



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 07:52 PM EDT

PDB ID : 3DBH  
Title : Structural Dissection of a Gating Mechanism Preventing Misactivation of Ubiquitin by NEDD8's E1 (APPBP1-UBA3Arg190Ala-NEDD8Ala72Arg)  
Authors : Souphron, J.; Schulman, B.A.  
Deposited on : 2008-05-31  
Resolution : 2.85 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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

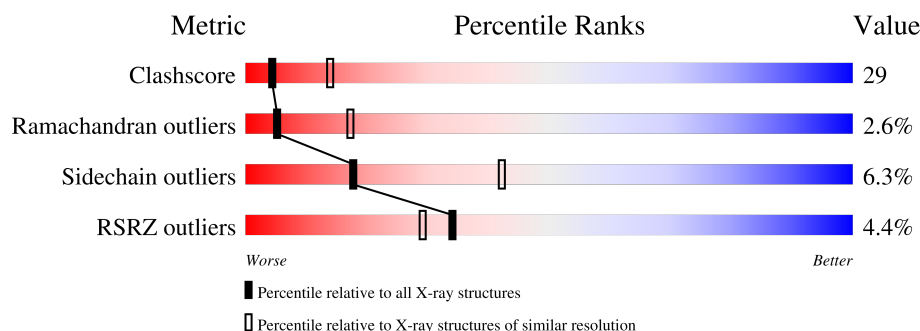
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	<div> <div>2%</div> <div>56%</div> <div>39%</div> <div>••</div> </div>
1	C	531	<div> <div>2%</div> <div>56%</div> <div>37%</div> <div>5%•</div> </div>
1	E	531	<div> <div>3%</div> <div>60%</div> <div>35%</div> <div>•••</div> </div>
1	G	531	<div> <div>4%</div> <div>55%</div> <div>37%</div> <div>5%•</div> </div>
2	B	434	<div> <div>5%</div> <div>52%</div> <div>42%</div> <div>5%</div> </div>
2	D	434	<div> <div>7%</div> <div>52%</div> <div>42%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	434	<div><div></div><div>6%</div><div>51%</div><div>42%</div><div>6% ..</div></div>
2	H	434	<div><div></div><div>7%</div><div>45%</div><div>44%</div><div>10% .</div></div>
3	I	88	<div><div></div><div>56%</div><div>38%</div><div>5% .</div></div>
3	J	88	<div><div></div><div>7%</div><div>40%</div><div>44%</div><div>. 14%</div></div>
3	K	88	<div><div></div><div>2%</div><div>39%</div><div>43%</div><div>5% 14%</div></div>
3	L	88	<div><div></div><div>5%</div><div>26%</div><div>55%</div><div>6% 14%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NEDD8-activating enzyme E1 regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4138	2621	704	797	16			
1	C	520	Total	C	N	O	S	0	0	0
			4125	2612	702	795	16			
1	E	523	Total	C	N	O	S	0	0	0
			4136	2618	705	798	15			
1	G	518	Total	C	N	O	S	0	0	0
			4113	2605	700	793	15			

There are 28 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	0	0
			3398	2172	574	635	17			
2	D	432	Total	C	N	O	S	0	0	0
			3402	2175	575	635	17			
2	F	431	Total	C	N	O	S	0	0	0
			3391	2169	573	632	17			
2	H	431	Total	C	N	O	S	0	0	0
			3383	2162	572	632	17			

There are 20 discrepancies between the modelled and reference sequences:

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

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

- Molecule 3 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	86	Total	C	N	O	S	0	0	0
			670	416	123	129	2			
3	J	76	Total	C	N	O	S	0	0	0
			606	381	107	116	2			
3	K	76	Total	C	N	O	S	0	0	0
			606	381	107	116	2			
3	L	76	Total	C	N	O	S	0	0	0
			606	381	107	116	2			

There are 52 discrepancies between the modelled and reference sequences:

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

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

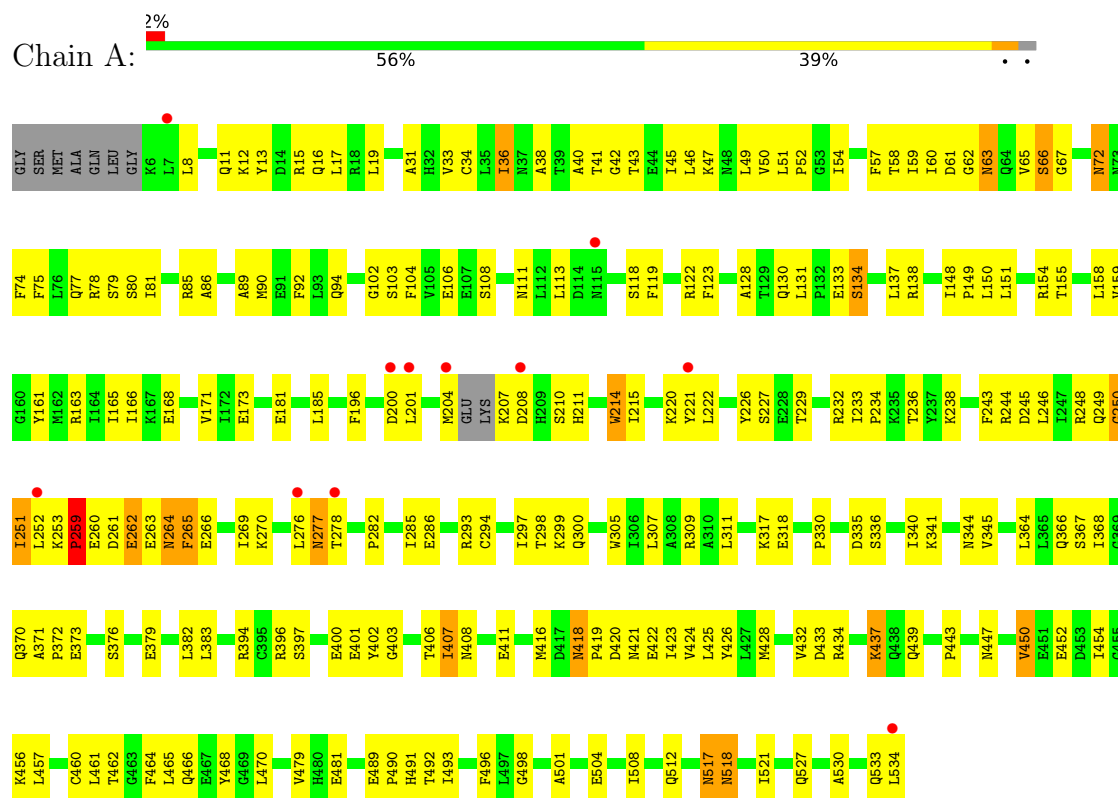
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

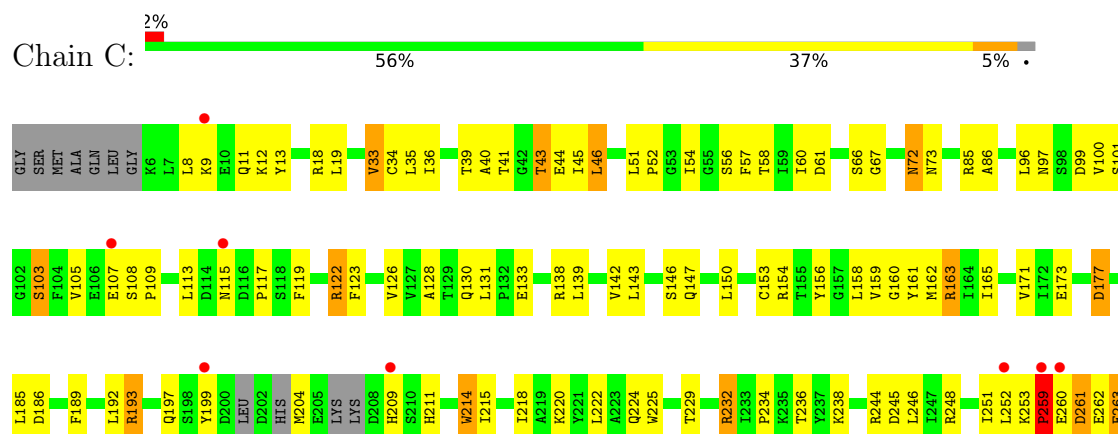
### 3 Residue-property plots

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.

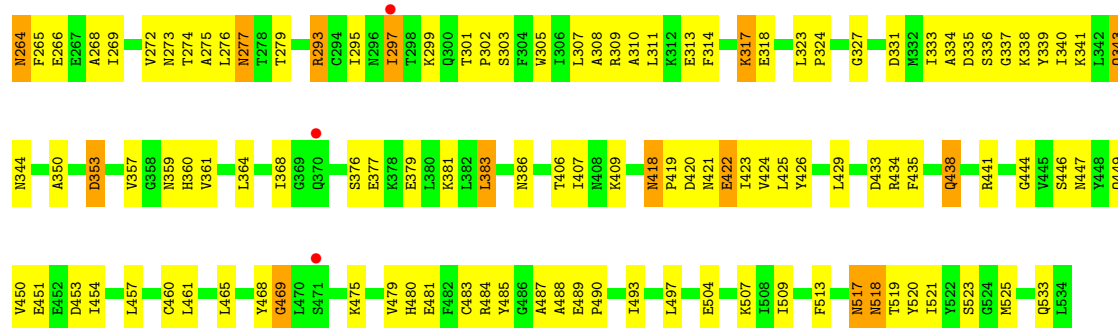
- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit



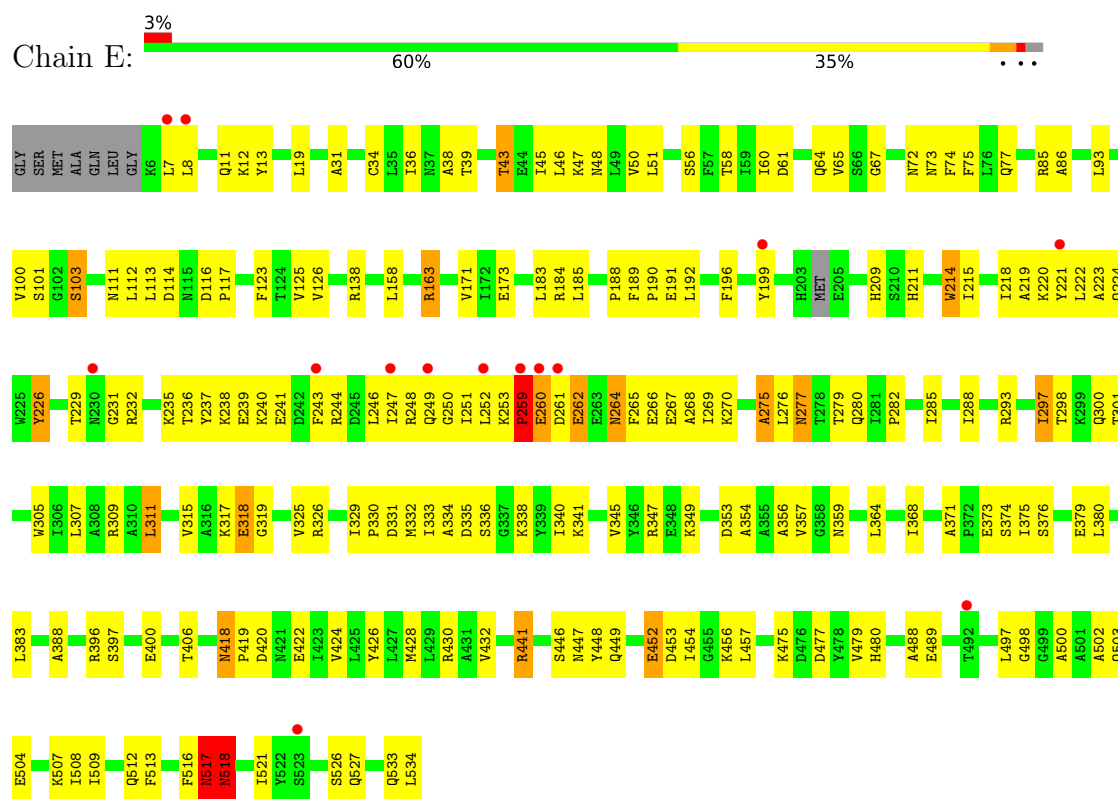
- Molecule 1: NEDD8-activating enzyme E1 regulatory subunit



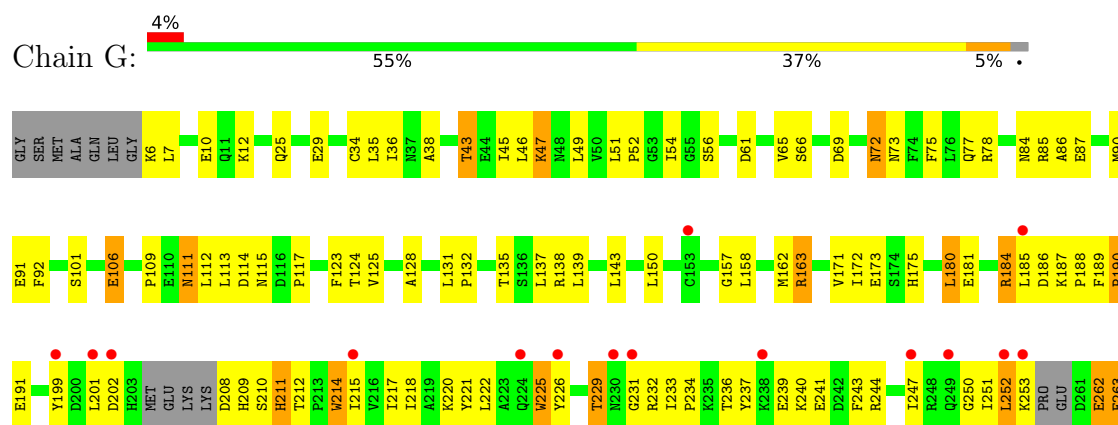


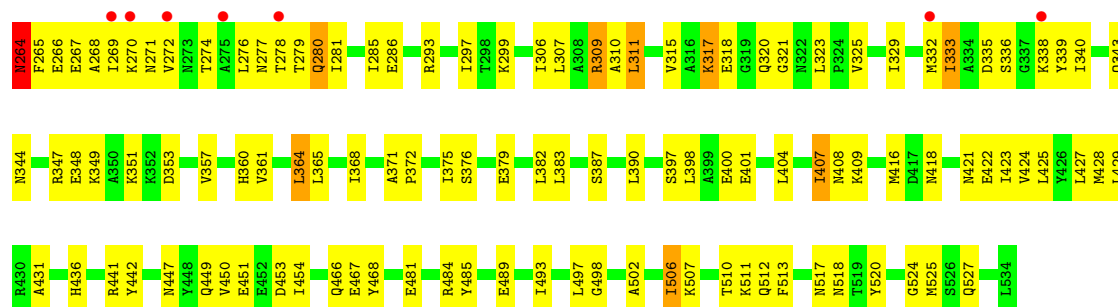


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

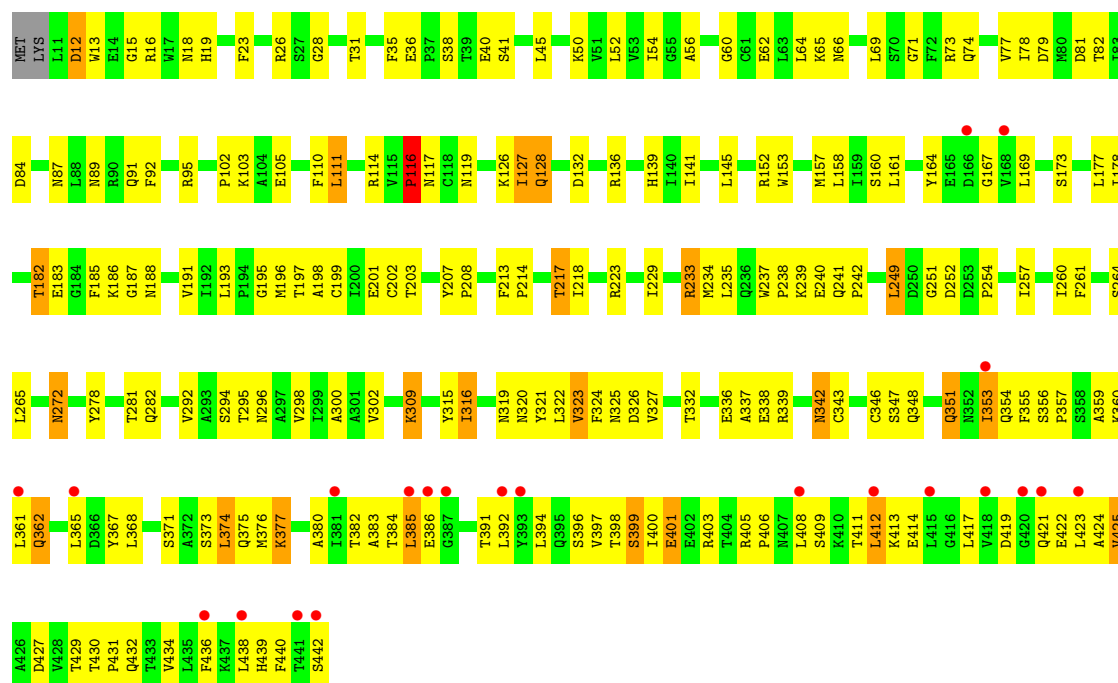


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

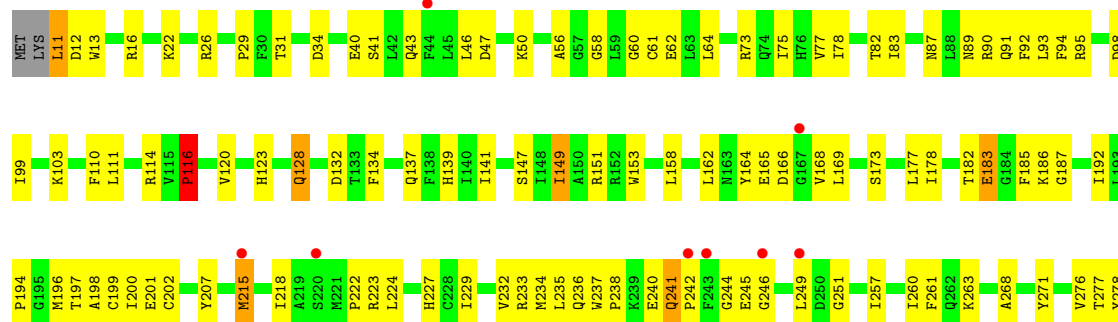


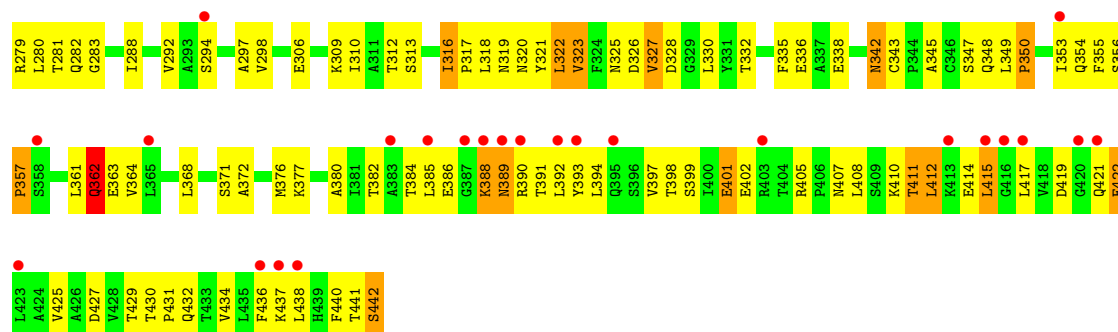


• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

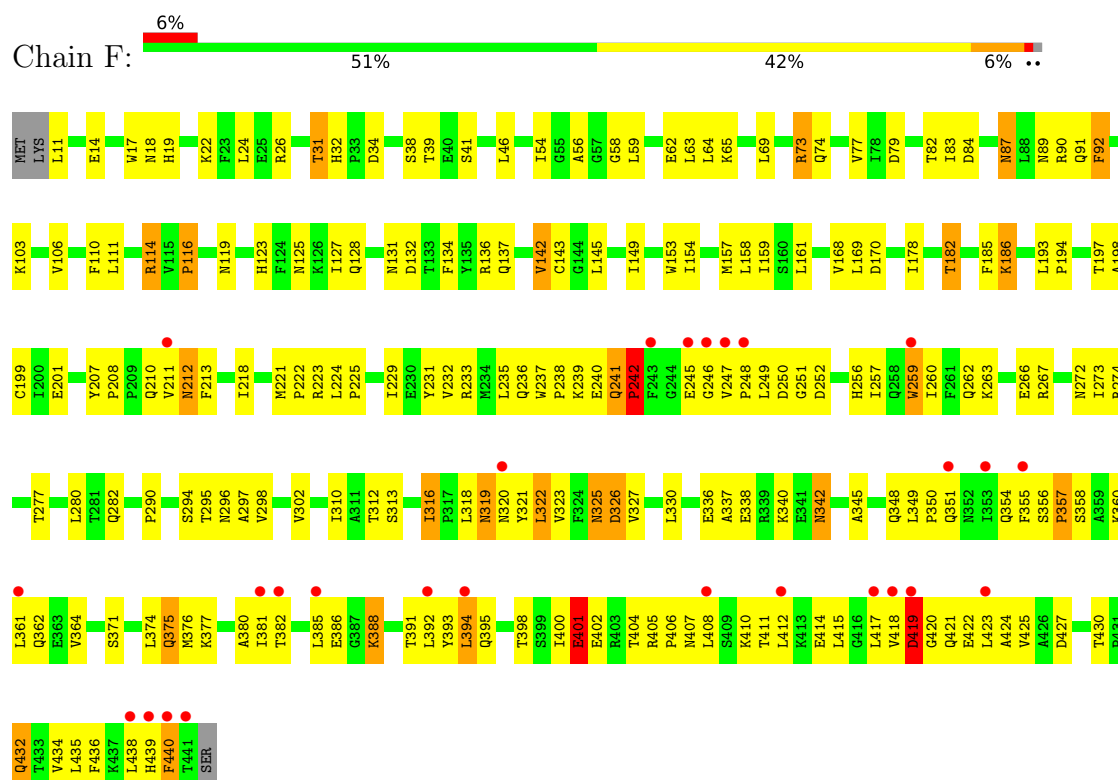


• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

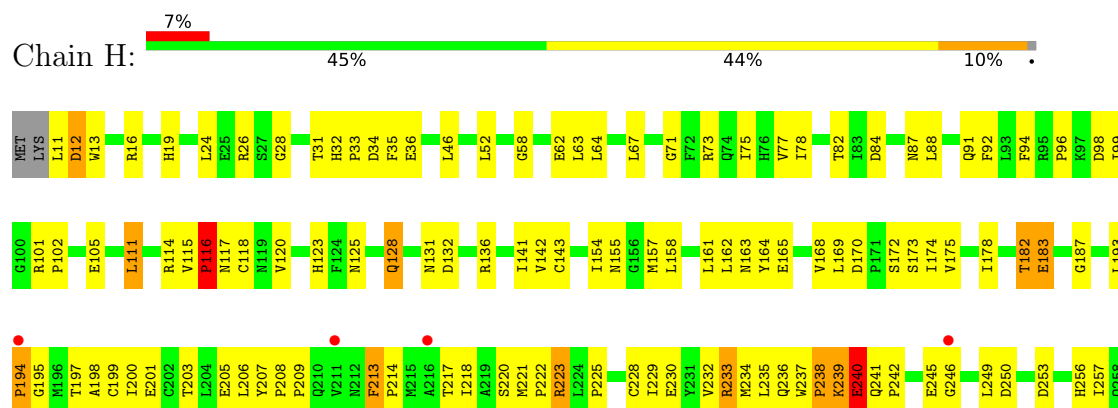


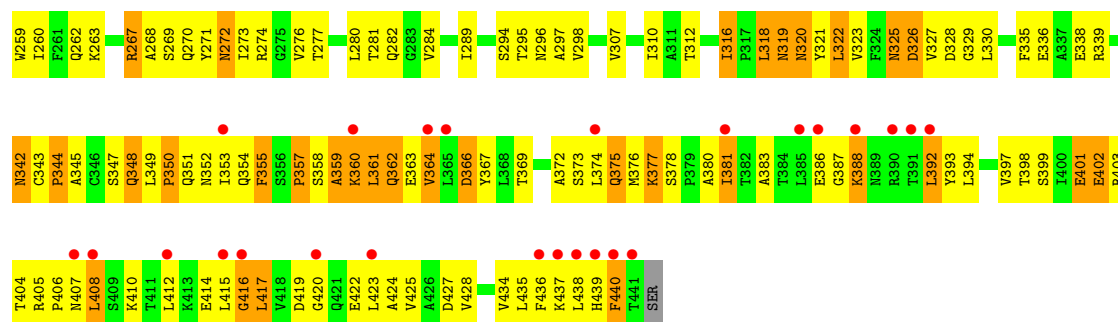


• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit



• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

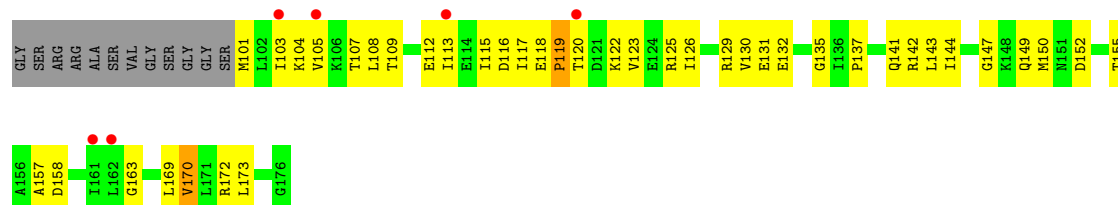




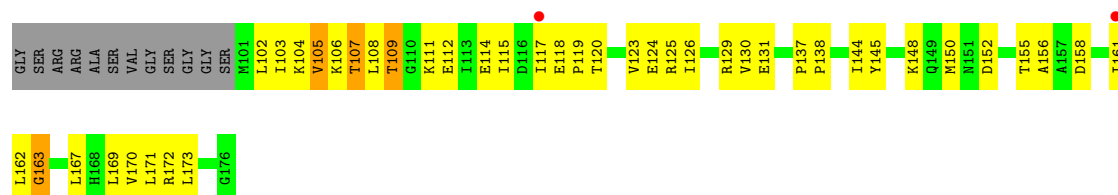
• Molecule 3: NEDD8



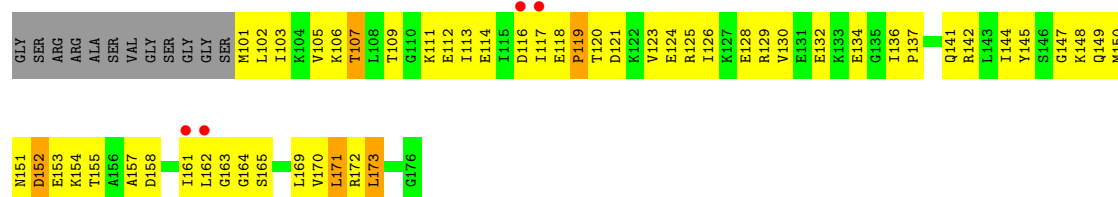
• Molecule 3: NEDD8



• 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, $\alpha$ , $\beta$ , $\gamma$	135.65Å 198.10Å 210.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 49.43 – 2.85	Depositor EDS
% Data completeness (in resolution range)	95.8 (50.00-2.85) 88.6 (49.43-2.85)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.224 , 0.274 0.222 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.9	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32578	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.43	0/4218	0.69	0/5706
1	C	0.41	0/4203	0.65	1/5682 (0.0%)
1	E	0.47	0/4216	0.71	2/5704 (0.0%)
1	G	0.45	0/4191	0.68	1/5668 (0.0%)
2	B	0.46	0/3476	0.76	5/4731 (0.1%)
2	D	0.47	1/3480 (0.0%)	0.72	4/4735 (0.1%)
2	F	0.48	0/3469	0.75	4/4723 (0.1%)
2	H	0.47	1/3461 (0.0%)	0.72	1/4713 (0.0%)
3	I	0.44	0/675	0.78	0/899
3	J	0.37	0/611	0.71	0/815
3	K	0.38	0/611	0.76	1/815 (0.1%)
3	L	0.36	0/611	0.72	0/815
All	All	0.45	2/33222 (0.0%)	0.71	19/45006 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	388	LYS	CE-NZ	6.17	1.64	1.49
2	H	143	CYS	CB-SG	-5.08	1.73	1.81

