



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:26 PM UTC

PDB ID : 3DBR / pdb_00003dbr
Title : Structural Dissection of a Gating Mechanism Preventing Misactivation of Ubiquitin by NEDD8's E1 (APPBP1-UBA3Arg190Gln-NEDD8Ala72Arg)
Authors : Souphron, J.; Schulman, B.A.
Deposited on : 2008-06-02
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

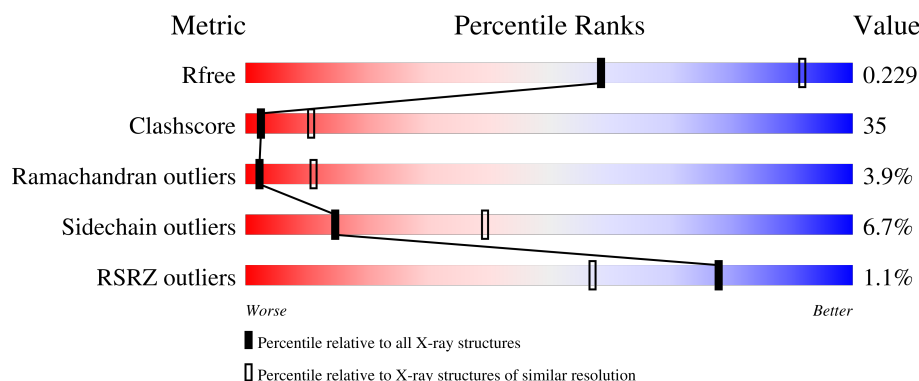
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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

Mol	Chain	Length	Quality of chain
1	A	531	% 44% 45% 7% ...
1	C	531	2% 45% 44% 8% ...
1	E	531	% 53% 36% 7% ...
1	G	531	% 48% 42% 5% .
2	B	434	% 47% 42% 9% .

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Mol	Chain	Length	Quality of chain					
2	D	434		%				
2	F	434		43%	46%	8%	..	
2	F	434		44%	48%	6%	..	
2	H	434		2%				
2	H	434		36%	50%	10%	..	
3	I	88		5%				
3	I	88		44%	43%	7%	. .	
3	J	88		35%	45%	7%	13%	
3	K	88		%				
3	K	88		40%	36%	10%	. 13%	
3	L	88		19%	57%	11%	. 11%	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32424 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 NEDD8-activating enzyme E1 regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			4104	2600	699	790	15			
1	C	516	Total	C	N	O	S	0	0	0
			4096	2596	698	787	15			
1	E	515	Total	C	N	O	S	0	0	0
			4093	2597	696	785	15			
1	G	508	Total	C	N	O	S	0	0	0
			4038	2563	686	774	15			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q13564
A	0	SER	-	expression tag	UNP Q13564
A	?	-	ASN	deletion	UNP Q13564
A	?	-	GLU	deletion	UNP Q13564
A	?	-	ASN	deletion	UNP Q13564
A	?	-	GLY	deletion	UNP Q13564
A	?	-	ALA	deletion	UNP Q13564
C	-1	GLY	-	expression tag	UNP Q13564
C	0	SER	-	expression tag	UNP Q13564
C	?	-	ASN	deletion	UNP Q13564
C	?	-	GLU	deletion	UNP Q13564
C	?	-	ASN	deletion	UNP Q13564
C	?	-	GLY	deletion	UNP Q13564
C	?	-	ALA	deletion	UNP Q13564
E	-1	GLY	-	expression tag	UNP Q13564
E	0	SER	-	expression tag	UNP Q13564
E	?	-	ASN	deletion	UNP Q13564
E	?	-	GLU	deletion	UNP Q13564
E	?	-	ASN	deletion	UNP Q13564
E	?	-	GLY	deletion	UNP Q13564
E	?	-	ALA	deletion	UNP Q13564

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP Q13564
G	0	SER	-	expression tag	UNP Q13564
G	?	-	ASN	deletion	UNP Q13564
G	?	-	GLU	deletion	UNP Q13564
G	?	-	ASN	deletion	UNP Q13564
G	?	-	GLY	deletion	UNP Q13564
G	?	-	ALA	deletion	UNP Q13564

- Molecule 2 is a protein called NEDD8-activating enzyme E1 catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	0	0
			3402	2174	575	636	17			
2	D	431	Total	C	N	O	S	0	0	0
			3399	2174	575	633	17			
2	F	431	Total	C	N	O	S	0	0	0
			3395	2171	574	633	17			
2	H	431	Total	C	N	O	S	0	0	0
			3387	2164	573	633	17			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	expression tag	UNP Q8TBC4
B	10	LYS	-	expression tag	UNP Q8TBC4
B	11	LEU	-	expression tag	UNP Q8TBC4
B	190	GLN	ARG	engineered mutation	UNP Q8TBC4
B	216	ALA	CYS	engineered mutation	UNP Q8TBC4
D	9	MET	-	expression tag	UNP Q8TBC4
D	10	LYS	-	expression tag	UNP Q8TBC4
D	11	LEU	-	expression tag	UNP Q8TBC4
D	190	GLN	ARG	engineered mutation	UNP Q8TBC4
D	216	ALA	CYS	engineered mutation	UNP Q8TBC4
F	9	MET	-	expression tag	UNP Q8TBC4
F	10	LYS	-	expression tag	UNP Q8TBC4
F	11	LEU	-	expression tag	UNP Q8TBC4
F	190	GLN	ARG	engineered mutation	UNP Q8TBC4
F	216	ALA	CYS	engineered mutation	UNP Q8TBC4
H	9	MET	-	expression tag	UNP Q8TBC4
H	10	LYS	-	expression tag	UNP Q8TBC4
H	11	LEU	-	expression tag	UNP Q8TBC4
H	190	GLN	ARG	engineered mutation	UNP Q8TBC4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	216	ALA	CYS	engineered mutation	UNP Q8TBC4

- Molecule 3 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	85	Total	C	N	O	S	0	0	0
			666	414	122	128	2			
3	J	77	Total	C	N	O	S	0	0	0
			612	384	108	118	2			
3	K	77	Total	C	N	O	S	0	0	0
			612	384	108	118	2			
3	L	78	Total	C	N	O	S	0	0	0
			616	386	109	119	2			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	89	GLY	-	expression tag	UNP Q15843
I	90	SER	-	expression tag	UNP Q15843
I	91	ARG	-	expression tag	UNP Q15843
I	92	ARG	-	expression tag	UNP Q15843
I	93	ALA	-	expression tag	UNP Q15843
I	94	SER	-	expression tag	UNP Q15843
I	95	VAL	-	expression tag	UNP Q15843
I	96	GLY	-	expression tag	UNP Q15843
I	97	SER	-	expression tag	UNP Q15843
I	98	GLY	-	expression tag	UNP Q15843
I	99	GLY	-	expression tag	UNP Q15843
I	100	SER	-	expression tag	UNP Q15843
I	172	ARG	ALA	engineered mutation	UNP Q15843
J	89	GLY	-	expression tag	UNP Q15843
J	90	SER	-	expression tag	UNP Q15843
J	91	ARG	-	expression tag	UNP Q15843
J	92	ARG	-	expression tag	UNP Q15843
J	93	ALA	-	expression tag	UNP Q15843
J	94	SER	-	expression tag	UNP Q15843
J	95	VAL	-	expression tag	UNP Q15843
J	96	GLY	-	expression tag	UNP Q15843
J	97	SER	-	expression tag	UNP Q15843
J	98	GLY	-	expression tag	UNP Q15843
J	99	GLY	-	expression tag	UNP Q15843
J	100	SER	-	expression tag	UNP Q15843

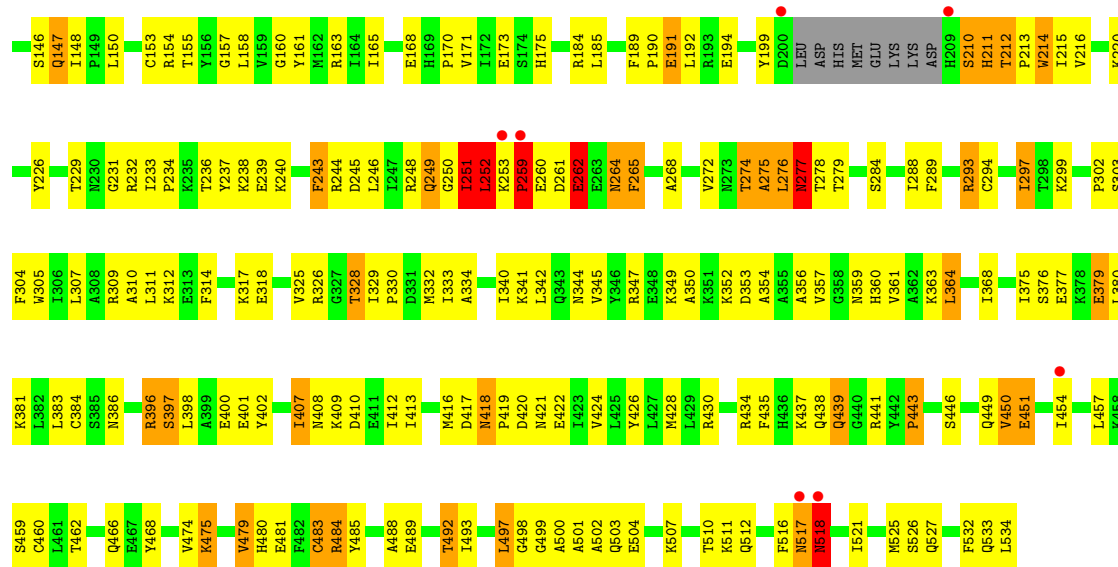
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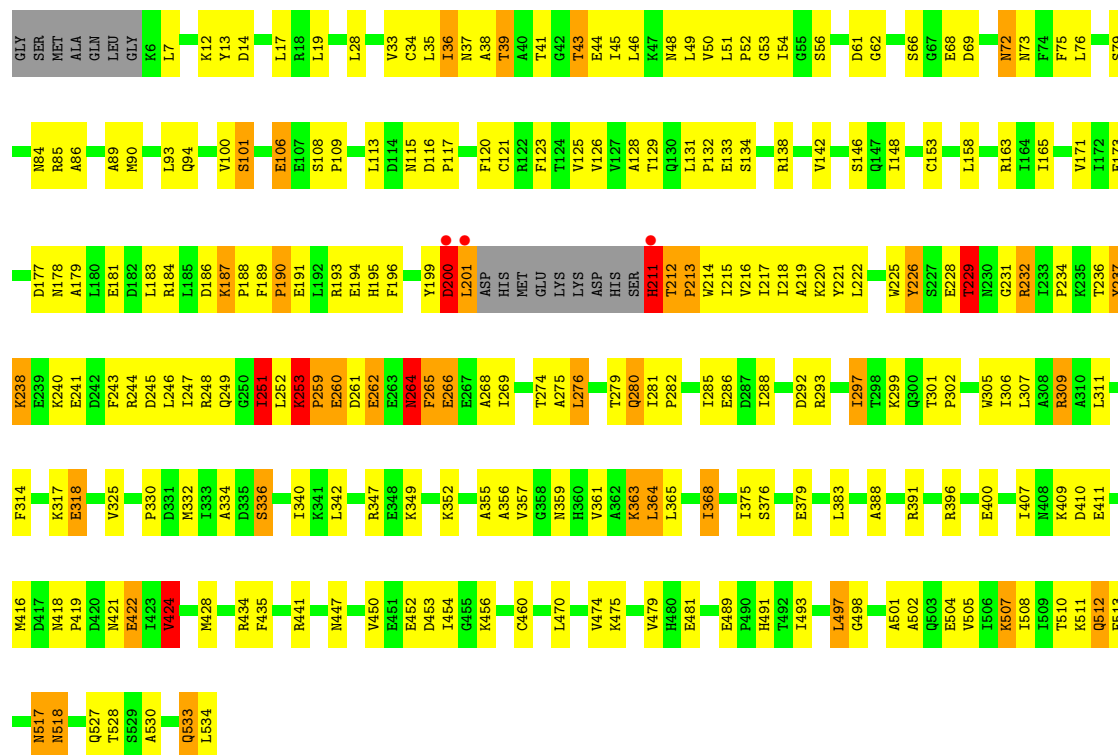
Chain	Residue	Modelled	Actual	Comment	Reference
J	172	ARG	ALA	engineered mutation	UNP Q15843
K	89	GLY	-	expression tag	UNP Q15843
K	90	SER	-	expression tag	UNP Q15843
K	91	ARG	-	expression tag	UNP Q15843
K	92	ARG	-	expression tag	UNP Q15843
K	93	ALA	-	expression tag	UNP Q15843
K	94	SER	-	expression tag	UNP Q15843
K	95	VAL	-	expression tag	UNP Q15843
K	96	GLY	-	expression tag	UNP Q15843
K	97	SER	-	expression tag	UNP Q15843
K	98	GLY	-	expression tag	UNP Q15843
K	99	GLY	-	expression tag	UNP Q15843
K	100	SER	-	expression tag	UNP Q15843
K	172	ARG	ALA	engineered mutation	UNP Q15843
L	89	GLY	-	expression tag	UNP Q15843
L	90	SER	-	expression tag	UNP Q15843
L	91	ARG	-	expression tag	UNP Q15843
L	92	ARG	-	expression tag	UNP Q15843
L	93	ALA	-	expression tag	UNP Q15843
L	94	SER	-	expression tag	UNP Q15843
L	95	VAL	-	expression tag	UNP Q15843
L	96	GLY	-	expression tag	UNP Q15843
L	97	SER	-	expression tag	UNP Q15843
L	98	GLY	-	expression tag	UNP Q15843
L	99	GLY	-	expression tag	UNP Q15843
L	100	SER	-	expression tag	UNP Q15843
L	172	ARG	ALA	engineered mutation	UNP Q15843

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

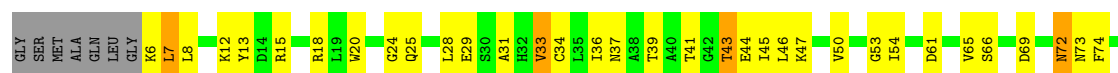
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0
4	H	1	Total Zn 1 1	0	0

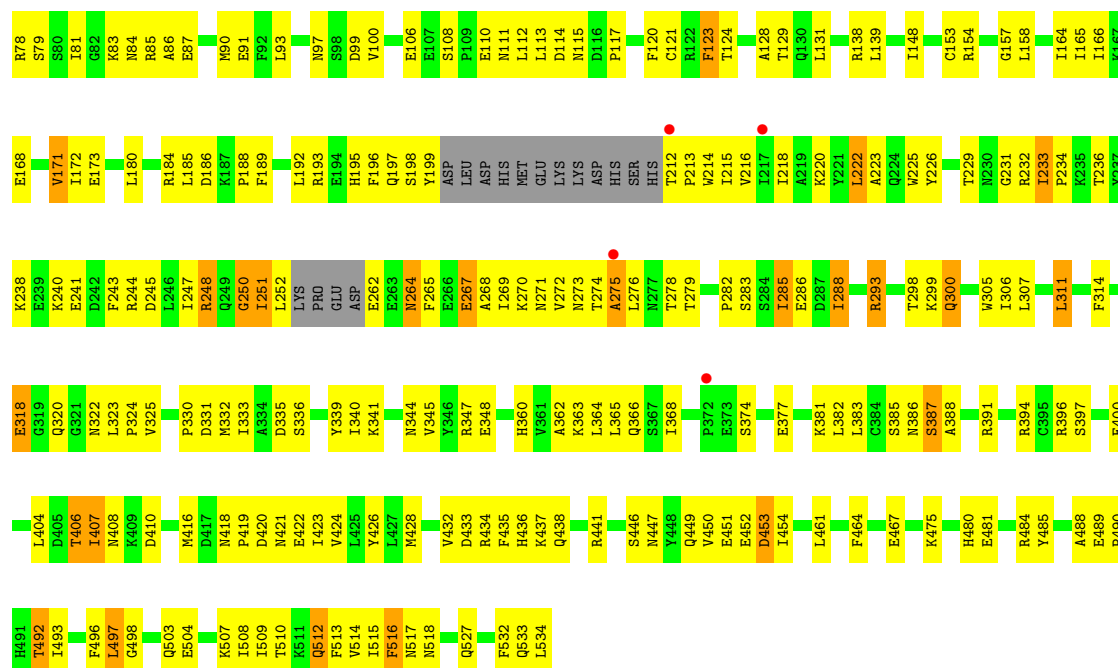


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

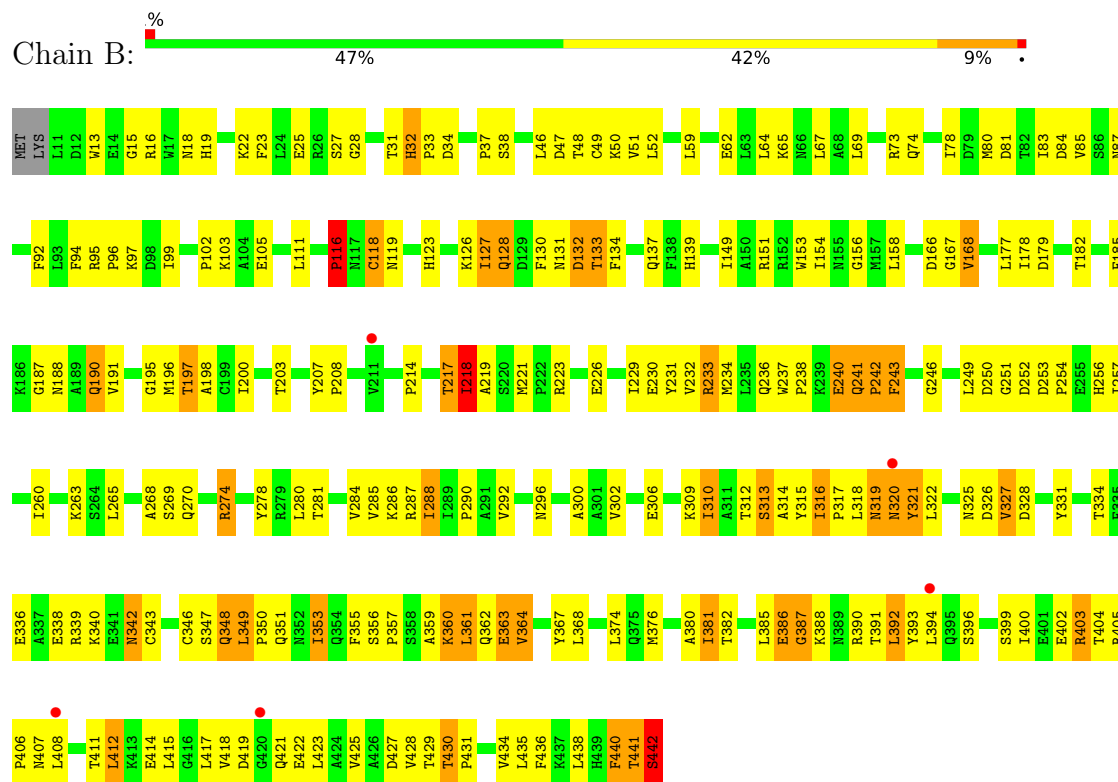


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

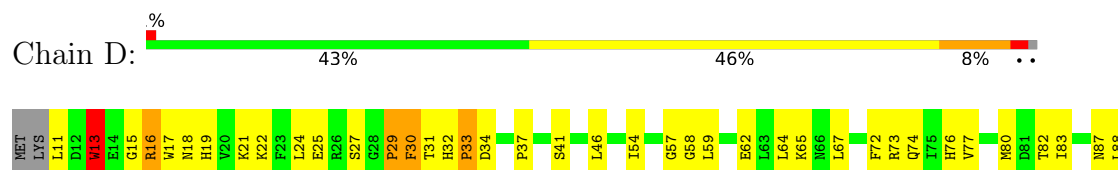


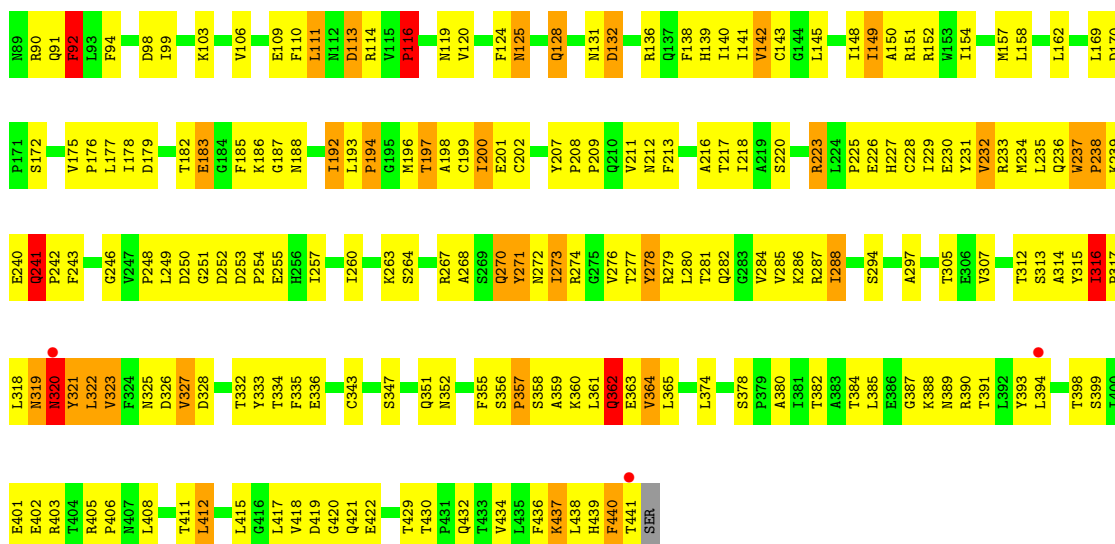


• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

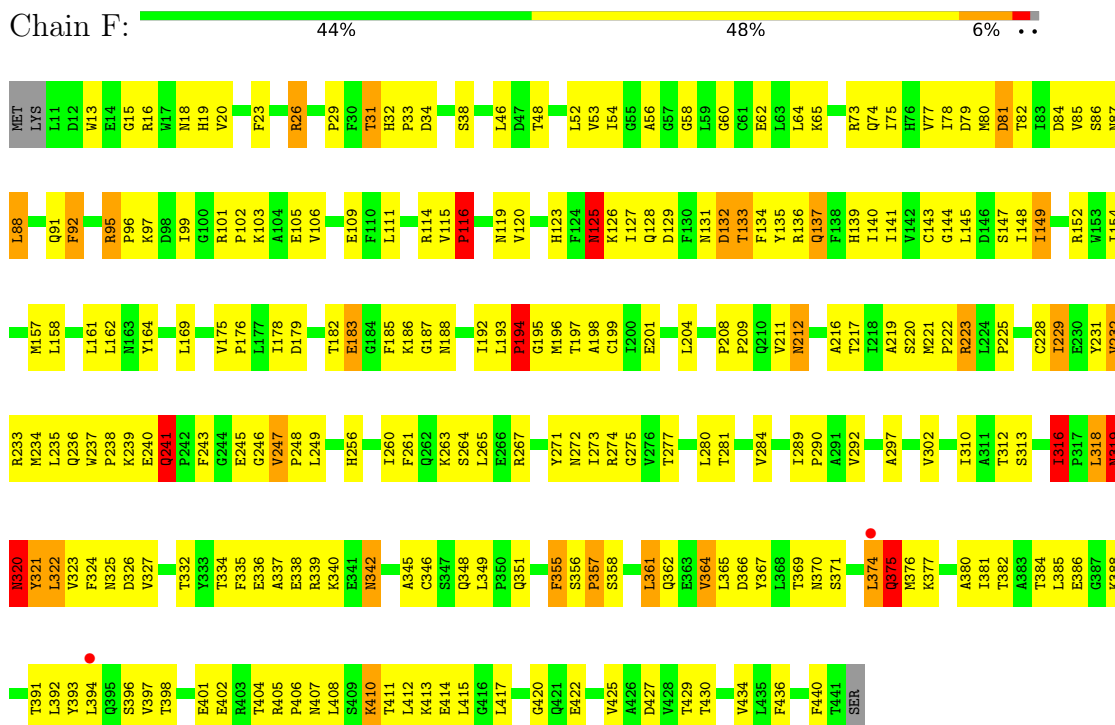


• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

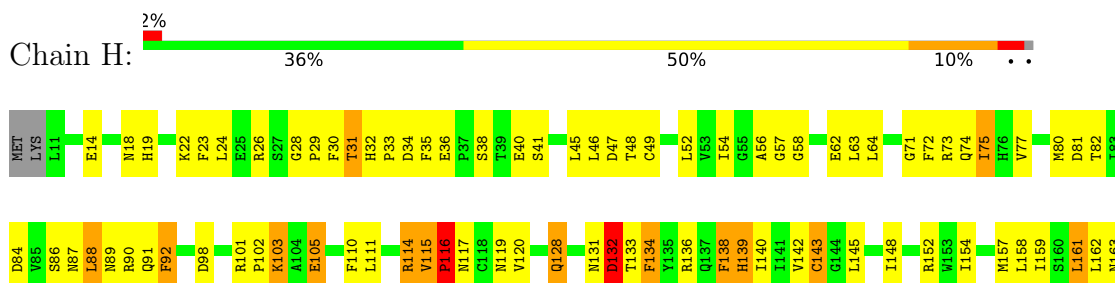


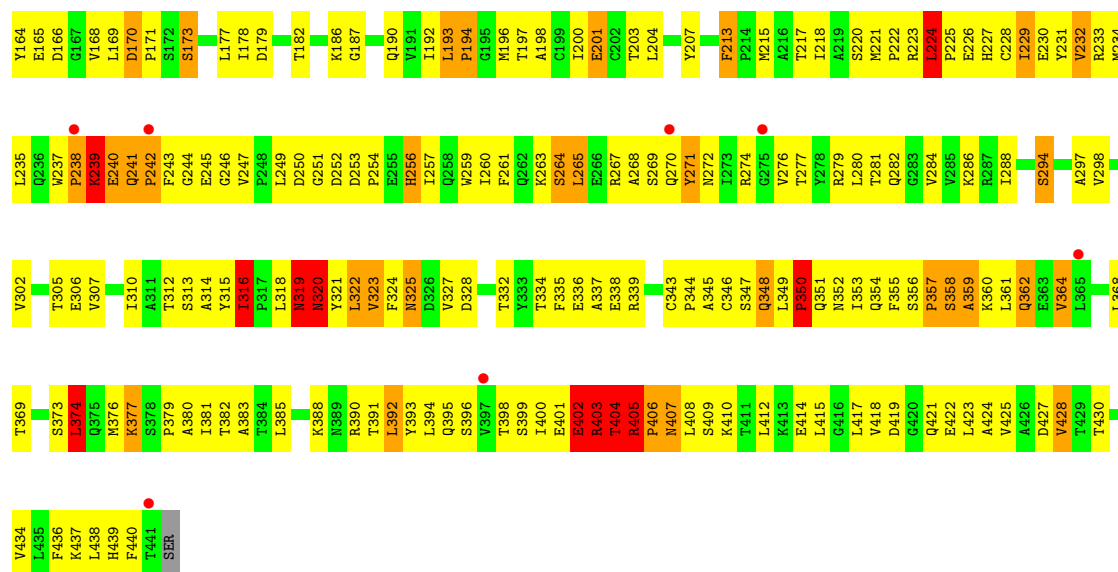


- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

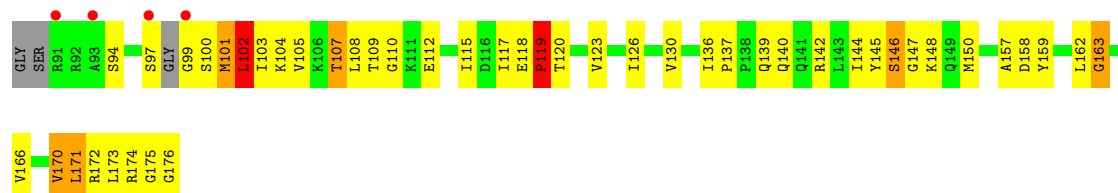
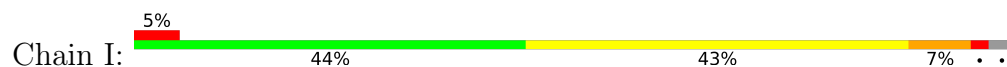


- Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

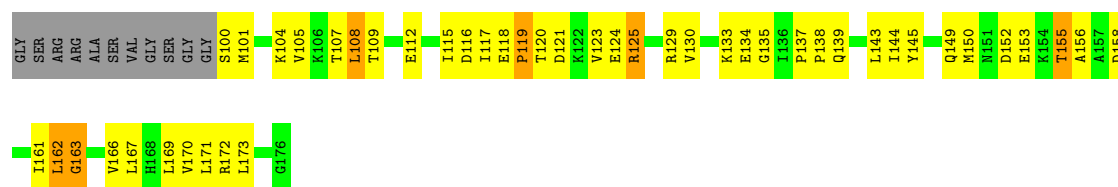




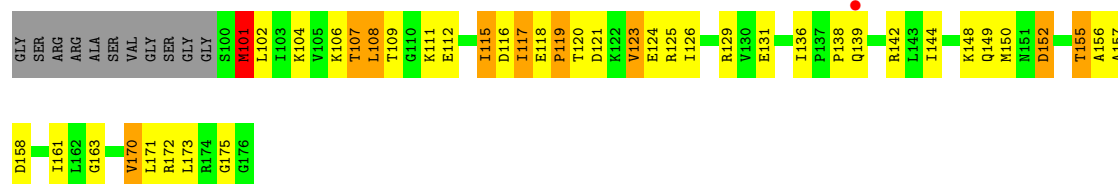
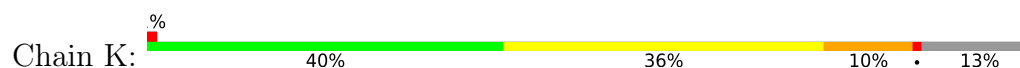
• Molecule 3: NEDD8



• Molecule 3: NEDD8

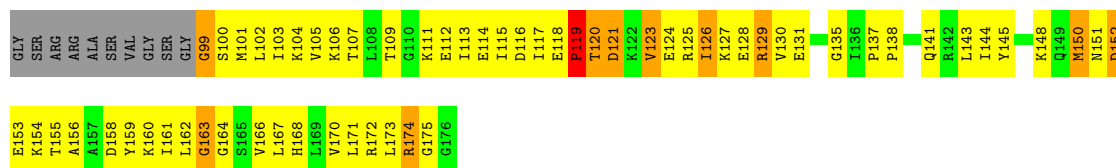
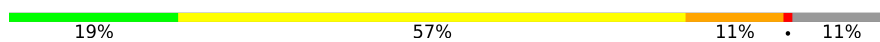


