



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:39 PM UTC

PDB ID : 3DBH / pdb_00003dbh
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

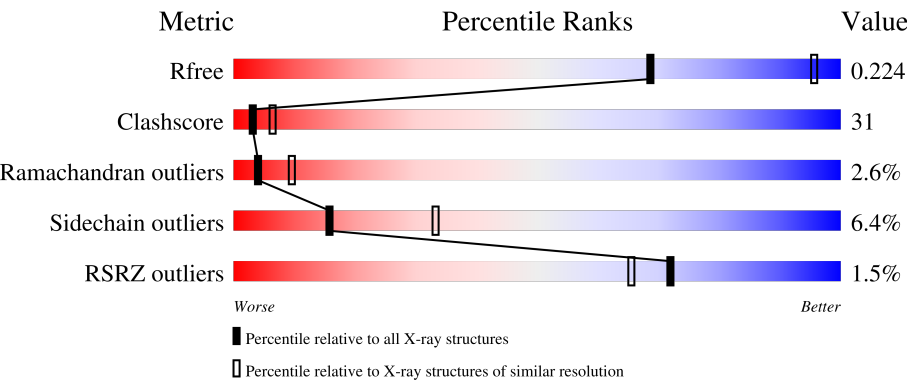
1 Overall quality at a glance i

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))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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

Mol	Chain	Length	Quality of chain
1	A	531	% 53%40%5%..
1	C	531	2% 53%38%6%..
1	E	531	% 57%36%5%..
1	G	531	2% 51%40%6%.
2	B	434	% 49%42%8%

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Mol	Chain	Length	Quality of chain
2	D	434	2% 48% 44% 7%
2	F	434	3% 47% 45% 7%
2	H	434	% 42% 43% 13%
3	I	88	% 53% 35% 9%
3	J	88	39% 41% 7% 14%
3	K	88	% 38% 41% 8% 14%
3	L	88	% 22% 56% 9% 14%

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

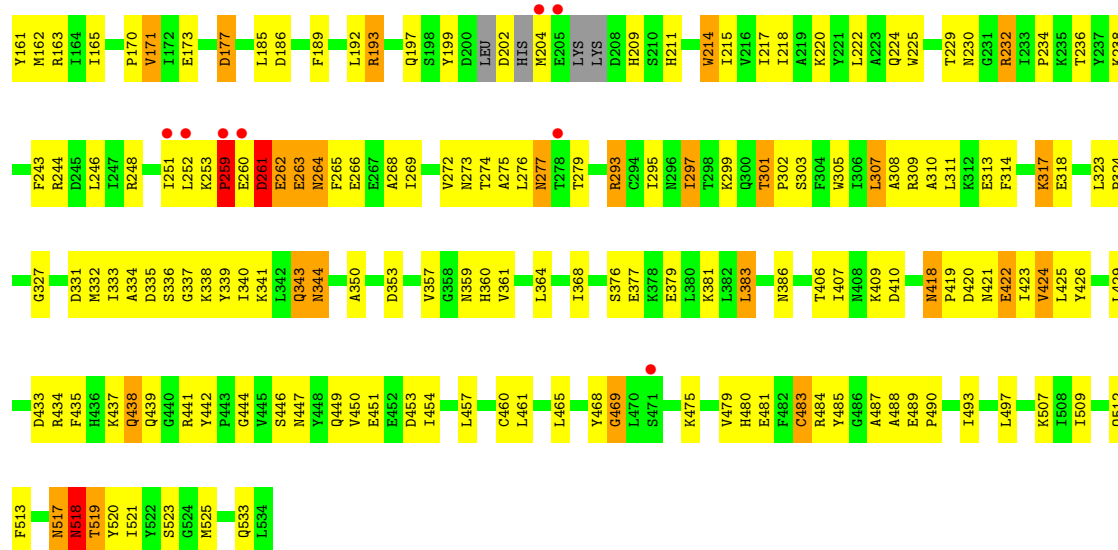
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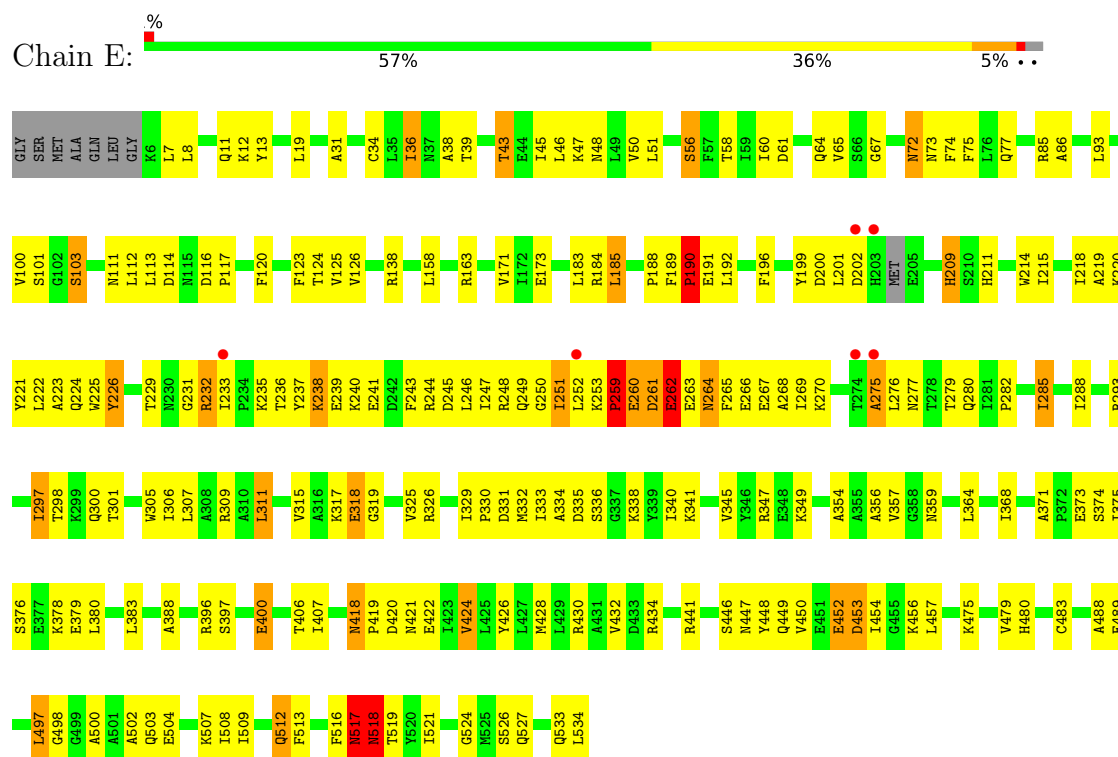
Chain	Residue	Modelled	Actual	Comment	Reference
J	172	ARG	ALA	engineered mutation	UNP Q15843
K	89	GLY	-	expression tag	UNP Q15843
K	90	SER	-	expression tag	UNP Q15843
K	91	ARG	-	expression tag	UNP Q15843
K	92	ARG	-	expression tag	UNP Q15843
K	93	ALA	-	expression tag	UNP Q15843
K	94	SER	-	expression tag	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 (CCD ID: ZN) (formula: Zn).

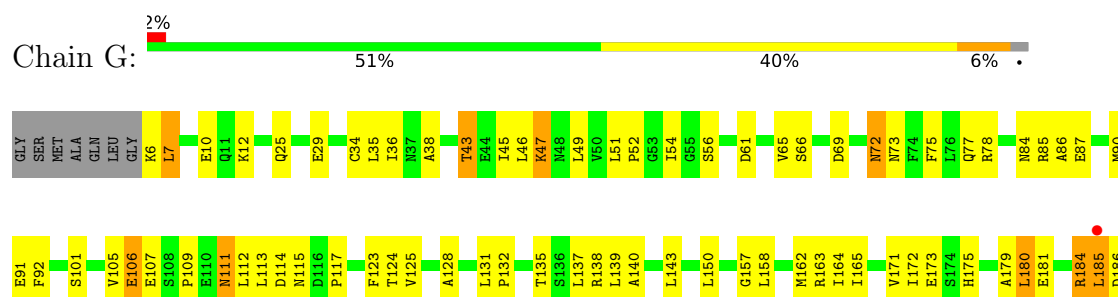
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0
4	H	1	Total Zn 1 1	0	0

