



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:41 AM UTC

PDB ID : 3IKO / pdb_00003iko
Title : Crystal structure of the heterotrimeric Sec13-Nup145C-Nup84 nucleoporin complex
Authors : Nagy, V.; Hsia, K.-C.; Debler, E.W.; Davenport, A.; Blobel, G.; Hoelz, A.
Deposited on : 2009-08-06
Resolution : 3.20 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

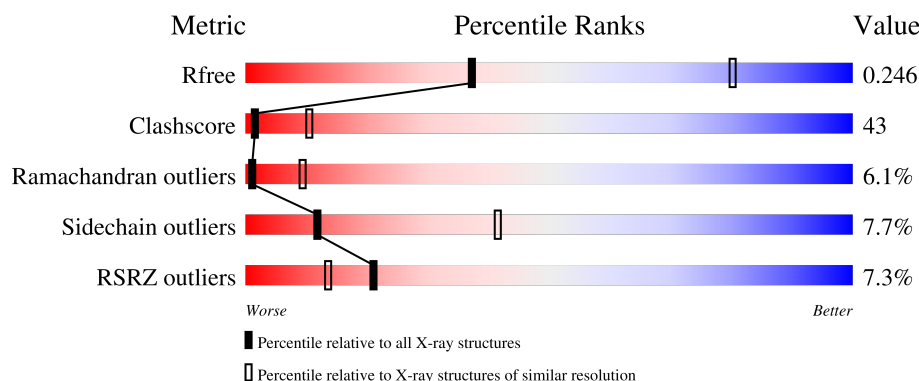
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	297	9% 30% 52% 9% 8%
1	D	297	15% 32% 50% 9% 8%
1	G	297	15% 30% 52% 10% 8%
2	B	442	5% 39% 45% 12% . .
2	E	442	7% 38% 43% 12% . .

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Mol	Chain	Length	Quality of chain
2	H	442	7% 38% 44% 12% 5%
3	C	460	4% 40% 38% 12% 9%
3	F	460	4% 39% 37% 14% 9%
3	I	460	2% 39% 38% 12% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27032 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 Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			
1	D	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			
1	G	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			

- Molecule 2 is a protein called Nucleoporin NUP145C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	434	Total	C	N	O	S	9	0	0
			3528	2254	587	675	12			
2	E	423	Total	C	N	O	S	9	0	0
			3438	2201	570	656	11			
2	H	420	Total	C	N	O	S	9	0	0
			3409	2182	566	650	11			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	111	MET	-	expression tag	UNP P49687
B	112	GLY	-	expression tag	UNP P49687
B	113	SER	-	expression tag	UNP P49687
B	114	SER	-	expression tag	UNP P49687
B	115	HIS	-	expression tag	UNP P49687
B	116	HIS	-	expression tag	UNP P49687
B	117	HIS	-	expression tag	UNP P49687
B	118	HIS	-	expression tag	UNP P49687
B	119	HIS	-	expression tag	UNP P49687
B	120	HIS	-	expression tag	UNP P49687
B	121	SER	-	expression tag	UNP P49687
B	122	GLN	-	expression tag	UNP P49687