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	420	GLY	N-CA-C	-9.28	89.91	113.10
2	B	12	ASP	N-CA-C	-8.11	89.11	111.00
2	B	241	GLN	N-CA-C	-7.56	90.58	111.00
2	D	12	ASP	N-CA-C	-6.68	92.95	111.00
2	B	385	LEU	CA-CB-CG	-6.61	100.09	115.30
1	E	517	ASN	C-N-CA	-6.53	105.39	121.70
2	D	13	TRP	N-CA-C	6.25	127.88	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	518	ASN	N-CA-C	6.03	127.28	111.00
2	D	441	THR	N-CA-C	-5.95	94.94	111.00
2	F	419	ASP	N-CA-C	5.88	126.89	111.00
2	F	440	PHE	N-CA-C	5.54	125.96	111.00
3	K	173	LEU	CA-CB-CG	-5.48	102.69	115.30
1	G	209	HIS	N-CA-C	-5.45	96.28	111.00
2	D	348	GLN	N-CA-C	5.44	125.69	111.00
1	C	259	PRO	N-CA-C	-5.22	98.52	112.10
2	B	240	GLU	N-CA-C	-5.19	96.98	111.00
2	F	394	LEU	CA-CB-CG	5.19	127.24	115.30
2	H	320	ASN	N-CA-C	5.10	124.77	111.00
2	B	414	GLU	N-CA-C	-5.03	97.41	111.00

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	210	0
1	C	4125	0	4065	196	0
1	E	4136	0	4065	206	0
1	G	4113	0	4058	223	0
2	B	3398	0	3377	225	0
2	D	3402	0	3388	216	0
2	F	3391	0	3372	260	0
2	H	3383	0	3351	301	0
3	I	670	0	707	38	0
3	J	606	0	643	42	0
3	K	606	0	643	43	0
3	L	606	0	643	58	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	32578	0	32392	1878	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 29.

