	N	554	VAL
3	M	11	ARG
3	M	35	MET
3	M	95	TYR
3	M	98	LEU
3	M	101	ARG
3	M	114	LEU
3	M	117	LEU
3	M	147	LEU
3	M	154	VAL
3	M	172	VAL
3	M	196	LEU
3	M	197	GLN
3	M	198	THR
3	M	218	THR
3	M	231	ASN

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Mol	Chain	Res	Type
3	M	239	ILE
3	M	250	ARG
3	M	257	LEU
3	M	289	ASP
3	M	297	LEU
4	P	3	THR
4	P	11	VAL
4	P	15	LEU
4	P	25	VAL
4	P	35	ASP
4	P	39	VAL
4	P	45	THR
4	P	46	THR
4	P	47	LEU
4	P	98	ASP
4	P	121	LEU
4	Q	6	PHE
4	Q	10	ILE
4	Q	26	ARG
4	Q	55	THR
4	Q	57	LEU
4	Q	100	LEU
4	Q	110	LEU
4	Q	112	ARG
4	Q	114	LEU
4	R	5	SER
4	R	6	PHE
4	R	7	ASP
4	R	10	ILE
4	R	17	THR
4	R	19	MET
4	R	25	VAL
4	R	45	THR
4	R	46	THR
4	R	51	THR
4	R	99	LYS
4	R	104	LEU
4	R	107	LEU
4	R	110	LEU
4	R	114	LEU
4	R	117	VAL
4	R	121	LEU

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Mol	Chain	Res	Type
4	R	125	ARG
4	S	10	ILE
4	S	11	VAL
4	S	13	SER
4	S	15	LEU
4	S	16	THR
4	S	17	THR
4	S	26	ARG
4	S	27	GLN
4	S	29	VAL
4	S	30	MET
4	S	33	SER
4	S	34	ILE
4	S	35	ASP
4	S	57	LEU
4	S	98	ASP
4	S	114	LEU
4	S	121	LEU
4	S	122	LEU
5	U	7	THR
5	U	29	THR
5	U	31	ILE
5	U	63	THR
5	U	90	VAL
5	U	91	LEU
5	U	168	ILE
5	U	173	THR
5	U	189	ILE
5	U	193	VAL
5	U	196	VAL
5	U	210	ASP
5	V	10	MET
5	V	12	SER
5	V	28	SER
5	V	29	THR
5	V	32	ASN
5	V	40	MET
5	V	44	VAL
5	V	52	ASN
5	V	62	THR
5	V	166	GLN
5	V	168	ILE

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Mol	Chain	Res	Type
5	V	171	LEU
5	V	213	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (373) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	131	ASN
1	A	171	GLN
1	A	279	ASN
1	A	310	ASN
1	A	322	ASN
1	A	340	ASN
1	A	351	GLN
1	A	356	ASN
1	A	365	ASN
1	A	403	ASN
1	A	412	ASN
1	A	456	ASN
1	A	536	ASN
1	A	537	HIS
1	A	540	ASN
1	A	561	GLN
1	A	584	ASN
1	A	624	HIS
1	A	639	ASN
1	A	644	ASN
1	A	715	ASN
1	A	755	ASN
1	A	779	GLN
1	A	797	ASN
1	A	816	GLN
1	A	824	ASN
1	A	825	ASN
1	A	840	GLN
1	A	890	GLN
1	B	14	HIS
1	B	131	ASN
1	B	167	HIS
1	B	171	GLN
1	B	210	GLN
1	B	253	GLN

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Mol	Chain	Res	Type
1	B	310	ASN
1	B	322	ASN
1	B	332	ASN
1	B	340	ASN
1	B	356	ASN
1	B	457	ASN
1	B	533	ASN
1	B	536	ASN
1	B	540	ASN
1	B	561	GLN
1	B	584	ASN
1	B	594	GLN
1	B	636	ASN
1	B	639	ASN
1	B	651	ASN
1	B	671	ASN
1	B	758	GLN
1	B	775	ASN
1	B	779	GLN
1	B	804	GLN
1	B	845	ASN
1	B	878	ASN
1	B	896	ASN
1	C	30	GLN
1	C	42	ASN
1	C	62	GLN
1	C	122	ASN
1	C	171	GLN
1	C	178	ASN
1	C	299	HIS
1	C	310	ASN
1	C	318	GLN
1	C	332	ASN
1	C	354	GLN
1	C	388	ASN
1	C	457	ASN
1	C	499	ASN
1	C	505	ASN
1	C	564	GLN
1	C	594	GLN
1	C	624	HIS
1	C	625	ASN