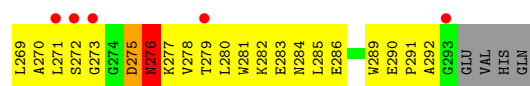
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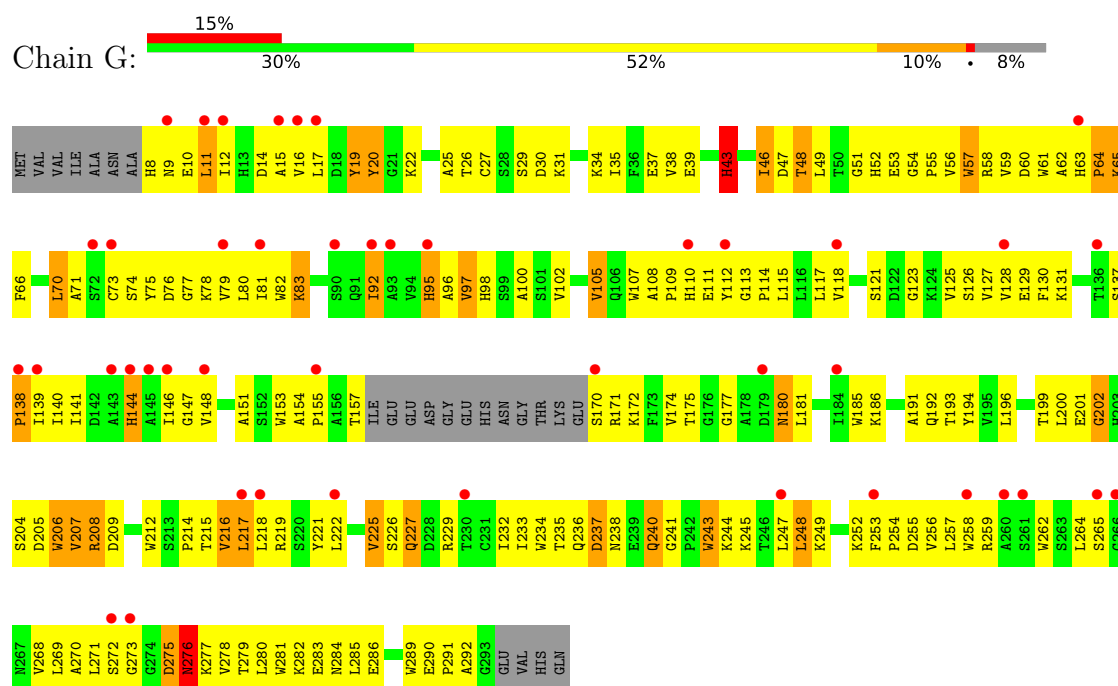
Chain	Residue	Modelled	Actual	Comment	Reference
B	123	ASP	-	expression tag	UNP P49687
B	124	PRO	-	expression tag	UNP P49687
E	111	MET	-	expression tag	UNP P49687
E	112	GLY	-	expression tag	UNP P49687
E	113	SER	-	expression tag	UNP P49687
E	114	SER	-	expression tag	UNP P49687
E	115	HIS	-	expression tag	UNP P49687
E	116	HIS	-	expression tag	UNP P49687
E	117	HIS	-	expression tag	UNP P49687
E	118	HIS	-	expression tag	UNP P49687
E	119	HIS	-	expression tag	UNP P49687
E	120	HIS	-	expression tag	UNP P49687
E	121	SER	-	expression tag	UNP P49687
E	122	GLN	-	expression tag	UNP P49687
E	123	ASP	-	expression tag	UNP P49687
E	124	PRO	-	expression tag	UNP P49687
H	111	MET	-	expression tag	UNP P49687
H	112	GLY	-	expression tag	UNP P49687
H	113	SER	-	expression tag	UNP P49687
H	114	SER	-	expression tag	UNP P49687
H	115	HIS	-	expression tag	UNP P49687
H	116	HIS	-	expression tag	UNP P49687
H	117	HIS	-	expression tag	UNP P49687
H	118	HIS	-	expression tag	UNP P49687
H	119	HIS	-	expression tag	UNP P49687
H	120	HIS	-	expression tag	UNP P49687
H	121	SER	-	expression tag	UNP P49687
H	122	GLN	-	expression tag	UNP P49687
H	123	ASP	-	expression tag	UNP P49687
H	124	PRO	-	expression tag	UNP P49687

- Molecule 3 is a protein called Nucleoporin NUP84.

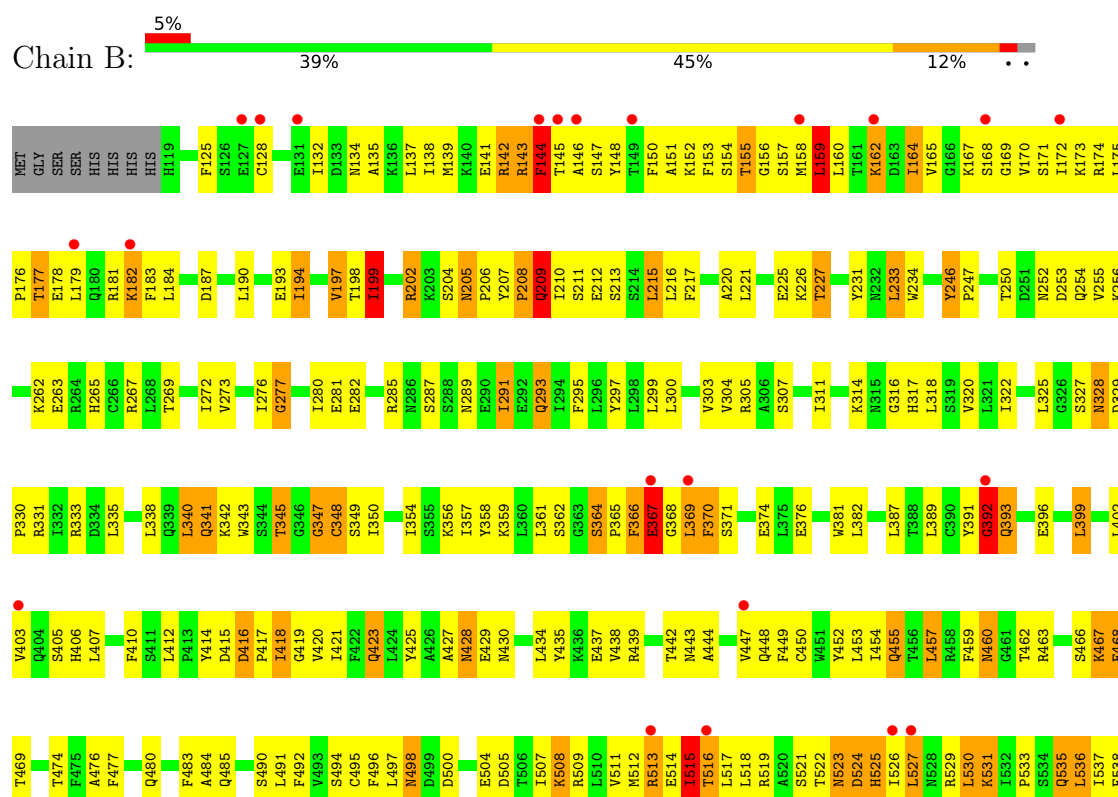
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	419	Total	C	N	O	S	0	0	0
			3404	2178	557	657	12			
3	F	419	Total	C	N	O	S	0	0	0
			3404	2178	558	656	12			
3	I	414	Total	C	N	O	S	0	0	0
			3369	2155	554	649	11			