All (1878) 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	1.09	1.17
2:D:357:PRO:HA	2:D:412:LEU:HD12	1.22	1.15
2:F:419:ASP:HB2	2:F:438:LEU:HB2	1.29	1.13
2:F:241:GLN:HG2	2:F:245:GLU:HA	1.26	1.12
2:F:425:VAL:HB	2:F:434:VAL:HG13	1.31	1.10
2:D:382:THR:HG22	2:D:391:THR:HA	1.28	1.06
1:E:253:LYS:O	1:E:260:GLU:N	1.88	1.05
2:H:344:PRO:HG3	2:H:374:LEU:HD22	1.37	1.05
1:A:248:ARG:HA	1:A:251:ILE:HG13	1.37	1.05
2:F:362:GLN:HG2	2:F:408:LEU:HD22	1.38	1.04
2:B:412:LEU:HD12	2:B:440:PHE:CE2	1.94	1.03
2:B:342:ASN:HD22	2:B:342:ASN:N	1.58	1.00
2:H:272:ASN:HD22	2:H:272:ASN:N	1.55	1.00
2:D:320:ASN:HB2	2:D:336:GLU:HA	1.44	0.99
1:C:229:THR:HG22	1:C:232:ARG:HB2	1.45	0.99
3:L:107:THR:HG23	3:L:109:THR:H	1.27	0.98
2:F:316:ILE:HD12	2:F:316:ILE:H	1.27	0.98
2:H:158:LEU:HA	2:H:161:LEU:HD12	1.45	0.97
2:D:380:ALA:CB	2:D:394:LEU:HD12	1.93	0.97
2:B:361:LEU:HD22	2:B:408:LEU:HD23	1.46	0.97
2:H:229:ILE:HD13	2:H:281:THR:HA	1.47	0.96
2:B:316:ILE:H	2:B:316:ILE:HD12	1.29	0.96
1:A:163:ARG:CZ	1:A:518:ASN:HD21	1.80	0.95
2:H:316:ILE:H	2:H:316:ILE:HD12	1.31	0.95
2:B:272:ASN:HD22	2:B:272:ASN:N	1.63	0.95
2:D:342:ASN:HD22	2:D:342:ASN:H	1.15	0.95
2:H:338:GLU:HG3	3:L:148:LYS:HD3	1.47	0.95
2:D:357:PRO:CA	2:D:412:LEU:HD12	1.97	0.94
2:F:423:LEU:HD11	2:F:438:LEU:HD21	1.47	0.94
2:B:213:PHE:HB2	2:B:218:ILE:HD11	1.50	0.94
2:B:342:ASN:H	2:B:342:ASN:ND2	1.65	0.94
1:C:39:THR:HG22	1:C:489:GLU:OE1	1.67	0.92
1:C:253:LYS:O	1:C:260:GLU:N	2.02	0.92
1:G:489:GLU:H	2:H:19:HIS:HD2	1.17	0.92
2:H:354:GLN:HE22	2:H:439:HIS:HB3	1.34	0.92
2:B:400:ILE:H	2:B:400:ILE:HD12	1.35	0.92
2:F:393:TYR:HD1	2:F:404:THR:HG1	1.10	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:342:ASN:H	2:H:342:ASN:HD22	1.18	0.91
3:K:103:ILE:HG12	3:K:117:ILE:HD12	1.52	0.91
1:C:277:ASN:C	1:C:277:ASN:HD22	1.73	0.91
2:B:320:ASN:HD22	2:B:336:GLU:HG3	1.35	0.91
1:G:229:THR:HG21	1:G:232:ARG:HH21	1.36	0.91
1:E:297:ILE:HB	1:E:368:ILE:HD11	1.53	0.90
1:G:421:ASN:O	1:G:424:VAL:HG23	1.71	0.90
2:F:325:ASN:HD21	2:F:327:VAL:HG23	1.32	0.90
2:B:412:LEU:HD12	2:B:440:PHE:HE2	1.31	0.90
2:H:412:LEU:HD23	2:H:438:LEU:HD21	1.53	0.90
1:A:163:ARG:NE	1:A:518:ASN:HD21	1.68	0.89
1:C:517:ASN:HD22	1:C:518:ASN:H	1.19	0.89
2:H:354:GLN:NE2	2:H:439:HIS:HB3	1.87	0.89
1:G:447:ASN:ND2	2:H:26:ARG:HE	1.69	0.89
1:E:489:GLU:H	2:F:19:HIS:HD2	1.21	0.89
2:H:58:GLY:H	2:H:91:GLN:HG2	1.35	0.89
2:H:236:GLN:O	2:H:240:GLU:HB3	1.71	0.88
1:C:229:THR:CG2	1:C:232:ARG:HB2	2.04	0.88
1:A:253:LYS:O	1:A:260:GLU:N	2.06	0.88
1:C:299:LYS:HA	1:C:368:ILE:HG23	1.54	0.87
2:F:277:THR:HG23	2:F:280:LEU:H	1.38	0.87
1:E:335:ASP:HB3	1:E:338:LYS:HB2	1.56	0.87
2:F:32:HIS:CD2	2:F:34:ASP:H	1.92	0.87
3:K:123:VAL:HB	3:K:152:ASP:HA	1.53	0.87
1:E:61:ASP:HB3	1:E:86:ALA:HB2	1.57	0.86
2:B:342:ASN:HD22	2:B:342:ASN:H	0.86	0.85
2:F:325:ASN:ND2	2:F:327:VAL:HG23	1.92	0.85
2:B:217:THR:HB	2:B:223:ARG:HH21	1.41	0.85
2:F:419:ASP:HB2	2:F:438:LEU:CB	2.07	0.85
2:D:412:LEU:O	2:D:417:LEU:HB2	1.78	0.84
2:F:425:VAL:HB	2:F:434:VAL:CG1	2.08	0.84
3:J:123:VAL:HB	3:J:152:ASP:HA	1.58	0.84
2:D:277:THR:HG23	2:D:280:LEU:H	1.42	0.83
1:G:36:ILE:HB	1:G:128:ALA:HA	1.58	0.83
2:D:50:LYS:H	2:D:139:HIS:HD2	1.24	0.83
2:F:318:LEU:O	2:F:319:ASN:O	1.96	0.83
3:K:107:THR:HG22	3:K:109:THR:H	1.42	0.83
2:B:359:ALA:O	2:B:412:LEU:HD23	1.78	0.83
2:D:380:ALA:HB1	2:D:394:LEU:HD12	1.60	0.83
2:F:74:GLN:HE22	2:F:119:ASN:HD22	1.26	0.83
1:C:66:SER:HB2	2:H:262:GLN:HE22	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:LEU:HB3	1:C:383:LEU:HD13	1.60	0.83
2:F:134:PHE:O	2:F:137:GLN:HG2	1.78	0.83
2:B:362:GLN:HG2	2:B:408:LEU:HB3	1.58	0.83
1:C:204:MET:SD	1:C:252:LEU:HD13	2.19	0.83
1:G:184:ARG:NH1	1:G:325:VAL:HG22	1.94	0.82
1:A:210:SER:HB2	1:A:262:GLU:HG3	1.60	0.82
1:E:489:GLU:H	2:F:19:HIS:CD2	1.98	0.82
1:A:12:LYS:HE3	1:A:13:TYR:CE2	2.14	0.82
2:D:405:ARG:O	2:D:408:LEU:HB2	1.78	0.82
2:D:410:LYS:HB2	2:D:415:LEU:HD23	1.59	0.82
1:A:527:GLN:NE2	2:B:302:VAL:HG13	1.95	0.82
1:C:446:SER:HB2	1:C:449:GLN:HG3	1.60	0.82
2:D:412:LEU:HD13	2:D:440:PHE:CE2	2.14	0.81
2:D:149:ILE:H	2:D:149:ILE:CD1	1.86	0.81
2:D:320:ASN:HD22	2:D:336:GLU:HG3	1.45	0.81
1:G:489:GLU:H	2:H:19:HIS:CD2	1.99	0.81
2:F:185:PHE:HB3	2:F:326:ASP:HB2	1.62	0.81
3:L:106:LYS:HG3	3:L:112:GLU:HB2	1.63	0.81
2:F:410:LYS:HD3	2:F:414:GLU:HG3	1.61	0.81
1:C:297:ILE:H	1:C:297:ILE:HD13	1.44	0.80
1:G:214:TRP:HB2	1:G:268:ALA:HB2	1.62	0.80
1:G:215:ILE:H	1:G:332:MET:HE1	1.46	0.80
2:B:394:LEU:HD11	2:B:396:SER:OG	1.80	0.80
1:A:163:ARG:NH1	1:A:165:ILE:HG12	1.95	0.80
2:B:217:THR:HB	2:B:223:ARG:NH2	1.96	0.80
1:C:261:ASP:O	1:C:262:GLU:HG3	1.81	0.80
2:H:419:ASP:OD2	2:H:440:PHE:HB2	1.82	0.80
2:F:132:ASP:HA	2:F:157:MET:HE2	1.62	0.79
1:G:450:VAL:O	1:G:454:ILE:HG13	1.81	0.79
2:B:64:LEU:HB3	2:B:111:LEU:HD13	1.64	0.79
2:B:320:ASN:HB2	2:B:336:GLU:HA	1.63	0.79
2:D:397:VAL:HG12	2:D:398:THR:H	1.45	0.79
3:K:144:ILE:HD13	3:K:170:VAL:HB	1.65	0.79
1:A:236:THR:HG22	1:A:238:LYS:H	1.47	0.79
1:E:333:ILE:HA	2:F:223:ARG:NH2	1.97	0.79
2:F:32:HIS:HD2	2:F:34:ASP:H	1.25	0.79
2:H:392:LEU:HD23	2:H:392:LEU:H	1.48	0.79
2:H:272:ASN:N	2:H:272:ASN:ND2	2.26	0.79
1:G:307:LEU:HB3	1:G:383:LEU:CD2	2.12	0.79
2:H:203:THR:HB	2:H:206:LEU:HD12	1.65	0.79
1:A:150:LEU:HD23	1:A:165:ILE:HD12	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:THR:HG22	2:B:391:THR:HA	1.63	0.79
1:C:421:ASN:O	1:C:423:ILE:N	2.16	0.79
2:D:64:LEU:HB3	2:D:111:LEU:CD1	2.13	0.79
1:G:184:ARG:HH11	1:G:325:VAL:HG22	1.47	0.78
1:E:317:LYS:HB3	1:E:318:GLU:OE1	1.83	0.78
2:D:64:LEU:HB3	2:D:111:LEU:HD12	1.65	0.78
2:F:342:ASN:O	2:F:351:GLN:NE2	2.17	0.78
3:J:107:THR:HG23	3:J:109:THR:H	1.49	0.78
2:D:320:ASN:ND2	2:D:336:GLU:HG3	1.98	0.78
2:H:102:PRO:HG2	2:H:105:GLU:HB3	1.66	0.78
2:H:350:PRO:HB2	2:H:437:LYS:HG3	1.65	0.78
2:B:356:SER:CB	2:B:442:SER:HB3	2.14	0.78
2:F:380:ALA:CB	2:F:394:LEU:HD12	2.13	0.78
2:B:357:PRO:HD2	2:B:442:SER:O	1.84	0.77
2:F:418:VAL:O	2:F:418:VAL:HG13	1.83	0.77
1:G:229:THR:HG21	1:G:232:ARG:NH2	1.97	0.77
2:F:405:ARG:O	2:F:408:LEU:HB2	1.85	0.77
1:G:210:SER:HB3	1:G:262:GLU:OE2	1.83	0.77
2:D:249:LEU:HD11	2:D:260:ILE:HD11	1.67	0.77
2:D:357:PRO:HA	2:D:412:LEU:CD1	2.11	0.77
2:H:362:GLN:HA	2:H:408:LEU:HD22	1.65	0.77
2:D:397:VAL:HG12	2:D:398:THR:N	2.00	0.77
2:D:322:LEU:HD12	2:D:323:VAL:N	2.00	0.76
1:E:38:ALA:O	1:E:85:ARG:HD3	1.85	0.76
2:F:357:PRO:HG3	2:F:412:LEU:HD12	1.66	0.76
3:I:107:THR:HG22	3:I:109:THR:H	1.48	0.76
2:D:232:VAL:HG11	2:D:263:LYS:HB2	1.68	0.76
1:E:163:ARG:NH1	1:E:518:ASN:HD21	1.83	0.76
1:G:234:PRO:HA	1:G:239:GLU:HG2	1.66	0.76
1:A:168:GLU:HG3	1:A:394:ARG:HE	1.50	0.76
1:G:211:HIS:O	1:G:338:LYS:HD2	1.85	0.76
1:E:264:ASN:ND2	1:E:265:PHE:H	1.83	0.76
2:F:340:LYS:HB3	2:F:342:ASN:HD21	1.50	0.76
1:G:332:MET:HG2	1:G:339:TYR:HE1	1.51	0.76
1:G:397:SER:OG	1:G:400:GLU:HG3	1.85	0.76
2:D:405:ARG:HB3	2:D:405:ARG:HH11	1.49	0.75
1:G:61:ASP:HB3	1:G:86:ALA:HB2	1.67	0.75
2:B:353:ILE:O	2:B:439:HIS:HB2	1.86	0.75
2:D:229:ILE:HD13	2:D:281:THR:HA	1.66	0.75
2:D:241:GLN:HG3	2:D:245:GLU:HA	1.65	0.75
2:D:411:THR:O	2:D:415:LEU:HG	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:ARG:HH22	2:F:274:ARG:NH1	1.83	0.75
1:G:266:GLU:HA	1:G:269:ILE:HD12	1.68	0.75
2:F:62:GLU:HG2	2:F:297:ALA:HA	1.69	0.75
2:B:64:LEU:HD21	2:B:77:VAL:CG2	2.17	0.75
2:F:201:GLU:HG3	2:F:345:ALA:HB2	1.69	0.75
2:D:149:ILE:HD12	2:D:149:ILE:N	1.95	0.75
1:A:452:GLU:HG2	1:A:456:LYS:HE3	1.68	0.74
1:A:266:GLU:O	1:A:270:LYS:HG3	1.87	0.74
3:L:107:THR:HG22	3:L:111:LYS:H	1.52	0.74
2:F:342:ASN:HD22	2:F:342:ASN:H	1.34	0.74
1:A:94:GLN:HE22	1:A:102:GLY:H	1.31	0.74
2:D:398:THR:HA	2:D:401:GLU:HB3	1.70	0.74
1:E:253:LYS:O	1:E:260:GLU:HB3	1.88	0.74
1:G:218:ILE:O	1:G:222:LEU:HB2	1.88	0.74
1:G:307:LEU:HD13	1:G:383:LEU:HD22	1.70	0.74
2:H:373:SER:C	2:H:374:LEU:HG	2.08	0.74
2:D:257:ILE:HG21	2:D:282:GLN:NE2	2.02	0.73
1:G:299:LYS:HE2	1:G:368:ILE:O	1.88	0.73
1:G:263:GLU:O	1:G:266:GLU:N	2.20	0.73
3:L:107:THR:HG22	3:L:111:LYS:N	2.03	0.73
2:D:412:LEU:HB3	2:D:440:PHE:CZ	2.23	0.73
2:H:412:LEU:HD22	2:H:440:PHE:CE2	2.23	0.73
2:B:272:ASN:N	2:B:272:ASN:ND2	2.37	0.73
2:D:185:PHE:HB3	2:D:326:ASP:HB2	1.71	0.73
2:B:74:GLN:HE22	2:B:119:ASN:HD22	1.35	0.73
1:C:189:PHE:CE1	1:C:192:LEU:HB2	2.24	0.73
1:E:297:ILE:HB	1:E:368:ILE:CD1	2.19	0.73
1:E:447:ASN:HD22	2:F:26:ARG:HH21	1.34	0.73
2:B:427:ASP:HB3	2:B:429:THR:HG22	1.70	0.73
2:D:50:LYS:H	2:D:139:HIS:CD2	2.07	0.72
2:D:322:LEU:HD12	2:D:322:LEU:C	2.09	0.72
2:D:335:PHE:HE2	3:J:170:VAL:HG21	1.52	0.72
2:D:327:VAL:HG23	2:D:328:ASP:H	1.54	0.72
1:E:214:TRP:HB2	1:E:268:ALA:HB2	1.72	0.72
2:H:322:LEU:HD12	2:H:323:VAL:N	2.04	0.72
1:C:507:LYS:HG2	1:C:513:PHE:HB2	1.70	0.72
1:G:251:ILE:HG23	1:G:262:GLU:HB2	1.70	0.72
2:H:223:ARG:O	2:H:273:ILE:HD13	1.90	0.72
2:F:318:LEU:HD12	2:F:319:ASN:N	2.05	0.72
1:G:49:LEU:O	1:G:52:PRO:HD2	1.89	0.72
2:H:380:ALA:HB2	2:H:394:LEU:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ASN:ND2	2:B:336:GLU:HG3	2.05	0.72
2:B:419:ASP:OD2	2:B:440:PHE:HB2	1.88	0.72
1:E:236:THR:HG22	1:E:237:TYR:N	2.04	0.72
2:H:123:HIS:HB3	2:H:125:ASN:HD22	1.55	0.72
1:G:226:TYR:CZ	1:G:233:ILE:HG22	2.25	0.71
1:A:489:GLU:H	2:B:19:HIS:CD2	2.07	0.71
1:C:163:ARG:NH1	1:C:165:ILE:HG12	2.04	0.71
2:D:46:LEU:O	2:D:73:ARG:HB2	1.91	0.71
1:E:43:THR:HG21	1:E:73:ASN:OD1	1.91	0.71
2:F:350:PRO:HG3	2:F:435:LEU:HB2	1.72	0.71
1:A:78:ARG:O	1:A:81:ILE:HG13	1.91	0.71
2:H:321:TYR:HE2	2:H:323:VAL:HG22	1.56	0.71
1:E:61:ASP:OD2	1:E:85:ARG:HD2	1.91	0.71
2:H:322:LEU:HD12	2:H:322:LEU:C	2.11	0.71
1:E:236:THR:HG22	1:E:238:LYS:H	1.54	0.71
1:E:248:ARG:O	1:E:251:ILE:HG13	1.91	0.71
2:F:64:LEU:HD11	2:F:77:VAL:HG21	1.73	0.71
2:D:386:GLU:C	2:D:388:LYS:H	1.95	0.70
1:E:418:ASN:HD22	1:E:419:PRO:HD2	1.56	0.70
1:E:426:TYR:HB2	1:E:521:ILE:CD1	2.21	0.70
2:F:362:GLN:HE21	2:F:408:LEU:CD2	2.03	0.70
1:G:262:GLU:OE1	1:G:262:GLU:HA	1.90	0.70
1:G:187:LYS:HD2	1:G:279:THR:HG21	1.73	0.70
2:B:62:GLU:HG2	2:B:300:ALA:HB3	1.74	0.70
2:B:316:ILE:H	2:B:316:ILE:CD1	2.00	0.70
2:H:380:ALA:CB	2:H:394:LEU:HD12	2.20	0.70
1:G:309:ARG:HG3	1:G:364:LEU:HD21	1.73	0.70
2:H:405:ARG:HB3	2:H:405:ARG:HH11	1.56	0.70
2:H:132:ASP:HB3	2:H:157:MET:HE1	1.74	0.70
1:A:489:GLU:H	2:B:19:HIS:HD2	1.37	0.70
1:G:7:LEU:O	1:G:7:LEU:HD23	1.91	0.70
2:H:325:ASN:HD22	2:H:326:ASP:H	1.40	0.70
2:B:325:ASN:HD21	2:B:327:VAL:HG13	1.56	0.70
2:B:355:PHE:O	2:B:440:PHE:HD2	1.75	0.70
2:D:380:ALA:HB2	2:D:394:LEU:HD12	1.71	0.70
1:G:407:ILE:HG23	1:G:409:LYS:HG3	1.72	0.70
3:L:153:GLU:HA	3:L:153:GLU:OE2	1.92	0.70
2:D:277:THR:HG22	2:D:280:LEU:HB2	1.73	0.70
1:E:229:THR:CG2	1:E:232:ARG:HB2	2.22	0.69
1:E:265:PHE:O	1:E:269:ILE:HG13	1.92	0.69
1:G:6:LYS:N	1:G:6:LYS:HD2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:376:MET:HB3	2:H:427:ASP:OD2	1.91	0.69
2:B:430:THR:HG22	2:B:432:GLN:H	1.57	0.69
2:F:361:LEU:HD22	2:F:408:LEU:HD23	1.73	0.69
2:D:411:THR:H	2:D:414:GLU:HB3	1.57	0.69
2:F:398:THR:O	2:F:401:GLU:HG3	1.91	0.69
1:G:307:LEU:HB3	1:G:383:LEU:HD22	1.72	0.69
2:F:74:GLN:NE2	2:F:74:GLN:HA	2.07	0.69
2:F:357:PRO:HA	2:F:412:LEU:HD12	1.73	0.69
2:H:233:ARG:HG2	2:H:233:ARG:HH11	1.56	0.69
2:H:343:CYS:H	2:H:347:SER:HB3	1.57	0.69
2:H:412:LEU:HB2	2:H:440:PHE:HZ	1.57	0.69
2:B:412:LEU:CD1	2:B:440:PHE:HE2	2.05	0.69
1:A:163:ARG:NE	1:A:518:ASN:ND2	2.41	0.69
1:E:252:LEU:HD12	1:E:252:LEU:O	1.93	0.69
1:C:426:TYR:HB2	1:C:521:ILE:HD11	1.75	0.69
1:E:418:ASN:HD22	1:E:419:PRO:CD	2.06	0.69
1:G:297:ILE:CG2	1:G:368:ILE:HD11	2.22	0.69
2:H:381:ILE:H	2:H:381:ILE:HD12	1.58	0.69
1:E:447:ASN:ND2	2:F:26:ARG:HE	1.90	0.69
2:H:207:TYR:CE1	3:L:172:ARG:HD3	2.28	0.69
3:L:155:THR:HG23	3:L:158:ASP:H	1.58	0.69
2:B:185:PHE:HB3	2:B:326:ASP:OD2	1.93	0.69
1:C:224:GLN:NE2	1:C:246:LEU:HD11	2.06	0.69
2:H:352:ASN:HB3	2:H:439:HIS:HD2	1.56	0.69
1:E:36:ILE:O	1:E:60:ILE:O	2.10	0.68
1:G:404:LEU:HD21	1:G:467:GLU:HG2	1.75	0.68
2:H:178:ILE:HD11	2:H:310:ILE:HD12	1.74	0.68
2:B:403:ARG:HG3	2:B:403:ARG:HH11	1.58	0.68
1:C:51:LEU:HD11	2:D:92:PHE:HB3	1.76	0.68
2:B:13:TRP:CZ3	2:B:116:PRO:HG2	2.28	0.68
1:C:119:PHE:O	1:C:122:ARG:HG2	1.93	0.68
2:D:357:PRO:HD2	2:D:442:SER:CB	2.24	0.68
2:F:242:PRO:HG3	2:F:259:TRP:CZ2	2.28	0.68
1:C:128:ALA:HB1	1:C:131:LEU:HD11	1.75	0.68
2:F:342:ASN:HD22	2:F:342:ASN:N	1.87	0.68
2:H:58:GLY:N	2:H:91:GLN:HG2	2.08	0.68
1:E:34:CYS:HB2	1:E:123:PHE:CD2	2.29	0.68
1:G:309:ARG:CG	1:G:364:LEU:HD21	2.23	0.68
2:H:84:ASP:H	2:H:87:ASN:ND2	1.91	0.68
1:E:236:THR:O	1:E:240:LYS:HG3	1.94	0.68
2:F:411:THR:H	2:F:414:GLU:HB3	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:344:PRO:CG	2:H:374:LEU:HD22	2.20	0.68
1:C:158:LEU:HA	1:C:493:ILE:HG13	1.76	0.67
1:C:309:ARG:HD2	1:C:313:GLU:OE2	1.93	0.67
2:D:357:PRO:HD2	2:D:442:SER:HB2	1.75	0.67
1:E:340:ILE:HD11	2:F:273:ILE:CG1	2.23	0.67
1:A:12:LYS:HE3	1:A:13:TYR:CZ	2.29	0.67
1:E:51:LEU:HD11	2:F:92:PHE:HB3	1.75	0.67
2:F:154:ILE:O	2:F:158:LEU:HD23	1.94	0.67
2:H:162:LEU:HA	2:H:173:SER:OG	1.93	0.67
2:H:381:ILE:HD12	2:H:381:ILE:N	2.07	0.67
1:E:376:SER:OG	1:E:379:GLU:HG3	1.95	0.67
1:E:447:ASN:ND2	2:F:26:ARG:HH21	1.91	0.67
2:H:325:ASN:HD22	2:H:326:ASP:N	1.92	0.67
2:D:241:GLN:HE21	2:D:246:GLY:H	1.41	0.67
2:F:362:GLN:HE21	2:F:408:LEU:HD22	1.60	0.67
2:H:412:LEU:HD22	2:H:440:PHE:HE2	1.59	0.67
1:A:61:ASP:OD2	1:A:85:ARG:HD2	1.94	0.67
1:C:277:ASN:C	1:C:277:ASN:ND2	2.46	0.67
2:B:356:SER:HB2	2:B:442:SER:HB3	1.76	0.67
1:C:177:ASP:OD1	2:D:327:VAL:HG11	1.95	0.67
2:F:237:TRP:HB3	2:F:238:PRO:HD3	1.77	0.67
1:E:218:ILE:O	1:E:222:LEU:HB2	1.95	0.67
1:E:253:LYS:O	1:E:259:PRO:C	2.33	0.67
2:F:342:ASN:H	2:F:342:ASN:ND2	1.91	0.67
2:H:357:PRO:HA	2:H:440:PHE:CE2	2.30	0.67
2:H:405:ARG:HB3	2:H:405:ARG:NH1	2.10	0.67
2:B:214:PRO:HG2	2:B:217:THR:HG23	1.76	0.67
1:E:426:TYR:HB2	1:E:521:ILE:HD11	1.77	0.67
1:G:267:GLU:O	1:G:270:LYS:HG2	1.95	0.67
2:H:349:LEU:HB3	2:H:350:PRO:HD2	1.76	0.67
2:D:236:GLN:HE22	2:D:263:LYS:HD2	1.61	0.66
1:G:35:LEU:HD22	1:G:46:LEU:HD22	1.75	0.66
1:A:299:LYS:HG2	1:A:368:ILE:O	1.95	0.66
2:B:50:LYS:H	2:B:139:HIS:HD2	1.41	0.66
1:E:340:ILE:HD11	2:F:273:ILE:HG12	1.75	0.66
1:G:447:ASN:HD21	2:H:26:ARG:HE	1.43	0.66
1:A:428:MET:HE1	1:A:479:VAL:HA	1.76	0.66
1:C:317:LYS:HB3	1:C:318:GLU:OE1	1.94	0.66
1:E:253:LYS:O	1:E:260:GLU:CB	2.43	0.66
1:E:307:LEU:HB3	1:E:383:LEU:HD22	1.77	0.66
1:A:77:GLN:HG3	1:A:92:PHE:CZ	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:362:GLN:CG	2:F:408:LEU:HD22	2.19	0.66
3:L:123:VAL:HB	3:L:152:ASP:HA	1.76	0.66
2:B:207:TYR:CE2	3:I:172:ARG:HG2	2.31	0.66
2:D:362:GLN:HG2	2:D:408:LEU:HD22	1.78	0.66
1:E:489:GLU:N	2:F:19:HIS:HD2	1.94	0.66
2:F:380:ALA:HB2	2:F:394:LEU:HD12	1.78	0.66
1:G:210:SER:HA	1:G:264:ASN:OD1	1.96	0.66
1:C:113:LEU:O	1:C:117:PRO:HG3	1.95	0.66
2:B:64:LEU:HB3	2:B:111:LEU:CD1	2.26	0.66
2:B:157:MET:O	2:B:160:SER:HB3	1.96	0.66
2:D:207:TYR:CE2	3:J:172:ARG:HG2	2.31	0.66
3:J:125:ARG:HD3	3:J:129:ARG:HH21	1.61	0.66
2:H:377:LYS:HG2	2:H:428:VAL:CG2	2.26	0.66
2:B:28:GLY:O	2:B:31:THR:HG22	1.96	0.66
2:F:361:LEU:HD22	2:F:408:LEU:CD2	2.26	0.66
1:A:45:ILE:HG13	1:A:498:GLY:HA2	1.78	0.66
2:H:118:CYS:SG	2:H:120:VAL:HG23	2.35	0.66
2:H:412:LEU:HB2	2:H:440:PHE:CZ	2.31	0.66
2:B:38:SER:HB3	2:B:41:SER:OG	1.96	0.65
1:C:236:THR:HG22	1:C:238:LYS:H	1.61	0.65
2:D:425:VAL:HB	2:D:434:VAL:HG13	1.78	0.65
1:E:452:GLU:HG2	1:E:456:LYS:HE3	1.77	0.65
1:C:133:GLU:HG3	1:C:433:ASP:HB3	1.77	0.65
2:F:340:LYS:HB3	2:F:342:ASN:ND2	2.12	0.65
2:H:380:ALA:HB1	2:H:394:LEU:CD1	2.26	0.65
2:H:343:CYS:SG	2:H:344:PRO:HD2	2.36	0.65
3:L:107:THR:HA	3:L:169:LEU:HD12	1.79	0.65
2:B:417:LEU:HD12	2:B:421:GLN:NE2	2.12	0.65
2:B:153:TRP:CE2	2:B:431:PRO:HG3	2.31	0.65
2:D:241:GLN:HE21	2:D:246:GLY:N	1.95	0.65
2:F:419:ASP:HA	2:F:421:GLN:HG2	1.77	0.65
1:A:250:GLY:O	1:A:252:LEU:N	2.30	0.65
2:B:213:PHE:CB	2:B:218:ILE:HD11	2.27	0.65
3:I:103:ILE:HD11	3:I:117:ILE:HD12	1.78	0.65
3:L:141:GLN:O	3:L:142:ARG:HD3	1.96	0.65
1:A:282:PRO:HB2	1:A:285:ILE:HD13	1.79	0.64
1:A:317:LYS:HB3	1:A:318:GLU:OE1	1.97	0.64
1:E:336:SER:HB2	2:F:221:MET:HA	1.77	0.64
2:F:131:ASN:HD22	2:H:131:ASN:HB3	1.61	0.64
2:D:414:GLU:HG2	2:D:414:GLU:O	1.98	0.64
2:F:357:PRO:CA	2:F:412:LEU:HD12	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:208:PRO:HG3	3:L:171:LEU:HD11	1.79	0.64
2:B:353:ILE:HD11	2:B:367:TYR:HE2	1.62	0.64
1:A:397:SER:OG	1:A:400:GLU:HG3	1.98	0.64
2:F:357:PRO:CG	2:F:412:LEU:HD12	2.27	0.64
1:A:336:SER:O	1:A:340:ILE:HG12	1.97	0.64
2:B:214:PRO:HG2	2:B:217:THR:CG2	2.27	0.64
2:B:377:LYS:HE2	2:B:377:LYS:O	1.98	0.64
3:I:117:ILE:HD11	3:I:126:ILE:HG23	1.80	0.64
2:D:357:PRO:HD2	2:D:442:SER:OG	1.98	0.64
2:F:380:ALA:CB	2:F:394:LEU:CD1	2.76	0.64
1:G:49:LEU:C	1:G:52:PRO:HD2	2.17	0.64
2:H:62:GLU:HG2	2:H:297:ALA:HA	1.80	0.64
2:H:397:VAL:HG12	2:H:399:SER:H	1.63	0.64
2:F:322:LEU:HD13	2:F:323:VAL:N	2.12	0.64
2:F:402:GLU:O	2:F:406:PRO:HD3	1.98	0.64
1:G:211:HIS:HB3	1:G:335:ASP:HB2	1.80	0.64
1:A:108:SER:HB3	1:A:111:ASN:HB2	1.80	0.64
2:B:353:ILE:HG23	2:B:355:PHE:HD1	1.62	0.64
2:B:361:LEU:HB3	2:B:408:LEU:HA	1.78	0.64
2:B:398:THR:HA	2:B:401:GLU:HB3	1.80	0.64
2:D:233:ARG:NH1	2:D:234:MET:HB2	2.13	0.64
1:E:56:SER:HB3	1:E:101:SER:HB2	1.80	0.64
2:H:318:LEU:HD12	2:H:319:ASN:N	2.13	0.64
2:H:398:THR:HA	2:H:401:GLU:HB3	1.80	0.64
1:A:58:THR:HA	1:A:103:SER:O	1.98	0.63
2:F:54:ILE:HG22	2:F:145:LEU:HD21	1.80	0.63
2:F:376:MET:HB3	2:F:427:ASP:OD1	1.98	0.63
2:F:405:ARG:HB3	2:F:406:PRO:HD3	1.78	0.63
2:H:361:LEU:O	2:H:364:VAL:HG23	1.97	0.63
2:H:412:LEU:HD12	2:H:412:LEU:N	2.13	0.63
1:A:173:GLU:O	1:A:512:GLN:O	2.15	0.63
2:B:233:ARG:HH12	2:B:234:MET:HB2	1.63	0.63
1:G:265:PHE:O	1:G:269:ILE:HG13	1.98	0.63
2:H:373:SER:O	2:H:374:LEU:HD23	1.98	0.63
2:B:419:ASP:HB2	2:B:440:PHE:CD1	2.33	0.63
3:J:117:ILE:HD11	3:J:126:ILE:HG23	1.80	0.63
2:H:361:LEU:C	2:H:363:GLU:H	2.00	0.63
2:B:400:ILE:H	2:B:400:ILE:CD1	2.11	0.63
2:H:128:GLN:NE2	2:H:128:GLN:H	1.97	0.63
3:L:155:THR:HG22	3:L:158:ASP:OD2	1.98	0.63
1:E:454:ILE:HD13	1:E:480:HIS:ND1	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:178:ILE:HD12	2:H:307:VAL:HG22	1.79	0.63
1:E:332:MET:O	2:F:223:ARG:CZ	2.47	0.63
2:H:267:ARG:HH11	2:H:267:ARG:HG3	1.64	0.63
2:B:380:ALA:HB1	2:B:394:LEU:HD13	1.81	0.63
2:F:382:THR:HG22	2:F:391:THR:HG23	1.81	0.63
1:G:263:GLU:O	1:G:265:PHE:N	2.32	0.63
2:H:380:ALA:CB	2:H:394:LEU:CD1	2.77	0.63
2:B:233:ARG:HG3	2:B:249:LEU:HD21	1.81	0.63
2:D:385:LEU:HD12	2:D:390:ARG:HB3	1.79	0.63
1:E:173:GLU:O	1:E:512:GLN:O	2.17	0.63
1:E:236:THR:HG22	1:E:237:TYR:H	1.62	0.63
1:G:210:SER:HA	1:G:264:ASN:CG	2.19	0.63
2:B:380:ALA:CB	2:B:394:LEU:HD13	2.28	0.62
1:C:177:ASP:OD2	2:D:186:LYS:NZ	2.31	0.62
1:E:229:THR:HG22	1:E:232:ARG:HB2	1.80	0.62
1:G:229:THR:HG22	1:G:229:THR:O	1.99	0.62
3:I:104:LYS:O	3:I:166:VAL:HA	1.98	0.62
2:H:249:LEU:HD11	2:H:260:ILE:HD11	1.81	0.62
2:B:257:ILE:HD13	2:B:282:GLN:HG2	1.82	0.62
2:B:320:ASN:HB2	2:B:337:ALA:H	1.64	0.62
2:D:327:VAL:HG23	2:D:328:ASP:N	2.15	0.62
1:G:317:LYS:HG2	1:G:318:GLU:N	2.15	0.62
2:H:200:ILE:HD13	3:L:172:ARG:NH2	2.15	0.62
2:F:393:TYR:HD1	2:F:404:THR:OG1	1.81	0.62
2:B:217:THR:CB	2:B:223:ARG:NH2	2.63	0.62
2:D:56:ALA:HA	2:D:60:GLY:HA3	1.82	0.62
3:K:107:THR:HG22	3:K:109:THR:N	2.13	0.62
1:G:347:ARG:HH22	2:H:274:ARG:HD2	1.64	0.62
1:A:66:SER:OG	1:A:67:GLY:N	2.31	0.62
2:F:123:HIS:HB3	2:F:125:ASN:HD22	1.63	0.62
2:F:417:LEU:HA	2:F:421:GLN:HE22	1.65	0.62
2:B:321:TYR:HE2	2:B:323:VAL:HG13	1.65	0.62
3:I:103:ILE:CD1	3:I:117:ILE:HD12	2.30	0.62
1:G:158:LEU:HD13	1:G:493:ILE:HD11	1.82	0.62
2:H:233:ARG:HG2	2:H:233:ARG:NH1	2.13	0.62
1:E:447:ASN:HD22	2:F:26:ARG:NH2	1.97	0.62
2:B:343:CYS:O	2:B:347:SER:HB3	1.99	0.62
2:D:356:SER:HB2	2:D:442:SER:OG	1.99	0.62
1:G:360:HIS:O	1:G:364:LEU:HB2	2.00	0.62
2:H:267:ARG:HA	2:H:270:GLN:HE21	1.64	0.62
2:B:365:LEU:HD22	2:B:408:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:389:ASN:OD1	2:D:389:ASN:N	2.34	0.61
1:E:61:ASP:CB	1:E:86:ALA:HB2	2.29	0.61
1:G:293:ARG:HG2	1:G:293:ARG:HH11	1.65	0.61
1:C:204:MET:SD	1:C:252:LEU:CD1	2.87	0.61
1:E:12:LYS:O	2:F:89:ASN:HB3	2.00	0.61
2:F:410:LYS:HD2	2:F:415:LEU:HG	1.82	0.61
1:A:418:ASN:ND2	1:A:420:ASP:H	1.98	0.61
1:G:87:GLU:O	1:G:91:GLU:HG3	1.99	0.61
1:A:40:ALA:O	1:A:43:THR:HG22	2.00	0.61
2:D:430:THR:OG1	2:D:432:GLN:HG2	1.99	0.61
2:H:380:ALA:HB1	2:H:394:LEU:HD13	1.83	0.61
1:A:297:ILE:HD12	1:A:297:ILE:N	2.15	0.61
1:A:163:ARG:HH11	1:A:165:ILE:HG12	1.66	0.61
1:A:264:ASN:HD22	1:A:265:PHE:H	1.47	0.61
2:B:84:ASP:H	2:B:87:ASN:ND2	1.99	0.61
2:B:425:VAL:HG23	2:B:434:VAL:O	1.99	0.61
1:C:60:ILE:HD11	1:C:119:PHE:HE2	1.64	0.61
1:G:35:LEU:CD2	1:G:46:LEU:HD22	2.30	0.61
1:A:207:LYS:O	1:A:211:HIS:HB2	2.00	0.61
2:B:342:ASN:N	2:B:342:ASN:ND2	2.32	0.61
2:B:357:PRO:HA	2:B:440:PHE:CE2	2.36	0.61
2:F:201:GLU:HG3	2:F:345:ALA:CB	2.30	0.61
2:H:32:HIS:CD2	2:H:34:ASP:H	2.17	0.61
2:H:373:SER:O	2:H:374:LEU:CD2	2.49	0.61
3:L:170:VAL:HG13	3:L:171:LEU:N	2.16	0.61
1:A:307:LEU:HD22	1:A:383:LEU:HD22	1.81	0.61
2:D:312:THR:O	2:D:313:SER:HB2	2.01	0.61
2:D:407:ASN:OD1	2:D:415:LEU:HD22	2.01	0.61
2:F:74:GLN:HA	2:F:74:GLN:HE21	1.64	0.61
1:G:349:LYS:HE3	1:G:353:ASP:OD1	2.00	0.61
2:B:233:ARG:NH1	2:B:234:MET:HB2	2.16	0.60
1:C:12:LYS:HE3	1:C:13:TYR:CZ	2.36	0.60
2:F:225:PRO:O	2:F:229:ILE:HG13	2.01	0.60
2:H:361:LEU:C	2:H:363:GLU:N	2.53	0.60
1:A:159:VAL:HG22	1:A:425:LEU:HD13	1.83	0.60
1:A:166:ILE:HD11	1:A:508:ILE:HD13	1.83	0.60
1:A:371:ALA:C	1:A:373:GLU:H	2.03	0.60
1:C:138:ARG:O	1:C:142:VAL:HG23	2.01	0.60
2:D:62:GLU:HG2	2:D:297:ALA:HA	1.82	0.60
2:H:174:ILE:HG23	2:H:194:PRO:HG2	1.83	0.60
2:H:272:ASN:HD22	2:H:272:ASN:H	1.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:342:ASN:HD22	2:D:342:ASN:N	1.90	0.60
1:E:500:ALA:HB1	2:F:330:LEU:HD21	1.82	0.60
1:A:248:ARG:C	1:A:250:GLY:H	2.05	0.60
1:A:403:GLY:O	1:A:407:ILE:HB	2.01	0.60
3:L:107:THR:HG23	3:L:109:THR:N	2.08	0.60
3:L:162:LEU:O	3:L:164:GLY:N	2.34	0.60
1:A:207:LYS:O	1:A:211:HIS:CG	2.55	0.60
1:C:224:GLN:HE22	1:C:246:LEU:HD11	1.66	0.60
1:E:248:ARG:C	1:E:250:GLY:H	2.05	0.60
2:H:234:MET:HG2	2:H:235:LEU:HD22	1.82	0.60
1:A:63:ASN:ND2	1:A:63:ASN:H	2.00	0.60
1:C:229:THR:HG22	1:C:232:ARG:CB	2.27	0.60
2:H:357:PRO:HA	2:H:440:PHE:CZ	2.37	0.60
2:B:203:THR:OG1	3:I:172:ARG:NH1	2.34	0.60
1:C:447:ASN:ND2	2:D:26:ARG:HE	1.99	0.60
3:J:103:ILE:HD11	3:J:117:ILE:HD12	1.84	0.60
2:F:32:HIS:HD2	2:F:34:ASP:N	1.96	0.60
2:F:89:ASN:OD1	2:F:90:ARG:HG2	2.00	0.60
2:F:132:ASP:CA	2:F:157:MET:HE2	2.31	0.60
3:K:155:THR:HG22	3:K:158:ASP:CG	2.21	0.60
3:I:144:ILE:HD12	3:I:170:VAL:HB	1.84	0.59
2:D:380:ALA:HB1	2:D:394:LEU:CD1	2.30	0.59
2:B:353:ILE:HD11	2:B:367:TYR:CE2	2.37	0.59
1:C:158:LEU:HD12	1:C:525:MET:HG2	1.83	0.59
2:F:241:GLN:CG	2:F:245:GLU:HA	2.17	0.59
2:F:349:LEU:HD12	2:F:349:LEU:N	2.17	0.59
1:A:366:GLN:C	1:A:368:ILE:H	2.04	0.59
2:D:277:THR:HG23	2:D:280:LEU:N	2.17	0.59
2:F:251:GLY:O	2:F:257:ILE:HD11	2.02	0.59
2:F:380:ALA:HB1	2:F:394:LEU:CD1	2.32	0.59
1:G:307:LEU:HB3	1:G:383:LEU:HD21	1.81	0.59
1:G:481:GLU:OE1	1:G:484:ARG:HD3	2.03	0.59
2:B:81:ASP:HB2	2:B:103:LYS:HD2	1.84	0.59
3:J:117:ILE:CD1	3:J:126:ILE:HG23	2.33	0.59
2:F:382:THR:OG1	2:F:424:ALA:HB3	2.02	0.59
2:F:423:LEU:CD1	2:F:438:LEU:HD21	2.28	0.59
1:G:201:LEU:HG	1:G:220:LYS:HG2	1.83	0.59
2:H:342:ASN:HD22	2:H:342:ASN:N	1.91	0.59
1:A:133:GLU:HG3	1:A:433:ASP:HB3	1.84	0.59
1:A:428:MET:O	1:A:432:VAL:HG23	2.02	0.59
2:B:405:ARG:HB3	2:B:406:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:125:ARG:O	3:K:129:ARG:HG2	2.02	0.59
1:G:78:ARG:HG3	2:H:13:TRP:CE3	2.37	0.59
1:G:347:ARG:HH22	2:H:274:ARG:HH11	1.50	0.59
1:A:264:ASN:HD22	1:A:265:PHE:N	2.00	0.59
2:B:74:GLN:NE2	2:B:119:ASN:HD22	2.01	0.59
2:B:237:TRP:HB3	2:B:238:PRO:HD3	1.84	0.59
1:C:108:SER:OG	1:C:109:PRO:HD2	2.03	0.59
1:C:438:GLN:O	1:C:438:GLN:HG2	2.02	0.59
2:D:342:ASN:H	2:D:342:ASN:ND2	1.95	0.59
2:D:382:THR:HA	2:D:392:LEU:HD13	1.83	0.59
2:F:349:LEU:CD1	2:F:349:LEU:H	2.15	0.59
2:H:419:ASP:OD1	2:H:420:GLY:N	2.35	0.59
1:A:46:LEU:O	1:A:50:VAL:HG23	2.03	0.59
2:B:380:ALA:HB2	2:B:394:LEU:CD1	2.32	0.59
1:C:34:CYS:HB2	1:C:123:PHE:CE2	2.38	0.59
1:C:61:ASP:OD2	1:C:85:ARG:HD2	2.03	0.59
1:A:229:THR:CG2	1:A:232:ARG:HB3	2.32	0.59
1:A:253:LYS:O	1:A:259:PRO:C	2.41	0.59
2:H:209:PRO:HD3	3:L:142:ARG:NH2	2.17	0.59
2:H:225:PRO:HB3	2:H:276:VAL:HG22	1.84	0.59
1:A:248:ARG:HA	1:A:251:ILE:CG1	2.24	0.59
2:B:356:SER:HB2	2:B:442:SER:CB	2.33	0.59
1:C:434:ARG:HD3	1:C:460:CYS:HB3	1.83	0.58
2:D:438:LEU:HD21	2:D:440:PHE:HE2	1.68	0.58
2:F:54:ILE:CG2	2:F:145:LEU:HD21	2.33	0.58
1:E:266:GLU:HG3	1:E:270:LYS:HE3	1.85	0.58
2:H:289:ILE:O	2:H:289:ILE:HG22	2.01	0.58
2:H:392:LEU:HD23	2:H:392:LEU:N	2.15	0.58
1:A:36:ILE:HB	1:A:128:ALA:HA	1.85	0.58
2:B:320:ASN:CB	2:B:337:ALA:H	2.17	0.58
2:H:253:ASP:HB3	2:H:256:HIS:HB2	1.84	0.58
1:C:311:LEU:HD13	1:C:383:LEU:HD21	1.84	0.58
2:F:362:GLN:NE2	2:F:408:LEU:HD13	2.19	0.58
1:C:307:LEU:HB3	1:C:383:LEU:CD1	2.33	0.58
1:G:56:SER:HB3	1:G:101:SER:HB2	1.85	0.58
2:F:208:PRO:HG3	3:K:171:LEU:HD11	1.85	0.58
1:G:347:ARG:HH22	2:H:274:ARG:NH1	2.01	0.58
2:B:50:LYS:H	2:B:139:HIS:CD2	2.21	0.58
2:D:165:GLU:N	2:D:168:VAL:O	2.37	0.58
1:E:196:PHE:CD1	1:E:219:ALA:HB1	2.39	0.58
2:F:197:THR:CG2	2:F:198:ALA:N	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:401:GLU:OE2	2:F:402:GLU:HG3	2.04	0.58
2:H:193:LEU:H	2:H:197:THR:HB	1.69	0.58
1:A:233:ILE:HD11	1:A:276:LEU:HD22	1.85	0.58
2:B:235:LEU:O	2:B:238:PRO:HD2	2.04	0.58
1:G:61:ASP:CB	1:G:86:ALA:HB2	2.34	0.58
1:G:241:GLU:O	1:G:244:ARG:HB2	2.03	0.58
1:A:78:ARG:HG3	1:A:81:ILE:HD11	1.85	0.58
2:B:357:PRO:HG3	2:B:440:PHE:CD1	2.38	0.58
2:F:131:ASN:HB3	2:H:131:ASN:HD22	1.68	0.58
3:K:170:VAL:HG13	3:K:171:LEU:N	2.19	0.58
2:H:217:THR:HG22	2:H:221:MET:HG3	1.84	0.58
2:H:63:LEU:HD22	2:H:142:VAL:HG11	1.86	0.57
2:B:35:PHE:O	2:B:36:GLU:HG3	2.04	0.57
2:F:357:PRO:HA	2:F:412:LEU:CD1	2.34	0.57
1:G:299:LYS:HG2	1:G:368:ILE:HG23	1.86	0.57
1:G:423:ILE:O	1:G:427:LEU:HG	2.05	0.57
2:H:158:LEU:HD23	2:H:161:LEU:CD1	2.33	0.57
2:H:201:GLU:HG2	2:H:345:ALA:HB2	1.86	0.57
2:B:13:TRP:HZ3	2:B:116:PRO:HG2	1.66	0.57
1:C:113:LEU:HB3	1:C:138:ARG:HH21	1.69	0.57
2:F:87:ASN:HD22	2:F:103:LYS:HE2	1.69	0.57
2:F:178:ILE:HD13	2:F:178:ILE:N	2.18	0.57
2:B:412:LEU:HD23	2:B:412:LEU:N	2.18	0.57
1:C:66:SER:HB2	2:H:262:GLN:NE2	2.16	0.57
2:H:342:ASN:H	2:H:342:ASN:ND2	1.97	0.57
3:I:117:ILE:HG22	3:I:118:GLU:N	2.19	0.57
1:C:126:VAL:O	1:C:150:LEU:HD12	2.04	0.57
1:A:61:ASP:CB	1:A:86:ALA:HB2	2.34	0.57
2:D:241:GLN:HB3	2:D:244:GLY:O	2.05	0.57
3:J:104:LYS:HE3	3:J:112:GLU:OE2	2.05	0.57
1:E:285:ILE:N	1:E:285:ILE:HD12	2.19	0.57
1:E:500:ALA:HB1	2:F:330:LEU:CD2	2.35	0.57
2:H:377:LYS:HG2	2:H:428:VAL:HG22	1.87	0.57
2:H:383:ALA:H	2:H:392:LEU:HD21	1.70	0.57
3:I:142:ARG:HB2	3:I:170:VAL:O	2.05	0.57
2:H:46:LEU:HD23	2:H:71:GLY:O	2.05	0.57
1:C:128:ALA:HB1	1:C:131:LEU:CD1	2.35	0.57
1:C:185:LEU:HD12	1:C:275:ALA:HB1	1.86	0.57
2:H:213:PHE:HB2	2:H:218:ILE:HD11	1.85	0.57
2:H:240:GLU:HG3	2:H:240:GLU:O	2.04	0.57
1:G:481:GLU:OE1	1:G:481:GLU:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:234:MET:C	2:H:235:LEU:HD22	2.24	0.57
2:B:325:ASN:ND2	2:B:327:VAL:HG13	2.18	0.57
1:C:34:CYS:HB2	1:C:123:PHE:CD2	2.40	0.57
1:G:43:THR:HG23	1:G:75:PHE:HD1	1.70	0.57
2:B:257:ILE:HG22	2:B:278:TYR:CE1	2.40	0.56
2:B:397:VAL:HG12	2:B:399:SER:H	1.69	0.56
2:D:64:LEU:HB3	2:D:111:LEU:HD11	1.87	0.56
1:E:356:ALA:O	1:E:359:ASN:HB2	2.05	0.56
3:K:107:THR:CG2	3:K:108:LEU:N	2.68	0.56
1:G:201:LEU:CD2	1:G:221:TYR:HE1	2.18	0.56
2:H:183:GLU:HB3	3:L:173:LEU:HD22	1.87	0.56
1:C:295:ILE:O	1:C:309:ARG:NH2	2.34	0.56
1:C:309:ARG:HB3	1:C:364:LEU:HD21	1.86	0.56
3:J:103:ILE:CD1	3:J:117:ILE:HD12	2.35	0.56
2:F:419:ASP:OD2	2:F:439:HIS:CA	2.53	0.56
2:B:128:GLN:NE2	2:B:128:GLN:H	2.03	0.56