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Mol	Chain	Res	Type
1	C	639	ASN
1	C	659	ASN
1	C	662	ASN
1	C	671	ASN
1	C	734	ASN
1	C	773	ASN
1	C	797	ASN
1	C	804	GLN
1	D	14	HIS
1	D	43	ASN
1	D	171	GLN
1	D	205	GLN
1	D	244	ASN
1	D	310	ASN
1	D	332	ASN
1	D	356	ASN
1	D	389	GLN
1	D	403	ASN
1	D	497	ASN
1	D	533	ASN
1	D	536	ASN
1	D	561	GLN
1	D	564	GLN
1	D	571	ASN
1	D	636	ASN
1	D	651	ASN
1	D	662	ASN
1	D	715	ASN
1	D	758	GLN
1	D	769	GLN
1	D	821	HIS
1	D	890	GLN
1	D	929	HIS
1	D	949	ASN
1	E	42	ASN
1	E	47	ASN
1	E	122	ASN
1	E	131	ASN
1	E	178	ASN
1	E	244	ASN
1	E	253	GLN
1	E	322	ASN

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Mol	Chain	Res	Type
1	E	332	ASN
1	E	354	GLN
1	E	422	ASN
1	E	437	ASN
1	E	463	ASN
1	E	465	ASN
1	E	471	ASN
1	E	519	ASN
1	E	552	ASN
1	E	561	GLN
1	E	571	ASN
1	E	590	ASN
1	E	594	GLN
1	E	639	ASN
1	E	671	ASN
1	E	779	GLN
1	E	797	ASN
1	E	824	ASN
1	E	878	ASN
1	F	122	ASN
1	F	185	GLN
1	F	201	GLN
1	F	244	ASN
1	F	265	GLN
1	F	299	HIS
1	F	340	ASN
1	F	351	GLN
1	F	362	GLN
1	F	365	ASN
1	F	371	GLN
1	F	412	ASN
1	F	437	ASN
1	F	450	ASN
1	F	457	ASN
1	F	465	ASN
1	F	538	HIS
1	F	540	ASN
1	F	559	HIS
1	F	564	GLN
1	F	584	ASN
1	F	594	GLN
1	F	651	ASN

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Mol	Chain	Res	Type
1	F	734	ASN
1	F	769	GLN
1	F	773	ASN
1	F	775	ASN
1	F	779	GLN
1	F	845	ASN
1	F	932	HIS
1	G	30	GLN
1	G	167	HIS
1	G	171	GLN
1	G	210	GLN
1	G	253	GLN
1	G	317	GLN
1	G	322	ASN
1	G	404	HIS
1	G	437	ASN
1	G	467	ASN
1	G	471	ASN
1	G	491	ASN
1	G	531	ASN
1	G	538	HIS
1	G	540	ASN
1	G	552	ASN
1	G	559	HIS
1	G	564	GLN
1	G	571	ASN
1	G	584	ASN
1	G	639	ASN
1	G	641	GLN
1	G	659	ASN
1	G	662	ASN
1	G	715	ASN
1	G	773	ASN
1	G	775	ASN
1	G	799	GLN
1	G	804	GLN
1	G	891	ASN
1	G	896	ASN
1	H	14	HIS
1	H	171	GLN
1	H	205	GLN
1	H	242	ASN