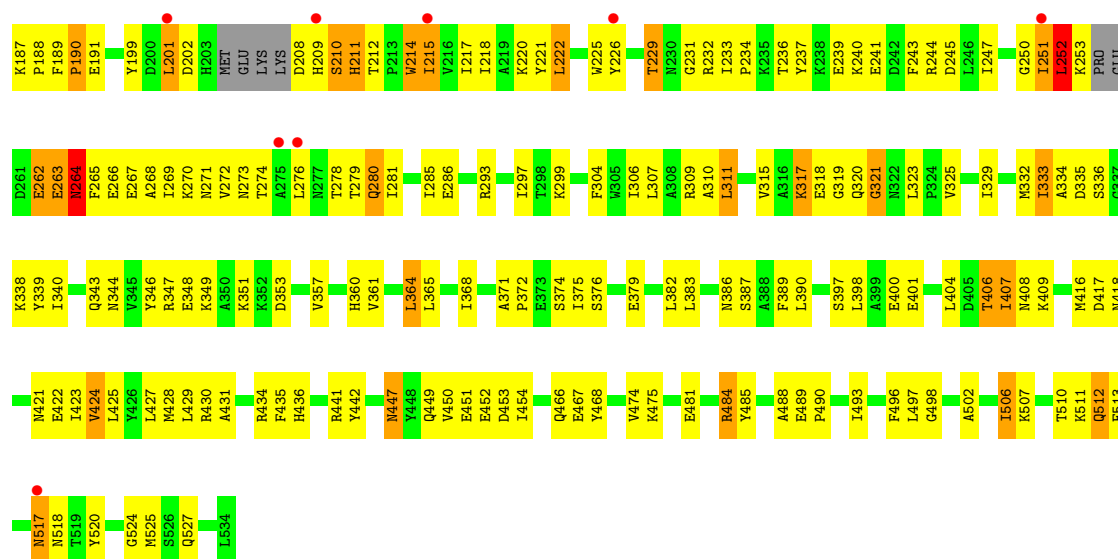


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit

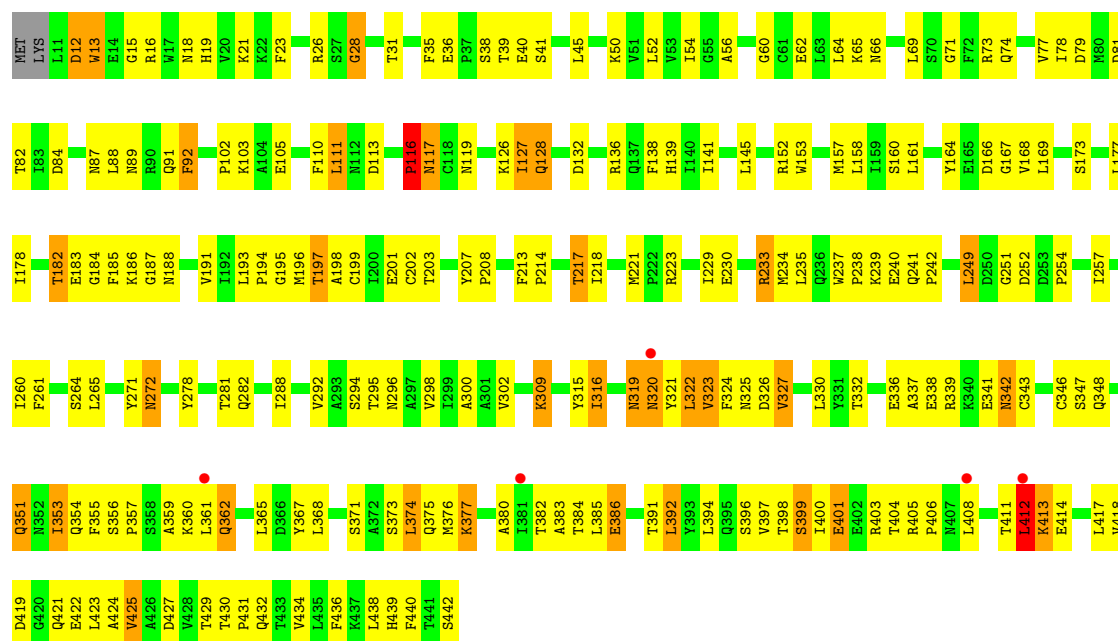


• Molecule 1: NEDD8-activating enzyme E1 regulatory subunit



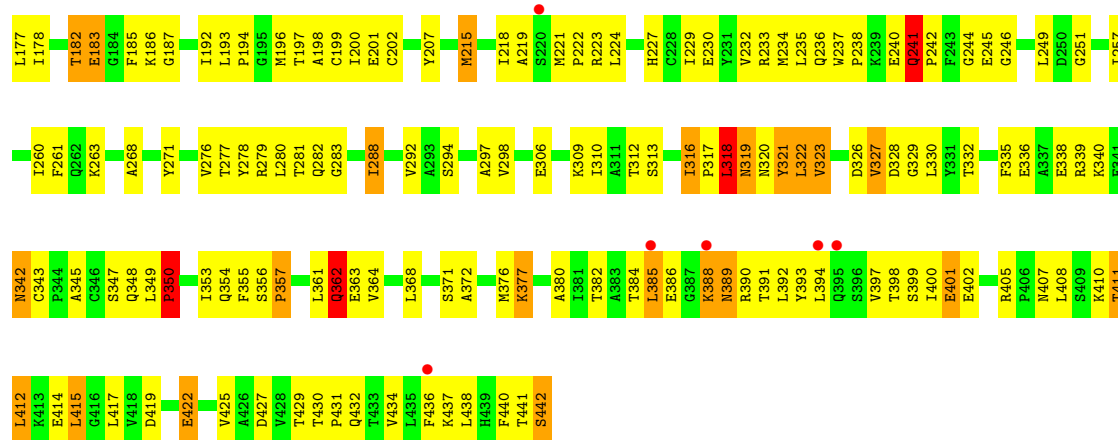


• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

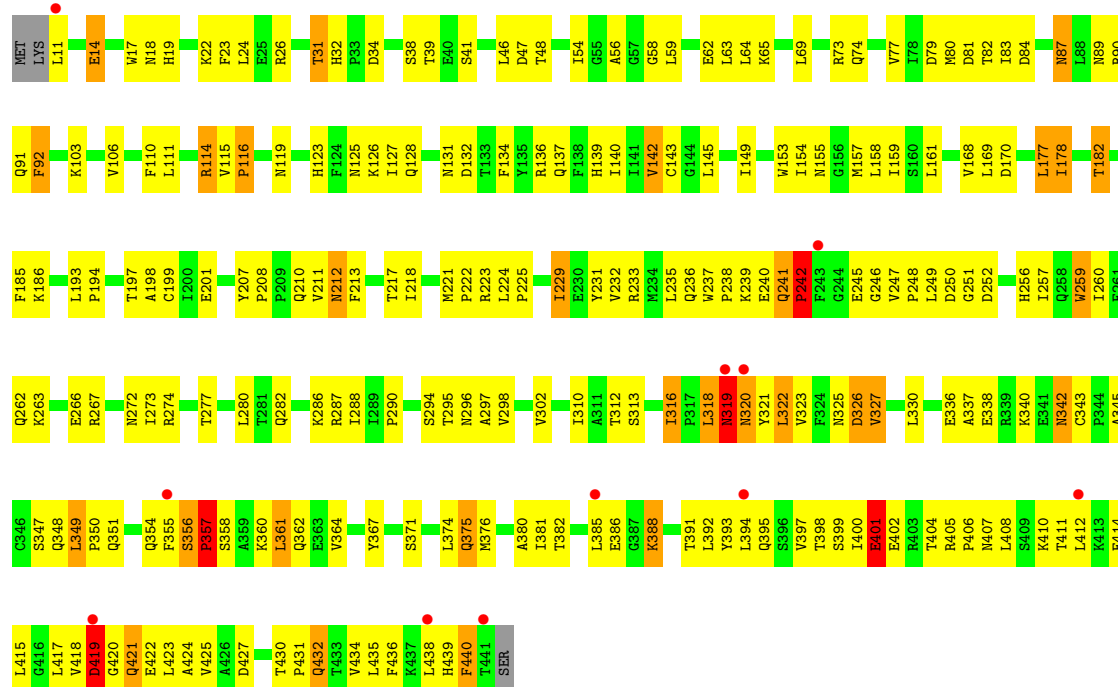


• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit

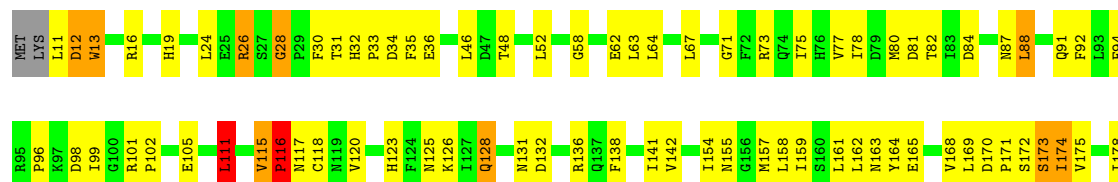


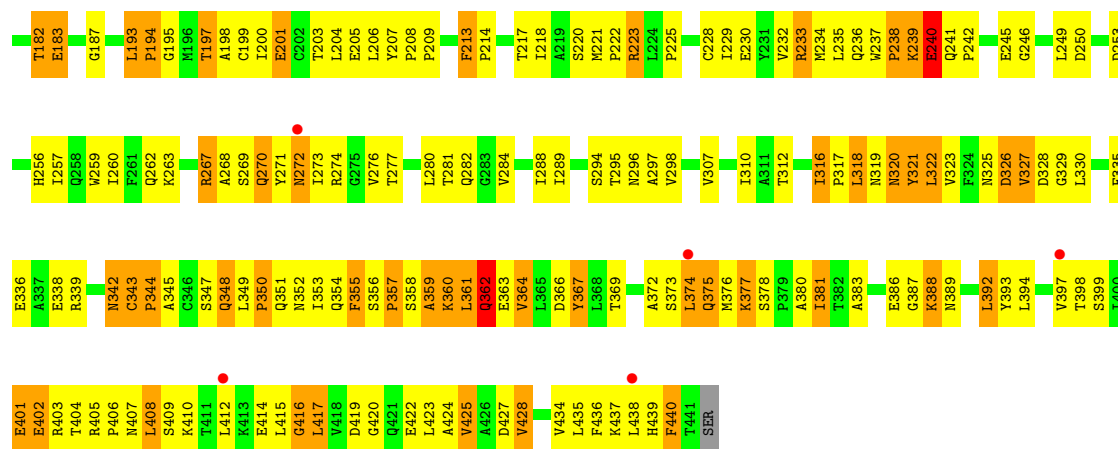


• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit



• Molecule 2: NEDD8-activating enzyme E1 catalytic subunit





• Molecule 3: NEDD8



• Molecule 3: NEDD8



• Molecule 3: NEDD8



M151	D152	E153	K154	T155	A156	A157	D158		I161	L162	G163	G164	S165	V166	L167	H168	L169	V170	L171	R172	L173	R174	G175	G176
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.65Å 198.10Å 210.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	95.8 (50.00-2.85) 88.6 (50.00-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.274 0.219 , 0.224	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	70.9	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	0/4218	1.06	26/5706 (0.5%)
1	C	0.51	0/4203	1.02	22/5682 (0.4%)
1	E	0.59	0/4216	1.11	32/5704 (0.6%)
1	G	0.55	0/4191	1.02	24/5668 (0.4%)
2	B	0.57	0/3476	1.14	21/4731 (0.4%)
2	D	0.56	1/3480 (0.0%)	1.13	29/4735 (0.6%)
2	F	0.58	0/3469	1.11	23/4723 (0.5%)
2	H	0.57	1/3461 (0.0%)	1.13	30/4713 (0.6%)
3	I	0.53	0/675	1.17	5/899 (0.6%)
3	J	0.48	0/611	1.06	5/815 (0.6%)
3	K	0.49	0/611	1.16	3/815 (0.4%)
3	L	0.45	0/611	1.14	4/815 (0.5%)
All	All	0.55	2/33222 (0.0%)	1.09	224/45006 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	80	MET	SD-CE	5.27	1.92	1.79
2	D	388	LYS	CE-NZ	5.04	1.64	1.49

