



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:19 PM UTC

PDB ID : 3DBL / pdb\_00003dbl  
Title : Structural Dissection of a Gating Mechanism Preventing Misactivation of Ubiquitin by NEDD8's E1 (APPBP1-UBA3Arg190wt-NEDD8Ala72Gln)  
Authors : Souphron, J.; Schulman, B.A.  
Deposited on : 2008-06-01  
Resolution : 2.90 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](mailto: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>.

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

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

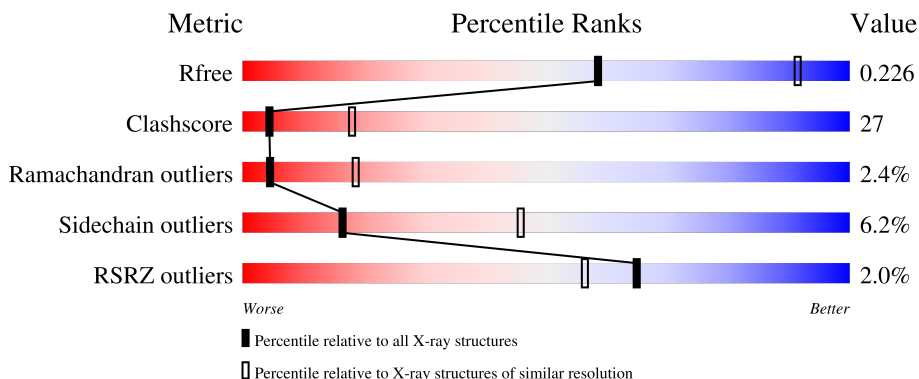
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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  $\geq 3$ , 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	 2% 55% 39% . .
1	C	531	 2% 57% 36% . .
1	E	531	 2% 57% 34% 6% .
1	G	531	 2% 56% 37% . .
2	B	434	 2% 47% 42% 9% .

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Mol	Chain	Length	Quality of chain
2	D	434	<p>3% 53% 42% . .</p>
2	F	434	<p>3% 50% 42% 6% ..</p>
2	H	434	<p>3% 45% 47% 7% ..</p>
3	I	88	<p>3% 53% 39% 6% .</p>
3	J	88	<p>2% 43% 35% 8% 14%</p>
3	K	88	<p>2% 39% 34% 14% 14%</p>
3	L	88	<p>5% 25% 55% 7% 14%</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32577 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
			Total	C	N	O	S			
1	A	522	4138	2621	704	797	16	0	0	0
1	C	520	4125	2612	702	795	16	0	0	0
1	E	521	4119	2609	703	792	15	0	0	0
1	G	518	4113	2605	700	793	15	0	0	0

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
			Total	C	N	O	S			
2	B	432	Total 3404	C 2175	N 577	O 635	S 17	0	0	0
2	D	432	Total 3408	C 2178	N 578	O 635	S 17	0	0	0
2	F	431	Total 3397	C 2172	N 576	O 632	S 17	0	0	0
2	H	431	Total 3389	C 2165	N 575	O 632	S 17	0	0	0

There are 16 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	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	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	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	216	ALA	CYS	engineered mutation	UNP Q8TBC4

- Molecule 3 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	86	668	415	121	130	2	0	0	0
3	J	76	604	380	105	117	2	0	0	0
3	K	76	604	380	105	117	2	0	0	0
3	L	76	604	380	105	117	2	0	0	0

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	GLN	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
J	172	GLN	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	GLN	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	GLN	ALA	engineered mutation	UNP Q15843

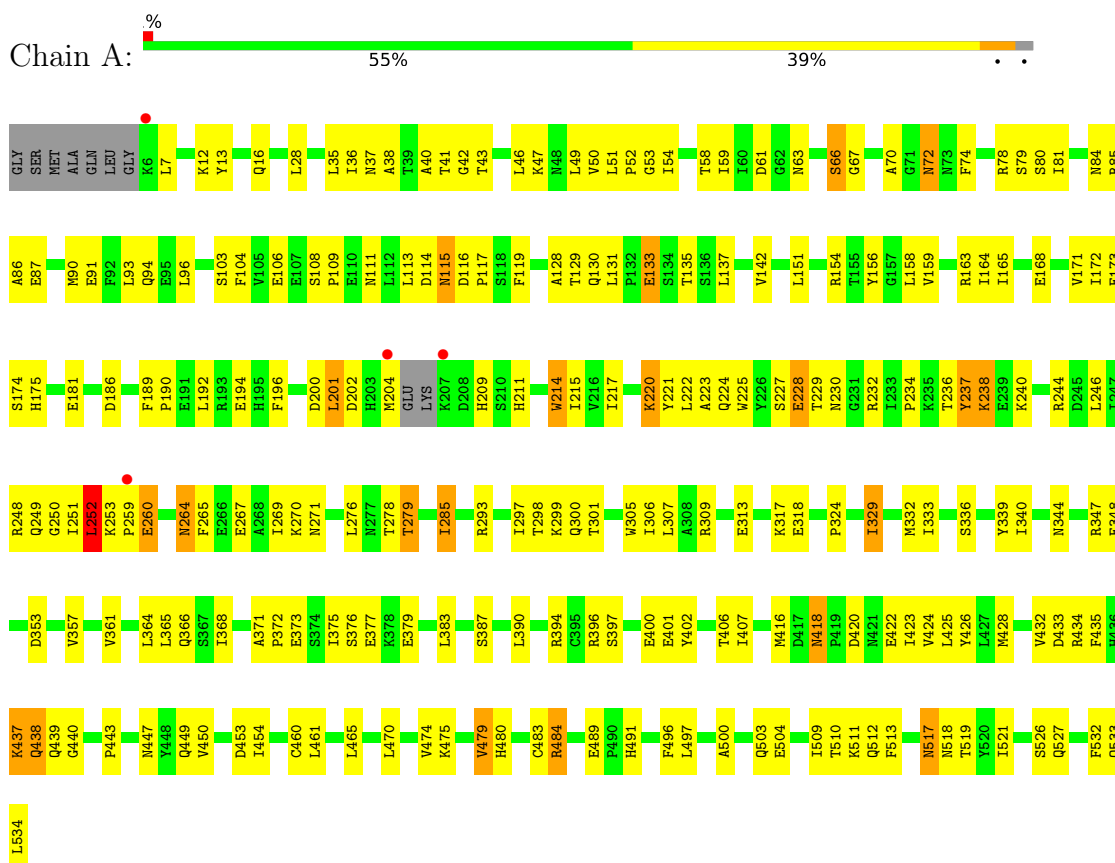
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

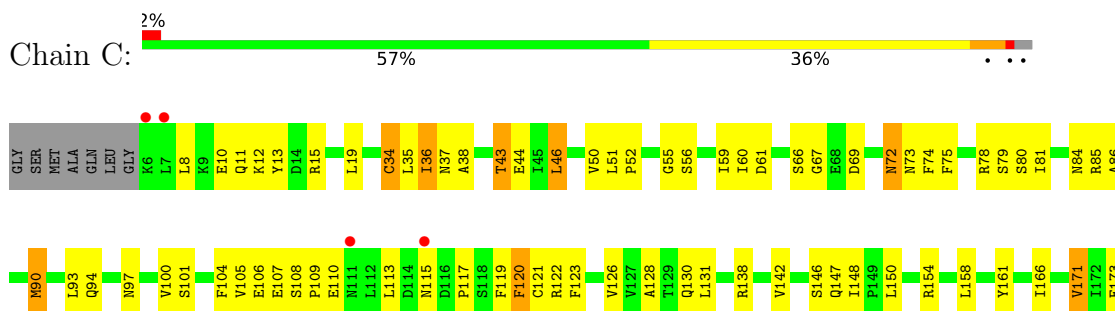
### 3 Residue-property plots [i](#)

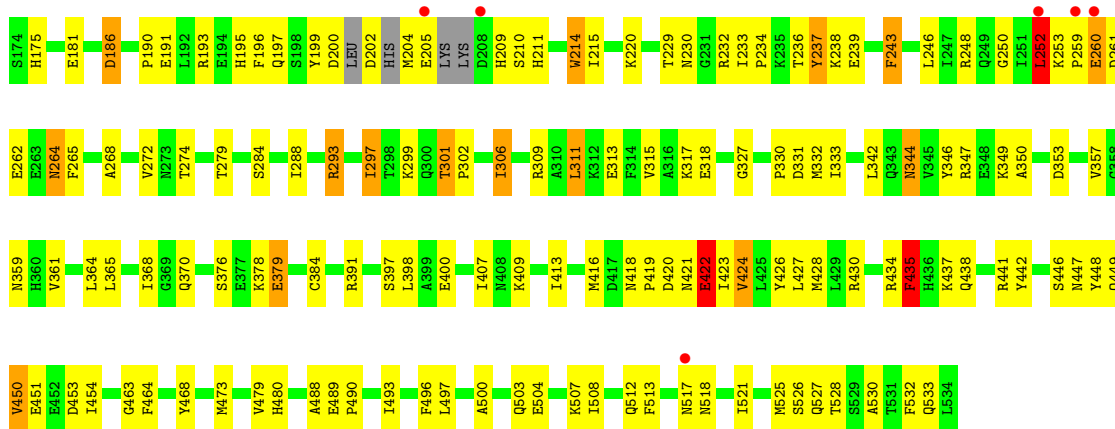
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

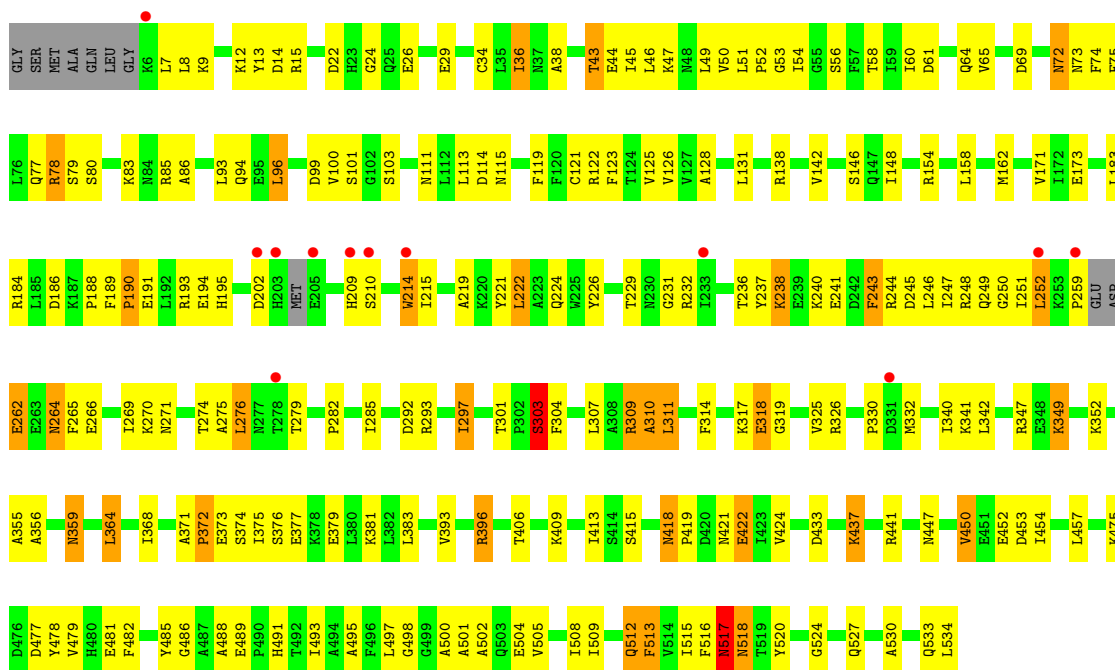


- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

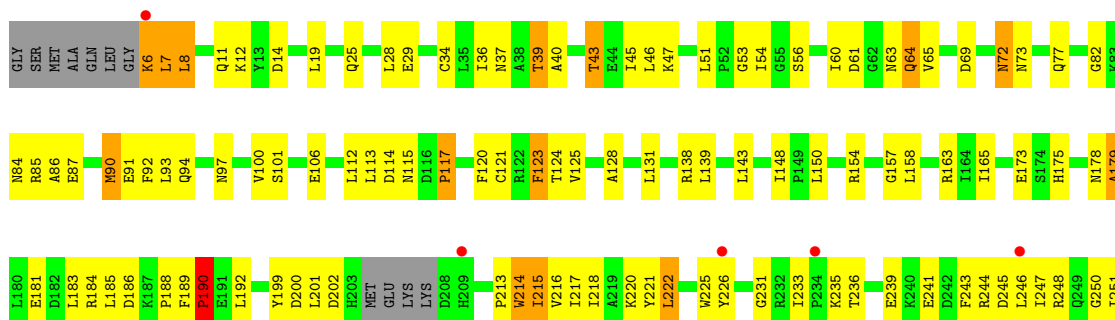


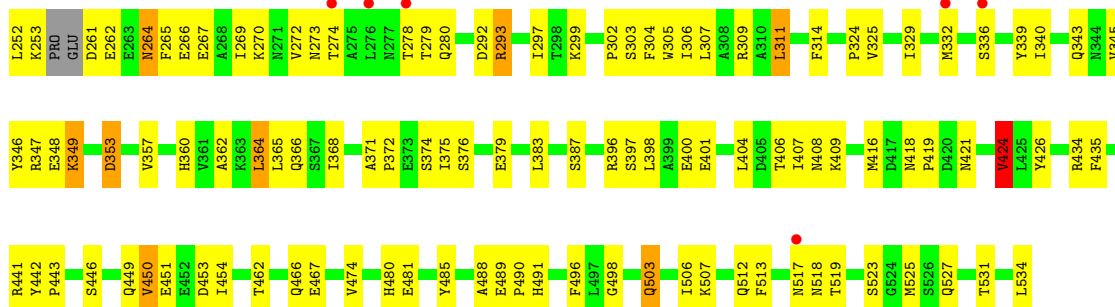


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

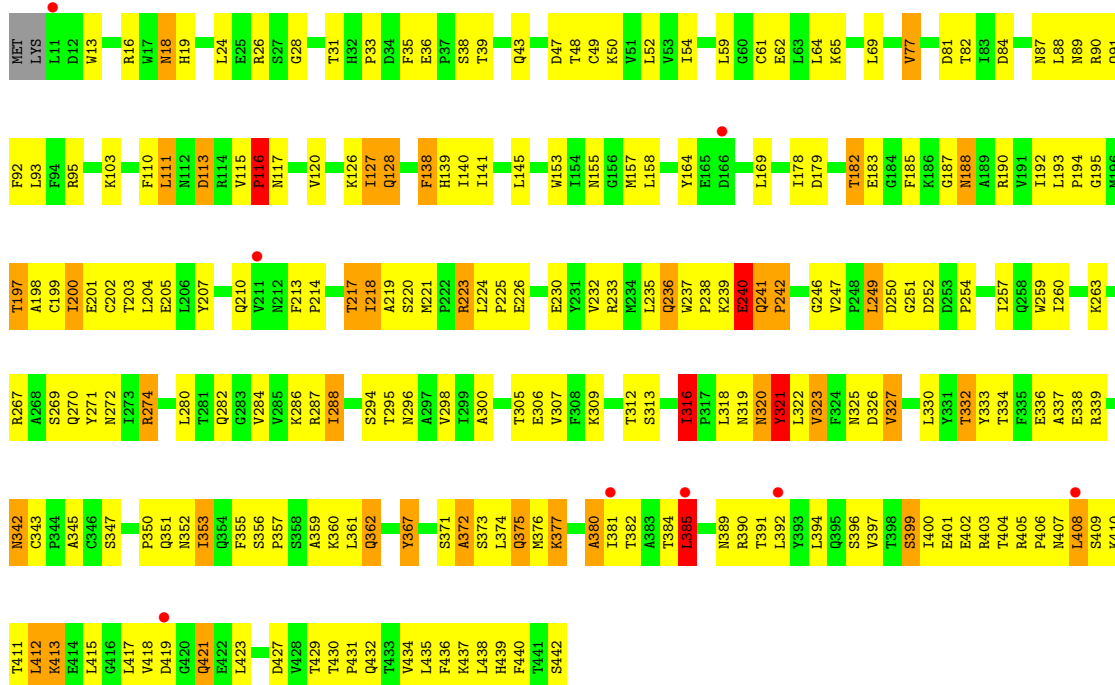


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

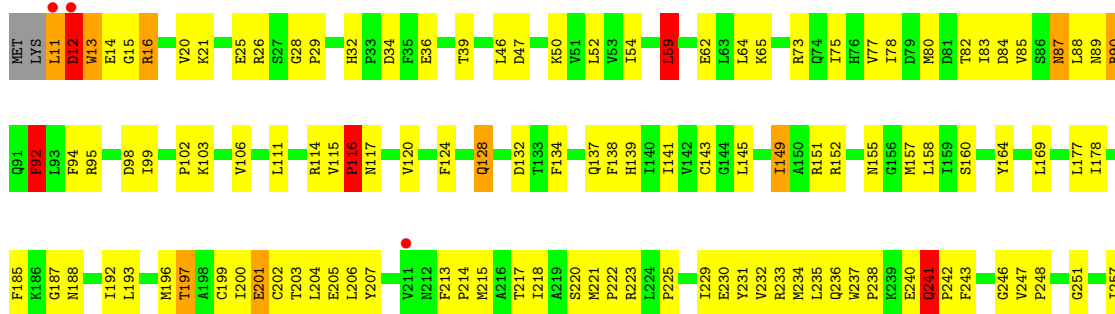


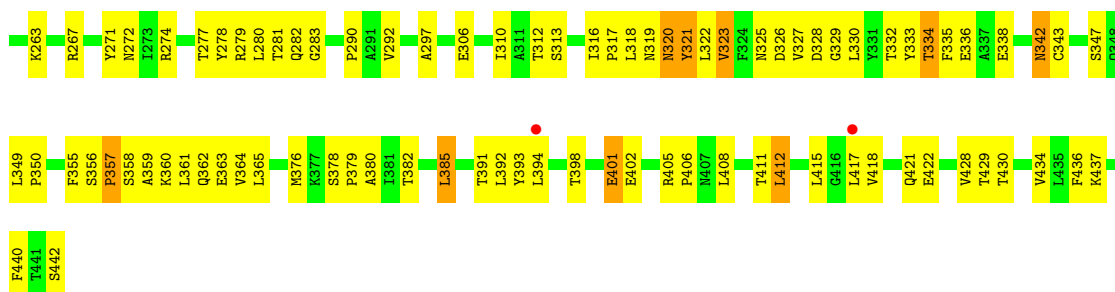


● Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

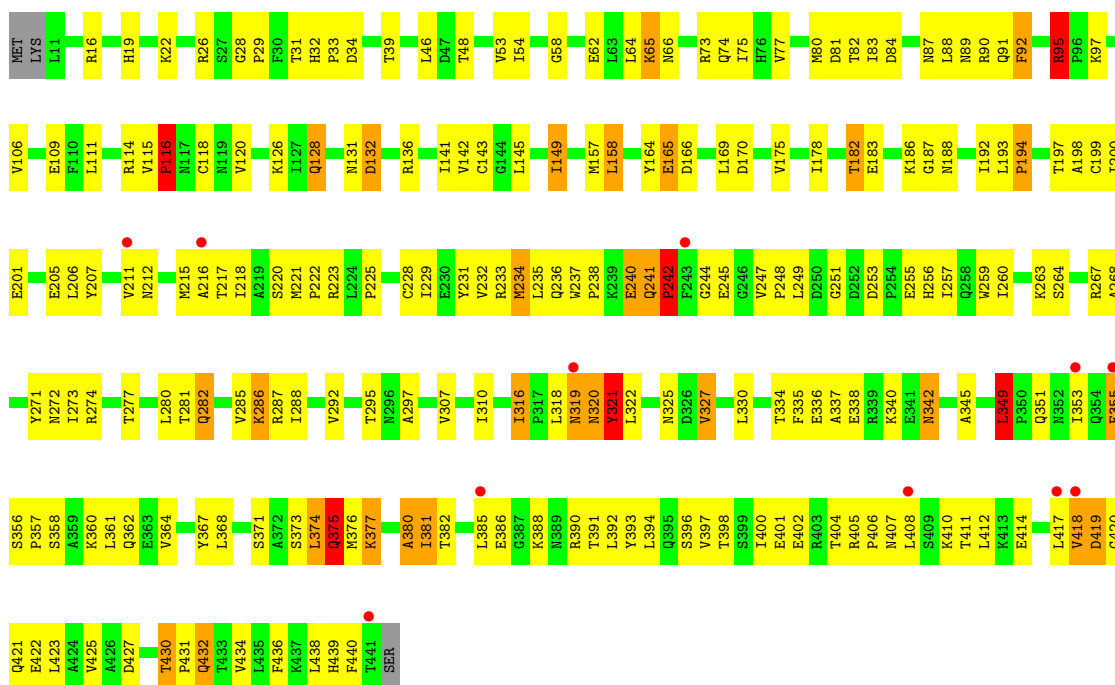


● Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

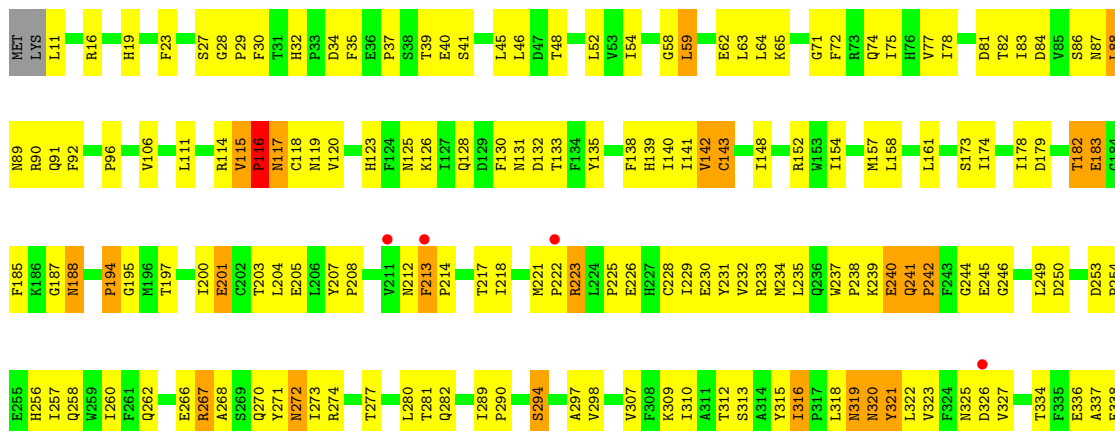


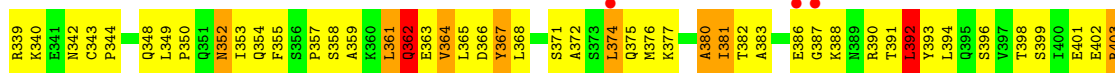


• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit



• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

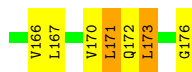




• Molecule 3: NEDD8



• Molecule 3: NEDD8



• Molecule 3: NEDD8



• Molecule 3: NEDD8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.12Å 198.95Å 210.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.2 (50.00-2.90) 92.6 (50.00-2.90)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.91Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.225 , 0.274 0.227 , 0.226	Depositor DCC
$R_{free}$ test set	5854 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.0	Xtrriage
Anisotropy	0.487	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	32577	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.52	0/4218	1.03	24/5706 (0.4%)
1	C	0.50	0/4203	1.01	20/5682 (0.4%)
1	E	0.54	0/4198	1.02	22/5678 (0.4%)
1	G	0.50	0/4191	1.01	14/5668 (0.2%)
2	B	0.58	1/3482 (0.0%)	1.12	25/4738 (0.5%)
2	D	0.54	0/3486	1.07	25/4742 (0.5%)
2	F	0.63	1/3475 (0.0%)	1.15	21/4730 (0.4%)
2	H	0.58	1/3467 (0.0%)	1.10	24/4720 (0.5%)
3	I	0.54	0/673	0.99	2/897 (0.2%)
3	J	0.49	0/609	1.05	5/813 (0.6%)
3	K	0.54	0/609	1.15	7/813 (0.9%)
3	L	0.49	0/609	1.06	5/813 (0.6%)
All	All	0.54	3/33220 (0.0%)	1.06	194/45000 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	380	ALA	CA-CB	-13.00	1.33	1.53
2	B	380	ALA	CA-CB	-7.94	1.40	1.53
2	H	380	ALA	CA-CB	-6.18	1.42	1.53