2:B:178:ILE:HD12	2:B:178:ILE:N	2.20	0.56
2:B:371:SER:C	2:B:373:SER:H	2.08	0.56
1:C:51:LEU:HB2	1:C:52:PRO:HD3	1.88	0.56
2:D:257:ILE:HG21	2:D:282:GLN:HE21	1.68	0.56
2:H:87:ASN:HB3	2:H:91:GLN:CD	2.26	0.56
2:H:267:ARG:HH11	2:H:267:ARG:CG	2.18	0.56
2:H:402:GLU:HG2	2:H:405:ARG:HH22	1.70	0.56
3:I:161:ILE:HG23	3:I:165:SER:CB	2.35	0.56
1:C:264:ASN:HD22	1:C:264:ASN:N	2.03	0.56
2:F:136:ARG:NH1	2:F:161:LEU:HD22	2.20	0.56
2:F:398:THR:HA	2:F:401:GLU:CG	2.35	0.56
1:G:268:ALA:HA	1:G:271:ASN:HD22	1.69	0.56
2:H:237:TRP:HB3	2:H:238:PRO:HD3	1.87	0.56
3:J:101:MET:HE1	3:J:119:PRO:HG3	1.87	0.56
2:F:199:CYS:SG	2:F:201:GLU:HB2	2.46	0.56
2:F:362:GLN:HE21	2:F:408:LEU:CD1	2.19	0.56
2:B:229:ILE:HD13	2:B:281:THR:HA	1.87	0.56
1:C:353:ASP:O	1:C:357:VAL:HG23	2.05	0.56
1:E:517:ASN:C	1:E:517:ASN:HD22	2.09	0.56
1:G:502:ALA:O	1:G:506:ILE:HD12	2.06	0.56
2:F:361:LEU:HB3	2:F:408:LEU:HD23	1.86	0.56
1:G:332:MET:HG2	1:G:339:TYR:CE1	2.35	0.56
2:H:417:LEU:HD22	2:H:438:LEU:HD23	1.88	0.56
2:F:257:ILE:HD13	2:F:282:GLN:HG2	1.87	0.56
1:G:447:ASN:HD22	2:H:26:ARG:HH21	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:GLU:HG3	1:A:261:ASP:HB2	1.86	0.56
2:B:15:GLY:HA2	2:B:18:ASN:OD1	2.06	0.56
1:C:377:GLU:O	1:C:381:LYS:HG2	2.06	0.56
2:D:283:GLY:HA2	2:D:288:ILE:HD12	1.88	0.56
2:F:207:TYR:CZ	3:K:172:ARG:HD3	2.41	0.56
1:G:527:GLN:OE1	1:G:527:GLN:HA	2.05	0.56
2:H:225:PRO:HB3	2:H:276:VAL:CG2	2.35	0.56
2:H:355:PHE:O	2:H:440:PHE:HD2	1.89	0.56
1:C:36:ILE:O	1:C:60:ILE:O	2.24	0.56
2:D:251:GLY:O	2:D:257:ILE:HD11	2.06	0.56
3:J:118:GLU:HB3	3:J:120:THR:HG22	1.86	0.56
1:E:183:LEU:CD2	1:E:329:ILE:HG22	2.36	0.56
1:E:219:ALA:O	1:E:222:LEU:HB3	2.05	0.56
1:G:56:SER:CB	1:G:101:SER:HB2	2.36	0.56
1:G:268:ALA:O	1:G:272:VAL:HG23	2.06	0.56
2:B:64:LEU:HD11	2:B:77:VAL:HG21	1.88	0.55
2:D:83:ILE:HD13	2:D:94:PHE:HB3	1.87	0.55
2:D:151:ARG:HB3	2:D:200:ILE:HD13	1.88	0.55
2:F:361:LEU:HB3	2:F:408:LEU:HA	1.86	0.55
3:K:103:ILE:CG1	3:K:117:ILE:HD12	2.30	0.55
1:G:281:ILE:HG21	1:G:286:GLU:OE2	2.06	0.55
1:G:311:LEU:O	1:G:315:VAL:HG23	2.05	0.55
2:H:267:ARG:HA	2:H:270:GLN:NE2	2.21	0.55
1:C:383:LEU:HG	1:C:383:LEU:O	2.05	0.55
2:D:405:ARG:HB3	2:D:405:ARG:NH1	2.20	0.55
1:A:437:LYS:HA	1:A:437:LYS:HZ3	1.71	0.55
1:E:77:GLN:OE1	2:F:114:ARG:HA	2.06	0.55
1:E:418:ASN:ND2	1:E:420:ASP:H	2.05	0.55
1:C:130:GLN:HA	1:C:154:ARG:HD2	1.89	0.55
1:C:303:SER:O	1:C:307:LEU:HG	2.07	0.55
1:G:173:GLU:HG3	1:G:382:LEU:HD21	1.88	0.55
2:H:351:GLN:HB3	2:H:436:PHE:CD2	2.42	0.55
1:A:416:MET:SD	1:A:424:VAL:HG22	2.47	0.55
2:B:251:GLY:O	2:B:257:ILE:HD11	2.06	0.55
1:G:264:ASN:O	1:G:267:GLU:HB3	2.07	0.55
3:L:119:PRO:O	3:L:157:ALA:HB2	2.06	0.55
1:C:163:ARG:HH11	1:C:165:ILE:HG12	1.71	0.55
2:D:316:ILE:H	2:D:316:ILE:HD12	1.72	0.55
1:E:12:LYS:HE3	1:E:13:TYR:CZ	2.42	0.55
2:H:201:GLU:HB3	2:H:343:CYS:SG	2.47	0.55
2:H:380:ALA:O	2:H:425:VAL:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LYS:O	1:A:260:GLU:HB3	2.07	0.55
3:I:105:VAL:HG13	3:I:113:ILE:HG12	1.89	0.55
1:C:488:ALA:C	1:C:490:PRO:HD3	2.27	0.55
3:J:115:ILE:HG22	3:J:117:ILE:HG13	1.88	0.55
1:E:260:GLU:HG3	1:E:261:ASP:HB2	1.87	0.55
1:G:208:ASP:HB3	1:G:338:LYS:HZ1	1.71	0.55
2:H:218:ILE:HD13	2:H:230:GLU:HG2	1.89	0.55
1:E:46:LEU:HD23	1:E:93:LEU:HD13	1.87	0.55
1:E:297:ILE:H	1:E:297:ILE:HD12	1.72	0.55
1:G:185:LEU:O	1:G:188:PRO:HD3	2.05	0.55
2:H:250:ASP:HB3	2:H:253:ASP:HB2	1.89	0.55
2:B:413:LYS:CG	2:B:413:LYS:O	2.54	0.55
2:F:361:LEU:HD13	2:F:408:LEU:HA	1.87	0.55
3:L:118:GLU:O	3:L:120:THR:N	2.39	0.55
2:B:56:ALA:HA	2:B:60:GLY:HA3	1.89	0.55
1:C:274:THR:HG22	3:J:132:GLU:HA	1.89	0.55
1:C:461:LEU:O	1:C:465:LEU:HG	2.07	0.55
1:E:229:THR:HG22	1:E:232:ARG:HD2	1.89	0.55
1:E:264:ASN:HD22	1:E:264:ASN:N	2.05	0.55
2:H:377:LYS:HG2	2:H:428:VAL:HG21	1.88	0.54
2:B:229:ILE:HA	2:B:264:SER:OG	2.07	0.54
2:B:361:LEU:HD22	2:B:408:LEU:CD2	2.30	0.54
1:C:305:TRP:O	1:C:308:ALA:HB3	2.07	0.54
1:E:192:LEU:HD12	1:E:345:VAL:HG11	1.88	0.54
1:E:243:PHE:O	1:E:247:ILE:HG13	2.08	0.54
2:F:87:ASN:ND2	2:F:103:LYS:HE2	2.21	0.54
2:D:361:LEU:HD23	2:D:408:LEU:HA	1.87	0.54
3:K:117:ILE:HG22	3:K:118:GLU:N	2.23	0.54
2:H:277:THR:HG23	2:H:280:LEU:H	1.73	0.54
2:B:399:SER:HB3	2:B:400:ILE:HD12	1.89	0.54
2:F:259:TRP:CH2	2:F:263:LYS:HG3	2.43	0.54
1:G:264:ASN:N	1:G:264:ASN:HD22	2.04	0.54
2:B:164:TYR:CE2	2:B:169:LEU:HB2	2.43	0.54
1:E:311:LEU:O	1:E:315:VAL:HG23	2.08	0.54
3:K:103:ILE:C	3:K:103:ILE:HD12	2.27	0.54
3:L:113:ILE:HD13	3:L:134:GLU:HG2	1.90	0.54
1:A:94:GLN:HE22	1:A:102:GLY:N	2.02	0.54
2:B:412:LEU:O	2:B:417:LEU:HD23	2.07	0.54
1:E:347:ARG:HH22	2:F:274:ARG:HH11	1.55	0.54
2:F:46:LEU:HD22	2:F:73:ARG:CZ	2.38	0.54
2:H:158:LEU:HD23	2:H:161:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:344:PRO:HB3	2:H:374:LEU:HD13	1.90	0.54
1:A:72:ASN:ND2	1:A:72:ASN:C	2.61	0.54
1:A:78:ARG:C	1:A:80:SER:H	2.10	0.54
2:B:157:MET:HA	2:B:157:MET:HE3	1.90	0.54
1:C:214:TRP:CD1	1:C:214:TRP:C	2.81	0.54
2:D:75:ILE:O	2:D:120:VAL:HA	2.08	0.54
2:D:376:MET:HB3	2:D:427:ASP:OD1	2.06	0.54
1:G:201:LEU:HD11	1:G:221:TYR:CD1	2.43	0.54
1:C:331:ASP:OD1	2:D:223:ARG:HD2	2.07	0.54
2:F:419:ASP:OD2	2:F:439:HIS:HA	2.07	0.54
1:A:229:THR:HG22	1:A:229:THR:O	2.07	0.54
2:D:64:LEU:HD21	2:D:77:VAL:HG22	1.89	0.54
2:D:128:GLN:HE21	2:D:128:GLN:H	1.56	0.54
2:H:336:GLU:O	3:L:147:GLY:HA2	2.08	0.54
3:L:170:VAL:CG1	3:L:171:LEU:N	2.71	0.54
2:B:357:PRO:HA	2:B:440:PHE:CZ	2.41	0.54
1:C:441:ARG:NH2	1:C:453:ASP:OD1	2.40	0.54
1:C:447:ASN:HD21	2:D:26:ARG:HE	1.56	0.54
1:G:47:LYS:HD3	1:G:51:LEU:HD12	1.90	0.54
1:G:407:ILE:CG2	1:G:409:LYS:HG3	2.38	0.54
3:I:107:THR:CG2	3:I:109:THR:H	2.17	0.53
1:C:277:ASN:ND2	1:C:277:ASN:O	2.40	0.53
2:F:193:LEU:H	2:F:197:THR:HB	1.71	0.53
2:F:197:THR:HG22	2:F:198:ALA:N	2.23	0.53
1:G:293:ARG:HG2	1:G:293:ARG:NH1	2.20	0.53
1:G:317:LYS:HB3	1:G:318:GLU:OE1	2.08	0.53
1:C:260:GLU:HG3	1:C:261:ASP:CG	2.29	0.53
2:D:128:GLN:H	2:D:128:GLN:NE2	2.05	0.53
2:D:237:TRP:HB3	2:D:238:PRO:HD3	1.90	0.53
3:J:155:THR:HG23	3:J:157:ALA:H	1.73	0.53
1:G:43:THR:HG23	1:G:75:PHE:CD1	2.43	0.53
1:G:252:LEU:HG	1:G:252:LEU:O	2.08	0.53
2:H:223:ARG:HH11	2:H:223:ARG:HG3	1.71	0.53
2:H:402:GLU:C	2:H:404:THR:H	2.11	0.53
1:A:368:ILE:CG2	1:A:370:GLN:HG3	2.37	0.53
1:C:360:HIS:O	1:C:364:LEU:HB2	2.08	0.53
1:E:311:LEU:CD2	1:E:383:LEU:HD11	2.38	0.53
3:K:123:VAL:HG13	3:K:150:MET:HE2	1.90	0.53
2:H:360:LYS:HB2	2:H:363:GLU:HG3	1.91	0.53
1:A:61:ASP:HB3	1:A:86:ALA:HB2	1.90	0.53
2:F:350:PRO:HB3	2:F:435:LEU:C	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:117:ASN:O	2:H:118:CYS:C	2.47	0.53
1:A:33:VAL:O	1:A:57:PHE:HA	2.07	0.53
1:A:163:ARG:HH11	1:A:163:ARG:HG2	1.72	0.53
1:C:43:THR:HG21	1:C:73:ASN:OD1	2.08	0.53
1:E:45:ILE:CG1	1:E:498:GLY:HA2	2.39	0.53
1:G:132:PRO:HG2	1:G:135:THR:OG1	2.09	0.53
2:H:164:TYR:CD2	2:H:169:LEU:HB2	2.44	0.53
2:H:220:SER:O	2:H:222:PRO:HD3	2.09	0.53
2:B:102:PRO:HG2	2:B:105:GLU:HB3	1.90	0.53
2:B:110:PHE:C	2:B:110:PHE:CD2	2.82	0.53
2:B:193:LEU:H	2:B:197:THR:HB	1.74	0.53
2:H:236:GLN:HE22	2:H:263:LYS:HD2	1.74	0.53
1:A:60:ILE:HD11	1:A:119:PHE:HE2	1.73	0.53
1:A:401:GLU:HG3	1:A:534:LEU:OXT	2.07	0.53
1:A:418:ASN:HD22	1:A:418:ASN:C	2.12	0.53
1:C:35:LEU:HD22	1:C:46:LEU:HD22	1.90	0.53
1:E:223:ALA:O	1:E:226:TYR:HD2	1.91	0.53
1:E:235:LYS:O	1:E:240:LYS:HE3	2.08	0.53
2:F:186:LYS:HE2	2:F:325:ASN:HD21	1.74	0.53
3:K:107:THR:CG2	3:K:109:THR:HG23	2.38	0.53
3:K:156:ALA:HA	3:K:161:ILE:HD12	1.91	0.53
1:G:347:ARG:NH2	2:H:274:ARG:HD2	2.24	0.53
1:G:447:ASN:ND2	2:H:26:ARG:NE	2.49	0.53
2:H:197:THR:HG22	2:H:198:ALA:N	2.24	0.53
1:A:447:ASN:ND2	2:B:26:ARG:HE	2.07	0.53
1:A:491:HIS:CD2	2:B:69:LEU:HD12	2.44	0.53
2:F:231:TYR:HD1	2:F:235:LEU:HD12	1.73	0.53
1:C:457:LEU:HD23	1:C:479:VAL:CG1	2.39	0.53
2:D:50:LYS:N	2:D:139:HIS:HD2	1.99	0.53
1:E:266:GLU:O	1:E:270:LYS:HG3	2.09	0.53
2:F:419:ASP:OD2	2:F:438:LEU:C	2.47	0.53
3:L:126:ILE:O	3:L:130:VAL:HG23	2.09	0.53
1:A:222:LEU:HG	1:A:226:TYR:CE1	2.44	0.53
1:A:421:ASN:O	1:A:424:VAL:HG23	2.09	0.53
1:C:307:LEU:CB	1:C:383:LEU:HD13	2.37	0.53
2:D:343:CYS:H	2:D:347:SER:CB	2.21	0.53
2:B:208:PRO:HD3	3:I:172:ARG:O	2.09	0.52
2:B:355:PHE:O	2:B:440:PHE:HA	2.09	0.52
1:C:36:ILE:HD13	1:C:60:ILE:HB	1.91	0.52
1:C:418:ASN:ND2	1:C:420:ASP:H	2.06	0.52
2:D:158:LEU:CD1	2:D:177:LEU:HB2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:405:ARG:HH11	2:D:405:ARG:CB	2.20	0.52
1:E:341:LYS:O	1:E:345:VAL:HG23	2.09	0.52
1:A:214:TRP:C	1:A:214:TRP:CD1	2.82	0.52
1:A:423:ILE:O	1:A:426:TYR:HB3	2.09	0.52
1:C:72:ASN:C	1:C:72:ASN:ND2	2.61	0.52
1:C:229:THR:HG21	1:C:232:ARG:HB2	1.91	0.52
2:D:235:LEU:O	2:D:238:PRO:HD2	2.10	0.52
1:E:264:ASN:ND2	1:E:265:PHE:N	2.56	0.52
1:G:210:SER:CB	1:G:262:GLU:OE2	2.55	0.52
1:G:236:THR:O	1:G:240:LYS:HG3	2.08	0.52
2:H:187:GLY:HA2	3:L:173:LEU:HD13	1.89	0.52
2:F:185:PHE:HB3	2:F:326:ASP:CB	2.36	0.52
2:H:101:ARG:HB3	2:H:102:PRO:HD2	1.90	0.52
2:H:158:LEU:HD22	2:H:175:VAL:HB	1.92	0.52
1:A:168:GLU:HG3	1:A:394:ARG:NE	2.23	0.52
2:B:235:LEU:C	2:B:238:PRO:HD2	2.29	0.52
1:C:177:ASP:OD2	2:D:186:LYS:CE	2.57	0.52
1:C:518:ASN:HB2	1:C:533:GLN:HA	1.91	0.52
2:D:405:ARG:NH1	2:D:405:ARG:CB	2.73	0.52
3:J:101:MET:HB2	3:J:117:ILE:O	2.09	0.52
1:E:236:THR:CG2	1:E:237:TYR:N	2.70	0.52
1:E:447:ASN:HD21	2:F:26:ARG:HE	1.55	0.52
2:F:355:PHE:CE1	2:F:364:VAL:HG22	2.44	0.52
1:C:154:ARG:HB3	1:C:161:TYR:HB3	1.92	0.52
1:C:214:TRP:CD1	1:C:215:ILE:N	2.77	0.52
1:C:407:ILE:HG23	1:C:409:LYS:HG3	1.91	0.52
2:D:386:GLU:C	2:D:388:LYS:N	2.62	0.52
3:J:144:ILE:HD12	3:J:170:VAL:HG11	1.91	0.52
1:E:340:ILE:HD11	2:F:273:ILE:HG13	1.91	0.52
1:G:157:GLY:HA3	1:G:485:TYR:CG	2.45	0.52
2:H:245:GLU:HG2	2:H:246:GLY:N	2.22	0.52
1:A:426:TYR:HB2	1:A:521:ILE:CD1	2.39	0.52
3:J:117:ILE:HD13	3:J:126:ILE:HG12	1.91	0.52
1:G:218:ILE:O	1:G:222:LEU:CB	2.57	0.52
1:G:226:TYR:CE2	1:G:233:ILE:HG22	2.45	0.52
2:H:294:SER:O	2:H:298:VAL:HG23	2.10	0.52
2:H:375:GLN:O	2:H:376:MET:HG2	2.08	0.52
1:A:128:ALA:HB1	1:A:131:LEU:HD11	1.90	0.52
1:A:204:MET:CE	1:A:208:ASP:HB3	2.39	0.52
2:D:320:ASN:ND2	2:D:336:GLU:CG	2.72	0.52
2:D:397:VAL:CG1	2:D:398:THR:H	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:232:VAL:O	2:F:232:VAL:HG12	2.08	0.52
2:H:241:GLN:HB3	2:H:245:GLU:HA	1.91	0.52
2:H:412:LEU:N	2:H:412:LEU:CD1	2.73	0.52
3:L:155:THR:HG23	3:L:157:ALA:HB3	1.91	0.52
2:B:405:ARG:O	2:B:408:LEU:HB2	2.10	0.52
2:D:73:ARG:HG3	2:D:73:ARG:HH11	1.74	0.52
1:E:46:LEU:O	1:E:50:VAL:HG23	2.09	0.52
1:E:50:VAL:HG13	1:E:100:VAL:HG21	1.91	0.52
3:K:155:THR:HG22	3:K:158:ASP:OD1	2.10	0.52
1:G:226:TYR:HE2	1:G:234:PRO:HD3	1.75	0.52
1:G:263:GLU:O	1:G:264:ASN:C	2.47	0.52
1:G:320:GLN:OE1	1:G:320:GLN:HA	2.09	0.52
2:H:222:PRO:O	2:H:273:ILE:HD11	2.09	0.52
1:A:66:SER:O	1:A:81:ILE:HG23	2.10	0.52
2:B:74:GLN:HE22	2:B:119:ASN:ND2	2.03	0.52
2:D:237:TRP:CE3	2:D:242:PRO:HG2	2.44	0.52
1:E:516:PHE:HB3	2:F:330:LEU:HD12	1.91	0.52
2:F:400:ILE:C	2:F:402:GLU:H	2.13	0.52
1:G:214:TRP:O	1:G:217:ILE:HB	2.09	0.52
2:B:197:THR:HG23	2:B:320:ASN:OD1	2.08	0.52
2:B:425:VAL:HG21	2:B:436:PHE:CE1	2.44	0.52
2:D:412:LEU:HD13	2:D:440:PHE:CD2	2.44	0.52
1:G:226:TYR:CE2	1:G:233:ILE:HA	2.45	0.52
2:H:164:TYR:CE2	2:H:169:LEU:HB2	2.45	0.52
2:D:321:TYR:HE2	2:D:323:VAL:HG13	1.75	0.51
1:E:426:TYR:O	1:E:430:ARG:HG2	2.10	0.51
2:F:157:MET:O	2:F:157:MET:HE3	2.10	0.51
2:H:92:PHE:H	2:H:92:PHE:HD2	1.55	0.51
1:A:77:GLN:HG3	1:A:92:PHE:CE2	2.45	0.51
1:A:400:GLU:O	1:A:406:THR:O	2.29	0.51
2:B:208:PRO:HG3	3:I:171:LEU:HD11	1.92	0.51
2:B:338:GLU:HG3	3:I:148:LYS:HD3	1.92	0.51
2:B:403:ARG:HG3	2:B:403:ARG:NH1	2.25	0.51
2:D:384:THR:HA	2:D:389:ASN:HB3	1.91	0.51
2:F:236:GLN:NE2	2:F:263:LYS:HD2	2.25	0.51
2:F:236:GLN:O	2:F:240:GLU:HG2	2.10	0.51
3:K:124:GLU:HB2	3:K:152:ASP:O	2.09	0.51
2:H:75:ILE:HB	2:H:120:VAL:HG22	1.93	0.51
1:A:371:ALA:O	1:A:373:GLU:N	2.42	0.51
2:D:16:ARG:NH2	2:D:116:PRO:HB2	2.24	0.51
1:E:236:THR:CG2	1:E:237:TYR:H	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:527:GLN:OE1	2:F:302:VAL:HG13	2.10	0.51
2:F:386:GLU:O	2:F:388:LYS:HG2	2.10	0.51
1:A:34:CYS:HB2	1:A:123:PHE:CD1	2.45	0.51
1:C:457:LEU:HD23	1:C:479:VAL:HG13	1.91	0.51
2:D:64:LEU:HD21	2:D:77:VAL:CG2	2.41	0.51
2:D:141:ILE:HD12	2:D:158:LEU:HD21	1.93	0.51
2:H:228:CYS:SG	2:H:268:ALA:HA	2.50	0.51
1:C:331:ASP:HB2	2:D:224:LEU:HD11	1.92	0.51
1:C:480:HIS:HB2	2:D:29:PRO:HG2	1.91	0.51
3:J:118:GLU:O	3:J:120:THR:N	2.44	0.51
2:F:398:THR:HA	2:F:401:GLU:HG3	1.92	0.51
1:G:344:ASN:O	1:G:348:GLU:HB2	2.09	0.51
1:C:54:ILE:HD11	1:C:509:ILE:HD13	1.93	0.51
1:C:218:ILE:O	1:C:222:LEU:HB2	2.11	0.51
2:H:349:LEU:HB3	2:H:350:PRO:CD	2.39	0.51
2:H:350:PRO:CB	2:H:437:LYS:HG3	2.39	0.51
1:A:244:ARG:HG2	1:A:269:ILE:HG23	1.93	0.51
1:A:517:ASN:HD22	1:A:517:ASN:C	2.12	0.51
2:B:187:GLY:CA	3:I:173:LEU:HD13	2.41	0.51
2:D:149:ILE:CD1	2:D:149:ILE:N	2.65	0.51
2:D:392:LEU:N	2:D:392:LEU:HD12	2.26	0.51
1:E:191:GLU:OE2	1:E:191:GLU:N	2.40	0.51
2:F:349:LEU:HD12	2:F:349:LEU:H	1.75	0.51
2:F:349:LEU:N	2:F:349:LEU:CD1	2.74	0.51
1:G:299:LYS:HG2	1:G:368:ILE:CG2	2.40	0.51
2:H:338:GLU:HG3	3:L:148:LYS:CD	2.31	0.51
2:B:249:LEU:HD13	2:B:260:ILE:HD11	1.93	0.51
2:B:322:LEU:O	2:B:322:LEU:HD23	2.10	0.51
2:B:368:LEU:HD13	2:B:425:VAL:HG11	1.93	0.51
2:B:374:LEU:O	2:B:376:MET:HG3	2.11	0.51
1:E:229:THR:CG2	1:E:232:ARG:HD2	2.41	0.51
2:H:64:LEU:HB3	2:H:111:LEU:HD13	1.91	0.51
2:H:267:ARG:HD2	2:H:271:TYR:CE1	2.46	0.51
2:H:422:GLU:O	2:H:423:LEU:HD23	2.11	0.51
1:A:428:MET:CE	1:A:479:VAL:HA	2.41	0.51
3:I:117:ILE:HD13	3:I:126:ILE:HG12	1.92	0.51
1:E:332:MET:O	2:F:223:ARG:NE	2.44	0.51
2:F:391:THR:O	2:F:404:THR:HG21	2.11	0.51
1:G:422:GLU:OE1	1:G:422:GLU:N	2.33	0.51
1:G:441:ARG:HH21	1:G:449:GLN:CD	2.14	0.51
2:H:344:PRO:HG2	2:H:345:ALA:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:350:PRO:HG3	2:H:435:LEU:CB	2.41	0.51
1:A:60:ILE:O	1:A:60:ILE:HG22	2.11	0.51
1:A:72:ASN:C	1:A:72:ASN:HD22	2.12	0.51
1:A:214:TRP:CD1	1:A:215:ILE:N	2.78	0.51
2:B:64:LEU:HD21	2:B:77:VAL:HG22	1.93	0.51
1:G:210:SER:HB3	1:G:262:GLU:CD	2.31	0.51
2:H:35:PHE:O	2:H:36:GLU:HG2	2.11	0.51
2:H:87:ASN:HB3	2:H:91:GLN:NE2	2.26	0.51
2:H:425:VAL:HB	2:H:434:VAL:CG1	2.41	0.51
1:A:113:LEU:HB3	1:A:138:ARG:NH2	2.26	0.50
1:A:181:GLU:OE1	1:A:330:PRO:HD3	2.11	0.50
2:D:316:ILE:H	2:D:316:ILE:CD1	2.24	0.50
2:F:430:THR:OG1	2:F:432:GLN:HB2	2.11	0.50
1:A:201:LEU:HD23	1:A:204:MET:SD	2.51	0.50
1:A:286:GLU:OE1	1:A:286:GLU:HA	2.11	0.50
1:C:209:HIS:CD2	1:C:252:LEU:HB2	2.46	0.50
1:C:253:LYS:O	1:C:259:PRO:C	2.44	0.50
1:E:184:ARG:HD2	1:E:325:VAL:HG22	1.91	0.50
1:E:199:TYR:O	1:E:220:LYS:HE2	2.12	0.50
1:E:248:ARG:O	1:E:250:GLY:N	2.42	0.50
1:E:331:ASP:HB2	2:F:224:LEU:HD11	1.93	0.50
2:F:235:LEU:O	2:F:238:PRO:HD2	2.10	0.50
2:F:294:SER:O	2:F:298:VAL:HG23	2.10	0.50
1:G:428:MET:O	1:G:431:ALA:HB3	2.11	0.50
2:H:239:LYS:HG3	2:H:239:LYS:O	2.11	0.50
1:C:9:LYS:C	1:C:11:GLN:H	2.15	0.50
2:D:232:VAL:CG1	2:D:263:LYS:HB2	2.39	0.50
1:G:77:GLN:HG3	1:G:92:PHE:CZ	2.46	0.50
2:H:233:ARG:NH1	2:H:234:MET:HB2	2.27	0.50
2:H:351:GLN:HB3	2:H:436:PHE:CE2	2.46	0.50
1:A:166:ILE:HD11	1:A:508:ILE:CD1	2.40	0.50
1:A:277:ASN:HD22	1:A:278:THR:N	2.10	0.50
1:C:444:GLY:O	2:D:26:ARG:NH1	2.43	0.50
2:D:215:MET:HA	2:D:218:ILE:HD12	1.93	0.50
2:D:357:PRO:HG3	2:D:440:PHE:CG	2.47	0.50
1:G:72:ASN:HD22	1:G:72:ASN:H	1.60	0.50
1:G:347:ARG:HH22	2:H:274:ARG:CD	2.24	0.50
2:H:92:PHE:CD2	2:H:92:PHE:N	2.79	0.50
1:C:41:THR:O	1:C:45:ILE:HG13	2.11	0.50
1:C:234:PRO:HB2	1:C:276:LEU:HD12	1.93	0.50
2:D:178:ILE:HD12	2:D:178:ILE:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:TRP:CZ3	1:E:332:MET:HG2	2.47	0.50
1:G:162:MET:HB3	1:G:520:TYR:HB3	1.93	0.50
2:H:187:GLY:CA	3:L:173:LEU:HD13	2.41	0.50
1:C:268:ALA:O	1:C:272:VAL:HG23	2.11	0.50
1:C:419:PRO:HB2	1:C:475:LYS:HE3	1.94	0.50
1:C:488:ALA:O	1:C:490:PRO:HD3	2.12	0.50
2:D:306:GLU:OE2	2:D:309:LYS:HD2	2.11	0.50
1:G:252:LEU:O	1:G:252:LEU:CG	2.57	0.50
1:G:262:GLU:OE1	1:G:262:GLU:CA	2.58	0.50
2:H:242:PRO:HG3	2:H:259:TRP:CH2	2.46	0.50
3:L:144:ILE:HD12	3:L:170:VAL:HG21	1.94	0.50
2:B:316:ILE:HD12	2:B:316:ILE:N	2.11	0.50
1:C:327:GLY:CA	1:C:350:ALA:HB2	2.41	0.50
1:C:517:ASN:HD22	1:C:518:ASN:N	1.99	0.50
2:D:277:THR:CG2	2:D:280:LEU:H	2.20	0.50
1:E:285:ILE:CD1	1:E:285:ILE:H	2.25	0.50
1:E:307:LEU:HB3	1:E:383:LEU:CD2	2.41	0.50
2:F:262:GLN:O	2:F:266:GLU:HG3	2.11	0.50
1:G:210:SER:HA	1:G:264:ASN:ND2	2.26	0.50
2:H:404:THR:O	2:H:407:ASN:HB2	2.11	0.50
2:B:322:LEU:HD23	2:B:322:LEU:C	2.32	0.50
1:C:186:ASP:OD2	1:C:279:THR:HB	2.11	0.50
1:E:446:SER:HB2	1:E:449:GLN:HG3	1.92	0.50
1:G:215:ILE:H	1:G:332:MET:CE	2.20	0.50
1:A:196:PHE:O	1:A:220:LYS:HE2	2.11	0.50
2:B:361:LEU:HD23	2:B:361:LEU:C	2.32	0.50
2:F:386:GLU:O	2:F:388:LYS:CG	2.60	0.50
2:H:223:ARG:O	2:H:273:ILE:HG21	2.11	0.50
3:L:117:ILE:HG23	3:L:121:ASP:OD1	2.12	0.50
1:A:298:THR:CA	1:A:368:ILE:HD11	2.42	0.49
1:C:163:ARG:CZ	1:C:518:ASN:OD1	2.60	0.49
2:D:134:PHE:O	2:D:137:GLN:HB3	2.12	0.49
2:D:397:VAL:CG1	2:D:398:THR:N	2.71	0.49
1:E:297:ILE:HG22	1:E:301:THR:HG21	1.94	0.49
2:F:321:TYR:OH	3:K:172:ARG:HG3	2.12	0.49
2:F:325:ASN:HD22	2:F:326:ASP:N	2.10	0.49
3:K:107:THR:HB	3:K:111:LYS:HB3	1.94	0.49
1:G:186:ASP:HB3	1:G:276:LEU:O	2.11	0.49
2:H:232:VAL:HG11	2:H:263:LYS:HB2	1.92	0.49
2:B:182:THR:HG21	2:B:296:ASN:OD1	2.12	0.49
2:D:368:LEU:HD22	2:D:436:PHE:HE1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:213:PHE:HB2	2:F:218:ILE:HD11	1.93	0.49
2:F:232:VAL:HG11	2:F:263:LYS:HB2	1.93	0.49
1:G:212:THR:OG1	1:G:217:ILE:HD11	2.11	0.49
2:H:63:LEU:O	2:H:67:LEU:HG	2.11	0.49
2:H:213:PHE:CD1	2:H:213:PHE:N	2.80	0.49
1:A:119:PHE:O	1:A:122:ARG:HG2	2.12	0.49
2:B:188:ASN:OD1	3:I:173:LEU:HD12	2.13	0.49
1:C:520:TYR:CE1	2:D:330:LEU:HB3	2.47	0.49
1:E:330:PRO:O	1:E:332:MET:HG3	2.11	0.49
2:F:357:PRO:HA	2:F:412:LEU:CG	2.43	0.49
1:G:189:PHE:HB2	1:G:190:PRO:HD2	1.94	0.49
2:H:257:ILE:HG21	2:H:282:GLN:HG2	1.94	0.49
1:C:481:GLU:OE1	1:C:484:ARG:HD3	2.12	0.49
2:F:74:GLN:HE22	2:F:119:ASN:ND2	2.04	0.49
1:G:315:VAL:O	1:G:321:GLY:N	2.43	0.49
1:A:12:LYS:O	2:B:89:ASN:HB3	2.13	0.49
1:A:137:LEU:HD11	1:A:402:TYR:CD2	2.48	0.49
2:B:183:GLU:HB2	3:I:173:LEU:HD23	1.94	0.49
2:B:348:GLN:OE1	2:B:348:GLN:HA	2.11	0.49
2:B:380:ALA:CB	2:B:394:LEU:CD1	2.90	0.49
2:B:398:THR:CA	2:B:401:GLU:HB3	2.42	0.49
2:D:236:GLN:HE22	2:D:263:LYS:CD	2.25	0.49
2:D:306:GLU:OE2	2:D:317:PRO:HA	2.12	0.49
2:F:402:GLU:HG2	2:F:405:ARG:NH2	2.27	0.49
1:G:262:GLU:O	1:G:265:PHE:HB2	2.11	0.49
1:G:441:ARG:NH2	1:G:453:ASP:OD2	2.44	0.49
2:B:339:ARG:NH2	2:B:346:CYS:O	2.44	0.49
2:D:397:VAL:HG12	2:D:399:SER:H	1.78	0.49
3:J:115:ILE:CG2	3:J:129:ARG:HG3	2.43	0.49
1:G:173:GLU:O	1:G:512:GLN:O	2.31	0.49
1:A:366:GLN:C	1:A:368:ILE:N	2.66	0.49
1:A:376:SER:OG	1:A:379:GLU:HG3	2.13	0.49
1:A:434:ARG:NH1	1:A:464:PHE:HA	2.28	0.49
2:B:126:LYS:O	2:B:128:GLN:N	2.46	0.49
1:C:18:ARG:HH22	2:D:282:GLN:HB2	1.76	0.49
1:C:39:THR:CG2	1:C:489:GLU:OE1	2.52	0.49
1:E:285:ILE:N	1:E:285:ILE:CD1	2.75	0.49
2:F:56:ALA:N	2:F:79:ASP:OD1	2.40	0.49
2:F:83:ILE:CD1	2:F:106:VAL:HG21	2.43	0.49
1:G:65:VAL:CG2	1:G:85:ARG:HA	2.42	0.49
2:B:74:GLN:NE2	2:B:74:GLN:HA	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:ASN:HD22	1:E:265:PHE:H	1.56	0.49
1:E:374:SER:O	1:E:375:ILE:HG13	2.13	0.49
2:F:385:LEU:HD21	2:F:417:LEU:HD12	1.95	0.49
2:F:422:GLU:O	2:F:423:LEU:HD23	2.13	0.49
3:K:144:ILE:CD1	3:K:170:VAL:HB	2.41	0.49
1:A:47:LYS:HG3	1:A:75:PHE:CZ	2.47	0.49
2:B:353:ILE:HG23	2:B:355:PHE:CD1	2.45	0.49
1:C:264:ASN:HD22	1:C:264:ASN:H	1.59	0.49
2:D:361:LEU:C	2:D:363:GLU:H	2.16	0.49
3:J:115:ILE:HG22	3:J:116:ASP:N	2.28	0.49
3:K:170:VAL:CG1	3:K:171:LEU:N	2.75	0.49
2:H:350:PRO:HG3	2:H:435:LEU:HB3	1.94	0.49
2:D:197:THR:HG22	2:D:198:ALA:O	2.12	0.49
1:E:45:ILE:HG12	1:E:498:GLY:HA2	1.95	0.49
2:H:157:MET:HE3	2:H:157:MET:O	2.12	0.49
3:L:125:ARG:HG3	3:L:128:GLU:OE1	2.13	0.49
3:L:155:THR:CG2	3:L:157:ALA:HB3	2.43	0.49
1:A:264:ASN:ND2	1:A:265:PHE:N	2.60	0.48
3:I:102:LEU:O	3:I:102:LEU:HD23	2.13	0.48
3:J:113:ILE:HD11	3:J:130:VAL:HG13	1.95	0.48
1:G:229:THR:CG2	1:G:232:ARG:NH2	2.72	0.48
2:H:182:THR:HG21	2:H:296:ASN:OD1	2.14	0.48
2:H:381:ILE:HA	2:H:424:ALA:O	2.13	0.48
2:H:405:ARG:NH1	2:H:405:ARG:CB	2.75	0.48
3:L:118:GLU:C	3:L:120:THR:H	2.17	0.48
1:A:8:LEU:HD12	1:A:11:GLN:OE1	2.13	0.48
2:B:400:ILE:HD12	2:B:400:ILE:N	2.15	0.48
2:F:110:PHE:CZ	2:F:114:ARG:NH1	2.81	0.48
1:G:236:THR:HG22	1:G:237:TYR:H	1.78	0.48
2:H:425:VAL:HB	2:H:434:VAL:HG13	1.95	0.48
1:A:163:ARG:HH12	1:A:165:ILE:HG12	1.75	0.48
1:A:461:LEU:O	1:A:465:LEU:HG	2.13	0.48
1:C:324:PRO:HB3	1:C:353:ASP:HB3	1.94	0.48
2:F:142:VAL:HG13	2:F:178:ILE:HB	1.95	0.48
2:F:207:TYR:CE1	3:K:172:ARG:HD3	2.47	0.48
2:F:362:GLN:NE2	2:F:408:LEU:HD22	2.27	0.48
2:H:11:LEU:HB2	2:H:12:ASP:H	1.43	0.48
2:H:31:THR:OG1	2:H:35:PHE:HB3	2.13	0.48
1:A:104:PHE:HE1	1:A:106:GLU:HG3	1.79	0.48
1:C:481:GLU:HG3	1:C:485:TYR:CZ	2.49	0.48
2:D:197:THR:CG2	2:D:198:ALA:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:106:LYS:HG2	3:K:112:GLU:HB2	1.94	0.48
1:G:221:TYR:CD2	1:G:247:ILE:HA	2.48	0.48
1:A:297:ILE:HG22	1:A:368:ILE:CD1	2.44	0.48
1:C:12:LYS:O	2:D:89:ASN:HB3	2.13	0.48
2:D:393:TYR:CE2	2:D:408:LEU:HD11	2.49	0.48
1:E:226:TYR:HD1	1:E:231:GLY:HA2	1.77	0.48
1:E:504:GLU:O	1:E:508:ILE:HG13	2.13	0.48
2:F:231:TYR:CD1	2:F:235:LEU:HD12	2.48	0.48
1:G:7:LEU:HG	1:G:10:GLU:OE1	2.12	0.48
1:G:497:LEU:O	1:G:498:GLY:C	2.52	0.48
2:H:318:LEU:HD12	2:H:319:ASN:H	1.76	0.48
1:A:299:LYS:HA	1:A:368:ILE:HG13	1.95	0.48
3:J:125:ARG:HD3	3:J:129:ARG:NH2	2.27	0.48
1:E:441:ARG:NH2	1:E:453:ASP:OD1	2.47	0.48
1:E:526:SER:O	1:E:527:GLN:HB2	2.14	0.48
2:F:213:PHE:CB	2:F:218:ILE:HD11	2.43	0.48
1:G:325:VAL:HG21	1:G:349:LYS:CG	2.43	0.48
1:G:347:ARG:O	1:G:351:LYS:HG3	2.14	0.48
2:H:386:GLU:O	2:H:388:LYS:HG2	2.12	0.48
1:A:294:CYS:HB2	1:A:305:TRP:CE3	2.49	0.48
2:B:371:SER:C	2:B:373:SER:N	2.65	0.48
3:I:117:ILE:CG2	3:I:118:GLU:N	2.76	0.48
1:C:450:VAL:O	1:C:454:ILE:HG13	2.14	0.48
3:J:155:THR:HG22	3:J:158:ASP:CG	2.34	0.48
1:E:34:CYS:HB2	1:E:123:PHE:CG	2.48	0.48
1:G:329:ILE:HD11	1:G:343:GLN:HG3	1.95	0.48
1:G:347:ARG:NH2	2:H:274:ARG:NH1	2.61	0.48
2:H:238:PRO:O	2:H:240:GLU:N	2.43	0.48
3:L:116:ASP:O	3:L:117:ILE:HG13	2.14	0.48
1:A:78:ARG:O	1:A:80:SER:N	2.45	0.48
2:B:391:THR:HG21	2:B:400:ILE:HG21	1.95	0.48
2:B:422:GLU:HA	2:B:436:PHE:O	2.13	0.48
2:D:83:ILE:HD12	2:D:98:ASP:HB3	1.96	0.48
2:D:349:LEU:N	2:D:349:LEU:HD23	2.28	0.48
1:E:262:GLU:O	1:E:264:ASN:ND2	2.47	0.48
1:G:111:ASN:C	1:G:111:ASN:OD1	2.50	0.48
2:H:316:ILE:HD12	2:H:316:ILE:N	2.15	0.48
3:L:102:LEU:HD21	3:L:114:GLU:OE1	2.13	0.48
3:I:150:MET:SD	3:I:167:LEU:HD22	2.53	0.48
3:J:135:GLY:O	3:J:137:PRO:HD3	2.14	0.48
1:G:158:LEU:HD12	1:G:524:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:285:ILE:HD11	1:G:387:SER:O	2.13	0.48
2:H:269:SER:C	2:H:271:TYR:N	2.67	0.48
2:B:87:ASN:HB3	2:B:91:GLN:CD	2.34	0.48
1:C:36:ILE:CD1	1:C:60:ILE:HB	2.44	0.48
1:C:293:ARG:HH11	1:C:293:ARG:CG	2.27	0.48
2:D:182:THR:CG2	2:D:183:GLU:N	2.77	0.48
1:G:199:TYR:O	1:G:220:LYS:HE2	2.14	0.48
2:H:237:TRP:O	2:H:242:PRO:HD3	2.14	0.48
1:A:419:PRO:O	1:A:424:VAL:HG21	2.13	0.47
3:I:107:THR:HB	3:I:111:LYS:O	2.14	0.47
1:C:105:VAL:HG12	1:C:107:GLU:H	1.79	0.47
1:E:253:LYS:O	1:E:260:GLU:CA	2.60	0.47
2:F:249:LEU:CD2	2:F:260:ILE:HD11	2.44	0.47
1:G:317:LYS:HG2	1:G:318:GLU:H	1.78	0.47
2:H:52:LEU:HD11	2:H:78:ILE:HG13	1.95	0.47
1:A:248:ARG:HG2	1:A:269:ILE:CD1	2.44	0.47
2:B:392:LEU:N	2:B:392:LEU:HD23	2.29	0.47
1:C:274:THR:CG2	3:J:131:GLU:HG2	2.44	0.47
1:G:376:SER:OG	1:G:379:GLU:HG3	2.14	0.47
1:C:153:CYS:SG	1:C:162:MET:HG3	2.54	0.47
1:E:185:LEU:CD1	1:E:275:ALA:HB1	2.43	0.47
1:E:223:ALA:O	1:E:226:TYR:CD2	2.66	0.47
2:F:31:THR:HG23	2:F:32:HIS:O	2.14	0.47
2:F:385:LEU:HA	2:F:385:LEU:HD23	1.55	0.47
1:A:207:LYS:O	1:A:211:HIS:CB	2.63	0.47
1:A:297:ILE:HG22	1:A:298:THR:N	2.29	0.47
1:A:418:ASN:ND2	1:A:418:ASN:C	2.68	0.47
2:B:81:ASP:CB	2:B:103:LYS:HD2	2.43	0.47
2:B:196:MET:O	2:B:339:ARG:HD2	2.14	0.47
3:I:161:ILE:HG23	3:I:165:SER:HB2	1.96	0.47
1:C:115:ASN:HD21	1:G:348:GLU:HG3	1.79	0.47
2:F:418:VAL:O	2:F:418:VAL:CG1	2.54	0.47
1:G:36:ILE:HG23	1:G:109:PRO:HG3	1.97	0.47
2:H:165:GLU:N	2:H:168:VAL:O	2.47	0.47
1:A:221:TYR:OH	1:A:250:GLY:HA3	2.14	0.47
1:A:252:LEU:HD12	1:A:252:LEU:O	2.15	0.47
1:A:407:ILE:HG23	1:A:407:ILE:O	2.15	0.47
2:B:62:GLU:HG2	2:B:300:ALA:CB	2.44	0.47
2:B:141:ILE:HD12	2:B:158:LEU:HD21	1.95	0.47
1:C:72:ASN:HD22	1:C:73:ASN:N	2.12	0.47
2:D:398:THR:CA	2:D:401:GLU:HB3	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:LEU:HD23	1:E:329:ILE:HG22	1.97	0.47
3:K:108:LEU:HD12	3:K:108:LEU:HA	1.70	0.47
1:G:485:TYR:OH	1:G:525:MET:SD	2.72	0.47
2:D:279:ARG:O	2:D:282:GLN:HB2	2.14	0.47
2:F:395:GLN:HA	2:F:401:GLU:HB3	1.97	0.47
1:G:409:LYS:HE2	1:G:468:TYR:O	2.14	0.47
2:H:381:ILE:N	2:H:381:ILE:CD1	2.76	0.47
1:A:47:LYS:HG3	1:A:75:PHE:HZ	1.79	0.47
1:A:104:PHE:CE1	1:A:106:GLU:HG3	2.49	0.47
1:A:229:THR:HG23	1:A:232:ARG:HH21	1.80	0.47
1:A:426:TYR:HB2	1:A:521:ILE:HD11	1.96	0.47
2:B:13:TRP:CZ2	2:B:16:ARG:HG3	2.50	0.47
1:C:139:LEU:HG	1:C:143:LEU:HD12	1.96	0.47
1:C:418:ASN:HD22	1:C:419:PRO:N	2.13	0.47
1:E:191:GLU:H	1:E:191:GLU:CD	2.18	0.47
1:E:214:TRP:HB2	1:E:268:ALA:CB	2.43	0.47
1:E:241:GLU:OE1	1:E:244:ARG:HD2	2.15	0.47
1:E:298:THR:OG1	1:E:300:GLN:HG2	2.15	0.47
2:F:168:VAL:HG12	2:F:169:LEU:N	2.30	0.47
2:F:316:ILE:HD12	2:F:316:ILE:N	2.11	0.47
2:F:319:ASN:C	2:F:320:ASN:HD22	2.18	0.47
1:G:72:ASN:ND2	1:G:72:ASN:C	2.66	0.47
1:G:325:VAL:HG21	1:G:349:LYS:HG2	1.96	0.47
2:H:257:ILE:HD13	2:H:282:GLN:HG2	1.96	0.47
2:H:325:ASN:ND2	2:H:327:VAL:HG22	2.30	0.47
2:B:13:TRP:CH2	2:B:116:PRO:HG2	2.50	0.47
2:B:199:CYS:O	2:B:202:CYS:HB2	2.15	0.47
2:D:277:THR:HG22	2:D:280:LEU:CB	2.45	0.47
2:D:343:CYS:H	2:D:347:SER:HB3	1.80	0.47
1:G:112:LEU:C	1:G:114:ASP:N	2.67	0.47
1:G:201:LEU:HD11	1:G:221:TYR:CE1	2.50	0.47
1:G:401:GLU:O	1:G:407:ILE:HD12	2.15	0.47
2:H:193:LEU:HD23	2:H:193:LEU:HA	1.79	0.47
2:H:322:LEU:C	2:H:322:LEU:CD1	2.82	0.47
2:H:357:PRO:HG3	2:H:440:PHE:CD1	2.50	0.47
1:A:78:ARG:HG3	1:A:81:ILE:CD1	2.44	0.47
1:A:200:ASP:O	1:A:204:MET:HG3	2.15	0.47
2:D:64:LEU:HD11	2:D:77:VAL:HG21	1.97	0.47
1:E:240:LYS:HE2	1:E:276:LEU:HD12	1.96	0.47
2:F:182:THR:OG1	2:F:295:THR:HG22	2.15	0.47
2:F:186:LYS:HE2	2:F:325:ASN:ND2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:325:ASN:HD21	2:F:327:VAL:CG2	2.14	0.47
1:G:113:LEU:HD21	1:G:139:LEU:CD1	2.45	0.47
1:G:225:TRP:CD1	1:G:225:TRP:C	2.87	0.47
2:H:249:LEU:CD1	2:H:260:ILE:HD11	2.44	0.47
3:L:129:ARG:O	3:L:132:GLU:HB3	2.14	0.47
1:A:62:GLY:O	1:A:63:ASN:O	2.33	0.47
1:A:155:THR:HG23	1:A:493:ILE:HG22	1.97	0.47
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.71	0.47
1:C:36:ILE:HB	1:C:128:ALA:HA	1.95	0.47
1:C:297:ILE:H	1:C:297:ILE:CD1	2.22	0.47
1:C:299:LYS:HA	1:C:368:ILE:CG2	2.37	0.47
1:E:518:ASN:CB	1:E:533:GLN:HA	2.45	0.47
2:F:237:TRP:C	2:F:239:LYS:H	2.18	0.47
1:C:335:ASP:HB3	1:C:338:LYS:HG3	1.97	0.46
1:C:426:TYR:HB2	1:C:521:ILE:CD1	2.43	0.46
2:D:384:THR:HA	2:D:389:ASN:HA	1.96	0.46
1:E:215:ILE:HG13	1:E:332:MET:SD	2.54	0.46
2:F:312:THR:O	2:F:313:SER:HB2	2.15	0.46
2:F:411:THR:OG1	2:F:414:GLU:HB2	2.14	0.46
2:F:417:LEU:HD12	2:F:417:LEU:N	2.30	0.46
1:G:112:LEU:C	1:G:114:ASP:H	2.17	0.46
1:G:507:LYS:HG2	1:G:513:PHE:HB2	1.97	0.46
2:H:354:GLN:NE2	2:H:354:GLN:HA	2.30	0.46
1:A:462:THR:O	1:A:466:GLN:HG3	2.15	0.46
2:B:186:LYS:HB3	3:I:173:LEU:HD21	1.95	0.46
3:J:122:LYS:HA	3:J:155:THR:HA	1.97	0.46
1:E:47:LYS:HG3	1:E:75:PHE:CZ	2.50	0.46
1:E:67:GLY:HA3	2:F:14:GLU:O	2.15	0.46
2:F:336:GLU:O	2:F:337:ALA:C	2.52	0.46
1:E:19:LEU:HG	2:F:290:PRO:HB3	1.96	0.46
1:E:211:HIS:HB3	1:E:335:ASP:HB2	1.97	0.46
2:F:380:ALA:HB1	2:F:394:LEU:HD13	1.96	0.46
3:K:125:ARG:HD3	3:K:129:ARG:HH21	1.80	0.46