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	348	GLN	N-CA-C	13.14	125.69	111.36
2	D	13	TRP	N-CA-C	12.83	127.88	110.55
2	B	414	GLU	N-CA-C	-11.86	97.41	113.30
1	A	208	ASP	N-CA-C	-11.51	98.61	112.89
2	D	385	LEU	N-CA-C	10.76	123.09	111.36
1	E	202	ASP	N-CA-C	-10.76	100.16	113.28
1	A	262	GLU	N-CA-C	10.41	122.69	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	12	ASP	N-CA-C	-10.18	89.11	110.80
2	F	440	PHE	N-CA-C	10.15	125.96	107.99
2	H	356	SER	CA-C-N	10.15	132.53	119.84
2	H	356	SER	C-N-CA	10.15	132.53	119.84
2	F	420	GLY	N-CA-C	-9.82	89.91	113.18
1	A	252	LEU	N-CA-C	9.77	122.94	111.02
2	D	12	ASP	N-CA-C	-9.08	92.95	107.93
2	B	241	GLN	N-CA-C	-8.70	90.58	109.81
2	H	193	LEU	CA-C-N	8.56	130.54	119.84
2	H	193	LEU	C-N-CA	8.56	130.54	119.84
1	E	517	ASN	CA-C-N	-8.46	105.39	121.54
1	E	517	ASN	C-N-CA	-8.46	105.39	121.54
1	A	329	ILE	CA-C-N	-8.44	111.95	120.98
1	A	329	ILE	C-N-CA	-8.44	111.95	120.98
2	B	413	LYS	N-CA-C	8.37	123.67	111.87
2	B	240	GLU	N-CA-C	-8.31	96.98	109.86
3	L	174	ARG	N-CA-C	8.22	120.02	111.14
1	G	185	LEU	N-CA-C	-8.20	103.41	113.41
2	B	88	LEU	N-CA-C	8.06	122.38	112.54
2	H	362	GLN	N-CA-C	-7.82	103.48	112.87
1	E	518	ASN	N-CA-C	7.74	127.28	110.80
1	A	7	LEU	N-CA-C	-7.64	103.84	113.01
1	C	301	THR	CA-C-N	7.64	128.24	120.14
1	C	301	THR	C-N-CA	7.64	128.24	120.14
2	B	92	PHE	N-CA-C	7.58	121.96	112.87
1	G	201	LEU	N-CA-C	7.56	122.19	113.19
2	F	419	ASP	N-CA-C	7.55	126.89	110.80
2	B	288	ILE	N-CA-C	7.45	120.35	109.63
1	E	450	VAL	N-CA-C	7.41	117.94	110.23
2	B	138	PHE	N-CA-C	7.40	121.44	110.48
1	E	262	GLU	N-CA-C	7.39	121.29	109.83
2	B	13	TRP	N-CA-C	7.37	119.48	110.41
2	D	441	THR	N-CA-C	-7.36	94.94	107.23
2	F	48	THR	N-CA-C	7.32	122.35	113.41
2	B	341	GLU	N-CA-C	7.25	121.23	112.38
2	H	173	SER	N-CA-C	-7.23	104.48	113.38
3	I	98	GLY	N-CA-C	-7.19	106.76	114.67
2	D	241	GLN	CA-C-N	7.17	126.66	118.85
2	D	241	GLN	C-N-CA	7.17	126.66	118.85
2	H	288	ILE	N-CA-C	7.14	118.22	109.30
1	E	524	GLY	N-CA-C	-7.10	105.85	114.66
2	D	288	ILE	N-CA-C	7.09	119.84	109.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	262	GLU	N-CA-C	7.09	121.34	111.56
2	H	81	ASP	N-CA-C	7.08	119.66	110.53
2	D	87	ASN	N-CA-C	-7.06	106.57	114.62
1	G	7	LEU	N-CA-C	-7.04	104.68	113.20
1	E	261	ASP	N-CA-C	7.02	122.48	107.67
1	G	406	THR	N-CA-C	6.97	121.78	113.28
2	F	115	VAL	CA-C-N	6.96	128.54	119.84
2	F	115	VAL	C-N-CA	6.96	128.54	119.84
1	E	424	VAL	N-CA-C	-6.90	103.79	110.42
2	H	88	LEU	N-CA-C	6.88	121.28	112.34
1	E	238	LYS	N-CA-C	-6.83	103.76	111.14
1	E	36	ILE	CA-C-N	-6.83	112.69	122.94
1	E	36	ILE	C-N-CA	-6.83	112.69	122.94
1	G	209	HIS	N-CA-C	-6.82	96.28	110.80
1	C	519	THR	N-CA-C	6.81	120.03	109.07
2	H	28	GLY	CA-C-N	6.79	127.34	119.47
2	H	28	GLY	C-N-CA	6.79	127.34	119.47
1	C	259	PRO	N-CA-C	-6.77	98.52	112.47
2	F	229	ILE	N-CA-C	-6.76	106.44	112.12
1	A	434	ARG	N-CA-C	-6.72	104.03	111.36
2	H	343	CYS	CA-C-N	6.71	126.40	119.82
2	H	343	CYS	C-N-CA	6.71	126.40	119.82
2	F	356	SER	CA-C-N	6.68	128.20	119.84
2	F	356	SER	C-N-CA	6.68	128.20	119.84
2	H	138	PHE	N-CA-C	6.66	120.89	110.17
1	G	430	ARG	N-CA-C	-6.62	104.14	111.36
2	H	321	TYR	N-CA-C	6.62	119.27	108.55
2	B	320	ASN	N-CA-C	6.62	122.02	113.88
2	D	81	ASP	N-CA-C	6.59	119.45	110.55
1	G	222	LEU	N-CA-C	-6.59	105.13	113.43
1	A	202	ASP	N-CA-C	-6.58	105.13	113.43
2	H	320	ASN	N-CA-C	6.56	124.77	110.80
2	D	28	GLY	CA-C-N	6.54	128.02	119.84
2	D	28	GLY	C-N-CA	6.54	128.02	119.84
1	G	517	ASN	N-CA-C	6.53	118.28	111.03
2	F	367	TYR	N-CA-C	-6.52	104.10	111.14
2	H	389	ASN	N-CA-C	6.50	118.72	110.33
1	E	512	GLN	N-CA-C	6.50	121.58	112.93
1	E	424	VAL	CB-CA-C	-6.46	103.70	111.97
2	H	115	VAL	CA-C-N	6.44	127.89	119.84
2	H	115	VAL	C-N-CA	6.44	127.89	119.84
2	F	320	ASN	N-CA-C	6.43	123.06	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	319	ASN	CA-C-N	-6.43	111.30	122.36
2	B	319	ASN	C-N-CA	-6.43	111.30	122.36
2	H	270	GLN	N-CA-C	-6.43	105.15	112.87
2	F	319	ASN	CA-C-N	-6.39	112.19	122.23
2	F	319	ASN	C-N-CA	-6.39	112.19	122.23
3	L	173	LEU	N-CA-C	6.36	119.84	109.59
3	J	150	MET	N-CA-C	6.36	119.71	110.42
1	A	493	ILE	N-CA-C	-6.36	104.07	111.00
2	D	92	PHE	N-CA-C	6.36	120.50	112.87
1	G	252	LEU	N-CA-C	6.33	124.28	110.80
2	B	117	ASN	N-CA-C	6.32	119.93	112.72
1	C	512	GLN	N-CA-C	6.31	121.83	112.94
1	E	306	ILE	N-CA-C	-6.30	104.37	110.42
2	H	13	TRP	N-CA-C	6.28	119.36	110.50
3	J	134	GLU	N-CA-C	6.28	121.07	113.41
1	E	200	ASP	N-CA-C	-6.27	101.00	110.28
1	C	148	ILE	N-CA-C	6.26	114.78	107.77
3	K	174	ARG	N-CA-C	6.20	120.87	113.12
2	D	59	LEU	N-CA-C	-6.19	104.45	111.07
1	G	251	ILE	N-CA-C	-6.17	100.70	108.84
1	A	49	LEU	N-CA-C	-6.16	106.31	113.88
1	A	261	ASP	N-CA-C	6.16	120.66	107.67
1	E	259	PRO	N-CA-C	-6.14	99.82	112.47
2	D	115	VAL	CA-C-N	6.13	127.51	119.84
2	D	115	VAL	C-N-CA	6.13	127.51	119.84
1	A	201	LEU	N-CA-C	6.13	123.86	110.80
1	A	518	ASN	N-CA-C	6.12	123.83	110.80
1	C	442	TYR	CA-C-N	6.08	125.83	119.76
1	C	442	TYR	C-N-CA	6.08	125.83	119.76
2	F	81	ASP	N-CA-C	6.08	118.75	110.55
2	B	28	GLY	CA-C-N	6.07	125.69	119.56
2	B	28	GLY	C-N-CA	6.07	125.69	119.56
1	C	518	ASN	N-CA-C	6.03	123.64	110.80
2	D	388	LYS	N-CA-C	-6.02	101.86	110.59
1	E	232	ARG	N-CA-C	6.02	117.81	110.41
1	E	512	GLN	CA-C-N	-5.96	111.60	123.99
1	E	512	GLN	C-N-CA	-5.96	111.60	123.99
1	G	512	GLN	N-CA-C	5.95	121.46	113.72
1	A	259	PRO	N-CA-C	-5.91	100.29	112.47
2	D	319	ASN	N-CA-C	5.91	117.41	110.97
1	G	374	SER	N-CA-C	-5.86	106.14	113.28
2	D	48	THR	N-CA-C	5.85	121.86	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	424	VAL	CB-CA-C	-5.82	104.40	112.02
2	F	361	LEU	N-CA-C	-5.80	104.96	112.68
3	I	150	MET	N-CA-C	5.80	119.00	110.30
1	G	484	ARG	N-CA-C	-5.79	104.87	111.07
1	A	512	GLN	N-CA-C	5.79	120.38	112.04
2	F	288	ILE	N-CA-C	5.79	117.05	109.58
1	A	276	LEU	CA-C-N	-5.78	114.90	123.11
1	A	276	LEU	C-N-CA	-5.78	114.90	123.11
1	E	453	ASP	N-CA-C	5.76	117.64	111.36
3	I	101	MET	N-CA-C	-5.76	100.66	109.41
1	G	424	VAL	CB-CA-C	-5.75	104.61	111.97
1	E	378	LYS	N-CA-C	-5.66	104.80	110.97
1	C	115	ASN	N-CA-C	5.64	117.88	111.11
2	H	327	VAL	N-CA-C	5.64	116.37	110.62
1	C	307	LEU	N-CA-C	-5.64	105.28	111.82
2	D	318	LEU	CA-C-N	-5.62	113.24	120.65
2	D	318	LEU	C-N-CA	-5.62	113.24	120.65
2	D	377	LYS	N-CA-C	5.61	117.26	111.03
1	C	261	ASP	CB-CA-C	-5.59	104.10	111.82
1	C	424	VAL	N-CA-C	-5.57	105.29	110.53
1	E	421	ASN	N-CA-C	-5.57	102.77	110.35
2	F	155	ASN	N-CA-C	-5.56	105.12	111.07
1	G	496	PHE	N-CA-C	-5.55	104.92	110.97
3	K	173	LEU	N-CA-C	5.55	119.03	110.42
1	A	318	GLU	N-CA-C	5.51	119.71	113.15
2	H	204	LEU	N-CA-C	5.49	117.98	111.33
2	F	14	GLU	N-CA-C	5.44	118.06	109.96
2	F	47	ASP	N-CA-C	5.43	118.25	111.24
3	L	115	ILE	N-CA-C	5.42	116.17	108.42
1	G	434	ARG	N-CA-C	-5.39	105.31	111.14
2	D	400	ILE	N-CA-C	-5.39	106.60	112.80
1	G	452	GLU	N-CA-C	5.38	116.82	111.07
2	H	367	TYR	N-CA-C	-5.36	105.10	111.69
1	G	417	ASP	N-CA-C	-5.36	106.81	113.19
1	C	483	CYS	N-CA-C	-5.35	106.44	113.12
1	C	123	PHE	N-CA-C	5.33	118.80	110.32
1	A	331	ASP	N-CA-C	-5.32	103.36	110.55
2	D	47	ASP	N-CA-C	5.31	119.86	112.90
2	B	39	THR	N-CA-C	-5.31	106.65	113.23
1	A	439	GLN	N-CA-C	5.29	119.59	113.18
1	E	483	CYS	N-CA-C	-5.29	105.59	111.36
2	D	111	LEU	N-CA-C	5.26	116.69	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	321	TYR	N-CA-CB	-5.23	103.29	111.56
3	J	115	ILE	N-CA-C	5.23	117.29	108.81
1	G	389	PHE	N-CA-C	5.23	119.21	112.41
1	A	442	TYR	CA-C-N	5.22	126.37	119.84
1	A	442	TYR	C-N-CA	5.22	126.37	119.84
2	F	431	PRO	N-CA-C	-5.22	107.23	114.27
2	D	144	GLY	N-CA-C	-5.21	100.83	113.18
1	E	185	LEU	N-CA-C	-5.21	105.20	112.45
2	F	217	THR	N-CA-C	5.21	116.96	111.28
2	H	197	THR	N-CA-C	-5.21	101.49	109.41
1	A	303	SER	N-CA-C	5.20	117.36	111.11
3	J	173	LEU	N-CA-C	5.19	118.53	110.17
1	E	201	LEU	N-CA-C	5.19	121.40	113.61
2	B	412	LEU	N-CA-C	-5.18	106.06	112.38
1	E	251	ILE	N-CA-C	-5.18	102.00	108.84
1	C	243	PHE	N-CA-C	-5.17	105.55	111.14
2	H	174	ILE	N-CA-C	5.17	116.03	108.58
1	A	78	ARG	N-CA-C	-5.17	105.33	111.69
2	H	126	LYS	N-CA-C	-5.17	101.85	110.17
1	E	120	PHE	N-CA-C	5.16	119.20	113.01
2	D	88	LEU	N-CA-C	5.15	119.05	112.87
1	C	301	THR	N-CA-C	5.15	115.90	109.57
3	K	123	VAL	N-CA-C	-5.14	105.52	110.72
2	H	111	LEU	N-CA-C	5.12	116.86	111.28
3	L	144	ILE	N-CA-C	5.12	115.84	107.24
1	E	124	THR	N-CA-C	-5.12	105.78	111.36
1	C	261	ASP	N-CA-C	5.11	117.94	107.37
1	E	233	ILE	CA-C-N	5.11	126.22	119.84
1	E	233	ILE	C-N-CA	5.11	126.22	119.84
3	I	174	ARG	N-CA-C	5.10	118.66	112.23
1	E	434	ARG	N-CA-C	-5.10	105.61	111.07
2	B	241	GLN	CA-C-N	5.10	126.22	119.84
2	B	241	GLN	C-N-CA	5.10	126.22	119.84
1	C	39	THR	N-CA-C	-5.10	103.31	110.35
1	G	321	GLY	N-CA-C	-5.10	107.22	115.08
2	F	23	PHE	N-CA-C	5.10	117.73	111.82
3	J	123	VAL	N-CA-C	-5.09	105.43	110.62
1	G	334	ALA	N-CA-C	5.07	115.89	107.73
3	I	173	LEU	N-CA-C	5.07	117.74	109.59
1	A	417	ASP	N-CA-C	-5.05	106.21	112.38
1	G	215	ILE	N-CA-C	-5.05	105.40	110.30
1	G	447	ASN	N-CA-C	5.05	117.52	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	210	SER	N-CA-C	5.05	117.68	111.82
2	D	138	PHE	N-CA-C	5.05	118.30	110.17
2	H	48	THR	N-CA-C	5.05	121.14	114.12
1	A	447	ASN	N-CA-C	5.04	117.42	111.33
1	C	95	GLU	N-CA-C	5.04	117.50	111.71
2	H	26	ARG	N-CA-C	5.02	117.08	108.90
2	F	421	GLN	N-CA-C	5.02	116.94	108.96