• Molecule 3: NEDD8



• Molecule 3: NEDD8

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.32Å 198.53Å 208.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.05 50.00 – 3.07	Depositor EDS
% Data completeness (in resolution range)	93.7 (50.00-3.05) 95.3 (50.00-3.07)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.07Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.280 0.232 , 0.229	Depositor DCC
R_{free} test set	4982 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32424	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.56	1/4184 (0.0%)	1.10	33/5660 (0.6%)
1	C	0.60	3/4176 (0.1%)	1.13	28/5649 (0.5%)
1	E	0.62	2/4172 (0.0%)	1.09	28/5643 (0.5%)
1	G	0.52	0/4114	1.06	23/5563 (0.4%)
2	B	0.64	2/3480 (0.1%)	1.11	21/4736 (0.4%)
2	D	0.54	0/3477	1.12	26/4732 (0.5%)
2	F	0.57	0/3473	1.12	26/4728 (0.5%)
2	H	0.64	5/3465 (0.1%)	1.30	53/4718 (1.1%)
3	I	0.62	0/670	1.15	5/891 (0.6%)
3	J	0.52	0/617	1.12	5/823 (0.6%)
3	K	0.58	0/617	1.10	3/823 (0.4%)
3	L	0.76	2/621 (0.3%)	1.46	16/828 (1.9%)
All	All	0.59	15/33066 (0.0%)	1.13	267/44794 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	211	HIS	CG-CD2	-9.87	1.25	1.35
2	B	441	THR	CA-C	9.51	1.58	1.52
2	B	442	SER	C-O	7.55	1.38	1.23
1	C	211	HIS	CG-CD2	-7.37	1.27	1.35
2	H	241	GLN	C-O	-7.09	1.15	1.24
3	L	100	SER	CA-C	-6.62	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	277	ASN	CA-CB	6.01	1.63	1.53
2	H	241	GLN	CA-C	-5.89	1.45	1.52
1	A	209	HIS	CG-CD2	-5.86	1.29	1.35
1	C	211	HIS	CB-CG	5.74	1.58	1.50
2	H	224	LEU	CA-C	5.54	1.59	1.52
2	H	239	LYS	CA-C	5.54	1.60	1.52
1	E	212	THR	CA-C	-5.27	1.48	1.52
3	L	99	GLY	N-CA	5.08	1.53	1.45
2	H	80	MET	SD-CE	5.05	1.92	1.79

All (267) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	100	SER	N-CA-C	16.36	136.40	108.76
2	H	320	ASN	N-CA-C	15.73	144.30	110.80
1	C	260	GLU	N-CA-C	-13.58	96.98	113.15
2	H	403	ARG	CA-C-N	-13.54	99.91	122.11
2	H	403	ARG	C-N-CA	-13.54	99.91	122.11
1	C	276	LEU	N-CA-C	12.72	129.20	113.17
2	D	320	ASN	N-CA-C	12.45	137.32	110.80
2	D	319	ASN	N-CA-C	-11.44	93.35	110.28
2	H	271	TYR	N-CA-C	-11.16	86.99	107.75
2	H	359	ALA	N-CA-C	11.14	126.62	110.24
1	E	260	GLU	N-CA-C	-11.12	101.19	112.97
2	B	320	ASN	N-CA-C	11.09	134.43	110.80
1	C	518	ASN	N-CA-C	10.63	133.44	110.80
2	D	241	GLN	CA-C-N	10.54	133.01	119.84
2	D	241	GLN	C-N-CA	10.54	133.01	119.84
2	H	240	GLU	N-CA-C	-10.45	89.43	107.61
1	A	519	THR	N-CA-C	10.44	125.58	110.24
1	C	278	THR	N-CA-C	10.33	124.50	112.72
1	A	260	GLU	N-CA-C	-10.14	99.41	113.20
1	G	273	ASN	N-CA-C	-10.03	101.04	113.18
1	G	517	ASN	CA-C-N	-9.83	110.74	122.44
1	G	517	ASN	C-N-CA	-9.83	110.74	122.44
2	B	442	SER	N-CA-C	-9.43	84.61	111.00
1	C	131	LEU	N-CA-C	9.26	123.64	110.40
3	L	120	THR	N-CA-C	9.24	125.29	112.72
3	I	174	ARG	N-CA-C	9.13	121.17	111.03
2	F	320	ASN	N-CA-C	8.97	129.91	110.80
1	E	232	ARG	N-CA-C	8.95	124.80	107.98
1	A	447	ASN	N-CA-C	8.84	123.16	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	316	ILE	CA-C-N	8.62	128.63	119.76
2	H	316	ILE	C-N-CA	8.62	128.63	119.76
2	H	404	THR	CB-CA-C	8.61	123.53	109.07
3	L	101	MET	N-CA-C	-8.46	92.78	110.80
2	F	375	GLN	N-CA-C	8.43	128.75	110.80
2	F	321	TYR	N-CA-C	8.27	122.95	109.72
2	B	386	GLU	N-CA-C	-8.26	94.94	108.07
1	C	210	SER	CA-C-N	-8.21	110.15	122.47
1	C	210	SER	C-N-CA	-8.21	110.15	122.47
3	L	99	GLY	CA-C-N	-8.14	110.21	122.74
3	L	99	GLY	C-N-CA	-8.14	110.21	122.74
2	H	239	LYS	N-CA-C	7.91	127.65	110.80
2	H	321	TYR	N-CA-C	7.89	122.65	110.42
1	A	7	LEU	N-CA-C	-7.89	103.66	113.20
1	C	252	LEU	N-CA-C	7.88	127.58	110.80
2	D	59	LEU	N-CA-C	-7.81	102.76	111.82
2	H	229	ILE	N-CA-C	-7.81	104.25	111.67
2	F	364	VAL	N-CA-C	-7.80	106.30	113.71
2	B	48	THR	N-CA-C	7.75	123.87	112.94
2	F	115	VAL	CA-C-N	7.73	129.50	119.84
2	F	115	VAL	C-N-CA	7.73	129.50	119.84
1	C	277	ASN	N-CA-CB	7.73	123.55	110.49
1	C	237	TYR	N-CA-C	-7.72	102.83	111.71
2	D	88	LEU	N-CA-C	7.63	120.48	111.71
1	G	233	ILE	N-CA-C	7.48	115.06	108.63
2	F	413	LYS	N-CA-C	-7.40	103.71	112.89
1	C	210	SER	N-CA-C	-7.33	95.20	110.80
1	G	517	ASN	N-CA-C	7.30	120.66	111.24
1	C	211	HIS	CB-CA-C	7.28	121.57	111.23
2	H	358	SER	N-CA-C	7.24	118.82	111.07
2	D	238	PRO	N-CA-C	-7.17	105.60	114.20
1	G	251	ILE	CB-CA-C	-7.14	104.23	111.80
2	D	120	VAL	N-CA-C	7.13	117.50	107.37
1	C	212	THR	N-CA-C	7.11	118.60	109.72
1	G	7	LEU	N-CA-C	-7.06	104.75	113.15
2	H	134	PHE	N-CA-C	7.05	118.75	111.14
3	K	123	VAL	N-CA-C	-7.04	103.61	110.72
2	H	319	ASN	CA-C-N	-7.03	108.12	121.54
2	H	319	ASN	C-N-CA	-7.03	108.12	121.54
2	F	316	ILE	CA-C-N	6.98	126.95	119.76
2	F	316	ILE	C-N-CA	6.98	126.95	119.76
1	C	511	LYS	N-CA-C	-6.97	103.32	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	173	SER	N-CA-C	-6.94	105.09	113.97
1	E	187	LYS	CA-C-N	6.92	127.31	119.83
1	E	187	LYS	C-N-CA	6.92	127.31	119.83
2	H	288	ILE	N-CA-C	6.92	117.97	108.84
2	H	240	GLU	CA-C-N	-6.90	104.97	121.80
2	H	240	GLU	C-N-CA	-6.90	104.97	121.80
2	B	240	GLU	N-CA-C	-6.89	95.50	107.49
2	B	440	PHE	N-CA-C	6.84	119.56	110.53
1	E	211	HIS	ND1-CG-CD2	6.80	112.90	106.10
2	D	192	ILE	N-CA-C	6.77	117.64	107.75
2	H	241	GLN	CA-C-N	6.74	128.27	119.84
2	H	241	GLN	C-N-CA	6.74	128.27	119.84
1	A	252	LEU	N-CA-C	6.73	120.27	107.75
2	D	288	ILE	N-CA-C	6.72	118.45	109.37
2	B	319	ASN	N-CA-C	-6.71	101.10	110.35
2	F	48	THR	N-CA-C	6.70	121.77	112.45
2	D	278	TYR	N-CA-C	-6.67	104.09	111.36
1	E	251	ILE	CA-C-N	-6.66	109.70	121.29
1	E	251	ILE	C-N-CA	-6.66	109.70	121.29
2	H	364	VAL	N-CA-C	-6.66	105.63	113.42
3	L	100	SER	O-C-N	6.65	131.09	123.31
2	H	92	PHE	N-CA-C	6.64	120.48	112.38
1	A	187	LYS	CA-C-N	6.63	126.59	119.76
1	A	187	LYS	C-N-CA	6.63	126.59	119.76
2	B	218	ILE	N-CA-C	6.58	116.74	110.42
1	G	461	LEU	N-CA-C	-6.57	104.12	111.28
2	H	294	SER	N-CA-C	6.55	119.01	111.02
1	C	129	THR	CA-C-N	-6.55	113.52	122.95
1	C	129	THR	C-N-CA	-6.55	113.52	122.95
2	B	321	TYR	N-CA-C	6.53	120.25	110.14
2	H	405	ARG	N-CA-C	6.51	124.19	109.81
2	D	316	ILE	CA-C-N	6.50	126.47	119.78
2	D	316	ILE	C-N-CA	6.50	126.47	119.78
1	E	266	GLU	N-CA-C	-6.47	104.42	112.90
2	H	369	THR	N-CA-C	6.46	117.98	111.07
1	E	251	ILE	N-CA-C	-6.43	100.24	108.93
2	H	81	ASP	N-CA-C	6.43	118.83	110.53
1	E	363	LYS	N-CA-C	-6.43	104.35	111.36
1	A	331	ASP	N-CA-C	-6.40	101.91	110.55
2	H	103	LYS	N-CA-C	6.38	117.90	111.07
2	B	59	LEU	N-CA-C	-6.38	104.25	111.07
2	B	310	ILE	N-CA-C	6.37	117.12	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	138	PHE	N-CA-C	6.37	120.45	110.32
2	H	314	ALA	N-CA-C	-6.37	105.33	113.23
1	G	212	THR	CA-C-N	6.37	126.13	119.76
1	G	212	THR	C-N-CA	6.37	126.13	119.76
2	D	440	PHE	CA-C-N	-6.33	110.31	121.70
2	D	440	PHE	C-N-CA	-6.33	110.31	121.70
1	E	517	ASN	N-CA-C	6.33	121.24	112.45
1	E	512	GLN	N-CA-C	6.32	121.12	113.41
1	G	267	GLU	N-CA-C	-6.30	102.96	112.04
1	A	120	PHE	N-CA-C	6.28	118.12	111.28
2	H	75	ILE	N-CA-C	6.26	117.49	108.48
1	A	36	ILE	CB-CA-C	6.25	119.81	111.94
1	A	281	ILE	N-CA-C	6.23	115.75	108.96
2	F	81	ASP	N-CA-C	6.18	119.67	110.52
3	K	106	LYS	N-CA-C	6.14	119.25	109.24
2	H	322	LEU	N-CA-C	6.14	118.29	107.61
2	B	32	HIS	N-CA-C	-6.12	101.86	109.64
3	J	100	SER	CA-C-N	6.10	132.61	122.73
3	J	100	SER	C-N-CA	6.10	132.61	122.73
1	E	37	ASN	N-CA-C	6.06	118.40	108.52
2	F	319	ASN	N-CA-CB	6.06	119.34	109.95
3	L	119	PRO	CA-C-N	-6.05	110.86	122.61
3	L	119	PRO	C-N-CA	-6.05	110.86	122.61
2	H	143	CYS	N-CA-C	6.02	119.52	109.95
1	C	483	CYS	N-CA-C	-6.01	106.11	113.50
2	H	241	GLN	N-CA-C	5.99	123.06	109.81
2	H	256	HIS	N-CA-C	-5.99	103.41	112.04
1	E	517	ASN	CA-C-N	-5.97	110.14	121.54
1	E	517	ASN	C-N-CA	-5.97	110.14	121.54
1	A	337	GLY	N-CA-C	5.96	119.85	112.64
2	B	179	ASP	N-CA-C	5.93	118.56	108.90
2	H	115	VAL	CA-C-N	5.92	127.25	119.84
2	H	115	VAL	C-N-CA	5.92	127.25	119.84
2	F	125	ASN	N-CA-C	5.91	117.25	107.73
1	A	361	VAL	N-CA-C	-5.90	104.87	110.42
1	C	265	PHE	N-CA-C	-5.90	104.93	111.71
1	G	512	GLN	N-CA-C	5.89	121.20	113.30
2	H	321	TYR	N-CA-CB	-5.88	101.38	110.56
1	C	262	GLU	N-CA-C	5.88	118.36	107.60
2	H	319	ASN	N-CA-C	-5.87	98.29	110.80
2	D	327	VAL	N-CA-C	5.86	116.32	110.23
1	E	306	ILE	N-CA-C	-5.86	104.80	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	PRO	N-CA-C	5.84	124.50	112.47
1	A	299	LYS	N-CA-C	-5.83	105.42	112.54
1	C	243	PHE	N-CA-C	-5.82	104.94	111.28
1	E	259	PRO	N-CA-C	5.82	124.45	112.47
1	C	199	TYR	N-CA-C	5.81	119.08	110.48
1	E	142	VAL	CB-CA-C	-5.79	104.46	111.88
2	D	321	TYR	N-CA-C	5.77	118.26	109.95
2	H	193	LEU	CA-C-N	5.75	127.02	119.84
2	H	193	LEU	C-N-CA	5.75	127.02	119.84
1	C	70	ALA	N-CA-C	-5.74	106.31	113.38
2	F	241	GLN	CA-C-N	5.73	125.26	119.19
2	F	241	GLN	C-N-CA	5.73	125.26	119.19
2	H	47	ASP	N-CA-C	5.71	118.71	111.69
1	G	248	ARG	N-CA-C	-5.69	105.17	111.71
3	L	126	ILE	N-CA-C	-5.67	103.96	111.05
3	L	120	THR	CA-C-N	-5.67	113.40	121.50
3	L	120	THR	C-N-CA	-5.67	113.40	121.50
3	I	175	GLY	N-CA-C	5.66	119.83	112.25
1	A	35	LEU	CA-C-N	-5.65	112.19	121.34
1	A	35	LEU	C-N-CA	-5.65	112.19	121.34
2	F	319	ASN	N-CA-C	-5.64	100.79	109.76
1	E	36	ILE	CA-C-N	-5.64	115.16	123.05
1	E	36	ILE	C-N-CA	-5.64	115.16	123.05
2	B	47	ASP	N-CA-C	5.62	117.21	111.14
1	E	507	LYS	N-CA-C	-5.61	105.07	111.07
2	H	48	THR	N-CA-C	5.59	120.99	113.72
2	D	285	VAL	N-CA-C	5.57	115.81	110.74
1	A	434	ARG	N-CA-C	-5.55	105.15	111.14
2	H	224	LEU	N-CA-C	5.54	122.05	109.81
2	D	378	SER	CA-C-N	5.53	125.51	120.03
2	D	378	SER	C-N-CA	5.53	125.51	120.03
1	E	238	LYS	N-CA-C	-5.53	105.33	112.68
1	E	281	ILE	N-CA-C	5.53	114.37	108.95
2	F	137	GLN	N-CA-C	5.51	119.85	113.18
2	H	161	LEU	N-CA-C	-5.49	106.42	113.23
1	A	442	TYR	CA-C-N	5.49	126.70	119.84
1	A	442	TYR	C-N-CA	5.49	126.70	119.84
2	F	26	ARG	N-CA-C	5.48	118.40	109.24
3	L	123	VAL	N-CA-C	-5.48	105.03	110.62
2	D	143	CYS	N-CA-C	5.46	118.36	109.24
1	G	223	ALA	N-CA-C	-5.46	105.44	111.71
1	A	377	GLU	N-CA-C	-5.45	104.57	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	332	THR	CB-CA-C	-5.45	103.97	110.94
2	B	243	PHE	N-CA-C	5.43	118.72	112.97
1	A	251	ILE	N-CA-C	-5.42	98.06	109.34
1	A	345	VAL	N-CA-C	-5.38	105.25	110.42
1	E	424	VAL	N-CA-C	-5.38	105.28	110.72
3	I	100	SER	N-CA-C	-5.37	100.90	109.23
2	B	414	GLU	N-CA-C	-5.36	106.24	112.89
3	J	153	GLU	N-CA-C	-5.36	106.05	113.18
1	G	222	LEU	N-CA-C	-5.36	105.86	112.72
1	G	123	PHE	N-CA-C	5.36	117.97	109.24
1	E	237	TYR	N-CA-C	-5.35	106.83	113.19
2	F	318	LEU	CA-C-N	-5.33	113.87	121.50
2	F	318	LEU	C-N-CA	-5.33	113.87	121.50
2	D	440	PHE	N-CA-C	5.32	117.38	108.23
1	C	484	ARG	N-CA-C	-5.32	105.38	111.07
1	G	78	ARG	N-CA-C	-5.32	105.65	111.82
1	E	14	ASP	N-CA-C	5.31	116.76	110.97
2	B	268	ALA	N-CA-C	-5.31	105.39	111.07
1	G	274	THR	N-CA-C	5.31	119.23	112.12
1	C	479	VAL	N-CA-C	-5.30	104.62	112.04
2	H	402	GLU	N-CA-C	-5.30	104.92	111.33
1	A	69	ASP	N-CA-C	-5.29	106.96	113.41
1	E	200	ASP	N-CA-C	5.28	122.04	110.80
1	E	288	ILE	N-CA-C	-5.26	105.20	110.30
1	A	281	ILE	CA-C-N	5.25	125.17	119.76
1	A	281	ILE	C-N-CA	5.25	125.17	119.76
2	H	264	SER	N-CA-C	-5.25	107.01	113.41
2	H	117	ASN	N-CA-C	5.24	118.80	112.93
2	D	92	PHE	N-CA-C	5.23	121.94	110.80
2	D	273	ILE	N-CA-C	5.20	116.19	108.23
1	C	211	HIS	ND1-CG-CD2	5.20	111.30	106.10
2	B	396	SER	N-CA-C	5.20	118.72	112.38
1	A	49	LEU	N-CA-C	-5.19	106.89	113.43
2	F	365	LEU	N-CA-C	-5.19	105.06	111.40
3	L	121	ASP	N-CA-C	-5.19	101.51	109.76
3	I	102	LEU	N-CA-C	5.19	117.10	108.02
3	L	129	ARG	N-CA-C	-5.19	105.80	111.82
1	A	209	HIS	N-CA-C	-5.18	105.12	111.75
1	A	70	ALA	N-CA-C	-5.17	106.97	113.28
2	F	346	CYS	N-CA-C	5.17	117.59	111.33
3	L	174	ARG	N-CA-C	5.17	119.48	112.04
2	B	288	ILE	N-CA-C	5.16	117.06	109.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	GLU	N-CA-C	-5.15	105.75	111.36
2	B	320	ASN	CA-CB-CG	-5.15	107.45	112.60
2	H	170	ASP	CA-C-N	5.14	124.31	118.97
2	H	170	ASP	C-N-CA	5.14	124.31	118.97
2	F	88	LEU	N-CA-C	5.13	121.73	110.80
2	F	247	VAL	CA-C-N	5.12	125.10	120.03
2	F	247	VAL	C-N-CA	5.12	125.10	120.03
3	I	94	SER	N-CA-C	5.12	116.85	109.07
3	J	125	ARG	N-CA-C	-5.11	105.62	111.14
1	A	263	GLU	N-CA-C	-5.11	105.34	112.45
1	G	406	THR	N-CA-C	5.10	119.21	112.89
2	H	240	GLU	N-CA-CB	5.08	118.48	110.71
1	G	288	ILE	N-CA-C	-5.08	105.59	110.72
1	G	74	PHE	N-CA-C	-5.08	106.87	113.16
1	C	443	PRO	N-CA-C	5.07	118.46	110.50
2	B	118	CYS	N-CA-C	-5.07	104.18	110.41
1	C	379	GLU	N-CA-C	-5.07	105.65	111.07
3	L	128	GLU	N-CA-C	-5.05	107.66	113.88
1	A	253	LYS	CA-C-N	-5.03	114.14	119.98
1	A	253	LYS	C-N-CA	-5.03	114.14	119.98
1	G	250	GLY	N-CA-C	-5.03	101.25	113.18
2	H	404	THR	N-CA-C	-5.03	107.53	113.97
2	D	364	VAL	N-CA-C	-5.03	105.52	111.00
1	A	342	LEU	N-CA-C	-5.03	105.69	111.07
1	G	374	SER	N-CA-C	-5.02	107.12	113.20
2	F	420	GLY	N-CA-C	-5.01	108.52	114.48
3	J	134	GLU	N-CA-C	5.01	120.23	113.72
3	K	101	MET	N-CA-C	-5.00	101.25	109.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	319	ASN	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4104	0	4052	284	0
1	C	4096	0	4048	278	0
1	E	4093	0	4059	235	0
1	G	4038	0	4009	238	0
2	B	3402	0	3380	269	0
2	D	3399	0	3386	251	0
2	F	3395	0	3375	282	0
2	H	3387	0	3354	326	0
3	I	666	0	703	55	0
3	J	612	0	648	49	0
3	K	612	0	648	49	0
3	L	616	0	651	80	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
All	All	32424	0	32313	2234	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 35.