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	165	GLU	N-CA-C	-14.32	88.48	109.96
2	F	321	TYR	N-CA-C	13.24	126.70	110.41
2	H	321	TYR	N-CA-C	12.50	127.03	110.53
2	B	321	TYR	N-CA-C	12.21	126.42	110.43
1	C	517	ASN	N-CA-C	11.71	124.12	111.36
2	B	240	GLU	N-CA-C	-11.67	91.61	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	241	GLN	CA-C-N	10.91	133.48	119.84
2	B	241	GLN	C-N-CA	10.91	133.48	119.84
2	F	115	VAL	CA-C-N	10.08	132.45	119.84
2	F	115	VAL	C-N-CA	10.08	132.45	119.84
1	A	517	ASN	N-CA-C	9.85	121.97	111.03
2	D	320	ASN	N-CA-C	9.47	124.48	108.67
1	C	378	LYS	N-CA-C	-9.43	102.14	114.31
2	D	59	LEU	N-CA-C	-9.04	101.43	111.28
2	D	12	ASP	N-CA-C	-8.94	91.75	110.80
2	B	385	LEU	N-CA-C	8.78	120.54	110.97
2	B	59	LEU	N-CA-C	-8.70	101.72	111.82
1	G	7	LEU	N-CA-C	-8.58	103.35	113.21
2	B	320	ASN	CB-CA-C	-8.42	106.86	116.63
1	A	7	LEU	N-CA-C	-8.15	103.34	113.20
2	F	81	ASP	N-CA-C	8.09	121.47	110.55
2	H	364	VAL	N-CA-C	-7.98	104.98	112.96
2	H	138	PHE	N-CA-C	7.92	122.91	110.32
2	H	126	LYS	N-CA-C	-7.78	97.95	110.32
1	E	512	GLN	N-CA-C	7.70	122.82	111.96
2	B	320	ASN	N-CA-C	7.60	120.93	108.08
2	H	362	GLN	N-CA-C	-7.59	103.91	113.01
2	D	321	TYR	N-CA-C	7.54	121.68	110.52
1	G	8	LEU	N-CA-C	-7.51	104.25	113.41
1	C	424	VAL	N-CA-C	-7.29	103.68	110.53
2	F	349	LEU	CA-C-N	7.27	128.92	119.84
2	F	349	LEU	C-N-CA	7.27	128.92	119.84
1	E	517	ASN	N-CA-C	7.18	120.50	111.24
2	H	28	GLY	CA-C-N	7.06	127.66	119.47
2	H	28	GLY	C-N-CA	7.06	127.66	119.47
2	B	88	LEU	N-CA-C	7.05	121.33	112.87
1	C	379	GLU	N-CA-C	-6.98	103.72	111.82
2	F	327	VAL	N-CA-C	6.96	117.05	110.30
2	D	28	GLY	CA-C-N	6.94	128.52	119.84
2	D	28	GLY	C-N-CA	6.94	128.52	119.84
2	D	320	ASN	CB-CA-C	-6.93	107.81	117.23
1	A	222	LEU	N-CA-C	-6.90	103.75	111.28
3	K	109	THR	N-CA-C	-6.83	103.37	113.61
1	A	175	HIS	CB-CA-C	-6.83	105.06	111.00
2	D	47	ASP	N-CA-C	6.83	121.94	112.45
2	F	48	THR	N-CA-C	6.79	122.55	113.72
2	F	420	GLY	N-CA-C	-6.78	105.24	115.00
2	H	320	ASN	CB-CA-C	-6.77	108.76	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	173	SER	N-CA-C	-6.75	103.43	112.94
1	C	237	TYR	N-CA-C	-6.71	103.21	111.33
1	C	398	LEU	N-CA-C	-6.71	104.03	111.82
1	A	329	ILE	CA-C-N	-6.64	113.88	120.98
1	A	329	ILE	C-N-CA	-6.64	113.88	120.98
1	G	14	ASP	N-CA-C	6.59	118.47	111.28
3	L	118	GLU	CA-C-N	6.58	128.07	119.84
3	L	118	GLU	C-N-CA	6.58	128.07	119.84
2	H	81	ASP	N-CA-C	6.58	119.02	110.53
2	F	16	ARG	N-CA-C	6.55	118.97	111.11
1	E	450	VAL	N-CA-C	6.53	117.22	110.36
2	D	143	CYS	N-CA-C	6.51	119.76	108.76
2	D	115	VAL	CA-C-N	6.49	127.95	119.84
2	D	115	VAL	C-N-CA	6.49	127.95	119.84
2	H	115	VAL	CA-C-N	6.49	127.95	119.84
2	H	115	VAL	C-N-CA	6.49	127.95	119.84
2	D	155	ASN	N-CA-C	-6.47	104.31	111.36
2	D	241	GLN	CA-C-N	6.47	127.92	119.84
2	D	241	GLN	C-N-CA	6.47	127.92	119.84
1	G	434	ARG	N-CA-C	-6.45	104.33	111.36
2	B	288	ILE	N-CA-C	6.43	117.87	109.58
2	B	412	LEU	N-CA-C	-6.39	105.87	113.21
1	C	435	PHE	N-CA-C	-6.35	104.23	112.23
2	H	320	ASN	N-CA-C	6.31	117.91	108.31
2	B	138	PHE	N-CA-C	6.29	120.31	110.32
1	C	384	CYS	N-CA-C	6.28	118.12	111.28
2	H	294	SER	N-CA-C	6.26	118.66	111.02
2	F	240	GLU	N-CA-C	-6.22	97.42	108.13
1	C	265	PHE	N-CA-C	-6.20	104.60	111.36
2	B	115	VAL	CA-C-N	6.15	127.53	119.84
2	B	115	VAL	C-N-CA	6.15	127.53	119.84
1	G	69	ASP	N-CA-C	-6.14	104.50	111.07
1	G	222	LEU	N-CA-C	-6.14	105.95	113.50
1	E	517	ASN	CA-C-N	-6.12	109.85	121.54
1	E	517	ASN	C-N-CA	-6.12	109.85	121.54
2	F	165	GLU	CB-CA-C	6.12	119.68	109.89
1	C	306	ILE	N-CA-C	-6.09	104.56	110.72
2	H	133	THR	N-CA-C	-6.09	104.56	111.07
1	A	49	LEU	N-CA-C	-6.08	106.50	114.04
1	E	14	ASP	N-CA-C	6.06	117.55	111.07
2	D	329	GLY	N-CA-C	-6.04	102.94	112.61
2	F	285	VAL	N-CA-C	6.02	117.49	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	135	TYR	N-CA-C	6.01	118.62	111.71
1	E	310	ALA	N-CA-C	-5.97	104.46	110.97
3	J	118	GLU	CA-C-N	5.96	127.30	119.84
3	J	118	GLU	C-N-CA	5.96	127.30	119.84
1	E	69	ASP	N-CA-C	-5.89	104.94	111.36
1	A	237	TYR	N-CA-C	-5.88	105.00	111.82
1	A	202	ASP	N-CA-C	-5.88	105.37	113.18
1	C	243	PHE	N-CA-C	-5.86	104.98	111.36
1	E	524	GLY	N-CA-C	-5.86	108.23	114.67
2	B	307	VAL	N-CA-C	-5.83	104.84	110.72
2	D	13	TRP	N-CA-C	5.82	123.20	110.80
2	B	220	SER	N-CA-C	5.78	120.06	112.13
1	E	303	SER	N-CA-C	5.74	118.02	111.02
3	J	134	GLU	N-CA-C	5.73	120.41	112.90
2	D	349	LEU	CA-C-N	5.71	125.72	119.89
2	D	349	LEU	C-N-CA	5.71	125.72	119.89
2	F	367	TYR	N-CA-C	-5.70	104.98	111.14
1	A	119	PHE	N-CA-C	-5.65	105.11	112.23
3	K	134	GLU	N-CA-C	5.64	118.28	111.40
3	L	173	LEU	N-CA-C	5.64	118.92	109.95
1	A	484	ARG	N-CA-C	-5.62	105.15	111.28
2	B	327	VAL	N-CA-C	-5.58	104.49	112.35
1	A	377	GLU	N-CA-C	-5.57	105.36	111.82
2	D	283	GLY	N-CA-C	5.57	119.42	112.73
1	E	349	LYS	N-CA-C	-5.57	105.11	111.07
1	E	96	LEU	N-CA-C	5.55	118.09	111.71
3	K	118	GLU	CA-C-N	5.55	126.77	119.84
3	K	118	GLU	C-N-CA	5.55	126.77	119.84
1	E	396	ARG	N-CA-C	-5.54	102.69	110.50
3	L	120	THR	N-CA-C	5.53	118.82	111.75
1	G	349	LYS	N-CA-C	-5.52	105.26	111.28
2	B	48	THR	N-CA-C	5.51	121.78	114.12
2	B	205	GLU	N-CA-C	5.50	119.98	113.16
2	H	367	TYR	N-CA-C	-5.48	105.33	112.23
2	H	48	THR	N-CA-C	5.47	120.63	113.30
2	H	387	GLY	N-CA-C	-5.46	100.24	113.18
3	I	173	LEU	N-CA-C	5.45	118.37	109.59
2	H	39	THR	N-CA-C	-5.45	106.63	113.28
2	F	419	ASP	N-CA-C	5.44	118.32	109.24
1	A	154	ARG	N-CA-C	5.43	117.22	108.32
2	H	117	ASN	N-CA-C	5.41	118.89	112.72
3	L	174	ARG	N-CA-C	5.40	117.99	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	PHE	N-CA-C	5.40	117.28	109.07
2	B	18	ASN	N-CA-C	5.39	116.84	111.07
2	H	240	GLU	N-CA-C	-5.39	99.32	110.80
1	A	435	PHE	N-CA-C	-5.38	105.11	110.97
1	A	217	ILE	N-CA-C	-5.37	105.48	110.53
2	D	385	LEU	N-CA-C	5.36	119.82	113.12
1	C	442	TYR	CA-C-N	5.36	125.28	119.76
1	C	442	TYR	C-N-CA	5.36	125.28	119.76
3	K	137	PRO	CA-C-N	5.35	126.52	119.84
3	K	137	PRO	C-N-CA	5.35	126.52	119.84
1	E	238	LYS	N-CA-C	-5.34	104.88	111.40
2	H	54	ILE	N-CA-C	5.34	114.06	106.53
1	E	24	GLY	N-CA-C	-5.34	106.32	112.73
1	G	39	THR	N-CA-C	-5.32	103.01	110.35
2	F	95	ARG	N-CA-C	-5.31	102.29	110.58
2	B	408	LEU	N-CA-C	-5.29	106.78	113.18
1	E	222	LEU	N-CA-C	-5.29	105.42	111.14
2	B	179	ASP	N-CA-C	5.28	117.69	108.76
3	J	166	VAL	N-CA-C	5.28	115.56	108.17
1	A	483	CYS	N-CA-C	-5.26	106.00	112.90
1	C	120	PHE	N-CA-C	5.26	118.80	112.38
1	G	374	SER	N-CA-C	-5.25	106.92	113.38
1	C	93	LEU	N-CA-C	-5.25	105.62	112.23
1	G	518	ASN	N-CA-C	5.25	121.97	110.80
2	D	87	ASN	N-CA-C	-5.24	106.21	113.18
1	A	279	THR	N-CA-C	5.22	117.26	108.96
2	H	59	LEU	N-CA-C	-5.22	105.48	111.07
1	G	63	ASN	N-CA-C	5.21	117.26	110.43
1	A	114	ASP	N-CA-C	5.21	116.77	111.14
1	E	512	GLN	CA-C-N	-5.20	113.11	122.15
1	E	512	GLN	C-N-CA	-5.20	113.11	122.15
1	E	243	PHE	N-CA-C	-5.19	106.05	112.38
2	D	20	VAL	N-CA-C	-5.17	106.76	111.67
2	F	282	GLN	N-CA-C	-5.16	105.65	111.28
1	G	406	THR	N-CA-C	5.15	119.66	113.17
2	F	431	PRO	N-CA-C	-5.15	108.02	114.20
3	J	150	MET	N-CA-C	5.12	117.99	110.30
1	A	174	SER	N-CA-C	5.11	119.27	113.19
1	G	424	VAL	CB-CA-C	-5.11	105.43	111.97
1	E	79	SER	N-CA-C	5.11	118.98	112.34
2	D	378	SER	CA-C-N	5.10	125.08	120.03
2	D	378	SER	C-N-CA	5.10	125.08	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	GLU	N-CA-C	-5.09	104.78	111.96
2	B	367	TYR	N-CA-C	-5.09	105.38	111.03
1	G	123	PHE	N-CA-C	5.09	118.36	110.17
2	B	316	ILE	CB-CA-C	-5.08	106.22	110.94
1	A	267	GLU	N-CA-C	-5.07	105.75	111.28
1	A	70	ALA	N-CA-C	-5.07	106.88	113.16
2	D	92	PHE	N-CA-C	5.07	121.59	110.80
1	E	342	LEU	N-CA-C	-5.07	105.85	112.23
1	C	424	VAL	CB-CA-C	-5.05	105.40	112.02
1	A	357	VAL	N-CA-C	-5.04	105.63	110.72
2	B	117	ASN	N-CA-C	5.04	118.91	112.26
2	F	66	ASN	N-CA-C	5.03	116.45	111.07
3	I	94	SER	N-CA-C	5.02	115.94	108.86
1	A	306	ILE	N-CA-C	-5.02	105.60	110.42
1	A	443	PRO	N-CA-C	5.02	118.38	110.80
1	E	8	LEU	N-CA-C	-5.02	105.94	111.71
3	K	153	GLU	N-CA-C	-5.01	108.20	114.56
1	C	301	THR	CA-C-N	5.00	124.91	119.85
1	C	301	THR	C-N-CA	5.00	124.91	119.85
2	F	88	LEU	N-CA-C	5.00	121.45	110.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4138	0	4080	193	0
1	C	4125	0	4065	200	0
1	E	4119	0	4054	212	0
1	G	4113	0	4058	184	0
2	B	3404	0	3385	218	0
2	D	3408	0	3396	186	0
2	F	3397	0	3380	245	0
2	H	3389	0	3359	250	0
3	I	668	0	702	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	604	0	638	38	0
3	K	604	0	638	40	0
3	L	604	0	638	55	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	32577	0	32393	1728	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 27.