1:G:340:ILE:HD11	2:H:273:ILE:HG12	1.96	0.46
2:H:128:GLN:H	2:H:128:GLN:HE21	1.63	0.46
1:C:199:TYR:O	1:C:220:LYS:NZ	2.40	0.46
2:D:335:PHE:CE2	3:J:170:VAL:HG21	2.42	0.46
1:E:221:TYR:CE2	1:E:247:ILE:HA	2.50	0.46
1:E:236:THR:HB	1:E:239:GLU:HG3	1.97	0.46
1:E:333:ILE:O	1:E:334:ALA:HB2	2.16	0.46
1:E:396:ARG:NH1	1:E:534:LEU:C	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:397:SER:OG	1:E:400:GLU:HB2	2.15	0.46
2:F:338:GLU:HG3	3:K:148:LYS:HG2	1.97	0.46
2:F:425:VAL:CB	2:F:434:VAL:HG13	2.23	0.46
2:D:355:PHE:CE1	2:D:364:VAL:HA	2.50	0.46
2:D:412:LEU:HD22	2:D:438:LEU:HD21	1.97	0.46
1:E:396:ARG:NH2	1:E:406:THR:O	2.48	0.46
3:I:171:LEU:HD12	3:I:172:ARG:H	1.80	0.46
2:D:58:GLY:N	2:D:91:GLN:HG2	2.31	0.46
1:E:58:THR:HA	1:E:103:SER:O	2.16	0.46
2:F:325:ASN:HD22	2:F:326:ASP:H	1.62	0.46
2:F:393:TYR:HA	2:F:404:THR:OG1	2.14	0.46
1:G:347:ARG:NH2	2:H:274:ARG:HH11	2.13	0.46
2:H:52:LEU:HD23	2:H:141:ILE:HD12	1.97	0.46
2:H:223:ARG:HG3	2:H:223:ARG:NH1	2.30	0.46
3:L:161:ILE:HG23	3:L:165:SER:OG	2.15	0.46
1:C:19:LEU:HD12	2:D:292:VAL:HG13	1.98	0.46
2:D:11:LEU:N	2:D:11:LEU:HD23	2.31	0.46
2:D:61:CYS:HB3	2:D:93:LEU:HG	1.98	0.46
2:D:326:ASP:O	2:D:327:VAL:C	2.54	0.46
3:J:105:VAL:HG13	3:J:113:ILE:HG12	1.98	0.46
1:E:243:PHE:CE2	1:E:247:ILE:HD11	2.51	0.46
1:E:297:ILE:H	1:E:297:ILE:CD1	2.28	0.46
1:E:311:LEU:HD21	1:E:383:LEU:HD11	1.97	0.46
1:E:418:ASN:HD22	1:E:418:ASN:C	2.19	0.46
2:F:231:TYR:CD2	2:F:267:ARG:HD3	2.51	0.46
1:G:34:CYS:HB2	1:G:123:PHE:CD2	2.50	0.46
2:H:335:PHE:CZ	3:L:144:ILE:HD13	2.50	0.46
1:A:16:GLN:HB3	2:B:292:VAL:HG12	1.98	0.46
1:A:294:CYS:O	1:A:297:ILE:HD11	2.15	0.46
1:A:341:LYS:O	1:A:345:VAL:HG23	2.15	0.46
2:B:320:ASN:HB2	2:B:337:ALA:N	2.29	0.46
2:B:362:GLN:HE21	2:B:362:GLN:C	2.19	0.46
1:C:333:ILE:HA	2:D:223:ARG:NH2	2.30	0.46
2:D:153:TRP:CE2	2:D:431:PRO:HB3	2.50	0.46
2:D:353:ILE:HG22	2:D:354:GLN:N	2.31	0.46
2:D:412:LEU:O	2:D:415:LEU:HD12	2.15	0.46
2:F:338:GLU:HG3	3:K:148:LYS:HA	1.98	0.46
1:A:368:ILE:HG23	1:A:370:GLN:HG3	1.98	0.46
2:D:199:CYS:O	2:D:202:CYS:HB2	2.16	0.46
2:F:355:PHE:O	2:F:357:PRO:HD3	2.16	0.46
2:H:348:GLN:HB3	2:H:349:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:HD11	2:B:92:PHE:HB3	1.98	0.46
1:A:248:ARG:HG2	1:A:269:ILE:HD11	1.98	0.46
2:B:355:PHE:O	2:B:440:PHE:CD2	2.63	0.46
2:F:356:SER:O	2:F:358:SER:N	2.49	0.46
2:H:203:THR:HB	2:H:206:LEU:CD1	2.42	0.46
2:H:229:ILE:HD12	2:H:284:VAL:HG21	1.97	0.46
2:B:182:THR:OG1	2:B:295:THR:HG22	2.15	0.45
2:B:252:ASP:O	2:B:254:PRO:HD3	2.16	0.45
2:B:354:GLN:OE1	2:B:439:HIS:HB3	2.15	0.45
1:C:54:ILE:HD11	1:C:509:ILE:CD1	2.46	0.45
2:D:90:ARG:HG2	2:D:90:ARG:HH11	1.80	0.45
2:D:343:CYS:C	2:D:345:ALA:H	2.17	0.45
1:E:185:LEU:O	1:E:188:PRO:HD3	2.16	0.45
2:F:242:PRO:HG3	2:F:259:TRP:CE2	2.50	0.45
1:G:72:ASN:HD22	1:G:72:ASN:N	2.13	0.45
1:G:335:ASP:HB3	1:G:338:LYS:HB2	1.98	0.45
1:G:336:SER:HB2	2:H:221:MET:HA	1.97	0.45
1:G:416:MET:C	1:G:418:ASN:H	2.20	0.45
2:H:96:PRO:O	2:H:99:ILE:HG13	2.15	0.45
2:H:373:SER:C	2:H:374:LEU:CG	2.79	0.45
1:A:74:PHE:CD1	2:B:65:LYS:HG3	2.51	0.45
1:A:434:ARG:HB3	1:A:460:CYS:HB3	1.98	0.45
2:B:217:THR:HG21	2:B:223:ARG:HH22	1.82	0.45
3:K:104:LYS:HG2	3:K:114:GLU:HG2	1.98	0.45
3:K:107:THR:HG23	3:K:108:LEU:N	2.31	0.45
2:H:12:ASP:OD2	2:H:16:ARG:HD3	2.16	0.45
2:H:398:THR:HA	2:H:401:GLU:CB	2.44	0.45
1:A:19:LEU:HD12	2:B:292:VAL:HG13	1.97	0.45
2:B:353:ILE:HD13	2:B:436:PHE:HD2	1.81	0.45
2:D:338:GLU:HG2	3:J:147:GLY:O	2.17	0.45
3:J:149:GLN:HG3	3:J:149:GLN:O	2.16	0.45
2:H:123:HIS:HB3	2:H:125:ASN:ND2	2.28	0.45
2:H:267:ARG:CG	2:H:267:ARG:NH1	2.79	0.45
2:H:321:TYR:HE1	3:L:172:ARG:NH1	2.14	0.45
2:H:393:TYR:HA	2:H:404:THR:HB	1.98	0.45
1:C:357:VAL:O	1:C:361:VAL:HG23	2.16	0.45
2:D:364:VAL:O	2:D:368:LEU:HG	2.17	0.45
2:D:417:LEU:HD23	2:D:417:LEU:HA	1.74	0.45
2:H:136:ARG:HG2	2:H:161:LEU:HD22	1.99	0.45
2:H:351:GLN:NE2	2:H:436:PHE:HE2	2.14	0.45
1:C:56:SER:HB3	1:C:101:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ASP:HB3	1:C:86:ALA:HB2	1.99	0.45
1:C:248:ARG:O	1:C:251:ILE:HG13	2.16	0.45
1:C:339:TYR:HE2	1:C:343:GLN:HE21	1.63	0.45
2:D:398:THR:O	2:D:402:GLU:HG3	2.16	0.45
2:F:362:GLN:C	2:F:364:VAL:H	2.19	0.45
2:F:374:LEU:HD12	2:F:374:LEU:O	2.16	0.45
1:G:45:ILE:HG13	1:G:498:GLY:HA2	1.98	0.45
1:G:306:ILE:HD13	1:G:365:LEU:HD23	1.98	0.45
2:H:142:VAL:HG21	2:H:307:VAL:HG21	1.97	0.45
2:H:360:LYS:HG3	2:H:363:GLU:OE1	2.16	0.45
1:A:38:ALA:HB2	1:A:59:ILE:CG2	2.47	0.45
1:A:227:SER:C	1:A:229:THR:H	2.19	0.45
1:A:407:ILE:C	1:A:407:ILE:HD13	2.37	0.45
2:B:360:LYS:HA	2:B:411:THR:HA	1.99	0.45
1:C:193:ARG:O	1:C:197:GLN:HG3	2.17	0.45
2:D:392:LEU:CD1	2:D:392:LEU:H	2.29	0.45
1:E:513:PHE:N	1:E:513:PHE:CD1	2.83	0.45
2:F:361:LEU:O	2:F:361:LEU:HD23	2.17	0.45
2:F:362:GLN:NE2	2:F:408:LEU:CD1	2.79	0.45
3:K:118:GLU:O	3:K:120:THR:N	2.50	0.45
1:G:201:LEU:CD1	1:G:221:TYR:CE1	3.00	0.45
2:H:98:ASP:OD1	2:H:101:ARG:NH1	2.50	0.45
2:H:269:SER:C	2:H:271:TYR:H	2.20	0.45
2:H:323:VAL:HG21	3:L:170:VAL:HG22	1.99	0.45
2:H:415:LEU:O	2:H:416:GLY:C	2.55	0.45
1:A:31:ALA:HB3	1:A:54:ILE:HD11	1.98	0.45
1:C:51:LEU:CB	1:C:52:PRO:HD3	2.46	0.45
1:C:337:GLY:HA2	1:C:340:ILE:HD12	1.99	0.45
2:D:158:LEU:HD12	2:D:177:LEU:HB2	1.98	0.45
2:D:187:GLY:CA	3:J:173:LEU:HD12	2.47	0.45
2:D:323:VAL:O	2:D:332:THR:HA	2.17	0.45
1:E:282:PRO:HG2	1:E:388:ALA:HB1	1.97	0.45
2:F:199:CYS:SG	2:F:201:GLU:N	2.89	0.45
1:G:226:TYR:O	1:G:231:GLY:N	2.48	0.45
2:H:362:GLN:O	2:H:362:GLN:NE2	2.50	0.45
1:C:8:LEU:O	1:C:11:GLN:HB2	2.17	0.45
1:C:314:PHE:CE1	1:C:318:GLU:HG2	2.52	0.45
2:D:197:THR:HG22	2:D:198:ALA:N	2.30	0.45
2:D:222:PRO:HD2	2:D:271:TYR:CE2	2.52	0.45
2:D:232:VAL:O	2:D:232:VAL:HG12	2.15	0.45
3:J:155:THR:HG23	3:J:158:ASP:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:83:ILE:HD12	2:F:106:VAL:HG21	1.99	0.45
2:H:178:ILE:HD12	2:H:307:VAL:CG2	2.45	0.45
2:H:238:PRO:O	2:H:241:GLN:NE2	2.50	0.45
2:H:353:ILE:HD12	2:H:367:TYR:CE2	2.52	0.45
2:H:362:GLN:HB2	2:H:408:LEU:HB3	1.98	0.45
2:H:366:ASP:HA	2:H:369:THR:HB	1.99	0.45
3:L:102:LEU:HD13	3:L:116:ASP:OD1	2.17	0.45
1:A:15:ARG:HA	1:A:15:ARG:HD3	1.77	0.45
1:A:185:LEU:HD11	1:A:215:ILE:HG23	1.99	0.45
1:A:207:LYS:O	1:A:211:HIS:ND1	2.50	0.45
1:A:422:GLU:HG3	1:A:530:ALA:HB3	1.99	0.45
2:B:272:ASN:HD22	2:B:272:ASN:H	1.58	0.45
2:B:323:VAL:O	2:B:332:THR:HA	2.17	0.45
2:D:268:ALA:HB2	2:D:276:VAL:HG21	1.98	0.45
1:E:518:ASN:HB3	1:E:533:GLN:HA	1.99	0.45
2:B:383:ALA:HB2	2:B:423:LEU:HD23	1.98	0.45
1:C:58:THR:HA	1:C:103:SER:O	2.16	0.45
2:D:361:LEU:HB3	2:D:408:LEU:HA	1.99	0.45
3:J:101:MET:CE	3:J:119:PRO:HG3	2.46	0.45
1:E:430:ARG:NH1	1:E:430:ARG:HB3	2.32	0.45
2:F:322:LEU:CD1	2:F:322:LEU:C	2.86	0.45
1:G:208:ASP:HA	1:G:211:HIS:HB2	1.99	0.45
2:H:200:ILE:HD13	3:L:172:ARG:HH21	1.82	0.45
1:A:233:ILE:HG13	1:A:234:PRO:HD2	1.98	0.44
2:B:197:THR:HG22	2:B:198:ALA:O	2.17	0.44
2:B:197:THR:CG2	2:B:198:ALA:N	2.79	0.44
2:B:380:ALA:HB2	2:B:394:LEU:HD12	1.98	0.44
1:C:40:ALA:O	1:C:44:GLU:HG2	2.16	0.44
1:E:264:ASN:O	1:E:267:GLU:HB2	2.17	0.44
2:F:242:PRO:CG	2:F:259:TRP:CZ2	2.99	0.44
1:G:310:ALA:CB	1:G:361:VAL:HG23	2.48	0.44
1:A:151:LEU:HD12	1:A:163:ARG:O	2.16	0.44
3:I:170:VAL:CG1	3:I:171:LEU:N	2.80	0.44
1:C:189:PHE:CE2	1:C:192:LEU:HD22	2.52	0.44
1:C:244:ARG:HH22	1:C:273:ASN:HB2	1.83	0.44
2:D:429:THR:HG22	2:D:430:THR:N	2.32	0.44
3:K:144:ILE:HD13	3:K:170:VAL:CB	2.41	0.44
1:G:180:LEU:HD23	1:G:274:THR:HG23	1.98	0.44
2:H:221:MET:H	2:H:221:MET:HG2	1.64	0.44
1:A:49:LEU:O	1:A:52:PRO:HG2	2.17	0.44
2:B:419:ASP:C	2:B:419:ASP:OD1	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:THR:HA	1:C:302:PRO:HD3	1.66	0.44
1:E:184:ARG:HG2	1:E:279:THR:OG1	2.17	0.44
3:K:103:ILE:HG21	3:K:161:ILE:CG2	2.47	0.44
1:G:115:ASN:O	1:G:117:PRO:HD3	2.16	0.44
1:G:436:HIS:CD2	1:G:442:TYR:CE1	3.06	0.44
1:G:447:ASN:HD22	2:H:26:ARG:NH2	2.15	0.44
2:H:267:ARG:HD2	2:H:271:TYR:HE1	1.80	0.44
3:L:145:TYR:CE1	3:L:165:SER:HB2	2.52	0.44
3:L:149:GLN:HG3	3:L:149:GLN:O	2.17	0.44
1:A:282:PRO:CB	1:A:285:ILE:HD13	2.46	0.44
1:A:396:ARG:HD3	1:A:534:LEU:O	2.17	0.44
2:B:161:LEU:O	2:B:173:SER:HB2	2.17	0.44
2:B:411:THR:C	2:B:413:LYS:N	2.69	0.44
1:C:113:LEU:HB3	1:C:138:ARG:NH2	2.33	0.44
1:C:211:HIS:HB3	1:C:335:ASP:HB2	1.99	0.44
1:E:288:ILE:HG23	1:E:305:TRP:CZ3	2.52	0.44
1:E:489:GLU:O	1:E:489:GLU:HG2	2.17	0.44
2:F:56:ALA:HB2	2:F:77:VAL:HG11	2.00	0.44
2:F:404:THR:O	2:F:407:ASN:HB2	2.17	0.44
2:H:342:ASN:O	2:H:342:ASN:CG	2.56	0.44
3:L:117:ILE:CD1	3:L:126:ILE:HG12	2.47	0.44
1:C:262:GLU:O	1:C:264:ASN:N	2.51	0.44
1:C:480:HIS:O	1:C:483:CYS:HB2	2.17	0.44
2:D:318:LEU:HD12	2:D:319:ASN:N	2.32	0.44
1:E:116:ASP:N	1:E:117:PRO:HD3	2.33	0.44
1:E:261:ASP:O	1:E:262:GLU:HG3	2.18	0.44
2:F:154:ILE:HG13	2:F:158:LEU:HD23	2.00	0.44
1:G:114:ASP:HA	1:G:138:ARG:NH2	2.33	0.44
1:G:243:PHE:O	1:G:247:ILE:HG13	2.17	0.44
2:H:132:ASP:O	2:H:136:ARG:HG3	2.16	0.44
3:L:161:ILE:O	3:L:162:LEU:HD23	2.17	0.44
2:B:31:THR:OG1	2:B:35:PHE:CB	2.66	0.44
2:B:207:TYR:O	3:I:142:ARG:NH1	2.51	0.44
1:C:33:VAL:CG1	1:C:54:ILE:HG12	2.48	0.44
1:E:335:ASP:HB3	1:E:338:LYS:CB	2.38	0.44
1:E:418:ASN:HD22	1:E:419:PRO:N	2.14	0.44
1:E:452:GLU:CG	1:E:456:LYS:HE3	2.46	0.44
2:F:221:MET:N	2:F:222:PRO:HD3	2.33	0.44
2:H:195:GLY:O	2:H:339:ARG:NH1	2.50	0.44
1:A:155:THR:HB	1:A:489:GLU:HG3	2.00	0.44
2:B:13:TRP:NE1	2:B:16:ARG:HB2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:GLN:CA	2:B:351:GLN:HE21	2.30	0.44
1:C:274:THR:HG21	3:J:131:GLU:HG2	2.00	0.44
1:C:504:GLU:OE2	1:C:507:LYS:NZ	2.47	0.44
2:D:224:LEU:O	2:D:227:HIS:HB2	2.18	0.44
2:F:232:VAL:HA	2:F:236:GLN:HB3	2.00	0.44
2:H:32:HIS:CG	2:H:33:PRO:HD2	2.53	0.44
2:H:280:LEU:O	2:H:284:VAL:HG23	2.17	0.44
1:A:371:ALA:C	1:A:373:GLU:N	2.71	0.44
2:B:64:LEU:HD21	2:B:77:VAL:HG21	1.96	0.44
2:B:187:GLY:HA2	3:I:173:LEU:HD13	2.00	0.44
1:C:225:TRP:NE1	1:C:234:PRO:HD3	2.33	0.44
1:C:263:GLU:O	1:C:266:GLU:HB3	2.18	0.44
2:D:162:LEU:HA	2:D:173:SER:OG	2.16	0.44
2:D:392:LEU:HD12	2:D:392:LEU:H	1.81	0.44
1:E:48:ASN:HB2	1:E:502:ALA:CB	2.48	0.44
1:E:317:LYS:O	1:E:319:GLY:N	2.51	0.44
2:F:249:LEU:CD1	2:F:256:HIS:HB3	2.47	0.44
1:G:353:ASP:O	1:G:357:VAL:HG23	2.18	0.44
3:L:124:GLU:HB2	3:L:152:ASP:O	2.18	0.44
1:A:253:LYS:O	1:A:260:GLU:CB	2.66	0.44
1:A:298:THR:OG1	1:A:300:GLN:HG2	2.18	0.44
2:B:351:GLN:HB3	2:B:436:PHE:CD2	2.53	0.44
2:B:356:SER:CA	2:B:442:SER:HB3	2.48	0.44
1:C:9:LYS:HE2	1:C:99:ASP:OD1	2.18	0.44
1:C:334:ALA:H	2:D:223:ARG:HH21	1.66	0.44
2:F:351:GLN:HB2	2:F:436:PHE:CD2	2.52	0.44
2:F:435:LEU:O	2:F:436:PHE:CD2	2.70	0.44
2:F:438:LEU:HD23	2:F:438:LEU:HA	1.75	0.44
1:G:210:SER:N	1:G:262:GLU:OE2	2.51	0.44
1:C:67:GLY:H	2:H:262:GLN:HE22	1.66	0.43
1:C:260:GLU:HG3	1:C:261:ASP:OD2	2.17	0.43
2:D:240:GLU:O	2:D:241:GLN:C	2.56	0.43
2:D:371:SER:OG	2:D:372:ALA:N	2.51	0.43
3:J:143:LEU:HB3	3:J:150:MET:HE2	2.00	0.43
1:E:336:SER:HB2	2:F:221:MET:CA	2.45	0.43
1:G:38:ALA:HB3	1:G:85:ARG:CD	2.48	0.43
2:H:267:ARG:O	2:H:271:TYR:HD1	2.01	0.43
3:L:136:ILE:O	3:L:137:PRO:C	2.55	0.43
1:A:408:ASN:OD1	1:A:411:GLU:HB3	2.18	0.43
3:I:107:THR:C	3:I:109:THR:H	2.21	0.43
2:D:147:SER:O	2:D:151:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:ILE:HD13	2:F:272:ASN:O	2.18	0.43
1:E:428:MET:O	1:E:432:VAL:HG23	2.18	0.43
3:K:103:ILE:HD11	3:K:115:ILE:HG22	2.00	0.43
1:G:527:GLN:HG3	2:H:318:LEU:HB2	1.99	0.43
2:H:31:THR:OG1	2:H:35:PHE:CB	2.66	0.43
2:H:237:TRP:CE3	2:H:242:PRO:HG2	2.53	0.43
2:H:362:GLN:HG2	2:H:408:LEU:HD22	2.00	0.43
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.81	0.43
2:B:54:ILE:CG2	2:B:145:LEU:HD21	2.48	0.43
1:C:488:ALA:HB2	2:D:22:LYS:HD2	2.00	0.43
1:E:373:GLU:C	1:E:375:ILE:H	2.20	0.43
1:G:46:LEU:HA	1:G:46:LEU:HD12	1.72	0.43
2:H:235:LEU:HD22	2:H:235:LEU:N	2.33	0.43
2:H:271:TYR:C	2:H:272:ASN:HD22	2.18	0.43
1:A:490:PRO:HG3	2:B:23:PHE:HE1	1.84	0.43
1:C:36:ILE:HD13	1:C:36:ILE:HA	1.67	0.43
1:C:299:LYS:HG2	1:C:368:ILE:O	2.19	0.43
2:D:349:LEU:HA	2:D:350:PRO:HD3	1.89	0.43
2:D:422:GLU:HA	2:D:437:LYS:HA	2.00	0.43
1:E:163:ARG:HD3	1:E:518:ASN:O	2.18	0.43
1:E:248:ARG:C	1:E:250:GLY:N	2.70	0.43
1:E:311:LEU:HD22	1:E:383:LEU:HD21	2.00	0.43
1:E:418:ASN:ND2	1:E:418:ASN:C	2.71	0.43
1:G:143:LEU:CD1	1:G:150:LEU:HD13	2.48	0.43
2:H:28:GLY:O	2:H:31:THR:HG22	2.19	0.43
2:H:193:LEU:HA	2:H:194:PRO:HD2	1.73	0.43
1:C:19:LEU:CD1	2:D:292:VAL:HG13	2.49	0.43
1:C:156:TYR:CE1	1:C:487:ALA:HA	2.54	0.43
2:D:415:LEU:CD1	2:D:417:LEU:HG	2.48	0.43
2:F:266:GLU:O	2:F:267:ARG:C	2.57	0.43
1:G:12:LYS:HG3	2:H:88:LEU:HB2	2.00	0.43
1:G:269:ILE:HG22	1:G:269:ILE:O	2.17	0.43
1:A:366:GLN:O	1:A:368:ILE:N	2.52	0.43
2:B:195:GLY:O	2:B:339:ARG:NH1	2.52	0.43
1:C:51:LEU:HA	1:C:51:LEU:HD23	1.75	0.43
2:D:40:GLU:O	2:D:41:SER:C	2.56	0.43
2:D:361:LEU:O	2:D:363:GLU:N	2.52	0.43
1:E:113:LEU:HD13	1:E:138:ARG:CG	2.48	0.43
1:E:447:ASN:ND2	2:F:26:ARG:NH2	2.61	0.43
3:K:117:ILE:HD13	3:K:126:ILE:HG12	2.01	0.43
1:G:191:GLU:CD	1:G:191:GLU:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:LEU:HD21	1:G:375:ILE:HG21	2.00	0.43
2:H:182:THR:OG1	2:H:295:THR:HG22	2.19	0.43
2:H:200:ILE:CD1	3:L:172:ARG:HH21	2.32	0.43
2:H:233:ARG:HH11	2:H:233:ARG:CG	2.26	0.43
2:H:321:TYR:HE2	2:H:323:VAL:CG2	2.29	0.43
2:H:361:LEU:O	2:H:364:VAL:CG2	2.65	0.43
2:H:402:GLU:CG	2:H:405:ARG:HH22	2.30	0.43
1:A:437:LYS:HA	1:A:437:LYS:NZ	2.32	0.43
2:B:52:LEU:HD11	2:B:78:ILE:HG13	2.00	0.43
2:B:158:LEU:CD1	2:B:177:LEU:HB2	2.49	0.43
2:B:412:LEU:CD1	2:B:438:LEU:HD11	2.49	0.43
1:C:160:GLY:HA3	1:C:497:LEU:HD11	2.01	0.43
1:C:310:ALA:CB	1:C:361:VAL:HG22	2.48	0.43
1:C:341:LYS:O	1:C:344:ASN:HB2	2.19	0.43
2:D:164:TYR:CE2	2:D:169:LEU:HB2	2.53	0.43
2:D:294:SER:O	2:D:298:VAL:HG23	2.17	0.43
2:F:169:LEU:HD12	2:F:170:ASP:N	2.33	0.43
2:F:223:ARG:O	2:F:273:ILE:HD13	2.18	0.43
2:F:231:TYR:CE1	2:F:235:LEU:HB2	2.54	0.43
2:H:64:LEU:HD21	2:H:77:VAL:HG22	1.99	0.43
3:L:103:ILE:HG21	3:L:161:ILE:CG2	2.49	0.43
3:L:151:ASN:C	3:L:153:GLU:H	2.22	0.43
3:L:170:VAL:HG13	3:L:171:LEU:H	1.83	0.43
1:A:234:PRO:HB2	1:A:276:LEU:CD1	2.48	0.43
2:B:403:ARG:NE	2:D:166:ASP:OD2	2.52	0.43
2:B:417:LEU:HD22	2:B:417:LEU:N	2.33	0.43
3:I:145:TYR:HB2	3:I:167:LEU:CD2	2.49	0.43
3:I:161:ILE:HD13	3:I:167:LEU:HD21	2.00	0.43
1:C:189:PHE:CD1	1:C:192:LEU:HB2	2.54	0.43
1:C:265:PHE:O	1:C:269:ILE:HG13	2.19	0.43
1:E:214:TRP:O	1:E:218:ILE:HG13	2.18	0.43
1:E:517:ASN:O	1:E:517:ASN:ND2	2.44	0.43
2:F:374:LEU:O	2:F:376:MET:HG3	2.18	0.43
2:H:24:LEU:CD2	2:H:312:THR:HB	2.48	0.43
2:H:412:LEU:CD1	2:H:412:LEU:H	2.31	0.43
1:A:130:GLN:OE1	1:A:154:ARG:HA	2.18	0.43
2:B:132:ASP:O	2:B:136:ARG:HB2	2.19	0.43
2:B:152:ARG:NH2	2:B:201:GLU:OE1	2.52	0.43
1:C:9:LYS:C	1:C:11:GLN:N	2.71	0.43
1:C:435:PHE:C	1:C:435:PHE:CD2	2.91	0.43
2:D:78:ILE:HG12	2:D:123:HIS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:ARG:HA	2:D:95:ARG:HD3	1.78	0.43
2:H:321:TYR:HE1	3:L:172:ARG:HH11	1.67	0.43
2:H:380:ALA:HB1	2:H:394:LEU:HD12	1.94	0.43
2:D:343:CYS:C	2:D:345:ALA:N	2.72	0.43
2:F:62:GLU:CG	2:F:297:ALA:HA	2.44	0.43
1:G:299:LYS:HA	1:G:368:ILE:CG2	2.49	0.43
1:A:128:ALA:HB1	1:A:131:LEU:CD1	2.49	0.42
1:A:492:THR:HG22	2:B:66:ASN:HB3	2.01	0.42
1:A:517:ASN:OD1	1:A:533:GLN:NE2	2.52	0.42
3:I:101:MET:SD	3:I:162:LEU:HA	2.59	0.42
3:I:118:GLU:O	3:I:121:ASP:HB2	2.19	0.42
2:F:385:LEU:HD21	2:F:417:LEU:CD1	2.49	0.42
1:G:25:GLN:O	1:G:29:GLU:HG3	2.19	0.42
1:G:124:THR:HG22	1:G:125:VAL:HG23	2.01	0.42
1:G:128:ALA:HB1	1:G:131:LEU:CD1	2.48	0.42
1:G:466:GLN:O	1:G:467:GLU:C	2.58	0.42
2:H:271:TYR:C	2:H:272:ASN:ND2	2.71	0.42
1:A:229:THR:HG22	1:A:232:ARG:HB3	2.01	0.42
3:I:137:PRO:HA	3:I:138:PRO:HD3	1.94	0.42
2:D:361:LEU:C	2:D:363:GLU:N	2.72	0.42
2:F:318:LEU:C	2:F:319:ASN:O	2.56	0.42
2:F:322:LEU:CD1	2:F:323:VAL:N	2.80	0.42
1:G:181:GLU:O	1:G:278:THR:HB	2.20	0.42
1:A:13:TYR:O	1:A:17:LEU:HG	2.18	0.42
1:A:34:CYS:HB2	1:A:123:PHE:CE1	2.55	0.42
1:A:148:ILE:HA	1:A:149:PRO:HD3	1.92	0.42
2:B:294:SER:O	2:B:298:VAL:HG23	2.19	0.42
2:B:430:THR:HA	2:B:431:PRO:HD3	1.93	0.42
2:D:261:PHE:CD1	2:D:278:TYR:HA	2.54	0.42
1:G:416:MET:C	1:G:418:ASN:N	2.72	0.42
1:A:222:LEU:HA	1:A:222:LEU:HD12	1.78	0.42
2:B:158:LEU:HD12	2:B:177:LEU:HB2	2.00	0.42
2:B:384:THR:C	2:B:385:LEU:O	2.55	0.42
1:C:252:LEU:O	1:C:252:LEU:HD12	2.19	0.42
1:C:423:ILE:HG13	1:C:423:ILE:O	2.19	0.42
1:E:224:GLN:HE21	1:E:246:LEU:HD11	1.84	0.42
1:E:396:ARG:NH1	1:E:534:LEU:O	2.49	0.42
2:F:182:THR:HG21	2:F:296:ASN:OD1	2.19	0.42
2:F:247:VAL:HA	2:F:248:PRO:HD3	1.88	0.42
2:F:250:ASP:OD2	2:F:252:ASP:HB2	2.19	0.42
2:F:423:LEU:O	2:F:435:LEU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:THR:O	1:G:280:GLN:HB2	2.19	0.42
2:H:352:ASN:N	2:H:352:ASN:HD22	2.16	0.42
2:B:40:GLU:HG2	2:B:40:GLU:O	2.20	0.42
1:E:163:ARG:NH1	1:E:518:ASN:ND2	2.62	0.42
1:E:357:VAL:HG12	1:E:380:LEU:HD11	2.02	0.42
2:H:310:ILE:O	2:H:310:ILE:HG22	2.19	0.42
2:B:309:LYS:HG2	2:B:315:TYR:HB2	2.01	0.42
1:C:57:PHE:C	1:C:57:PHE:CD1	2.93	0.42
1:C:327:GLY:HA3	1:C:350:ALA:HB2	2.01	0.42
1:E:419:PRO:HB2	1:E:475:LYS:HE3	2.01	0.42
1:E:457:LEU:HD23	1:E:479:VAL:HG13	2.01	0.42
2:F:84:ASP:HB3	2:F:87:ASN:OD1	2.18	0.42
1:G:163:ARG:NH2	1:G:518:ASN:HD21	2.17	0.42
2:H:84:ASP:H	2:H:87:ASN:HD21	1.66	0.42
2:H:354:GLN:NE2	2:H:439:HIS:CB	2.72	0.42
2:H:398:THR:CA	2:H:401:GLU:HB3	2.49	0.42
1:A:396:ARG:NH2	1:A:406:THR:O	2.50	0.42
2:B:152:ARG:NE	2:B:201:GLU:OE1	2.53	0.42
2:B:233:ARG:HG3	2:B:249:LEU:CD2	2.47	0.42
1:C:454:ILE:HD13	1:C:480:HIS:ND1	2.34	0.42
2:D:73:ARG:HG3	2:D:73:ARG:NH1	2.35	0.42
2:D:322:LEU:C	2:D:322:LEU:CD1	2.81	0.42
1:E:447:ASN:ND2	2:F:26:ARG:NE	2.62	0.42
3:K:162:LEU:HB3	3:K:163:GLY:H	1.65	0.42
1:G:214:TRP:CD1	1:G:214:TRP:C	2.92	0.42
2:H:155:ASN:OD1	2:H:199:CYS:HB2	2.19	0.42
2:B:239:LYS:HD2	2:B:239:LYS:HA	1.83	0.42
2:D:64:LEU:C	2:D:111:LEU:HD11	2.39	0.42
1:E:125:VAL:HG12	1:E:126:VAL:N	2.34	0.42
3:K:137:PRO:HA	3:K:138:PRO:HD3	1.87	0.42
1:G:66:SER:O	1:G:69:ASP:HB2	2.20	0.42
1:G:236:THR:HG22	1:G:237:TYR:N	2.34	0.42
1:A:282:PRO:CG	1:A:285:ILE:HD13	2.49	0.42
2:B:237:TRP:CE3	2:B:242:PRO:HG3	2.54	0.42
1:C:67:GLY:H	2:H:262:GLN:NE2	2.18	0.42
1:C:177:ASP:OD1	2:D:327:VAL:HG21	2.20	0.42
2:D:405:ARG:HG3	2:D:408:LEU:HD12	2.01	0.42
2:F:24:LEU:CD2	2:F:312:THR:HB	2.49	0.42
2:F:231:TYR:C	2:F:233:ARG:H	2.23	0.42
2:F:357:PRO:HG3	2:F:412:LEU:CD1	2.43	0.42
1:G:281:ILE:CG2	1:G:286:GLU:OE2	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:333:ILE:H	1:G:333:ILE:HG13	1.59	0.42
2:H:201:GLU:HG2	2:H:345:ALA:CB	2.50	0.42
2:H:213:PHE:O	2:H:214:PRO:C	2.58	0.42
3:L:107:THR:CG2	3:L:111:LYS:H	2.27	0.42
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.93	0.42
1:A:468:TYR:HB2	1:A:470:LEU:HD11	2.02	0.42
2:B:157:MET:HA	2:B:157:MET:CE	2.49	0.42
2:B:385:LEU:HD23	2:B:385:LEU:HA	1.56	0.42
1:C:481:GLU:HG3	1:C:485:TYR:CE2	2.55	0.42
3:J:105:VAL:HG13	3:J:105:VAL:O	2.20	0.42
1:E:38:ALA:C	1:E:85:ARG:HD3	2.40	0.42
2:F:38:SER:HB3	2:F:41:SER:OG	2.20	0.42
2:F:392:LEU:O	2:F:393:TYR:HB2	2.20	0.42
1:G:175:HIS:HD2	1:G:512:GLN:O	2.02	0.42
1:G:201:LEU:HD22	1:G:221:TYR:HE1	1.85	0.42
1:G:208:ASP:O	1:G:212:THR:HG23	2.20	0.42
1:A:250:GLY:O	1:A:251:ILE:C	2.58	0.41
2:B:79:ASP:OD2	2:B:81:ASP:HB2	2.20	0.41
2:B:361:LEU:HD23	2:B:361:LEU:O	2.19	0.41
1:C:97:ASN:HB3	1:C:100:VAL:HG23	2.02	0.41
1:C:159:VAL:HG22	1:C:425:LEU:HD13	2.02	0.41
1:C:425:LEU:HD11	1:C:523:SER:HB2	2.02	0.41
3:J:123:VAL:CB	3:J:152:ASP:HA	2.40	0.41
2:F:69:LEU:HD23	2:F:69:LEU:HA	1.87	0.41
2:F:351:GLN:HB2	2:F:436:PHE:CE2	2.55	0.41
3:K:169:LEU:HD23	3:K:169:LEU:HA	1.83	0.41
2:H:32:HIS:HD2	2:H:34:ASP:H	1.60	0.41
2:H:270:GLN:HB2	2:H:271:TYR:CE1	2.55	0.41
2:H:329:GLY:C	2:H:330:LEU:HD12	2.40	0.41
1:A:407:ILE:HD13	1:A:408:ASN:N	2.34	0.41
2:B:324:PHE:HD1	2:B:332:THR:HG22	1.84	0.41
2:D:187:GLY:HA2	3:J:173:LEU:HD12	2.03	0.41
3:J:107:THR:HA	3:J:169:LEU:HD12	2.02	0.41
1:E:209:HIS:CD2	1:E:252:LEU:H	2.38	0.41
1:E:241:GLU:OE1	1:E:241:GLU:HA	2.20	0.41
2:F:59:LEU:O	2:F:63:LEU:HG	2.20	0.41
1:G:137:LEU:HD23	1:G:137:LEU:HA	1.84	0.41
1:G:251:ILE:O	1:G:253:LYS:N	2.52	0.41
2:H:163:ASN:O	2:H:163:ASN:OD1	2.39	0.41
1:A:344:ASN:CG	1:E:111:ASN:HD22	2.24	0.41
1:A:434:ARG:HD3	1:A:460:CYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ARG:HG2	1:C:519:THR:OG1	2.21	0.41
2:D:58:GLY:O	2:D:62:GLU:HB2	2.21	0.41
2:D:178:ILE:HD11	2:D:310:ILE:HD12	2.02	0.41
2:D:233:ARG:HH12	2:D:234:MET:HB2	1.85	0.41
1:E:240:LYS:HG2	1:E:276:LEU:CD1	2.51	0.41
1:G:34:CYS:HB2	1:G:123:PHE:CG	2.55	0.41
2:H:46:LEU:O	2:H:73:ARG:HB3	2.20	0.41
2:H:197:THR:CG2	2:H:198:ALA:N	2.83	0.41
2:H:199:CYS:SG	2:H:201:GLU:HB2	2.60	0.41
1:A:249:GLN:HG2	1:A:249:GLN:O	2.20	0.41
1:A:297:ILE:N	1:A:297:ILE:CD1	2.84	0.41
2:B:126:LYS:O	2:B:127:ILE:C	2.59	0.41
2:B:191:VAL:O	2:B:197:THR:HG21	2.20	0.41
1:C:335:ASP:OD2	1:C:336:SER:N	2.53	0.41
1:C:376:SER:OG	1:C:379:GLU:HG3	2.20	0.41
1:E:113:LEU:HD13	1:E:138:ARG:HG2	2.02	0.41
1:E:277:ASN:C	1:E:277:ASN:HD22	2.23	0.41
2:F:58:GLY:N	2:F:91:GLN:HG2	2.34	0.41
2:F:127:ILE:HD12	2:F:153:TRP:CE3	2.55	0.41
2:F:380:ALA:HB1	2:F:394:LEU:HD12	1.94	0.41
2:H:205:GLU:OE1	2:H:372:ALA:HB1	2.20	0.41
3:L:105:VAL:HG13	3:L:105:VAL:O	2.19	0.41
1:E:12:LYS:HE3	1:E:13:TYR:CE2	2.56	0.41
1:E:354:ALA:O	1:E:380:LEU:HD21	2.20	0.41
2:F:381:ILE:H	2:F:381:ILE:HG13	1.75	0.41
2:F:386:GLU:C	2:F:388:LYS:N	2.74	0.41
1:G:43:THR:HG21	1:G:73:ASN:OD1	2.19	0.41
1:G:84:ASN:CG	1:G:106:GLU:HG2	2.40	0.41
2:H:88:LEU:HD22	2:H:94:PHE:O	2.20	0.41
2:H:335:PHE:CD1	2:H:335:PHE:C	2.94	0.41
3:L:101:MET:CE	3:L:119:PRO:HG3	2.50	0.41
1:A:104:PHE:CD1	1:A:104:PHE:C	2.93	0.41
1:A:155:THR:HG23	1:A:493:ILE:CG2	2.50	0.41
2:B:73:ARG:HD3	2:B:117:ASN:O	2.21	0.41
2:D:192:ILE:CD1	2:D:200:ILE:HG13	2.51	0.41
1:E:503:GLN:O	1:E:507:LYS:HG3	2.21	0.41
2:F:193:LEU:HD23	2:F:193:LEU:HA	1.80	0.41
2:F:319:ASN:C	2:F:320:ASN:ND2	2.74	0.41
1:G:128:ALA:HB1	1:G:131:LEU:HD11	2.03	0.41
1:G:447:ASN:ND2	2:H:26:ARG:HH21	2.17	0.41
2:H:358:SER:O	2:H:359:ALA:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:O	1:A:42:GLY:C	2.58	0.41
1:A:154:ARG:HB3	1:A:161:TYR:HB3	2.03	0.41
2:B:13:TRP:CD1	2:B:16:ARG:HB2	2.56	0.41
2:D:87:ASN:ND2	2:D:103:LYS:HE2	2.36	0.41
1:E:261:ASP:O	1:E:262:GLU:CG	2.69	0.41
2:F:17:TRP:O	2:F:18:ASN:C	2.58	0.41
1:G:199:TYR:O	1:G:220:LYS:NZ	2.51	0.41
2:H:64:LEU:HB3	2:H:111:LEU:CD1	2.51	0.41
2:H:316:ILE:H	2:H:316:ILE:CD1	2.08	0.41
2:H:410:LYS:HA	2:H:414:GLU:OE1	2.20	0.41
2:B:45:LEU:HG	2:B:71:GLY:O	2.21	0.41
2:B:382:THR:OG1	2:B:424:ALA:HB3	2.20	0.41
3:I:117:ILE:CD1	3:I:126:ILE:HG23	2.48	0.41
3:K:145:TYR:CD1	3:K:167:LEU:HD23	2.55	0.41
1:G:210:SER:C	1:G:212:THR:H	2.24	0.41
1:G:425:LEU:O	1:G:429:LEU:HG	2.21	0.41
2:H:207:TYR:HA	2:H:208:PRO:HD3	1.93	0.41
2:H:412:LEU:O	2:H:417:LEU:HB2	2.20	0.41
1:A:45:ILE:HG12	1:A:501:ALA:HB3	2.03	0.41
1:A:54:ILE:HD12	1:A:54:ILE:HA	1.86	0.41
1:A:229:THR:HG21	1:A:232:ARG:HB3	2.00	0.41
1:A:248:ARG:HG3	1:A:248:ARG:NH1	2.35	0.41
1:A:434:ARG:HD3	1:A:460:CYS:HB3	2.03	0.41
1:A:450:VAL:O	1:A:454:ILE:HG13	2.21	0.41
2:B:413:LYS:O	2:B:413:LYS:HG2	2.19	0.41
1:C:204:MET:SD	1:C:252:LEU:HD22	2.60	0.41
2:D:43:GLN:HG3	2:D:47:ASP:OD2	2.21	0.41
2:D:98:ASP:O	2:D:99:ILE:C	2.60	0.41
3:J:118:GLU:C	3:J:120:THR:H	2.25	0.41
1:E:65:VAL:HG23	1:E:85:ARG:HA	2.03	0.41
1:E:325:VAL:O	1:E:326:ARG:C	2.59	0.41
1:E:347:ARG:NH2	2:F:274:ARG:NH1	2.61	0.41
1:E:488:ALA:HB2	2:F:22:LYS:HG3	2.01	0.41
2:F:259:TRP:CZ2	2:F:263:LYS:HE3	2.56	0.41
2:F:407:ASN:HA	2:F:410:LYS:HG3	2.03	0.41
3:K:107:THR:HG22	3:K:109:THR:HG23	2.01	0.41
1:G:172:ILE:HA	1:G:390:LEU:HD23	2.02	0.41
1:G:189:PHE:CE1	1:G:349:LYS:HB2	2.56	0.41
2:H:170:ASP:O	2:H:173:SER:HB3	2.20	0.41
2:H:440:PHE:HD2	2:H:440:PHE:HA	1.79	0.41
1:A:439:GLN:HE21	1:A:439:GLN:HB3	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLU:OE1	2:B:315:TYR:OH	2.28	0.41
1:C:96:LEU:HD23	2:D:95:ARG:HH21	1.86	0.41
1:C:146:SER:O	1:C:147:GLN:HB2	2.21	0.41
1:E:39:THR:O	1:E:43:THR:HB	2.21	0.41
1:E:189:PHE:CZ	1:E:349:LYS:HG2	2.55	0.41
2:F:74:GLN:NE2	2:F:74:GLN:CA	2.72	0.41
2:F:178:ILE:HD11	2:F:310:ILE:HD12	2.02	0.41
2:F:210:GLN:HG3	2:F:210:GLN:O	2.21	0.41
2:F:212:ASN:HD22	2:F:212:ASN:HA	1.62	0.41
2:F:357:PRO:HG3	2:F:440:PHE:CE2	2.55	0.41
1:G:340:ILE:CD1	2:H:271:TYR:O	2.69	0.41
2:H:245:GLU:CG	2:H:246:GLY:N	2.83	0.41
1:A:504:GLU:O	1:A:508:ILE:HG13	2.21	0.40
3:I:151:ASN:OD1	3:I:153:GLU:N	2.48	0.40
1:C:189:PHE:CZ	1:C:192:LEU:HB2	2.55	0.40
2:D:90:ARG:HG2	2:D:90:ARG:NH1	2.36	0.40
2:D:162:LEU:HD21	2:D:194:PRO:HB2	2.03	0.40
1:E:7:LEU:O	1:E:7:LEU:HD23	2.21	0.40
1:E:8:LEU:HD12	1:E:11:GLN:OE1	2.21	0.40
1:E:114:ASP:OD1	1:E:138:ARG:NH2	2.53	0.40
1:E:282:PRO:HB2	1:E:285:ILE:HD13	2.02	0.40
1:E:368:ILE:O	1:E:368:ILE:CG2	2.69	0.40
2:F:87:ASN:HB3	2:F:91:GLN:OE1	2.21	0.40
2:F:423:LEU:HD11	2:F:438:LEU:CD2	2.32	0.40
3:K:105:VAL:HG11	3:K:130:VAL:HG22	2.03	0.40
1:G:187:LYS:HD2	1:G:279:THR:CG2	2.45	0.40
1:G:226:TYR:HE2	1:G:233:ILE:HA	1.86	0.40
1:G:407:ILE:HG13	1:G:408:ASN:N	2.36	0.40
3:L:106:LYS:HA	3:L:112:GLU:HA	2.03	0.40
1:A:229:THR:CG2	1:A:229:THR:O	2.68	0.40
1:C:173:GLU:HA	1:C:386:ASN:ND2	2.37	0.40
2:D:377:LYS:N	2:D:427:ASP:OD1	2.54	0.40
2:D:412:LEU:HB3	2:D:440:PHE:CE2	2.56	0.40
1:E:31:ALA:HB2	1:E:509:ILE:HG23	2.02	0.40
1:E:74:PHE:CD1	2:F:65:LYS:HG3	2.57	0.40
1:E:229:THR:HG22	1:E:229:THR:O	2.21	0.40
1:E:448:TYR:CE1	1:E:449:GLN:HG2	2.56	0.40
2:F:178:ILE:HD11	2:F:310:ILE:CD1	2.51	0.40
1:G:285:ILE:HD12	1:G:323:LEU:HD11	2.04	0.40
1:G:510:THR:O	1:G:511:LYS:HB2	2.22	0.40
2:H:237:TRP:CZ2	2:H:249:LEU:HA	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ILE:HD12	1:A:368:ILE:HA	1.97	0.40
1:A:496:PHE:CD2	1:A:496:PHE:C	2.94	0.40
1:C:368:ILE:CG2	1:C:368:ILE:O	2.70	0.40
1:C:418:ASN:HD22	1:C:418:ASN:C	2.24	0.40
1:C:468:TYR:O	1:C:469:GLY:C	2.60	0.40
2:D:327:VAL:CG2	2:D:328:ASP:H	2.29	0.40
1:E:184:ARG:NH1	1:E:325:VAL:HG22	2.35	0.40
1:G:297:ILE:HD11	1:G:309:ARG:HG2	2.03	0.40
2:H:115:VAL:HA	2:H:116:PRO:HD2	1.96	0.40
1:A:447:ASN:ND2	2:B:26:ARG:NE	2.69	0.40
2:B:261:PHE:CZ	2:B:265:LEU:HD11	2.56	0.40
2:D:241:GLN:CG	2:D:245:GLU:HA	2.43	0.40
3:J:141:GLN:O	3:J:142:ARG:NH1	2.47	0.40
2:F:24:LEU:HD21	2:F:312:THR:HB	2.03	0.40
2:F:159:ILE:HG22	2:F:432:GLN:OE1	2.22	0.40
3:K:131:GLU:OE2	3:K:138:PRO:HD3	2.22	0.40
1:G:72:ASN:HD22	1:G:72:ASN:C	2.24	0.40
1:G:264:ASN:ND2	1:G:265:PHE:H	2.18	0.40
1:G:371:ALA:HA	1:G:372:PRO:HD3	1.90	0.40
2:H:405:ARG:HB3	2:H:406:PRO:HD3	2.03	0.40
2:H:415:LEU:HD23	2:H:415:LEU:HA	1.92	0.40
1:A:45:ILE:CG1	1:A:498:GLY:HA2	2.50	0.40
1:A:89:ALA:O	1:A:90:MET:C	2.58	0.40
1:A:243:PHE:O	1:A:246:LEU:HB3	2.20	0.40
1:A:457:LEU:HD23	1:A:479:VAL:HG12	2.02	0.40
1:A:527:GLN:OE1	1:A:527:GLN:HA	2.22	0.40
2:B:356:SER:HA	2:B:442:SER:HB3	2.04	0.40
2:B:412:LEU:CB	2:B:440:PHE:HZ	2.35	0.40
1:C:323:LEU:HB3	1:C:324:PRO:CD	2.51	0.40
1:E:45:ILE:HG13	1:E:498:GLY:HA2	2.03	0.40
1:E:371:ALA:O	1:E:374:SER:N	2.53	0.40
1:E:418:ASN:ND2	1:E:419:PRO:HD2	2.31	0.40
2:F:354:GLN:O	2:F:355:PHE:CD2	2.74	0.40
2:F:381:ILE:HA	2:F:424:ALA:O	2.22	0.40
1:G:54:ILE:HD12	1:G:54:ILE:HA	1.93	0.40
1:G:398:LEU:HD12	1:G:398:LEU:HA	1.91	0.40
2:H:321:TYR:CD2	2:H:322:LEU:N	2.89	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/531 (98%)	442 (85%)	61 (12%)	15 (3%)	4	15
1	C	513/531 (97%)	448 (87%)	56 (11%)	9 (2%)	8	25
1	E	519/531 (98%)	465 (90%)	47 (9%)	7 (1%)	12	33
1	G	512/531 (96%)	437 (85%)	62 (12%)	13 (2%)	5	18
2	B	430/434 (99%)	373 (87%)	51 (12%)	6 (1%)	11	31
2	D	430/434 (99%)	366 (85%)	53 (12%)	11 (3%)	5	17
2	F	429/434 (99%)	359 (84%)	55 (13%)	15 (4%)	3	12
2	H	429/434 (99%)	347 (81%)	63 (15%)	19 (4%)	2	8
3	I	84/88 (96%)	76 (90%)	4 (5%)	4 (5%)	2	6
3	J	74/88 (84%)	67 (90%)	5 (7%)	2 (3%)	5	16
3	K	74/88 (84%)	66 (89%)	6 (8%)	2 (3%)	5	16
3	L	74/88 (84%)	64 (86%)	5 (7%)	5 (7%)	1	2
All	All	4086/4212 (97%)	3510 (86%)	468 (12%)	108 (3%)	5	17