All (2234) 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:C:252:LEU:O	1:C:259:PRO:HD2	1.17	1.33
1:A:252:LEU:O	1:A:259:PRO:HD2	1.25	1.30
1:C:517:ASN:ND2	1:C:518:ASN:H	1.31	1.28
2:F:371:SER:CB	2:F:374:LEU:HD11	1.64	1.26
1:C:517:ASN:HD22	1:C:518:ASN:N	1.35	1.24
2:F:371:SER:HB3	2:F:374:LEU:HD11	1.20	1.12
1:A:259:PRO:HB2	1:A:262:GLU:OE1	1.51	1.11
3:K:123:VAL:HB	3:K:152:ASP:HA	1.29	1.11
2:F:149:ILE:HD12	2:F:149:ILE:H	1.06	1.10
1:G:333:ILE:HG22	2:H:223:ARG:NH2	1.66	1.10
1:A:36:ILE:HD12	1:A:60:ILE:HB	1.25	1.10
3:J:123:VAL:HB	3:J:152:ASP:HA	1.33	1.09
2:D:149:ILE:H	2:D:149:ILE:HD12	1.11	1.09
2:B:338:GLU:HG3	3:I:148:LYS:HG2	1.30	1.09
2:F:325:ASN:HD21	2:F:327:VAL:HG23	0.98	1.08
2:D:207:TYR:CE1	3:J:172:ARG:HD3	1.89	1.07
1:E:226:TYR:CD1	1:E:231:GLY:HA2	1.89	1.07
1:A:208:ASP:N	1:A:211:HIS:HB2	1.69	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:PRO:HD2	2:B:442:SER:O	1.56	1.05
1:C:35:LEU:HD11	1:C:129:THR:CG2	1.87	1.05
1:G:333:ILE:HG22	2:H:223:ARG:HH22	1.13	1.04
1:A:518:ASN:HD22	1:A:534:LEU:N	1.56	1.03
2:H:362:GLN:HG2	2:H:408:LEU:HB3	1.36	1.03
1:C:35:LEU:HD11	1:C:129:THR:HG21	1.42	1.01
2:H:403:ARG:HG2	2:H:403:ARG:O	1.54	1.01
2:H:232:VAL:HG21	2:H:264:SER:HA	1.39	1.00
1:C:252:LEU:O	1:C:259:PRO:CD	2.10	1.00
1:E:226:TYR:HD1	1:E:231:GLY:HA2	1.23	1.00
1:A:252:LEU:C	1:A:259:PRO:HD2	1.87	0.99
1:A:236:THR:HB	1:A:239:GLU:HG3	1.43	0.99
2:F:325:ASN:ND2	2:F:327:VAL:HG23	1.77	0.98
1:G:489:GLU:H	2:H:19:HIS:HD2	1.00	0.98
2:F:380:ALA:CB	2:F:394:LEU:HD12	1.93	0.98
2:H:380:ALA:CB	2:H:394:LEU:HD12	1.93	0.98
1:A:518:ASN:ND2	1:A:534:LEU:N	2.12	0.97
1:C:130:GLN:OE1	1:C:155:THR:HB	1.63	0.97
2:D:402:GLU:HA	2:D:405:ARG:HH12	1.26	0.97
3:K:155:THR:HG22	3:K:158:ASP:OD1	1.63	0.97
1:E:184:ARG:HH12	1:E:325:VAL:HG22	1.27	0.97
2:F:362:GLN:HG2	2:F:408:LEU:HD22	1.45	0.96
1:C:259:PRO:HB2	1:C:262:GLU:OE1	1.66	0.96
2:H:128:GLN:HE21	2:H:128:GLN:H	1.12	0.96
2:F:361:LEU:HB3	2:F:408:LEU:HD23	1.48	0.96
2:B:386:GLU:O	2:B:388:LYS:N	1.99	0.95
1:A:518:ASN:ND2	1:A:534:LEU:H	1.64	0.95
2:B:207:TYR:CE2	3:I:172:ARG:HG2	2.02	0.95
1:E:211:HIS:CE1	2:F:221:MET:SD	2.60	0.94
1:E:347:ARG:HH22	2:F:274:ARG:HD2	1.30	0.94
2:F:376:MET:HE2	2:F:427:ASP:HB2	1.48	0.94
2:F:376:MET:HB3	2:F:427:ASP:OD1	1.67	0.94
2:F:374:LEU:H	2:F:374:LEU:HD12	1.33	0.94
1:G:489:GLU:H	2:H:19:HIS:CD2	1.85	0.94
1:G:293:ARG:HG2	1:G:293:ARG:HH11	1.29	0.94
2:F:371:SER:HB3	2:F:374:LEU:CD1	1.98	0.93
3:I:99:GLY:O	3:I:118:GLU:CB	2.16	0.93
1:A:252:LEU:O	1:A:259:PRO:CD	2.16	0.93
2:D:257:ILE:HD13	2:D:282:GLN:HG2	1.50	0.93
3:I:107:THR:HG22	3:I:109:THR:H	1.31	0.92
2:D:149:ILE:H	2:D:149:ILE:CD1	1.81	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:PRO:HG2	2:B:217:THR:HG23	1.52	0.92
1:C:35:LEU:CD1	1:C:129:THR:CG2	2.48	0.92
1:E:201:LEU:N	1:E:201:LEU:HD23	1.85	0.91
2:F:64:LEU:HD11	2:F:77:VAL:HG21	1.51	0.91
2:F:362:GLN:HE21	2:F:408:LEU:HD13	1.35	0.90
2:B:236:GLN:HE22	2:B:263:LYS:HD2	1.35	0.90
3:L:107:THR:HG23	3:L:109:THR:H	1.35	0.90
2:F:342:ASN:HD22	2:F:342:ASN:H	1.18	0.90
2:F:149:ILE:H	2:F:149:ILE:CD1	1.82	0.90
2:F:380:ALA:HB1	2:F:394:LEU:HA	1.54	0.90
2:B:342:ASN:H	2:B:342:ASN:HD22	1.18	0.89
2:F:74:GLN:HE22	2:F:119:ASN:HD22	1.15	0.89
2:H:223:ARG:HB2	2:H:227:HIS:CE1	2.08	0.89
1:G:121:CYS:HA	1:G:148:ILE:HD11	1.53	0.89
2:D:380:ALA:HB2	2:D:394:LEU:HD12	1.53	0.89
3:K:118:GLU:HG2	3:K:121:ASP:OD1	1.73	0.88
1:G:180:LEU:H	1:G:180:LEU:HD12	1.39	0.88
2:B:380:ALA:HB2	2:B:394:LEU:HD12	1.56	0.88
2:H:128:GLN:H	2:H:128:GLN:NE2	1.72	0.87
3:L:120:THR:HA	3:L:155:THR:OG1	1.73	0.87
2:F:131:ASN:HB3	2:H:131:ASN:HD22	1.35	0.87
2:B:380:ALA:CB	2:B:394:LEU:HD12	2.04	0.87
2:F:340:LYS:HB3	2:F:342:ASN:HD21	1.38	0.87
2:B:327:VAL:HG23	2:B:328:ASP:H	1.39	0.87
2:D:232:VAL:HG11	2:D:263:LYS:HB2	1.56	0.86
2:F:380:ALA:HB1	2:F:394:LEU:HD12	1.56	0.86
3:J:161:ILE:HD11	3:J:167:LEU:HD21	1.56	0.86
1:E:211:HIS:N	1:E:211:HIS:CD2	2.39	0.86
2:H:58:GLY:H	2:H:91:GLN:HG2	1.40	0.86
1:E:184:ARG:NH1	1:E:325:VAL:HG22	1.89	0.86
2:H:318:LEU:HD11	2:H:334:THR:CG2	2.06	0.86
2:F:325:ASN:HD21	2:F:327:VAL:CG2	1.87	0.85
2:B:343:CYS:O	2:B:347:SER:HB3	1.76	0.85
1:C:36:ILE:HB	1:C:128:ALA:HA	1.58	0.85
1:E:297:ILE:H	1:E:297:ILE:HD12	1.41	0.85
1:A:307:LEU:HB3	1:A:383:LEU:HD22	1.57	0.85
1:E:212:THR:OG1	1:E:217:ILE:HD11	1.76	0.85
3:L:170:VAL:HG12	3:L:171:LEU:H	1.40	0.85
1:E:307:LEU:HD13	1:E:383:LEU:HD22	1.58	0.85
2:H:380:ALA:HB2	2:H:394:LEU:HD12	1.59	0.85
1:G:421:ASN:O	1:G:424:VAL:HG23	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:ILE:HD11	2:B:230:GLU:HG2	1.59	0.85
1:C:37:ASN:O	1:C:129:THR:OG1	1.94	0.84
1:E:252:LEU:C	1:E:259:PRO:HD2	2.01	0.84
2:F:134:PHE:O	2:F:137:GLN:HG2	1.77	0.84
1:E:51:LEU:HD11	2:F:92:PHE:HB3	1.58	0.84
2:H:271:TYR:N	2:H:271:TYR:CD2	2.42	0.84
2:B:355:PHE:O	2:B:440:PHE:HA	1.76	0.84
2:F:411:THR:H	2:F:414:GLU:HB3	1.40	0.84
3:K:125:ARG:HD3	3:K:129:ARG:HH21	1.41	0.83
2:B:361:LEU:HD23	2:B:408:LEU:HD23	1.60	0.83
2:D:141:ILE:HD12	2:D:158:LEU:HD21	1.58	0.83
2:F:149:ILE:HD12	2:F:149:ILE:N	1.90	0.83
2:F:411:THR:H	2:F:414:GLU:CB	1.91	0.83
1:A:229:THR:CG2	1:A:232:ARG:HB3	2.08	0.83
2:F:371:SER:OG	2:F:374:LEU:HD11	1.79	0.83
2:H:318:LEU:HG	2:H:319:ASN:O	1.79	0.83
1:E:248:ARG:O	1:E:251:ILE:CG1	2.27	0.83
1:G:518:ASN:HB3	1:G:533:GLN:HA	1.61	0.83
3:J:143:LEU:HB3	3:J:150:MET:HE2	1.60	0.82
2:B:316:ILE:H	2:B:316:ILE:HD12	1.42	0.82
3:L:123:VAL:HG11	3:L:150:MET:HB3	1.60	0.82
2:D:380:ALA:CB	2:D:394:LEU:HD12	2.08	0.82
2:B:342:ASN:H	2:B:342:ASN:ND2	1.75	0.82
1:G:518:ASN:CB	1:G:533:GLN:HA	2.10	0.81
2:H:318:LEU:HD11	2:H:334:THR:HG23	1.61	0.81
1:A:215:ILE:HD11	1:A:332:MET:HE1	1.61	0.81
1:A:418:ASN:ND2	1:A:420:ASP:H	1.79	0.81
1:C:35:LEU:CD1	1:C:129:THR:HG21	2.08	0.81
1:C:299:LYS:HA	1:C:368:ILE:HG23	1.63	0.81
2:D:149:ILE:HD12	2:D:149:ILE:N	1.94	0.81
1:A:224:GLN:NE2	1:A:246:LEU:HD11	1.96	0.81
1:C:35:LEU:CD1	1:C:129:THR:HG23	2.10	0.80
3:J:101:MET:SD	3:J:162:LEU:HA	2.21	0.80
2:B:13:TRP:CZ3	2:B:116:PRO:HG2	2.16	0.80
1:C:527:GLN:HB2	2:D:318:LEU:HD13	1.64	0.80
2:B:240:GLU:O	2:B:242:PRO:CD	2.30	0.80
1:E:211:HIS:N	1:E:211:HIS:HD2	1.76	0.79
2:D:318:LEU:HG	2:D:319:ASN:O	1.82	0.79
2:F:74:GLN:NE2	2:F:119:ASN:HD22	1.79	0.79
3:J:118:GLU:HG3	3:J:120:THR:HG22	1.62	0.79
2:H:277:THR:HG23	2:H:280:LEU:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:99:GLY:O	3:I:118:GLU:HB2	1.81	0.79
1:C:229:THR:CG2	1:C:232:ARG:HB2	2.12	0.79
3:J:170:VAL:HG22	3:J:171:LEU:H	1.48	0.79
1:C:259:PRO:HB2	1:C:262:GLU:CD	2.07	0.79
3:I:99:GLY:O	3:I:118:GLU:HB3	1.81	0.79
1:C:252:LEU:C	1:C:259:PRO:HD2	2.06	0.79
1:E:201:LEU:N	1:E:201:LEU:CD2	2.45	0.79
2:F:412:LEU:HD13	2:F:440:PHE:HE2	1.49	0.78
1:G:6:LYS:N	1:G:6:LYS:HD2	1.97	0.78
2:H:231:TYR:HA	2:H:235:LEU:HD23	1.64	0.78
1:A:462:THR:O	1:A:466:GLN:HG3	1.83	0.78
2:H:380:ALA:HB1	2:H:394:LEU:HD12	1.64	0.78
1:C:518:ASN:HB2	1:C:533:GLN:HA	1.63	0.78
1:G:360:HIS:O	1:G:364:LEU:HD13	1.83	0.78
1:C:297:ILE:H	1:C:297:ILE:HD13	1.48	0.78
1:E:262:GLU:OE2	1:E:262:GLU:HA	1.83	0.78
1:A:125:VAL:HG12	1:A:149:PRO:HB2	1.65	0.78
1:A:259:PRO:CB	1:A:262:GLU:OE1	2.31	0.78
2:F:87:ASN:ND2	2:F:103:LYS:HE2	1.99	0.78
1:E:186:ASP:OD2	1:E:279:THR:HB	1.84	0.78
2:H:241:GLN:OE1	2:H:245:GLU:HA	1.83	0.77
1:A:418:ASN:HD22	1:A:420:ASP:H	1.29	0.77
2:D:402:GLU:HA	2:D:405:ARG:NH1	1.98	0.77
2:B:240:GLU:O	2:B:242:PRO:HD3	1.84	0.77
2:H:351:GLN:H	2:H:436:PHE:HA	1.47	0.77
2:F:277:THR:HG23	2:F:280:LEU:H	1.47	0.77
1:G:333:ILE:HA	2:H:223:ARG:CZ	2.15	0.77
1:A:317:LYS:HB3	1:A:318:GLU:OE1	1.85	0.77
1:C:35:LEU:HD11	1:C:129:THR:HG23	1.65	0.77
2:B:356:SER:HB3	2:B:441:THR:OG1	1.84	0.77
2:F:340:LYS:HB3	2:F:342:ASN:ND2	2.00	0.77
1:G:489:GLU:N	2:H:19:HIS:HD2	1.81	0.77
2:H:162:LEU:HA	2:H:173:SER:OG	1.83	0.77
2:H:403:ARG:O	2:H:403:ARG:CG	2.33	0.77
1:G:447:ASN:HD22	2:H:26:ARG:HH21	1.30	0.77
2:H:316:ILE:H	2:H:316:ILE:HD12	1.48	0.77
1:A:28:LEU:HD12	1:A:509:ILE:HG21	1.67	0.76
1:G:226:TYR:OH	1:G:233:ILE:HG22	1.85	0.76
3:L:105:VAL:HG23	3:L:167:LEU:HB2	1.67	0.76
1:A:259:PRO:C	1:A:261:ASP:H	1.94	0.76
1:C:163:ARG:CZ	1:C:518:ASN:OD1	2.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ASN:ND2	1:C:420:ASP:H	1.81	0.76
1:C:51:LEU:HD11	2:D:92:PHE:HB3	1.68	0.76
1:E:248:ARG:O	1:E:251:ILE:HG13	1.84	0.76
2:H:164:TYR:CE2	2:H:169:LEU:HB2	2.21	0.76
1:G:267:GLU:OE2	1:G:333:ILE:HG12	1.85	0.76
3:L:120:THR:CA	3:L:155:THR:OG1	2.34	0.76
1:A:75:PHE:O	1:A:76:LEU:HD23	1.85	0.75
2:B:357:PRO:CD	2:B:442:SER:O	2.34	0.75
1:G:41:THR:O	1:G:45:ILE:HG13	1.85	0.75
2:H:217:THR:HG21	2:H:223:ARG:HH21	1.50	0.75
1:C:129:THR:O	1:C:153:CYS:O	2.03	0.75
3:J:101:MET:HE2	3:J:119:PRO:HG3	1.66	0.75
1:E:253:LYS:HA	1:E:253:LYS:HE3	1.69	0.75
2:D:380:ALA:CB	2:D:394:LEU:CD1	2.64	0.75
1:E:489:GLU:H	2:F:19:HIS:CD2	2.04	0.75
2:H:318:LEU:C	2:H:319:ASN:O	2.24	0.75
2:F:62:GLU:HG2	2:F:297:ALA:HA	1.68	0.74
1:A:112:LEU:H	1:A:112:LEU:HD22	1.50	0.74
1:A:229:THR:HG21	1:A:232:ARG:HB3	1.68	0.74
1:E:409:LYS:HG2	1:E:470:LEU:HD21	1.68	0.74
1:A:518:ASN:CG	1:A:519:THR:H	1.94	0.74
2:B:342:ASN:HD22	2:B:342:ASN:N	1.79	0.74
1:E:61:ASP:HB3	1:E:86:ALA:HB2	1.70	0.74
1:G:341:LYS:O	1:G:345:VAL:HG23	1.87	0.74
2:H:62:GLU:HG2	2:H:297:ALA:HA	1.69	0.74
2:B:81:ASP:HB2	2:B:103:LYS:HD2	1.68	0.74
1:C:115:ASN:O	1:C:117:PRO:HD3	1.88	0.74
1:A:34:CYS:SG	1:A:36:ILE:HD11	2.28	0.74
2:B:214:PRO:HG2	2:B:217:THR:CG2	2.18	0.74
1:C:396:ARG:HD2	1:C:534:LEU:O	1.88	0.74
2:B:419:ASP:OD1	2:B:440:PHE:HD1	1.71	0.74
2:B:229:ILE:HD13	2:B:281:THR:HA	1.69	0.73
1:C:259:PRO:C	1:C:261:ASP:H	1.93	0.73
1:G:293:ARG:HG2	1:G:293:ARG:NH1	2.00	0.73
2:B:95:ARG:HH11	2:B:95:ARG:HG3	1.52	0.73
1:C:229:THR:HG21	1:C:232:ARG:HB2	1.69	0.73
2:H:240:GLU:O	2:H:242:PRO:HD3	1.88	0.73
2:H:339:ARG:HH21	2:H:346:CYS:HB3	1.52	0.73
2:B:13:TRP:HZ3	2:B:116:PRO:HG2	1.53	0.73
1:C:84:ASN:HB3	1:C:87:GLU:HB3	1.71	0.73
1:C:397:SER:OG	1:C:400:GLU:HG3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:316:ILE:HD12	2:F:316:ILE:H	1.52	0.73
1:A:36:ILE:CD1	1:A:60:ILE:HB	2.11	0.73
1:C:143:LEU:HD22	1:C:148:ILE:HB	1.70	0.73
2:H:252:ASP:O	2:H:254:PRO:HD3	1.88	0.73
2:H:356:SER:O	2:H:358:SER:N	2.21	0.73
1:A:236:THR:CB	1:A:239:GLU:HG3	2.19	0.73
1:E:307:LEU:HB3	1:E:383:LEU:HD22	1.71	0.73
2:F:217:THR:HG21	2:F:223:ARG:NH2	2.03	0.73
2:F:382:THR:HG22	2:F:391:THR:HA	1.70	0.73
2:H:223:ARG:HB2	2:H:227:HIS:HE1	1.52	0.73
2:F:348:GLN:O	2:F:349:LEU:HD12	1.89	0.73
2:F:199:CYS:SG	2:F:201:GLU:HB2	2.29	0.73
1:A:61:ASP:HB3	1:A:86:ALA:HB2	1.69	0.73
2:B:200:ILE:HD13	3:I:172:ARG:HH22	1.54	0.73
1:C:130:GLN:HG2	1:C:154:ARG:HA	1.71	0.72
2:D:223:ARG:HB2	2:D:223:ARG:HH11	1.52	0.72
2:B:318:LEU:HD11	2:B:334:THR:CG2	2.19	0.72
2:F:371:SER:O	2:F:374:LEU:HD12	1.90	0.72
2:H:404:THR:HG22	2:H:407:ASN:HD22	1.54	0.72
1:E:259:PRO:C	1:E:261:ASP:H	1.96	0.72
1:A:236:THR:HG22	1:A:238:LYS:H	1.55	0.72
2:B:353:ILE:HG23	2:B:355:PHE:HD1	1.54	0.72
2:D:322:LEU:HD12	2:D:322:LEU:C	2.14	0.72
2:H:38:SER:HB3	2:H:41:SER:OG	1.90	0.72
1:C:248:ARG:C	1:C:250:GLY:H	1.98	0.72
2:F:58:GLY:H	2:F:91:GLN:HG2	1.54	0.72
2:F:351:GLN:HB2	2:F:436:PHE:CD2	2.24	0.72
1:G:45:ILE:HG12	1:G:498:GLY:HA2	1.72	0.72
2:D:162:LEU:HD22	2:D:169:LEU:HD11	1.71	0.72
1:G:215:ILE:HG13	1:G:332:MET:HE1	1.72	0.72
1:A:489:GLU:H	2:B:19:HIS:CD2	2.08	0.71
1:E:347:ARG:NH2	2:F:274:ARG:HD2	2.04	0.71
2:D:16:ARG:HD3	2:D:17:TRP:NE1	2.05	0.71
1:E:211:HIS:HE1	2:F:221:MET:SD	2.13	0.71
2:B:217:THR:HA	2:B:221:MET:HG3	1.70	0.71
2:B:253:ASP:HB3	2:B:256:HIS:HB2	1.70	0.71
1:C:409:LYS:HE2	1:C:468:TYR:O	1.91	0.71
2:H:224:LEU:HG	2:H:227:HIS:CE1	2.26	0.71
2:F:220:SER:C	2:F:222:PRO:HD3	2.15	0.71
2:H:207:TYR:CE1	3:L:172:ARG:HD3	2.25	0.71
3:L:170:VAL:HG12	3:L:171:LEU:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLU:O	1:A:270:LYS:HG3	1.91	0.71
1:G:446:SER:HB2	1:G:449:GLN:HG3	1.73	0.71
2:H:325:ASN:ND2	2:H:327:VAL:HG23	2.06	0.71
1:G:112:LEU:C	1:G:114:ASP:H	1.96	0.70
1:A:397:SER:OG	1:A:400:GLU:HG3	1.90	0.70
1:C:251:ILE:HG22	1:C:262:GLU:OE1	1.90	0.70
2:H:235:LEU:O	2:H:238:PRO:HD2	1.91	0.70
2:B:217:THR:HB	2:B:223:ARG:NH2	2.06	0.70
2:D:232:VAL:CG1	2:D:263:LYS:HB2	2.20	0.70
1:G:196:PHE:O	1:G:220:LYS:HE3	1.91	0.70
1:E:184:ARG:HG3	1:E:184:ARG:HH11	1.55	0.70
2:F:374:LEU:HD12	2:F:374:LEU:N	1.98	0.70
1:A:264:ASN:HD22	1:A:264:ASN:N	1.89	0.70
2:B:240:GLU:O	2:B:240:GLU:HG3	1.91	0.70
2:B:325:ASN:HD21	2:B:327:VAL:HG22	1.56	0.70
2:D:231:TYR:C	2:D:233:ARG:H	1.98	0.70
2:F:411:THR:OG1	2:F:414:GLU:HB2	1.91	0.70
2:H:239:LYS:HG3	2:H:239:LYS:O	1.91	0.70
2:H:74:GLN:HE22	2:H:119:ASN:HD22	1.39	0.70
1:A:299:LYS:HG2	1:A:368:ILE:O	1.90	0.70
2:B:74:GLN:HE22	2:B:119:ASN:HD22	1.40	0.70
2:F:241:GLN:HG2	2:F:245:GLU:HA	1.72	0.70
3:K:116:ASP:O	3:K:117:ILE:HD12	1.92	0.70
1:A:297:ILE:HD12	1:A:297:ILE:N	2.06	0.70
1:C:248:ARG:O	1:C:251:ILE:HG13	1.92	0.70
2:H:234:MET:O	2:H:235:LEU:HD13	1.92	0.70
2:D:157:MET:O	2:D:157:MET:HE3	1.91	0.70
2:D:325:ASN:HD21	2:D:327:VAL:HG22	1.56	0.70
2:F:32:HIS:CD2	2:F:34:ASP:H	2.10	0.70
1:A:84:ASN:OD1	1:A:106:GLU:HG2	1.92	0.69
2:B:64:LEU:HB3	2:B:111:LEU:CD1	2.22	0.69
2:H:148:ILE:HG12	3:L:174:ARG:HG2	1.73	0.69
2:H:157:MET:HE3	2:H:157:MET:O	1.92	0.69
2:H:164:TYR:CD2	2:H:169:LEU:HB2	2.27	0.69
2:H:187:GLY:HA2	3:L:173:LEU:HD13	1.74	0.69
2:H:294:SER:O	2:H:298:VAL:HG23	1.92	0.69
2:H:398:THR:O	2:H:402:GLU:HG3	1.92	0.69
2:D:318:LEU:HD11	2:D:334:THR:CG2	2.22	0.69
1:A:36:ILE:O	1:A:60:ILE:O	2.08	0.69
1:C:317:LYS:HB3	1:C:318:GLU:OE1	1.93	0.69
2:D:141:ILE:CD1	2:D:158:LEU:HD21	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:380:ALA:HB1	2:D:394:LEU:CD1	2.21	0.69
2:F:237:TRP:HB3	2:F:238:PRO:HD3	1.75	0.69
1:G:507:LYS:HG2	1:G:513:PHE:HB2	1.73	0.69
2:B:356:SER:HB3	2:B:442:SER:H	1.55	0.69
2:B:380:ALA:CB	2:B:394:LEU:CD1	2.71	0.69
1:C:146:SER:O	1:C:147:GLN:HB2	1.90	0.69
1:G:185:LEU:HD12	1:G:275:ALA:HB1	1.73	0.69
2:B:361:LEU:HB3	2:B:408:LEU:HA	1.74	0.69
1:A:527:GLN:HB2	2:B:318:LEU:HD13	1.75	0.69
1:C:215:ILE:HG13	1:C:332:MET:HE1	1.74	0.69
1:E:297:ILE:H	1:E:297:ILE:CD1	2.03	0.69
2:F:125:ASN:HD22	2:F:125:ASN:N	1.91	0.69
1:A:154:ARG:HB3	1:A:161:TYR:HB3	1.76	0.68
2:B:64:LEU:HB3	2:B:111:LEU:HD11	1.74	0.68
2:B:203:THR:OG1	3:I:172:ARG:NH1	2.25	0.68
1:C:274:THR:O	1:C:276:LEU:N	2.26	0.68
2:F:131:ASN:HD22	2:H:131:ASN:HB3	1.58	0.68
1:G:33:VAL:CG2	1:G:54:ILE:HG12	2.22	0.68
1:C:163:ARG:NH1	1:C:165:ILE:HG12	2.07	0.68
2:D:17:TRP:O	2:D:21:LYS:HB2	1.92	0.68
3:K:104:LYS:HD2	3:K:112:GLU:OE2	1.91	0.68
3:K:172:ARG:C	3:K:173:LEU:HG	2.17	0.68
2:H:355:PHE:O	2:H:440:PHE:HA	1.93	0.68
1:C:259:PRO:C	1:C:261:ASP:N	2.49	0.68
2:D:125:ASN:HD22	2:D:125:ASN:N	1.92	0.68
2:F:217:THR:HG21	2:F:223:ARG:HH22	1.56	0.68
2:F:355:PHE:CE1	2:F:364:VAL:HG22	2.28	0.68
1:A:61:ASP:OD2	1:A:85:ARG:HB3	1.92	0.68
2:D:74:GLN:NE2	2:D:119:ASN:HD22	1.92	0.68
2:F:54:ILE:HG22	2:F:145:LEU:HD21	1.75	0.68
2:H:271:TYR:N	2:H:271:TYR:HD2	1.90	0.68
1:C:46:LEU:O	1:C:50:VAL:HG23	1.94	0.68
1:G:248:ARG:O	1:G:251:ILE:HG13	1.93	0.68
2:H:232:VAL:HG21	2:H:264:SER:CA	2.21	0.68
2:B:182:THR:HG21	2:B:296:ASN:OD1	1.94	0.68
2:D:322:LEU:HD12	2:D:323:VAL:N	2.08	0.68
1:E:309:ARG:HH11	1:E:309:ARG:HG3	1.59	0.68
2:F:362:GLN:NE2	2:F:408:LEU:HD13	2.08	0.68
1:A:87:GLU:O	1:A:91:GLU:HG3	1.94	0.68
2:H:192:ILE:HG22	2:H:194:PRO:HD3	1.76	0.68
1:C:163:ARG:HD2	1:C:518:ASN:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:THR:C	1:C:276:LEU:H	2.01	0.68
1:C:42:GLY:HA2	1:C:129:THR:HG21	1.77	0.67
2:D:62:GLU:HG2	2:D:297:ALA:HA	1.77	0.67
2:F:229:ILE:HD13	2:F:281:THR:HA	1.75	0.67
2:F:357:PRO:HA	2:F:412:LEU:HB2	1.76	0.67
2:H:228:CYS:O	2:H:232:VAL:HG23	1.94	0.67
2:H:357:PRO:HA	2:H:440:PHE:CE2	2.29	0.67
2:H:362:GLN:OE1	2:H:408:LEU:HD13	1.93	0.67
2:H:361:LEU:O	2:H:364:VAL:HG22	1.95	0.67
1:A:446:SER:HB2	1:A:449:GLN:NE2	2.10	0.67
1:C:226:TYR:CE1	1:C:231:GLY:HA2	2.29	0.67
2:H:64:LEU:HD21	2:H:77:VAL:CG2	2.25	0.67
1:C:421:ASN:O	1:C:424:VAL:HG22	1.95	0.67
2:H:325:ASN:HD21	2:H:327:VAL:HG23	1.58	0.67
1:E:297:ILE:HB	1:E:368:ILE:HD11	1.75	0.67
2:F:380:ALA:CB	2:F:394:LEU:HA	2.25	0.67
1:G:518:ASN:HD22	1:G:534:LEU:H	1.43	0.67
2:B:400:ILE:H	2:B:400:ILE:HD12	1.58	0.67
3:J:143:LEU:CB	3:J:150:MET:HE2	2.23	0.67
1:A:461:LEU:O	1:A:465:LEU:HG	1.95	0.66
2:F:139:HIS:C	2:F:140:ILE:HD12	2.20	0.66
2:H:253:ASP:HB3	2:H:256:HIS:HB2	1.77	0.66
2:B:361:LEU:HB2	2:B:407:ASN:O	1.95	0.66
1:C:264:ASN:HD22	1:C:264:ASN:H	1.44	0.66
1:G:333:ILE:HG22	2:H:223:ARG:CZ	2.25	0.66
2:H:128:GLN:HE21	2:H:128:GLN:N	1.91	0.66
2:D:380:ALA:HB1	2:D:394:LEU:HD13	1.78	0.66
2:F:398:THR:O	2:F:401:GLU:HG2	1.96	0.66
1:A:446:SER:HB2	1:A:449:GLN:HE21	1.59	0.66
1:E:307:LEU:HB3	1:E:383:LEU:CD2	2.25	0.66
1:E:422:GLU:HG3	1:E:530:ALA:HB3	1.78	0.66
2:F:362:GLN:HE21	2:F:408:LEU:CD1	2.06	0.66
3:L:117:ILE:HD13	3:L:126:ILE:HG12	1.76	0.66
2:D:411:THR:O	2:D:415:LEU:HG	1.96	0.66
2:D:412:LEU:HD22	2:D:417:LEU:HD12	1.77	0.66
2:H:348:GLN:HB3	2:H:349:LEU:HD12	1.77	0.66
1:A:366:GLN:C	1:A:368:ILE:H	2.04	0.66
2:D:192:ILE:CD1	2:D:200:ILE:HG13	2.26	0.66
2:D:418:VAL:HG22	2:D:421:GLN:NE2	2.10	0.66
1:A:125:VAL:HG21	1:A:505:VAL:HG13	1.77	0.66
1:A:430:ARG:HB3	1:A:430:ARG:NH1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:241:GLN:HE21	2:F:246:GLY:H	1.42	0.66
1:G:61:ASP:OD2	1:G:85:ARG:HD2	1.95	0.66
1:E:252:LEU:C	1:E:259:PRO:CD	2.69	0.66
1:G:307:LEU:HB3	1:G:383:LEU:CD2	2.25	0.66
2:H:412:LEU:HD22	2:H:440:PHE:CE2	2.31	0.66
2:B:407:ASN:ND2	2:B:415:LEU:HD22	2.10	0.65
3:K:156:ALA:HA	3:K:161:ILE:HD12	1.78	0.65
1:A:58:THR:HA	1:A:103:SER:O	1.96	0.65
1:A:61:ASP:OD2	1:A:85:ARG:HD2	1.95	0.65
2:B:385:LEU:HD12	2:B:390:ARG:HD3	1.78	0.65
2:D:360:LYS:HA	2:D:411:THR:HA	1.77	0.65
2:H:234:MET:C	2:H:235:LEU:HD22	2.20	0.65
3:L:123:VAL:HA	3:L:126:ILE:HD12	1.78	0.65
2:B:400:ILE:HD12	2:B:400:ILE:N	2.12	0.65
2:B:427:ASP:HB3	2:B:429:THR:HG22	1.77	0.65
1:C:43:THR:HG21	1:C:73:ASN:OD1	1.97	0.65
1:C:407:ILE:HG13	1:C:408:ASN:N	2.12	0.65
2:D:200:ILE:HG12	3:J:172:ARG:HH22	1.61	0.65
2:F:125:ASN:N	2:F:125:ASN:ND2	2.41	0.65
2:H:128:GLN:NE2	2:H:128:GLN:N	2.42	0.65
3:L:107:THR:CG2	3:L:111:LYS:HB3	2.26	0.65
3:I:104:LYS:HD3	3:I:112:GLU:OE2	1.96	0.65
3:K:124:GLU:HB2	3:K:152:ASP:O	1.96	0.65
3:K:125:ARG:HD3	3:K:129:ARG:NH2	2.09	0.65
1:G:226:TYR:HB3	1:G:231:GLY:HA2	1.79	0.65
1:A:220:LYS:HE2	1:A:220:LYS:HA	1.78	0.65
2:B:200:ILE:CD1	3:I:172:ARG:HH22	2.09	0.65
3:I:101:MET:N	3:I:117:ILE:O	2.23	0.65
2:F:154:ILE:O	2:F:158:LEU:HD23	1.97	0.65
2:F:384:THR:C	2:F:385:LEU:HD23	2.22	0.65
3:K:117:ILE:HG12	3:K:126:ILE:HG12	1.77	0.65
1:A:311:LEU:O	1:A:315:VAL:HG23	1.97	0.65
2:H:354:GLN:HE22	2:H:439:HIS:HB3	1.61	0.65
2:B:442:SER:O	2:B:442:SER:OG	2.12	0.65
2:H:405:ARG:HB3	2:H:406:PRO:HD3	1.77	0.65
1:A:518:ASN:HD21	1:A:534:LEU:HB2	1.60	0.64
2:B:380:ALA:HB1	2:B:394:LEU:CD1	2.28	0.64
2:D:343:CYS:O	2:D:347:SER:HB3	1.98	0.64
1:A:150:LEU:HD23	1:A:165:ILE:HD12	1.79	0.64
1:A:248:ARG:HA	1:A:251:ILE:HD11	1.79	0.64
2:B:318:LEU:HG	2:B:319:ASN:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:VAL:O	1:C:361:VAL:HG23	1.97	0.64
1:E:45:ILE:HG12	1:E:498:GLY:HA2	1.79	0.64
1:A:229:THR:O	1:A:230:ASN:HB2	1.98	0.64
1:A:252:LEU:HD22	1:A:253:LYS:N	2.12	0.64
2:B:102:PRO:HG2	2:B:105:GLU:HB3	1.78	0.64
2:B:425:VAL:HB	2:B:434:VAL:HG13	1.77	0.64
1:A:430:ARG:HB3	1:A:430:ARG:HH11	1.62	0.64
2:H:32:HIS:HD2	2:H:34:ASP:H	1.43	0.64
3:L:99:GLY:O	3:L:116:ASP:HB3	1.97	0.64
3:L:125:ARG:HD3	3:L:129:ARG:NH2	2.12	0.64
2:B:302:VAL:HG11	2:B:322:LEU:HD23	1.79	0.64
1:C:163:ARG:NH2	1:C:518:ASN:OD1	2.31	0.64
2:D:29:PRO:HG2	2:D:30:PHE:H	1.63	0.64
2:D:357:PRO:HG3	2:D:440:PHE:CG	2.33	0.64
1:G:527:GLN:HB2	2:H:318:LEU:HD13	1.79	0.64
1:E:211:HIS:HB2	1:E:334:ALA:HA	1.79	0.64