All (1728) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:ILE:H	2:D:149:ILE:HD12	1.01	1.14
2:H:359:ALA:HB3	2:H:412:LEU:HD11	1.26	1.13
2:F:149:ILE:HD12	2:F:149:ILE:H	1.15	1.11
3:J:150:MET:HE1	3:J:167:LEU:HD13	1.33	1.08
1:E:184:ARG:HH12	1:E:325:VAL:HG22	1.11	1.07
3:J:143:LEU:HB3	3:J:150:MET:HE3	1.39	1.04
3:J:123:VAL:HB	3:J:152:ASP:HA	1.39	1.04
2:B:382:THR:HG22	2:B:391:THR:HA	1.40	1.03
2:D:149:ILE:H	2:D:149:ILE:CD1	1.72	1.02
2:H:316:ILE:H	2:H:316:ILE:HD12	1.21	1.01
2:F:325:ASN:HD21	2:F:327:VAL:HG23	1.22	1.00
1:E:297:ILE:HB	1:E:368:ILE:HD11	1.40	1.00
2:F:342:ASN:HD22	2:F:342:ASN:H	1.10	0.99
2:F:84:ASP:H	2:F:87:ASN:ND2	1.62	0.97
2:F:316:ILE:HD12	2:F:316:ILE:H	1.27	0.96
2:F:277:THR:HG23	2:F:280:LEU:H	1.30	0.95
3:K:123:VAL:HB	3:K:152:ASP:HA	1.46	0.95
2:H:386:GLU:C	2:H:388:LYS:H	1.74	0.94
1:E:184:ARG:NH1	1:E:325:VAL:HG22	1.81	0.94
2:H:320:ASN:HD22	2:H:336:GLU:C	1.75	0.93
3:L:107:THR:HG23	3:L:109:THR:H	1.34	0.93
2:B:342:ASN:H	2:B:342:ASN:HD22	0.93	0.93
1:C:297:ILE:H	1:C:297:ILE:HD13	1.33	0.93
1:E:252:LEU:O	1:E:259:PRO:HD3	1.69	0.92
2:F:325:ASN:ND2	2:F:327:VAL:HG23	1.84	0.92
2:H:412:LEU:H	2:H:412:LEU:HD12	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:MET:HB3	2:B:427:ASP:OD2	1.70	0.92
1:A:297:ILE:HG22	1:A:368:ILE:HD11	1.52	0.91
2:F:183:GLU:HG3	3:K:173:LEU:HB3	1.52	0.91
2:B:338:GLU:HG3	3:I:148:LYS:HD3	1.51	0.91
3:I:107:THR:HG22	3:I:109:THR:H	1.37	0.90
2:B:418:VAL:HG23	2:B:421:GLN:HG2	1.53	0.90
2:F:361:LEU:HD23	2:F:408:LEU:HA	1.54	0.90
2:B:342:ASN:HD22	2:B:342:ASN:N	1.70	0.89
1:A:365:LEU:HD11	1:A:375:ILE:HD13	1.53	0.89
1:E:447:ASN:HD22	2:F:26:ARG:HH21	1.20	0.89
1:A:236:THR:HG22	1:A:238:LYS:H	1.37	0.89
2:D:149:ILE:HD12	2:D:149:ILE:N	1.86	0.88
2:D:50:LYS:H	2:D:139:HIS:HD2	1.20	0.88
1:A:253:LYS:O	1:A:260:GLU:N	2.07	0.88
2:B:400:ILE:H	2:B:400:ILE:HD12	1.40	0.87
2:H:213:PHE:HB2	2:H:218:ILE:HD11	1.55	0.87
2:H:277:THR:HG23	2:H:280:LEU:H	1.37	0.87
1:C:447:ASN:ND2	2:D:26:ARG:HE	1.73	0.86
2:H:350:PRO:HB2	2:H:437:LYS:HG3	1.57	0.86
1:C:66:SER:HB2	2:H:262:GLN:HE22	1.37	0.85
2:B:355:PHE:O	2:B:440:PHE:HA	1.75	0.85
2:F:412:LEU:HD13	2:F:440:PHE:HE2	1.38	0.85
2:H:132:ASP:HB3	2:H:157:MET:HE1	1.59	0.85
3:L:117:ILE:HD13	3:L:126:ILE:HG12	1.59	0.84
2:F:377:LYS:HE2	2:F:377:LYS:HA	1.58	0.84
2:D:342:ASN:HD22	2:D:342:ASN:H	1.26	0.83
2:H:380:ALA:HB2	2:H:394:LEU:HD12	1.58	0.83
1:E:377:GLU:HG2	1:E:381:LYS:HE3	1.61	0.83
2:F:411:THR:H	2:F:414:GLU:CB	1.91	0.83
2:B:359:ALA:O	2:B:412:LEU:HG	1.79	0.83
2:B:413:LYS:HA	2:B:413:LYS:HE3	1.61	0.83
2:F:380:ALA:CB	2:F:394:LEU:HD12	2.08	0.83
2:B:385:LEU:HD22	2:B:390:ARG:HB3	1.61	0.83
2:F:149:ILE:H	2:F:149:ILE:CD1	1.88	0.83
1:G:527:GLN:HB2	2:H:318:LEU:HD13	1.60	0.83
2:H:62:GLU:HG2	2:H:297:ALA:HA	1.61	0.82
1:E:224:GLN:HE21	1:E:246:LEU:HD11	1.44	0.82
2:F:84:ASP:H	2:F:87:ASN:HD22	1.28	0.82
2:H:320:ASN:HD22	2:H:337:ALA:N	1.77	0.82
2:F:80:MET:HE2	2:F:126:LYS:HB2	1.60	0.81
2:F:362:GLN:HE21	2:F:408:LEU:HD22	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LYS:O	1:C:260:GLU:N	2.13	0.81
2:F:401:GLU:HG3	2:F:402:GLU:HG3	1.61	0.81
2:H:217:THR:HG21	2:H:223:ARG:HH21	1.44	0.81
2:H:338:GLU:HG3	3:L:148:LYS:HD3	1.60	0.81
2:D:359:ALA:O	2:D:412:LEU:HG	1.81	0.81
2:H:229:ILE:HD13	2:H:281:THR:HA	1.62	0.81
2:H:325:ASN:ND2	2:H:327:VAL:HG22	1.95	0.81
1:E:347:ARG:HH12	2:F:274:ARG:HD2	1.46	0.80
2:H:267:ARG:HA	2:H:270:GLN:HE21	1.43	0.80
2:B:13:TRP:HH2	2:B:116:PRO:HG2	1.45	0.80
2:B:407:ASN:OD1	2:B:415:LEU:HD21	1.82	0.80
1:G:183:LEU:HD22	1:G:215:ILE:HD11	1.64	0.80
2:B:418:VAL:HG23	2:B:421:GLN:CG	2.12	0.79
3:J:143:LEU:HB3	3:J:150:MET:CE	2.10	0.79
1:G:36:ILE:HB	1:G:128:ALA:HA	1.62	0.79
1:G:46:LEU:HD23	1:G:93:LEU:HD13	1.62	0.79
2:B:342:ASN:H	2:B:342:ASN:ND2	1.77	0.79
2:F:342:ASN:HD22	2:F:342:ASN:N	1.80	0.79
1:E:518:ASN:HB2	1:E:533:GLN:HA	1.64	0.79
2:D:277:THR:HG23	2:D:280:LEU:H	1.47	0.79
1:G:397:SER:OG	1:G:400:GLU:HG3	1.83	0.79
1:G:37:ASN:HB3	1:G:39:THR:HG23	1.65	0.79
2:D:213:PHE:HB2	2:D:218:ILE:HD11	1.66	0.78
2:F:392:LEU:H	2:F:392:LEU:HD12	1.49	0.78
2:F:411:THR:H	2:F:414:GLU:HB3	1.47	0.78
1:C:299:LYS:HA	1:C:368:ILE:HG23	1.66	0.78
1:E:374:SER:C	1:E:375:ILE:HD12	2.09	0.78
1:G:421:ASN:O	1:G:424:VAL:HG23	1.83	0.78
2:F:418:VAL:HG22	2:F:419:ASP:H	1.49	0.78
2:D:134:PHE:O	2:D:137:GLN:HG2	1.84	0.77
1:C:421:ASN:O	1:C:424:VAL:HG23	1.85	0.77
1:C:43:THR:HG21	1:C:73:ASN:OD1	1.83	0.77
2:H:320:ASN:ND2	2:H:337:ALA:N	2.33	0.77
2:B:188:ASN:OD1	3:I:173:LEU:HD12	1.85	0.76
2:B:240:GLU:O	2:B:241:GLN:HG2	1.85	0.76
1:C:261:ASP:O	1:C:262:GLU:HG3	1.85	0.76
1:E:56:SER:HB3	1:E:101:SER:HB2	1.66	0.76
1:G:340:ILE:HD11	2:H:273:ILE:HG12	1.67	0.76
2:D:325:ASN:HD22	2:D:326:ASP:N	1.84	0.76
1:C:446:SER:HB2	1:C:449:GLN:HG3	1.68	0.76
1:A:347:ARG:HH22	2:B:274:ARG:HH22	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:382:THR:HG22	2:F:391:THR:HA	1.66	0.75
2:F:64:LEU:HD11	2:F:77:VAL:HG21	1.69	0.75
2:B:13:TRP:CH2	2:B:116:PRO:HG2	2.21	0.75
1:C:66:SER:HB2	2:H:262:GLN:NE2	2.02	0.75
2:H:178:ILE:HD11	2:H:310:ILE:HD12	1.69	0.74
2:H:320:ASN:HB2	2:H:336:GLU:HA	1.67	0.74
2:B:325:ASN:HD21	2:B:327:VAL:HG13	1.52	0.74
2:D:193:LEU:H	2:D:197:THR:HG22	1.50	0.74
1:C:416:MET:HE2	1:C:427:LEU:HD12	1.69	0.74
2:D:50:LYS:H	2:D:139:HIS:CD2	2.05	0.74
1:C:202:ASP:N	1:C:204:MET:HB3	2.03	0.74
2:F:54:ILE:CG2	2:F:145:LEU:HD21	2.17	0.74
1:E:262:GLU:HB3	1:E:265:PHE:HB2	1.70	0.74
1:C:347:ARG:NH1	2:D:274:ARG:HD2	2.02	0.73
1:G:307:LEU:HB3	1:G:383:LEU:CD2	2.18	0.73
1:A:36:ILE:HB	1:A:128:ALA:HA	1.70	0.73
1:A:299:LYS:HA	1:A:368:ILE:HG23	1.69	0.73
1:E:317:LYS:HB3	1:E:318:GLU:OE1	1.88	0.73
1:A:229:THR:CG2	1:A:232:ARG:HB3	2.18	0.73
1:G:407:ILE:HG23	1:G:409:LYS:HG3	1.70	0.73
3:L:125:ARG:HG3	3:L:128:GLU:OE1	1.88	0.73
2:B:356:SER:HB3	2:B:442:SER:HB3	1.70	0.73
1:G:61:ASP:HB3	1:G:86:ALA:HB2	1.69	0.73
2:H:323:VAL:HG21	3:L:170:VAL:HG13	1.69	0.73
2:D:237:TRP:HB3	2:D:238:PRO:HD3	1.71	0.73
2:F:421:GLN:HG3	2:F:423:LEU:HD21	1.68	0.73
2:H:386:GLU:C	2:H:388:LYS:N	2.46	0.73
1:A:201:LEU:HD22	1:A:209:HIS:ND1	2.03	0.73
3:J:143:LEU:CB	3:J:150:MET:HE3	2.19	0.73
2:D:357:PRO:HG3	2:D:440:PHE:CG	2.23	0.72
2:F:361:LEU:HD23	2:F:408:LEU:HD23	1.70	0.72
2:H:368:LEU:HB3	2:H:376:MET:HG3	1.70	0.72
2:D:193:LEU:H	2:D:197:THR:CG2	2.02	0.72
2:D:380:ALA:HB1	2:D:394:LEU:HD12	1.68	0.72
3:K:104:LYS:HG2	3:K:114:GLU:HG2	1.71	0.72
2:H:325:ASN:HD21	2:H:327:VAL:HG22	1.52	0.72
2:B:322:LEU:HD23	2:B:322:LEU:C	2.15	0.72
1:E:340:ILE:HG21	2:F:272:ASN:ND2	2.03	0.72
1:G:360:HIS:O	1:G:364:LEU:HB2	1.90	0.72
2:H:380:ALA:CB	2:H:394:LEU:HD12	2.19	0.72
2:F:131:ASN:HB3	2:H:131:ASN:HD22	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:450:VAL:O	1:G:454:ILE:HG13	1.90	0.72
2:B:35:PHE:O	2:B:36:GLU:HG3	1.89	0.72
1:G:226:TYR:OH	1:G:233:ILE:HG22	1.90	0.72
2:H:267:ARG:HH11	2:H:267:ARG:HG3	1.54	0.72
2:D:325:ASN:ND2	2:D:327:VAL:HG22	2.06	0.71
2:B:316:ILE:H	2:B:316:ILE:HD12	1.52	0.71
1:A:518:ASN:HD22	1:A:534:LEU:H	1.36	0.71
1:C:126:VAL:O	1:C:150:LEU:HD12	1.91	0.71
1:E:78:ARG:HG3	1:E:78:ARG:HH11	1.53	0.71
2:F:242:PRO:HG3	2:F:259:TRP:CZ2	2.25	0.71
2:D:320:ASN:HB2	2:D:336:GLU:HA	1.71	0.71
2:B:362:GLN:HB2	2:B:408:LEU:O	1.91	0.71
1:E:251:ILE:HG23	1:E:262:GLU:HB2	1.72	0.71
1:A:437:LYS:HA	1:A:437:LYS:HZ3	1.54	0.70
1:E:491:HIS:NE2	2:F:65:LYS:HE2	2.06	0.70
2:H:234:MET:C	2:H:235:LEU:HD22	2.15	0.70
2:F:32:HIS:CD2	2:F:34:ASP:H	2.08	0.70
1:E:447:ASN:ND2	2:F:26:ARG:HH21	1.88	0.70
1:A:227:SER:C	1:A:229:THR:H	1.99	0.70
1:E:307:LEU:HD13	1:E:383:LEU:HD22	1.73	0.70
1:E:210:SER:HB3	1:E:262:GLU:OE2	1.90	0.70
2:F:237:TRP:HB3	2:F:238:PRO:HD3	1.74	0.70
1:E:72:ASN:HD22	1:E:73:ASN:N	1.89	0.70
2:H:381:ILE:H	2:H:381:ILE:HD12	1.56	0.70
1:C:454:ILE:HD13	1:C:480:HIS:ND1	2.06	0.70
1:G:376:SER:OG	1:G:379:GLU:HG3	1.92	0.70
2:H:320:ASN:HD22	2:H:336:GLU:CA	2.04	0.70
1:C:299:LYS:HA	1:C:368:ILE:CG2	2.22	0.70
1:E:236:THR:HG22	1:E:237:TYR:H	1.57	0.69
2:F:142:VAL:HG21	2:F:307:VAL:HG21	1.71	0.69
1:E:226:TYR:CD1	1:E:231:GLY:HA2	2.26	0.69
1:A:90:MET:HE3	1:A:94:GLN:OE1	1.92	0.69
3:L:155:THR:HG23	3:L:158:ASP:H	1.57	0.69
1:E:186:ASP:OD2	1:E:279:THR:HB	1.92	0.69
1:A:61:ASP:HB3	1:A:86:ALA:HB2	1.75	0.69
2:B:380:ALA:CB	2:B:394:LEU:HD12	2.22	0.69
2:D:380:ALA:CB	2:D:394:LEU:HD12	2.22	0.69
1:E:421:ASN:O	1:E:424:VAL:HG23	1.93	0.68
1:G:332:MET:HG2	1:G:339:TYR:HE1	1.56	0.68
1:E:190:PRO:HG2	1:E:191:GLU:OE2	1.93	0.68
2:F:62:GLU:HG2	2:F:297:ALA:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:LEU:H	2:B:197:THR:HB	1.58	0.68
2:D:151:ARG:HB3	2:D:200:ILE:HD13	1.75	0.68
1:E:236:THR:HG22	1:E:237:TYR:N	2.08	0.68
2:F:201:GLU:HG3	2:F:345:ALA:HB2	1.74	0.68
3:K:116:ASP:C	3:K:117:ILE:HD12	2.18	0.68
1:C:215:ILE:CD1	1:C:332:MET:HE1	2.23	0.68
3:K:107:THR:CG2	3:K:109:THR:H	2.06	0.68
3:K:155:THR:HG22	3:K:158:ASP:CG	2.18	0.68
1:G:246:LEU:HD23	1:G:246:LEU:O	1.93	0.68
2:B:338:GLU:HG3	3:I:148:LYS:CD	2.22	0.68
2:H:250:ASP:HB3	2:H:253:ASP:HB2	1.75	0.68
1:A:437:LYS:HA	1:A:437:LYS:NZ	2.09	0.68
2:F:382:THR:HA	2:F:392:LEU:HD13	1.76	0.68
1:C:397:SER:OG	1:C:400:GLU:HG3	1.93	0.68
2:B:351:GLN:HB3	2:B:436:PHE:CD2	2.28	0.68
1:G:309:ARG:CG	1:G:364:LEU:HD21	2.24	0.68
1:C:293:ARG:HG2	1:C:293:ARG:HH11	1.58	0.68
2:D:16:ARG:NH2	2:D:116:PRO:HB2	2.09	0.68
1:E:226:TYR:CE1	1:E:231:GLY:HA2	2.28	0.68
2:B:237:TRP:HB3	2:B:238:PRO:HD3	1.76	0.67
1:A:61:ASP:OD2	1:A:85:ARG:HD2	1.94	0.67
1:A:264:ASN:HD22	1:A:264:ASN:N	1.91	0.67
2:F:54:ILE:HB	2:F:143:CYS:HB2	1.75	0.67
2:F:425:VAL:HB	2:F:434:VAL:HG13	1.76	0.67
2:B:343:CYS:O	2:B:347:SER:HB3	1.95	0.67
1:E:209:HIS:CD2	1:E:252:LEU:HB2	2.28	0.67
2:H:316:ILE:HD12	2:H:316:ILE:N	2.04	0.67
1:C:317:LYS:HB3	1:C:318:GLU:OE1	1.94	0.67
1:G:481:GLU:HG2	1:G:525:MET:HE1	1.75	0.67
2:B:207:TYR:O	3:I:142:ARG:NH1	2.27	0.67
1:C:347:ARG:NH2	2:D:274:ARG:HE	1.92	0.67
2:D:322:LEU:HD23	2:D:322:LEU:C	2.19	0.67
1:E:309:ARG:HD2	1:E:364:LEU:HD21	1.76	0.67
1:G:340:ILE:HD13	2:H:272:ASN:O	1.95	0.67
1:A:461:LEU:O	1:A:465:LEU:HG	1.95	0.67
1:A:253:LYS:C	1:A:260:GLU:H	2.02	0.67
1:C:61:ASP:OD2	1:C:85:ARG:HD2	1.94	0.67
2:D:73:ARG:HD3	2:D:117:ASN:O	1.94	0.67
2:D:325:ASN:HD21	2:D:327:VAL:HG22	1.59	0.67
1:G:201:LEU:HD21	1:G:220:LYS:HB2	1.77	0.67
2:H:402:GLU:HG3	2:H:405:ARG:HH22	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:102:LEU:HD13	3:L:116:ASP:OD1	1.94	0.67
2:B:217:THR:HB	2:B:223:ARG:NH2	2.11	0.66
2:F:54:ILE:HG22	2:F:145:LEU:HD21	1.76	0.66
3:L:117:ILE:HD11	3:L:126:ILE:HA	1.77	0.66
2:D:360:LYS:HA	2:D:411:THR:HA	1.78	0.66
3:I:103:ILE:CD1	3:I:117:ILE:HD12	2.26	0.66
1:A:173:GLU:O	1:A:512:GLN:O	2.13	0.66
2:B:257:ILE:HD13	2:B:282:GLN:HG2	1.78	0.66
1:C:36:ILE:HG22	1:C:37:ASN:N	2.09	0.66
2:D:355:PHE:HE1	2:D:364:VAL:HA	1.59	0.66
1:E:311:LEU:HD21	1:E:383:LEU:HD11	1.78	0.66
1:E:340:ILE:HG21	2:F:272:ASN:HD21	1.58	0.66
1:E:43:THR:HG21	1:E:73:ASN:OD1	1.96	0.66
1:G:43:THR:HG21	1:G:73:ASN:OD1	1.94	0.66
2:D:241:GLN:NE2	2:D:246:GLY:H	1.93	0.66
2:F:240:GLU:O	2:F:242:PRO:HD3	1.95	0.66
2:F:438:LEU:HD13	2:F:439:HIS:N	2.10	0.66
1:C:311:LEU:O	1:C:315:VAL:HG23	1.96	0.66
1:E:34:CYS:HB2	1:E:123:PHE:CD2	2.31	0.66
1:E:489:GLU:H	2:F:19:HIS:CD2	2.14	0.66
1:C:236:THR:HG22	1:C:238:LYS:H	1.60	0.65
1:E:193:ARG:HG3	1:E:193:ARG:HH11	1.60	0.65
2:H:257:ILE:HD13	2:H:282:GLN:HG2	1.78	0.65
2:F:242:PRO:HG3	2:F:259:TRP:CE2	2.31	0.65
2:H:266:GLU:C	2:H:268:ALA:H	2.03	0.65
2:F:218:ILE:HD13	2:F:234:MET:HE1	1.78	0.65
1:C:297:ILE:H	1:C:297:ILE:CD1	2.07	0.65
2:F:286:LYS:O	2:F:288:ILE:HG13	1.97	0.65
2:D:327:VAL:HG23	2:D:328:ASP:N	2.12	0.65
1:E:297:ILE:HG22	1:E:301:THR:HG21	1.78	0.65
2:F:355:PHE:O	2:F:440:PHE:HA	1.97	0.65
2:D:192:ILE:HA	2:D:197:THR:HG21	1.79	0.65
1:E:22:ASP:O	1:E:26:GLU:HG3	1.97	0.65
2:D:422:GLU:HG2	2:D:437:LYS:HG3	1.77	0.65
3:K:107:THR:HG23	3:K:109:THR:H	1.62	0.65
1:G:236:THR:OG1	1:G:239:GLU:HB2	1.97	0.65
2:B:64:LEU:HB3	2:B:111:LEU:HD22	1.79	0.65
2:D:214:PRO:HB2	2:D:217:THR:HG23	1.79	0.65
1:E:396:ARG:HG3	1:E:396:ARG:HH11	1.62	0.65
2:B:380:ALA:HB1	2:B:394:LEU:HD12	1.79	0.64
2:F:381:ILE:HD12	2:F:381:ILE:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:143:LEU:HD12	1:G:150:LEU:HD22	1.79	0.64
1:C:507:LYS:HG2	1:C:513:PHE:HB2	1.78	0.64
1:E:447:ASN:HD22	2:F:26:ARG:NH2	1.94	0.64
2:B:427:ASP:CG	2:B:429:THR:HG22	2.22	0.64
1:E:184:ARG:HG3	1:E:184:ARG:HH11	1.62	0.64
1:A:133:GLU:HG3	1:A:433:ASP:HB3	1.79	0.64
1:E:240:LYS:NZ	1:E:276:LEU:HD12	2.11	0.64
3:I:170:VAL:CG1	3:I:171:LEU:N	2.60	0.64
2:F:80:MET:HE2	2:F:126:LYS:CB	2.27	0.64
2:F:316:ILE:H	2:F:316:ILE:CD1	2.05	0.64
2:B:153:TRP:CE2	2:B:431:PRO:HG3	2.33	0.64
1:C:236:THR:HB	1:C:239:GLU:HG3	1.79	0.64
2:D:342:ASN:HD22	2:D:342:ASN:N	1.93	0.64
1:C:204:MET:HE1	1:C:252:LEU:HG	1.78	0.64
1:E:377:GLU:O	1:E:381:LYS:HG3	1.97	0.64
1:A:317:LYS:HB3	1:A:318:GLU:OE1	1.98	0.64
2:D:64:LEU:HD21	2:D:77:VAL:CG2	2.28	0.64
2:H:267:ARG:HA	2:H:270:GLN:NE2	2.11	0.64
1:A:137:LEU:HD11	1:A:402:TYR:CD2	2.34	0.63
2:B:357:PRO:HG3	2:B:440:PHE:CD2	2.33	0.63
1:A:344:ASN:HB3	1:E:111:ASN:ND2	2.14	0.63
1:A:371:ALA:C	1:A:373:GLU:H	2.06	0.63
1:G:199:TYR:CD2	1:G:216:VAL:HG11	2.32	0.63
1:A:248:ARG:HH11	1:A:248:ARG:HG3	1.64	0.63
3:I:102:LEU:HD23	3:I:102:LEU:H	1.63	0.63
1:C:72:ASN:H	1:C:72:ASN:HD22	1.44	0.63
1:G:489:GLU:H	2:H:19:HIS:CD2	2.17	0.63
2:H:362:GLN:HA	2:H:408:LEU:HD22	1.80	0.63
1:A:87:GLU:O	1:A:91:GLU:HG3	1.97	0.63
1:C:293:ARG:HG2	1:C:293:ARG:NH1	2.12	0.63
1:C:441:ARG:NH2	1:C:453:ASP:OD1	2.32	0.63
1:G:45:ILE:HG12	1:G:498:GLY:HA2	1.81	0.63
1:G:307:LEU:HB3	1:G:383:LEU:HD22	1.78	0.63
2:B:320:ASN:HB2	2:B:336:GLU:HA	1.80	0.63
2:F:325:ASN:HD21	2:F:327:VAL:CG2	2.04	0.63
2:H:201:GLU:HB3	2:H:343:CYS:SG	2.39	0.63
2:B:214:PRO:HG2	2:B:217:THR:HG23	1.80	0.63
1:C:236:THR:HB	1:C:239:GLU:H	1.63	0.63
1:E:12:LYS:O	2:F:89:ASN:HB3	1.98	0.63
1:E:311:LEU:CD2	1:E:383:LEU:HD11	2.29	0.63
2:H:412:LEU:HD23	2:H:438:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLU:HG3	1:A:394:ARG:HE	1.63	0.63
3:J:170:VAL:HG22	3:J:171:LEU:H	1.63	0.63
2:F:141:ILE:HD12	2:F:158:LEU:HD11	1.80	0.63
1:G:54:ILE:O	1:G:100:VAL:HG13	1.98	0.63
3:L:107:THR:HG22	3:L:111:LYS:N	2.13	0.63
1:A:181:GLU:O	1:A:278:THR:HB	1.98	0.62
2:D:229:ILE:HD13	2:D:281:THR:HA	1.80	0.62
2:H:27:SER:HB3	2:H:37:PRO:CG	2.30	0.62
2:F:398:THR:O	2:F:401:GLU:HG2	1.99	0.62
2:H:377:LYS:HD3	2:H:428:VAL:HG21	1.81	0.62
2:D:185:PHE:HB3	2:D:326:ASP:HB2	1.81	0.62
2:F:362:GLN:NE2	2:F:408:LEU:HD13	2.13	0.62
2:F:381:ILE:HD12	2:F:381:ILE:N	2.14	0.62
1:A:371:ALA:O	1:A:373:GLU:N	2.31	0.62
2:D:327:VAL:HG23	2:D:328:ASP:H	1.63	0.62
1:E:248:ARG:O	1:E:251:ILE:HG13	1.99	0.62
2:D:62:GLU:HG2	2:D:297:ALA:HA	1.82	0.62
3:L:154:LYS:HD2	3:L:159:TYR:OH	1.98	0.62
1:A:209:HIS:CD2	1:A:252:LEU:HD13	2.34	0.62
2:B:81:ASP:HB3	2:B:103:LYS:HE3	1.80	0.62
1:E:184:ARG:HH12	1:E:325:VAL:CG2	2.00	0.62
2:F:131:ASN:HD22	2:H:131:ASN:HB3	1.64	0.62
3:J:155:THR:HG22	3:J:158:ASP:OD2	2.00	0.61
2:F:169:LEU:HD12	2:F:170:ASP:H	1.64	0.61
2:F:229:ILE:HD13	2:F:281:THR:HA	1.82	0.61
1:G:248:ARG:HG3	1:G:248:ARG:HH11	1.65	0.61
1:A:428:MET:HE1	1:A:479:VAL:HA	1.82	0.61
1:A:518:ASN:ND2	1:A:534:LEU:H	1.97	0.61
1:C:115:ASN:O	1:C:117:PRO:HD3	2.00	0.61
2:D:102:PRO:O	2:D:106:VAL:HG23	1.99	0.61
1:G:307:LEU:HB3	1:G:383:LEU:HD21	1.82	0.61
2:D:141:ILE:HD12	2:D:158:LEU:HD21	1.82	0.61
3:J:144:ILE:HD13	3:J:149:GLN:HA	1.81	0.61
1:E:46:LEU:O	1:E:50:VAL:HG23	2.01	0.61
1:E:516:PHE:HB3	2:F:330:LEU:HD12	1.81	0.61
1:G:214:TRP:CD1	1:G:214:TRP:C	2.78	0.61
2:H:132:ASP:HB3	2:H:157:MET:CE	2.29	0.61
1:C:43:THR:HG23	1:C:75:PHE:CD1	2.36	0.61
1:C:268:ALA:O	1:C:272:VAL:HG23	2.00	0.61
3:I:107:THR:CG2	3:I:109:THR:HG23	2.30	0.61
2:F:411:THR:H	2:F:414:GLU:HB2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:381:ILE:HD12	2:H:381:ILE:N	2.16	0.61
2:D:330:LEU:H	2:D:330:LEU:HD12	1.64	0.61
1:E:409:LYS:O	1:E:413:ILE:HG13	2.00	0.61
1:C:229:THR:CG2	1:C:232:ARG:HB2	2.31	0.61
1:C:449:GLN:HB3	1:C:453:ASP:OD2	2.01	0.61
2:B:305:THR:HG22	2:B:309:LYS:NZ	2.15	0.61
2:F:393:TYR:HD1	2:F:404:THR:OG1	1.83	0.61
2:H:402:GLU:C	2:H:404:THR:H	2.09	0.61
1:C:297:ILE:HD13	1:C:297:ILE:N	2.12	0.60
2:D:342:ASN:H	2:D:342:ASN:ND2	1.95	0.60
1:A:307:LEU:HB3	1:A:383:LEU:HD22	1.81	0.60
2:B:413:LYS:HE3	2:B:413:LYS:CA	2.30	0.60
1:C:518:ASN:CB	1:C:533:GLN:HA	2.31	0.60
3:J:124:GLU:HB2	3:J:152:ASP:O	2.01	0.60
1:G:297:ILE:HG21	1:G:368:ILE:HD11	1.84	0.60
2:D:355:PHE:CE1	2:D:364:VAL:HA	2.36	0.60
2:D:50:LYS:N	2:D:139:HIS:HD2	1.93	0.60
2:B:320:ASN:HD22	2:B:336:GLU:C	2.10	0.60
2:B:384:THR:HG23	2:B:384:THR:O	1.99	0.60
2:B:418:VAL:O	2:B:421:GLN:HG3	2.02	0.60
2:D:323:VAL:HG21	3:J:170:VAL:HG23	1.84	0.60
2:F:380:ALA:HB2	2:F:394:LEU:HD12	1.84	0.60
2:B:318:LEU:HD11	2:B:334:THR:CG2	2.32	0.60
2:B:320:ASN:HD22	2:B:337:ALA:N	1.97	0.60
2:D:325:ASN:HD22	2:D:326:ASP:H	1.50	0.60
2:F:249:LEU:HD11	2:F:260:ILE:HD11	1.83	0.60
3:J:105:VAL:HG11	3:J:130:VAL:HG22	1.83	0.60
1:G:266:GLU:HA	1:G:269:ILE:HD12	1.84	0.60
3:L:170:VAL:HG12	3:L:171:LEU:N	2.16	0.60
2:F:385:LEU:HD12	2:F:390:ARG:HG2	1.84	0.60
3:K:124:GLU:HB2	3:K:152:ASP:O	2.01	0.60
1:G:332:MET:HG2	1:G:339:TYR:CE1	2.36	0.60
1:G:454:ILE:HD13	1:G:480:HIS:ND1	2.17	0.60
1:C:138:ARG:O	1:C:142:VAL:HG23	2.02	0.59
2:F:362:GLN:HE21	2:F:408:LEU:CD2	2.15	0.59
2:F:392:LEU:H	2:F:392:LEU:CD1	2.15	0.59
1:G:12:LYS:HG3	2:H:88:LEU:HB2	1.84	0.59
1:G:25:GLN:O	1:G:29:GLU:HG3	2.02	0.59
2:H:143:CYS:HB3	2:H:179:ASP:OD2	2.01	0.59
1:E:240:LYS:HZ2	1:E:276:LEU:HD12	1.67	0.59
2:D:393:TYR:CZ	2:D:408:LEU:HD11	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:54:ILE:HG21	2:F:145:LEU:HD21	1.83	0.59
2:H:438:LEU:HD12	2:H:439:HIS:H	1.67	0.59
1:A:215:ILE:CD1	1:A:332:MET:HE1	2.32	0.59
2:D:157:MET:O	2:D:160:SER:HB3	2.02	0.59
2:F:361:LEU:CD2	2:F:408:LEU:HA	2.29	0.59
1:G:6:LYS:C	1:G:8:LEU:H	2.09	0.59
2:H:207:TYR:CE2	3:L:172:GLN:HG2	2.37	0.59
2:B:405:ARG:HB3	2:B:406:PRO:HD3	1.84	0.59
2:D:128:GLN:NE2	2:D:128:GLN:H	1.99	0.59
2:H:217:THR:CG2	2:H:221:MET:HE3	2.33	0.59
1:C:376:SER:OG	1:C:379:GLU:HG3	2.02	0.59
1:E:229:THR:HG22	1:E:232:ARG:HD2	1.85	0.59
2:F:321:TYR:OH	3:K:172:GLN:HG3	2.01	0.59
1:E:189:PHE:HB2	1:E:190:PRO:HD2	1.85	0.59
2:F:136:ARG:HH11	2:F:136:ARG:HG3	1.68	0.59
2:H:187:GLY:HA2	3:L:173:LEU:HD13	1.85	0.59
2:F:95:ARG:HA	2:F:95:ARG:HE	1.67	0.59
2:F:430:THR:OG1	2:F:432:GLN:HB2	2.03	0.59
1:A:401:GLU:OE2	1:A:534:LEU:HB2	2.02	0.59
1:A:470:LEU:HD12	1:A:470:LEU:O	2.02	0.59
2:B:312:THR:O	2:B:313:SER:HB2	2.03	0.59
1:E:347:ARG:NH1	2:F:274:ARG:HD2	2.16	0.59
2:F:53:VAL:HB	2:F:77:VAL:HG22	1.84	0.59
2:F:236:GLN:HE22	2:F:263:LYS:HD2	1.68	0.59
2:F:368:LEU:HA	2:F:374:LEU:HD11	1.85	0.59
1:G:246:LEU:HD23	1:G:246:LEU:C	2.28	0.59
2:H:222:PRO:O	2:H:273:ILE:HD11	2.02	0.59
1:A:214:TRP:C	1:A:214:TRP:CD1	2.81	0.59
2:H:349:LEU:HB3	2:H:350:PRO:HD2	1.85	0.59
2:B:418:VAL:CG2	2:B:421:GLN:HG2	2.28	0.58
1:G:121:CYS:HA	1:G:148:ILE:HD11	1.85	0.58
1:G:297:ILE:CG2	1:G:368:ILE:HD11	2.33	0.58
2:H:309:LYS:HD3	2:H:315:TYR:HB2	1.85	0.58
3:L:107:THR:HG21	3:L:111:LYS:HB3	1.85	0.58
3:L:126:ILE:O	3:L:130:VAL:HG23	2.03	0.58
1:C:78:ARG:HH12	2:D:11:LEU:HD22	1.68	0.58
2:F:92:PHE:H	2:F:92:PHE:HD2	1.52	0.58
2:B:178:ILE:HD12	2:B:178:ILE:N	2.19	0.58
1:C:447:ASN:HD21	2:D:26:ARG:HE	1.51	0.58
2:D:59:LEU:HB2	3:J:176:GLY:O	2.04	0.58
1:E:447:ASN:ND2	2:F:26:ARG:HE	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:241:GLU:O	1:G:244:ARG:HB2	2.03	0.58
2:H:350:PRO:CB	2:H:437:LYS:HG3	2.31	0.58
1:A:434:ARG:O	1:A:437:LYS:HB3	2.04	0.58
2:D:257:ILE:HG22	2:D:278:TYR:CE1	2.39	0.58
2:F:32:HIS:HD2	2:F:34:ASP:H	1.49	0.58
1:A:61:ASP:CB	1:A:86:ALA:HB2	2.33	0.58
1:C:376:SER:HG	1:C:379:GLU:HG3	1.68	0.58
1:C:422:GLU:HG3	1:C:530:ALA:HB3	1.86	0.58
2:F:197:THR:CG2	2:F:198:ALA:N	2.66	0.58
1:C:215:ILE:HD11	1:C:332:MET:HE1	1.85	0.58
1:E:224:GLN:NE2	1:E:246:LEU:HD11	2.15	0.58
2:F:89:ASN:OD1	2:F:90:ARG:HG2	2.03	0.58
2:B:64:LEU:HB3	2:B:111:LEU:CD2	2.34	0.58
2:B:376:MET:HE1	2:B:434:VAL:HG11	1.86	0.58
1:C:236:THR:CB	1:C:239:GLU:HG3	2.34	0.58
1:E:78:ARG:HG3	1:E:78:ARG:NH1	2.19	0.58
2:H:376:MET:HB3	2:H:427:ASP:OD2	2.04	0.58
1:C:214:TRP:CZ3	1:C:332:MET:HB3	2.39	0.58
2:H:182:THR:O	2:H:183:GLU:HB2	2.04	0.58
2:H:185:PHE:HB3	2:H:326:ASP:HB3	1.86	0.58
2:H:412:LEU:HD22	2:H:440:PHE:CE2	2.38	0.58
3:L:104:LYS:HD3	3:L:112:GLU:OE2	2.03	0.58
1:A:519:THR:HG22	1:A:521:ILE:CD1	2.34	0.58
1:C:423:ILE:HG13	1:C:423:ILE:O	2.02	0.58
1:G:84:ASN:CG	1:G:106:GLU:HG2	2.28	0.58
2:H:253:ASP:HB3	2:H:256:HIS:HB2	1.86	0.58
2:B:356:SER:CB	2:B:442:SER:HB3	2.32	0.57
1:G:61:ASP:CB	1:G:86:ALA:HB2	2.35	0.57
2:H:237:TRP:HB3	2:H:238:PRO:HD3	1.86	0.57
2:B:325:ASN:ND2	2:B:327:VAL:HG13	2.19	0.57
2:B:412:LEU:O	2:B:417:LEU:HB2	2.04	0.57
1:G:114:ASP:HA	1:G:138:ARG:HH22	1.68	0.57
1:A:58:THR:HA	1:A:103:SER:O	2.04	0.57
3:I:104:LYS:HD2	3:I:112:GLU:OE2	2.04	0.57
2:F:410:LYS:HB3	2:F:414:GLU:HB3	1.86	0.57
1:G:267:GLU:O	1:G:270:LYS:HG2	2.04	0.57
1:A:434:ARG:HD3	1:A:460:CYS:HB3	1.86	0.57
1:C:128:ALA:HB1	1:C:131:LEU:HD11	1.86	0.57
2:D:75:ILE:O	2:D:120:VAL:HA	2.04	0.57
2:F:241:GLN:CG	2:F:245:GLU:HA	2.35	0.57
1:A:236:THR:HG22	1:A:238:LYS:N	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:HD22	1:C:46:LEU:HD22	1.85	0.57
1:E:371:ALA:O	1:E:373:GLU:N	2.37	0.57
2:F:182:THR:OG1	2:F:295:THR:HG22	2.04	0.57
1:G:244:ARG:HH11	1:G:244:ARG:HG3	1.68	0.57
2:H:412:LEU:C	2:H:417:LEU:HB2	2.29	0.57
2:B:360:LYS:HA	2:B:411:THR:HA	1.86	0.57
1:E:356:ALA:O	1:E:359:ASN:HB2	2.04	0.57
2:F:405:ARG:HB3	2:F:406:PRO:HD3	1.85	0.57
3:L:105:VAL:HG13	3:L:105:VAL:O	2.04	0.57
1:A:159:VAL:HG22	1:A:425:LEU:HD13	1.86	0.57
2:D:240:GLU:O	2:D:241:GLN:C	2.48	0.57
1:G:185:LEU:O	1:G:188:PRO:HD3	2.04	0.57
2:B:380:ALA:HB1	2:B:394:LEU:CD1	2.33	0.57
1:C:61:ASP:CB	1:C:86:ALA:HB2	2.34	0.57
3:K:117:ILE:HG12	3:K:126:ILE:HG12	1.86	0.57
2:H:320:ASN:ND2	2:H:336:GLU:C	2.56	0.57
2:B:407:ASN:HB3	2:B:415:LEU:HD11	1.86	0.57
2:F:249:LEU:CD1	2:F:260:ILE:HD11	2.34	0.57
1:E:46:LEU:HD23	1:E:93:LEU:HD13	1.87	0.57
1:C:12:LYS:O	2:D:89:ASN:HB3	2.04	0.56
1:C:19:LEU:HD12	2:D:292:VAL:HG13	1.86	0.56
3:K:155:THR:HG22	3:K:158:ASP:OD2	2.05	0.56
1:G:264:ASN:N	1:G:264:ASN:HD22	2.02	0.56
2:H:178:ILE:HD12	2:H:307:VAL:HG22	1.87	0.56
2:B:182:THR:O	3:I:175:GLY:HA3	2.05	0.56
2:F:228:CYS:SG	2:F:268:ALA:HA	2.45	0.56
2:H:217:THR:HG22	2:H:221:MET:HE3	1.87	0.56
2:H:249:LEU:HD13	2:H:260:ILE:HD11	1.87	0.56
1:A:248:ARG:HG3	1:A:248:ARG:NH1	2.20	0.56
2:B:157:MET:HA	2:B:157:MET:HE3	1.88	0.56
1:C:46:LEU:O	1:C:50:VAL:HG23	2.05	0.56
2:F:132:ASP:HB3	2:F:157:MET:HE1	1.87	0.56
2:H:87:ASN:HB3	2:H:91:GLN:CD	2.30	0.56
2:H:368:LEU:HD22	2:H:376:MET:HE2	1.88	0.56
2:H:390:ARG:HH22	2:H:407:ASN:HD21	1.53	0.56
2:H:390:ARG:NH2	2:H:407:ASN:HD21	2.03	0.56
3:L:117:ILE:HD12	3:L:126:ILE:HG23	1.88	0.56
1:A:366:GLN:C	1:A:368:ILE:H	2.12	0.56
1:E:309:ARG:CD	1:E:364:LEU:HD21	2.35	0.56
1:G:184:ARG:HH12	1:G:325:VAL:HG22	1.70	0.56
1:G:264:ASN:HD22	1:G:265:PHE:H	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:412:LEU:HA	2:H:417:LEU:HD12	1.87	0.56
1:A:113:LEU:HD22	1:A:142:VAL:HG21	1.88	0.56
1:A:240:LYS:O	1:A:244:ARG:HG3	2.06	0.56
2:B:270:GLN:HG3	2:B:271:TYR:CD1	2.40	0.56
1:C:115:ASN:C	1:C:117:PRO:HD3	2.29	0.56
2:H:398:THR:O	2:H:401:GLU:HB3	2.06	0.56
2:B:201:GLU:HG3	2:B:345:ALA:HB2	1.86	0.56
1:C:264:ASN:HD22	1:C:264:ASN:N	2.04	0.56
1:G:480:HIS:HB2	2:H:29:PRO:HG2	1.88	0.56
2:H:75:ILE:O	2:H:120:VAL:HA	2.06	0.56
1:A:484:ARG:HG2	1:A:484:ARG:HH11	1.71	0.56
2:D:356:SER:HB2	2:D:442:SER:OG	2.05	0.56
2:F:188:ASN:OD1	3:K:173:LEU:HD12	2.06	0.56
2:H:58:GLY:N	2:H:91:GLN:HG2	2.21	0.56
3:L:117:ILE:HG23	3:L:121:ASP:HB2	1.87	0.56
1:A:78:ARG:C	1:A:80:SER:H	2.13	0.56
1:A:186:ASP:OD2	1:A:279:THR:HB	2.06	0.56
2:B:54:ILE:HG22	2:B:145:LEU:HD21	1.87	0.56
2:B:213:PHE:HB3	2:B:218:ILE:HD13	1.87	0.56
2:B:350:PRO:HG2	2:B:437:LYS:HG3	1.88	0.56
2:B:352:ASN:O	2:B:353:ILE:HD12	2.06	0.56
1:E:243:PHE:O	1:E:247:ILE:HG13	2.06	0.56
1:G:64:GLN:HG2	1:G:82:GLY:O	2.06	0.56
1:G:87:GLU:O	1:G:91:GLU:HG3	2.05	0.56
1:G:307:LEU:HD21	1:G:375:ILE:HG21	1.88	0.56
1:E:500:ALA:HB1	2:F:330:LEU:CD2	2.36	0.56
2:H:218:ILE:HD13	2:H:230:GLU:HG2	1.88	0.56
1:C:489:GLU:HG2	1:C:489:GLU:O	2.05	0.56
2:D:357:PRO:HD2	2:D:442:SER:OG	2.06	0.56
2:H:212:ASN:O	2:H:214:PRO:HD3	2.06	0.56
2:H:354:GLN:HE22	2:H:439:HIS:HB3	1.70	0.56
2:H:382:THR:HA	2:H:392:LEU:HG	1.88	0.56
2:B:430:THR:HG22	2:B:432:GLN:H	1.70	0.55
3:I:123:VAL:HG22	3:I:150:MET:HE2	1.88	0.55
2:F:374:LEU:O	2:F:375:GLN:C	2.49	0.55
3:L:124:GLU:HB2	3:L:152:ASP:O	2.06	0.55
1:A:307:LEU:HD22	1:A:383:LEU:CD2	2.36	0.55
2:B:400:ILE:H	2:B:400:ILE:CD1	2.16	0.55
1:C:36:ILE:HB	1:C:128:ALA:HA	1.87	0.55
1:E:72:ASN:HD22	1:E:72:ASN:C	2.13	0.55
2:F:241:GLN:O	2:F:242:PRO:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ILE:CG2	1:A:368:ILE:HD11	2.30	0.55
2:D:203:THR:O	2:D:205:GLU:N	2.39	0.55
1:G:77:GLN:HG3	1:G:92:PHE:CZ	2.41	0.55
3:L:154:LYS:HD2	3:L:159:TYR:CZ	2.41	0.55
1:E:340:ILE:HD11	2:F:273:ILE:HG12	1.89	0.55
1:G:72:ASN:ND2	1:G:72:ASN:C	2.63	0.55
1:A:307:LEU:HD22	1:A:383:LEU:HD22	1.89	0.55
1:E:56:SER:CB	1:E:101:SER:HB2	2.35	0.55
2:F:28:GLY:O	2:F:31:THR:HG22	2.07	0.55
3:L:170:VAL:CG1	3:L:171:LEU:N	2.70	0.55
1:A:251:ILE:O	1:A:252:LEU:C	2.49	0.55
2:D:128:GLN:H	2:D:128:GLN:HE21	1.55	0.55
1:E:9:LYS:HE3	1:E:99:ASP:OD1	2.06	0.55
1:C:34:CYS:HB2	1:C:123:PHE:CE2	2.42	0.55
3:L:117:ILE:CD1	3:L:126:ILE:HG12	2.32	0.55
2:B:164:TYR:CE2	2:B:169:LEU:HB2	2.42	0.55
1:C:15:ARG:HG3	2:D:90:ARG:NH1	2.22	0.55
1:E:347:ARG:HH22	2:F:274:ARG:NH1	2.04	0.55
2:H:320:ASN:ND2	2:H:336:GLU:CG	2.70	0.55
2:H:362:GLN:O	2:H:362:GLN:NE2	2.39	0.55
1:A:201:LEU:HD13	1:A:209:HIS:CE1	2.42	0.55
3:I:170:VAL:HG13	3:I:171:LEU:H	1.72	0.55
2:H:402:GLU:HG3	2:H:405:ARG:NH2	2.21	0.55
2:B:419:ASP:HB2	2:B:440:PHE:CD1	2.42	0.55
1:E:282:PRO:HB2	1:E:285:ILE:HD13	1.88	0.55
1:C:518:ASN:HB3	1:C:532:PHE:O	2.07	0.54
2:D:187:GLY:HA2	3:J:173:LEU:HD13	1.89	0.54
1:E:61:ASP:HB3	1:E:86:ALA:HB2	1.89	0.54
2:F:64:LEU:HD21	2:F:77:VAL:CG2	2.37	0.54
2:B:353:ILE:HG23	2:B:355:PHE:HD1	1.73	0.54
1:E:513:PHE:N	1:E:513:PHE:CD1	2.74	0.54
1:C:409:LYS:O	1:C:413:ILE:HG13	2.07	0.54
2:D:241:GLN:HE21	2:D:246:GLY:H	1.53	0.54
1:E:307:LEU:HD22	1:E:383:LEU:CD2	2.38	0.54
2:B:187:GLY:HA2	3:I:173:LEU:HD13	1.88	0.54
2:D:158:LEU:HD12	2:D:177:LEU:HD22	1.89	0.54
2:F:319:ASN:O	2:F:320:ASN:HB2	2.07	0.54
2:H:235:LEU:HD22	2:H:235:LEU:N	2.22	0.54
2:H:348:GLN:HB3	2:H:349:LEU:HD12	1.89	0.54
1:C:264:ASN:HD22	1:C:264:ASN:H	1.55	0.54
1:E:505:VAL:O	1:E:509:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:234:MET:HG2	2:F:234:MET:O	2.06	0.54
2:F:404:THR:HA	2:F:407:ASN:HD22	1.71	0.54
3:K:101:MET:HB3	3:K:117:ILE:O	2.07	0.54
1:A:201:LEU:HD23	1:A:204:MET:SD	2.47	0.54
2:B:380:ALA:HB2	2:B:394:LEU:HD12	1.88	0.54
1:C:500:ALA:HB1	2:D:330:LEU:HD21	1.90	0.54
2:D:376:MET:HE1	2:D:434:VAL:HG11	1.89	0.54
2:F:64:LEU:HD21	2:F:77:VAL:HG23	1.89	0.54
1:G:175:HIS:HD2	1:G:512:GLN:O	1.90	0.54
1:G:309:ARG:HG3	1:G:364:LEU:HD21	1.89	0.54
2:H:27:SER:HB3	2:H:37:PRO:HG3	1.88	0.54
2:H:357:PRO:HG3	2:H:440:PHE:CD2	2.42	0.54
1:A:46:LEU:O	1:A:50:VAL:HG23	2.07	0.54
1:C:146:SER:O	1:C:147:GLN:HB2	2.08	0.54
1:E:422:GLU:H	1:E:422:GLU:CD	2.15	0.54
2:F:251:GLY:O	2:F:286:LYS:HD3	2.07	0.54
2:H:417:LEU:HD23	2:H:421:GLN:NE2	2.23	0.54
1:A:53:GLY:O	1:A:54:ILE:C	2.49	0.54
1:C:56:SER:HB3	1:C:101:SER:HB3	1.90	0.54
1:E:72:ASN:C	1:E:72:ASN:ND2	2.65	0.54
1:E:264:ASN:HD22	1:E:265:PHE:H	1.55	0.54
1:E:264:ASN:ND2	1:E:265:PHE:N	2.56	0.54
2:F:425:VAL:HB	2:F:434:VAL:CG1	2.37	0.54
2:H:46:LEU:HD23	2:H:71:GLY:O	2.08	0.54
2:H:392:LEU:HD23	2:H:392:LEU:H	1.73	0.54
2:B:397:VAL:HG12	2:B:399:SER:H	1.72	0.53
1:E:437:LYS:O	1:E:437:LYS:HE3	2.08	0.53
2:F:218:ILE:CD1	2:F:234:MET:HE1	2.37	0.53
2:F:417:LEU:HB3	2:F:421:GLN:OE1	2.08	0.53
1:G:184:ARG:NH1	1:G:325:VAL:HG22	2.23	0.53
1:A:215:ILE:HD12	1:A:332:MET:HE1	1.89	0.53
1:A:518:ASN:HB3	1:A:532:PHE:O	2.08	0.53
2:D:225:PRO:HB2	2:D:280:LEU:HD21	1.89	0.53
2:F:183:GLU:HB2	3:K:173:LEU:HD22	1.89	0.53
1:A:74:PHE:CD1	2:B:65:LYS:HG3	2.43	0.53
2:B:49:CYS:HA	2:B:139:HIS:HD2	1.71	0.53
1:C:72:ASN:ND2	1:C:73:ASN:N	2.56	0.53
3:J:125:ARG:HD3	3:J:129:ARG:NH2	2.23	0.53
1:E:188:PRO:HG2	1:E:193:ARG:NH2	2.23	0.53
1:G:488:ALA:C	1:G:490:PRO:HD3	2.33	0.53
2:H:322:LEU:C	2:H:322:LEU:HD23	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:PRO:HG2	2:B:217:THR:CG2	2.38	0.53
2:D:16:ARG:HH22	2:D:116:PRO:HB2	1.72	0.53
1:E:450:VAL:O	1:E:454:ILE:HG13	2.08	0.53
1:A:423:ILE:O	1:A:426:TYR:HB3	2.09	0.53
2:B:235:LEU:O	2:B:238:PRO:HD2	2.09	0.53
2:B:323:VAL:HG23	2:B:333:TYR:HB3	1.89	0.53
3:I:122:LYS:HA	3:I:155:THR:HA	1.91	0.53
2:F:197:THR:HG22	2:F:198:ALA:N	2.23	0.53
1:C:368:ILE:O	1:C:368:ILE:HG22	2.07	0.53
1:E:162:MET:HE1	1:E:501:ALA:HA	1.91	0.53
2:F:74:GLN:NE2	2:F:74:GLN:HA	2.23	0.53
2:F:178:ILE:HD11	2:F:310:ILE:CD1	2.39	0.53
2:H:88:LEU:HD13	2:H:96:PRO:HG3	1.91	0.53
2:H:267:ARG:HH11	2:H:267:ARG:CG	2.21	0.53
1:A:227:SER:O	1:A:229:THR:N	2.37	0.53
2:B:320:ASN:ND2	2:B:337:ALA:O	2.41	0.53
1:C:66:SER:H	1:C:69:ASP:HB2	1.74	0.53
1:C:214:TRP:CE3	1:C:332:MET:HB3	2.44	0.53
1:C:447:ASN:ND2	2:D:26:ARG:NE	2.53	0.53
1:E:325:VAL:HG21	1:E:349:LYS:HG3	1.90	0.53
2:F:386:GLU:C	2:F:388:LYS:H	2.17	0.53
2:H:405:ARG:HB3	2:H:405:ARG:HH11	1.74	0.53
1:A:248:ARG:C	1:A:250:GLY:H	2.17	0.53
1:C:209:HIS:NE2	1:C:252:LEU:HD23	2.24	0.53
1:G:201:LEU:HD22	1:G:221:TYR:HE1	1.73	0.53
2:H:32:HIS:HD2	2:H:34:ASP:H	1.57	0.53
2:B:411:THR:C	2:B:413:LYS:H	2.17	0.53
1:E:347:ARG:HH22	2:F:274:ARG:HH11	1.57	0.53
1:G:213:PRO:HB3	1:G:332:MET:SD	2.49	0.53
2:H:32:HIS:CD2	2:H:34:ASP:H	2.25	0.53
2:B:381:ILE:CG2	2:B:423:LEU:HD22	2.39	0.52
2:D:412:LEU:O	2:D:415:LEU:HD12	2.10	0.52
2:F:95:ARG:HG3	2:F:97:LYS:NZ	2.24	0.52
3:K:123:VAL:HG22	3:K:150:MET:HE2	1.91	0.52
1:G:503:GLN:NE2	2:H:185:PHE:CE2	2.77	0.52
2:H:325:ASN:HD22	2:H:326:ASP:H	1.56	0.52
1:A:189:PHE:CE1	1:A:192:LEU:HB2	2.44	0.52
1:C:518:ASN:HB2	1:C:533:GLN:HA	1.90	0.52
2:D:405:ARG:HB3	2:D:405:ARG:NH1	2.23	0.52
2:F:376:MET:HE2	2:F:427:ASP:HB2	1.91	0.52
2:F:380:ALA:HB1	2:F:394:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:231:TYR:CD2	2:H:267:ARG:HG2	2.44	0.52
2:H:413:LYS:C	2:H:415:LEU:H	2.16	0.52
1:A:418:ASN:HD22	1:A:418:ASN:C	2.17	0.52
1:E:377:GLU:CG	1:E:381:LYS:HE3	2.37	0.52
1:A:366:GLN:C	1:A:368:ILE:N	2.67	0.52
1:C:438:GLN:O	1:C:438:GLN:HG2	2.08	0.52
1:E:49:LEU:O	1:E:52:PRO:HG2	2.10	0.52
3:K:118:GLU:O	3:K:120:THR:N	2.43	0.52
1:G:124:THR:HG22	1:G:125:VAL:HG23	1.90	0.52
1:A:450:VAL:O	1:A:454:ILE:HG13	2.09	0.52
2:B:183:GLU:HG3	3:I:173:LEU:HB3	1.91	0.52
1:C:434:ARG:HH11	1:C:464:PHE:HA	1.74	0.52
1:E:222:LEU:O	1:E:226:TYR:HB3	2.09	0.52
2:H:228:CYS:SG	2:H:268:ALA:HA	2.48	0.52
1:A:66:SER:OG	1:A:67:GLY:N	2.43	0.52
2:B:326:ASP:HB3	2:B:330:LEU:HD23	1.91	0.52
1:C:61:ASP:HB3	1:C:86:ALA:HB2	1.91	0.52
2:D:64:LEU:HD21	2:D:77:VAL:HG22	1.91	0.52
2:D:330:LEU:HD12	2:D:330:LEU:N	2.25	0.52
2:D:411:THR:O	2:D:415:LEU:HG	2.09	0.52
1:E:45:ILE:HG12	1:E:498:GLY:HA2	1.92	0.52
1:E:65:VAL:HG22	1:E:85:ARG:HG3	1.91	0.52
2:F:316:ILE:HD12	2:F:316:ILE:N	2.10	0.52
2:H:178:ILE:HD12	2:H:307:VAL:CG2	2.39	0.52
2:B:182:THR:HG21	2:B:296:ASN:OD1	2.10	0.52
1:C:121:CYS:HA	1:C:148:ILE:HD11	1.92	0.52
2:D:306:GLU:CD	2:D:318:LEU:H	2.17	0.52
1:E:504:GLU:O	1:E:508:ILE:HG13	2.09	0.52
1:G:115:ASN:O	1:G:117:PRO:HD3	2.10	0.52
2:H:440:PHE:O	2:H:441:THR:HG23	2.09	0.52
2:B:321:TYR:HH	3:I:172:GLN:CD	2.17	0.52
2:B:361:LEU:HB3	2:B:407:ASN:O	2.10	0.52
2:D:251:GLY:O	2:D:257:ILE:HD11	2.10	0.52
2:H:240:GLU:O	2:H:242:PRO:HD3	2.09	0.52
2:H:267:ARG:HG3	2:H:267:ARG:O	2.10	0.52
1:A:196:PHE:O	1:A:220:LYS:HE2	2.10	0.52
2:D:178:ILE:HD11	2:D:310:ILE:HD12	1.92	0.52
2:F:282:GLN:O	2:F:286:LYS:HG3	2.10	0.52
1:G:158:LEU:HD22	1:G:158:LEU:N	2.24	0.52
1:G:262:GLU:HB2	1:G:265:PHE:HB2	1.91	0.52
2:H:123:HIS:HB3	2:H:125:ASN:HD22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ASN:ND2	1:A:420:ASP:H	2.08	0.52
1:A:428:MET:CE	1:A:479:VAL:HA	2.39	0.52
2:B:61:CYS:HB3	2:B:93:LEU:HG	1.91	0.52
3:I:117:ILE:HD11	3:I:126:ILE:HG23	1.91	0.52
1:C:72:ASN:HD22	1:C:73:ASN:N	2.08	0.52
2:H:249:LEU:HA	2:H:256:HIS:ND1	2.24	0.52
2:H:266:GLU:C	2:H:268:ALA:N	2.68	0.52
1:E:47:LYS:HG2	1:E:96:LEU:HD11	1.92	0.51
2:H:52:LEU:HD11	2:H:78:ILE:HG13	1.91	0.51
3:L:161:ILE:HG23	3:L:165:SER:OG	2.10	0.51
2:B:197:THR:HG22	2:B:198:ALA:O	2.10	0.51
1:C:357:VAL:O	1:C:361:VAL:HG23	2.09	0.51
2:H:354:GLN:NE2	2:H:354:GLN:HA	2.25	0.51
1:A:224:GLN:NE2	1:A:246:LEU:HD11	2.25	0.51
2:B:427:ASP:OD1	2:B:429:THR:HG22	2.10	0.51
1:E:36:ILE:HG21	1:E:131:LEU:HD21	1.91	0.51
3:K:104:LYS:HD2	3:K:112:GLU:OE2	2.10	0.51
1:G:441:ARG:HH22	1:G:453:ASP:CG	2.18	0.51
2:H:16:ARG:NH2	2:H:116:PRO:HB2	2.25	0.51
1:A:298:THR:C	1:A:300:GLN:H	2.18	0.51
2:B:81:ASP:CB	2:B:103:LYS:HE3	2.40	0.51
1:E:158:LEU:HA	1:E:493:ILE:HG12	1.93	0.51
2:F:199:CYS:SG	2:F:201:GLU:HB2	2.51	0.51
2:H:233:ARG:HG2	2:H:233:ARG:HH11	1.75	0.51
2:B:188:ASN:HD22	2:B:188:ASN:C	2.18	0.51
1:C:51:LEU:N	1:C:52:PRO:HD2	2.25	0.51
1:E:376:SER:OG	1:E:379:GLU:HG2	2.10	0.51
2:F:259:TRP:CH2	2:F:263:LYS:HG3	2.45	0.51
1:A:253:LYS:C	1:A:260:GLU:N	2.60	0.51
2:B:232:VAL:HA	2:B:236:GLN:HB2	1.93	0.51
2:B:353:ILE:HG22	2:B:438:LEU:HD12	1.91	0.51
2:D:87:ASN:HD21	2:D:103:LYS:HE2	1.76	0.51
2:D:319:ASN:ND2	2:D:336:GLU:HG3	2.25	0.51
1:E:162:MET:CE	1:E:501:ALA:HA	2.41	0.51
2:F:75:ILE:O	2:F:120:VAL:HA	2.11	0.51
1:A:527:GLN:HG3	2:B:306:GLU:OE1	2.09	0.51
2:B:267:ARG:HA	2:B:270:GLN:HE21	1.76	0.51
2:B:353:ILE:HD11	2:B:367:TYR:HE2	1.74	0.51
1:C:130:GLN:HA	1:C:154:ARG:HD2	1.92	0.51
1:C:430:ARG:HB3	1:C:430:ARG:HH11	1.75	0.51
2:D:418:VAL:HG22	2:D:421:GLN:CD	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:LEU:HB3	1:E:383:LEU:CD2	2.41	0.51
2:F:232:VAL:HG11	2:F:263:LYS:HB2	1.93	0.51
1:A:163:ARG:HG2	1:A:163:ARG:HH11	1.76	0.51
2:D:361:LEU:HD21	2:D:392:LEU:HB3	1.93	0.51
2:D:393:TYR:CE2	2:D:408:LEU:HD11	2.45	0.51
3:J:115:ILE:HG23	3:J:129:ARG:HB3	1.92	0.51
1:E:264:ASN:HD22	1:E:264:ASN:N	2.07	0.51
2:F:398:THR:C	2:F:401:GLU:HG2	2.36	0.51
2:F:411:THR:N	2:F:414:GLU:HB3	2.22	0.51
1:A:225:TRP:CE2	1:A:234:PRO:HG3	2.46	0.51
1:A:416:MET:HE1	1:A:424:VAL:HG22	1.93	0.51
1:C:430:ARG:HB3	1:C:430:ARG:NH1	2.25	0.51
2:D:84:ASP:O	2:D:87:ASN:HB2	2.10	0.51
2:H:354:GLN:HA	2:H:354:GLN:HE21	1.76	0.51
1:A:454:ILE:HD13	1:A:480:HIS:CD2	2.45	0.51
1:C:229:THR:HG21	1:C:232:ARG:HB2	1.92	0.51
1:C:293:ARG:HH11	1:C:293:ARG:CG	2.24	0.51
1:E:352:LYS:O	1:E:355:ALA:HB3	2.10	0.51
2:F:231:TYR:CE2	2:F:267:ARG:HD3	2.46	0.51
1:G:53:GLY:O	1:G:54:ILE:C	2.54	0.51
1:G:336:SER:HB2	2:H:221:MET:HA	1.93	0.51
2:H:84:ASP:H	2:H:87:ASN:ND2	2.08	0.51
2:H:197:THR:CG2	2:H:320:ASN:OD1	2.59	0.51
1:A:474:VAL:O	1:A:475:LYS:C	2.54	0.50
1:C:435:PHE:C	1:C:435:PHE:CD2	2.88	0.50
1:E:264:ASN:HD22	1:E:265:PHE:N	2.09	0.50
2:F:349:LEU:CD1	2:F:349:LEU:H	2.24	0.50
3:L:104:LYS:O	3:L:166:VAL:HA	2.11	0.50
1:C:84:ASN:OD1	1:C:106:GLU:HG2	2.11	0.50
1:C:528:THR:HG22	2:D:334:THR:OG1	2.11	0.50
2:D:141:ILE:CD1	2:D:158:LEU:HD21	2.41	0.50
3:J:138:PRO:O	3:J:141:GLN:HB2	2.11	0.50
1:E:74:PHE:CD1	2:F:65:LYS:HG3	2.45	0.50
1:G:407:ILE:HG13	1:G:408:ASN:N	2.26	0.50
1:G:441:ARG:NH2	1:G:453:ASP:OD2	2.43	0.50
1:A:13:TYR:O	1:A:16:GLN:HG2	2.12	0.50
1:A:108:SER:HB3	1:A:111:ASN:HB2	1.92	0.50
1:A:116:ASP:N	1:A:117:PRO:HD3	2.26	0.50
1:A:376:SER:OG	1:A:379:GLU:HG3	2.11	0.50
2:B:64:LEU:HD21	2:B:77:VAL:HG22	1.92	0.50
3:I:139:GLN:O	3:I:142:ARG:NH2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:GLY:H	2:H:262:GLN:NE2	2.09	0.50
1:C:67:GLY:H	2:H:262:GLN:HE22	1.59	0.50
2:H:223:ARG:HH11	2:H:223:ARG:HG3	1.76	0.50
3:L:107:THR:CG2	3:L:111:LYS:HB3	2.41	0.50
1:A:35:LEU:HD21	1:A:42:GLY:C	2.37	0.50
1:C:407:ILE:HG23	1:C:409:LYS:HG3	1.93	0.50
2:D:357:PRO:HG3	2:D:440:PHE:CD1	2.46	0.50
2:F:241:GLN:HG3	2:F:245:GLU:HA	1.94	0.50
2:H:376:MET:HE3	2:H:425:VAL:HG11	1.93	0.50
1:A:38:ALA:HB2	1:A:59:ILE:HG21	1.93	0.50
1:C:214:TRP:CD1	1:C:215:ILE:N	2.79	0.50
1:E:241:GLU:OE1	1:E:244:ARG:HD2	2.12	0.50
1:G:90:MET:HE3	1:G:94:GLN:OE1	2.12	0.50
3:L:105:VAL:HG23	3:L:167:LEU:HB2	1.92	0.50
1:A:204:MET:O	1:A:209:HIS:HB2	2.11	0.50
2:B:251:GLY:O	2:B:257:ILE:HD11	2.11	0.50
2:B:267:ARG:HA	2:B:270:GLN:HG2	1.93	0.50
1:C:34:CYS:HB2	1:C:123:PHE:CZ	2.46	0.50
1:C:434:ARG:NH1	1:C:463:GLY:C	2.69	0.50
1:E:58:THR:HA	1:E:103:SER:O	2.11	0.50
2:F:205:GLU:O	2:F:207:TYR:N	2.45	0.50
2:F:257:ILE:HG21	2:F:282:GLN:HG2	1.94	0.50
1:C:214:TRP:CD1	1:C:214:TRP:C	2.89	0.50
1:E:502:ALA:O	1:E:505:VAL:HB	2.11	0.50
2:F:158:LEU:HD12	2:F:175:VAL:HB	1.92	0.50
2:H:372:ALA:HA	2:H:375:GLN:NE2	2.27	0.50
1:A:163:ARG:NH1	1:A:165:ILE:HG12	2.27	0.50
1:A:229:THR:O	1:A:230:ASN:HB2	2.12	0.50
2:B:54:ILE:CG2	2:B:145:LEU:HD21	2.42	0.50
2:B:226:GLU:CD	2:B:226:GLU:H	2.19	0.50
2:B:434:VAL:HG13	2:B:436:PHE:HE1	1.77	0.50
2:F:319:ASN:C	2:F:319:ASN:HD22	2.20	0.50
2:F:374:LEU:O	2:F:376:MET:HG3	2.12	0.50
2:F:412:LEU:HD23	2:F:417:LEU:HD13	1.93	0.50
2:H:139:HIS:C	2:H:140:ILE:HG13	2.36	0.50
2:H:383:ALA:HB2	2:H:423:LEU:CD2	2.42	0.50
1:A:168:GLU:HG3	1:A:394:ARG:CG	2.41	0.50
1:A:264:ASN:HD22	1:A:265:PHE:H	1.60	0.50
3:I:103:ILE:HD11	3:I:117:ILE:HD12	1.91	0.50
2:D:398:THR:O	2:D:402:GLU:HG3	2.12	0.50
3:J:115:ILE:HG22	3:J:116:ASP:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:201:LEU:HD22	1:G:221:TYR:CE1	2.47	0.50
2:H:63:LEU:HD22	2:H:142:VAL:HG11	1.93	0.50
1:A:221:TYR:OH	1:A:250:GLY:HA3	2.11	0.49
1:A:227:SER:C	1:A:229:THR:N	2.65	0.49
1:A:517:ASN:HD22	1:A:517:ASN:C	2.20	0.49
1:G:233:ILE:O	1:G:235:LYS:HG3	2.12	0.49
1:G:264:ASN:ND2	1:G:265:PHE:H	2.08	0.49
3:L:103:ILE:C	3:L:103:ILE:HD12	2.36	0.49
1:A:489:GLU:H	2:B:19:HIS:HD2	1.60	0.49
1:A:491:HIS:CD2	2:B:69:LEU:HD12	2.47	0.49
2:D:206:LEU:HB2	3:J:172:GLN:NE2	2.27	0.49
2:F:62:GLU:OE2	2:F:65:LYS:NZ	2.45	0.49
2:F:434:VAL:HG13	2:F:436:PHE:HE1	1.76	0.49
2:H:438:LEU:HD12	2:H:439:HIS:N	2.27	0.49
1:C:78:ARG:C	1:C:80:SER:H	2.20	0.49
2:F:216:ALA:O	2:F:220:SER:HB2	2.12	0.49
2:F:217:THR:HG22	2:F:221:MET:HE3	1.94	0.49
2:F:392:LEU:HD12	2:F:392:LEU:N	2.22	0.49
2:H:240:GLU:O	2:H:242:PRO:CD	2.60	0.49
1:A:190:PRO:O	1:A:194:GLU:HG3	2.13	0.49
1:G:19:LEU:HG	2:H:290:PRO:HB3	1.94	0.49
2:B:197:THR:CG2	2:B:198:ALA:N	2.75	0.49
3:I:117:ILE:HG22	3:I:118:GLU:N	2.27	0.49
1:C:503:GLN:CD	2:D:185:PHE:HE2	2.21	0.49
2:F:229:ILE:HA	2:F:264:SER:OG	2.12	0.49
1:G:84:ASN:OD1	1:G:86:ALA:HB3	2.11	0.49
1:G:299:LYS:HE2	1:G:368:ILE:O	2.13	0.49
2:H:241:GLN:O	2:H:242:PRO:C	2.55	0.49
2:H:349:LEU:HB3	2:H:350:PRO:CD	2.42	0.49
1:A:214:TRP:CZ3	1:A:332:MET:HG2	2.46	0.49
1:A:248:ARG:HG2	1:A:269:ILE:HD11	1.94	0.49
1:C:8:LEU:O	1:C:11:GLN:HB2	2.13	0.49
1:C:66:SER:CB	2:H:262:GLN:HE22	2.19	0.49
2:D:220:SER:HB2	2:D:221:MET:HE3	1.95	0.49
2:D:323:VAL:HG23	2:D:333:TYR:HB3	1.95	0.49
2:D:429:THR:HG23	2:D:430:THR:HG22	1.93	0.49
3:J:170:VAL:HG22	3:J:171:LEU:N	2.28	0.49
3:J:171:LEU:HD12	3:J:172:GLN:H	1.78	0.49
2:H:232:VAL:HG11	2:H:260:ILE:HA	1.93	0.49
3:L:123:VAL:HB	3:L:152:ASP:HA	1.92	0.49
1:A:332:MET:O	1:A:333:ILE:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:LEU:HD12	1:C:525:MET:HG2	1.94	0.49
1:C:309:ARG:HD2	1:C:313:GLU:OE2	2.12	0.49
1:C:426:TYR:HB2	1:C:521:ILE:CD1	2.43	0.49
2:D:415:LEU:CD1	2:D:417:LEU:HG	2.43	0.49
1:E:340:ILE:HD13	2:F:272:ASN:O	2.13	0.49
2:F:54:ILE:HG22	2:F:145:LEU:CD2	2.42	0.49
2:H:319:ASN:HD22	2:H:320:ASN:N	2.10	0.49
2:B:62:GLU:HG2	2:B:300:ALA:HB3	1.95	0.49
2:F:338:GLU:HG3	3:K:148:LYS:HA	1.95	0.49
1:G:186:ASP:OD2	1:G:279:THR:HB	2.13	0.49
1:G:349:LYS:O	1:G:353:ASP:HB2	2.13	0.49
2:H:35:PHE:HB2	2:H:313:SER:O	2.13	0.49
2:H:158:LEU:HA	2:H:161:LEU:HD12	1.94	0.49
2:H:270:GLN:HB2	2:H:271:TYR:CE1	2.48	0.49
2:H:318:LEU:HD11	2:H:334:THR:CG2	2.43	0.49
2:H:380:ALA:CB	2:H:394:LEU:CD1	2.89	0.49
2:B:62:GLU:OE2	2:B:65:LYS:NZ	2.36	0.49
1:C:80:SER:O	1:C:81:ILE:C	2.55	0.49
3:K:107:THR:HG22	3:K:109:THR:H	1.78	0.49
2:H:357:PRO:HA	2:H:440:PHE:CE2	2.47	0.49
1:A:104:PHE:CE1	1:A:106:GLU:HG3	2.48	0.49
2:B:190:ARG:HH22	2:B:203:THR:CG2	2.24	0.49
2:B:207:TYR:CE2	3:I:172:GLN:HG2	2.48	0.49
2:D:85:VAL:C	2:D:87:ASN:H	2.21	0.49
1:E:309:ARG:O	1:E:309:ARG:HD3	2.13	0.49
2:H:394:LEU:HG	2:H:396:SER:H	1.78	0.49
1:A:36:ILE:HG22	1:A:36:ILE:O	2.13	0.48
1:A:78:ARG:HD2	2:B:13:TRP:CE3	2.48	0.48
1:A:201:LEU:HD22	1:A:209:HIS:CE1	2.47	0.48
1:A:253:LYS:CB	1:A:260:GLU:HG3	2.43	0.48
2:B:399:SER:HB3	2:B:400:ILE:HD12	1.95	0.48
2:D:187:GLY:CA	3:J:173:LEU:HD13	2.42	0.48
3:K:104:LYS:CG	3:K:114:GLU:HG2	2.42	0.48
2:H:361:LEU:C	2:H:363:GLU:H	2.21	0.48
3:I:102:LEU:H	3:I:102:LEU:CD2	2.27	0.48
1:A:51:LEU:N	1:A:52:PRO:HD2	2.28	0.48
1:A:526:SER:O	1:A:527:GLN:HB2	2.13	0.48
2:D:271:TYR:O	2:D:272:ASN:HB2	2.12	0.48
2:F:419:ASP:N	2:F:419:ASP:OD1	2.45	0.48
3:K:131:GLU:OE2	3:K:138:PRO:HD3	2.13	0.48
1:A:41:THR:CG2	1:A:497:LEU:HD23	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:170:VAL:HG12	3:I:171:LEU:N	2.28	0.48
2:D:237:TRP:CE3	2:D:242:PRO:HG3	2.48	0.48
2:F:205:GLU:C	2:F:207:TYR:H	2.21	0.48
1:G:264:ASN:ND2	1:G:265:PHE:N	2.61	0.48
1:A:519:THR:HG22	1:A:521:ILE:HD12	1.96	0.48
1:C:90:MET:O	1:C:94:GLN:HB2	2.13	0.48
1:C:202:ASP:HA	1:C:204:MET:HE2	1.95	0.48
1:E:38:ALA:O	1:E:85:ARG:HD3	2.13	0.48
2:F:192:ILE:HG22	2:F:194:PRO:HD3	1.95	0.48
1:G:181:GLU:O	1:G:278:THR:HB	2.13	0.48
1:G:265:PHE:O	1:G:269:ILE:HG13	2.14	0.48
2:H:125:ASN:ND2	2:H:130:PHE:HZ	2.10	0.48
2:H:320:ASN:HD22	2:H:336:GLU:HA	1.77	0.48
2:H:325:ASN:HD22	2:H:326:ASP:N	2.12	0.48
2:B:16:ARG:NH2	2:B:116:PRO:HB2	2.29	0.48
1:C:344:ASN:HD21	1:C:347:ARG:NH2	2.12	0.48
1:E:500:ALA:HB1	2:F:330:LEU:HD21	1.95	0.48
1:G:40:ALA:O	1:G:43:THR:HG22	2.14	0.48
2:H:213:PHE:H	2:H:213:PHE:HD1	1.61	0.48
2:H:223:ARG:O	2:H:273:ILE:HD13	2.12	0.48
2:H:354:GLN:NE2	2:H:439:HIS:HB3	2.28	0.48
1:A:298:THR:C	1:A:300:GLN:N	2.70	0.48
1:A:484:ARG:HG2	1:A:484:ARG:NH1	2.27	0.48
2:B:197:THR:HG23	2:B:320:ASN:OD1	2.14	0.48
2:B:321:TYR:OH	3:I:172:GLN:HG3	2.13	0.48
1:C:74:PHE:CE2	2:D:92:PHE:HE1	2.30	0.48
1:C:428:MET:CE	1:C:479:VAL:HA	2.44	0.48
2:D:279:ARG:O	2:D:282:GLN:HB2	2.14	0.48
1:E:307:LEU:HB3	1:E:383:LEU:HD22	1.95	0.48
3:I:107:THR:CG2	3:I:109:THR:H	2.19	0.48
3:I:117:ILE:HD13	3:I:126:ILE:HG12	1.96	0.48
3:L:125:ARG:C	3:L:127:LYS:N	2.70	0.48
2:B:126:LYS:O	2:B:128:GLN:N	2.47	0.48
2:B:413:LYS:HA	2:B:413:LYS:CE	2.34	0.48
1:C:50:VAL:HG13	1:C:100:VAL:HG21	1.96	0.48
1:C:158:LEU:HA	1:C:493:ILE:HG13	1.96	0.48
3:J:105:VAL:HG13	3:J:113:ILE:CG1	2.44	0.48
1:E:34:CYS:HB2	1:E:123:PHE:CE2	2.49	0.48
2:F:178:ILE:HD11	2:F:310:ILE:HD12	1.95	0.48
1:G:65:VAL:CG2	1:G:85:ARG:HA	2.43	0.48
1:A:361:VAL:HG12	1:A:365:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:LEU:HD11	1:C:346:TYR:HE1	1.79	0.48
1:E:325:VAL:O	1:E:326:ARG:C	2.55	0.48
3:K:103:ILE:HG12	3:K:117:ILE:HD13	1.96	0.48
1:G:226:TYR:CZ	1:G:233:ILE:HG22	2.48	0.48
1:G:496:PHE:C	1:G:496:PHE:CD2	2.92	0.48
2:H:405:ARG:HB3	2:H:405:ARG:NH1	2.29	0.48
2:B:415:LEU:O	2:B:417:LEU:HD22	2.14	0.47
2:B:434:VAL:HG13	2:B:436:PHE:CE1	2.49	0.47
1:C:38:ALA:HB2	1:C:59:ILE:CG2	2.44	0.47
1:E:303:SER:O	1:E:304:PHE:C	2.57	0.47
3:L:149:GLN:HG3	3:L:149:GLN:O	2.15	0.47
1:C:36:ILE:HG21	1:C:131:LEU:HD21	1.96	0.47
1:C:105:VAL:HG12	1:C:107:GLU:H	1.79	0.47
1:C:229:THR:HG22	1:C:232:ARG:HB2	1.94	0.47
1:C:500:ALA:O	1:C:504:GLU:HG2	2.13	0.47
1:E:190:PRO:O	1:E:191:GLU:C	2.57	0.47
1:E:236:THR:CG2	1:E:237:TYR:N	2.77	0.47
2:F:58:GLY:H	2:F:91:GLN:HG2	1.79	0.47
2:F:92:PHE:CD2	2:F:92:PHE:N	2.79	0.47
2:F:217:THR:HG21	2:F:223:ARG:HH22	1.79	0.47
3:K:143:LEU:O	3:K:144:ILE:HD12	2.14	0.47
2:H:270:GLN:HB2	2:H:271:TYR:CD1	2.49	0.47
2:H:316:ILE:H	2:H:316:ILE:CD1	1.99	0.47
1:A:375:ILE:HD12	1:A:375:ILE:N	2.29	0.47
2:B:190:ARG:NH2	2:B:203:THR:CG2	2.77	0.47
2:D:231:TYR:CD1	2:D:235:LEU:HD12	2.48	0.47
2:D:306:GLU:OE2	2:D:317:PRO:HA	2.14	0.47
2:D:319:ASN:HD22	2:D:319:ASN:C	2.21	0.47
1:E:121:CYS:HA	1:E:148:ILE:HD11	1.95	0.47
2:F:225:PRO:HG3	2:F:274:ARG:O	2.15	0.47
1:G:192:LEU:HD12	1:G:345:VAL:HG11	1.94	0.47
1:G:347:ARG:HH22	2:H:274:ARG:HD2	1.78	0.47
1:A:264:ASN:N	1:A:264:ASN:ND2	2.59	0.47
2:B:371:SER:O	2:B:373:SER:N	2.48	0.47
3:I:103:ILE:HD13	3:I:117:ILE:HD12	1.95	0.47
1:C:158:LEU:HD22	1:C:493:ILE:HD11	1.95	0.47
1:C:500:ALA:HB1	2:D:330:LEU:CD2	2.45	0.47
2:D:87:ASN:ND2	2:D:103:LYS:HE2	2.29	0.47
2:D:355:PHE:O	2:D:440:PHE:HA	2.14	0.47
1:E:191:GLU:O	1:E:194:GLU:HB2	2.13	0.47
2:F:320:ASN:OD1	2:F:337:ALA:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:LEU:HB2	3:L:176:GLY:O	2.15	0.47
1:A:156:TYR:CZ	1:A:432:VAL:HG11	2.49	0.47
1:A:518:ASN:CB	1:A:533:GLN:HA	2.44	0.47
2:B:353:ILE:O	2:B:439:HIS:HB2	2.13	0.47
2:B:384:THR:HA	2:B:389:ASN:ND2	2.28	0.47
2:D:21:LYS:HD3	2:D:25:GLU:OE2	2.15	0.47
1:G:226:TYR:O	1:G:231:GLY:N	2.41	0.47
2:D:325:ASN:ND2	2:D:327:VAL:H	2.11	0.47
2:F:215:MET:SD	2:F:218:ILE:HD12	2.54	0.47
2:F:371:SER:C	2:F:373:SER:N	2.71	0.47
3:L:145:TYR:HB2	3:L:167:LEU:HD22	1.97	0.47
1:C:252:LEU:HA	1:C:252:LEU:HD13	1.67	0.47
1:C:332:MET:O	1:C:333:ILE:C	2.58	0.47
2:D:343:CYS:O	2:D:347:SER:HB3	2.14	0.47
1:E:307:LEU:HD22	1:E:383:LEU:HD22	1.96	0.47
2:F:142:VAL:HG21	2:F:307:VAL:CG2	2.42	0.47
2:F:235:LEU:O	2:F:238:PRO:HD2	2.15	0.47
1:G:7:LEU:O	1:G:7:LEU:HD23	2.14	0.47
1:G:113:LEU:HD11	1:G:139:LEU:HB2	1.97	0.47
1:G:424:VAL:CG1	1:G:474:VAL:HG13	2.44	0.47
1:G:462:THR:O	1:G:466:GLN:HG3	2.15	0.47
2:H:213:PHE:CD1	2:H:213:PHE:N	2.82	0.47
2:H:266:GLU:O	2:H:270:GLN:HG3	2.15	0.47
1:A:336:SER:O	1:A:340:ILE:HG12	2.14	0.47
2:B:126:LYS:O	2:B:127:ILE:C	2.58	0.47
1:C:233:ILE:O	1:C:234:PRO:C	2.57	0.47
2:D:132:ASP:HB3	2:D:157:MET:HE2	1.96	0.47
2:F:193:LEU:H	2:F:197:THR:HB	1.80	0.47
2:F:241:GLN:OE1	2:F:245:GLU:HA	2.15	0.47
2:H:245:GLU:HG2	2:H:246:GLY:N	2.30	0.47
1:C:12:LYS:HE3	1:C:13:TYR:CZ	2.50	0.47
2:D:188:ASN:HA	2:D:322:LEU:O	2.14	0.47
2:D:325:ASN:CG	2:D:327:VAL:HG22	2.39	0.47
2:D:359:ALA:HB1	2:D:363:GLU:CD	2.40	0.47
1:E:418:ASN:C	1:E:418:ASN:HD22	2.23	0.47
2:F:232:VAL:HG12	2:F:260:ILE:HG23	1.97	0.47
3:K:102:LEU:HD12	3:K:116:ASP:OD1	2.15	0.47
2:B:64:LEU:HD21	2:B:77:VAL:CG2	2.45	0.47
2:B:350:PRO:HB3	2:B:435:LEU:CB	2.45	0.47
1:C:426:TYR:O	1:C:430:ARG:HG2	2.15	0.47
2:H:218:ILE:HD13	2:H:230:GLU:CG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:361:LEU:C	2:H:363:GLU:N	2.74	0.47
2:F:349:LEU:CD1	2:F:349:LEU:N	2.78	0.46
2:H:312:THR:O	2:H:313:SER:HB2	2.14	0.46
1:A:96:LEU:HD23	2:B:95:ARG:NH2	2.30	0.46
1:A:348:GLU:HG3	1:E:115:ASN:ND2	2.30	0.46
2:B:155:ASN:HB2	2:B:200:ILE:HD13	1.96	0.46
2:B:233:ARG:NH1	2:B:287:ARG:HH12	2.13	0.46
2:B:284:VAL:O	2:B:287:ARG:NH1	2.48	0.46
2:B:419:ASP:HB2	2:B:440:PHE:HD1	1.80	0.46
1:C:36:ILE:HD13	1:C:60:ILE:HD12	1.98	0.46
1:C:418:ASN:C	1:C:420:ASP:H	2.22	0.46
1:E:162:MET:HB2	1:E:520:TYR:HB3	1.97	0.46
3:K:105:VAL:HG22	3:K:113:ILE:HG12	1.97	0.46
1:G:97:ASN:HB3	1:G:100:VAL:HG23	1.97	0.46
2:H:16:ARG:HH22	2:H:116:PRO:HB2	1.80	0.46
2:H:203:THR:O	2:H:205:GLU:N	2.48	0.46
2:H:249:LEU:HA	2:H:256:HIS:CE1	2.50	0.46
2:H:419:ASP:HB2	2:H:440:PHE:HD1	1.80	0.46
3:L:152:ASP:OD1	3:L:152:ASP:N	2.46	0.46
2:B:195:GLY:C	2:B:339:ARG:HH12	2.24	0.46
2:B:232:VAL:HG11	2:B:263:LYS:HB2	1.98	0.46
2:D:52:LEU:HB2	2:D:138:PHE:CE2	2.50	0.46
1:G:128:ALA:HB1	1:G:131:LEU:CD1	2.45	0.46
2:H:140:ILE:C	2:H:141:ILE:HD12	2.41	0.46
2:H:223:ARG:HG3	2:H:223:ARG:NH1	2.30	0.46
1:A:151:LEU:HD13	1:A:164:ILE:HD13	1.97	0.46
1:A:489:GLU:H	2:B:19:HIS:CD2	2.34	0.46
2:B:271:TYR:O	2:B:272:ASN:HB2	2.14	0.46
1:C:108:SER:OG	1:C:109:PRO:HD2	2.14	0.46
2:D:222:PRO:HD2	2:D:271:TYR:CE2	2.50	0.46
2:D:335:PHE:HE2	3:J:170:VAL:HG21	1.80	0.46
1:E:61:ASP:CB	1:E:86:ALA:HB2	2.45	0.46
2:F:74:GLN:HA	2:F:74:GLN:HE21	1.79	0.46
2:B:192:ILE:CD1	2:B:200:ILE:HD12	2.46	0.46
1:C:173:GLU:O	1:C:512:GLN:O	2.33	0.46
1:E:47:LYS:HG3	1:E:75:PHE:CZ	2.50	0.46
1:E:188:PRO:HG2	1:E:193:ARG:CZ	2.45	0.46
2:F:362:GLN:HG2	2:F:408:LEU:HD22	1.98	0.46
2:H:174:ILE:HG23	2:H:194:PRO:HG2	1.97	0.46
2:B:87:ASN:HB3	2:B:91:GLN:CD	2.40	0.46
1:C:248:ARG:C	1:C:250:GLY:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:ASN:O	1:C:423:ILE:N	2.49	0.46
2:D:356:SER:O	2:D:358:SER:N	2.49	0.46
1:E:138:ARG:HG2	1:E:138:ARG:HH11	1.80	0.46
1:E:314:PHE:CE2	1:E:319:GLY:HA3	2.50	0.46
2:F:83:ILE:CD1	2:F:106:VAL:HG21	2.45	0.46
2:F:340:LYS:HB3	2:F:342:ASN:ND2	2.30	0.46
1:G:47:LYS:HZ1	2:H:65:LYS:HE2	1.79	0.46
1:A:36:ILE:O	1:A:36:ILE:CG2	2.64	0.46
1:A:214:TRP:CD1	1:A:215:ILE:N	2.84	0.46
1:A:299:LYS:HG2	1:A:368:ILE:O	2.16	0.46
1:C:72:ASN:HD22	1:C:72:ASN:N	2.08	0.46
1:C:119:PHE:O	1:C:122:ARG:HG2	2.16	0.46
2:D:385:LEU:HD23	2:D:385:LEU:HA	1.74	0.46
1:E:527:GLN:OE1	1:E:527:GLN:HA	2.14	0.46
2:F:95:ARG:HE	2:F:95:ARG:CA	2.29	0.46
2:F:418:VAL:HG22	2:F:419:ASP:N	2.25	0.46
1:G:245:ASP:HA	1:G:248:ARG:HG3	1.98	0.46
2:D:46:LEU:O	2:D:73:ARG:HB2	2.15	0.46
1:E:44:GLU:OE2	2:F:65:LYS:HE3	2.15	0.46
1:E:113:LEU:HD13	1:E:138:ARG:HG2	1.97	0.46
1:E:219:ALA:O	1:E:222:LEU:HB3	2.16	0.46
2:F:253:ASP:OD1	2:F:255:GLU:HB2	2.16	0.46
2:F:259:TRP:CZ2	2:F:263:LYS:HG3	2.51	0.46
1:G:28:LEU:HD11	1:G:506:ILE:HD13	1.98	0.46
1:G:244:ARG:NH1	1:G:272:VAL:HB	2.30	0.46
1:A:264:ASN:ND2	1:A:265:PHE:H	2.13	0.46
1:A:407:ILE:HG23	1:A:407:ILE:O	2.16	0.46
2:B:185:PHE:HB3	2:B:326:ASP:OD2	2.16	0.46
2:B:199:CYS:O	2:B:202:CYS:HB2	2.15	0.46
2:B:321:TYR:OH	3:I:172:GLN:CG	2.64	0.46
2:B:326:ASP:CB	2:B:330:LEU:HD23	2.46	0.46
1:C:243:PHE:O	1:C:246:LEU:HB3	2.16	0.46
2:D:192:ILE:HA	2:D:197:THR:CG2	2.45	0.46
2:D:355:PHE:CE1	2:D:364:VAL:HG22	2.51	0.46
2:D:392:LEU:HD21	2:D:417:LEU:HD21	1.98	0.46
1:E:489:GLU:O	1:E:489:GLU:HG2	2.15	0.46
1:E:489:GLU:C	2:F:19:HIS:HD2	2.24	0.46
2:H:64:LEU:HD21	2:H:77:VAL:HG22	1.98	0.46
3:I:103:ILE:HD11	3:I:117:ILE:CD1	2.45	0.46
1:C:171:VAL:HG13	1:C:391:ARG:HB2	1.97	0.46
2:D:90:ARG:HG2	2:D:90:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:149:ILE:HD12	2:F:149:ILE:N	2.01	0.46
2:F:322:LEU:HD23	2:F:322:LEU:C	2.41	0.46
1:G:72:ASN:C	1:G:72:ASN:HD22	2.23	0.46
1:G:398:LEU:HD12	1:G:401:GLU:OE2	2.16	0.46
3:L:102:LEU:O	3:L:163:GLY:O	2.34	0.46
1:A:396:ARG:NH2	1:A:406:THR:O	2.41	0.45
2:B:28:GLY:O	2:B:31:THR:HG23	2.15	0.45
1:C:527:GLN:HG3	2:D:306:GLU:OE1	2.15	0.45
2:D:230:GLU:O	2:D:234:MET:HB3	2.16	0.45
2:F:410:LYS:HB3	2:F:414:GLU:CG	2.46	0.45
3:K:145:TYR:HB2	3:K:167:LEU:HD22	1.98	0.45
2:H:45:LEU:HD11	2:H:72:PHE:CE2	2.52	0.45
2:H:254:PRO:O	2:H:258:GLN:HB2	2.16	0.45
2:D:429:THR:CG2	2:D:430:THR:HG22	2.46	0.45
1:E:318:GLU:HG3	1:E:356:ALA:HB1	1.99	0.45
1:G:158:LEU:HD21	2:H:23:PHE:CE2	2.51	0.45
1:G:264:ASN:HD22	1:G:265:PHE:N	2.14	0.45
1:G:299:LYS:HG2	1:G:368:ILE:HG23	1.98	0.45
1:A:72:ASN:ND2	1:A:72:ASN:C	2.73	0.45
1:A:329:ILE:HD12	1:A:332:MET:HE3	1.98	0.45
2:B:249:LEU:HD13	2:B:260:ILE:HD11	1.98	0.45
3:I:156:ALA:HA	3:I:161:ILE:HD12	1.97	0.45
1:C:128:ALA:HB1	1:C:131:LEU:CD1	2.45	0.45
1:C:166:ILE:HD11	1:C:508:ILE:HD13	1.98	0.45
1:C:418:ASN:C	1:C:420:ASP:N	2.73	0.45
2:D:405:ARG:HB3	2:D:405:ARG:HH11	1.81	0.45
2:D:405:ARG:O	2:D:408:LEU:HB2	2.17	0.45
1:E:396:ARG:NH1	1:E:534:LEU:O	2.49	0.45
2:F:232:VAL:HA	2:F:236:GLN:HB3	1.96	0.45
1:G:112:LEU:C	1:G:114:ASP:N	2.73	0.45
2:H:125:ASN:ND2	2:H:130:PHE:CZ	2.84	0.45
2:H:237:TRP:CE2	2:H:249:LEU:HB3	2.51	0.45
2:H:353:ILE:O	2:H:439:HIS:HB2	2.16	0.45
2:H:399:SER:HB2	2:H:403:ARG:HH22	1.81	0.45
3:L:138:PRO:HA	3:L:141:GLN:NE2	2.32	0.45
3:L:143:LEU:C	3:L:144:ILE:HD12	2.42	0.45
1:A:518:ASN:HB3	1:A:533:GLN:HA	1.99	0.45
2:B:239:LYS:HD2	2:B:239:LYS:HA	1.76	0.45
1:C:204:MET:HE1	1:C:252:LEU:CG	2.46	0.45
2:F:280:LEU:HD12	2:F:280:LEU:O	2.16	0.45
2:F:361:LEU:HB3	2:F:408:LEU:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:371:SER:C	2:F:373:SER:H	2.24	0.45
2:F:405:ARG:O	2:F:408:LEU:HB2	2.16	0.45
2:H:239:LYS:HG3	2:H:239:LYS:O	2.15	0.45
3:L:155:THR:HG22	3:L:158:ASP:CG	2.40	0.45
1:A:285:ILE:HG12	1:A:387:SER:O	2.16	0.45
2:B:427:ASP:HB3	2:B:429:THR:HG22	1.99	0.45
1:C:327:GLY:CA	1:C:350:ALA:HB2	2.46	0.45
1:E:113:LEU:HD13	1:E:138:ARG:CG	2.47	0.45
2:H:233:ARG:HG2	2:H:233:ARG:NH1	2.31	0.45
2:H:392:LEU:HD23	2:H:392:LEU:N	2.30	0.45
2:B:50:LYS:H	2:B:139:HIS:CD2	2.34	0.45
2:D:164:TYR:CE2	2:D:169:LEU:HB2	2.51	0.45
2:F:321:TYR:O	2:F:334:THR:HG23	2.17	0.45
2:F:336:GLU:O	2:F:337:ALA:C	2.60	0.45
2:F:412:LEU:HA	2:F:417:LEU:HD12	1.98	0.45
3:K:107:THR:HG22	3:K:111:LYS:H	1.81	0.45
1:G:416:MET:C	1:G:418:ASN:N	2.75	0.45
2:H:59:LEU:HD12	3:L:176:GLY:CA	2.46	0.45
2:B:318:LEU:HD11	2:B:334:THR:HG21	1.96	0.45
2:B:374:LEU:O	2:B:375:GLN:C	2.59	0.45
1:C:428:MET:HE1	1:C:479:VAL:HA	1.98	0.45
1:C:434:ARG:NH1	1:C:464:PHE:HA	2.31	0.45
2:D:94:PHE:N	2:D:94:PHE:CD2	2.82	0.45
1:E:209:HIS:CD2	1:E:252:LEU:H	2.35	0.45
1:E:209:HIS:CG	1:E:252:LEU:HB2	2.52	0.45
1:E:371:ALA:C	1:E:373:GLU:H	2.24	0.45
2:B:187:GLY:CA	3:I:173:LEU:HD13	2.47	0.45
2:D:54:ILE:HG22	2:D:145:LEU:HD21	1.98	0.45
1:E:154:ARG:HH12	1:E:433:ASP:CG	2.25	0.45
1:A:78:ARG:O	1:A:80:SER:N	2.46	0.45
2:B:351:GLN:O	2:B:436:PHE:HA	2.16	0.45
2:D:149:ILE:CD1	2:D:149:ILE:N	2.54	0.45
1:E:138:ARG:HG2	1:E:138:ARG:NH1	2.32	0.45
1:E:236:THR:CG2	1:E:237:TYR:H	2.26	0.45
1:E:317:LYS:HD3	1:E:318:GLU:OE1	2.16	0.45
2:F:349:LEU:N	2:F:349:LEU:HD12	2.32	0.45
2:F:357:PRO:HD3	2:F:440:PHE:CD2	2.52	0.45
3:K:155:THR:HG22	3:K:158:ASP:OD1	2.17	0.45
1:G:7:LEU:O	1:G:11:GLN:HG3	2.17	0.45
1:G:485:TYR:OH	1:G:525:MET:SD	2.75	0.45
2:H:218:ILE:CD1	2:H:230:GLU:HG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:320:ASN:ND2	2:H:336:GLU:HG2	2.32	0.45
2:H:344:PRO:HG3	2:H:374:LEU:HD22	1.98	0.45
1:C:38:ALA:HB2	1:C:59:ILE:HG21	1.99	0.45
2:D:232:VAL:HG11	2:D:263:LYS:HB2	1.99	0.45
1:E:447:ASN:HD22	1:E:447:ASN:N	2.13	0.45
1:G:120:PHE:O	1:G:148:ILE:HD13	2.16	0.45
1:G:503:GLN:O	1:G:507:LYS:HG3	2.17	0.45
2:H:74:GLN:HE22	2:H:119:ASN:HD22	1.64	0.45
2:H:320:ASN:CB	2:H:336:GLU:HA	2.44	0.45
1:A:236:THR:HG22	1:A:237:TYR:N	2.32	0.44
1:A:397:SER:OG	1:A:400:GLU:HG3	2.17	0.44
2:B:84:ASP:H	2:B:87:ASN:ND2	2.16	0.44
1:C:109:PRO:HG2	1:C:110:GLU:H	1.82	0.44
1:C:512:GLN:HE21	1:C:512:GLN:HB2	1.55	0.44
2:D:338:GLU:HG3	3:J:148:LYS:HD3	1.99	0.44
1:E:47:LYS:HG2	1:E:96:LEU:CD1	2.46	0.44
1:E:93:LEU:O	1:E:94:GLN:C	2.60	0.44
1:E:125:VAL:HG12	1:E:126:VAL:N	2.31	0.44
1:E:340:ILE:HD12	2:F:271:TYR:O	2.17	0.44
1:G:340:ILE:HD11	2:H:273:ILE:CG1	2.42	0.44
2:H:40:GLU:O	2:H:40:GLU:HG2	2.16	0.44
2:H:266:GLU:O	2:H:268:ALA:N	2.48	0.44
3:L:105:VAL:HA	3:L:167:LEU:O	2.17	0.44
3:L:129:ARG:O	3:L:132:GLU:HB3	2.17	0.44
1:A:371:ALA:C	1:A:373:GLU:N	2.75	0.44
1:E:310:ALA:O	1:E:311:LEU:C	2.60	0.44
2:F:106:VAL:O	2:F:109:GLU:HB3	2.16	0.44
2:F:221:MET:N	2:F:222:PRO:HD3	2.33	0.44
1:G:157:GLY:HA3	1:G:485:TYR:CG	2.52	0.44
1:G:225:TRP:CD1	1:G:225:TRP:C	2.94	0.44
1:G:325:VAL:HG21	1:G:349:LYS:CG	2.47	0.44
2:H:225:PRO:HD2	2:H:226:GLU:OE1	2.17	0.44
1:E:359:ASN:HD22	1:E:359:ASN:HA	1.63	0.44
1:E:422:GLU:HG3	1:E:530:ALA:HB3	1.99	0.44
1:G:311:LEU:O	1:G:314:PHE:HB3	2.18	0.44
1:G:396:ARG:HD3	1:G:534:LEU:O	2.18	0.44
1:G:426:TYR:CE2	1:G:534:LEU:HD13	2.52	0.44
1:G:435:PHE:C	1:G:435:PHE:CD2	2.95	0.44
1:G:503:GLN:OE1	1:G:506:ILE:HB	2.17	0.44
2:B:217:THR:HB	2:B:223:ARG:HH21	1.81	0.44
2:B:342:ASN:N	2:B:342:ASN:ND2	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:PRO:HD3	2:B:440:PHE:HB3	1.99	0.44
1:C:480:HIS:HB2	2:D:29:PRO:HG2	1.97	0.44
1:C:518:ASN:HB3	1:C:533:GLN:HA	1.99	0.44
1:E:173:GLU:O	1:E:512:GLN:O	2.34	0.44
1:E:457:LEU:HD23	1:E:479:VAL:HG13	1.98	0.44
2:F:398:THR:HA	2:F:401:GLU:HG2	1.99	0.44
3:K:113:ILE:O	3:K:113:ILE:HG13	2.17	0.44
1:G:311:LEU:HD21	1:G:387:SER:HB2	1.98	0.44
1:A:12:LYS:HE3	1:A:13:TYR:CE2	2.52	0.44
2:B:225:PRO:HB2	2:B:280:LEU:HD21	1.99	0.44
2:B:374:LEU:O	2:B:376:MET:HG3	2.18	0.44
2:D:15:GLY:O	2:D:16:ARG:C	2.60	0.44
1:E:12:LYS:HG3	1:E:13:TYR:CD2	2.52	0.44
1:E:15:ARG:HG3	2:F:90:ARG:NH1	2.33	0.44
2:F:164:TYR:O	2:F:165:GLU:C	2.57	0.44
2:F:320:ASN:HB3	2:F:321:TYR:H	1.26	0.44
2:F:362:GLN:HG2	2:F:408:LEU:HB3	1.99	0.44
1:G:120:PHE:HA	1:G:123:PHE:CD1	2.53	0.44
1:G:490:PRO:O	1:G:491:HIS:C	2.61	0.44
1:A:500:ALA:O	1:A:504:GLU:HG2	2.17	0.44
2:B:139:HIS:C	2:B:140:ILE:HG13	2.42	0.44
2:B:323:VAL:O	2:B:332:THR:HA	2.17	0.44
1:C:72:ASN:HD22	1:C:73:ASN:H	1.65	0.44
1:C:236:THR:O	1:C:237:TYR:C	2.61	0.44
2:D:203:THR:C	2:D:205:GLU:N	2.76	0.44
2:D:230:GLU:OE2	2:D:233:ARG:NH1	2.51	0.44
2:D:243:PHE:O	2:D:247:VAL:HG21	2.17	0.44
1:E:221:TYR:H	1:E:221:TYR:HD1	1.65	0.44
1:E:265:PHE:O	1:E:269:ILE:HG13	2.18	0.44
1:G:371:ALA:HA	1:G:372:PRO:HD3	1.89	0.44
1:G:424:VAL:HG13	1:G:474:VAL:HG13	2.00	0.44
2:H:233:ARG:NH1	2:H:234:MET:HB2	2.32	0.44
2:H:294:SER:O	2:H:298:VAL:HG23	2.17	0.44
3:L:117:ILE:CD1	3:L:126:ILE:HA	2.45	0.44
1:A:229:THR:HG22	1:A:232:ARG:H	1.83	0.44
2:B:350:PRO:CG	2:B:437:LYS:HG3	2.47	0.44
3:I:108:LEU:CD2	3:I:171:LEU:HD23	2.47	0.44
3:I:113:ILE:HD13	3:I:134:GLU:HG2	2.00	0.44
1:C:349:LYS:HE3	1:C:353:ASP:OD1	2.17	0.44
2:D:325:ASN:ND2	2:D:326:ASP:N	2.59	0.44
1:E:36:ILE:HB	1:E:128:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:LYS:N	1:G:6:LYS:HD2	2.33	0.44
1:G:114:ASP:HA	1:G:138:ARG:NH2	2.32	0.44
1:A:211:HIS:CE1	2:B:221:MET:HE1	2.52	0.44
1:A:248:ARG:HG2	1:A:269:ILE:CD1	2.48	0.44
1:A:434:ARG:HD3	1:A:460:CYS:CB	2.47	0.44
1:C:74:PHE:CD2	2:D:65:LYS:HD3	2.53	0.44
2:D:13:TRP:HZ3	2:D:116:PRO:HG2	1.83	0.44
1:E:393:VAL:HG11	1:E:515:ILE:HD11	2.00	0.44
2:F:353:ILE:O	2:F:353:ILE:HG22	2.16	0.44
2:F:376:MET:HB3	2:F:427:ASP:OD1	2.18	0.44
1:G:442:TYR:HB3	1:G:443:PRO:HD2	1.99	0.44
2:H:83:ILE:CD1	2:H:106:VAL:HG21	2.48	0.44
1:A:416:MET:C	1:A:418:ASN:N	2.74	0.44
1:C:19:LEU:HG	2:D:290:PRO:HB3	2.00	0.44
2:D:231:TYR:HD1	2:D:235:LEU:HD12	1.83	0.44
1:E:183:LEU:HD22	1:E:215:ILE:HD11	2.00	0.44
1:G:34:CYS:SG	1:G:60:ILE:HD13	2.57	0.44
1:G:325:VAL:HG23	1:G:353:ASP:OD2	2.17	0.44
2:H:27:SER:HB3	2:H:37:PRO:HG2	2.00	0.44
2:H:123:HIS:O	2:H:125:ASN:N	2.51	0.44
2:H:340:LYS:C	2:H:342:ASN:H	2.23	0.44
2:H:352:ASN:HD22	2:H:437:LYS:HB2	1.83	0.44
2:H:402:GLU:C	2:H:404:THR:N	2.76	0.44
2:B:246:GLY:O	2:B:247:VAL:C	2.61	0.43
3:I:118:GLU:O	3:I:119:PRO:C	2.61	0.43
2:F:187:GLY:HA2	3:K:173:LEU:HD13	2.00	0.43
2:F:318:LEU:HD12	2:F:319:ASN:N	2.33	0.43
1:G:303:SER:O	1:G:304:PHE:C	2.61	0.43
1:G:466:GLN:O	1:G:467:GLU:C	2.61	0.43
2:H:365:LEU:O	2:H:365:LEU:HG	2.18	0.43
2:H:407:ASN:C	2:H:409:SER:H	2.26	0.43
1:A:285:ILE:HD11	1:A:390:LEU:H	1.82	0.43
2:B:182:THR:OG1	2:B:295:THR:HG22	2.17	0.43
2:B:241:GLN:HA	2:B:242:PRO:HD2	1.68	0.43
1:E:50:VAL:HG13	1:E:100:VAL:HG21	2.00	0.43
1:E:415:SER:HB3	1:E:421:ASN:OD1	2.18	0.43
2:H:267:ARG:CG	2:H:267:ARG:NH1	2.81	0.43
3:L:170:VAL:CG1	3:L:171:LEU:H	2.31	0.43
1:A:50:VAL:HA	1:A:54:ILE:HG22	1.99	0.43
1:A:192:LEU:HD11	1:A:196:PHE:CZ	2.53	0.43
2:B:371:SER:C	2:B:373:SER:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ASN:OD1	1:C:86:ALA:HB3	2.19	0.43
2:D:401:GLU:HG3	2:D:402:GLU:N	2.33	0.43
1:E:54:ILE:HD12	1:E:54:ILE:HA	1.73	0.43
1:E:184:ARG:HD3	1:E:279:THR:OG1	2.17	0.43
1:G:253:LYS:CB	1:G:261:ASP:N	2.81	0.43
2:H:338:GLU:HG3	3:L:148:LYS:CD	2.41	0.43
3:L:101:MET:HB3	3:L:117:ILE:O	2.17	0.43
3:L:103:ILE:HD12	3:L:103:ILE:O	2.18	0.43
3:L:144:ILE:HD13	3:L:170:VAL:HB	2.00	0.43
1:A:339:TYR:CD2	2:B:223:ARG:HB3	2.53	0.43
2:D:199:CYS:O	2:D:202:CYS:HB2	2.18	0.43
3:J:105:VAL:HG11	3:J:115:ILE:HD11	2.00	0.43
1:E:418:ASN:HD22	1:E:419:PRO:HD2	1.82	0.43
2:F:267:ARG:HG2	2:F:267:ARG:HH11	1.83	0.43
3:K:137:PRO:HA	3:K:138:PRO:HD3	1.87	0.43
1:G:297:ILE:HD11	1:G:309:ARG:HG2	1.99	0.43
1:G:507:LYS:HG2	1:G:513:PHE:HB2	2.01	0.43
2:H:232:VAL:HG12	2:H:260:ILE:HG23	1.99	0.43
1:A:36:ILE:HG23	1:A:109:PRO:HG3	2.00	0.43
1:A:84:ASN:OD1	1:A:86:ALA:HB3	2.19	0.43
1:A:298:THR:C	1:A:368:ILE:HD12	2.44	0.43
2:B:113:ASP:C	2:B:113:ASP:OD1	2.61	0.43
3:I:104:LYS:O	3:I:166:VAL:HA	2.18	0.43
2:D:393:TYR:CD2	2:D:408:LEU:HD21	2.53	0.43
1:E:248:ARG:C	1:E:250:GLY:H	2.26	0.43
1:E:340:ILE:HD11	2:F:273:ILE:CG1	2.48	0.43
1:E:475:LYS:C	1:E:477:ASP:N	2.76	0.43
1:G:184:ARG:HH11	1:G:184:ARG:HG3	1.84	0.43
1:G:362:ALA:O	1:G:366:GLN:HG3	2.18	0.43
1:A:527:GLN:HB2	2:B:318:LEU:HD13	2.00	0.43
3:J:105:VAL:CG1	3:J:115:ILE:HD11	2.49	0.43
1:E:51:LEU:HD11	2:F:92:PHE:HB3	1.99	0.43
1:E:138:ARG:O	1:E:142:VAL:HG23	2.19	0.43
2:F:422:GLU:O	2:F:423:LEU:HD23	2.18	0.43
1:G:329:ILE:HD11	1:G:343:GLN:HA	2.01	0.43
2:H:390:ARG:HH11	2:H:390:ARG:HG3	1.83	0.43
2:H:412:LEU:O	2:H:417:LEU:HB2	2.19	0.43
1:A:513:PHE:CZ	2:B:185:PHE:HE1	2.36	0.43
1:A:517:ASN:OD1	1:A:533:GLN:NE2	2.52	0.43
2:B:224:LEU:HB3	2:B:226:GLU:OE1	2.19	0.43
2:B:322:LEU:C	2:B:322:LEU:CD2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ARG:CZ	2:D:13:TRP:HB3	2.48	0.43
1:C:344:ASN:HD22	1:C:344:ASN:HA	1.53	0.43
1:C:527:GLN:HA	1:C:527:GLN:OE1	2.18	0.43
1:G:324:PRO:HA	1:G:353:ASP:OD2	2.18	0.43
2:H:30:PHE:N	2:H:30:PHE:CD1	2.85	0.43
1:A:324:PRO:HB3	1:A:353:ASP:HB3	1.99	0.43
1:A:517:ASN:C	1:A:517:ASN:ND2	2.76	0.43
2:B:111:LEU:HD23	2:B:120:VAL:HG21	2.01	0.43
2:B:141:ILE:HD12	2:B:158:LEU:HD21	2.00	0.43
1:C:199:TYR:HB3	1:C:200:ASP:H	1.61	0.43
1:C:301:THR:HA	1:C:302:PRO:HD3	1.82	0.43
1:E:128:ALA:HB1	1:E:131:LEU:CD1	2.48	0.43
1:E:214:TRP:CE2	1:E:271:ASN:ND2	2.86	0.43
2:F:54:ILE:HB	2:F:143:CYS:CB	2.48	0.43
1:G:215:ILE:C	1:G:217:ILE:N	2.76	0.43
2:H:115:VAL:HA	2:H:116:PRO:HD2	1.90	0.43
2:B:95:ARG:HA	2:B:95:ARG:HD3	1.73	0.43
2:D:59:LEU:HD12	3:J:176:GLY:HA3	2.01	0.43
2:D:312:THR:O	2:D:313:SER:HB2	2.18	0.43
1:E:15:ARG:HG3	2:F:90:ARG:HH12	1.83	0.43
1:G:51:LEU:HD11	2:H:92:PHE:HB3	2.01	0.43
2:H:367:TYR:O	2:H:371:SER:CB	2.67	0.43
2:H:383:ALA:HB2	2:H:423:LEU:HD22	2.00	0.43
1:A:42:GLY:HA2	1:A:129:THR:HG21	2.00	0.43
1:A:309:ARG:HD2	1:A:313:GLU:HG2	2.01	0.43
1:A:447:ASN:ND2	2:B:26:ARG:HE	2.17	0.43
1:C:43:THR:HG22	1:C:44:GLU:N	2.34	0.43
1:C:419:PRO:HB3	1:C:473:MET:HE1	2.00	0.43
1:C:488:ALA:C	1:C:490:PRO:HD3	2.44	0.43
1:C:507:LYS:NZ	2:D:326:ASP:O	2.50	0.43
2:D:152:ARG:NE	2:D:201:GLU:OE1	2.52	0.43
2:F:400:ILE:O	2:F:400:ILE:HG22	2.18	0.43
3:K:155:THR:N	3:K:158:ASP:OD2	2.43	0.43
2:H:187:GLY:CA	3:L:173:LEU:HD13	2.48	0.43
1:A:78:ARG:C	1:A:80:SER:N	2.77	0.42
1:A:438:GLN:O	1:A:440:GLY:N	2.52	0.42
2:B:89:ASN:OD1	2:B:90:ARG:NH1	2.47	0.42
2:B:353:ILE:HD13	2:B:436:PHE:HD2	1.84	0.42
2:B:384:THR:HA	2:B:389:ASN:HD22	1.83	0.42
1:C:441:ARG:HG2	1:C:441:ARG:HH11	1.84	0.42
1:C:496:PHE:CD2	1:C:496:PHE:C	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:ASN:HD22	2:D:325:ASN:C	2.23	0.42
2:D:382:THR:HG22	2:D:391:THR:HA	2.00	0.42
2:F:182:THR:O	2:F:183:GLU:HG2	2.19	0.42
1:G:173:GLU:O	1:G:512:GLN:O	2.37	0.42
1:G:449:GLN:O	1:G:450:VAL:C	2.61	0.42
2:H:382:THR:HG22	2:H:391:THR:HA	2.00	0.42
1:A:128:ALA:HB1	1:A:131:LEU:HD11	2.02	0.42
1:A:246:LEU:O	1:A:249:GLN:HB3	2.19	0.42
1:C:186:ASP:OD2	1:C:279:THR:HB	2.19	0.42
2:D:203:THR:C	2:D:205:GLU:H	2.27	0.42
3:J:155:THR:HG22	3:J:158:ASP:CG	2.44	0.42
1:E:114:ASP:OD1	1:E:138:ARG:NH2	2.48	0.42
2:F:397:VAL:O	2:F:397:VAL:HG23	2.19	0.42
1:G:307:LEU:HD13	1:G:383:LEU:HD22	2.01	0.42
2:H:320:ASN:ND2	2:H:336:GLU:HG3	2.34	0.42
2:H:393:TYR:CG	2:H:394:LEU:N	2.87	0.42
2:B:145:LEU:O	3:I:176:GLY:HA2	2.19	0.42
1:C:46:LEU:HD12	1:C:46:LEU:HA	1.86	0.42
1:C:78:ARG:C	1:C:80:SER:N	2.78	0.42
1:C:146:SER:O	1:C:147:GLN:CB	2.67	0.42
1:E:184:ARG:NH1	1:E:184:ARG:HG3	2.29	0.42
1:E:214:TRP:CD1	1:E:214:TRP:C	2.97	0.42
2:F:58:GLY:N	2:F:91:GLN:HG2	2.35	0.42
2:F:74:GLN:NE2	2:F:74:GLN:CA	2.83	0.42
2:F:212:ASN:HD22	2:F:212:ASN:HA	1.62	0.42
2:F:233:ARG:HG2	2:F:234:MET:N	2.35	0.42
2:F:335:PHE:CE2	3:K:170:VAL:HG21	2.54	0.42
2:F:356:SER:C	2:F:358:SER:H	2.27	0.42
1:G:272:VAL:C	1:G:274:THR:H	2.27	0.42
2:H:188:ASN:OD1	3:L:173:LEU:HD12	2.18	0.42
1:A:35:LEU:CD2	1:A:46:LEU:HD22	2.49	0.42
1:A:269:ILE:O	1:A:270:LYS:C	2.61	0.42
2:B:43:GLN:HG3	2:B:47:ASP:OD2	2.19	0.42
2:B:235:LEU:C	2:B:238:PRO:HD2	2.44	0.42
2:B:250:ASP:OD1	2:B:250:ASP:C	2.62	0.42
1:C:181:GLU:OE1	1:C:330:PRO:HD3	2.19	0.42
1:E:221:TYR:N	1:E:221:TYR:CD1	2.85	0.42
2:F:220:SER:C	2:F:222:PRO:HD3	2.44	0.42
2:F:236:GLN:NE2	2:F:263:LYS:HD2	2.32	0.42
2:F:256:HIS:O	2:F:260:ILE:HG13	2.19	0.42
2:F:342:ASN:N	2:F:342:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:ILE:O	1:G:165:ILE:HG22	2.20	0.42
1:G:221:TYR:CD2	1:G:247:ILE:HA	2.55	0.42
2:H:319:ASN:HD22	2:H:319:ASN:C	2.28	0.42
2:B:233:ARG:HH11	2:B:287:ARG:HH12	1.65	0.42
2:B:380:ALA:CB	2:B:394:LEU:CD1	2.92	0.42
1:C:504:GLU:O	1:C:508:ILE:HG13	2.19	0.42
1:E:193:ARG:HG3	1:E:193:ARG:NH1	2.30	0.42
1:E:274:THR:O	1:E:276:LEU:N	2.53	0.42
2:F:257:ILE:HD13	2:F:282:GLN:HG2	2.00	0.42
2:H:411:THR:OG1	2:H:414:GLU:HB2	2.19	0.42
1:A:28:LEU:HA	1:A:509:ILE:HG21	2.02	0.42
2:B:128:GLN:HG3	2:B:153:TRP:CE2	2.54	0.42
2:B:185:PHE:HB2	2:B:327:VAL:HG12	2.02	0.42
2:B:294:SER:O	2:B:298:VAL:HG23	2.19	0.42
2:B:322:LEU:HD23	2:B:323:VAL:N	2.35	0.42
3:I:124:GLU:HB2	3:I:152:ASP:O	2.19	0.42
2:D:196:MET:HE2	2:D:196:MET:HB3	1.81	0.42
3:J:156:ALA:O	3:J:161:ILE:HB	2.20	0.42
1:E:119:PHE:O	1:E:122:ARG:HG2	2.19	0.42
1:E:297:ILE:HB	1:E:368:ILE:CD1	2.30	0.42
1:E:309:ARG:HD3	1:E:309:ARG:C	2.45	0.42
1:E:374:SER:O	1:E:375:ILE:HD12	2.20	0.42
2:F:128:GLN:HE21	2:F:128:GLN:H	1.66	0.42
2:F:320:ASN:HD22	2:F:320:ASN:HA	1.56	0.42
2:F:364:VAL:O	2:F:368:LEU:HG	2.19	0.42
2:H:132:ASP:OD1	2:H:132:ASP:N	2.52	0.42
1:A:510:THR:O	1:A:511:LYS:HB2	2.19	0.42
2:B:33:PRO:C	2:B:35:PHE:H	2.28	0.42
1:C:331:ASP:OD2	2:D:223:ARG:NH1	2.53	0.42
1:E:236:THR:HG22	1:E:238:LYS:H	1.83	0.42
2:F:95:ARG:HG3	2:F:97:LYS:HZ3	1.84	0.42
2:F:128:GLN:H	2:F:128:GLN:NE2	2.18	0.42
1:G:407:ILE:CG2	1:G:409:LYS:HE3	2.49	0.42
1:G:523:SER:OG	1:G:525:MET:HG2	2.20	0.42
2:H:183:GLU:HG3	2:H:289:ILE:CG2	2.49	0.42
3:L:157:ALA:C	3:L:159:TYR:H	2.28	0.42
2:B:385:LEU:HA	2:B:385:LEU:HD12	1.77	0.42
2:B:391:THR:O	2:B:392:LEU:C	2.62	0.42
1:C:441:ARG:HH21	1:C:453:ASP:CG	2.27	0.42
2:D:95:ARG:HG3	2:D:95:ARG:HH11	1.85	0.42
3:K:115:ILE:HG13	3:K:117:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:ARG:NH1	1:G:165:ILE:HG12	2.34	0.42
2:H:235:LEU:O	2:H:238:PRO:HD2	2.19	0.42
2:D:350:PRO:HB2	2:D:437:LYS:HD3	2.01	0.42
3:K:105:VAL:HG22	3:K:113:ILE:CG1	2.50	0.42
1:G:47:LYS:NZ	2:H:65:LYS:HE2	2.34	0.42
1:G:251:ILE:HG12	1:G:265:PHE:HB3	2.02	0.42
2:H:77:VAL:HG23	2:H:120:VAL:CG1	2.50	0.42
1:A:229:THR:HG21	1:A:232:ARG:HB3	2.01	0.42
1:A:236:THR:CG2	1:A:238:LYS:HB3	2.49	0.42
1:A:276:LEU:HA	1:A:276:LEU:HD23	1.83	0.42
1:C:67:GLY:HA3	2:D:14:GLU:O	2.20	0.42
2:D:335:PHE:CE2	3:J:170:VAL:HG21	2.55	0.42
1:E:34:CYS:HB2	1:E:123:PHE:CG	2.55	0.42
2:F:114:ARG:O	2:F:116:PRO:HD3	2.20	0.42
3:K:107:THR:HG23	3:K:108:LEU:N	2.34	0.42
1:G:226:TYR:CE2	1:G:233:ILE:HG22	2.55	0.42
1:G:306:ILE:HD13	1:G:365:LEU:HD23	2.02	0.42
1:G:324:PRO:CG	1:G:357:VAL:HG21	2.50	0.42
3:L:135:GLY:O	3:L:137:PRO:HD3	2.20	0.42
1:A:168:GLU:HG3	1:A:394:ARG:NE	2.34	0.41
1:A:248:ARG:C	1:A:250:GLY:N	2.78	0.41
3:I:131:GLU:CD	3:I:138:PRO:HD3	2.44	0.41
1:C:51:LEU:HD11	2:D:92:PHE:HB3	2.02	0.41
2:D:32:HIS:CD2	2:D:34:ASP:H	2.38	0.41
2:D:80:MET:O	2:D:124:PHE:HE1	2.03	0.41
2:D:241:GLN:HA	2:D:242:PRO:HD2	1.89	0.41
3:J:162:LEU:O	3:J:163:GLY:C	2.63	0.41
1:E:330:PRO:O	1:E:332:MET:HG3	2.20	0.41
2:F:34:ASP:N	2:F:34:ASP:OD1	2.53	0.41
1:G:244:ARG:HH11	1:G:244:ARG:CG	2.32	0.41
2:H:117:ASN:O	2:H:118:CYS:C	2.63	0.41
2:H:427:ASP:C	2:H:429:THR:H	2.28	0.41
1:A:301:THR:CG2	1:A:305:TRP:HB2	2.50	0.41
2:B:213:PHE:HD1	2:B:230:GLU:HG2	1.85	0.41
1:C:418:ASN:HD22	1:C:419:PRO:HD2	1.84	0.41
1:C:437:LYS:HA	1:C:437:LYS:HD2	1.73	0.41
2:D:98:ASP:O	2:D:99:ILE:C	2.64	0.41
2:D:318:LEU:HD11	2:D:334:THR:CG2	2.50	0.41
2:F:32:HIS:CG	2:F:33:PRO:HD2	2.55	0.41
1:G:90:MET:O	1:G:94:GLN:HB2	2.19	0.41
2:H:207:TYR:HA	2:H:208:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:245:GLU:CG	2:H:246:GLY:N	2.83	0.41
3:L:162:LEU:O	3:L:164:GLY:N	2.53	0.41
1:A:172:ILE:HA	1:A:390:LEU:HD23	2.01	0.41
1:A:236:THR:HG21	1:A:238:LYS:HB3	2.02	0.41
1:A:366:GLN:O	1:A:368:ILE:N	2.54	0.41
2:B:286:LYS:HB2	2:B:288:ILE:HG13	2.00	0.41
2:B:401:GLU:HG3	2:B:402:GLU:N	2.35	0.41
2:B:403:ARG:HG3	2:B:403:ARG:HH11	1.85	0.41
2:B:413:LYS:HE3	2:B:413:LYS:O	2.20	0.41
1:C:74:PHE:HE2	2:D:92:PHE:HE1	1.69	0.41
1:C:284:SER:O	1:C:288:ILE:HG13	2.21	0.41
1:E:486:GLY:HA3	2:F:22:LYS:HD3	2.02	0.41
2:F:319:ASN:HD22	2:F:320:ASN:N	2.18	0.41
2:F:351:GLN:HB2	2:F:436:PHE:CD2	2.56	0.41
1:G:90:MET:CE	1:G:94:GLN:OE1	2.68	0.41
1:G:218:ILE:O	1:G:222:LEU:HB2	2.20	0.41
1:G:404:LEU:HD21	1:G:467:GLU:HG2	2.02	0.41
1:G:519:THR:O	1:G:531:THR:HA	2.20	0.41
2:H:392:LEU:H	2:H:392:LEU:CD2	2.30	0.41
2:H:402:GLU:O	2:H:404:THR:N	2.54	0.41
2:H:405:ARG:HB3	2:H:406:PRO:HD3	2.01	0.41
3:L:136:ILE:O	3:L:137:PRO:C	2.62	0.41
2:B:218:ILE:HD12	2:B:218:ILE:HA	1.91	0.41
2:B:402:GLU:C	2:B:404:THR:H	2.29	0.41
2:D:207:TYR:CE2	3:J:172:GLN:HG2	2.55	0.41
1:E:44:GLU:HG3	1:E:495:ALA:HA	2.03	0.41
1:E:53:GLY:O	1:E:54:ILE:C	2.62	0.41
1:E:229:THR:CG2	1:E:232:ARG:HD2	2.49	0.41
1:E:332:MET:O	2:F:223:ARG:NE	2.54	0.41
1:E:488:ALA:HB2	2:F:22:LYS:HD2	2.03	0.41
1:G:189:PHE:HB2	1:G:190:PRO:HD2	2.02	0.41
1:G:346:TYR:C	1:G:348:GLU:N	2.78	0.41
2:H:84:ASP:OD1	2:H:86:SER:N	2.47	0.41
2:H:89:ASN:OD1	2:H:90:ARG:NH1	2.50	0.41
1:A:78:ARG:O	1:A:81:ILE:HG13	2.20	0.41
1:A:496:PHE:CD2	1:A:496:PHE:C	2.98	0.41
2:B:24:LEU:HD21	2:B:312:THR:HG21	2.01	0.41
2:B:110:PHE:C	2:B:110:PHE:CD2	2.98	0.41
2:B:385:LEU:CD2	2:B:390:ARG:HB3	2.40	0.41
1:C:195:HIS:O	1:C:196:PHE:C	2.64	0.41
2:D:405:ARG:N	2:D:406:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:GLN:O	1:E:78:ARG:C	2.64	0.41
1:E:341:LYS:HE2	1:E:341:LYS:HB3	1.93	0.41
2:F:222:PRO:O	2:F:273:ILE:HD11	2.20	0.41
2:F:361:LEU:CD2	2:F:408:LEU:HD23	2.45	0.41
2:F:402:GLU:HG2	2:F:405:ARG:NH2	2.34	0.41
2:F:410:LYS:HB3	2:F:414:GLU:HG2	2.03	0.41
1:G:251:ILE:O	1:G:253:LYS:N	2.54	0.41
1:G:299:LYS:HG2	1:G:368:ILE:CG2	2.50	0.41
2:H:195:GLY:O	2:H:339:ARG:NH1	2.53	0.41
2:H:249:LEU:CD1	2:H:260:ILE:HD11	2.49	0.41
2:B:217:THR:CB	2:B:223:ARG:NH2	2.81	0.41
1:C:97:ASN:HB3	1:C:100:VAL:HG23	2.01	0.41
1:C:175:HIS:HD2	1:C:512:GLN:O	2.03	0.41
2:D:319:ASN:HD22	2:D:320:ASN:N	2.19	0.41
2:D:323:VAL:O	2:D:332:THR:HA	2.21	0.41
2:D:365:LEU:HD12	2:D:379:PRO:HG2	2.01	0.41
3:J:118:GLU:O	3:J:120:THR:N	2.54	0.41
2:F:377:LYS:HE2	2:F:377:LYS:CA	2.39	0.41
1:G:45:ILE:CG1	1:G:498:GLY:HA2	2.48	0.41
1:G:178:ASN:O	1:G:179:ALA:HB2	2.20	0.41
1:G:302:PRO:O	1:G:303:SER:C	2.64	0.41
2:H:355:PHE:O	2:H:440:PHE:HA	2.20	0.41
1:A:40:ALA:O	1:A:43:THR:HG22	2.20	0.41
1:A:51:LEU:HD11	2:B:92:PHE:HB3	2.03	0.41
1:A:93:LEU:O	1:A:94:GLN:C	2.64	0.41
1:C:365:LEU:O	1:C:370:GLN:HB2	2.19	0.41
1:E:418:ASN:C	1:E:418:ASN:ND2	2.77	0.41
1:E:424:VAL:HG11	1:E:478:TYR:CD1	2.55	0.41
1:E:482:PHE:HA	1:E:485:TYR:CD1	2.55	0.41
2:F:46:LEU:HD22	2:F:73:ARG:CZ	2.50	0.41
2:F:142:VAL:CG2	2:F:307:VAL:CG2	2.99	0.41
2:F:247:VAL:HA	2:F:248:PRO:HD3	1.87	0.41
3:K:150:MET:CE	3:K:161:ILE:HD11	2.50	0.41
1:G:248:ARG:HG3	1:G:248:ARG:NH1	2.31	0.41
1:G:396:ARG:HH21	1:G:400:GLU:HB3	1.86	0.41
1:G:488:ALA:O	1:G:490:PRO:HD3	2.20	0.41
2:H:352:ASN:ND2	2:H:437:LYS:HB2	2.35	0.41
2:H:362:GLN:C	2:H:362:GLN:HE21	2.28	0.41
2:H:391:THR:O	2:H:392:LEU:C	2.64	0.41
1:A:72:ASN:C	1:A:72:ASN:HD22	2.28	0.41
1:A:115:ASN:OD1	1:A:115:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:SER:OG	2:B:39:THR:N	2.53	0.41
3:I:150:MET:HE3	3:I:161:ILE:HD11	2.03	0.41
1:C:120:PHE:C	1:C:122:ARG:H	2.28	0.41
1:C:450:VAL:O	1:C:451:GLU:C	2.64	0.41
2:D:36:GLU:HA	2:D:36:GLU:OE1	2.21	0.41
2:D:246:GLY:O	2:D:248:PRO:HD3	2.21	0.41
3:J:140:GLN:O	3:J:140:GLN:HG3	2.20	0.41
1:E:64:GLN:HA	1:E:83:LYS:O	2.20	0.41
1:E:266:GLU:HG3	1:E:270:LYS:NZ	2.36	0.41
2:F:237:TRP:CD1	2:F:237:TRP:C	2.99	0.41
1:G:222:LEU:HD13	1:G:243:PHE:CZ	2.55	0.41
2:H:117:ASN:C	2:H:118:CYS:O	2.61	0.41
1:A:307:LEU:HB3	1:A:383:LEU:CD2	2.49	0.41
1:A:368:ILE:HD13	1:A:368:ILE:HA	1.86	0.41
1:A:449:GLN:HB3	1:A:453:ASP:OD2	2.20	0.41
2:B:218:ILE:HG22	2:B:219:ALA:N	2.36	0.41
2:B:240:GLU:OE1	2:B:259:TRP:HZ2	2.03	0.41
2:B:394:LEU:HG	2:B:396:SER:H	1.86	0.41
2:B:427:ASP:CB	2:B:429:THR:HG22	2.50	0.41
1:C:113:LEU:C	1:C:138:ARG:HH21	2.29	0.41
1:C:193:ARG:O	1:C:197:GLN:HG3	2.21	0.41
1:C:204:MET:HG3	1:C:205:GLU:N	2.36	0.41
1:C:409:LYS:HE2	1:C:468:TYR:O	2.19	0.41
2:D:52:LEU:HD11	2:D:78:ILE:HG13	2.02	0.41
2:D:83:ILE:HD12	2:D:98:ASP:HB3	2.03	0.41
2:D:231:TYR:CD2	2:D:267:ARG:HD2	2.56	0.41
1:E:7:LEU:HD23	1:E:7:LEU:O	2.21	0.41
1:E:422:GLU:C	1:E:424:VAL:N	2.78	0.41
2:F:192:ILE:CD1	2:F:200:ILE:HG12	2.51	0.41
1:G:235:LYS:NZ	1:G:235:LYS:HB3	2.35	0.41
1:G:446:SER:HB2	1:G:449:GLN:HG3	2.02	0.41
2:H:139:HIS:O	2:H:140:ILE:HG13	2.21	0.41
2:H:200:ILE:HD13	2:H:200:ILE:HA	1.96	0.41
2:H:354:GLN:HE21	2:H:354:GLN:CA	2.31	0.41
2:H:412:LEU:H	2:H:412:LEU:CD1	2.13	0.41
1:A:130:GLN:OE1	1:A:130:GLN:HA	2.21	0.41
2:B:193:LEU:O	2:B:194:PRO:C	2.63	0.41
2:B:371:SER:O	2:B:372:ALA:C	2.63	0.41
1:C:261:ASP:C	1:C:262:GLU:HG3	2.44	0.41
1:C:448:TYR:CD1	1:C:448:TYR:C	2.99	0.41
3:J:105:VAL:O	3:J:113:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:ILE:O	1:E:60:ILE:O	2.38	0.41
1:E:43:THR:HG23	1:E:75:PHE:CD1	2.56	0.41
1:E:297:ILE:HD12	1:E:297:ILE:O	2.21	0.41
1:E:441:ARG:NH2	1:E:453:ASP:OD1	2.54	0.41
1:G:214:TRP:O	1:G:217:ILE:HB	2.21	0.41
1:A:35:LEU:HD23	1:A:46:LEU:HD22	2.03	0.40
1:C:119:PHE:CE1	1:C:122:ARG:NH1	2.89	0.40
1:C:347:ARG:HH12	2:D:274:ARG:HD2	1.84	0.40
2:D:408:LEU:HD23	2:D:408:LEU:HA	1.94	0.40
3:J:115:ILE:CG2	3:J:129:ARG:HB3	2.51	0.40
1:E:65:VAL:HB	1:E:80:SER:O	2.20	0.40
1:E:195:HIS:HE1	1:E:341:LYS:HE2	1.86	0.40
1:E:377:GLU:HG2	1:E:381:LYS:CE	2.41	0.40
2:F:231:TYR:CG	2:F:267:ARG:NH1	2.89	0.40
3:K:108:LEU:HD21	3:K:171:LEU:HB2	2.03	0.40
3:K:170:VAL:HG13	3:K:171:LEU:N	2.36	0.40
1:G:293:ARG:HG2	1:G:305:TRP:NE1	2.36	0.40
1:G:407:ILE:CG2	1:G:409:LYS:HG3	2.48	0.40
1:G:416:MET:C	1:G:418:ASN:H	2.27	0.40
2:H:374:LEU:O	2:H:374:LEU:HD12	2.21	0.40
3:L:102:LEU:HG	3:L:114:GLU:HG2	2.02	0.40
1:A:229:THR:HG22	1:A:232:ARG:HB3	1.99	0.40
2:B:190:ARG:HH22	2:B:203:THR:HG23	1.87	0.40
2:B:252:ASP:O	2:B:254:PRO:HD3	2.21	0.40
2:B:350:PRO:HB3	2:B:435:LEU:HB3	2.02	0.40
2:B:409:SER:O	2:B:410:LYS:C	2.64	0.40
1:C:220:LYS:HD2	1:C:220:LYS:HA	1.90	0.40
1:C:301:THR:HG22	1:C:306:ILE:HG13	2.04	0.40
3:J:154:LYS:HB3	3:J:158:ASP:OD2	2.21	0.40
2:F:205:GLU:C	2:F:207:TYR:N	2.79	0.40
1:G:269:ILE:O	1:G:269:ILE:HG22	2.20	0.40
2:H:250:ASP:N	2:H:256:HIS:ND1	2.59	0.40
2:H:267:ARG:CG	2:H:267:ARG:O	2.69	0.40
1:C:248:ARG:C	1:C:250:GLY:N	2.78	0.40
1:C:311:LEU:HD12	1:C:311:LEU:HA	1.85	0.40
2:D:54:ILE:CG2	2:D:145:LEU:HD21	2.51	0.40
1:E:340:ILE:O	1:E:340:ILE:HG22	2.22	0.40
1:E:481:GLU:OE1	2:F:29:PRO:HD2	2.21	0.40
1:G:56:SER:HB3	1:G:101:SER:OG	2.21	0.40
2:H:125:ASN:HD22	2:H:130:PHE:HZ	1.69	0.40
2:H:148:ILE:O	2:H:152:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LEU:HD21	1:A:375:ILE:HG21	2.03	0.40
1:C:154:ARG:HB3	1:C:161:TYR:HB3	2.03	0.40
2:D:13:TRP:CZ3	2:D:116:PRO:HG2	2.56	0.40
2:D:52:LEU:HB2	2:D:138:PHE:CD2	2.56	0.40
2:D:422:GLU:HA	2:D:436:PHE:O	2.22	0.40
1:E:183:LEU:HD22	1:E:215:ILE:CD1	2.51	0.40
1:E:245:ASP:C	1:E:247:ILE:N	2.79	0.40
1:E:371:ALA:C	1:E:373:GLU:N	2.78	0.40
3:K:139:GLN:H	3:K:139:GLN:HG2	1.61	0.40
1:G:273:ASN:O	1:G:273:ASN:CG	2.64	0.40
2:H:386:GLU:O	2:H:388:LYS:N	2.49	0.40
3:L:107:THR:HG22	3:L:111:LYS:H	1.82	0.40
1:A:223:ALA:O	1:A:224:GLN:C	2.64	0.40
1:A:344:ASN:HB3	1:E:111:ASN:HD21	1.83	0.40
2:B:52:LEU:HB2	2:B:138:PHE:CE2	2.57	0.40
2:B:230:GLU:OE2	2:B:233:ARG:NH1	2.54	0.40
1:C:210:SER:O	1:C:211:HIS:HD2	2.05	0.40
1:C:526:SER:O	1:C:527:GLN:HB2	2.19	0.40
3:J:113:ILE:O	3:J:113:ILE:HG13	2.21	0.40
1:E:517:ASN:C	1:E:517:ASN:HD22	2.29	0.40
2:H:358:SER:O	2:H:359:ALA:C	2.63	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	518/531 (98%)	451 (87%)	54 (10%)	13 (2%)	4	17
1	C	513/531 (97%)	452 (88%)	52 (10%)	9 (2%)	6	25
1	E	515/531 (97%)	464 (90%)	42 (8%)	9 (2%)	7	26
1	G	512/531 (96%)	447 (87%)	56 (11%)	9 (2%)	6	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	430/434 (99%)	376 (87%)	46 (11%)	8 (2%)	6	23
2	D	430/434 (99%)	370 (86%)	50 (12%)	10 (2%)	5	19
2	F	429/434 (99%)	360 (84%)	55 (13%)	14 (3%)	3	13
2	H	429/434 (99%)	355 (83%)	60 (14%)	14 (3%)	3	13
3	I	84/88 (96%)	78 (93%)	4 (5%)	2 (2%)	4	18
3	J	74/88 (84%)	70 (95%)	1 (1%)	3 (4%)	2	9
3	K	74/88 (84%)	65 (88%)	6 (8%)	3 (4%)	2	9
3	L	74/88 (84%)	65 (88%)	5 (7%)	4 (5%)	1	5
All	All	4082/4212 (97%)	3553 (87%)	431 (11%)	98 (2%)	4	18