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	230	0
1	C	4125	0	4065	216	0
1	E	4136	0	4065	221	0
1	G	4113	0	4058	247	0
2	B	3398	0	3377	242	0
2	D	3402	0	3388	233	0
2	F	3391	0	3372	274	0
2	H	3383	0	3351	314	0
3	I	670	0	707	41	0
3	J	606	0	643	47	0
3	K	606	0	643	45	0
3	L	606	0	643	62	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	2027	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 31.

All (2027) 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:C:277:ASN:C	1:C:277:ASN:HD22	1.73	0.95
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:F:393:TYR:HD1	2:F:404:THR:HG1	1.23	0.82
1:G:184:ARG:NH1	1:G:325:VAL:HG22	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:394:LEU:HD11	2:B:396:SER:OG	1.80	0.80
2:F:132:ASP:HB3	2:F:157:MET:HE1	1.64	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
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
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:H:373:SER:C	2:H:374:LEU:HG	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:322:LEU:HD12	2:D:322:LEU:C	2.09	0.77
1:A:90:MET:HE3	1:A:94:GLN:OE1	1.85	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:215:ILE:HG13	1:G:332:MET:HE1	1.66	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:H:322:LEU:C	2:H:322:LEU:HD12	2.11	0.76
2:B:157:MET:HA	2:B:157:MET:HE3	1.68	0.75
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:386:GLU:C	2:D:388:LYS:H	1.95	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:411:THR:O	2:D:415:LEU:HG	1.87	0.75
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: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: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
3:J:143:LEU:HB3	3:J:150:MET:HE2	1.70	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
2:H:132:ASP:HB3	2:H:157:MET:HE1	1.72	0.72
1:E:253:LYS:O	1:E:259:PRO:C	2.33	0.71
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
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
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:A:204:MET:HE2	1:A:208:ASP:HB3	1.72	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
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: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:215:ILE:CD1	1:C:332:MET:HE1	2.22	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
1:A:215:ILE:HD11	1:A:332:MET:HE1	1.75	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
1:G:49:LEU:C	1:G:52:PRO:HD2	2.17	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
1:C:211:HIS:CE1	2:D:221:MET:HE1	2.28	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
2:F:74:GLN:NE2	2:F:74:GLN:HA	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:G:210:SER:HA	1:G:264:ASN:CG	2.19	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:F:157:MET:O	2:F:157:MET:HE3	1.94	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
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
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:C:317:LYS:HB3	1:C:318:GLU:OE1	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:101:MET:HE2	3:J:119:PRO:HG3	1.78	0.66
3:J:125:ARG:HD3	3:J:129:ARG:HH21	1.61	0.66
2:H:361:LEU:C	2:H:363:GLU:H	2.00	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
1:A:366:GLN:C	1:A:368:ILE:H	2.04	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:248:ARG:C	1:A:250:GLY:H	2.05	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
1:E:248:ARG:C	1:E:250:GLY:H	2.05	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:371:ALA:C	1:A:373:GLU:H	2.03	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
3:K:155:THR:HG22	3:K:158:ASP:CG	2.21	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
2:H:208:PRO:HG3	3:L:171:LEU:HD11	1.79	0.64
2:H:361:LEU:C	2:H:363:GLU:N	2.53	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
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
1:A:253:LYS:O	1:A:259:PRO:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
2:H:200:ILE:HD13	3:L:172:ARG:NH2	2.15	0.62
1:A:428:MET:HE1	1:A:479:VAL:HA	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:371:SER:C	2:B:373:SER:H	2.08	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
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
2:H:234:MET:C	2:H:235:LEU:HD22	2.24	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:G:317:LYS:HG2	1:G:318:GLU: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:H:87:ASN:HB3	2:H:91:GLN:CD	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:517:ASN:C	1:E:517:ASN:HD22	2.09	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:F:80:MET:HE2	2:F:126:LYS:HB3	1.82	0.60
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
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:C:138:ARG:O	1:C:142:VAL:HG23	2.01	0.60
1:C:277:ASN:C	1:C:277:ASN:ND2	2.46	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
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: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
2:H:234:MET:HG2	2:H:235:LEU:HD22	1.82	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
3:I:144:ILE:HD12	3:I:170:VAL:HB	1.84	0.59
1:C:488:ALA:C	1:C:490:PRO:HD3	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:215:ILE:H	1:G:332:MET:HE1	1.65	0.59
1:G:347:ARG:HH22	2:H:274:ARG:HH11	1.50	0.59
1:A:63:ASN:ND2	1:A:63:ASN:H	2.00	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
3:K:103:ILE:C	3:K:103:ILE:HD12	2.27	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:A:78:ARG:C	1:A:80:SER:H	2.10	0.58
1:C:214:TRP:CD1	1:C:214:TRP:C	2.81	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:402:GLU:C	2:H:404:THR:H	2.11	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
2:F:350:PRO:HB3	2:F:435:LEU:C	2.29	0.58
2:F:401:GLU:OE2	2:F:402:GLU:HG3	2.04	0.58
2:H:117:ASN:O	2:H:118:CYS:C	2.47	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:110:PHE:C	2:B:110:PHE:CD2	2.82	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
1:A:418:ASN:HD22	1:A:418:ASN:C	2.12	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
1:C:260:GLU:HG3	1:C:261:ASP:CG	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:419:ASP:OD2	2:F:438:LEU:C	2.47	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
1:A:214:TRP:C	1:A:214:TRP:CD1	2.82	0.57
1:C:253:LYS:O	1:C:259:PRO:C	2.44	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
2:B:235:LEU:C	2:B:238:PRO:HD2	2.29	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
1:A:72:ASN:C	1:A:72:ASN:HD22	2.12	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
2:D:386:GLU:C	2:D:388:LYS:N	2.62	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:400:ILE:C	2:F:402:GLU:H	2.13	0.56
2:F:419:ASP:OD2	2:F:439:HIS:CA	2.53	0.56
1:G:263:GLU:O	1:G:264:ASN:C	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:376:MET:HE1	2:D:434:VAL:HG11	1.87	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
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: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
1:A:72:ASN:C	1:A:72:ASN:ND2	2.61	0.56
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
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
1:G:527:GLN:OE1	1:G:527:GLN:HA	2.05	0.56
2:H:373:SER:C	2:H:374:LEU:CG	2.79	0.56
2:B:64:LEU:HD11	2:B:77:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:80:MET:HE2	2:F:126:LYS:CB	2.36	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
1:G:441:ARG:HH21	1:G:449:GLN:CD	2.14	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:A:517:ASN:HD22	1:A:517:ASN:C	2.12	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:G:210:SER:HB3	1:G:262:GLU:CD	2.31	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:211:HIS:NE2	2:H:221:MET:HE1	2.21	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:215:ILE:H	1:G:332:MET:CE	2.20	0.55
2:B:322:LEU:HD23	2:B:322:LEU:C	2.32	0.54
2:B:361:LEU:HD23	2:B:361:LEU:C	2.32	0.54
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
1:C:9:LYS:C	1:C:11:GLN:H	2.15	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
1:A:211:HIS:CE1	2:B:221:MET:HE1	2.43	0.54
2:B:164:TYR:CE2	2:B:169:LEU:HB2	2.43	0.54
1:C:72:ASN:C	1:C:72:ASN:ND2	2.61	0.54
1:E:311:LEU:O	1:E:315:VAL:HG23	2.08	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:C:202:ASP:HA	1:C:204:MET:HE3	1.90	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
2:H:344:PRO:HB3	2:H:374:LEU:HD13	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:J:101:MET:HE2	3:J:119:PRO:CG	2.38	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:214:TRP:N	1:G:332:MET:HE2	2.23	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:D:361:LEU:C	2:D:363:GLU:H	2.16	0.53
3:J:143:LEU:CB	3:J:150:MET:HE2	2.36	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
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
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
2:H:360:LYS:HB2	2:H:363:GLU:HG3	1.91	0.53
3:L:118:GLU:C	3:L:120:THR:H	2.17	0.53
1:A:61:ASP:HB3	1:A:86:ALA:HB2	1.90	0.53
3:K:123:VAL:HG13	3:K:150:MET:HE2	1.90	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
2:D:215:MET:HE2	2:D:215:MET:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:LEU:H	2:B:197:THR:HB	1.74	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: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
1:G:497:LEU:O	1:G:498:GLY:C	2.52	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:A:366:GLN:C	1:A:368:ILE:N	2.66	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
3:J:155:THR:HG22	3:J:158:ASP:CG	2.34	0.53
1:E:266:GLU:O	1:E:270:LYS:HG3	2.09	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
1:G:111:ASN:C	1:G:111:ASN:OD1	2.50	0.53
2:B:87:ASN:HB3	2:B:91:GLN:CD	2.34	0.52
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
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:423:ILE:O	1:A:426:TYR:HB3	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:72:ASN:ND2	1:G:72:ASN:C	2.66	0.52
1:G:208:ASP:HB3	1:G:338:LYS:HZ1	1.72	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
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:418:ASN:ND2	1:A:418:ASN:C	2.68	0.52
1:A:426:TYR:HB2	1:A:521:ILE:CD1	2.39	0.52
2:B:371:SER:C	2:B:373:SER:N	2.65	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
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
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
1:C:90:MET:HE3	1:C:94:GLN:OE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:E:191:GLU:H	1:E:191:GLU:CD	2.18	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:319:ASN:C	2:F:320:ASN:HD22	2.18	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