2:F:201:GLU:HG3	2:F:345:ALA:HB2	1.80	0.64
2:B:233:ARG:HB3	2:B:233:ARG:HH11	1.63	0.64
2:D:124:PHE:C	2:D:125:ASN:HD22	2.05	0.64
2:F:16:ARG:HH22	2:F:116:PRO:HB2	1.63	0.64
2:F:412:LEU:HD23	2:F:417:LEU:HD22	1.78	0.64
2:B:188:ASN:OD1	3:I:173:LEU:HD12	1.98	0.64
3:J:161:ILE:CD1	3:J:167:LEU:HD21	2.26	0.64
2:B:200:ILE:CD1	3:I:172:ARG:NH2	2.61	0.63
1:C:84:ASN:HB3	1:C:87:GLU:CB	2.27	0.63
2:D:237:TRP:HB3	2:D:238:PRO:HD3	1.79	0.63
2:F:371:SER:CB	2:F:374:LEU:CD1	2.58	0.63
1:C:396:ARG:HG3	1:C:518:ASN:HD21	1.62	0.63
2:F:132:ASP:HB3	2:F:157:MET:HE1	1.78	0.63
2:H:35:PHE:HD1	2:H:313:SER:O	1.80	0.63
2:H:344:PRO:HG3	2:H:374:LEU:HD13	1.80	0.63
1:C:51:LEU:HB2	1:C:52:PRO:HD3	1.81	0.63
3:L:107:THR:HG21	3:L:111:LYS:HB3	1.79	0.63
2:H:132:ASP:OD1	2:H:132:ASP:N	2.30	0.63
2:F:342:ASN:H	2:F:342:ASN:ND2	1.92	0.63
2:H:270:GLN:O	2:H:272:ASN:OD1	2.16	0.63
2:B:430:THR:HG22	2:B:431:PRO:HD2	1.79	0.63
2:D:268:ALA:HB2	2:D:276:VAL:HG21	1.80	0.63
2:H:318:LEU:HD11	2:H:334:THR:HG21	1.80	0.63
1:E:200:ASP:C	1:E:201:LEU:HD23	2.24	0.63
2:H:238:PRO:O	2:H:241:GLN:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:ASN:ND2	1:C:518:ASN:N	2.10	0.63
3:J:155:THR:HG23	3:J:158:ASP:OD1	1.99	0.63
2:F:384:THR:O	2:F:385:LEU:HD23	1.99	0.63
2:H:178:ILE:HD11	2:H:310:ILE:CD1	2.29	0.63
2:H:187:GLY:CA	3:L:173:LEU:HD13	2.29	0.63
1:A:409:LYS:HE2	1:A:468:TYR:O	1.99	0.62
1:A:458:LYS:O	1:A:458:LYS:HD3	1.99	0.62
2:B:96:PRO:O	2:B:99:ILE:HG13	1.99	0.62
3:I:170:VAL:HG13	3:I:171:LEU:N	2.13	0.62
1:C:33:VAL:HG22	1:C:34:CYS:N	2.12	0.62
2:D:380:ALA:HB2	2:D:394:LEU:CD1	2.26	0.62
2:D:207:TYR:CE1	3:J:172:ARG:CD	2.76	0.62
1:A:178:ASN:ND2	3:I:136:ILE:HG12	2.14	0.62
1:C:503:GLN:O	1:C:507:LYS:HG3	1.99	0.62
2:D:250:ASP:OD2	2:D:253:ASP:HB2	1.99	0.62
2:H:404:THR:HG22	2:H:407:ASN:ND2	2.14	0.62
1:E:113:LEU:O	1:E:117:PRO:HG3	1.99	0.62
1:E:309:ARG:HB3	1:E:364:LEU:HD21	1.81	0.62
1:G:488:ALA:C	1:G:490:PRO:HD3	2.25	0.62
1:A:418:ASN:HD22	1:A:418:ASN:C	2.08	0.62
1:C:434:ARG:HD3	1:C:460:CYS:HB3	1.80	0.62
2:D:232:VAL:O	2:D:232:VAL:HG12	1.99	0.62
2:F:46:LEU:HD22	2:F:73:ARG:CZ	2.30	0.62
2:F:267:ARG:HG2	2:F:267:ARG:HH11	1.64	0.62
1:G:6:LYS:C	1:G:8:LEU:H	2.08	0.62
1:G:158:LEU:HD12	1:G:493:ILE:HD11	1.80	0.62
1:G:311:LEU:O	1:G:314:PHE:HB3	2.00	0.62
1:G:397:SER:OG	1:G:400:GLU:HG3	1.98	0.62
2:B:356:SER:CB	2:B:441:THR:OG1	2.47	0.62
3:I:107:THR:HG22	3:I:109:THR:N	2.09	0.62
1:C:61:ASP:OD1	1:C:63:ASN:HB2	1.99	0.62
1:E:36:ILE:HG21	1:E:131:LEU:HD21	1.82	0.62
1:E:243:PHE:O	1:E:247:ILE:HG13	1.99	0.62
1:G:264:ASN:HB3	1:G:333:ILE:HG13	1.80	0.62
2:H:270:GLN:C	2:H:272:ASN:OD1	2.43	0.62
1:G:332:MET:HG2	1:G:339:TYR:HE1	1.65	0.62
1:G:333:ILE:N	2:H:223:ARG:NH1	2.46	0.62
2:F:183:GLU:HG3	2:F:289:ILE:HG21	1.80	0.62
1:E:253:LYS:N	1:E:259:PRO:HD2	2.14	0.62
2:F:342:ASN:HD22	2:F:342:ASN:N	1.85	0.62
2:H:58:GLY:N	2:H:91:GLN:HG2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:237:TRP:HB3	2:H:238:PRO:HD3	1.81	0.62
1:A:112:LEU:H	1:A:112:LEU:CD2	2.13	0.61
1:C:294:CYS:O	1:C:309:ARG:HD3	2.00	0.61
3:K:155:THR:HG23	3:K:157:ALA:H	1.65	0.61
2:H:391:THR:O	2:H:404:THR:HG21	1.99	0.61
3:L:123:VAL:HA	3:L:126:ILE:CD1	2.29	0.61
2:B:74:GLN:NE2	2:B:119:ASN:HD22	1.97	0.61
1:E:214:TRP:O	1:E:218:ILE:HG13	1.99	0.61
2:F:31:THR:HG23	2:F:32:HIS:O	2.00	0.61
2:F:232:VAL:O	2:F:232:VAL:HG12	1.99	0.61
2:H:233:ARG:NH1	2:H:234:MET:HB2	2.15	0.61
2:F:192:ILE:HG22	2:F:194:PRO:HD3	1.82	0.61
1:G:185:LEU:CD1	1:G:275:ALA:HB1	2.30	0.61
1:G:199:TYR:CD2	1:G:216:VAL:HG11	2.35	0.61
2:H:237:TRP:CE3	2:H:242:PRO:HG2	2.35	0.61
1:A:234:PRO:HB2	1:A:276:LEU:CD1	2.30	0.61
2:D:390:ARG:HG2	2:D:391:THR:N	2.14	0.61
1:E:447:ASN:ND2	2:F:26:ARG:HH21	1.97	0.61
1:G:50:VAL:HG13	1:G:100:VAL:HG21	1.82	0.61
1:G:241:GLU:O	1:G:244:ARG:HB2	1.99	0.61
1:A:450:VAL:O	1:A:454:ILE:HG13	1.99	0.61
2:B:415:LEU:HB2	2:B:417:LEU:CD2	2.30	0.61
3:J:104:LYS:HB2	3:J:166:VAL:HG12	1.81	0.61
2:F:316:ILE:H	2:F:316:ILE:CD1	2.09	0.61
2:B:316:ILE:H	2:B:316:ILE:CD1	2.08	0.61
1:C:58:THR:HA	1:C:103:SER:O	2.01	0.61
1:C:492:THR:HB	2:D:305:THR:OG1	2.01	0.61
1:G:61:ASP:HB3	1:G:86:ALA:HB2	1.83	0.61
1:G:72:ASN:HD22	1:G:72:ASN:H	1.48	0.61
2:H:320:ASN:HD22	2:H:337:ALA:HB3	1.66	0.61
1:A:211:HIS:CE1	2:B:221:MET:HE1	2.36	0.61
2:B:368:LEU:HD21	2:B:436:PHE:CE2	2.35	0.61
2:D:15:GLY:HA2	2:D:18:ASN:ND2	2.16	0.61
2:F:362:GLN:CG	2:F:408:LEU:HD22	2.27	0.61
2:H:92:PHE:H	2:H:92:PHE:HD2	1.48	0.61
2:H:405:ARG:CB	2:H:405:ARG:HH11	2.13	0.61
1:A:423:ILE:O	1:A:426:TYR:HB3	2.01	0.61
2:H:58:GLY:H	2:H:91:GLN:CG	2.14	0.61
2:H:422:GLU:C	2:H:423:LEU:HD12	2.25	0.61
1:A:281:ILE:HD11	1:A:315:VAL:HG11	1.82	0.61
2:B:131:ASN:HB3	2:D:131:ASN:HD22	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:185:PHE:HB3	2:D:326:ASP:HB2	1.83	0.61
2:D:192:ILE:HD11	2:D:200:ILE:HG13	1.83	0.61
3:L:150:MET:CE	3:L:167:LEU:HD13	2.31	0.61
1:A:36:ILE:HD12	1:A:60:ILE:CB	2.16	0.61
1:C:418:ASN:C	1:C:418:ASN:HD22	2.07	0.61
1:G:192:LEU:O	1:G:195:HIS:HB3	2.01	0.61
2:H:32:HIS:CG	2:H:33:PRO:HD2	2.36	0.61
2:H:405:ARG:HB3	2:H:405:ARG:HH11	1.65	0.61
2:H:419:ASP:OD2	2:H:440:PHE:HB2	2.01	0.61
1:A:168:GLU:HG3	1:A:394:ARG:HE	1.66	0.60
1:C:376:SER:OG	1:C:379:GLU:HG3	2.01	0.60
1:C:501:ALA:O	1:C:504:GLU:N	2.34	0.60
1:G:214:TRP:HB2	1:G:268:ALA:HB2	1.82	0.60
1:G:336:SER:HB2	2:H:221:MET:HA	1.83	0.60
2:B:49:CYS:HA	2:B:139:HIS:HD2	1.65	0.60
2:B:233:ARG:HD2	2:B:285:VAL:HG13	1.82	0.60
2:B:353:ILE:HG23	2:B:355:PHE:CD1	2.35	0.60
2:B:374:LEU:O	2:B:376:MET:HG3	2.01	0.60
1:C:90:MET:HE3	1:C:94:GLN:OE1	2.01	0.60
1:C:430:ARG:NH1	1:C:430:ARG:HB3	2.16	0.60
3:J:101:MET:HB2	3:J:117:ILE:O	1.99	0.60
1:G:229:THR:HG21	1:G:232:ARG:HH21	1.65	0.60
2:H:217:THR:HG21	2:H:223:ARG:HE	1.65	0.60
2:B:218:ILE:CD1	2:B:230:GLU:HG2	2.29	0.60
1:C:6:LYS:O	1:C:9:LYS:HG2	2.01	0.60
1:C:438:GLN:O	1:C:438:GLN:HG2	2.01	0.60
2:F:178:ILE:HD11	2:F:310:ILE:HD12	1.82	0.60
1:G:306:ILE:HD13	1:G:365:LEU:CD2	2.31	0.60
2:H:178:ILE:N	2:H:178:ILE:HD12	2.16	0.60
2:H:349:LEU:HB3	2:H:350:PRO:HD2	1.83	0.60
1:A:371:ALA:C	1:A:373:GLU:H	2.08	0.60
1:A:407:ILE:HD13	1:A:408:ASN:N	2.16	0.60
2:B:412:LEU:O	2:B:417:LEU:HB2	2.02	0.60
1:E:240:LYS:HE2	1:E:276:LEU:HD12	1.84	0.60
1:E:489:GLU:H	2:F:19:HIS:HD2	1.46	0.60
2:F:223:ARG:HH11	2:F:223:ARG:HG3	1.67	0.60
1:G:306:ILE:HD13	1:G:365:LEU:HD23	1.83	0.60
2:H:390:ARG:NH2	2:H:407:ASN:HD21	1.99	0.60
3:L:124:GLU:HB2	3:L:152:ASP:O	2.00	0.60
1:A:147:GLN:N	1:A:147:GLN:HE21	1.99	0.60
1:C:284:SER:O	1:C:288:ILE:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:GLY:C	2:D:91:GLN:HG2	2.26	0.60
2:D:236:GLN:HE22	2:D:263:LYS:HD2	1.67	0.60
1:G:307:LEU:HB3	1:G:383:LEU:HD22	1.84	0.60
2:H:356:SER:C	2:H:358:SER:H	2.08	0.60
2:D:199:CYS:O	2:D:202:CYS:HB2	2.02	0.60
1:E:365:LEU:HD11	1:E:375:ILE:HD13	1.83	0.60
2:H:400:ILE:O	2:H:404:THR:N	2.35	0.60
2:D:325:ASN:ND2	2:D:327:VAL:HG22	2.17	0.60
3:J:144:ILE:HD13	3:J:149:GLN:HA	1.84	0.60
2:H:158:LEU:CD1	2:H:177:LEU:HD22	2.32	0.60
1:E:212:THR:O	1:E:213:PRO:C	2.44	0.60
2:F:425:VAL:HB	2:F:434:VAL:HG13	1.82	0.60
1:G:265:PHE:O	1:G:269:ILE:HG13	2.02	0.60
2:H:237:TRP:CD2	2:H:242:PRO:HG2	2.37	0.60
2:F:131:ASN:HB3	2:H:131:ASN:ND2	2.14	0.60
2:F:361:LEU:HD12	2:F:407:ASN:O	2.02	0.60
2:D:158:LEU:HD22	2:D:175:VAL:HB	1.84	0.59
1:E:219:ALA:O	1:E:222:LEU:HB3	2.02	0.59
3:K:144:ILE:HD11	3:K:170:VAL:HG11	1.83	0.59
1:C:126:VAL:O	1:C:150:LEU:HD12	2.02	0.59
1:C:360:HIS:O	1:C:364:LEU:HD23	2.02	0.59
1:G:184:ARG:HD3	1:G:279:THR:OG1	2.02	0.59
2:H:38:SER:C	2:H:40:GLU:H	2.10	0.59
2:B:435:LEU:C	2:B:436:PHE:HD1	2.10	0.59
1:C:407:ILE:HG13	1:C:408:ASN:H	1.66	0.59
1:G:36:ILE:HB	1:G:128:ALA:HA	1.85	0.59
2:H:90:ARG:HH11	2:H:90:ARG:HG2	1.68	0.59
2:H:131:ASN:O	2:H:133:THR:N	2.35	0.59
3:L:150:MET:HE1	3:L:167:LEU:HD22	1.84	0.59
1:C:113:LEU:HD13	1:C:138:ARG:HG2	1.84	0.59
1:E:39:THR:O	1:E:43:THR:HB	2.01	0.59
1:E:447:ASN:ND2	2:F:26:ARG:HE	2.00	0.59
2:F:410:LYS:HB3	2:F:414:GLU:HG2	1.84	0.59
2:B:158:LEU:HD12	2:B:177:LEU:HB2	1.85	0.59
1:C:61:ASP:CB	1:C:86:ALA:HB2	2.33	0.59
1:C:277:ASN:O	1:C:277:ASN:ND2	2.36	0.59
2:F:241:GLN:CG	2:F:245:GLU:HA	2.32	0.59
3:L:117:ILE:CD1	3:L:126:ILE:HG23	2.32	0.59
1:A:47:LYS:HG3	1:A:75:PHE:HZ	1.67	0.59
3:I:103:ILE:CD1	3:I:117:ILE:HD12	2.33	0.59
1:C:113:LEU:O	1:C:117:PRO:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:422:GLU:OE1	1:G:422:GLU:N	2.33	0.59
1:G:492:THR:HB	2:H:305:THR:OG1	2.02	0.59
2:B:385:LEU:CD1	2:B:390:ARG:HD3	2.32	0.59
1:C:158:LEU:HA	1:C:493:ILE:HG13	1.82	0.59
2:D:200:ILE:HG12	3:J:172:ARG:NH2	2.17	0.59
3:L:117:ILE:HG23	3:L:121:ASP:HB2	1.82	0.59
1:C:232:ARG:C	1:C:233:ILE:HD12	2.28	0.59
2:F:15:GLY:HA2	2:F:18:ASN:HD21	1.67	0.59
2:H:335:PHE:HE2	3:L:170:VAL:HG11	1.67	0.59
1:A:252:LEU:C	1:A:259:PRO:CD	2.72	0.59
2:B:286:LYS:HB2	2:B:288:ILE:HG13	1.85	0.59
1:C:42:GLY:CA	1:C:129:THR:HG21	2.32	0.59
1:E:13:TYR:O	1:E:17:LEU:HG	2.03	0.59
1:E:226:TYR:CD1	1:E:231:GLY:CA	2.78	0.59
2:F:219:ALA:HA	2:F:267:ARG:HH22	1.67	0.59
2:F:411:THR:O	2:F:414:GLU:HB3	2.02	0.59
3:K:149:GLN:HG3	3:K:149:GLN:O	2.03	0.59
2:H:356:SER:C	2:H:358:SER:N	2.57	0.59
1:A:178:ASN:CG	3:I:136:ILE:HG12	2.28	0.59
3:I:117:ILE:HG22	3:I:118:GLU:N	2.17	0.59
2:D:237:TRP:CE3	2:D:242:PRO:HG2	2.38	0.59
2:F:249:LEU:CD1	2:F:260:ILE:HD11	2.33	0.59
1:G:264:ASN:HA	1:G:333:ILE:HD11	1.85	0.58
3:L:143:LEU:C	3:L:144:ILE:HD12	2.28	0.58
1:C:173:GLU:HA	1:C:386:ASN:ND2	2.18	0.58
1:C:441:ARG:HB3	2:H:270:GLN:OE1	2.03	0.58
1:E:220:LYS:C	1:E:222:LEU:H	2.11	0.58
1:E:248:ARG:O	1:E:251:ILE:HG12	2.00	0.58
1:E:340:ILE:HG21	2:F:272:ASN:ND2	2.18	0.58
2:H:224:LEU:H	2:H:227:HIS:CE1	2.20	0.58
2:H:368:LEU:HD13	2:H:425:VAL:HG11	1.84	0.58
1:A:211:HIS:ND1	2:B:221:MET:HE1	2.17	0.58
1:C:262:GLU:HG2	1:C:265:PHE:CD1	2.38	0.58
1:C:274:THR:C	1:C:276:LEU:N	2.61	0.58
2:D:128:GLN:NE2	2:D:128:GLN:H	2.01	0.58
1:E:282:PRO:HB2	1:E:285:ILE:HD13	1.84	0.58
3:L:120:THR:HA	3:L:155:THR:HG1	1.66	0.58
2:B:393:TYR:CE2	2:B:408:LEU:HD21	2.39	0.58
2:D:384:THR:HA	2:D:389:ASN:HB3	1.83	0.58
1:E:236:THR:HG22	1:E:238:LYS:H	1.67	0.58
1:E:507:LYS:HG2	1:E:513:PHE:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:222:PRO:O	2:F:273:ILE:HD11	2.01	0.58
1:A:307:LEU:HB3	1:A:383:LEU:CD2	2.32	0.58
2:B:380:ALA:HB1	2:B:394:LEU:HD12	1.84	0.58
2:D:430:THR:OG1	2:D:432:GLN:HG2	2.02	0.58
2:F:225:PRO:O	2:F:229:ILE:HG13	2.03	0.58
2:H:35:PHE:CD1	2:H:313:SER:O	2.57	0.58
3:L:106:LYS:HG2	3:L:112:GLU:HG2	1.84	0.58
1:A:518:ASN:OD1	1:A:519:THR:N	2.35	0.58
1:C:229:THR:HG22	1:C:232:ARG:HD2	1.85	0.58
3:J:105:VAL:CG1	3:J:115:ILE:HD11	2.34	0.58
2:F:366:ASP:HB3	2:F:370:ASN:HD22	1.68	0.58
2:H:177:LEU:HG	2:H:177:LEU:O	2.03	0.58
2:H:249:LEU:CD1	2:H:260:ILE:HD11	2.34	0.58
3:L:126:ILE:O	3:L:130:VAL:HG23	2.04	0.58
1:A:19:LEU:HD21	2:B:290:PRO:HB2	1.86	0.58
1:A:49:LEU:O	1:A:52:PRO:HG2	2.03	0.58
1:A:214:TRP:C	1:A:214:TRP:CD1	2.82	0.58
2:B:15:GLY:HA2	2:B:18:ASN:OD1	2.03	0.58
2:B:196:MET:O	2:B:339:ARG:HD2	2.03	0.58
2:D:320:ASN:HB2	2:D:336:GLU:HA	1.86	0.58
1:E:41:THR:O	1:E:45:ILE:HG13	2.04	0.58
2:F:221:MET:N	2:F:222:PRO:HD3	2.19	0.58
3:L:103:ILE:HD12	3:L:103:ILE:O	2.04	0.58
1:C:130:GLN:CD	1:C:155:THR:H	2.12	0.58
1:C:236:THR:HB	1:C:239:GLU:HG3	1.86	0.58
2:F:325:ASN:HD22	2:F:326:ASP:N	2.01	0.58
2:H:238:PRO:O	2:H:241:GLN:CG	2.51	0.58
1:C:130:GLN:OE1	1:C:155:THR:CB	2.48	0.58
2:D:13:TRP:HZ3	2:D:116:PRO:HG2	1.67	0.58
2:F:356:SER:C	2:F:358:SER:H	2.12	0.58
1:A:436:HIS:HA	1:A:441:ARG:O	2.04	0.58
1:A:518:ASN:HD22	1:A:534:LEU:H	1.29	0.58
2:B:153:TRP:CE2	2:B:431:PRO:HG3	2.39	0.58
1:E:184:ARG:HD3	1:E:279:THR:OG1	2.04	0.58
2:F:376:MET:HE2	2:F:427:ASP:CB	2.31	0.58
3:K:107:THR:HG22	3:K:109:THR:H	1.69	0.58
1:G:226:TYR:HE2	1:G:233:ILE:HA	1.67	0.58
2:H:84:ASP:H	2:H:87:ASN:ND2	2.02	0.58
2:D:193:LEU:H	2:D:197:THR:HB	1.68	0.57
2:F:239:LYS:O	2:F:240:GLU:HG2	2.04	0.57
2:B:325:ASN:ND2	2:B:327:VAL:HG22	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:PHE:C	1:C:122:ARG:H	2.12	0.57
2:F:410:LYS:CB	2:F:414:GLU:HG2	2.33	0.57
3:K:115:ILE:HG23	3:K:117:ILE:HD13	1.85	0.57
1:G:84:ASN:OD1	1:G:106:GLU:HG3	2.04	0.57
2:H:32:HIS:CD2	2:H:34:ASP:H	2.22	0.57
2:B:241:GLN:O	2:B:242:PRO:C	2.47	0.57
1:C:72:ASN:OD1	1:C:489:GLU:HG2	2.04	0.57
1:C:88:ALA:O	1:C:91:GLU:HB2	2.05	0.57
2:D:132:ASP:HB3	2:D:157:MET:HE1	1.85	0.57
1:G:65:VAL:HB	1:G:81:ILE:HA	1.86	0.57
3:L:102:LEU:HD11	3:L:114:GLU:HB3	1.85	0.57
2:H:318:LEU:O	2:H:319:ASN:O	2.22	0.57
2:B:327:VAL:HG23	2:B:328:ASP:N	2.17	0.57
2:F:152:ARG:CZ	2:F:429:THR:HG21	2.35	0.57
2:F:187:GLY:CA	3:K:173:LEU:HD13	2.35	0.57
2:F:236:GLN:HE22	2:F:263:LYS:HB3	1.70	0.57
2:F:371:SER:O	2:F:374:LEU:CD1	2.52	0.57
1:A:72:ASN:C	1:A:72:ASN:HD22	2.11	0.57
1:A:224:GLN:HE21	1:A:246:LEU:HD11	1.70	0.57
2:F:187:GLY:HA2	3:K:173:LEU:HD13	1.87	0.57
1:G:20:TRP:O	1:G:24:GLY:HA3	2.04	0.57
1:A:484:ARG:HH12	2:B:31:THR:HG22	1.68	0.57
1:C:438:GLN:O	1:C:439:GLN:HG2	2.04	0.57
2:F:178:ILE:HD11	2:F:310:ILE:CD1	2.34	0.57
2:F:381:ILE:HD12	2:F:381:ILE:H	1.70	0.57
2:B:353:ILE:HD11	2:B:367:TYR:CE2	2.40	0.57
1:C:97:ASN:HB3	1:C:100:VAL:HG23	1.87	0.57
2:D:316:ILE:H	2:D:316:ILE:HD12	1.70	0.57
2:D:335:PHE:HE2	3:J:170:VAL:HG21	1.70	0.57
3:K:118:GLU:HG3	3:K:120:THR:HG22	1.86	0.57
1:G:33:VAL:HG22	1:G:54:ILE:HG12	1.86	0.57
2:H:201:GLU:HB3	2:H:343:CYS:SG	2.44	0.57
2:H:359:ALA:O	2:H:412:LEU:HD12	2.05	0.57
3:L:102:LEU:HD12	3:L:115:ILE:O	2.04	0.57
1:A:248:ARG:C	1:A:250:GLY:H	2.12	0.57
2:B:318:LEU:HD11	2:B:334:THR:HG21	1.87	0.57
1:C:163:ARG:CD	1:C:518:ASN:O	2.52	0.57
1:C:189:PHE:CE1	1:C:192:LEU:HB2	2.39	0.57
1:C:418:ASN:HD22	1:C:419:PRO:N	2.02	0.57
2:F:411:THR:N	2:F:414:GLU:HB3	2.16	0.57
1:G:275:ALA:O	1:G:278:THR:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:TYR:CE1	1:A:487:ALA:HA	2.40	0.56
2:B:385:LEU:HD12	2:B:390:ARG:CD	2.34	0.56
2:F:385:LEU:HD11	2:F:392:LEU:HD21	1.86	0.56
1:G:518:ASN:ND2	1:G:534:LEU:H	2.03	0.56
2:H:231:TYR:C	2:H:233:ARG:H	2.14	0.56
2:D:252:ASP:O	2:D:254:PRO:HD3	2.05	0.56
2:H:376:MET:HB3	2:H:427:ASP:OD1	2.04	0.56
1:A:441:ARG:HG2	1:A:441:ARG:HH11	1.71	0.56
1:A:527:GLN:HG3	2:B:306:GLU:OE1	2.05	0.56
1:C:492:THR:HB	2:D:305:THR:HG1	1.69	0.56
2:F:222:PRO:HG2	2:F:267:ARG:NH2	2.19	0.56
2:F:236:GLN:O	2:F:240:GLU:HG3	2.05	0.56
1:G:215:ILE:O	1:G:218:ILE:HG22	2.05	0.56
1:G:434:ARG:NH1	1:G:464:PHE:HA	2.19	0.56
2:H:338:GLU:CD	3:L:148:LYS:HE3	2.29	0.56
1:A:484:ARG:NH1	2:B:31:THR:HG22	2.21	0.56
2:B:427:ASP:OD2	2:B:428:VAL:N	2.38	0.56
2:D:216:ALA:O	2:D:220:SER:HB2	2.06	0.56
2:D:352:ASN:HB3	2:D:439:HIS:CD2	2.39	0.56
2:F:96:PRO:O	2:F:99:ILE:HG13	2.05	0.56
1:C:49:LEU:C	1:C:52:PRO:HD2	2.30	0.56
1:C:59:ILE:HG22	1:C:60:ILE:H	1.69	0.56
1:C:307:LEU:HD22	1:C:383:LEU:HD22	1.88	0.56
1:E:215:ILE:HG13	1:E:332:MET:SD	2.46	0.56
2:H:383:ALA:HB3	2:H:392:LEU:HD21	1.87	0.56
2:B:132:ASP:O	2:B:133:THR:C	2.49	0.56
1:C:430:ARG:HB3	1:C:430:ARG:HH11	1.70	0.56
2:F:164:TYR:CZ	2:F:348:GLN:HG3	2.41	0.56
1:G:331:ASP:OD1	2:H:223:ARG:HB3	2.04	0.56
2:H:46:LEU:HD23	2:H:71:GLY:O	2.05	0.56
1:A:72:ASN:C	1:A:72:ASN:ND2	2.62	0.56
1:E:193:ARG:HG3	1:E:193:ARG:HH11	1.70	0.56
1:E:416:MET:HE1	1:E:424:VAL:HG13	1.88	0.56
1:G:299:LYS:HA	1:G:368:ILE:CG2	2.36	0.56
2:H:229:ILE:HD13	2:H:281:THR:HA	1.88	0.56
2:D:148:ILE:HG12	2:D:207:TYR:CE2	2.40	0.56
1:E:218:ILE:O	1:E:222:LEU:HB2	2.06	0.56
1:E:264:ASN:HD22	1:E:265:PHE:N	2.04	0.56
3:L:155:THR:HG23	3:L:158:ASP:H	1.70	0.56
1:A:147:GLN:HE21	1:A:147:GLN:CA	2.18	0.56
1:C:435:PHE:O	1:C:439:GLN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:147:SER:HB2	2:F:149:ILE:HD13	1.87	0.56
3:K:107:THR:HG22	3:K:109:THR:N	2.20	0.56
1:G:112:LEU:C	1:G:114:ASP:N	2.64	0.56
2:H:324:PHE:HD1	2:H:332:THR:HG22	1.70	0.56
2:B:425:VAL:HB	2:B:434:VAL:CG1	2.35	0.56
1:C:297:ILE:H	1:C:297:ILE:CD1	2.16	0.56
2:D:158:LEU:HD13	2:D:177:LEU:HB2	1.86	0.56
2:D:270:GLN:C	2:D:272:ASN:H	2.13	0.56
3:J:116:ASP:O	3:J:117:ILE:HD13	2.06	0.56
1:E:518:ASN:HB2	1:E:533:GLN:HA	1.87	0.56
2:F:16:ARG:NH2	2:F:116:PRO:HB2	2.21	0.56
2:F:312:THR:O	2:F:313:SER:HB2	2.05	0.56
2:F:376:MET:HE1	2:F:425:VAL:HG12	1.88	0.56
2:H:350:PRO:HB3	2:H:436:PHE:C	2.31	0.56
2:B:198:ALA:H	2:B:320:ASN:HD21	1.54	0.55
2:B:252:ASP:O	2:B:254:PRO:HD3	2.06	0.55
2:B:441:THR:C	2:B:442:SER:OXT	2.44	0.55
1:C:233:ILE:HD12	1:C:233:ILE:N	2.21	0.55
1:E:299:LYS:HE2	1:E:368:ILE:O	2.06	0.55
2:F:256:HIS:O	2:F:260:ILE:HG13	2.06	0.55
1:A:66:SER:O	1:A:81:ILE:HG23	2.06	0.55
1:A:264:ASN:HD22	1:A:264:ASN:H	1.53	0.55
1:C:426:TYR:O	1:C:430:ARG:HG2	2.06	0.55
1:E:158:LEU:HD12	1:E:158:LEU:N	2.21	0.55
1:E:447:ASN:HD22	2:F:26:ARG:NH2	2.04	0.55
2:F:381:ILE:HG22	2:F:382:THR:N	2.20	0.55
1:G:7:LEU:O	1:G:7:LEU:HD23	2.06	0.55
2:H:52:LEU:HD22	2:H:138:PHE:CE1	2.42	0.55
2:B:197:THR:CG2	2:B:198:ALA:N	2.70	0.55
2:B:356:SER:N	2:B:441:THR:OG1	2.38	0.55
1:C:61:ASP:HB2	1:C:86:ALA:HB2	1.88	0.55
1:C:481:GLU:OE2	2:D:29:PRO:HD2	2.05	0.55
2:F:348:GLN:O	2:F:348:GLN:HG2	2.06	0.55
2:F:351:GLN:H	2:F:436:PHE:HA	1.70	0.55
2:F:412:LEU:HD13	2:F:440:PHE:CE2	2.35	0.55
1:G:407:ILE:HG13	1:G:408:ASN:N	2.21	0.55
1:A:19:LEU:HD21	2:B:290:PRO:CB	2.36	0.55
1:C:119:PHE:O	1:C:122:ARG:HG2	2.07	0.55
1:C:259:PRO:CB	1:C:262:GLU:OE1	2.47	0.55
1:E:84:ASN:OD1	1:E:106:GLU:HG2	2.06	0.55
1:E:234:PRO:HG2	1:E:243:PHE:CD1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:15:GLY:HA2	2:F:18:ASN:ND2	2.21	0.55
2:F:234:MET:O	2:F:235:LEU:HD23	2.06	0.55
2:F:320:ASN:ND2	2:F:337:ALA:O	2.40	0.55
1:G:18:ARG:HH12	2:H:279:ARG:HG3	1.71	0.55
1:A:74:PHE:CD1	2:B:65:LYS:HG3	2.42	0.55
2:D:230:GLU:HG3	2:D:230:GLU:O	2.07	0.55
1:E:357:VAL:O	1:E:361:VAL:HG23	2.06	0.55
3:K:107:THR:C	3:K:109:THR:H	2.13	0.55
1:G:180:LEU:H	1:G:180:LEU:CD1	2.17	0.55
1:G:267:GLU:O	1:G:270:LYS:HG2	2.06	0.55
3:L:113:ILE:HG13	3:L:113:ILE:O	2.06	0.55
1:A:14:ASP:O	1:A:18:ARG:HG3	2.07	0.55
1:A:112:LEU:HD22	1:A:112:LEU:N	2.19	0.55
1:G:164:ILE:HD11	1:G:166:ILE:HD11	1.89	0.55
1:G:299:LYS:HG2	1:G:368:ILE:HG22	1.89	0.55
1:A:193:ARG:O	1:A:197:GLN:HG3	2.07	0.55
1:C:248:ARG:C	1:C:250:GLY:N	2.65	0.55
3:J:170:VAL:HG22	3:J:171:LEU:N	2.18	0.55
1:E:396:ARG:NH2	1:E:400:GLU:HB3	2.22	0.55
2:F:425:VAL:HB	2:F:434:VAL:CG1	2.37	0.55
2:D:240:GLU:HG3	2:D:240:GLU:O	2.07	0.55
2:H:270:GLN:C	2:H:271:TYR:HD2	2.14	0.55
1:A:47:LYS:HG3	1:A:75:PHE:CZ	2.42	0.55
2:B:319:ASN:CG	2:B:336:GLU:HG3	2.32	0.55
2:B:353:ILE:HD11	2:B:367:TYR:HE2	1.71	0.55
3:J:123:VAL:CB	3:J:152:ASP:HA	2.22	0.55
1:E:173:GLU:O	1:E:512:GLN:O	2.25	0.55
1:G:279:THR:HG22	1:G:322:ASN:ND2	2.22	0.55
2:H:217:THR:HG21	2:H:223:ARG:NH2	2.19	0.55
1:A:227:SER:C	1:A:229:THR:H	2.15	0.54
2:D:74:GLN:HE22	2:D:119:ASN:HD22	1.52	0.54
2:H:228:CYS:SG	2:H:268:ALA:HB2	2.47	0.54
1:A:418:ASN:HD22	1:A:419:PRO:N	2.05	0.54
1:C:412:ILE:O	1:C:416:MET:HB2	2.07	0.54
2:F:236:GLN:HE22	2:F:263:LYS:HD2	1.72	0.54
1:G:87:GLU:O	1:G:91:GLU:HG3	2.07	0.54
1:G:248:ARG:O	1:G:251:ILE:CG1	2.55	0.54
1:G:516:PHE:H	1:G:516:PHE:HD2	1.54	0.54
1:C:243:PHE:O	1:C:246:LEU:HB3	2.08	0.54
2:D:229:ILE:HD13	2:D:281:THR:HA	1.89	0.54
1:E:252:LEU:O	1:E:259:PRO:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:ASN:HD21	2:F:103:LYS:HE2	1.70	0.54
2:H:200:ILE:HD13	3:L:172:ARG:HH22	1.72	0.54
2:H:412:LEU:HD23	2:H:438:LEU:HD21	1.88	0.54
1:A:215:ILE:CD1	1:A:332:MET:HE1	2.36	0.54
2:B:182:THR:HG22	3:I:176:GLY:HA2	1.90	0.54
1:C:154:ARG:HB3	1:C:161:TYR:HB3	1.88	0.54
2:D:231:TYR:C	2:D:233:ARG:N	2.64	0.54
2:F:318:LEU:HD11	2:F:334:THR:CG2	2.37	0.54
3:K:123:VAL:CB	3:K:152:ASP:HA	2.21	0.54
1:G:37:ASN:HB3	1:G:39:THR:HG23	1.89	0.54
1:G:518:ASN:HB3	1:G:532:PHE:O	2.07	0.54
1:E:171:VAL:CG1	1:E:391:ARG:HB2	2.37	0.54
1:E:332:MET:O	2:F:223:ARG:NE	2.40	0.54
1:G:215:ILE:H	1:G:332:MET:CE	2.20	0.54
1:A:45:ILE:HG12	1:A:498:GLY:HA2	1.90	0.54