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	LEU
1	C	252	LEU
2	D	116	PRO
2	D	204	LEU
1	E	202	ASP
1	E	252	LEU
1	E	275	ALA
2	F	396	SER
3	K	119	PRO
2	H	116	PRO
2	H	204	LEU
2	H	241	GLN
2	H	244	GLY
2	H	361	LEU
3	L	119	PRO
3	L	163	GLY
1	A	63	ASN
1	A	79	SER
1	A	228	GLU
1	A	439	GLN
2	B	116	PRO
2	B	127	ILE
3	I	147	GLY
3	I	163	GLY
1	C	230	ASN
1	C	422	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	12	ASP
2	D	92	PHE
2	D	412	LEU
3	J	119	PRO
3	J	163	GLY
1	E	249	GLN
1	E	318	GLU
1	E	372	PRO
2	F	92	PHE
2	F	116	PRO
2	F	206	LEU
2	F	244	GLY
2	F	287	ARG
2	F	360	LYS
2	F	418	VAL
1	G	252	LEU
1	G	451	GLU
2	H	183	GLU
2	H	392	LEU
2	H	403	ARG
1	A	201	LEU
1	A	260	GLU
1	A	372	PRO
1	A	438	GLN
2	B	372	ALA
2	B	399	SER
1	C	36	ILE
1	C	259	PRO
2	D	357	PRO
2	F	132	ASP
2	F	166	ASP
3	K	152	ASP
1	G	190	PRO
1	G	517	ASN
2	H	88	LEU
2	H	267	ARG
3	L	124	GLU
1	A	271	ASN
2	B	204	LEU
2	B	375	GLN
1	C	79	SER
1	C	450	VAL