1:G:225:TRP:CD1	1:G:225:TRP:C	2.87	0.51
2:H:75:ILE:HB	2:H:120:VAL:HG22	1.93	0.51
1:A:204:MET:CE	1:A:208:ASP:HB3	2.39	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:237:TRP:C	2:F:239:LYS:H	2.18	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:336:GLU:O	2:F:337:ALA:C	2.52	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
1:G:112:LEU:C	1:G:114:ASP:H	2.17	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
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
1:E:396:ARG:NH1	1:E:534:LEU:C	2.69	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:112:LEU:C	1:G:114:ASP:N	2.67	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:HD23	2:B:322:LEU:O	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
2:D:343:CYS:C	2:D:345:ALA:H	2.17	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
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:214:TRP:CD1	1:A:215:ILE:N	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LEU:HD21	2:B:77:VAL:HG22	1.93	0.51
2:D:326:ASP:O	2:D:327:VAL:C	2.54	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:B:362:GLN:HE21	2:B:362:GLN:C	2.19	0.50
2:D:316:ILE:H	2:D:316:ILE:CD1	2.24	0.50
3:J:101:MET:HE2	3:J:119:PRO:CD	2.41	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: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
2:H:269:SER:C	2:H:271:TYR:N	2.67	0.50
2:D:232:VAL:CG1	2:D:263:LYS:HB2	2.39	0.50
1:E:418:ASN:HD22	1:E:418:ASN:C	2.19	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:322:LEU:C	2:H:322:LEU:CD1	2.82	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
1:G:416:MET:C	1:G:418:ASN:H	2.20	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:E:248:ARG:C	1:E:250:GLY:N	2.70	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
3:L:150:MET:HE1	3:L:167:LEU:HD13	1.94	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
2:F:362:GLN:C	2:F:364:VAL:H	2.19	0.50
2:H:269:SER:C	2:H:271:TYR:H	2.20	0.50
1:A:196:PHE:O	1:A:220:LYS:HE2	2.11	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
2:H:415:LEU:O	2:H:416:GLY:C	2.55	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:A:407:ILE:C	1:A:407:ILE:HD13	2.37	0.49
2:B:376:MET:HE1	2:B:434:VAL:HG11	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:227:SER:C	1:A:229:THR:H	2.19	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
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
2:F:322:LEU:CD1	2:F:322:LEU:C	2.86	0.49
1:G:315:VAL:O	1:G:321:GLY:N	2.43	0.49
2:H:344:PRO:HG2	2:H:345:ALA:N	2.25	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:132:ASP:CB	2:F:157:MET:HE1	2.39	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:B:419:ASP:C	2:B:419:ASP:OD1	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:H:342:ASN:O	2:H:342:ASN:CG	2.56	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:215:ILE:HD12	1:C:332:MET:HE1	1.95	0.49
1:C:264:ASN:HD22	1:C:264:ASN:H	1.59	0.49
3:J:115:ILE:HG22	3:J:116:ASP:N	2.28	0.49
2:F:343:CYS:O	2:F:347:SER:OG	2.17	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:B:230:GLU:OE2	2:B:234:MET:HE3	2.12	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
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
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:371:ALA:C	1:A:373:GLU:N	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LEU:O	1:A:465:LEU:HG	2.13	0.48
3:I:101:MET:HE2	3:I:119:PRO:HD3	1.95	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
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
3:L:136:ILE:O	3:L:137:PRO:C	2.55	0.48
1:A:297:ILE:HG22	1:A:368:ILE:CD1	2.44	0.48
1:A:416:MET:O	1:A:416:MET:HE3	2.14	0.48
3:I:107:THR:C	3:I:109:THR:H	2.21	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
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
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:271:TYR:C	2:H:272:ASN:ND2	2.71	0.48
2:H:271:TYR:C	2:H:272:ASN:HD22	2.18	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:373:GLU:C	1:E:375:ILE:H	2.20	0.48
1:E:418:ASN:ND2	1:E:418:ASN:C	2.71	0.48
2:F:266:GLU:O	2:F:267:ARG:C	2.57	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
2:D:40:GLU:O	2:D:41:SER:C	2.56	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
1:G:191:GLU:CD	1:G:191:GLU:H	2.21	0.48
1:G:285:ILE:HD11	1:G:387:SER:O	2.13	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
2:D:240:GLU:O	2:D:241:GLN:C	2.56	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
3:L:151:ASN:C	3:L:153:GLU:H	2.22	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:C:435:PHE:C	1:C:435:PHE:CD2	2.91	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
1:E:526:SER:O	1:E:527:GLN:HB2	2.14	0.47
2:F:31:THR:HG23	2:F:32:HIS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:343:CYS:C	2:D:345:ALA:N	2.72	0.47
2:F:318:LEU:C	2:F:319:ASN:O	2.56	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
1:G:466:GLN:O	1:G:467:GLU:C	2.58	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
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
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:416:MET:C	1:G:418:ASN:N	2.72	0.47
1:G:485:TYR:OH	1:G:525:MET:SD	2.72	0.47
2:H:157:MET:HE3	2:H:157:MET:O	2.14	0.47
2:B:384:THR:C	2:B:385:LEU:O	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:407:ILE:HG23	1:A:407:ILE:O	2.15	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:B:411:THR:C	2:B:413:LYS:N	2.69	0.47
1:C:9:LYS:C	1:C:11:GLN:N	2.71	0.47
1:C:57:PHE:C	1:C:57:PHE:CD1	2.93	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: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
1:G:525:MET:HE3	2:H:30:PHE:CD2	2.49	0.47
2:H:193:LEU:HD23	2:H:193:LEU:HA	1.79	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:C	2:D:111:LEU:HD11	2.39	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
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:214:TRP:CD1	1:G:214:TRP:C	2.92	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:H:213:PHE:O	2:H:214:PRO:C	2.58	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:231:TYR:C	2:F:233:ARG:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:376:SER:HG	1:G:379:GLU:HG3	1.80	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:38:ALA:C	1:E:85:ARG:HD3	2.40	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
1:A:250:GLY:O	1:A:251:ILE:C	2.58	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
2:H:329:GLY:C	2:H:330:LEU:HD12	2.40	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: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
1:A:344:ASN:CG	1:E:111:ASN:HD22	2.24	0.46
2:D:322:LEU:C	2:D:322:LEU:CD1	2.81	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
2:B:126:LYS:O	2:B:127:ILE:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:CD1	2:H:335:PHE:C	2.94	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:104:PHE:CD1	1:A:104:PHE:C	2.93	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
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:319:ASN:C	2:F:320:ASN:ND2	2.74	0.46
2:F:338:GLU:HG3	3:K:148:LYS:HA	1.98	0.46
2:H:358:SER:O	2:H:359:ALA:C	2.58	0.46
1:A:41:THR:O	1:A:42:GLY:C	2.58	0.46
1:A:368:ILE:HG23	1:A:370:GLN:HG3	1.98	0.46
1:A:376:SER:HG	1:A:379:GLU:HG3	1.81	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:ARG:HG2	2:D:90:ARG:HH11	1.80	0.45
2:D:98:ASP:O	2:D:99:ILE:C	2.60	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
2:H:96:PRO:O	2:H:99:ILE:HG13	2.15	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:J:118:GLU:C	3:J:120:THR:H	2.25	0.45
3:J:141:GLN:C	3:J:142:ARG:HH11	2.24	0.45
1:E:325:VAL:O	1:E:326:ARG:C	2.59	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
1:G:84:ASN:CG	1:G:106:GLU:HG2	2.40	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
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
1:C:468:TYR:O	1:C:469:GLY:C	2.60	0.45
2:D:398:THR:O	2:D:402:GLU:HG3	2.16	0.45
1:E:277:ASN:HD22	1:E:277:ASN:C	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:496:PHE:C	1:A:496:PHE:CD2	2.94	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:177:LEU:C	2:F:178:ILE:HD13	2.42	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:323:VAL:HG21	3:L:170:VAL:HG22	1.99	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
1:C:418:ASN:HD22	1:C:418:ASN:C	2.24	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
2:F:386:GLU:C	2:F:388:LYS:N	2.74	0.45
1:G:226:TYR:O	1:G:231:GLY:N	2.48	0.45
2:H:343:CYS:C	2:H:345:ALA:H	2.24	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
2:F:83:ILE:HD12	2:F:106:VAL:HG21	1.99	0.45
2:F:231:TYR:C	2:F:233:ARG:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:322:LEU:HD12	2:D:323:VAL:C	2.42	0.45
1:E:518:ASN:HB3	1:E:533:GLN:HA	1.99	0.45
2:F:386:GLU:C	2:F:388:LYS:H	2.24	0.45
1:G:72:ASN:C	1:G:72:ASN:HD22	2.24	0.45
1:G:179:ALA:O	1:G:180:LEU:C	2.58	0.45
1:G:304:PHE:CD2	1:G:304:PHE:C	2.95	0.45
2:H:238:PRO:C	2:H:240:GLU:H	2.23	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
1:G:208:ASP:HA	1:G:211:HIS:HB2	1.99	0.45
1:G:210:SER:C	1:G:212:THR:H	2.24	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: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:C:421:ASN:C	1:C:423:ILE:H	2.24	0.44
2:D:361:LEU:C	2:D:363:GLU:N	2.72	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:89:ALA:O	1:A:90:MET:C	2.58	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
1:E:72:ASN:C	1:E:72:ASN:ND2	2.74	0.44
3:K:144:ILE:HD13	3:K:170:VAL:CB	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:H:317:PRO:O	2:H:318:LEU:C	2.60	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
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
1:E:497:LEU:O	1:E:498:GLY:C	2.60	0.44
2:F:56:ALA:HB2	2:F:77:VAL:HG11	2.00	0.44
2:F:139:HIS:C	2:F:140:ILE:HG13	2.42	0.44
2:F:404:THR:O	2:F:407:ASN:HB2	2.17	0.44
3:L:117:ILE:CD1	3:L:126:ILE:HG12	2.47	0.44
3:L:118:GLU:C	3:L:120:THR:N	2.76	0.44
1:C:72:ASN:C	1:C:72:ASN:HD22	2.26	0.44
1:C:262:GLU:O	1:C:264:ASN:N	2.51	0.44
1:C:409:LYS:O	1:C:410:ASP:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:LYS:C	1:E:319:GLY:H	2.24	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
1:G:406:THR:O	1:G:407:ILE:C	2.60	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
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
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:171:PRO:C	2:H:173:SER:H	2.26	0.44