1:A:461:LEU:HD21	1:A:474:VAL:HG11	1.89	0.54
1:C:34:CYS:HB2	1:C:123:PHE:CD2	2.42	0.54
1:A:78:ARG:HA	1:A:81:ILE:HG13	1.90	0.54
1:C:248:ARG:O	1:C:250:GLY:N	2.41	0.54
2:D:32:HIS:ND1	2:D:33:PRO:HD2	2.23	0.54
1:E:302:PRO:HG2	1:E:305:TRP:HD1	1.72	0.54
1:G:434:ARG:O	1:G:438:GLN:HG2	2.08	0.54
2:H:229:ILE:HD12	2:H:284:VAL:HG21	1.88	0.54
1:A:96:LEU:HD23	2:B:95:ARG:HH21	1.73	0.54
1:E:260:GLU:O	1:E:261:ASP:OD1	2.25	0.54
2:F:54:ILE:CG2	2:F:145:LEU:HD21	2.37	0.54
2:F:415:LEU:HB2	2:F:417:LEU:CD1	2.38	0.54
1:G:307:LEU:HB3	1:G:383:LEU:HD21	1.89	0.54
2:H:132:ASP:HB3	2:H:157:MET:HE1	1.90	0.54
2:H:259:TRP:CE2	2:H:263:LYS:HG3	2.42	0.54
1:A:396:ARG:HD3	1:A:534:LEU:O	2.08	0.54
2:B:226:GLU:HG3	2:B:280:LEU:HD11	1.90	0.54
2:D:357:PRO:HG3	2:D:440:PHE:CD2	2.43	0.54
2:H:231:TYR:O	2:H:233:ARG:N	2.41	0.54
1:A:12:LYS:HG3	1:A:13:TYR:CD2	2.43	0.54
1:A:214:TRP:CZ3	1:A:332:MET:HB3	2.43	0.54
2:B:359:ALA:O	2:B:412:LEU:HD23	2.08	0.54
1:E:163:ARG:NH1	1:E:518:ASN:HD21	2.05	0.54
3:K:118:GLU:HG2	3:K:121:ASP:CG	2.33	0.54
1:G:215:ILE:H	1:G:332:MET:HE1	1.73	0.54
1:G:269:ILE:HG22	1:G:269:ILE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ARG:O	1:A:81:ILE:HG13	2.08	0.53
2:B:62:GLU:HG2	2:B:300:ALA:HB3	1.89	0.53
2:D:362:GLN:NE2	2:D:365:LEU:HD23	2.23	0.53
3:L:117:ILE:CG2	3:L:121:ASP:HB2	2.38	0.53
2:B:46:LEU:HD22	2:B:73:ARG:CZ	2.38	0.53
2:B:241:GLN:OE1	2:B:246:GLY:N	2.40	0.53
2:B:351:GLN:HB3	2:B:436:PHE:CG	2.43	0.53
2:B:419:ASP:HA	2:B:440:PHE:HE1	1.72	0.53
2:D:183:GLU:HB3	3:J:173:LEU:HD22	1.89	0.53
2:D:415:LEU:HD11	2:D:417:LEU:HG	1.90	0.53
2:D:415:LEU:CD1	2:D:417:LEU:HG	2.38	0.53
1:E:72:ASN:C	1:E:72:ASN:ND2	2.65	0.53
1:E:422:GLU:H	1:E:422:GLU:CD	2.15	0.53
3:K:119:PRO:O	3:K:157:ALA:HB2	2.08	0.53
1:A:162:MET:HB3	1:A:520:TYR:HB3	1.90	0.53
3:J:118:GLU:HG3	3:J:120:THR:CG2	2.37	0.53
1:E:158:LEU:HD11	2:F:23:PHE:CE2	2.43	0.53
2:F:125:ASN:HB2	2:F:129:ASP:OD2	2.07	0.53
2:H:207:TYR:OH	3:L:172:ARG:NE	2.40	0.53
2:H:224:LEU:N	2:H:227:HIS:ND1	2.55	0.53
2:H:344:PRO:HG3	2:H:374:LEU:HD22	1.90	0.53
1:A:282:PRO:HB2	1:A:285:ILE:HD13	1.91	0.53
2:B:74:GLN:HE22	2:B:119:ASN:ND2	2.06	0.53
2:F:322:LEU:CD1	2:F:322:LEU:C	2.82	0.53
2:F:322:LEU:HD13	2:F:323:VAL:N	2.23	0.53
3:I:101:MET:HE2	3:I:119:PRO:HD3	1.90	0.53
1:E:246:LEU:O	1:E:246:LEU:HD23	2.08	0.53
2:H:402:GLU:HA	2:H:405:ARG:HH12	1.73	0.53
2:H:407:ASN:C	2:H:409:SER:H	2.15	0.53
1:A:35:LEU:C	1:A:36:ILE:HD13	2.33	0.53
1:A:437:LYS:HA	1:A:437:LYS:NZ	2.24	0.53
2:B:49:CYS:HA	2:B:139:HIS:CD2	2.43	0.53
2:B:195:GLY:O	2:B:339:ARG:NH1	2.41	0.53
1:C:59:ILE:O	1:C:60:ILE:HG13	2.08	0.53
1:C:297:ILE:HD13	1:C:297:ILE:N	2.19	0.53
1:E:171:VAL:HG12	1:E:391:ARG:HB2	1.89	0.53
1:E:220:LYS:C	1:E:222:LEU:N	2.66	0.53
2:F:391:THR:HG21	2:F:394:LEU:HB2	1.90	0.53
1:G:333:ILE:CA	2:H:223:ARG:NH1	2.71	0.53
2:B:251:GLY:O	2:B:257:ILE:HD11	2.09	0.53
2:B:361:LEU:O	2:B:364:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:LYS:O	1:C:345:VAL:HG23	2.08	0.53
1:E:68:GLU:HG2	2:F:18:ASN:HD22	1.73	0.53
1:A:172:ILE:HA	1:A:390:LEU:HD23	1.91	0.53
1:E:447:ASN:HD22	2:F:26:ARG:HH21	1.55	0.53
1:E:527:GLN:HB2	2:F:318:LEU:HD13	1.89	0.53
2:H:322:LEU:C	2:H:322:LEU:HD12	2.34	0.53
1:A:130:GLN:OE1	1:A:154:ARG:HA	2.09	0.53
1:A:425:LEU:HD21	1:A:525:MET:HE1	1.90	0.53
1:C:36:ILE:CB	1:C:128:ALA:HA	2.36	0.53
1:A:437:LYS:HA	1:A:437:LYS:HZ3	1.73	0.53
2:B:178:ILE:HD11	2:B:310:ILE:CD1	2.39	0.53
2:B:207:TYR:O	3:I:142:ARG:NH1	2.42	0.53
1:C:59:ILE:HG22	1:C:60:ILE:N	2.23	0.53
1:C:132:PRO:HD2	1:C:135:THR:HB	1.90	0.53
2:D:398:THR:O	2:D:402:GLU:HG3	2.09	0.53
1:E:113:LEU:HB3	1:E:138:ARG:NH2	2.23	0.53
2:F:231:TYR:C	2:F:233:ARG:H	2.16	0.53
1:G:404:LEU:HD21	1:G:467:GLU:HG2	1.89	0.53
3:L:126:ILE:HD11	3:L:156:ALA:HB2	1.91	0.53
1:A:518:ASN:ND2	1:A:534:LEU:CA	2.72	0.52
2:D:13:TRP:CD1	2:D:13:TRP:C	2.87	0.52
2:D:405:ARG:HB3	2:D:405:ARG:HH11	1.73	0.52
2:H:234:MET:O	2:H:234:MET:HG2	2.08	0.52
2:H:243:PHE:O	2:H:247:VAL:HB	2.09	0.52
2:H:380:ALA:HB1	2:H:394:LEU:CD1	2.35	0.52
2:H:382:THR:OG1	2:H:424:ALA:HB3	2.08	0.52
2:B:51:VAL:HG11	2:B:67:LEU:HD13	1.89	0.52
2:B:360:LYS:O	2:B:363:GLU:HB2	2.09	0.52
2:B:407:ASN:HB3	2:B:415:LEU:HD11	1.91	0.52
2:B:422:GLU:HG3	2:B:436:PHE:O	2.10	0.52
3:I:102:LEU:O	3:I:102:LEU:HD23	2.09	0.52
1:G:226:TYR:CZ	1:G:233:ILE:HG22	2.44	0.52
2:H:348:GLN:CA	2:H:348:GLN:HE21	2.21	0.52
3:L:150:MET:HE3	3:L:167:LEU:HD13	1.92	0.52
1:A:186:ASP:C	1:A:188:PRO:HD3	2.35	0.52
1:A:518:ASN:CG	1:A:519:THR:N	2.65	0.52
1:E:194:GLU:O	1:E:196:PHE:N	2.42	0.52
3:K:123:VAL:HB	3:K:152:ASP:CA	2.21	0.52
1:G:299:LYS:HE2	1:G:368:ILE:O	2.09	0.52
1:G:518:ASN:HB2	1:G:533:GLN:HA	1.89	0.52
2:H:412:LEU:HD22	2:H:440:PHE:HE2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:246:GLY:O	2:D:248:PRO:HD3	2.09	0.52
2:F:195:GLY:O	2:F:196:MET:HG2	2.10	0.52
3:K:102:LEU:O	3:K:163:GLY:O	2.28	0.52
1:G:244:ARG:HH11	1:G:244:ARG:HG3	1.74	0.52
2:H:343:CYS:O	2:H:347:SER:HB3	2.10	0.52
1:A:119:PHE:O	1:A:122:ARG:HG2	2.10	0.52
1:C:457:LEU:C	1:C:459:SER:H	2.16	0.52
3:J:105:VAL:HG11	3:J:115:ILE:HD11	1.90	0.52
2:H:102:PRO:HG2	2:H:105:GLU:HB2	1.91	0.52
2:B:83:ILE:HD13	2:B:94:PHE:HB3	1.91	0.52
2:B:434:VAL:HG22	2:B:436:PHE:HE1	1.75	0.52
1:E:307:LEU:HD21	1:E:375:ILE:HG21	1.91	0.52
1:E:376:SER:OG	1:E:379:GLU:HG3	2.09	0.52
2:F:183:GLU:HG3	2:F:289:ILE:CG2	2.39	0.52
2:F:324:PHE:HD1	2:F:332:THR:HG22	1.74	0.52
1:G:25:GLN:O	1:G:29:GLU:HG3	2.10	0.52
1:G:377:GLU:OE2	1:G:381:LYS:HE2	2.09	0.52
2:H:381:ILE:HD12	2:H:381:ILE:N	2.25	0.52
2:B:80:MET:HE2	2:B:126:LYS:HB2	1.92	0.52
2:B:419:ASP:CA	2:B:440:PHE:HE1	2.23	0.52
3:I:115:ILE:HD11	3:I:126:ILE:HG23	1.90	0.52
1:C:416:MET:HE1	1:C:424:VAL:CG1	2.40	0.52
2:D:322:LEU:C	2:D:322:LEU:CD1	2.82	0.52
2:H:385:LEU:HD12	2:H:390:ARG:HD3	1.92	0.52
1:A:309:ARG:HG3	1:A:364:LEU:HD21	1.92	0.52
1:A:516:PHE:CD1	1:A:518:ASN:O	2.63	0.52
2:B:232:VAL:CG1	2:B:260:ILE:HG23	2.40	0.52
1:C:66:SER:H	1:C:69:ASP:HB2	1.74	0.52
2:D:152:ARG:CZ	2:D:429:THR:HG21	2.40	0.52
2:D:152:ARG:HB3	2:D:429:THR:CG2	2.39	0.52
2:D:231:TYR:CD1	2:D:235:LEU:HD12	2.45	0.52
2:D:318:LEU:HD11	2:D:334:THR:HG21	1.89	0.52
1:E:194:GLU:C	1:E:196:PHE:H	2.18	0.52
1:G:333:ILE:HA	2:H:223:ARG:NH1	2.24	0.52
1:A:128:ALA:HB1	1:A:131:LEU:CD1	2.40	0.52
2:B:190:GLN:HG3	2:B:191:VAL:N	2.23	0.52
1:C:521:ILE:HD12	1:C:532:PHE:HE1	1.75	0.52
2:D:327:VAL:HG23	2:D:328:ASP:H	1.75	0.52
2:D:362:GLN:HG2	2:D:408:LEU:HB3	1.92	0.52
1:E:309:ARG:HG3	1:E:309:ARG:NH1	2.24	0.52
1:E:450:VAL:O	1:E:454:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:142:ARG:HB2	3:K:170:VAL:HG12	1.92	0.52
2:H:231:TYR:C	2:H:233:ARG:N	2.66	0.52
1:C:226:TYR:CZ	1:C:231:GLY:HA2	2.45	0.51
1:C:462:THR:O	1:C:466:GLN:HB2	2.09	0.51
2:H:148:ILE:HD11	3:L:174:ARG:HD3	1.91	0.51
2:H:306:GLU:O	2:H:307:VAL:C	2.53	0.51
1:A:252:LEU:C	1:A:252:LEU:HD22	2.35	0.51
2:B:13:TRP:CH2	2:B:116:PRO:HG2	2.44	0.51
1:C:33:VAL:CG2	1:C:34:CYS:N	2.74	0.51
1:C:214:TRP:CD1	1:C:214:TRP:C	2.88	0.51
1:E:121:CYS:HA	1:E:148:ILE:HD11	1.92	0.51
1:E:317:LYS:HD3	1:E:318:GLU:OE1	2.10	0.51
1:G:298:THR:OG1	1:G:300:GLN:HG2	2.09	0.51
1:G:331:ASP:OD1	2:H:224:LEU:HD21	2.10	0.51
1:A:516:PHE:CE1	1:A:518:ASN:O	2.64	0.51
2:F:228:CYS:SG	2:F:273:ILE:HD12	2.50	0.51
2:H:350:PRO:HB2	2:H:437:LYS:HG3	1.91	0.51
1:A:35:LEU:O	1:A:36:ILE:HD13	2.11	0.51
1:A:432:VAL:HG21	1:A:482:PHE:HD2	1.75	0.51
1:A:448:TYR:CE1	1:A:449:GLN:HG3	2.45	0.51
2:B:64:LEU:CB	2:B:111:LEU:HD11	2.41	0.51
2:B:309:LYS:HG2	2:B:315:TYR:HB2	1.92	0.51
2:B:318:LEU:HD11	2:B:334:THR:HG23	1.93	0.51
1:C:397:SER:HG	1:C:400:GLU:HG3	1.74	0.51
1:E:43:THR:HG21	1:E:73:ASN:OD1	2.10	0.51
1:E:72:ASN:C	1:E:72:ASN:HD22	2.19	0.51
1:E:72:ASN:HD22	1:E:73:ASN:N	2.08	0.51
2:F:64:LEU:HD21	2:F:77:VAL:CG2	2.41	0.51
2:H:382:THR:HG1	2:H:424:ALA:HB3	1.75	0.51
1:A:12:LYS:HE3	1:A:13:TYR:CE2	2.46	0.51
2:B:32:HIS:ND1	2:B:33:PRO:HD2	2.26	0.51
2:D:223:ARG:HB2	2:D:223:ARG:NH1	2.24	0.51
1:E:317:LYS:HB3	1:E:318:GLU:OE1	2.10	0.51
2:H:87:ASN:HB3	2:H:91:GLN:CD	2.35	0.51
2:H:355:PHE:O	2:H:440:PHE:HD2	1.94	0.51
1:C:426:TYR:CE2	1:C:534:LEU:HD13	2.45	0.51
2:D:152:ARG:HB3	2:D:429:THR:HG23	1.90	0.51
1:E:245:ASP:C	1:E:247:ILE:H	2.19	0.51
2:F:348:GLN:C	2:F:349:LEU:HD12	2.34	0.51
1:G:168:GLU:HG3	1:G:394:ARG:HE	1.74	0.51
2:H:24:LEU:HD21	2:H:312:THR:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:90:ARG:HG2	2:H:90:ARG:NH1	2.24	0.51
1:A:78:ARG:C	1:A:80:SER:H	2.19	0.51
1:C:48:ASN:O	1:C:52:PRO:HG2	2.11	0.51
1:C:215:ILE:CG1	1:C:332:MET:HE1	2.40	0.51
3:J:108:LEU:HD22	3:J:169:LEU:O	2.10	0.51
1:E:265:PHE:O	1:E:269:ILE:HG13	2.10	0.51
1:G:197:GLN:C	1:G:199:TYR:H	2.19	0.51
1:A:229:THR:HG22	1:A:232:ARG:HB3	1.88	0.51
1:A:445:VAL:O	2:B:22:LYS:HE2	2.11	0.51
1:C:185:LEU:HD12	1:C:275:ALA:HB1	1.92	0.51
1:C:446:SER:HB2	1:C:449:GLN:HB3	1.93	0.51
1:E:184:ARG:NH1	1:E:184:ARG:HG3	2.23	0.51
2:F:366:ASP:HB3	2:F:370:ASN:ND2	2.26	0.51
1:G:199:TYR:CE2	1:G:216:VAL:HG11	2.45	0.51
2:H:136:ARG:HG2	2:H:161:LEU:HD22	1.93	0.51
2:H:316:ILE:H	2:H:316:ILE:CD1	2.14	0.51
1:A:176:PRO:HG2	1:A:389:PHE:CD2	2.45	0.51
2:B:27:SER:HB3	2:B:37:PRO:HG3	1.93	0.51
2:B:84:ASP:OD1	2:B:85:VAL:N	2.44	0.51
2:B:187:GLY:HA2	3:I:173:LEU:HD13	1.93	0.51
1:C:236:THR:HG22	1:C:238:LYS:H	1.76	0.51
2:D:25:GLU:O	2:D:37:PRO:HB2	2.11	0.51
1:E:116:ASP:N	1:E:117:PRO:HD3	2.26	0.51
1:G:386:ASN:O	1:G:387:SER:C	2.54	0.51
1:G:408:ASN:OD1	1:G:408:ASN:O	2.29	0.51
2:H:339:ARG:HE	2:H:346:CYS:HB3	1.75	0.51
2:H:339:ARG:NH2	2:H:346:CYS:HB3	2.25	0.51
2:H:380:ALA:CB	2:H:394:LEU:CD1	2.78	0.51
1:A:215:ILE:HD12	1:A:342:LEU:HD21	1.93	0.51
1:A:248:ARG:HA	1:A:251:ILE:CD1	2.39	0.51
1:C:113:LEU:HD22	1:C:142:VAL:HG21	1.91	0.51
1:C:344:ASN:HD22	1:C:347:ARG:HH12	1.58	0.51
1:G:447:ASN:HD22	2:H:26:ARG:NH2	2.05	0.51
2:H:74:GLN:NE2	2:H:119:ASN:HD22	2.07	0.51
2:H:320:ASN:HB2	2:H:337:ALA:N	2.26	0.51
2:H:418:VAL:HG22	2:H:421:GLN:OE1	2.11	0.51
1:A:65:VAL:HB	1:A:82:GLY:H	1.75	0.50
1:A:330:PRO:HG2	1:A:332:MET:HE2	1.92	0.50
2:B:422:GLU:O	2:B:423:LEU:HG	2.10	0.50
1:C:259:PRO:CB	1:C:262:GLU:CD	2.83	0.50
2:D:419:ASP:CG	2:D:420:GLY:N	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:ASN:HD22	1:G:72:ASN:N	2.06	0.50
1:G:330:PRO:O	1:G:339:TYR:OH	2.24	0.50
2:H:350:PRO:HB3	2:H:436:PHE:O	2.11	0.50
2:B:95:ARG:HH11	2:B:95:ARG:CG	2.22	0.50
1:C:216:VAL:O	1:C:220:LYS:HG2	2.11	0.50
1:E:61:ASP:CB	1:E:86:ALA:HB2	2.40	0.50
2:F:197:THR:HG23	2:F:320:ASN:OD1	2.12	0.50
1:G:184:ARG:NH1	1:G:325:VAL:HG22	2.26	0.50
1:C:259:PRO:CB	1:C:262:GLU:OE2	2.59	0.50
1:E:108:SER:HB2	1:E:109:PRO:HD2	1.92	0.50
2:F:320:ASN:HD22	2:F:337:ALA:N	2.09	0.50
1:G:214:TRP:CZ3	1:G:332:MET:HB3	2.46	0.50
2:H:64:LEU:HD21	2:H:77:VAL:HG21	1.92	0.50
2:H:320:ASN:HB2	2:H:337:ALA:H	1.77	0.50
1:A:112:LEU:O	1:A:116:ASP:O	2.29	0.50
1:C:268:ALA:O	1:C:272:VAL:HG23	2.12	0.50
1:E:132:PRO:O	1:E:133:GLU:C	2.54	0.50
1:E:187:LYS:HD2	1:E:279:THR:HG21	1.93	0.50
1:E:441:ARG:NH2	1:E:453:ASP:OD1	2.44	0.50
1:G:396:ARG:NH2	1:G:406:THR:O	2.44	0.50
2:B:237:TRP:HB3	2:B:238:PRO:HD3	1.93	0.50
1:C:264:ASN:ND2	1:C:265:PHE:N	2.60	0.50
1:A:474:VAL:O	1:A:475:LYS:C	2.53	0.50
2:D:16:ARG:HD3	2:D:17:TRP:HE1	1.75	0.50
1:E:66:SER:H	1:E:69:ASP:HB2	1.75	0.50
1:E:264:ASN:ND2	1:E:265:PHE:N	2.60	0.50
2:F:232:VAL:HG21	2:F:264:SER:HA	1.93	0.50
2:F:236:GLN:NE2	2:F:263:LYS:HB3	2.26	0.50
2:F:280:LEU:O	2:F:284:VAL:HG23	2.11	0.50
1:G:214:TRP:CD1	1:G:214:TRP:C	2.90	0.50
2:H:250:ASP:HB3	2:H:253:ASP:HB2	1.94	0.50
2:D:314:ALA:O	2:D:315:TYR:CD1	2.65	0.50
1:E:236:THR:C	1:E:238:LYS:H	2.20	0.50
2:F:338:GLU:OE1	3:K:148:LYS:HE3	2.12	0.50
3:K:123:VAL:HG13	3:K:150:MET:HE2	1.94	0.50
1:G:226:TYR:O	1:G:231:GLY:N	2.44	0.50
1:G:450:VAL:O	1:G:454:ILE:HG13	2.11	0.50
2:H:220:SER:O	2:H:222:PRO:HD3	2.11	0.50
2:H:322:LEU:HD12	2:H:323:VAL:O	2.12	0.50
1:A:491:HIS:CD2	2:B:69:LEU:HD12	2.46	0.50
1:C:215:ILE:HD12	1:C:342:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:VAL:HG21	1:C:349:LYS:HG2	1.94	0.50
2:D:24:LEU:CD2	2:D:312:THR:HB	2.41	0.50
2:D:142:VAL:HG12	2:D:178:ILE:HB	1.93	0.50
1:E:375:ILE:N	1:E:375:ILE:HD12	2.27	0.50
3:K:102:LEU:C	3:K:102:LEU:HD23	2.37	0.50
2:B:376:MET:HB3	2:B:427:ASP:OD1	2.12	0.50
2:D:83:ILE:HD12	2:D:98:ASP:HB3	1.92	0.50
2:D:277:THR:HG22	2:D:278:TYR:N	2.27	0.50
1:E:447:ASN:HD21	2:F:26:ARG:HE	1.59	0.50
2:F:401:GLU:HG3	2:F:402:GLU:N	2.27	0.50
2:H:393:TYR:HA	2:H:404:THR:HB	1.93	0.50
2:B:430:THR:HG22	2:B:431:PRO:CD	2.41	0.49
3:I:103:ILE:HD11	3:I:117:ILE:HD12	1.94	0.49
3:I:104:LYS:O	3:I:166:VAL:HA	2.12	0.49
1:C:34:CYS:SG	1:C:60:ILE:HD12	2.51	0.49
3:K:101:MET:HE3	3:K:117:ILE:HG22	1.93	0.49
3:L:120:THR:CB	3:L:155:THR:OG1	2.60	0.49
2:B:197:THR:HG23	2:B:198:ALA:N	2.27	0.49
2:B:391:THR:HG21	2:B:400:ILE:HG21	1.94	0.49
2:B:415:LEU:HB2	2:B:417:LEU:HD21	1.93	0.49
1:C:454:ILE:HD13	1:C:480:HIS:ND1	2.27	0.49
1:E:19:LEU:HG	2:F:290:PRO:HB2	1.94	0.49
1:E:199:TYR:CD2	1:E:216:VAL:HG11	2.46	0.49
1:E:309:ARG:HB3	1:E:364:LEU:CD2	2.42	0.49
1:G:218:ILE:O	1:G:222:LEU:HB2	2.12	0.49
2:B:284:VAL:O	2:B:287:ARG:NH1	2.45	0.49
1:C:418:ASN:ND2	1:C:418:ASN:C	2.69	0.49
2:D:152:ARG:NE	2:D:429:THR:HG21	2.27	0.49
2:D:352:ASN:HB3	2:D:439:HIS:HD2	1.78	0.49
3:J:162:LEU:O	3:J:163:GLY:C	2.55	0.49
1:G:43:THR:HG21	1:G:73:ASN:OD1	2.11	0.49
2:H:240:GLU:O	2:H:242:PRO:CD	2.59	0.49
2:H:322:LEU:HD12	2:H:323:VAL:N	2.26	0.49
3:L:105:VAL:HG13	3:L:105:VAL:O	2.11	0.49
2:B:197:THR:HG23	2:B:320:ASN:HD21	1.78	0.49
1:C:409:LYS:O	1:C:413:ILE:HG13	2.11	0.49
2:F:342:ASN:ND2	2:F:342:ASN:N	2.57	0.49
1:G:34:CYS:HB2	1:G:123:PHE:CG	2.48	0.49
1:G:288:ILE:HG23	1:G:305:TRP:CZ3	2.47	0.49
2:H:344:PRO:CD	2:H:374:LEU:HD22	2.42	0.49
2:B:37:PRO:O	2:B:38:SER:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:PRO:HB2	2:B:436:PHE:C	2.38	0.49
3:I:171:LEU:HD12	3:I:172:ARG:H	1.76	0.49
2:D:234:MET:O	2:D:235:LEU:HD23	2.13	0.49
2:F:188:ASN:OD1	3:K:173:LEU:HD12	2.12	0.49
1:G:12:LYS:HE3	1:G:13:TYR:CZ	2.48	0.49
2:H:233:ARG:HH12	2:H:234:MET:HB2	1.76	0.49
1:A:49:LEU:C	1:A:52:PRO:HD2	2.38	0.49
1:A:133:GLU:HG3	1:A:433:ASP:HB3	1.95	0.49
1:A:416:MET:HE1	1:A:424:VAL:HG22	1.94	0.49
2:B:348:GLN:OE1	2:B:348:GLN:HA	2.13	0.49
3:I:126:ILE:O	3:I:130:VAL:HG23	2.11	0.49
1:C:36:ILE:HG22	1:C:37:ASN:N	2.27	0.49
2:D:18:ASN:O	2:D:22:LYS:HG3	2.13	0.49
2:D:232:VAL:HA	2:D:236:GLN:HB3	1.94	0.49
2:D:434:VAL:HG13	2:D:436:PHE:HE1	1.77	0.49
3:J:104:LYS:HD3	3:J:112:GLU:OE2	2.12	0.49
2:F:275:GLY:O	2:F:280:LEU:HD23	2.13	0.49
1:G:12:LYS:HG3	2:H:88:LEU:HB2	1.94	0.49
2:H:357:PRO:HG3	2:H:440:PHE:CG	2.48	0.49
3:I:123:VAL:HG13	3:I:150:MET:HE2	1.93	0.49
1:C:35:LEU:HD12	1:C:129:THR:HG23	1.94	0.49
1:C:157:GLY:HA3	1:C:485:TYR:CD1	2.47	0.49
2:F:102:PRO:HG2	2:F:105:GLU:CB	2.43	0.49
2:F:401:GLU:O	2:F:405:ARG:N	2.44	0.49
1:G:518:ASN:ND2	1:G:534:LEU:N	2.61	0.49
2:H:18:ASN:O	2:H:22:LYS:HG2	2.12	0.49
2:H:45:LEU:HD11	2:H:72:PHE:CE2	2.48	0.49
3:L:162:LEU:O	3:L:164:GLY:N	2.45	0.49
3:I:118:GLU:O	3:I:120:THR:N	2.46	0.49
1:C:131:LEU:HB3	1:C:132:PRO:CD	2.43	0.49
1:C:137:LEU:HA	1:C:398:LEU:HD23	1.95	0.49
2:F:132:ASP:HB3	2:F:157:MET:CE	2.42	0.49
1:G:34:CYS:HB2	1:G:123:PHE:CD2	2.47	0.49
2:H:391:THR:O	2:H:392:LEU:C	2.55	0.49
2:H:401:GLU:HG3	2:H:402:GLU:N	2.28	0.49
1:A:409:LYS:O	1:A:413:ILE:HG13	2.12	0.49
2:D:286:LYS:HB2	2:D:288:ILE:HG13	1.94	0.49
3:J:107:THR:HG23	3:J:109:THR:H	1.77	0.49
1:E:336:SER:OG	2:F:221:MET:HA	2.12	0.49
1:A:64:GLN:HA	1:A:83:LYS:O	2.13	0.49
1:A:164:ILE:HD11	1:A:166:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:418:VAL:HG22	2:B:421:GLN:HG3	1.95	0.49
1:C:220:LYS:HA	1:C:220:LYS:HE3	1.95	0.49
2:D:178:ILE:HD12	2:D:307:VAL:HG22	1.94	0.49
1:E:297:ILE:HD12	1:E:297:ILE:N	2.19	0.49
1:G:214:TRP:CD2	1:G:332:MET:HE3	2.48	0.49
2:H:148:ILE:O	2:H:152:ARG:HG3	2.13	0.49
1:A:323:LEU:HB3	1:A:324:PRO:HD2	1.95	0.48
1:A:425:LEU:HD11	1:A:523:SER:HB2	1.95	0.48
1:C:229:THR:HG22	1:C:232:ARG:HB2	1.91	0.48
2:D:268:ALA:CB	2:D:276:VAL:HG21	2.43	0.48
1:E:307:LEU:CD1	1:E:383:LEU:HD22	2.39	0.48
1:G:164:ILE:HD13	1:G:515:ILE:HD12	1.95	0.48
2:H:98:ASP:OD1	2:H:101:ARG:NH1	2.46	0.48
2:H:170:ASP:O	2:H:173:SER:HB3	2.12	0.48
2:H:349:LEU:HB3	2:H:350:PRO:CD	2.42	0.48
1:A:348:GLU:HG3	1:E:115:ASN:ND2	2.27	0.48
2:B:353:ILE:CG2	2:B:355:PHE:HD1	2.23	0.48
2:B:386:GLU:O	2:B:387:GLY:C	2.54	0.48
3:J:124:GLU:HB3	3:J:152:ASP:O	2.12	0.48
1:E:12:LYS:HE3	1:E:13:TYR:CZ	2.47	0.48
1:E:49:LEU:C	1:E:52:PRO:HD2	2.37	0.48
1:E:158:LEU:HA	1:E:493:ILE:HG13	1.95	0.48
1:E:194:GLU:C	1:E:196:PHE:N	2.71	0.48
2:F:197:THR:CG2	2:F:198:ALA:N	2.75	0.48
3:K:118:GLU:O	3:K:120:THR:N	2.46	0.48
2:H:320:ASN:HB2	2:H:336:GLU:HA	1.95	0.48
1:A:211:HIS:HB3	1:A:335:ASP:HB3	1.96	0.48
1:A:297:ILE:HG22	1:A:298:THR:N	2.29	0.48
2:B:353:ILE:HG22	2:B:438:LEU:HB2	1.95	0.48
1:C:19:LEU:HD22	2:D:185:PHE:CE1	2.48	0.48
1:C:293:ARG:HB3	1:C:305:TRP:CD2	2.48	0.48
1:C:526:SER:O	1:C:527:GLN:HB2	2.13	0.48
2:D:207:TYR:CD1	3:J:172:ARG:HD3	2.46	0.48
2:D:225:PRO:HG3	2:D:274:ARG:O	2.13	0.48
1:E:527:GLN:CB	2:F:318:LEU:HD13	2.42	0.48
1:A:401:GLU:O	1:A:407:ILE:HG12	2.13	0.48
3:I:107:THR:CG2	3:I:108:LEU:N	2.76	0.48
1:C:240:LYS:O	1:C:244:ARG:HG3	2.13	0.48
2:D:29:PRO:C	2:D:31:THR:H	2.22	0.48
2:D:208:PRO:HB2	2:D:209:PRO:HD2	1.95	0.48
2:F:240:GLU:O	2:F:241:GLN:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:ILE:HD11	1:G:272:VAL:HG22	1.95	0.48
1:G:416:MET:C	1:G:418:ASN:H	2.22	0.48
2:H:56:ALA:O	2:H:103:LYS:HD3	2.12	0.48
1:A:181:GLU:O	1:A:278:THR:HB	2.13	0.48
2:B:400:ILE:H	2:B:400:ILE:CD1	2.27	0.48
2:B:402:GLU:C	2:B:404:THR:H	2.21	0.48
2:B:417:LEU:CD1	2:B:421:GLN:HE22	2.26	0.48
1:C:190:PRO:O	1:C:194:GLU:HG3	2.13	0.48
1:C:354:ALA:HA	1:C:384:CYS:SG	2.52	0.48
1:C:481:GLU:HG2	1:C:525:MET:SD	2.53	0.48
1:C:521:ILE:HD12	1:C:532:PHE:CE1	2.49	0.48
2:D:419:ASP:HB2	2:D:440:PHE:CD1	2.49	0.48
1:E:34:CYS:HB2	1:E:123:PHE:CD2	2.48	0.48
1:E:259:PRO:CB	1:E:261:ASP:O	2.62	0.48
1:G:108:SER:HB3	1:G:111:ASN:HB3	1.94	0.48
2:H:52:LEU:HB2	2:H:138:PHE:CD2	2.48	0.48
1:A:401:GLU:OE2	1:A:534:LEU:HB2	2.13	0.48
1:C:416:MET:HE3	1:C:416:MET:O	2.13	0.48
1:E:48:ASN:HB2	1:E:502:ALA:CB	2.43	0.48
2:H:158:LEU:HD13	2:H:177:LEU:HD22	1.96	0.48
1:A:236:THR:O	1:A:240:LYS:HG3	2.13	0.48
2:B:198:ALA:HB3	2:B:320:ASN:ND2	2.28	0.48
1:C:349:LYS:O	1:C:350:ALA:C	2.57	0.48
2:D:87:ASN:ND2	2:D:103:LYS:HE2	2.29	0.48
2:D:98:ASP:O	2:D:99:ILE:C	2.56	0.48
2:D:249:LEU:HD11	2:D:260:ILE:HD11	1.95	0.48
1:E:481:GLU:OE1	2:F:29:PRO:HD2	2.13	0.48
1:G:47:LYS:C	1:G:47:LYS:HD2	2.39	0.48
1:G:165:ILE:HG22	1:G:165:ILE:O	2.11	0.48
2:H:382:THR:HA	2:H:392:LEU:HG	1.96	0.48
3:L:170:VAL:CG1	3:L:171:LEU:H	2.18	0.48
2:B:312:THR:C	2:B:314:ALA:N	2.72	0.48
2:B:405:ARG:HB3	2:B:406:PRO:HD3	1.95	0.48
1:C:50:VAL:HG13	1:C:100:VAL:HG21	1.95	0.48
2:D:361:LEU:O	2:D:363:GLU:N	2.47	0.48
1:E:422:GLU:HG3	1:E:530:ALA:CB	2.42	0.48
1:E:435:PHE:HE1	1:E:456:LYS:HB2	1.78	0.48
2:F:231:TYR:CG	2:F:267:ARG:NH1	2.81	0.48
1:A:47:LYS:HD2	1:A:47:LYS:O	2.14	0.48
2:D:361:LEU:C	2:D:363:GLU:N	2.70	0.48
2:D:393:TYR:CZ	2:D:408:LEU:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:115:ILE:CG2	3:K:117:ILE:HD13	2.43	0.48
2:H:89:ASN:OD1	2:H:90:ARG:NH1	2.47	0.48
2:H:377:LYS:HD3	2:H:428:VAL:HG21	1.96	0.48
2:H:414:GLU:O	2:H:414:GLU:HG2	2.14	0.48
3:L:161:ILE:O	3:L:162:LEU:HD23	2.14	0.48
1:A:527:GLN:NE2	2:B:302:VAL:HG13	2.28	0.48
2:B:391:THR:O	2:B:391:THR:HG22	2.13	0.48
2:B:391:THR:O	2:B:392:LEU:C	2.56	0.48
3:I:157:ALA:C	3:I:159:TYR:H	2.22	0.48
2:D:356:SER:C	2:D:358:SER:H	2.21	0.48
1:E:491:HIS:NE2	2:F:65:LYS:HE3	2.29	0.48
2:F:102:PRO:HG2	2:F:105:GLU:HB3	1.95	0.48
2:H:251:GLY:O	2:H:286:LYS:HD2	2.13	0.48
2:B:166:ASP:C	2:B:168:VAL:H	2.22	0.47
2:B:208:PRO:HG3	3:I:171:LEU:HD11	1.95	0.47