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Mol	Chain	Res	Type
1	E	36	ILE
1	E	190	PRO
1	E	276	LEU
2	F	375	GLN
1	G	250	GLY
2	H	272	ASN
1	A	133	GLU
1	A	200	ASP
2	B	242	PRO
2	B	377	LYS
2	D	88	LEU
2	D	90	ARG
3	J	152	ASP
2	F	211	VAL
2	F	242	PRO
2	F	320	ASN
3	K	163	GLY
1	G	179	ALA
2	H	352	ASN
1	A	259	PRO
2	D	16	ARG
2	D	241	GLN
1	G	280	GLN
2	H	194	PRO
3	L	154	LYS
1	G	419	PRO
2	H	242	PRO
1	C	55	GLY
1	C	190	PRO
1	G	450	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	452/462 (98%)	430 (95%)	22 (5%)	22 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	451/462 (98%)	429 (95%)	22 (5%)	22	54
1	E	448/462 (97%)	421 (94%)	27 (6%)	17	47
1	G	450/462 (97%)	430 (96%)	20 (4%)	25	59
2	B	378/382 (99%)	346 (92%)	32 (8%)	10	31
2	D	379/382 (99%)	357 (94%)	22 (6%)	18	49
2	F	377/382 (99%)	347 (92%)	30 (8%)	11	34
2	H	375/382 (98%)	351 (94%)	24 (6%)	16	44
3	I	73/74 (99%)	66 (90%)	7 (10%)	8	26
3	J	67/74 (90%)	62 (92%)	5 (8%)	12	37
3	K	67/74 (90%)	59 (88%)	8 (12%)	5	16
3	L	67/74 (90%)	65 (97%)	2 (3%)	36	70
All	All	3584/3672 (98%)	3363 (94%)	221 (6%)	16	46