2:H:280:LEU:O	2:H:284:VAL:HG23	2.17	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:230:ASN:C	1:C:230:ASN:OD1	2.61	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:166:ASP:C	2:B:168:VAL:H	2.26	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:223:ARG:C	2:F:273:ILE:HD13	2.43	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:G:317:LYS:C	1:G:319:GLY:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:488:ALA:C	1:G:490:PRO:HD3	2.43	0.44
1:A:449:GLN:O	1:A:450:VAL:C	2.61	0.43
1:C:39:THR:HG22	1:C:489:GLU:CD	2.41	0.43
1:C:67:GLY:H	2:H:262:GLN:HE22	1.66	0.43
2:D:371:SER:OG	2:D:372:ALA:N	2.51	0.43
1:E:336:SER:HB2	2:F:221:MET:CA	2.45	0.43
2:F:361:LEU:HD23	2:F:361:LEU:C	2.42	0.43
1:G:38:ALA:HB3	1:G:85:ARG:CD	2.48	0.43
1:G:164:ILE:C	1:G:165:ILE:HG13	2.42	0.43
2:H:240:GLU:O	2:H:241:GLN:C	2.61	0.43
2:H:267:ARG:O	2:H:271:TYR:HD1	2.01	0.43
1:A:408:ASN:OD1	1:A:411:GLU:HB3	2.18	0.43
2:D:147:SER:O	2:D:151:ARG:HG3	2.18	0.43
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
3:L:150:MET:HE1	3:L:167:LEU:CD1	2.48	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:245:ASP:C	1:E:247:ILE:N	2.75	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
1:A:277:ASN:HD22	1:A:277:ASN:C	2.26	0.43
1:A:490:PRO:HG3	2:B:23:PHE:HE1	1.84	0.43
2:B:110:PHE:C	2:B:110:PHE:HD2	2.25	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:190:PRO:O	1:E:191:GLU:C	2.61	0.43
1:E:311:LEU:HD22	1:E:383:LEU:HD21	2.00	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
2:H:343:CYS:C	2:H:345:ALA:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ARG:C	1:A:80:SER:N	2.75	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
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:117:PRO:C	1:A:119:PHE:H	2.27	0.43
1:A:366:GLN:O	1:A:368:ILE:N	2.52	0.43
1:A:517:ASN:C	1:A:517:ASN:ND2	2.77	0.43
2:B:195:GLY:O	2:B:339:ARG:NH1	2.52	0.43
2:B:197:THR:CG2	2:B:198:ALA:N	2.79	0.43
1:C:51:LEU:HA	1:C:51:LEU:HD23	1.75	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: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:298:THR:C	1:A:300:GLN:N	2.76	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:187:GLY:C	3:I:173:LEU:HD13	2.43	0.43
2:B:412:LEU:CD1	2:B:438:LEU:HD11	2.49	0.43
2:B:418:VAL:O	2:B:419:ASP:C	2.61	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:D:328:ASP:O	2:D:329:GLY:C	2.61	0.43
1:E:252:LEU:HD12	1:E:252:LEU:C	2.43	0.43
1:E:263:GLU:O	1:E:264:ASN:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:113:ASP:C	2:B:113:ASP:OD1	2.61	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:260:GLU:HG3	1:C:261:ASP:OD2	2.17	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:F:398:THR:O	2:F:399:SER:C	2.62	0.43
1:G:435:PHE:C	1:G:435:PHE:CD2	2.97	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:47:LYS:HD2	1:C:47:LYS:C	2.43	0.43
2:D:78:ILE:HG12	2:D:123:HIS:HB2	2.00	0.43
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:F:17:TRP:O	2:F:18:ASN:C	2.58	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
2:B:193:LEU:O	2:B:194:PRO:C	2.60	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
2:H:159:ILE:C	2:H:161:LEU:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:82:GLY:O	1:C:83:LYS:C	2.62	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
2:H:402:GLU:C	2:H:404:THR:N	2.76	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:132:PRO:O	1:A:133:GLU:C	2.61	0.42
1:A:148:ILE:HA	1:A:149:PRO:HD3	1.92	0.42
1:A:416:MET:C	1:A:418:ASN:N	2.76	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
2:H:343:CYS:O	2:H:347:SER:OG	2.33	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:183:GLU:O	2:B:184:GLY:C	2.62	0.42
1:C:252:LEU:O	1:C:252:LEU:HD12	2.19	0.42
1:C:421:ASN:C	1:C:423:ILE:N	2.78	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
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
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
2:B:357:PRO:HD2	2:B:442:SER:C	2.43	0.42
2:D:157:MET:HA	2:D:157:MET:HE3	2.01	0.42
3:J:118:GLU:C	3:J:120:THR:N	2.78	0.42
1:E:163:ARG:NH1	1:E:518:ASN:ND2	2.62	0.42
1:E:189:PHE:O	1:E:190:PRO:C	2.61	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
1:A:422:GLU:CD	1:A:422:GLU:H	2.27	0.42
2:B:309:LYS:HG2	2:B:315:TYR:HB2	2.01	0.42
1:C:217:ILE:O	1:C:218:ILE:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:K:107:THR:C	3:K:109:THR:H	2.28	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
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
2:H:155:ASN:OD1	2:H:199:CYS:HB2	2.19	0.42
2:H:407:ASN:C	2:H:409:SER:H	2.28	0.42
2:B:239:LYS:HD2	2:B:239:LYS:HA	1.83	0.42
1:E:125:VAL:HG12	1:E:126:VAL:N	2.34	0.42
2:F:419:ASP:OD1	2:F:419:ASP:C	2.62	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:G:265:PHE:C	1:G:267:GLU:H	2.28	0.42
1:A:66:SER:HB3	1:A:69:ASP:CG	2.45	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
3:I:107:THR:C	3:I:109:THR:N	2.78	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:318:LEU:HD12	2:F:318:LEU:C	2.44	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:105:VAL:HG13	3:J:105:VAL:O	2.20	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:105:VAL:C	1:G:107:GLU:H	2.28	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
2:H:98:ASP:O	2:H:99:ILE:C	2.63	0.42
2:B:79:ASP:OD2	2:B:81:ASP:HB2	2.20	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
1:E:396:ARG:HH11	1:E:534:LEU:C	2.28	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
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:214:TRP:CD2	1:G:332:MET:HE3	2.55	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:434:ARG:HD3	1:A:460:CYS:HA	2.02	0.41
1:A:435:PHE:O	1:A:436:HIS:C	2.63	0.41
2:B:361:LEU:HD23	2:B:361:LEU:O	2.19	0.41
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
2:D:339:ARG:O	2:D:340:LYS:C	2.63	0.41
2:D:376:MET:HE1	2:D:434:VAL:CG1	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:421:ASN:O	1:G:422:GLU:C	2.63	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:191:VAL:O	2:B:197:THR:HG21	2.20	0.41
1:C:133:GLU:O	1:C:134:SER:C	2.64	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:245:ASP:C	1:E:247:ILE:H	2.26	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
2:D:230:GLU:OE2	2:D:234:MET:HE3	2.20	0.41
2:D:342:ASN:CG	2:D:342:ASN:O	2.63	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
1:G:43:THR:HG21	1:G:73:ASN:OD1	2.19	0.41
2:H:88:LEU:HD22	2:H:94:PHE:O	2.20	0.41
3:L:101:MET:CE	3:L:119:PRO:HG3	2.50	0.41
1:A:155:THR:HG23	1:A:493:ILE:CG2	2.50	0.41
1:A:488:ALA:C	1:A:490:PRO:HD3	2.45	0.41
2:B:73:ARG:HD3	2:B:117:ASN:O	2.21	0.41
1:C:113:LEU:C	1:C:138:ARG:HH21	2.29	0.41
1:C:437:LYS:C	1:C:439:GLN:H	2.28	0.41
2:D:192:ILE:CD1	2:D:200:ILE:HG13	2.51	0.41
2:D:411:THR:O	2:D:412:LEU:C	2.63	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
1:G:128:ALA:HB1	1:G:131:LEU:HD11	2.03	0.41
1:G:245:ASP:C	1:G:247:ILE:H	2.29	0.41
1:G:447:ASN:ND2	2:H:26:ARG:HH21	2.17	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:B:398:THR:C	2:B:401:GLU:HB3	2.46	0.41
2:D:87:ASN:ND2	2:D:103:LYS:HE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:ASP:O	1:E:262:GLU:CG	2.69	0.41
1:E:297:ILE:C	1:E:368:ILE:HD11	2.46	0.41
1:E:448:TYR:CD1	1:E:448:TYR:C	2.99	0.41
2:F:286:LYS:O	2:F:287:ARG:C	2.63	0.41
1:G:199:TYR:O	1:G:220:LYS:NZ	2.51	0.41
1:G:273:ASN:O	1:G:273:ASN:CG	2.63	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:346:TYR:C	1:G:348:GLU:N	2.79	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:26:GLU:O	1:A:27:ALA:C	2.64	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:144:TRP:CD1	1:A:144:TRP:C	2.99	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:237:TRP:CD1	2:B:237:TRP:C	2.98	0.41
2:B:385:LEU:O	2:B:386:GLU:C	2.64	0.41
2:B:404:THR:O	2:B:405:ARG:C	2.64	0.41
2:B:413:LYS:O	2:B:413:LYS:HG2	2.19	0.41
1:C:49:LEU:C	1:C:52:PRO:HD2	2.45	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:193:LEU:O	2:D:194:PRO:C	2.62	0.41
2:D:215:MET:HE3	2:D:219:ALA:HB2	2.03	0.41
1:E:65:VAL:HG23	1:E:85:ARG:HA	2.03	0.41
1:E:225:TRP:O	1:E:229:THR:OG1	2.36	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:397:VAL:O	2:F:398:THR:C	2.64	0.41
2:F:407:ASN:HA	2:F:410:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:263:GLU:C	1:G:265:PHE:N	2.78	0.41
1:G:474:VAL:O	1:G:475:LYS:C	2.63	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:162:MET:HE1	2:B:330:LEU:HD11	2.03	0.41
1:A:439:GLN:HE21	1:A:439:GLN:HB3	1.68	0.41
2:B:230:GLU:CD	2:B:233:ARG:NH1	2.79	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
2:D:131:ASN:O	2:D:132:ASP:C	2.64	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
3:K:103:ILE:C	3:K:103:ILE:CD1	2.93	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
2:B:271:TYR:C	2:B:272:ASN:HD22	2.26	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:110:PHE:C	2:D:110:PHE:CD2	2.99	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:214:TRP:CD1	1:E:214:TRP:C	2.98	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
1:E:396:ARG:NH1	1:E:534:LEU:O	2.49	0.40
1:E:517:ASN:C	1:E:517:ASN:ND2	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:54:ILE:O	1:C:55:GLY:C	2.64	0.40
1:C:170:PRO:C	1:C:171:VAL:HG12	2.46	0.40
1:C:173:GLU:HA	1:C:386:ASN:ND2	2.37	0.40
2:D:18:ASN:C	2:D:20:VAL:H	2.30	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:245:ASP:C	1:G:247:ILE:N	2.80	0.40
1:G:285:ILE:HD12	1:G:323:LEU:HD11	2.04	0.40
1:G:386:ASN:O	1:G:387:SER:C	2.65	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
1:A:368:ILE:HD12	1:A:368:ILE:HA	1.97	0.40
2:B:21:LYS:C	2:B:23:PHE:H	2.29	0.40
1:C:229:THR:O	1:C:230:ASN:C	2.64	0.40
1:C:368:ILE:CG2	1:C:368:ILE:O	2.70	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:139:LEU:O	1:G:140:ALA:C	2.64	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
3:L:155:THR:O	3:L:156:ALA:C	2.64	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:D:33:PRO:C	2:D:35:PHE:H	2.29	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%)	3	8
1	C	513/531 (97%)	448 (87%)	56 (11%)	9 (2%)	6	15
1	E	519/531 (98%)	465 (90%)	47 (9%)	7 (1%)	9	21
1	G	512/531 (96%)	437 (85%)	62 (12%)	13 (2%)	4	10
2	B	430/434 (99%)	373 (87%)	51 (12%)	6 (1%)	9	19
2	D	430/434 (99%)	366 (85%)	53 (12%)	11 (3%)	4	9
2	F	429/434 (99%)	359 (84%)	55 (13%)	15 (4%)	3	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	429/434 (99%)	347 (81%)	63 (15%)	19 (4%)	2	3
3	I	84/88 (96%)	76 (90%)	4 (5%)	4 (5%)	2	3
3	J	74/88 (84%)	67 (90%)	5 (7%)	2 (3%)	4	9
3	K	74/88 (84%)	66 (89%)	6 (8%)	2 (3%)	4	9
3	L	74/88 (84%)	64 (86%)	5 (7%)	5 (7%)	1	1
All	All	4086/4212 (97%)	3510 (86%)	468 (12%)	108 (3%)	4	9