1:C:175:HIS:HD2	1:C:512:GLN:O	1.97	0.47
1:C:418:ASN:HD22	1:C:419:PRO:CD	2.27	0.47
2:D:73:ARG:HG3	2:D:73:ARG:NH1	2.29	0.47
2:D:419:ASP:CG	2:D:420:GLY:H	2.21	0.47
3:J:115:ILE:HG23	3:J:129:ARG:HB3	1.95	0.47
1:E:34:CYS:HB2	1:E:123:PHE:CE2	2.49	0.47
1:E:187:LYS:HD2	1:E:279:THR:CG2	2.44	0.47
2:F:158:LEU:HD12	2:F:175:VAL:HB	1.96	0.47
1:G:18:ARG:NH1	2:H:279:ARG:HG3	2.28	0.47
2:H:197:THR:HG22	2:H:198:ALA:N	2.29	0.47
1:A:40:ALA:O	1:A:43:THR:HG22	2.14	0.47
2:B:187:GLY:CA	3:I:173:LEU:HD13	2.44	0.47
2:B:403:ARG:HG3	2:B:403:ARG:HH11	1.80	0.47
1:C:168:GLU:HG2	1:C:170:PRO:HD3	1.96	0.47
1:C:264:ASN:HD22	1:C:264:ASN:N	2.10	0.47
1:E:75:PHE:O	1:E:76:LEU:HD23	2.14	0.47
2:F:80:MET:HE2	2:F:126:LYS:HG2	1.96	0.47
1:G:36:ILE:HG21	1:G:131:LEU:HD11	1.96	0.47
1:G:43:THR:HG22	1:G:44:GLU:N	2.29	0.47
1:G:120:PHE:O	1:G:148:ILE:HD13	2.14	0.47
1:G:225:TRP:CE2	1:G:234:PRO:HG3	2.49	0.47
2:H:57:GLY:HA2	2:H:91:GLN:HG2	1.96	0.47
2:H:249:LEU:HD11	2:H:260:ILE:HD11	1.95	0.47
2:B:351:GLN:H	2:B:436:PHE:HA	1.78	0.47
1:C:25:GLN:O	1:C:29:GLU:HG3	2.14	0.47
2:D:73:ARG:HG3	2:D:73:ARG:HH11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:LEU:HD22	2:F:185:PHE:CE1	2.48	0.47
1:E:43:THR:HG22	1:E:44:GLU:N	2.29	0.47
1:E:163:ARG:HH11	1:E:165:ILE:HG12	1.79	0.47
1:E:236:THR:HG22	1:E:237:TYR:N	2.28	0.47
2:H:267:ARG:O	2:H:267:ARG:HD3	2.14	0.47
1:A:32:HIS:HD2	1:A:56:SER:O	1.97	0.47
1:A:435:PHE:O	1:A:438:GLN:N	2.48	0.47
1:C:428:MET:HE1	1:C:479:VAL:HA	1.96	0.47
1:C:474:VAL:O	1:C:475:LYS:C	2.57	0.47
2:D:182:THR:CG2	2:D:183:GLU:N	2.77	0.47
1:E:190:PRO:O	1:E:191:GLU:C	2.58	0.47
2:H:190:GLN:OE1	3:L:172:ARG:NH1	2.47	0.47
2:H:348:GLN:HE21	2:H:348:GLN:C	2.22	0.47
2:H:423:LEU:HD12	2:H:423:LEU:N	2.29	0.47
2:B:274:ARG:HD3	1:E:62:GLY:O	2.14	0.47
2:B:421:GLN:HB2	2:B:438:LEU:HD21	1.96	0.47
1:C:130:GLN:NE2	1:C:155:THR:O	2.47	0.47
1:C:409:LYS:O	1:C:410:ASP:C	2.56	0.47
3:J:156:ALA:O	3:J:161:ILE:HB	2.14	0.47
1:E:183:LEU:O	1:E:184:ARG:HB2	2.14	0.47
2:H:354:GLN:NE2	2:H:354:GLN:HA	2.29	0.47
2:H:402:GLU:HA	2:H:405:ARG:NH1	2.30	0.47
2:H:412:LEU:O	2:H:417:LEU:HB2	2.15	0.47
2:B:81:ASP:CB	2:B:103:LYS:HD2	2.42	0.47
1:C:484:ARG:HD2	2:D:27:SER:O	2.13	0.47
2:D:225:PRO:HB2	2:D:280:LEU:HD21	1.97	0.47
2:D:286:LYS:O	2:D:287:ARG:C	2.57	0.47
2:H:270:GLN:C	2:H:271:TYR:CD2	2.92	0.47
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.79	0.47
1:A:424:VAL:HA	1:A:427:LEU:HD12	1.97	0.47
1:A:516:PHE:HD2	1:A:516:PHE:H	1.62	0.47
2:B:166:ASP:O	2:B:168:VAL:N	2.45	0.47
2:B:230:GLU:CD	2:B:233:ARG:HH12	2.22	0.47
1:C:163:ARG:NE	1:C:518:ASN:OD1	2.46	0.47
1:C:326:ARG:HG2	1:C:328:THR:HG23	1.96	0.47
2:D:152:ARG:NH2	2:D:374:LEU:O	2.48	0.47
2:D:197:THR:CG2	2:D:198:ALA:N	2.77	0.47
2:D:280:LEU:O	2:D:284:VAL:HG23	2.15	0.47
3:J:145:TYR:HB2	3:J:167:LEU:CD2	2.44	0.47
2:F:123:HIS:HB3	2:F:125:ASN:HD21	1.79	0.47
2:F:136:ARG:NH1	2:F:161:LEU:HD22	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:361:LEU:O	2:F:364:VAL:N	2.42	0.47
2:F:380:ALA:HB3	2:F:394:LEU:HD12	1.90	0.47
2:F:422:GLU:HA	2:F:436:PHE:O	2.15	0.47
2:F:425:VAL:O	2:F:434:VAL:HG12	2.15	0.47
1:G:97:ASN:OD1	1:G:99:ASP:HB2	2.13	0.47
1:G:158:LEU:CD2	2:H:23:PHE:CE2	2.98	0.47
1:G:184:ARG:NH2	1:G:323:LEU:O	2.47	0.47
2:H:87:ASN:HB3	2:H:91:GLN:NE2	2.29	0.47
2:H:159:ILE:HG23	2:H:162:LEU:HD12	1.96	0.47
2:H:351:GLN:HB3	2:H:436:PHE:CD2	2.50	0.47
2:H:412:LEU:CD2	2:H:438:LEU:HD21	2.44	0.47
2:H:419:ASP:HB2	2:H:440:PHE:HD1	1.79	0.47
3:L:123:VAL:HA	3:L:126:ILE:CG1	2.45	0.47
3:L:155:THR:O	3:L:158:ASP:HB2	2.14	0.47
1:A:89:ALA:O	1:A:90:MET:C	2.58	0.47
1:A:467:GLU:HG2	1:A:467:GLU:O	2.15	0.47
3:I:123:VAL:O	3:I:126:ILE:N	2.45	0.47
2:D:382:THR:HG22	2:D:391:THR:HA	1.96	0.47
2:F:141:ILE:HD12	2:F:158:LEU:HD11	1.97	0.47
2:H:207:TYR:CE1	3:L:172:ARG:CD	2.97	0.47
1:A:128:ALA:HB1	1:A:131:LEU:HD12	1.97	0.47
1:A:262:GLU:HG2	1:A:265:PHE:HD1	1.79	0.47
1:A:265:PHE:O	1:A:269:ILE:HG13	2.15	0.47
2:B:218:ILE:HG22	2:B:219:ALA:N	2.29	0.47
2:B:321:TYR:OH	3:I:172:ARG:CG	2.63	0.47
2:B:427:ASP:CB	2:B:429:THR:HG22	2.45	0.47
1:C:75:PHE:CD2	1:C:93:LEU:HD23	2.50	0.47
1:C:138:ARG:O	1:C:142:VAL:HG23	2.15	0.47
2:D:209:PRO:HG3	3:J:139:GLN:HG2	1.96	0.47
2:D:312:THR:O	2:D:313:SER:HB3	2.14	0.47
2:F:225:PRO:HG2	2:F:275:GLY:HA3	1.97	0.47
1:G:53:GLY:O	1:G:54:ILE:C	2.58	0.47
2:H:63:LEU:HD22	2:H:142:VAL:HG11	1.97	0.47
1:A:34:CYS:SG	1:A:36:ILE:CD1	3.02	0.47
1:A:262:GLU:HG2	1:A:265:PHE:CD1	2.50	0.47
1:A:489:GLU:HG2	1:A:489:GLU:O	2.14	0.47
1:A:504:GLU:O	1:A:508:ILE:HG13	2.15	0.47
2:B:230:GLU:OE2	2:B:234:MET:HE3	2.15	0.47
1:C:307:LEU:HB3	1:C:383:LEU:HD22	1.97	0.47
1:C:401:GLU:OE1	1:C:426:TYR:OH	2.29	0.47
1:C:449:GLN:O	1:C:449:GLN:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:359:ALA:HB1	2:D:363:GLU:CD	2.40	0.47
1:E:447:ASN:ND2	2:F:26:ARG:NH2	2.62	0.47
2:F:129:ASP:HB3	2:H:134:PHE:HB2	1.95	0.47
2:F:386:GLU:CB	2:F:388:LYS:HE2	2.45	0.47
1:G:180:LEU:HD12	1:G:180:LEU:N	2.19	0.47
1:A:371:ALA:O	1:A:373:GLU:N	2.47	0.46
2:B:126:LYS:O	2:B:128:GLN:N	2.48	0.46
2:B:312:THR:O	2:B:314:ALA:N	2.48	0.46
2:D:192:ILE:O	2:D:194:PRO:HD3	2.15	0.46
2:F:355:PHE:O	2:F:440:PHE:HA	2.16	0.46
1:G:433:ASP:O	1:G:436:HIS:HB3	2.15	0.46
1:G:510:THR:OG1	1:G:512:GLN:HB2	2.16	0.46
3:L:104:LYS:HB2	3:L:166:VAL:HG22	1.98	0.46
2:B:380:ALA:HB1	2:B:394:LEU:HD13	1.94	0.46
1:C:131:LEU:HB3	1:C:132:PRO:HD2	1.97	0.46
2:D:412:LEU:HD22	2:D:417:LEU:CD1	2.44	0.46
1:G:480:HIS:HB2	2:H:29:PRO:HG2	1.98	0.46
1:C:184:ARG:HD3	1:C:279:THR:OG1	2.14	0.46
2:D:237:TRP:C	2:D:239:LYS:H	2.23	0.46
2:F:335:PHE:HE2	3:K:170:VAL:HG21	1.80	0.46
2:F:381:ILE:HG13	2:F:425:VAL:HG22	1.96	0.46
1:A:366:GLN:O	1:A:368:ILE:N	2.47	0.46
1:A:518:ASN:HD21	1:A:534:LEU:CB	2.26	0.46
2:B:16:ARG:HH22	2:B:116:PRO:HB2	1.80	0.46
2:B:27:SER:HB3	2:B:37:PRO:CG	2.46	0.46
1:C:72:ASN:HB2	2:D:19:HIS:ND1	2.31	0.46
1:C:481:GLU:OE1	2:D:315:TYR:OH	2.32	0.46
1:C:489:GLU:HG2	1:C:489:GLU:O	2.16	0.46
2:D:187:GLY:CA	3:J:173:LEU:HD12	2.46	0.46
1:E:347:ARG:HH22	2:F:274:ARG:CD	2.15	0.46
1:G:124:THR:HG21	1:G:509:ILE:HG12	1.96	0.46
1:G:447:ASN:HA	2:H:26:ARG:HH21	1.80	0.46
2:H:257:ILE:HD13	2:H:282:GLN:HG2	1.98	0.46
3:L:151:ASN:O	3:L:153:GLU:N	2.48	0.46
3:L:151:ASN:C	3:L:153:GLU:H	2.23	0.46
2:B:207:TYR:HE2	3:I:172:ARG:HG2	1.72	0.46
3:J:105:VAL:HG11	3:J:130:VAL:HG22	1.97	0.46
2:F:106:VAL:O	2:F:109:GLU:HB3	2.16	0.46
2:F:312:THR:O	2:F:313:SER:CB	2.63	0.46
2:F:356:SER:O	2:F:358:SER:N	2.48	0.46
2:F:357:PRO:HD3	2:F:440:PHE:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:121:ASP:HB3	3:K:125:ARG:HD2	1.98	0.46
2:B:240:GLU:O	2:B:240:GLU:CG	2.62	0.46
2:B:418:VAL:CG2	2:B:421:GLN:HG3	2.46	0.46
1:C:137:LEU:HD21	1:C:402:TYR:CG	2.51	0.46
1:C:146:SER:O	1:C:147:GLN:CB	2.61	0.46
1:C:488:ALA:HB2	2:D:22:LYS:HD2	1.98	0.46
2:D:67:LEU:O	2:D:72:PHE:HB2	2.15	0.46
1:E:245:ASP:C	1:E:247:ILE:N	2.74	0.46
1:G:6:LYS:C	1:G:8:LEU:N	2.74	0.46
1:G:225:TRP:CD1	1:G:225:TRP:C	2.92	0.46
2:H:158:LEU:HD13	2:H:177:LEU:HB2	1.97	0.46
2:H:213:PHE:O	2:H:218:ILE:HD11	2.16	0.46
1:A:130:GLN:HA	1:A:154:ARG:HD2	1.98	0.46
1:C:214:TRP:CD1	1:C:215:ILE:N	2.84	0.46
1:C:264:ASN:ND2	1:C:265:PHE:H	2.12	0.46
2:D:405:ARG:N	2:D:406:PRO:CD	2.79	0.46
1:E:44:GLU:OE1	2:F:65:LYS:NZ	2.48	0.46
3:L:155:THR:HG22	3:L:158:ASP:CG	2.41	0.46
3:I:142:ARG:HA	3:I:142:ARG:HD3	1.82	0.46
2:D:125:ASN:N	2:D:125:ASN:ND2	2.60	0.46
3:J:135:GLY:O	3:J:137:PRO:HD3	2.16	0.46
2:F:85:VAL:HG13	2:F:86:SER:N	2.31	0.46
1:G:248:ARG:O	1:G:251:ILE:CD1	2.64	0.46
2:H:163:ASN:O	2:H:163:ASN:OD1	2.33	0.46
2:B:28:GLY:O	2:B:31:THR:HG23	2.16	0.46
2:B:349:LEU:HD23	2:B:349:LEU:N	2.30	0.46
2:D:438:LEU:HD12	2:D:439:HIS:H	1.81	0.46
1:E:301:THR:HG23	1:E:305:TRP:HB2	1.98	0.46
2:F:366:ASP:HA	2:F:369:THR:HB	1.98	0.46
1:G:157:GLY:HA3	1:G:485:TYR:CG	2.51	0.46
1:G:347:ARG:HH12	2:H:274:ARG:HD2	1.81	0.46
1:G:396:ARG:HH21	1:G:400:GLU:HB3	1.80	0.46
2:H:233:ARG:HG2	2:H:234:MET:N	2.31	0.46
3:L:125:ARG:C	3:L:127:LYS:N	2.72	0.46
1:A:324:PRO:HB3	1:A:353:ASP:HB3	1.98	0.46
2:D:228:CYS:O	2:D:231:TYR:HB3	2.16	0.46
3:J:125:ARG:HG3	3:J:125:ARG:HH11	1.81	0.46
1:E:178:ASN:O	1:E:179:ALA:HB2	2.15	0.46
2:F:412:LEU:HB3	2:F:440:PHE:CZ	2.51	0.46
2:H:373:SER:OG	2:H:374:LEU:HD23	2.16	0.46
3:L:170:VAL:CG1	3:L:171:LEU:N	2.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ARG:HA	1:A:81:ILE:CG1	2.46	0.45
1:A:348:GLU:O	1:A:352:LYS:HG3	2.16	0.45
1:A:490:PRO:HG3	2:B:23:PHE:HE1	1.81	0.45
1:C:119:PHE:HE1	1:C:122:ARG:NH1	2.14	0.45
2:D:186:LYS:C	3:J:173:LEU:HD13	2.41	0.45
1:E:49:LEU:O	1:E:52:PRO:HG2	2.14	0.45
1:G:28:LEU:HD12	1:G:28:LEU:HA	1.77	0.45
1:G:173:GLU:CG	1:G:382:LEU:HD11	2.46	0.45
1:G:215:ILE:N	1:G:332:MET:HE1	2.31	0.45
1:G:251:ILE:C	1:G:252:LEU:O	2.58	0.45
2:H:75:ILE:O	2:H:120:VAL:HA	2.15	0.45
2:H:193:LEU:HB3	2:H:196:MET:HE2	1.98	0.45
2:H:357:PRO:HD3	2:H:440:PHE:HB3	1.96	0.45
2:H:417:LEU:HD23	2:H:421:GLN:NE2	2.31	0.45
1:A:38:ALA:O	1:A:85:ARG:HD3	2.16	0.45
1:A:164:ILE:HG23	1:A:164:ILE:O	2.15	0.45
1:A:165:ILE:C	1:A:166:ILE:HG13	2.40	0.45
1:C:310:ALA:CB	1:C:361:VAL:HG22	2.47	0.45
2:D:76:HIS:CD2	2:D:138:PHE:HE2	2.34	0.45
1:E:181:GLU:HG3	1:E:330:PRO:HD3	1.96	0.45
2:F:32:HIS:CG	2:F:33:PRO:HD2	2.51	0.45
2:F:131:ASN:O	2:F:133:THR:N	2.49	0.45
2:F:393:TYR:CE2	2:F:408:LEU:HD11	2.52	0.45
2:H:74:GLN:HE22	2:H:119:ASN:ND2	2.12	0.45
2:H:158:LEU:HD12	2:H:177:LEU:HD22	1.98	0.45
2:H:171:PRO:C	2:H:173:SER:H	2.24	0.45
2:B:130:PHE:HE2	2:D:125:ASN:OD1	1.99	0.45
2:B:217:THR:HG21	2:B:223:ARG:HH22	1.80	0.45
3:I:139:GLN:O	3:I:142:ARG:NH2	2.36	0.45
1:C:28:LEU:HD12	1:C:54:ILE:HD12	1.97	0.45
1:C:94:GLN:HE22	1:C:102:GLY:H	1.64	0.45
1:C:443:PRO:HB2	1:C:483:CYS:SG	2.56	0.45
2:D:158:LEU:CD1	2:D:177:LEU:HB2	2.46	0.45
2:D:356:SER:C	2:D:358:SER:N	2.75	0.45
1:E:46:LEU:HD23	1:E:93:LEU:HD13	1.97	0.45
1:E:474:VAL:O	1:E:475:LYS:C	2.59	0.45
2:F:13:TRP:CZ3	2:F:116:PRO:HG2	2.50	0.45
2:F:316:ILE:HD12	2:F:316:ILE:N	2.27	0.45
1:G:512:GLN:C	1:G:513:PHE:CD1	2.94	0.45
2:H:381:ILE:HD12	2:H:381:ILE:H	1.81	0.45
1:A:453:ASP:C	1:A:455:GLY:N	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:THR:CB	1:C:239:GLU:HG3	2.45	0.45
1:C:318:GLU:HG3	1:C:356:ALA:HB1	1.98	0.45
2:D:257:ILE:HG21	2:D:282:GLN:HG2	1.97	0.45
1:E:527:GLN:OE1	2:F:302:VAL:HG13	2.16	0.45
2:F:204:LEU:HD21	2:F:375:GLN:CG	2.46	0.45
2:F:231:TYR:C	2:F:233:ARG:N	2.75	0.45
2:F:356:SER:C	2:F:358:SER:N	2.75	0.45
3:K:131:GLU:CD	3:K:138:PRO:HD3	2.41	0.45
1:G:158:LEU:HA	1:G:493:ILE:HG13	1.99	0.45
1:G:504:GLU:O	1:G:508:ILE:HG13	2.17	0.45
3:L:103:ILE:HG22	3:L:163:GLY:O	2.17	0.45
1:A:344:ASN:HA	1:A:347:ARG:HB2	1.97	0.45
1:A:371:ALA:C	1:A:373:GLU:N	2.75	0.45
1:A:430:ARG:CZ	1:A:464:PHE:CE1	3.00	0.45
2:B:405:ARG:HG3	2:B:405:ARG:HH11	1.82	0.45
2:B:421:GLN:O	2:B:438:LEU:HD23	2.17	0.45
2:F:87:ASN:HD22	2:F:103:LYS:HE2	1.78	0.45
2:F:325:ASN:HD22	2:F:326:ASP:H	1.65	0.45
3:K:156:ALA:CA	3:K:161:ILE:HD12	2.45	0.45
1:G:172:ILE:N	1:G:172:ILE:HD12	2.32	0.45
1:G:262:GLU:HG3	1:G:264:ASN:ND2	2.32	0.45
3:L:107:THR:HG22	3:L:111:LYS:HB3	1.97	0.45
1:A:163:ARG:HG2	1:A:163:ARG:HH11	1.82	0.45
1:A:489:GLU:H	2:B:19:HIS:HD2	1.61	0.45
1:C:110:GLU:O	1:C:113:LEU:N	2.49	0.45
2:D:11:LEU:N	2:D:11:LEU:HD23	2.32	0.45
2:D:58:GLY:O	2:D:62:GLU:HB2	2.17	0.45
2:D:136:ARG:NH1	2:D:136:ARG:HG2	2.31	0.45
2:D:229:ILE:HA	2:D:264:SER:OG	2.16	0.45
2:D:270:GLN:O	2:D:272:ASN:N	2.50	0.45
1:E:286:GLU:HA	1:E:286:GLU:OE1	2.16	0.45
2:F:101:ARG:HB3	2:F:102:PRO:HD2	1.98	0.45
2:F:158:LEU:CD1	2:F:175:VAL:HB	2.47	0.45
3:K:107:THR:CG2	3:K:108:LEU:N	2.79	0.45
3:L:107:THR:HG22	3:L:111:LYS:N	2.32	0.45
2:B:25:GLU:O	2:B:37:PRO:HB3	2.16	0.45
2:D:54:ILE:HG22	2:D:145:LEU:HD21	1.97	0.45
2:D:145:LEU:HD12	2:D:151:ARG:HG3	1.99	0.45
1:E:220:LYS:O	1:E:222:LEU:N	2.50	0.45
1:E:266:GLU:C	1:E:268:ALA:H	2.23	0.45
1:G:340:ILE:HD13	1:G:340:ILE:HA	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:178:ILE:HD11	2:H:310:ILE:HD13	1.96	0.45
1:A:36:ILE:HD11	1:A:60:ILE:HD12	1.99	0.45
1:A:513:PHE:N	1:A:513:PHE:CD1	2.85	0.45
2:B:64:LEU:HB3	2:B:111:LEU:HD13	1.97	0.45
2:B:226:GLU:OE1	2:B:226:GLU:N	2.44	0.45
2:B:342:ASN:ND2	2:B:342:ASN:N	2.43	0.45
3:I:117:ILE:CG2	3:I:118:GLU:N	2.79	0.45
2:D:270:GLN:C	2:D:272:ASN:N	2.75	0.45
1:E:236:THR:C	1:E:238:LYS:N	2.74	0.45
2:H:110:PHE:CE2	2:H:114:ARG:NH1	2.85	0.45
1:A:113:LEU:O	1:A:138:ARG:NH2	2.50	0.45
1:A:418:ASN:HB3	1:A:421:ASN:HB2	1.99	0.45
2:B:83:ILE:HB	2:B:99:ILE:HA	1.99	0.45
2:B:185:PHE:HE2	2:B:292:VAL:HG21	1.82	0.45
2:B:217:THR:CG2	2:B:223:ARG:HH22	2.30	0.45
2:B:356:SER:CA	2:B:441:THR:OG1	2.65	0.45
1:C:500:ALA:O	1:C:504:GLU:HG2	2.17	0.45
2:D:151:ARG:HG2	2:D:179:ASP:OD2	2.17	0.45
2:D:188:ASN:HA	2:D:322:LEU:O	2.17	0.45
2:F:131:ASN:O	2:F:132:ASP:C	2.59	0.45
2:F:185:PHE:HB3	2:F:326:ASP:HB3	1.98	0.45
1:G:453:ASP:O	1:G:454:ILE:C	2.60	0.45
1:A:335:ASP:O	1:A:336:SER:C	2.59	0.45
2:B:32:HIS:CD2	2:B:34:ASP:HB2	2.52	0.45
1:C:78:ARG:C	1:C:80:SER:H	2.24	0.45
1:C:90:MET:O	1:C:94:GLN:HB2	2.17	0.45
1:C:262:GLU:HB3	1:C:265:PHE:HB2	1.99	0.45
1:C:407:ILE:HG23	1:C:409:LYS:HG3	1.99	0.45
2:D:15:GLY:O	2:D:16:ARG:C	2.59	0.45
2:D:64:LEU:HB3	2:D:111:LEU:CD1	2.47	0.45
2:D:207:TYR:HE1	3:J:172:ARG:HD3	1.64	0.45
2:D:356:SER:O	2:D:358:SER:N	2.50	0.45
1:E:178:ASN:ND2	3:K:136:ILE:HG12	2.32	0.45
2:F:32:HIS:CD2	2:F:34:ASP:HB2	2.52	0.45
1:G:271:ASN:O	1:G:275:ALA:N	2.47	0.45
2:H:215:MET:HE1	2:H:235:LEU:HD11	1.99	0.45
2:H:232:VAL:O	2:H:232:VAL:HG12	2.17	0.45
1:A:47:LYS:HD2	1:A:47:LYS:C	2.42	0.44
3:I:145:TYR:O	3:I:146:SER:C	2.60	0.44
1:C:501:ALA:O	1:C:502:ALA:C	2.59	0.44
2:D:149:ILE:CD1	2:D:149:ILE:N	2.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:ILE:HB	1:E:128:ALA:HA	1.99	0.44
1:E:51:LEU:N	1:E:52:PRO:HD2	2.32	0.44
1:G:72:ASN:ND2	1:G:72:ASN:C	2.74	0.44
1:G:113:LEU:HD11	1:G:139:LEU:HB2	1.99	0.44
2:H:225:PRO:HG3	2:H:274:ARG:O	2.17	0.44
2:H:402:GLU:HG3	2:H:402:GLU:H	1.51	0.44
3:L:138:PRO:HA	3:L:141:GLN:NE2	2.31	0.44
1:A:28:LEU:CD1	1:A:509:ILE:HG21	2.44	0.44
1:A:376:SER:OG	1:A:379:GLU:HG3	2.18	0.44
2:B:87:ASN:ND2	2:B:103:LYS:HE3	2.33	0.44
2:B:419:ASP:HA	2:B:440:PHE:CE1	2.52	0.44
2:D:226:GLU:OE2	2:D:226:GLU:N	2.49	0.44
1:E:264:ASN:ND2	1:E:264:ASN:C	2.73	0.44
2:F:208:PRO:HG3	3:K:171:LEU:HD11	2.00	0.44
1:G:428:MET:O	1:G:432:VAL:HG23	2.17	0.44
3:L:123:VAL:HA	3:L:126:ILE:HG13	1.98	0.44
1:A:229:THR:O	1:A:229:THR:HG22	2.17	0.44
1:A:259:PRO:CG	1:A:262:GLU:OE1	2.65	0.44
1:A:419:PRO:HB2	1:A:475:LYS:HE3	2.00	0.44
1:C:504:GLU:HG3	1:C:516:PHE:CE2	2.51	0.44
1:E:229:THR:O	1:E:232:ARG:HG3	2.18	0.44
1:E:259:PRO:HB3	1:E:261:ASP:O	2.17	0.44
2:H:230:GLU:HA	2:H:230:GLU:OE1	2.17	0.44
2:H:230:GLU:O	2:H:234:MET:HB3	2.17	0.44
2:H:344:PRO:HD3	2:H:374:LEU:HD22	1.98	0.44
3:L:103:ILE:HD12	3:L:103:ILE:C	2.42	0.44
1:A:78:ARG:NH2	2:B:13:TRP:HB3	2.32	0.44
1:A:347:ARG:HH12	2:B:274:ARG:HH22	1.65	0.44
1:A:439:GLN:HE21	1:A:441:ARG:HH12	1.65	0.44
1:C:252:LEU:C	1:C:259:PRO:CD	2.78	0.44
3:J:101:MET:HE2	3:J:119:PRO:CG	2.43	0.44
1:E:125:VAL:HG12	1:E:126:VAL:N	2.31	0.44
3:K:170:VAL:HG13	3:K:171:LEU:N	2.33	0.44
1:G:320:GLN:OE1	1:G:320:GLN:HA	2.17	0.44
1:G:363:LYS:O	1:G:366:GLN:HB2	2.16	0.44
2:H:132:ASP:O	2:H:136:ARG:HG3	2.18	0.44
2:H:139:HIS:C	2:H:140:ILE:HG13	2.42	0.44
2:H:318:LEU:O	2:H:319:ASN:C	2.55	0.44
3:L:155:THR:O	3:L:158:ASP:N	2.50	0.44
1:A:32:HIS:HD2	1:A:56:SER:C	2.26	0.44
2:B:399:SER:HB3	2:B:400:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:GLN:HE22	2:D:119:ASN:ND2	2.15	0.44
2:D:237:TRP:C	2:D:239:LYS:N	2.74	0.44
2:D:251:GLY:O	2:D:257:ILE:HD11	2.17	0.44
2:D:405:ARG:NH1	2:D:405:ARG:CB	2.80	0.44
2:F:261:PHE:O	2:F:264:SER:HB2	2.17	0.44
2:F:320:ASN:HD22	2:F:336:GLU:C	2.26	0.44
1:G:193:ARG:C	1:G:195:HIS:N	2.73	0.44
1:G:534:LEU:N	1:G:534:LEU:HD23	2.32	0.44
2:H:245:GLU:CG	2:H:246:GLY:N	2.80	0.44
2:H:269:SER:O	2:H:272:ASN:OD1	2.36	0.44
1:A:409:LYS:HB3	1:A:413:ILE:HD11	1.98	0.44
1:A:412:ILE:HG21	1:A:427:LEU:HD21	2.00	0.44
1:E:46:LEU:O	1:E:50:VAL:HG23	2.18	0.44
1:E:61:ASP:OD2	1:E:85:ARG:HD2	2.18	0.44
2:F:84:ASP:OD1	2:F:85:VAL:N	2.49	0.44
2:F:355:PHE:CZ	2:F:364:VAL:HG22	2.51	0.44
1:G:426:TYR:CE2	1:G:534:LEU:HD13	2.53	0.44
2:H:54:ILE:HG22	2:H:145:LEU:HD21	2.00	0.44
2:H:186:LYS:HG2	2:H:325:ASN:ND2	2.32	0.44
1:A:60:ILE:O	1:A:60:ILE:HG22	2.16	0.44
1:A:210:SER:O	1:A:211:HIS:HD2	2.01	0.44
1:A:441:ARG:HG2	1:A:441:ARG:NH1	2.32	0.44
1:A:449:GLN:O	1:A:450:VAL:C	2.59	0.44
1:A:458:LYS:HD3	1:A:458:LYS:C	2.43	0.44
1:C:333:ILE:O	1:C:334:ALA:HB2	2.16	0.44
1:C:368:ILE:O	1:C:368:ILE:HG22	2.17	0.44
2:D:124:PHE:C	2:D:125:ASN:ND2	2.72	0.44
2:D:237:TRP:CZ2	2:D:249:LEU:HA	2.53	0.44
1:G:283:SER:O	1:G:286:GLU:HB2	2.18	0.44
3:L:143:LEU:HB3	3:L:150:MET:HE2	2.00	0.44
1:A:430:ARG:CZ	1:A:464:PHE:HE1	2.31	0.44
2:B:237:TRP:CE2	2:B:249:LEU:HB2	2.52	0.44
1:C:450:VAL:O	1:C:451:GLU:C	2.61	0.44
2:D:327:VAL:HG23	2:D:328:ASP:N	2.33	0.44
1:E:50:VAL:HG13	1:E:100:VAL:HG21	1.99	0.44
2:F:192:ILE:O	2:F:193:LEU:HD23	2.18	0.44
1:G:222:LEU:HD13	1:G:243:PHE:CZ	2.53	0.44
2:H:213:PHE:CD1	2:H:213:PHE:N	2.79	0.44
2:H:380:ALA:O	2:H:425:VAL:HA	2.17	0.44
2:B:405:ARG:O	2:B:406:PRO:C	2.61	0.44
1:C:349:LYS:O	1:C:352:LYS:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:ARG:O	2:D:119:ASN:HB3	2.18	0.44
1:E:359:ASN:HB3	1:E:363:LYS:HE3	1.99	0.44
2:F:53:VAL:HB	2:F:77:VAL:HG22	1.99	0.44
1:G:46:LEU:HD23	1:G:93:LEU:HD13	1.99	0.44
1:G:293:ARG:NH1	1:G:293:ARG:CG	2.77	0.44
2:H:84:ASP:OD1	2:H:86:SER:N	2.44	0.44
2:H:136:ARG:CG	2:H:161:LEU:HD22	2.48	0.44
2:H:353:ILE:HG22	2:H:355:PHE:CD1	2.53	0.44
2:H:379:PRO:HD2	2:H:395:GLN:NE2	2.33	0.44
2:H:410:LYS:CB	2:H:415:LEU:HD21	2.48	0.44
1:C:61:ASP:HB3	1:C:86:ALA:HB2	2.00	0.43
2:D:58:GLY:N	2:D:91:GLN:HG2	2.32	0.43
2:D:113:ASP:OD1	2:D:113:ASP:C	2.60	0.43
2:D:141:ILE:HD12	2:D:158:LEU:HD11	2.00	0.43
2:D:223:ARG:HH12	2:D:227:HIS:CE1	2.36	0.43
3:J:123:VAL:HG13	3:J:150:MET:HE3	1.99	0.43
1:E:252:LEU:O	1:E:253:LYS:C	2.61	0.43
2:F:56:ALA:HA	2:F:60:GLY:HA3	1.99	0.43
1:G:214:TRP:CE2	1:G:271:ASN:ND2	2.86	0.43
1:G:386:ASN:O	1:G:388:ALA:N	2.51	0.43
2:H:165:GLU:O	2:H:166:ASP:HB2	2.18	0.43
2:H:348:GLN:C	2:H:349:LEU:HD12	2.43	0.43
3:L:104:LYS:HG2	3:L:114:GLU:HG2	2.00	0.43
3:L:105:VAL:HA	3:L:167:LEU:O	2.18	0.43
2:B:339:ARG:O	2:B:340:LYS:C	2.61	0.43
2:B:362:GLN:OE1	2:B:362:GLN:HA	2.17	0.43
1:C:34:CYS:HB2	1:C:123:PHE:CE2	2.54	0.43
1:C:56:SER:HB2	1:C:101:SER:O	2.17	0.43
1:C:65:VAL:HG22	1:C:85:ARG:HA	1.99	0.43
1:E:505:VAL:O	1:E:508:ILE:HB	2.18	0.43
2:F:377:LYS:HD2	2:F:377:LYS:O	2.18	0.43
3:K:170:VAL:HG22	3:K:171:LEU:H	1.83	0.43
1:G:226:TYR:CB	1:G:231:GLY:HA2	2.46	0.43
3:L:159:TYR:O	3:L:160:LYS:HB2	2.18	0.43
1:A:214:TRP:CD1	1:A:215:ILE:N	2.87	0.43
1:A:215:ILE:HG13	1:A:332:MET:SD	2.58	0.43
1:A:457:LEU:HD23	1:A:479:VAL:O	2.18	0.43
2:B:123:HIS:CE1	2:D:125:ASN:HD21	2.36	0.43
1:C:293:ARG:HH11	1:C:293:ARG:HG3	1.84	0.43
1:C:437:LYS:HD2	1:C:437:LYS:HA	1.90	0.43
1:C:503:GLN:CD	2:D:185:PHE:CE2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:408:LEU:HD23	2:D:408:LEU:HA	1.86	0.43
2:D:412:LEU:CD1	2:D:440:PHE:HE2	2.31	0.43
1:E:215:ILE:HD12	1:E:332:MET:HE1	2.01	0.43
1:E:259:PRO:C	1:E:261:ASP:N	2.66	0.43
1:E:314:PHE:HB2	1:E:357:VAL:HG22	1.99	0.43
1:E:411:GLU:OE1	1:E:411:GLU:HA	2.18	0.43
2:F:162:LEU:HD22	2:F:169:LEU:HD11	2.00	0.43
2:F:367:TYR:O	2:F:371:SER:HB3	2.18	0.43
1:G:504:GLU:OE2	1:G:507:LYS:NZ	2.42	0.43
2:H:170:ASP:OD1	2:H:170:ASP:C	2.61	0.43
2:H:265:LEU:HD23	2:H:276:VAL:CG1	2.48	0.43
3:L:120:THR:O	3:L:120:THR:OG1	2.31	0.43
1:A:159:VAL:HG21	1:A:425:LEU:HD22	2.00	0.43
1:A:189:PHE:CE1	1:A:192:LEU:HB2	2.54	0.43
2:B:226:GLU:CG	2:B:280:LEU:HD11	2.48	0.43
2:D:106:VAL:O	2:D:109:GLU:HG2	2.18	0.43