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	47	LYS
1	A	66	SER
1	A	72	ASN
1	A	115	ASN
1	A	135	THR
1	A	158	LEU
1	A	171	VAL
1	A	214	TRP
1	A	220	LYS
1	A	228	GLU
1	A	238	LYS
1	A	252	LEU
1	A	264	ASN
1	A	285	ILE
1	A	293	ARG
1	A	364	LEU
1	A	418	ASN
1	A	422	GLU
1	A	437	LYS
1	A	479	VAL
1	A	503	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	18	ASN
2	B	77	VAL
2	B	82	THR
2	B	111	LEU
2	B	113	ASP
2	B	116	PRO
2	B	128	GLN
2	B	182	THR
2	B	188	ASN
2	B	197	THR
2	B	200	ILE
2	B	210	GLN
2	B	217	THR
2	B	218	ILE
2	B	223	ARG
2	B	236	GLN
2	B	240	GLU
2	B	249	LEU
2	B	269	SER
2	B	274	ARG
2	B	316	ILE
2	B	319	ASN
2	B	321	TYR
2	B	323	VAL
2	B	332	THR
2	B	342	ASN
2	B	353	ILE
2	B	362	GLN
2	B	377	LYS
2	B	385	LEU
2	B	413	LYS
2	B	421	GLN
3	I	101	MET
3	I	105	VAL
3	I	107	THR
3	I	109	THR
3	I	165	SER
3	I	170	VAL
3	I	171	LEU
1	C	10	GLU
1	C	34	CYS
1	C	43	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	46	LEU
1	C	72	ASN
1	C	90	MET
1	C	171	VAL
1	C	186	ASP
1	C	191	GLU
1	C	214	TRP
1	C	252	LEU
1	C	264	ASN
1	C	274	THR
1	C	293	ARG
1	C	297	ILE
1	C	311	LEU
1	C	344	ASN
1	C	359	ASN
1	C	364	LEU
1	C	422	GLU
1	C	435	PHE
1	C	497	LEU
2	D	11	LEU
2	D	12	ASP
2	D	39	THR
2	D	59	LEU
2	D	82	THR
2	D	111	LEU
2	D	114	ARG
2	D	116	PRO
2	D	128	GLN
2	D	149	ILE
2	D	197	THR
2	D	201	GLU
2	D	215	MET
2	D	236	GLN
2	D	316	ILE
2	D	321	TYR
2	D	323	VAL
2	D	334	THR
2	D	342	ASN
2	D	362	GLN
2	D	401	GLU
2	D	428	VAL
3	J	108	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	J	129	ARG
3	J	133	LYS
3	J	171	LEU
3	J	173	LEU
1	E	29	GLU
1	E	43	THR
1	E	72	ASN
1	E	78	ARG
1	E	146	SER
1	E	171	VAL
1	E	214	TRP
1	E	262	GLU
1	E	264	ASN
1	E	292	ASP
1	E	293	ARG
1	E	297	ILE
1	E	303	SER
1	E	309	ARG
1	E	311	LEU
1	E	359	ASN
1	E	364	LEU
1	E	372	PRO
1	E	406	THR
1	E	418	ASN
1	E	422	GLU
1	E	437	LYS
1	E	452	GLU
1	E	497	LEU
1	E	513	PHE
1	E	517	ASN
1	E	518	ASN
2	F	39	THR
2	F	65	LYS
2	F	82	THR
2	F	95	ARG
2	F	111	LEU
2	F	116	PRO
2	F	118	CYS
2	F	128	GLN
2	F	149	ILE
2	F	158	LEU
2	F	182	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	186	LYS
2	F	194	PRO
2	F	234	MET
2	F	241	GLN
2	F	242	PRO
2	F	286	LYS
2	F	292	VAL
2	F	316	ILE
2	F	319	ASN
2	F	321	TYR
2	F	342	ASN
2	F	349	LEU
2	F	355	PHE
2	F	374	LEU
2	F	375	GLN
2	F	377	LYS
2	F	381	ILE
2	F	430	THR
2	F	432	GLN
3	K	102	LEU
3	K	105	VAL
3	K	107	THR
3	K	119	PRO
3	K	144	ILE
3	K	170	VAL
3	K	171	LEU
3	K	173	LEU
1	G	6	LYS
1	G	43	THR
1	G	64	GLN
1	G	72	ASN
1	G	90	MET
1	G	117	PRO
1	G	154	ARG
1	G	190	PRO
1	G	200	ASP
1	G	202	ASP
1	G	214	TRP
1	G	215	ILE
1	G	264	ASN
1	G	292	ASP
1	G	293	ARG