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	430 (95%)	22 (5%)	22	45
1	C	451/462 (98%)	425 (94%)	26 (6%)	18	38
1	E	450/462 (97%)	420 (93%)	30 (7%)	15	31
1	G	450/462 (97%)	434 (96%)	16 (4%)	31	56
2	B	377/381 (99%)	350 (93%)	27 (7%)	13	28
2	D	378/381 (99%)	353 (93%)	25 (7%)	15	32
2	F	376/381 (99%)	345 (92%)	31 (8%)	10	23
2	H	374/381 (98%)	338 (90%)	36 (10%)	8	17
3	I	73/74 (99%)	67 (92%)	6 (8%)	10	23
3	J	67/74 (90%)	65 (97%)	2 (3%)	36	61
3	K	67/74 (90%)	61 (91%)	6 (9%)	9	19
3	L	67/74 (90%)	64 (96%)	3 (4%)	24	48
All	All	3582/3668 (98%)	3352 (94%)	230 (6%)	16	33

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	63	ASN
1	A	72	ASN
1	A	134	SER
1	A	158	LEU
1	A	171	VAL
1	A	214	TRP
1	A	220	LYS
1	A	259	PRO
1	A	262	GLU
1	A	264	ASN
1	A	293	ARG
1	A	311	LEU
1	A	364	LEU
1	A	368	ILE
1	A	407	ILE
1	A	418	ASN
1	A	422	GLU
1	A	429	LEU