1:E:214:TRP:CD1	1:E:214:TRP:C	2.96	0.43
1:E:252:LEU:O	1:E:259:PRO:CD	2.65	0.43
2:F:139:HIS:O	2:F:176:PRO:HD2	2.19	0.43
1:G:164:ILE:HD11	1:G:508:ILE:HD11	2.00	0.43
1:G:264:ASN:N	1:G:264:ASN:HD22	2.16	0.43
1:G:264:ASN:CA	1:G:333:ILE:HD11	2.48	0.43
3:L:145:TYR:HB2	3:L:167:LEU:HD22	2.00	0.43
1:A:311:LEU:HD12	1:A:311:LEU:HA	1.89	0.43
1:C:457:LEU:C	1:C:459:SER:N	2.75	0.43
2:D:237:TRP:O	2:D:241:GLN:HG2	2.18	0.43
2:F:249:LEU:HD13	2:F:260:ILE:HD11	1.99	0.43
1:G:111:ASN:OD1	1:G:111:ASN:C	2.62	0.43
1:G:516:PHE:CD2	1:G:516:PHE:N	2.86	0.43
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.85	0.43
2:B:351:GLN:N	2:B:436:PHE:HA	2.33	0.43
2:B:360:LYS:O	2:B:361:LEU:C	2.62	0.43
2:B:418:VAL:HG22	2:B:421:GLN:OE1	2.19	0.43
1:C:47:LYS:HD2	1:C:47:LYS:C	2.43	0.43
1:C:115:ASN:C	1:C:117:PRO:HD3	2.44	0.43
1:E:416:MET:C	1:E:418:ASN:N	2.76	0.43
2:F:195:GLY:C	2:F:196:MET:HG2	2.44	0.43
2:H:241:GLN:O	2:H:242:PRO:C	2.61	0.43
2:H:393:TYR:CG	2:H:394:LEU:N	2.86	0.43
1:A:361:VAL:O	1:A:362:ALA:C	2.62	0.43
2:B:249:LEU:HD12	2:B:250:ASP:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:LEU:HA	1:E:28:LEU:HD12	1.81	0.43
2:F:401:GLU:O	2:F:405:ARG:HB2	2.19	0.43
2:F:412:LEU:O	2:F:417:LEU:HB2	2.18	0.43
3:L:120:THR:OG1	3:L:155:THR:OG1	2.37	0.43
2:B:253:ASP:O	2:B:256:HIS:HB2	2.19	0.43
2:B:407:ASN:HD22	2:B:415:LEU:HD13	1.83	0.43
1:E:76:LEU:HD21	1:E:89:ALA:HB2	1.99	0.43
1:E:251:ILE:C	1:E:252:LEU:O	2.61	0.43
1:G:129:THR:HA	1:G:153:CYS:O	2.19	0.43
2:H:92:PHE:CD2	2:H:92:PHE:N	2.80	0.43
2:B:331:TYR:CE1	3:I:110:GLY:HA2	2.54	0.43
2:D:243:PHE:N	2:D:243:PHE:CD1	2.87	0.43
1:E:396:ARG:HH21	1:E:400:GLU:HB3	1.82	0.43
1:E:421:ASN:O	1:E:424:VAL:HG22	2.19	0.43
1:E:447:ASN:ND2	2:F:26:ARG:NE	2.65	0.43
1:G:157:GLY:HA3	1:G:485:TYR:CD1	2.54	0.43
2:H:46:LEU:O	2:H:73:ARG:HB3	2.19	0.43
2:H:398:THR:O	2:H:401:GLU:HB3	2.19	0.43
1:A:225:TRP:O	1:A:229:THR:HB	2.18	0.43
1:A:364:LEU:HD12	1:A:364:LEU:HA	1.80	0.43
2:B:128:GLN:HE21	2:B:128:GLN:HB2	1.63	0.43
2:B:385:LEU:HD23	2:B:385:LEU:HA	1.53	0.43
1:C:435:PHE:CE2	1:C:439:GLN:HG3	2.54	0.43
2:D:76:HIS:CD2	2:D:138:PHE:CE2	3.07	0.43
2:D:139:HIS:O	2:D:176:PRO:HD2	2.19	0.43
2:D:325:ASN:OD1	2:D:327:VAL:HG22	2.19	0.43
2:D:422:GLU:HA	2:D:437:LYS:HA	2.01	0.43
1:E:56:SER:HB3	1:E:101:SER:HB2	2.00	0.43
1:E:214:TRP:CH2	1:E:332:MET:HG2	2.54	0.43
2:F:102:PRO:O	2:F:103:LYS:C	2.62	0.43
2:F:231:TYR:O	2:F:233:ARG:N	2.52	0.43
2:F:357:PRO:HB3	2:F:440:PHE:CZ	2.54	0.43
1:G:31:ALA:HB3	1:G:54:ILE:HD11	2.01	0.43
1:G:110:GLU:OE2	1:G:138:ARG:NH1	2.52	0.43
2:H:200:ILE:HD13	3:L:172:ARG:NH2	2.34	0.43
2:H:233:ARG:HG2	2:H:233:ARG:HH11	1.84	0.43
1:A:139:LEU:HD12	1:A:143:LEU:HG	2.01	0.42
1:A:140:ALA:CB	1:A:398:LEU:HD23	2.48	0.42
1:A:181:GLU:OE1	1:A:330:PRO:HD3	2.19	0.42
1:A:279:THR:O	1:A:280:GLN:HB2	2.17	0.42
1:A:430:ARG:O	1:A:433:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLU:O	1:A:484:ARG:HB3	2.18	0.42
1:A:518:ASN:HD21	1:A:534:LEU:CA	2.31	0.42
2:B:156:GLY:HA3	2:B:430:THR:CG2	2.49	0.42
2:B:217:THR:CB	2:B:223:ARG:NH2	2.79	0.42
2:B:356:SER:HA	2:B:441:THR:H	1.84	0.42
3:I:170:VAL:CG1	3:I:171:LEU:N	2.82	0.42
2:D:90:ARG:HG2	2:D:90:ARG:HH11	1.84	0.42
2:D:351:GLN:O	2:D:436:PHE:HA	2.19	0.42
2:D:390:ARG:CG	2:D:391:THR:N	2.80	0.42
1:E:53:GLY:O	1:E:54:ILE:C	2.62	0.42
1:E:120:PHE:HA	1:E:123:PHE:CD1	2.54	0.42
2:F:256:HIS:CD2	2:F:256:HIS:N	2.87	0.42
2:F:405:ARG:N	2:F:406:PRO:CD	2.82	0.42
1:G:171:VAL:HG12	1:G:391:ARG:O	2.19	0.42
2:H:272:ASN:OD1	2:H:272:ASN:N	2.49	0.42
1:A:171:VAL:HG13	1:A:391:ARG:HB2	2.01	0.42
1:A:248:ARG:O	1:A:251:ILE:HG13	2.20	0.42
1:A:260:GLU:O	1:A:261:ASP:OD1	2.37	0.42
1:A:403:GLY:HA3	1:A:406:THR:OG1	2.19	0.42
2:B:151:ARG:HH11	2:B:151:ARG:HG3	1.83	0.42
1:C:25:GLN:HE21	1:C:29:GLU:CG	2.31	0.42
2:D:405:ARG:HB3	2:D:406:PRO:HD3	2.00	0.42
1:E:279:THR:O	1:E:280:GLN:HB2	2.20	0.42
2:F:148:ILE:O	2:F:152:ARG:HG3	2.20	0.42
2:F:237:TRP:CD1	2:F:237:TRP:C	2.97	0.42
1:G:447:ASN:ND2	2:H:26:ARG:HE	2.17	0.42
2:H:226:GLU:OE1	2:H:226:GLU:N	2.53	0.42
1:A:238:LYS:O	1:A:238:LYS:HD3	2.19	0.42
1:A:396:ARG:NH2	1:A:406:THR:O	2.47	0.42
2:B:415:LEU:HB2	2:B:417:LEU:HD23	2.01	0.42
2:B:417:LEU:HD22	2:B:417:LEU:N	2.35	0.42
2:D:321:TYR:OH	3:J:172:ARG:HA	2.20	0.42
2:D:399:SER:HB2	2:D:403:ARG:HH12	1.83	0.42
2:D:418:VAL:HG22	2:D:421:GLN:CD	2.43	0.42
1:E:48:ASN:O	1:E:52:PRO:HG3	2.19	0.42
1:A:225:TRP:CE2	1:A:234:PRO:HG3	2.54	0.42
1:C:71:GLY:HA3	2:D:16:ARG:O	2.19	0.42
1:C:354:ALA:O	1:C:380:LEU:HD21	2.18	0.42
1:C:377:GLU:O	1:C:381:LYS:HG2	2.19	0.42
1:C:446:SER:HB2	1:C:449:GLN:CB	2.50	0.42
2:D:406:PRO:C	2:D:408:LEU:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:428:MET:HE2	1:E:479:VAL:HA	2.01	0.42
2:F:204:LEU:HD21	2:F:375:GLN:HG2	2.01	0.42
1:G:236:THR:O	1:G:240:LYS:HG3	2.19	0.42
1:G:318:GLU:OE1	1:G:360:HIS:NE2	2.52	0.42
1:G:484:ARG:NH1	2:H:315:TYR:CZ	2.88	0.42
1:G:514:VAL:HB	2:H:328:ASP:OD1	2.20	0.42
2:H:373:SER:C	2:H:374:LEU:HD23	2.45	0.42
1:A:165:ILE:HD13	1:A:398:LEU:HB2	2.01	0.42
1:C:160:GLY:HA3	1:C:497:LEU:HD11	2.01	0.42
1:C:299:LYS:HA	1:C:368:ILE:CG2	2.43	0.42
2:D:32:HIS:HB3	2:D:313:SER:O	2.19	0.42
3:J:137:PRO:HA	3:J:138:PRO:HD3	1.89	0.42
1:G:270:LYS:C	1:G:272:VAL:H	2.26	0.42
2:H:260:ILE:O	2:H:264:SER:HB2	2.20	0.42
2:B:231:TYR:CD2	2:B:231:TYR:C	2.98	0.42
3:I:103:ILE:HD11	3:I:117:ILE:CD1	2.49	0.42
2:D:217:THR:CG2	2:D:223:ARG:HH22	2.33	0.42
1:E:352:LYS:O	1:E:355:ALA:N	2.52	0.42
1:E:504:GLU:O	1:E:508:ILE:HG13	2.20	0.42
1:G:214:TRP:CG	1:G:332:MET:HE3	2.55	0.42
2:H:169:LEU:HD12	2:H:170:ASP:N	2.34	0.42
2:H:423:LEU:HD11	2:H:438:LEU:HB2	2.02	0.42
1:A:53:GLY:O	1:A:54:ILE:C	2.62	0.42
1:A:236:THR:HB	1:A:239:GLU:H	1.85	0.42
1:A:318:GLU:OE1	1:A:318:GLU:N	2.50	0.42
2:B:312:THR:O	2:B:313:SER:C	2.62	0.42
3:I:102:LEU:O	3:I:102:LEU:CG	2.67	0.42
1:C:210:SER:C	1:C:211:HIS:CG	2.98	0.42
1:C:416:MET:CE	1:C:419:PRO:HA	2.50	0.42
2:D:316:ILE:HA	2:D:317:PRO:HD3	1.84	0.42
3:J:169:LEU:HD23	3:J:169:LEU:HA	1.87	0.42
1:E:211:HIS:HE1	2:F:221:MET:CE	2.33	0.42
1:E:259:PRO:HB2	1:E:261:ASP:O	2.20	0.42
1:G:299:LYS:HA	1:G:368:ILE:HG21	2.01	0.42
2:H:425:VAL:O	2:H:434:VAL:HG12	2.19	0.42
3:L:154:LYS:HB3	3:L:158:ASP:OD1	2.19	0.42
1:A:259:PRO:C	1:A:261:ASP:N	2.59	0.42
1:A:307:LEU:HD21	1:A:375:ILE:HG21	2.02	0.42
2:B:351:GLN:HB3	2:B:436:PHE:CD1	2.54	0.42
3:I:137:PRO:O	3:I:140:GLN:HG2	2.20	0.42
1:C:252:LEU:HA	1:C:252:LEU:HD23	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:316:ILE:H	2:D:316:ILE:CD1	2.32	0.42
1:E:428:MET:CE	1:E:479:VAL:HA	2.50	0.42
2:F:127:ILE:O	2:F:135:TYR:OH	2.38	0.42
2:F:212:ASN:HD22	2:F:212:ASN:HA	1.58	0.42
2:F:217:THR:CG2	2:F:223:ARG:NH2	2.79	0.42
3:K:107:THR:HB	3:K:111:LYS:HB3	2.02	0.42
1:G:311:LEU:HD21	1:G:387:SER:HB2	2.02	0.42
2:H:30:PHE:N	2:H:30:PHE:CD1	2.87	0.42
2:H:356:SER:O	2:H:357:PRO:C	2.62	0.42
2:H:356:SER:OG	2:H:358:SER:HB3	2.19	0.42
3:L:118:GLU:O	3:L:119:PRO:C	2.63	0.42
1:A:96:LEU:HD23	2:B:95:ARG:NH2	2.34	0.42
1:A:457:LEU:HD22	1:A:483:CYS:SG	2.60	0.42
2:B:52:LEU:HD11	2:B:78:ILE:HG13	2.02	0.42
2:B:357:PRO:O	2:B:411:THR:HB	2.20	0.42
2:B:381:ILE:CG2	2:B:423:LEU:HD22	2.50	0.42
2:B:417:LEU:HD12	2:B:421:GLN:HE22	1.84	0.42
1:C:189:PHE:O	1:C:192:LEU:N	2.52	0.42
1:C:359:ASN:O	1:C:363:LYS:HG3	2.20	0.42
1:C:417:ASP:O	1:C:418:ASN:C	2.63	0.42
1:C:446:SER:HB2	1:C:449:GLN:HE21	1.84	0.42
2:D:46:LEU:HB3	2:D:73:ARG:NH1	2.34	0.42
2:D:412:LEU:HD12	2:D:440:PHE:HE2	1.84	0.42
1:E:214:TRP:CZ3	1:E:332:MET:HG2	2.54	0.42
1:E:396:ARG:HD3	1:E:534:LEU:O	2.20	0.42
2:F:393:TYR:HD1	2:F:404:THR:OG1	2.03	0.42
1:G:185:LEU:O	1:G:188:PRO:HD3	2.19	0.42
1:G:282:PRO:HG2	1:G:285:ILE:HD13	2.02	0.42
1:G:323:LEU:HB3	1:G:324:PRO:HD2	2.02	0.42
1:G:434:ARG:O	1:G:435:PHE:C	2.61	0.42
2:H:178:ILE:N	2:H:178:ILE:CD1	2.82	0.42
2:H:201:GLU:C	2:H:203:THR:N	2.77	0.42
1:A:78:ARG:HB2	1:A:81:ILE:HD11	2.02	0.42
2:B:178:ILE:HD12	2:B:178:ILE:N	2.34	0.42
2:B:419:ASP:OD1	2:B:440:PHE:CD1	2.62	0.42
1:C:120:PHE:C	1:C:122:ARG:N	2.77	0.42
1:C:250:GLY:C	1:C:252:LEU:H	2.27	0.42
1:E:215:ILE:HD12	1:E:342:LEU:HD21	2.01	0.42
2:F:52:LEU:HD11	2:F:78:ILE:HG13	2.01	0.42
2:F:239:LYS:C	2:F:240:GLU:CG	2.92	0.42
1:G:197:GLN:C	1:G:199:TYR:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:362:ALA:O	1:G:366:GLN:HG3	2.20	0.42
1:G:481:GLU:OE1	1:G:481:GLU:HA	2.20	0.42
2:H:193:LEU:HD23	2:H:193:LEU:HA	1.74	0.42
1:A:42:GLY:HA2	1:A:129:THR:HG21	2.02	0.41
1:A:84:ASN:HB3	1:A:87:GLU:HB3	2.02	0.41
3:I:107:THR:CG2	3:I:109:THR:HG23	2.50	0.41
1:C:143:LEU:HD22	1:C:148:ILE:CB	2.45	0.41
1:C:157:GLY:HA3	1:C:485:TYR:CG	2.55	0.41
1:C:340:ILE:CD1	2:D:271:TYR:O	2.68	0.41
1:C:437:LYS:C	1:C:439:GLN:H	2.27	0.41
2:D:64:LEU:HB3	2:D:111:LEU:HD13	2.02	0.41
1:E:43:THR:CG2	1:E:44:GLU:N	2.83	0.41
1:E:240:LYS:HG2	1:E:276:LEU:CD1	2.49	0.41
2:F:154:ILE:O	2:F:154:ILE:HG13	2.20	0.41
2:F:243:PHE:O	2:F:247:VAL:HG21	2.19	0.41
1:G:416:MET:C	1:G:418:ASN:N	2.76	0.41
2:H:245:GLU:C	2:H:247:VAL:H	2.28	0.41
3:L:135:GLY:O	3:L:137:PRO:HD3	2.20	0.41
1:A:416:MET:CE	1:A:424:VAL:HG22	2.50	0.41
1:A:426:TYR:O	1:A:429:LEU:HB2	2.19	0.41
1:A:514:VAL:HB	2:B:328:ASP:HA	2.01	0.41
2:B:339:ARG:NH2	2:B:346:CYS:O	2.44	0.41
1:C:39:THR:O	1:C:43:THR:HB	2.19	0.41
1:C:329:ILE:HB	1:C:330:PRO:HD2	2.02	0.41
2:D:110:PHE:C	2:D:110:PHE:CD2	2.98	0.41
3:J:121:ASP:CG	3:J:125:ARG:HD2	2.45	0.41
1:E:187:LYS:N	1:E:188:PRO:CD	2.82	0.41
1:E:282:PRO:HG2	1:E:388:ALA:HB1	2.03	0.41
2:F:75:ILE:O	2:F:120:VAL:HA	2.19	0.41
2:F:143:CYS:HB2	2:F:179:ASP:HA	2.01	0.41
2:F:320:ASN:HB2	2:F:336:GLU:HA	2.02	0.41
1:G:196:PHE:O	1:G:199:TYR:HB2	2.20	0.41
1:G:238:LYS:O	1:G:241:GLU:HB3	2.20	0.41
1:G:264:ASN:HD22	1:G:265:PHE:N	2.18	0.41
2:H:148:ILE:CG1	3:L:174:ARG:HG2	2.46	0.41
3:L:106:LYS:CG	3:L:112:GLU:HG2	2.49	0.41
3:L:123:VAL:HG23	3:L:154:LYS:O	2.20	0.41
1:A:105:VAL:C	1:A:107:GLU:H	2.28	0.41
2:B:132:ASP:O	2:B:134:PHE:N	2.53	0.41
2:B:207:TYR:CE2	3:I:172:ARG:CG	2.91	0.41
2:B:325:ASN:HD22	2:B:326:ASP:N	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:ARG:HG3	2:D:91:GLN:HG3	2.02	0.41
2:D:277:THR:HG22	2:D:279:ARG:H	1.85	0.41
2:F:357:PRO:HD3	2:F:440:PHE:CD2	2.54	0.41
1:G:115:ASN:C	1:G:117:PRO:HD3	2.45	0.41
1:A:186:ASP:OD2	1:A:187:LYS:N	2.53	0.41
1:A:248:ARG:C	1:A:250:GLY:N	2.78	0.41
1:C:59:ILE:C	1:C:60:ILE:HG13	2.45	0.41
1:C:212:THR:HA	1:C:213:PRO:HD3	1.94	0.41
1:E:364:LEU:HD12	1:E:364:LEU:HA	1.84	0.41
2:F:241:GLN:CB	2:F:245:GLU:HA	2.51	0.41
1:G:333:ILE:CG2	2:H:223:ARG:NH1	2.83	0.41
2:H:217:THR:HG21	2:H:223:ARG:NE	2.31	0.41
2:H:220:SER:O	2:H:222:PRO:CD	2.68	0.41
2:H:427:ASP:OD2	2:H:428:VAL:N	2.49	0.41
1:C:47:LYS:NZ	2:D:65:LYS:HE2	2.36	0.41
1:C:245:ASP:O	1:C:249:GLN:HG3	2.21	0.41
1:C:314:PHE:HZ	1:C:353:ASP:OD2	2.04	0.41
2:D:268:ALA:O	2:D:273:ILE:N	2.53	0.41
2:D:418:VAL:CG2	2:D:421:GLN:NE2	2.80	0.41
3:J:125:ARG:HG3	3:J:125:ARG:NH1	2.35	0.41
1:E:311:LEU:HD22	1:E:383:LEU:HD11	2.02	0.41
1:G:214:TRP:N	1:G:332:MET:HE2	2.35	0.41
1:G:344:ASN:O	1:G:348:GLU:HB2	2.20	0.41
2:H:221:MET:HE2	2:H:221:MET:HB3	1.94	0.41
2:H:354:GLN:NE2	2:H:439:HIS:HB3	2.34	0.41
1:A:154:ARG:HG2	1:A:154:ARG:NH1	2.36	0.41
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.84	0.41
1:A:428:MET:SD	1:A:461:LEU:HD22	2.61	0.41
2:B:434:VAL:HG22	2:B:436:PHE:CE1	2.55	0.41
3:I:117:ILE:HD13	3:I:126:ILE:HG12	2.03	0.41
1:C:40:ALA:O	1:C:43:THR:HG22	2.21	0.41
1:E:241:GLU:OE1	1:E:244:ARG:HD2	2.21	0.41
1:E:419:PRO:HB2	1:E:475:LYS:HE3	2.03	0.41
1:E:501:ALA:O	1:E:505:VAL:HG23	2.20	0.41
2:F:79:ASP:OD2	2:F:81:ASP:HB2	2.20	0.41
2:F:271:TYR:O	2:F:272:ASN:OD1	2.37	0.41
3:K:107:THR:C	3:K:109:THR:N	2.78	0.41
1:G:282:PRO:HG2	1:G:285:ILE:HB	2.02	0.41
1:G:497:LEU:HD12	1:G:497:LEU:HA	1.92	0.41
2:H:35:PHE:O	2:H:36:GLU:HG2	2.19	0.41
2:H:249:LEU:CD2	2:H:260:ILE:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:349:LEU:O	2:H:350:PRO:O	2.38	0.41
1:A:37:ASN:HB2	1:A:129:THR:O	2.21	0.41
1:A:297:ILE:N	1:A:297:ILE:CD1	2.76	0.41
1:A:427:LEU:O	1:A:428:MET:C	2.63	0.41
2:B:50:LYS:H	2:B:139:HIS:CD2	2.38	0.41
1:C:499:GLY:O	2:D:294:SER:HB2	2.20	0.41
2:D:228:CYS:SG	2:D:267:ARG:HG2	2.61	0.41
2:D:385:LEU:O	2:D:387:GLY:N	2.52	0.41
1:E:318:GLU:HG3	1:E:356:ALA:HB1	2.02	0.41
2:F:136:ARG:HH11	2:F:136:ARG:HG3	1.85	0.41
2:F:261:PHE:CZ	2:F:265:LEU:HD11	2.55	0.41
1:G:15:ARG:HA	1:G:15:ARG:HD3	1.92	0.41
1:G:311:LEU:HD12	1:G:311:LEU:HA	1.83	0.41
1:G:333:ILE:CG2	2:H:223:ARG:HH12	2.34	0.41
1:G:333:ILE:HD13	1:G:333:ILE:HG21	1.74	0.41
2:H:204:LEU:HG	2:H:204:LEU:O	2.20	0.41
3:L:151:ASN:C	3:L:153:GLU:N	2.77	0.41
1:A:97:ASN:HB3	1:A:100:VAL:HG23	2.02	0.41
1:A:261:ASP:O	1:A:262:GLU:CG	2.69	0.41
1:A:353:ASP:O	1:A:357:VAL:HG23	2.20	0.41
1:A:359:ASN:HD22	1:A:359:ASN:HA	1.60	0.41
2:B:309:LYS:HD3	2:B:317:PRO:HA	2.03	0.41
2:B:357:PRO:CD	2:B:442:SER:C	2.94	0.41
3:I:102:LEU:O	3:I:163:GLY:O	2.39	0.41
1:C:289:PHE:HB3	1:C:312:LYS:HD2	2.03	0.41
1:C:481:GLU:HG3	1:C:485:TYR:CE2	2.56	0.41
2:D:29:PRO:C	2:D:31:THR:N	2.79	0.41
2:D:231:TYR:HD1	2:D:235:LEU:HD12	1.85	0.41
2:D:333:TYR:CE2	2:D:335:PHE:HB3	2.56	0.41
1:E:518:ASN:CB	1:E:533:GLN:HA	2.50	0.41
2:F:209:PRO:HG2	3:K:139:GLN:O	2.20	0.41
2:F:247:VAL:HA	2:F:248:PRO:HD3	1.81	0.41
1:G:66:SER:N	1:G:69:ASP:HB2	2.35	0.41
1:G:248:ARG:O	1:G:251:ILE:HD12	2.21	0.41
2:H:57:GLY:O	2:H:58:GLY:C	2.63	0.41
3:L:131:GLU:O	3:L:131:GLU:HG2	2.19	0.41
2:B:16:ARG:NH2	2:B:116:PRO:HB2	2.36	0.41
2:B:126:LYS:O	2:B:127:ILE:C	2.62	0.41
2:B:441:THR:O	2:B:442:SER:OXT	2.38	0.41
1:C:47:LYS:HZ1	2:D:65:LYS:HE2	1.85	0.41
1:C:113:LEU:C	1:C:138:ARG:HH21	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:PHE:O	1:C:122:ARG:N	2.54	0.41
1:C:158:LEU:HD12	1:C:525:MET:HG2	2.01	0.41
1:C:163:ARG:HH12	1:C:165:ILE:HG12	1.81	0.41
1:C:293:ARG:HB3	1:C:305:TRP:CE3	2.55	0.41
2:D:141:ILE:HD12	2:D:158:LEU:CD2	2.41	0.41
2:D:213:PHE:HB2	2:D:218:ILE:HD11	2.02	0.41
2:D:406:PRO:C	2:D:408:LEU:N	2.79	0.41
1:E:35:LEU:HD12	1:E:36:ILE:N	2.36	0.41
1:E:45:ILE:CG1	1:E:498:GLY:HA2	2.49	0.41
1:E:177:ASP:CG	2:F:186:LYS:HZ1	2.29	0.41
1:E:241:GLU:O	1:E:244:ARG:HB2	2.21	0.41
1:E:247:ILE:O	1:E:248:ARG:C	2.63	0.41
1:E:274:THR:O	1:E:276:LEU:N	2.54	0.41
2:F:74:GLN:NE2	2:F:74:GLN:HA	2.36	0.41
2:F:196:MET:HE3	2:F:196:MET:HB3	1.99	0.41
2:F:410:LYS:HD3	2:F:415:LEU:HG	2.03	0.41
1:G:213:PRO:CB	1:G:332:MET:HE2	2.51	0.41
1:G:418:ASN:C	1:G:420:ASP:H	2.29	0.41
1:G:422:GLU:O	1:G:424:VAL:N	2.54	0.41
1:G:496:PHE:C	1:G:496:PHE:CD2	2.98	0.41
2:H:385:LEU:CD1	2:H:390:ARG:HD3	2.51	0.41
3:L:106:LYS:HB2	3:L:168:HIS:CD2	2.55	0.41
3:L:120:THR:OG1	3:L:155:THR:CB	2.68	0.41
1:A:213:PRO:HG3	1:A:334:ALA:CB	2.50	0.41
1:A:510:THR:O	1:A:511:LYS:HB2	2.21	0.41
2:B:257:ILE:HG22	2:B:278:TYR:CE1	2.56	0.41
3:I:102:LEU:O	3:I:102:LEU:HG	2.21	0.41
3:I:162:LEU:O	3:I:163:GLY:C	2.64	0.41
1:C:9:LYS:HE2	1:C:9:LYS:HB3	1.90	0.41
2:D:15:GLY:O	2:D:17:TRP:N	2.54	0.41
2:D:32:HIS:CE1	2:D:33:PRO:HD2	2.56	0.41
2:D:140:ILE:HG22	2:D:141:ILE:N	2.35	0.41
2:D:150:ALA:O	2:D:154:ILE:HG22	2.21	0.41
2:D:249:LEU:CD1	2:D:260:ILE:HD11	2.50	0.41
2:D:253:ASP:OD1	2:D:255:GLU:HB2	2.20	0.41
2:D:405:ARG:NH1	2:D:405:ARG:HB3	2.35	0.41
2:F:152:ARG:HH21	2:F:201:GLU:CD	2.28	0.41
2:F:321:TYR:OH	3:K:172:ARG:HG3	2.21	0.41
1:G:245:ASP:C	1:G:247:ILE:H	2.27	0.41
1:G:286:GLU:OE1	1:G:286:GLU:HA	2.20	0.41
1:G:437:LYS:HA	1:G:437:LYS:HD2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:64:LEU:HD11	2:H:77:VAL:HG21	2.03	0.41
2:H:115:VAL:HA	2:H:116:PRO:HD2	1.88	0.41
2:H:233:ARG:NH1	2:H:233:ARG:HG2	2.35	0.41
2:H:241:GLN:HA	2:H:242:PRO:HD3	1.57	0.41
2:H:352:ASN:HD22	2:H:439:HIS:CD2	2.39	0.41
1:A:140:ALA:HB3	1:A:398:LEU:HD23	2.03	0.40
1:A:424:VAL:HG11	1:A:478:TYR:CD1	2.56	0.40
2:B:250:ASP:OD1	2:B:250:ASP:C	2.64	0.40
2:B:265:LEU:HD13	1:E:66:SER:HA	2.02	0.40
2:B:269:SER:O	2:B:270:GLN:C	2.63	0.40
3:I:172:ARG:C	3:I:173:LEU:HG	2.46	0.40
1:C:302:PRO:O	1:C:304:PHE:N	2.54	0.40
1:E:178:ASN:CG	3:K:136:ILE:HG12	2.45	0.40
1:E:528:THR:HG22	2:F:334:THR:OG1	2.20	0.40
2:F:95:ARG:HB2	2:F:97:LYS:HG2	2.03	0.40
2:F:219:ALA:HB2	2:F:231:TYR:CD1	2.56	0.40
1:G:421:ASN:O	1:G:422:GLU:C	2.63	0.40
1:A:144:TRP:CD1	1:A:144:TRP:C	2.98	0.40
1:A:248:ARG:HH11	1:A:248:ARG:HG3	1.87	0.40
1:A:252:LEU:C	1:A:252:LEU:CD2	2.92	0.40
1:A:366:GLN:C	1:A:368:ILE:N	2.70	0.40
1:A:430:ARG:NH2	1:A:464:PHE:HE1	2.18	0.40
2:B:131:ASN:OD1	2:B:131:ASN:C	2.64	0.40
2:B:328:ASP:OD1	2:B:328:ASP:C	2.65	0.40
3:I:157:ALA:C	3:I:159:TYR:N	2.79	0.40
1:C:9:LYS:HA	1:C:12:LYS:HB3	2.03	0.40
1:C:190:PRO:HG2	1:C:191:GLU:OE2	2.21	0.40
2:D:323:VAL:HG21	3:J:170:VAL:HG23	2.03	0.40
1:E:129:THR:HA	1:E:153:CYS:O	2.21	0.40
1:E:201:LEU:H	1:E:201:LEU:HG	1.34	0.40
1:E:241:GLU:OE1	1:E:241:GLU:HA	2.21	0.40
1:E:434:ARG:HD3	1:E:460:CYS:O	2.21	0.40
2:F:18:ASN:C	2:F:20:VAL:H	2.29	0.40
2:F:195:GLY:HA2	2:F:339:ARG:NH2	2.35	0.40
2:H:143:CYS:HB3	2:H:179:ASP:OD2	2.20	0.40
1:A:51:LEU:N	1:A:52:PRO:HD2	2.36	0.40
1:A:238:LYS:HD3	1:A:238:LYS:C	2.46	0.40
2:B:87:ASN:ND2	2:B:103:LYS:CE	2.85	0.40
2:B:355:PHE:CE2	2:B:363:GLU:O	2.74	0.40
2:B:402:GLU:C	2:B:404:THR:N	2.79	0.40
1:C:161:TYR:OH	1:C:163:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ASP:O	1:C:262:GLU:OE2	2.39	0.40
1:E:225:TRP:CD1	1:E:225:TRP:C	2.99	0.40
1:E:497:LEU:O	1:E:498:GLY:C	2.65	0.40
2:F:65:LYS:HE2	2:F:65:LYS:HB3	1.91	0.40
1:G:66:SER:H	1:G:69:ASP:HB2	1.86	0.40
1:G:111:ASN:O	1:G:114:ASP:HB3	2.22	0.40
1:G:158:LEU:HA	1:G:158:LEU:HD13	1.83	0.40
1:G:243:PHE:CE2	1:G:247:ILE:HD11	2.56	0.40
2:H:28:GLY:O	2:H:31:THR:HG22	2.22	0.40
1:A:288:ILE:O	1:A:289:PHE:C	2.64	0.40
1:A:332:MET:O	1:A:333:ILE:C	2.63	0.40
1:C:132:PRO:O	1:C:133:GLU:C	2.65	0.40
1:C:361:VAL:CG1	1:C:375:ILE:HD12	2.51	0.40
1:C:419:PRO:O	1:C:424:VAL:HG11	2.21	0.40
1:C:497:LEU:O	1:C:498:GLY:C	2.64	0.40
1:C:510:THR:C	1:C:512:GLN:N	2.75	0.40
2:D:170:ASP:OD2	2:D:172:SER:HB2	2.21	0.40
2:D:351:GLN:HG2	2:D:352:ASN:N	2.36	0.40
2:D:361:LEU:C	2:D:363:GLU:H	2.29	0.40
1:E:33:VAL:HG12	1:E:34:CYS:N	2.36	0.40
1:E:90:MET:O	1:E:94:GLN:HB2	2.20	0.40
1:E:189:PHE:CE1	1:E:349:LYS:HB2	2.56	0.40
1:G:65:VAL:HG23	1:G:83:LYS:O	2.21	0.40
1:G:84:ASN:CG	1:G:106:GLU:HG3	2.46	0.40
1:G:441:ARG:NH2	1:G:453:ASP:OD2	2.55	0.40
2:H:302:VAL:HG11	2:H:322:LEU:HD23	2.04	0.40
1:A:192:LEU:HD11	1:A:196:PHE:CZ	2.57	0.40
1:A:454:ILE:HG21	1:A:480:HIS:CE1	2.56	0.40
2:B:230:GLU:CD	2:B:233:ARG:NH1	2.79	0.40
2:B:243:PHE:N	2:B:243:PHE:CD1	2.90	0.40
1:C:233:ILE:O	1:C:234:PRO:C	2.62	0.40
1:C:309:ARG:HH11	1:C:309:ARG:HG3	1.86	0.40
2:D:21:LYS:O	2:D:25:GLU:HG3	2.22	0.40
2:D:94:PHE:N	2:D:94:PHE:CD2	2.87	0.40
2:D:325:ASN:HD21	2:D:327:VAL:CG2	2.29	0.40
2:D:355:PHE:CZ	2:D:364:VAL:HA	2.57	0.40
1:E:7:LEU:O	1:E:7:LEU:HD23	2.20	0.40
1:E:229:THR:HG22	1:E:232:ARG:HB2	2.04	0.40
1:E:251:ILE:HG13	1:E:251:ILE:H	1.44	0.40
1:E:510:THR:O	1:E:511:LYS:C	2.64	0.40
2:F:335:PHE:CZ	3:K:144:ILE:HD13	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:351:GLN:HB2	2:F:436:PHE:HD2	1.77	0.40
2:H:166:ASP:C	2:H:168:VAL:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	513/531 (97%)	433 (84%)	64 (12%)	16 (3%)	3	14
1	C	512/531 (96%)	432 (84%)	59 (12%)	21 (4%)	2	10
1	E	511/531 (96%)	447 (88%)	46 (9%)	18 (4%)	3	13
1	G	502/531 (94%)	434 (86%)	54 (11%)	14 (3%)	4	16
2	B	430/434 (99%)	362 (84%)	56 (13%)	12 (3%)	4	16
2	D	429/434 (99%)	347 (81%)	62 (14%)	20 (5%)	2	9
2	F	429/434 (99%)	362 (84%)	51 (12%)	16 (4%)	2	12
2	H	429/434 (99%)	344 (80%)	60 (14%)	25 (6%)	1	6
3	I	81/88 (92%)	71 (88%)	5 (6%)	5 (6%)	1	5
3	J	75/88 (85%)	66 (88%)	7 (9%)	2 (3%)	4	16
3	K	75/88 (85%)	63 (84%)	8 (11%)	4 (5%)	1	7
3	L	76/88 (86%)	60 (79%)	12 (16%)	4 (5%)	1	7
All	All	4062/4212 (96%)	3421 (84%)	484 (12%)	157 (4%)	2	11