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Mol	Chain	Res	Type
1	G	311	LEU
1	G	353	ASP
1	G	364	LEU
1	G	424	VAL
1	G	503	GLN
2	H	11	LEU
2	H	41	SER
2	H	82	THR
2	H	111	LEU
2	H	114	ARG
2	H	116	PRO
2	H	128	GLN
2	H	142	VAL
2	H	143	CYS
2	H	154	ILE
2	H	182	THR
2	H	188	ASN
2	H	201	GLU
2	H	213	PHE
2	H	223	ARG
2	H	316	ILE
2	H	319	ASN
2	H	321	TYR
2	H	362	GLN
2	H	364	VAL
2	H	366	ASP
2	H	374	LEU
2	H	381	ILE
2	H	392	LEU
3	L	119	PRO
3	L	171	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (163) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	64	GLN
1	A	72	ASN
1	A	77	GLN
1	A	175	HIS
1	A	178	ASN
1	A	197	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	209	HIS
1	A	224	GLN
1	A	264	ASN
1	A	277	ASN
1	A	320	GLN
1	A	322	ASN
1	A	359	ASN
1	A	418	ASN
1	A	438	GLN
1	A	447	ASN
1	A	480	HIS
1	A	518	ASN
1	A	533	GLN
2	B	19	HIS
2	B	74	GLN
2	B	87	ASN
2	B	128	GLN
2	B	139	HIS
2	B	210	GLN
2	B	270	GLN
2	B	272	ASN
2	B	320	ASN
2	B	325	ASN
2	B	342	ASN
2	B	351	GLN
2	B	389	ASN
2	B	395	GLN
2	B	439	HIS
3	I	168	HIS
1	C	11	GLN
1	C	37	ASN
1	C	48	ASN
1	C	72	ASN
1	C	195	HIS
1	C	211	HIS
1	C	224	GLN
1	C	264	ASN
1	C	280	GLN
1	C	320	GLN
1	C	344	ASN
1	C	359	ASN
1	C	370	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	386	ASN
1	C	418	ASN
1	C	439	GLN
1	C	447	ASN
1	C	512	GLN
2	D	18	ASN
2	D	74	GLN
2	D	87	ASN
2	D	128	GLN
2	D	139	HIS
2	D	210	GLN
2	D	212	ASN
2	D	241	GLN
2	D	270	GLN
2	D	282	GLN
2	D	296	ASN
2	D	319	ASN
2	D	325	ASN
2	D	342	ASN
2	D	351	GLN
2	D	362	GLN
2	D	375	GLN
2	D	421	GLN
2	D	432	GLN
3	J	141	GLN
3	J	151	ASN
3	J	168	HIS
1	E	37	ASN
1	E	48	ASN
1	E	64	GLN
1	E	72	ASN
1	E	111	ASN
1	E	115	ASN
1	E	195	HIS
1	E	197	GLN
1	E	211	HIS
1	E	224	GLN
1	E	264	ASN
1	E	271	ASN
1	E	273	ASN
1	E	277	ASN
1	E	296	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	322	ASN
1	E	359	ASN
1	E	360	HIS
1	E	386	ASN
1	E	418	ASN
1	E	436	HIS
1	E	438	GLN
1	E	439	GLN
1	E	447	ASN
1	E	517	ASN
1	E	518	ASN
2	F	18	ASN
2	F	19	HIS
2	F	32	HIS
2	F	74	GLN
2	F	87	ASN
2	F	128	GLN
2	F	131	ASN
2	F	210	GLN
2	F	212	ASN
2	F	236	GLN
2	F	272	ASN
2	F	319	ASN
2	F	325	ASN
2	F	342	ASN
2	F	352	ASN
2	F	362	GLN
2	F	375	GLN
2	F	395	GLN
2	F	407	ASN
2	F	439	HIS
3	K	172	GLN
1	G	37	ASN
1	G	72	ASN
1	G	178	ASN
1	G	197	GLN
1	G	264	ASN
1	G	271	ASN
1	G	277	ASN
1	G	343	GLN
1	G	344	ASN
1	G	359	ASN