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	450	VAL
2	B	116	PRO
1	C	263	GLU
1	C	422	GLU
1	C	518	ASN
2	D	116	PRO
1	E	275	ALA
2	F	116	PRO
2	F	242	PRO
2	F	319	ASN
2	F	348	GLN

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Mol	Chain	Res	Type
2	F	357	PRO
2	F	360	LYS
2	F	419	ASP
1	G	263	GLU
1	G	264	ASN
2	H	116	PRO
3	L	163	GLY
1	A	66	SER
1	A	79	SER
1	A	118	SER
1	A	134	SER
1	A	263	GLU
2	B	127	ILE
2	B	319	ASN
1	C	438	GLN
1	C	451	GLU
2	D	412	LEU
3	J	163	GLY
1	E	190	PRO
1	E	249	GLN
1	E	259	PRO
1	E	318	GLU
2	F	375	GLN
3	K	163	GLY
1	G	190	PRO
2	H	239	LYS
2	H	357	PRO
2	H	361	LEU
3	L	119	PRO
2	B	386	GLU
3	I	147	GLY
1	C	317	LYS
2	D	31	THR
2	D	34	ASP
2	D	132	ASP
2	D	362	GLN
1	G	184	ARG
1	G	250	GLY
1	G	252	LEU
1	G	280	GLN
1	G	317	LYS
2	H	240	GLU