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Mol	Chain	Res	Type
1	A	437	LYS
1	A	497	LEU
1	A	518	ASN
2	B	12	ASP
2	B	82	THR
2	B	111	LEU
2	B	116	PRO
2	B	128	GLN
2	B	182	THR
2	B	197	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	322	LEU
2	B	323	VAL
2	B	327	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
2	B	392	LEU
2	B	401	GLU
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	170	VAL
3	I	171	LEU
1	C	33	VAL
1	C	36	ILE
1	C	43	THR
1	C	46	LEU
1	C	72	ASN
1	C	103	SER

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Mol	Chain	Res	Type
1	C	171	VAL
1	C	177	ASP
1	C	193	ARG
1	C	214	TRP
1	C	259	PRO
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	344	ASN
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	33	PRO
2	D	82	THR
2	D	114	ARG
2	D	116	PRO
2	D	128	GLN
2	D	149	ILE
2	D	182	THR
2	D	201	GLU
2	D	215	MET
2	D	316	ILE
2	D	318	LEU
2	D	322	LEU
2	D	323	VAL
2	D	342	ASN
2	D	350	PRO
2	D	357	PRO
2	D	362	GLN
2	D	389	ASN
2	D	401	GLU
2	D	411	THR
2	D	415	LEU

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Mol	Chain	Res	Type
2	D	419	ASP
2	D	422	GLU
2	D	442	SER
3	J	108	LEU
3	J	170	VAL
1	E	43	THR
1	E	56	SER
1	E	64	GLN
1	E	72	ASN
1	E	103	SER
1	E	112	LEU
1	E	158	LEU
1	E	171	VAL
1	E	190	PRO
1	E	209	HIS
1	E	226	TYR
1	E	259	PRO
1	E	262	GLU
1	E	264	ASN
1	E	285	ILE
1	E	293	ARG
1	E	297	ILE
1	E	309	ARG
1	E	311	LEU
1	E	364	LEU
1	E	400	GLU
1	E	407	ILE
1	E	418	ASN
1	E	422	GLU
1	E	424	VAL
1	E	452	GLU
1	E	497	LEU
1	E	517	ASN
1	E	518	ASN
1	E	519	THR
2	F	11	LEU
2	F	31	THR
2	F	39	THR
2	F	82	THR
2	F	87	ASN
2	F	111	LEU
2	F	114	ARG

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Mol	Chain	Res	Type
2	F	116	PRO
2	F	128	GLN
2	F	142	VAL
2	F	143	CYS
2	F	149	ILE
2	F	177	LEU
2	F	178	ILE
2	F	182	THR
2	F	212	ASN
2	F	241	GLN
2	F	242	PRO
2	F	316	ILE
2	F	318	LEU
2	F	322	LEU
2	F	326	ASP
2	F	327	VAL
2	F	342	ASN
2	F	349	LEU
2	F	357	PRO
2	F	375	GLN
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
3	K	115	ILE
3	K	170	VAL
1	G	43	THR
1	G	47	LYS
1	G	72	ASN
1	G	90	MET
1	G	111	ASN
1	G	171	VAL
1	G	180	LEU
1	G	202	ASP
1	G	214	TRP
1	G	262	GLU
1	G	264	ASN
1	G	311	LEU

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Mol	Chain	Res	Type
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	116	PRO
2	H	128	GLN
2	H	154	ILE
2	H	182	THR
2	H	201	GLU
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	322	LEU
2	H	326	ASP
2	H	328	ASP
2	H	342	ASN
2	H	344	PRO
2	H	348	GLN
2	H	355	PHE
2	H	362	GLN
2	H	364	VAL
2	H	374	LEU
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	425	VAL
2	H	428	VAL
2	H	440	PHE
3	L	107	THR
3	L	170	VAL

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Mol	Chain	Res	Type
3	L	171	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (158) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	37	ASN
1	A	63	ASN
1	A	64	GLN
1	A	72	ASN
1	A	94	GLN
1	A	169	HIS
1	A	178	ASN
1	A	195	HIS
1	A	197	GLN
1	A	211	HIS
1	A	264	ASN
1	A	277	ASN
1	A	320	GLN
1	A	322	ASN
1	A	359	ASN
1	A	418	ASN
1	A	439	GLN
1	A	447	ASN
1	A	518	ASN
1	A	533	GLN
2	B	19	HIS
2	B	74	GLN
2	B	76	HIS
2	B	87	ASN
2	B	119	ASN
2	B	128	GLN
2	B	139	HIS
2	B	212	ASN
2	B	236	GLN
2	B	241	GLN
2	B	272	ASN
2	B	319	ASN
2	B	320	ASN
2	B	325	ASN
2	B	342	ASN
2	B	351	GLN

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Mol	Chain	Res	Type
2	B	352	ASN
2	B	362	GLN
2	B	370	ASN
2	B	389	ASN
2	B	395	GLN
2	B	421	GLN
3	I	149	GLN
1	C	48	ASN
1	C	72	ASN
1	C	175	HIS
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	322	ASN
1	C	343	GLN
1	C	344	ASN
1	C	359	ASN
1	C	370	GLN
1	C	386	ASN
1	C	418	ASN
1	C	439	GLN
1	C	447	ASN
1	C	517	ASN
2	D	74	GLN
2	D	128	GLN
2	D	139	HIS
2	D	210	GLN
2	D	212	ASN
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

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Mol	Chain	Res	Type
2	D	421	GLN
2	D	432	GLN
3	J	141	GLN
3	J	151	ASN
1	E	37	ASN
1	E	64	GLN
1	E	72	ASN
1	E	111	ASN
1	E	115	ASN
1	E	197	GLN
1	E	211	HIS
1	E	224	GLN
1	E	264	ASN
1	E	271	ASN
1	E	277	ASN
1	E	322	ASN
1	E	343	GLN
1	E	344	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	128	GLN
2	F	131	ASN
2	F	139	HIS
2	F	212	ASN
2	F	236	GLN
2	F	320	ASN
2	F	325	ASN
2	F	342	ASN
2	F	348	GLN
2	F	354	GLN
2	F	362	GLN
2	F	375	GLN
2	F	395	GLN
2	F	407	ASN
2	F	421	GLN

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Mol	Chain	Res	Type
2	F	439	HIS
1	G	37	ASN
1	G	72	ASN
1	G	115	ASN
1	G	178	ASN
1	G	195	HIS
1	G	197	GLN
1	G	264	ASN
1	G	271	ASN
1	G	277	ASN
1	G	343	GLN
1	G	344	ASN
1	G	359	ASN
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	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	352	ASN
2	H	354	GLN
2	H	362	GLN
2	H	395	GLN
2	H	439	HIS
3	L	140	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	522/531 (98%)	-0.07	6 (1%) 78 73	49, 84, 116, 147	0
1	C	520/531 (97%)	0.11	10 (1%) 66 59	58, 89, 123, 157	0
1	E	523/531 (98%)	-0.11	6 (1%) 78 73	46, 71, 137, 158	0
1	G	518/531 (97%)	0.04	9 (1%) 69 63	49, 80, 143, 157	0
2	B	432/434 (99%)	-0.00	5 (1%) 76 71	47, 76, 116, 130	0
2	D	432/434 (99%)	0.12	7 (1%) 70 64	55, 92, 122, 143	0
2	F	431/434 (99%)	0.08	11 (2%) 57 48	50, 76, 124, 147	0
2	H	431/434 (99%)	0.22	5 (1%) 76 71	52, 83, 133, 152	0
3	I	86/88 (97%)	0.03	1 (1%) 76 71	61, 87, 106, 117	0
3	J	76/88 (86%)	0.15	0 100 100	75, 101, 119, 124	0
3	K	76/88 (86%)	0.04	1 (1%) 75 68	68, 91, 111, 121	0
3	L	76/88 (86%)	0.27	1 (1%) 75 68	75, 112, 132, 140	0
All	All	4123/4212 (97%)	0.05	62 (1%) 72 65	46, 84, 126, 158	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	252	LEU	3.4
2	D	11	LEU	3.4
2	D	388	LYS	3.3
1	A	276	LEU	3.3
2	F	419	ASP	3.3
1	C	6	LYS	3.3
2	F	243	PHE	3.1
2	H	397	VAL	3.1
2	D	385	LEU	3.1
1	E	202	ASP	3.0
2	H	272	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
3	L	116	ASP	3.0
1	E	233	ILE	2.9
1	C	260	GLU	2.9
2	B	320	ASN	2.9
2	B	412	LEU	2.8
1	C	259	PRO	2.8
2	F	385	LEU	2.7
1	C	251	ILE	2.7
2	F	412	LEU	2.7
2	F	438	LEU	2.7
2	D	220	SER	2.7
1	A	6	LYS	2.6
1	G	275	ALA	2.6
1	E	203	HIS	2.6
1	A	278	THR	2.5
2	B	361	LEU	2.5
1	G	215	ILE	2.5
1	C	7	LEU	2.4
2	F	320	ASN	2.4
1	G	209	HIS	2.4
2	B	381	ILE	2.4
1	A	117	PRO	2.4
1	E	274	THR	2.3
2	F	441	THR	2.3
1	C	471	SER	2.3
3	K	117	ILE	2.3
2	D	394	LEU	2.3
1	G	226	TYR	2.3
2	F	394	LEU	2.3
1	E	252	LEU	2.2
1	A	200	ASP	2.2
2	F	11	LEU	2.2
2	D	436	PHE	2.2
1	G	185	LEU	2.2
1	G	201	LEU	2.2
1	C	205	GLU	2.2
1	C	278	THR	2.2
2	H	438	LEU	2.1
3	I	176	GLY	2.1
2	F	355	PHE	2.1
2	H	412	LEU	2.1
2	D	395	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	276	LEU	2.1
1	C	204	MET	2.1
1	E	275	ALA	2.1
1	A	259	PRO	2.0
2	H	374	LEU	2.0
2	B	408	LEU	2.0
1	G	517	ASN	2.0
2	F	319	ASN	2.0
1	G	251	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	B	1	1/1	0.99	0.04	79,79,79,79	0
4	ZN	F	4	1/1	0.99	0.04	74,74,74,74	0
4	ZN	H	2	1/1	0.99	0.05	84,84,84,84	0
4	ZN	D	3	1/1	1.00	0.03	93,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.