All (157) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	LYS
2	B	116	PRO

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Mol	Chain	Res	Type
2	B	127	ILE
2	B	241	GLN
2	B	387	GLY
1	C	253	LYS
2	D	13	TRP
2	D	16	ARG
2	D	41	SER
2	D	92	PHE
2	D	116	PRO
2	D	320	ASN
1	E	253	LYS
1	E	275	ALA
1	E	276	LEU
2	F	116	PRO
2	F	132	ASP
2	F	375	GLN
1	G	276	LEU
2	H	116	PRO
2	H	132	ASP
2	H	242	PRO
2	H	320	ASN
2	H	350	PRO
2	H	377	LYS
2	H	396	SER
3	L	163	GLY
1	A	228	GLU
1	A	336	SER
1	A	367	SER
1	A	450	VAL
3	I	147	GLY
3	I	163	GLY
1	C	36	ILE
1	C	79	SER
1	C	249	GLN
1	C	275	ALA
1	C	451	GLU
2	D	270	GLN
2	D	271	TYR
1	E	195	HIS
1	E	200	ASP
1	E	280	GLN
2	F	320	ASN

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Mol	Chain	Res	Type
1	G	171	VAL
1	G	335	ASP
1	G	451	GLU
1	G	453	ASP
1	G	475	LYS
2	H	88	LEU
2	H	244	GLY
2	H	319	ASN
2	H	362	GLN
2	H	399	SER
2	H	407	ASN
3	L	119	PRO
1	A	90	MET
1	A	106	GLU
1	A	280	GLN
2	B	92	PHE
2	B	133	THR
2	B	313	SER
2	B	403	ARG
3	I	119	PRO
3	I	158	ASP
1	C	121	CYS
1	C	252	LEU
1	C	475	LYS
1	C	518	ASN
2	D	29	PRO
2	D	30	PHE
2	D	237	TRP
2	D	362	GLN
1	E	134	SER
1	E	229	THR
1	E	249	GLN
1	E	264	ASN
1	E	318	GLU
1	E	336	SER
2	F	183	GLU
2	F	232	VAL
2	F	396	SER
2	F	410	LYS
3	K	119	PRO
3	K	152	ASP
1	G	452	GLU

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Mol	Chain	Res	Type
2	H	194	PRO
2	H	232	VAL
2	H	239	LYS
2	H	265	LEU
2	H	345	ALA
2	H	357	PRO
3	L	152	ASP
1	A	79	SER
1	A	198	SER
1	A	230	ASN
1	A	435	PHE
2	B	361	LEU
3	I	146	SER
1	C	72	ASN
1	C	147	GLN
1	C	251	ILE
2	D	34	ASP
2	D	183	GLU
2	D	412	LEU
3	J	163	GLY
1	E	38	ALA
1	E	106	GLU
2	F	88	LEU
2	F	194	PRO
2	F	211	VAL
2	F	216	ALA
2	F	357	PRO
1	G	198	SER
1	G	275	ALA
1	G	387	SER
2	H	31	THR
2	H	374	LEU
2	H	388	LYS
1	A	249	GLN
2	B	242	PRO
1	C	106	GLU
1	C	303	SER
1	C	397	SER
2	D	241	GLN
1	E	190	PRO
2	F	92	PHE
3	K	108	LEU

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Mol	Chain	Res	Type
3	K	175	GLY
1	G	250	GLY
2	H	261	PHE
1	A	372	PRO
2	B	348	GLN
1	C	259	PRO
1	E	221	TYR
1	E	228	GLU
1	G	407	ILE
1	C	109	PRO
2	D	357	PRO
2	F	144	GLY
1	C	407	ILE
2	D	232	VAL
1	E	213	PRO
1	G	423	ILE
2	H	405	ARG
1	C	450	VAL
2	D	211	VAL
1	G	419	PRO
2	H	238	PRO
1	A	333	ILE
1	A	443	PRO
2	B	167	GLY
1	C	60	ILE
2	D	194	PRO
3	L	175	GLY
3	J	119	PRO
2	F	229	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	449/462 (97%)	418 (93%)	31 (7%)	14	38
1	C	448/462 (97%)	422 (94%)	26 (6%)	18	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	448/462 (97%)	418 (93%)	30 (7%)	15	39
1	G	442/462 (96%)	422 (96%)	20 (4%)	24	52
2	B	378/382 (99%)	349 (92%)	29 (8%)	12	35
2	D	378/382 (99%)	350 (93%)	28 (7%)	13	36
2	F	377/382 (99%)	351 (93%)	26 (7%)	14	38
2	H	375/382 (98%)	345 (92%)	30 (8%)	11	33
3	I	73/74 (99%)	64 (88%)	9 (12%)	4	16
3	J	68/74 (92%)	64 (94%)	4 (6%)	18	44
3	K	68/74 (92%)	62 (91%)	6 (9%)	9	30
3	L	68/74 (92%)	67 (98%)	1 (2%)	57	73
All	All	3572/3672 (97%)	3332 (93%)	240 (7%)	15	39

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	A	39	THR
1	A	43	THR
1	A	69	ASP
1	A	72	ASN
1	A	90	MET
1	A	147	GLN
1	A	158	LEU
1	A	165	ILE
1	A	171	VAL
1	A	208	ASP
1	A	214	TRP
1	A	218	ILE
1	A	245	ASP
1	A	251	ILE
1	A	252	LEU
1	A	262	GLU
1	A	264	ASN
1	A	285	ILE
1	A	297	ILE
1	A	335	ASP
1	A	364	LEU
1	A	368	ILE

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Mol	Chain	Res	Type
1	A	395	CYS
1	A	407	ILE
1	A	418	ASN
1	A	422	GLU
1	A	437	LYS
1	A	439	GLN
1	A	458	LYS
1	A	480	HIS
2	B	97	LYS
2	B	116	PRO
2	B	118	CYS
2	B	128	GLN
2	B	132	ASP
2	B	137	GLN
2	B	149	ILE
2	B	154	ILE
2	B	168	VAL
2	B	190	GLN
2	B	197	THR
2	B	217	THR
2	B	218	ILE
2	B	233	ARG
2	B	274	ARG
2	B	316	ILE
2	B	327	VAL
2	B	342	ASN
2	B	349	LEU
2	B	353	ILE
2	B	360	LYS
2	B	363	GLU
2	B	364	VAL
2	B	381	ILE
2	B	382	THR
2	B	392	LEU
2	B	412	LEU
2	B	430	THR
2	B	442	SER
3	I	97	SER
3	I	101	MET
3	I	102	LEU
3	I	105	VAL
3	I	107	THR

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Mol	Chain	Res	Type
3	I	119	PRO
3	I	144	ILE
3	I	170	VAL
3	I	171	LEU
1	C	10	GLU
1	C	34	CYS
1	C	37	ASN
1	C	39	THR
1	C	43	THR
1	C	112	LEU
1	C	171	VAL
1	C	191	GLU
1	C	214	TRP
1	C	251	ILE
1	C	262	GLU
1	C	264	ASN
1	C	274	THR
1	C	277	ASN
1	C	293	ARG
1	C	297	ILE
1	C	311	LEU
1	C	328	THR
1	C	364	LEU
1	C	396	ARG
1	C	418	ASN
1	C	422	GLU
1	C	439	GLN
1	C	492	THR
1	C	497	LEU
1	C	517	ASN
2	D	13	TRP
2	D	33	PRO
2	D	77	VAL
2	D	80	MET
2	D	82	THR
2	D	111	LEU
2	D	113	ASP
2	D	114	ARG
2	D	116	PRO
2	D	125	ASN
2	D	128	GLN
2	D	132	ASP

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Mol	Chain	Res	Type
2	D	142	VAL
2	D	149	ILE
2	D	196	MET
2	D	197	THR
2	D	200	ILE
2	D	201	GLU
2	D	212	ASN
2	D	223	ARG
2	D	316	ILE
2	D	322	LEU
2	D	323	VAL
2	D	362	GLN
2	D	388	LYS
2	D	401	GLU
2	D	437	LYS
2	D	441	THR
3	J	108	LEU
3	J	133	LYS
3	J	155	THR
3	J	162	LEU
1	E	39	THR
1	E	43	THR
1	E	72	ASN
1	E	79	SER
1	E	101	SER
1	E	146	SER
1	E	201	LEU
1	E	211	HIS
1	E	226	TYR
1	E	229	THR
1	E	251	ILE
1	E	253	LYS
1	E	262	GLU
1	E	264	ASN
1	E	265	PHE
1	E	292	ASP
1	E	293	ARG
1	E	297	ILE
1	E	309	ARG
1	E	364	LEU
1	E	368	ILE
1	E	407	ILE

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Mol	Chain	Res	Type
1	E	410	ASP
1	E	422	GLU
1	E	424	VAL
1	E	452	GLU
1	E	497	LEU
1	E	517	ASN
1	E	518	ASN
1	E	533	GLN
2	F	31	THR
2	F	38	SER
2	F	82	THR
2	F	95	ARG
2	F	111	LEU
2	F	114	ARG
2	F	116	PRO
2	F	125	ASN
2	F	128	GLN
2	F	133	THR
2	F	149	ILE
2	F	182	THR
2	F	194	PRO
2	F	212	ASN
2	F	223	ARG
2	F	241	GLN
2	F	292	VAL
2	F	316	ILE
2	F	319	ASN
2	F	322	LEU
2	F	342	ASN
2	F	355	PHE
2	F	361	LEU
2	F	374	LEU
2	F	397	VAL
2	F	430	THR
3	K	101	MET
3	K	107	THR
3	K	115	ILE
3	K	117	ILE
3	K	155	THR
3	K	170	VAL
1	G	33	VAL
1	G	43	THR

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Mol	Chain	Res	Type
1	G	72	ASN
1	G	79	SER
1	G	90	MET
1	G	154	ARG
1	G	186	ASP
1	G	189	PHE
1	G	264	ASN
1	G	285	ILE
1	G	293	ARG
1	G	300	GLN
1	G	311	LEU
1	G	318	GLU
1	G	385	SER
1	G	410	ASP
1	G	492	THR
1	G	497	LEU
1	G	503	GLN
1	G	516	PHE
2	H	14	GLU
2	H	49	CYS
2	H	82	THR
2	H	105	GLU
2	H	111	LEU
2	H	114	ARG
2	H	116	PRO
2	H	128	GLN
2	H	132	ASP
2	H	139	HIS
2	H	154	ILE
2	H	182	THR
2	H	201	GLU
2	H	213	PHE
2	H	224	LEU
2	H	316	ILE
2	H	323	VAL
2	H	325	ASN
2	H	348	GLN
2	H	350	PRO
2	H	360	LYS
2	H	374	LEU
2	H	392	LEU
2	H	402	GLU

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Mol	Chain	Res	Type
2	H	403	ARG
2	H	404	THR
2	H	405	ARG
2	H	406	PRO
2	H	428	VAL
2	H	430	THR
3	L	150	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (150) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	37	ASN
1	A	111	ASN
1	A	147	GLN
1	A	169	HIS
1	A	178	ASN
1	A	197	GLN
1	A	211	HIS
1	A	224	GLN
1	A	264	ASN
1	A	277	ASN
1	A	320	GLN
1	A	359	ASN
1	A	418	ASN
1	A	439	GLN
1	A	480	HIS
1	A	512	GLN
1	A	518	ASN
2	B	19	HIS
2	B	66	ASN
2	B	119	ASN
2	B	137	GLN
2	B	139	HIS
2	B	210	GLN
2	B	212	ASN
2	B	236	GLN
2	B	319	ASN
2	B	325	ASN
2	B	342	ASN
2	B	351	GLN
2	B	389	ASN

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Mol	Chain	Res	Type
2	B	395	GLN
2	B	407	ASN
3	I	149	GLN
1	C	11	GLN
1	C	48	ASN
1	C	94	GLN
1	C	197	GLN
1	C	224	GLN
1	C	230	ASN
1	C	264	ASN
1	C	271	ASN
1	C	320	GLN
1	C	344	ASN
1	C	359	ASN
1	C	418	ASN
1	C	436	HIS
1	C	439	GLN
1	C	447	ASN
1	C	512	GLN
1	C	517	ASN
2	D	18	ASN
2	D	74	GLN
2	D	125	ASN
2	D	128	GLN
2	D	131	ASN
2	D	139	HIS
2	D	210	GLN
2	D	236	GLN
2	D	270	GLN
2	D	282	GLN
2	D	325	ASN
2	D	342	ASN
2	D	348	GLN
2	D	362	GLN
2	D	375	GLN
2	D	421	GLN
2	D	432	GLN
1	E	64	GLN
1	E	72	ASN
1	E	115	ASN
1	E	178	ASN
1	E	197	GLN

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Mol	Chain	Res	Type
1	E	211	HIS
1	E	264	ASN
1	E	271	ASN
1	E	277	ASN
1	E	344	ASN
1	E	359	ASN
1	E	370	GLN
1	E	418	ASN
1	E	436	HIS
1	E	439	GLN
1	E	447	ASN
1	E	466	GLN
1	E	518	ASN
2	F	18	ASN
2	F	19	HIS
2	F	32	HIS
2	F	74	GLN
2	F	125	ASN
2	F	128	GLN
2	F	131	ASN
2	F	139	HIS
2	F	212	ASN
2	F	236	GLN
2	F	241	GLN
2	F	319	ASN
2	F	320	ASN
2	F	325	ASN
2	F	342	ASN
2	F	354	GLN
2	F	362	GLN
2	F	370	ASN
2	F	395	GLN
2	F	407	ASN
3	K	141	GLN
1	G	37	ASN
1	G	64	GLN
1	G	72	ASN
1	G	195	HIS
1	G	197	GLN
1	G	264	ASN
1	G	271	ASN
1	G	277	ASN

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Mol	Chain	Res	Type
1	G	300	GLN
1	G	322	ASN
1	G	343	GLN
1	G	344	ASN
1	G	359	ASN
1	G	366	GLN
1	G	386	ASN
1	G	438	GLN
1	G	439	GLN
1	G	447	ASN
1	G	449	GLN
1	G	527	GLN
2	H	18	ASN
2	H	19	HIS
2	H	32	HIS
2	H	74	GLN
2	H	87	ASN
2	H	119	ASN
2	H	125	ASN
2	H	128	GLN
2	H	131	ASN
2	H	163	ASN
2	H	236	GLN
2	H	258	GLN
2	H	296	ASN
2	H	325	ASN
2	H	348	GLN
2	H	351	GLN
2	H	352	ASN
2	H	354	GLN
2	H	362	GLN
2	H	395	GLN
2	H	407	ASN
3	L	141	GLN
3	L	149	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	517/531 (97%)	-0.11	5 (0%) 79 59	46, 76, 107, 130	0
1	C	516/531 (97%)	-0.02	11 (2%) 63 40	53, 82, 116, 140	0
1	E	515/531 (96%)	-0.24	3 (0%) 85 69	36, 62, 128, 141	0
1	G	508/531 (95%)	-0.11	4 (0%) 82 63	44, 71, 135, 147	0
2	B	432/434 (99%)	-0.07	5 (1%) 76 55	46, 68, 122, 131	0
2	D	431/434 (99%)	0.02	3 (0%) 84 66	47, 85, 118, 131	0
2	F	431/434 (99%)	-0.07	2 (0%) 87 72	41, 70, 121, 134	0
2	H	431/434 (99%)	0.11	7 (1%) 70 47	45, 79, 127, 140	0
3	I	85/88 (96%)	0.05	4 (4%) 36 19	54, 77, 99, 110	0
3	J	77/88 (87%)	0.02	0 100 100	58, 90, 106, 116	0
3	K	77/88 (87%)	-0.07	1 (1%) 75 53	56, 81, 99, 104	0
3	L	78/88 (88%)	0.23	0 100 100	70, 105, 125, 129	0
All	All	4098/4212 (97%)	-0.06	45 (1%) 78 57	36, 76, 122, 147	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	211	VAL	3.8
2	D	320	ASN	3.4
1	C	72	ASN	3.3
1	C	129	THR	3.3
2	D	441	THR	3.1
2	F	374	LEU	3.1
3	I	91	ARG	2.9
1	A	200	ASP	2.8
1	G	212	THR	2.7
2	D	394	LEU	2.7
1	C	518	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	320	ASN	2.7
1	C	259	PRO	2.6
1	C	209	HIS	2.5
1	C	253	LYS	2.5
3	I	99	GLY	2.5
2	B	394	LEU	2.4
1	C	200	ASP	2.4
1	A	209	HIS	2.4
2	F	394	LEU	2.4
1	G	275	ALA	2.3
1	E	211	HIS	2.3
1	C	454	ILE	2.3
1	C	131	LEU	2.3
1	E	200	ASP	2.2
2	H	275	GLY	2.2
3	I	97	SER	2.2
1	G	217	ILE	2.2
2	B	420	GLY	2.2
2	H	441	THR	2.2
1	G	372	PRO	2.2
2	H	238	PRO	2.2
2	H	397	VAL	2.1
2	B	408	LEU	2.1
2	H	365	LEU	2.1
1	E	201	LEU	2.1
1	A	252	LEU	2.1
3	K	139	GLN	2.1
3	I	93	ALA	2.1
2	H	242	PRO	2.1
1	C	6	LYS	2.1
1	A	6	LYS	2.0
1	C	517	ASN	2.0
1	A	160	GLY	2.0
2	H	270	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	F	4	1/1	0.99	0.03	67,67,67,67	0
4	ZN	H	2	1/1	0.99	0.05	84,84,84,84	0
4	ZN	B	1	1/1	1.00	0.03	70,70,70,70	0
4	ZN	D	3	1/1	1.00	0.02	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.