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Mol	Chain	Res	Type
2	H	320	ASN
2	H	350	PRO
2	H	388	LYS
2	H	403	ARG
2	H	416	GLY
3	L	150	MET
1	A	259	PRO
1	A	367	SER
2	B	399	SER
3	I	146	SER
1	C	232	ARG
2	D	183	GLU
3	J	119	PRO
2	F	92	PHE
2	F	371	SER
2	F	401	GLU
3	K	119	PRO
1	G	211	HIS
2	H	194	PRO
2	H	359	ALA
2	H	360	LYS
3	L	152	ASP
3	L	154	LYS
1	A	65	VAL
1	A	251	ILE
1	A	372	PRO
1	A	443	PRO
2	B	167	GLY
3	I	108	LEU
1	C	259	PRO
2	D	196	MET
2	F	211	VAL
2	F	259	TRP
1	G	106	GLU
1	G	451	GLU
2	H	183	GLU
2	H	238	PRO
2	H	401	GLU
2	H	408	LEU
3	I	163	GLY
1	E	260	GLU
1	E	280	GLN

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Mol	Chain	Res	Type
1	G	229	THR
2	H	172	SER
2	H	387	GLY
1	A	36	ILE
2	D	241	GLN
2	D	327	VAL
2	D	350	PRO
1	C	469	GLY
1	G	407	ILE
2	F	246	GLY
1	A	250	GLY
2	F	194	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	452/462 (98%)	431 (95%)	21 (5%)	27	56
1	C	451/462 (98%)	424 (94%)	27 (6%)	19	45
1	E	450/462 (97%)	421 (94%)	29 (6%)	17	41
1	G	450/462 (97%)	430 (96%)	20 (4%)	28	58
2	B	377/381 (99%)	351 (93%)	26 (7%)	15	38
2	D	378/381 (99%)	354 (94%)	24 (6%)	18	42
2	F	376/381 (99%)	347 (92%)	29 (8%)	13	32
2	H	374/381 (98%)	338 (90%)	36 (10%)	8	22
3	I	73/74 (99%)	67 (92%)	6 (8%)	11	29
3	J	67/74 (90%)	65 (97%)	2 (3%)	41	72
3	K	67/74 (90%)	63 (94%)	4 (6%)	19	45
3	L	67/74 (90%)	64 (96%)	3 (4%)	27	57
All	All	3582/3668 (98%)	3355 (94%)	227 (6%)	18	42