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Mol	Chain	Res	Type
1	H	299	HIS
1	H	310	ASN
1	H	325	ASN
1	H	354	GLN
1	H	389	GLN
1	H	422	ASN
1	H	465	ASN
1	H	471	ASN
1	H	561	GLN
1	H	590	ASN
1	H	594	GLN
1	H	624	HIS
1	H	641	GLN
1	H	651	ASN
1	H	671	ASN
1	H	716	HIS
1	H	758	GLN
1	H	775	ASN
1	H	779	GLN
1	H	861	GLN
1	H	890	GLN
1	H	932	HIS
1	I	42	ASN
1	I	47	ASN
1	I	122	ASN
1	I	201	GLN
1	I	205	GLN
1	I	299	HIS
1	I	310	ASN
1	I	317	GLN
1	I	322	ASN
1	I	325	ASN
1	I	371	GLN
1	I	388	ASN
1	I	403	ASN
1	I	404	HIS
1	I	412	ASN
1	I	463	ASN
1	I	467	ASN
1	I	552	ASN
1	I	571	ASN
1	I	590	ASN

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Mol	Chain	Res	Type
1	I	639	ASN
1	I	644	ASN
1	I	662	ASN
1	I	755	ASN
1	I	769	GLN
1	I	779	GLN
1	I	797	ASN
1	I	878	ASN
1	I	890	GLN
1	I	896	ASN
1	J	47	ASN
1	J	131	ASN
1	J	210	GLN
1	J	265	GLN
1	J	310	ASN
1	J	317	GLN
1	J	322	ASN
1	J	450	ASN
1	J	456	ASN
1	J	465	ASN
1	J	471	ASN
1	J	531	ASN
1	J	536	ASN
1	J	552	ASN
1	J	571	ASN
1	J	639	ASN
1	J	662	ASN
1	J	671	ASN
1	J	741	ASN
1	J	755	ASN
1	J	758	GLN
1	J	769	GLN
1	J	779	GLN
1	J	797	ASN
1	J	799	GLN
1	J	822	GLN
1	J	825	ASN
1	K	122	ASN
1	K	167	HIS
1	K	317	GLN
1	K	322	ASN
1	K	362	GLN

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Mol	Chain	Res	Type
1	K	404	HIS
1	K	437	ASN
1	K	450	ASN
1	K	471	ASN
1	K	531	ASN
1	K	533	ASN
1	K	536	ASN
1	K	540	ASN
1	K	552	ASN
1	K	564	GLN
1	K	599	ASN
1	K	636	ASN
1	K	639	ASN
1	K	641	GLN
1	K	644	ASN
1	K	734	ASN
1	K	755	ASN
1	K	758	GLN
1	K	760	ASN
1	K	775	ASN
1	K	797	ASN
1	K	799	GLN
1	K	823	HIS
1	L	18	GLN
1	L	47	ASN
1	L	62	GLN
1	L	178	ASN
1	L	261	GLN
1	L	322	ASN
1	L	332	ASN
1	L	389	GLN
1	L	412	ASN
1	L	437	ASN
1	L	471	ASN
1	L	476	ASN
1	L	499	ASN
1	L	540	ASN
1	L	594	GLN
1	L	599	ASN
1	L	639	ASN
1	L	662	ASN
1	L	758	GLN

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Mol	Chain	Res	Type
1	L	824	ASN
2	N	86	ASN
2	N	90	ASN
2	N	141	ASN
2	N	157	ASN
2	N	174	ASN
2	N	185	ASN
2	N	191	HIS
2	N	199	ASN
2	N	233	ASN
2	N	282	ASN
2	N	396	ASN
2	N	488	GLN
2	N	497	ASN
3	M	17	GLN
3	M	22	ASN
3	M	144	ASN
3	M	158	GLN
3	M	200	ASN
3	M	203	GLN
3	M	209	GLN
3	M	231	ASN
3	M	267	GLN
3	M	287	GLN
4	P	27	GLN
4	P	28	ASN
4	P	43	ASN
4	P	115	ASN
4	R	28	ASN
4	R	43	ASN
4	S	28	ASN
4	S	106	GLN
5	U	25	GLN
5	U	39	HIS
5	U	52	ASN
5	U	70	ASN
5	U	107	GLN
5	U	187	GLN
5	U	211	GLN
5	V	16	GLN
5	V	32	ASN
5	V	107	GLN

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Mol	Chain	Res	Type
5	V	187	GLN

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.