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Mol	Chain	Res	Type
1	G	360	HIS
1	G	436	HIS
1	G	438	GLN
1	G	517	ASN
1	G	533	GLN
2	H	19	HIS
2	H	74	GLN
2	H	87	ASN
2	H	125	ASN
2	H	128	GLN
2	H	131	ASN
2	H	212	ASN
2	H	236	GLN
2	H	262	GLN
2	H	270	GLN
2	H	272	ASN
2	H	319	ASN
2	H	320	ASN
2	H	325	ASN
2	H	351	GLN
2	H	352	ASN
2	H	354	GLN
2	H	362	GLN
2	H	375	GLN
2	H	389	ASN
2	H	407	ASN
2	H	421	GLN
2	H	432	GLN
2	H	439	HIS
3	L	141	GLN

### 5.3.3 RNA [i](#)

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 i

### 6.1 Protein, DNA and RNA chains i

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	522/531 (98%)	0.06	4 (0%) 82 77	33, 67, 99, 122	0
1	C	520/531 (97%)	0.11	10 (1%) 66 58	41, 68, 102, 130	0
1	E	521/531 (98%)	-0.01	12 (2%) 61 52	32, 56, 116, 134	0
1	G	518/531 (97%)	0.15	11 (2%) 63 54	34, 64, 124, 137	0
2	B	432/434 (99%)	0.06	8 (1%) 66 58	36, 59, 109, 117	0
2	D	432/434 (99%)	0.19	5 (1%) 76 69	40, 70, 109, 117	0
2	F	431/434 (99%)	0.24	11 (2%) 57 48	37, 61, 116, 124	0
2	H	431/434 (99%)	0.35	11 (2%) 57 48	37, 69, 116, 122	0
3	I	86/88 (97%)	0.14	3 (3%) 47 38	47, 68, 93, 97	0
3	J	76/88 (86%)	0.31	2 (2%) 57 48	58, 77, 96, 98	0
3	K	76/88 (86%)	0.22	2 (2%) 57 48	56, 73, 90, 91	0
3	L	76/88 (86%)	0.64	4 (5%) 32 25	67, 93, 115, 121	0
All	All	4121/4212 (97%)	0.15	83 (2%) 65 56	32, 66, 113, 137	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	176	GLY	3.8
2	B	211	VAL	3.7
3	L	116	ASP	3.6
1	E	203	HIS	3.4
3	K	117	ILE	3.3
2	D	11	LEU	3.3
2	H	441	THR	3.3
1	C	259	PRO	3.2
1	E	252	LEU	3.1
1	E	233	ILE	3.0
1	C	6	LYS	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	211	VAL	3.0
1	C	517	ASN	2.9
3	L	117	ILE	2.8
1	A	6	LYS	2.8
2	H	213	PHE	2.8
1	G	209	HIS	2.8
2	H	386	GLU	2.7
2	F	319	ASN	2.7
1	G	276	LEU	2.7
2	B	11	LEU	2.7
2	B	381	ILE	2.7
1	A	259	PRO	2.7
1	E	278	THR	2.7
2	H	326	ASP	2.7
1	C	252	LEU	2.7
2	F	408	LEU	2.7
1	G	336	SER	2.6
2	F	211	VAL	2.6
2	F	385	LEU	2.6
2	H	211	VAL	2.6
3	I	91	ARG	2.5
1	E	209	HIS	2.5
2	H	374	LEU	2.5
1	E	202	ASP	2.5
1	E	331	ASP	2.5
2	H	408	LEU	2.5
2	B	408	LEU	2.4
1	C	111	ASN	2.4
1	C	260	GLU	2.4
1	E	210	SER	2.4
2	H	436	PHE	2.4
1	C	115	ASN	2.4
1	E	259	PRO	2.4
1	E	205	GLU	2.4
1	E	214	TRP	2.3
2	F	441	THR	2.3
2	H	438	LEU	2.3
1	G	332	MET	2.3
1	G	278	THR	2.3
1	E	6	LYS	2.3
2	D	394	LEU	2.3
2	F	418	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	222	PRO	2.3
2	B	392	LEU	2.3
1	G	234	PRO	2.3
1	G	517	ASN	2.2
2	F	417	LEU	2.2
2	F	243	PHE	2.2
2	B	419	ASP	2.2
2	D	417	LEU	2.2
2	D	12	ASP	2.2
2	B	385	LEU	2.2
1	C	7	LEU	2.2
3	J	162	LEU	2.2
1	A	207	LYS	2.1
2	F	216	ALA	2.1
1	C	208	ASP	2.1
2	B	166	ASP	2.1
2	H	387	GLY	2.1
3	K	176	GLY	2.1
3	I	93	ALA	2.1
2	F	353	ILE	2.1
2	F	355	PHE	2.1
3	J	115	ILE	2.1
1	C	205	GLU	2.1
1	G	226	TYR	2.1
1	G	246	LEU	2.0
1	A	204	MET	2.0
3	L	108	LEU	2.0
1	G	274	THR	2.0
3	L	156	ALA	2.0
1	G	6	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	ZN	B	1	1/1	0.99	0.05	65,65,65,65	0
4	ZN	D	3	1/1	0.99	0.06	74,74,74,74	0
4	ZN	F	4	1/1	0.99	0.04	62,62,62,62	0
4	ZN	H	2	1/1	0.99	0.05	80,80,80,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.