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	134	SER
1	A	158	LEU
1	A	171	VAL
1	A	214	TRP
1	A	245	ASP
1	A	259	PRO
1	A	262	GLU
1	A	264	ASN
1	A	265	PHE
1	A	277	ASN
1	A	293	ARG
1	A	309	ARG
1	A	311	LEU
1	A	335	ASP
1	A	364	LEU
1	A	407	ILE
1	A	418	ASN
1	A	437	LYS
1	A	517	ASN
1	A	518	ASN
2	B	12	ASP
2	B	82	THR
2	B	95	ARG
2	B	111	LEU
2	B	114	ARG
2	B	116	PRO
2	B	128	GLN
2	B	182	THR
2	B	217	THR
2	B	233	ARG
2	B	249	LEU
2	B	272	ASN
2	B	309	LYS
2	B	316	ILE
2	B	323	VAL
2	B	342	ASN
2	B	351	GLN
2	B	353	ILE
2	B	362	GLN
2	B	374	LEU
2	B	375	GLN
2	B	377	LYS

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Mol	Chain	Res	Type
2	B	401	GLU
2	B	409	SER
2	B	412	LEU
2	B	425	VAL
3	I	97	SER
3	I	102	LEU
3	I	107	THR
3	I	153	GLU
3	I	158	ASP
3	I	171	LEU
1	C	33	VAL
1	C	43	THR
1	C	46	LEU
1	C	72	ASN
1	C	103	SER
1	C	122	ARG
1	C	163	ARG
1	C	171	VAL
1	C	177	ASP
1	C	193	ARG
1	C	214	TRP
1	C	245	ASP
1	C	261	ASP
1	C	264	ASN
1	C	277	ASN
1	C	293	ARG
1	C	297	ILE
1	C	343	GLN
1	C	353	ASP
1	C	359	ASN
1	C	383	LEU
1	C	406	THR
1	C	418	ASN
1	C	422	GLU
1	C	424	VAL
1	C	429	LEU
1	C	517	ASN
2	D	11	LEU
2	D	82	THR
2	D	110	PHE
2	D	114	ARG
2	D	116	PRO

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Mol	Chain	Res	Type
2	D	128	GLN
2	D	149	ILE
2	D	201	GLU
2	D	215	MET
2	D	316	ILE
2	D	322	LEU
2	D	323	VAL
2	D	325	ASN
2	D	342	ASN
2	D	357	PRO
2	D	362	GLN
2	D	389	ASN
2	D	401	GLU
2	D	411	THR
2	D	415	LEU
2	D	419	ASP
2	D	421	GLN
2	D	422	GLU
2	D	442	SER
3	J	108	LEU
3	J	170	VAL
1	E	43	THR
1	E	64	GLN
1	E	72	ASN
1	E	103	SER
1	E	112	LEU
1	E	158	LEU
1	E	163	ARG
1	E	171	VAL
1	E	214	TRP
1	E	226	TYR
1	E	259	PRO
1	E	262	GLU
1	E	264	ASN
1	E	277	ASN
1	E	293	ARG
1	E	297	ILE
1	E	309	ARG
1	E	311	LEU
1	E	353	ASP
1	E	364	LEU
1	E	418	ASN

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Mol	Chain	Res	Type
1	E	422	GLU
1	E	424	VAL
1	E	441	ARG
1	E	452	GLU
1	E	477	ASP
1	E	497	LEU
1	E	517	ASN
1	E	518	ASN
2	F	11	LEU
2	F	31	THR
2	F	39	THR
2	F	73	ARG
2	F	82	THR
2	F	87	ASN
2	F	111	LEU
2	F	114	ARG
2	F	116	PRO
2	F	128	GLN
2	F	142	VAL
2	F	143	CYS
2	F	149	ILE
2	F	182	THR
2	F	186	LYS
2	F	212	ASN
2	F	241	GLN
2	F	242	PRO
2	F	316	ILE
2	F	322	LEU
2	F	325	ASN
2	F	326	ASP
2	F	342	ASN
2	F	375	GLN
2	F	377	LYS
2	F	388	LYS
2	F	401	GLU
2	F	419	ASP
2	F	432	GLN
3	K	102	LEU
3	K	105	VAL
3	K	107	THR
3	K	109	THR
1	G	43	THR

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Mol	Chain	Res	Type
1	G	47	LYS
1	G	72	ASN
1	G	90	MET
1	G	111	ASN
1	G	163	ARG
1	G	171	VAL
1	G	180	LEU
1	G	202	ASP
1	G	214	TRP
1	G	225	TRP
1	G	262	GLU
1	G	264	ASN
1	G	277	ASN
1	G	309	ARG
1	G	311	LEU
1	G	333	ILE
1	G	364	LEU
1	G	506	ILE
1	G	517	ASN
2	H	12	ASP
2	H	82	THR
2	H	111	LEU
2	H	114	ARG
2	H	116	PRO
2	H	128	GLN
2	H	154	ILE
2	H	182	THR
2	H	213	PHE
2	H	223	ARG
2	H	233	ARG
2	H	240	GLU
2	H	267	ARG
2	H	272	ASN
2	H	316	ILE
2	H	318	LEU
2	H	319	ASN
2	H	322	LEU
2	H	325	ASN
2	H	326	ASP
2	H	328	ASP
2	H	342	ASN
2	H	344	PRO

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Mol	Chain	Res	Type
2	H	348	GLN
2	H	355	PHE
2	H	362	GLN
2	H	364	VAL
2	H	366	ASP
2	H	375	GLN
2	H	377	LYS
2	H	378	SER
2	H	381	ILE
2	H	392	LEU
2	H	402	GLU
2	H	417	LEU
2	H	440	PHE
3	L	107	THR
3	L	171	LEU
3	L	173	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	37	ASN
1	A	63	ASN
1	A	72	ASN
1	A	197	GLN
1	A	264	ASN
1	A	277	ASN
1	A	320	GLN
1	A	322	ASN
1	A	359	ASN
1	A	370	GLN
1	A	418	ASN
1	A	439	GLN
1	A	447	ASN
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	236	GLN

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Mol	Chain	Res	Type
2	B	241	GLN
2	B	272	ASN
2	B	320	ASN
2	B	325	ASN
2	B	342	ASN
2	B	351	GLN
2	B	362	GLN
2	B	389	ASN
2	B	395	GLN
3	I	149	GLN
1	C	72	ASN
1	C	197	GLN
1	C	209	HIS
1	C	211	HIS
1	C	224	GLN
1	C	264	ASN
1	C	271	ASN
1	C	277	ASN
1	C	320	GLN
1	C	343	GLN
1	C	344	ASN
1	C	359	ASN
1	C	386	ASN
1	C	418	ASN
1	C	439	GLN
1	C	447	ASN
1	C	512	GLN
1	C	517	ASN
2	D	74	GLN
2	D	128	GLN
2	D	139	HIS
2	D	210	GLN
2	D	236	GLN
2	D	241	GLN
2	D	270	GLN
2	D	282	GLN
2	D	320	ASN
2	D	325	ASN
2	D	342	ASN
2	D	362	GLN
2	D	375	GLN
2	D	421	GLN

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Mol	Chain	Res	Type
2	D	432	GLN
1	E	37	ASN
1	E	63	ASN
1	E	64	GLN
1	E	72	ASN
1	E	111	ASN
1	E	115	ASN
1	E	197	GLN
1	E	209	HIS
1	E	211	HIS
1	E	224	GLN
1	E	264	ASN
1	E	271	ASN
1	E	277	ASN
1	E	296	ASN
1	E	359	ASN
1	E	418	ASN
1	E	439	GLN
1	E	447	ASN
1	E	466	GLN
1	E	518	ASN
2	F	19	HIS
2	F	32	HIS
2	F	74	GLN
2	F	125	ASN
2	F	128	GLN
2	F	212	ASN
2	F	236	GLN
2	F	320	ASN
2	F	325	ASN
2	F	342	ASN
2	F	354	GLN
2	F	362	GLN
2	F	375	GLN
2	F	395	GLN
2	F	407	ASN
2	F	439	HIS
1	G	37	ASN
1	G	72	ASN
1	G	115	ASN
1	G	197	GLN
1	G	264	ASN

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Mol	Chain	Res	Type
1	G	271	ASN
1	G	277	ASN
1	G	343	GLN
1	G	344	ASN
1	G	359	ASN
1	G	436	HIS
1	G	438	GLN
1	G	439	GLN
1	G	447	ASN
1	G	517	ASN
2	H	19	HIS
2	H	32	HIS
2	H	74	GLN
2	H	87	ASN
2	H	123	HIS
2	H	125	ASN
2	H	128	GLN
2	H	236	GLN
2	H	258	GLN
2	H	262	GLN
2	H	270	GLN
2	H	272	ASN
2	H	325	ASN
2	H	342	ASN
2	H	351	GLN
2	H	352	ASN
2	H	354	GLN
2	H	362	GLN
2	H	395	GLN
2	H	439	HIS
3	L	140	GLN
3	L	141	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.03	11 (2%) 63 60	49, 84, 116, 147	0
1	C	520/531 (97%)	0.12	11 (2%) 63 60	58, 89, 123, 157	0
1	E	523/531 (98%)	0.09	14 (2%) 54 50	46, 71, 137, 158	0
1	G	518/531 (97%)	0.19	22 (4%) 36 31	49, 80, 143, 157	0
2	B	432/434 (99%)	0.20	22 (5%) 28 23	47, 76, 116, 130	0
2	D	432/434 (99%)	0.39	32 (7%) 14 10	55, 92, 122, 143	0
2	F	431/434 (99%)	0.36	27 (6%) 20 15	50, 76, 124, 147	0
2	H	431/434 (99%)	0.33	29 (6%) 17 13	52, 83, 133, 152	0
3	I	86/88 (97%)	0.01	0 100 100	61, 87, 106, 117	0
3	J	76/88 (86%)	0.42	6 (7%) 12 9	75, 101, 119, 124	0
3	K	76/88 (86%)	0.16	2 (2%) 56 52	68, 91, 111, 121	0
3	L	76/88 (86%)	0.44	4 (5%) 26 22	75, 112, 132, 140	0
All	All	4123/4212 (97%)	0.21	180 (4%) 34 29	46, 84, 126, 158	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	385	LEU	6.6
1	E	252	LEU	5.6
1	C	259	PRO	5.6
2	F	385	LEU	5.4
2	D	438	LEU	5.1
1	E	259	PRO	5.1
1	C	260	GLU	5.1
2	F	441	THR	4.9
2	F	392	LEU	4.8
3	L	116	ASP	4.6
2	D	389	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
2	H	407	ASN	4.4
1	G	252	LEU	4.4
2	D	436	PHE	4.4
3	L	161	ILE	4.3
2	B	381	ILE	4.3
2	D	423	LEU	4.2
1	C	252	LEU	4.2
2	F	412	LEU	4.1
2	H	438	LEU	4.1
2	B	361	LEU	4.1
1	G	249	GLN	4.1
2	F	438	LEU	4.0
1	G	201	LEU	3.9
1	E	261	ASP	3.9
2	H	408	LEU	3.9
2	F	353	ILE	3.9
1	G	253	LYS	3.9
2	F	419	ASP	3.9
2	D	388	LYS	3.9
2	D	220	SER	3.7
2	B	408	LEU	3.7
2	B	420	GLY	3.6
2	F	417	LEU	3.6
2	F	211	VAL	3.5
2	F	248	PRO	3.5
2	H	441	THR	3.5
3	J	103	ILE	3.5
2	D	353	ILE	3.4
2	D	395	GLN	3.4
2	B	385	LEU	3.4
2	H	440	PHE	3.4
1	G	226	TYR	3.3
2	D	392	LEU	3.3
2	H	436	PHE	3.3
1	G	185	LEU	3.3
2	D	415	LEU	3.3
2	H	392	LEU	3.3
2	H	364	VAL	3.2
2	B	438	LEU	3.2
2	B	436	PHE	3.2
2	D	416	GLY	3.2
1	A	208	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	374	LEU	3.2
2	F	381	ILE	3.1
2	F	418	VAL	3.1
2	H	423	LEU	3.1
2	H	412	LEU	3.1
2	H	381	ILE	3.1
1	A	115	ASN	3.1
2	D	390	ARG	3.1
1	A	534	LEU	3.1
2	F	246	GLY	3.1
2	B	353	ILE	3.0
1	G	338	LYS	3.0
2	D	387	GLY	3.0
2	B	166	ASP	3.0
1	A	252	LEU	3.0
3	L	162	LEU	2.9
1	G	230	ASN	2.9
1	G	275	ALA	2.9
2	B	386	GLU	2.9
2	D	243	PHE	2.9
1	E	260	GLU	2.9
1	G	247	ILE	2.8
1	A	276	LEU	2.8
1	A	201	LEU	2.8
2	F	361	LEU	2.8
2	B	412	LEU	2.8
3	L	117	ILE	2.8
1	C	199	TYR	2.8
1	G	153	CYS	2.8
2	D	242	PRO	2.8
2	H	437	LYS	2.8
2	F	243	PHE	2.8
2	B	415	LEU	2.8
2	D	393	TYR	2.8
2	F	439	HIS	2.8
1	C	471	SER	2.7
1	G	215	ILE	2.7
2	H	385	LEU	2.7
1	E	230	ASN	2.7
2	D	246	GLY	2.7
2	D	413	LYS	2.7
1	E	249	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	417	LEU	2.7
2	H	365	LEU	2.6
1	A	204	MET	2.6
2	D	249	LEU	2.6
2	H	439	HIS	2.6
2	F	440	PHE	2.6
2	H	246	GLY	2.6
2	D	167	GLY	2.6
2	H	360	LYS	2.6
2	D	421	GLN	2.5
2	B	442	SER	2.5
2	F	245	GLU	2.5
2	H	194	PRO	2.5
2	B	423	LEU	2.5
2	F	382	THR	2.5
1	A	221	TYR	2.5
2	F	423	LEU	2.5
1	E	247	ILE	2.5
3	J	113	ILE	2.5
1	G	272	VAL	2.4
2	B	387	GLY	2.4
1	A	278	THR	2.4
2	D	403	ARG	2.4
2	F	394	LEU	2.4
2	H	211	VAL	2.4
1	E	7	LEU	2.4
2	B	418	VAL	2.3
1	G	278	THR	2.3
2	D	294	SER	2.3
3	J	162	LEU	2.3
1	C	209	HIS	2.3
2	B	168	VAL	2.3
1	G	231	GLY	2.3
1	E	199	TYR	2.3
1	E	243	PHE	2.3
2	F	355	PHE	2.3
3	J	120	THR	2.3
1	C	107	GLU	2.3
1	C	370	GLN	2.3
2	D	420	GLY	2.3
2	H	386	GLU	2.3
2	H	388	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	9	LYS	2.2
2	H	216	ALA	2.2
1	G	199	TYR	2.2
3	K	161	ILE	2.2
2	H	415	LEU	2.2
2	F	247	VAL	2.2
2	D	437	LYS	2.2
2	F	259	TRP	2.2
2	B	392	LEU	2.2
1	E	221	TYR	2.2
2	H	390	ARG	2.2
2	D	365	LEU	2.2
2	B	441	THR	2.2
1	A	7	LEU	2.2
2	D	215	MET	2.2
1	G	332	MET	2.1
1	G	224	GLN	2.1
1	E	8	LEU	2.1
2	F	408	LEU	2.1
2	B	421	GLN	2.1
1	C	115	ASN	2.1
1	G	238	LYS	2.1
2	B	393	TYR	2.1
1	C	297	ILE	2.1
1	G	270	LYS	2.1
1	G	202	ASP	2.1
2	D	44	PHE	2.1
2	D	383	ALA	2.1
2	H	353	ILE	2.1
1	G	269	ILE	2.1
2	H	391	THR	2.1
2	F	351	GLN	2.0
3	J	161	ILE	2.0
2	H	420	GLY	2.0
3	J	105	VAL	2.0
2	H	416	GLY	2.0
1	E	492	THR	2.0
1	A	200	ASP	2.0
1	E	523	SER	2.0
2	F	320	ASN	2.0
3	K	117	ILE	2.0
2	D	358	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	365	LEU	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 monosaccharides 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	F	4	1/1	0.96	0.19	74,74,74,74	0
4	ZN	H	2	1/1	0.97	0.16	84,84,84,84	0
4	ZN	B	1	1/1	0.98	0.16	79,79,79,79	0
4	ZN	D	3	1/1	0.99	0.17	93,93,93,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.