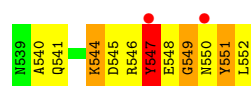


• Molecule 1: Protein transport protein SEC13

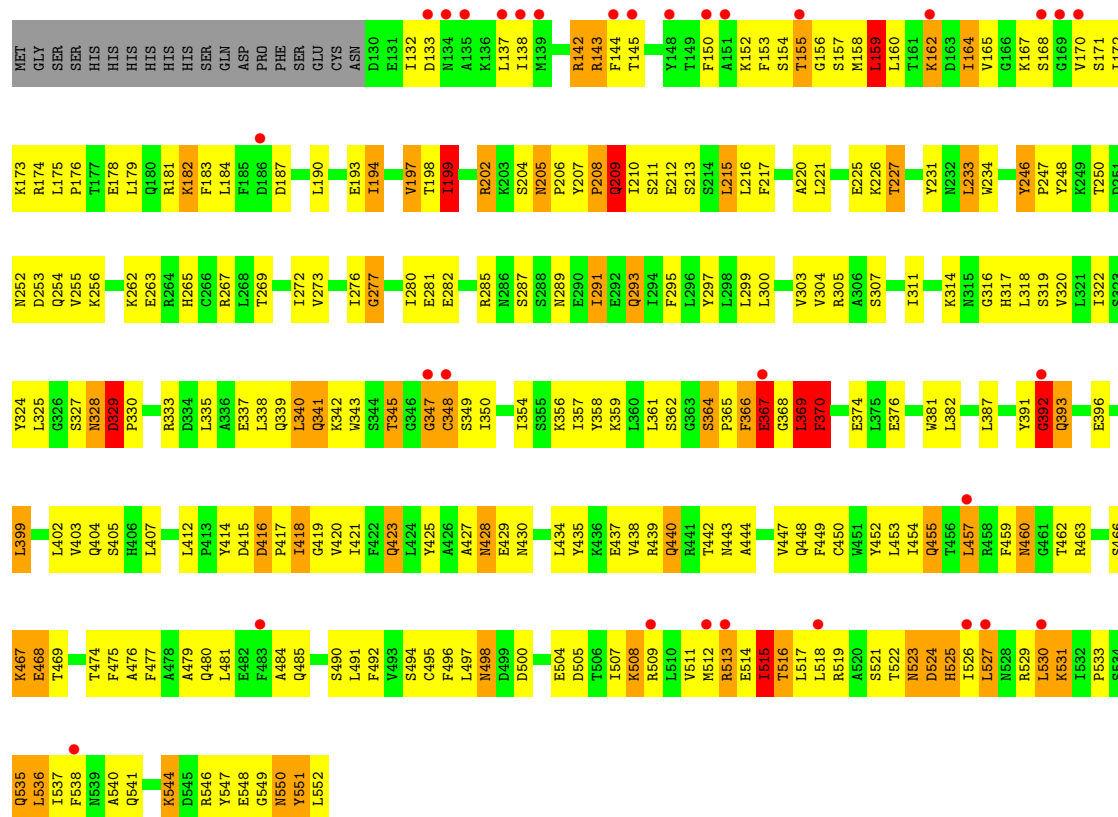


• Molecule 2: Nucleoporin NUP145C

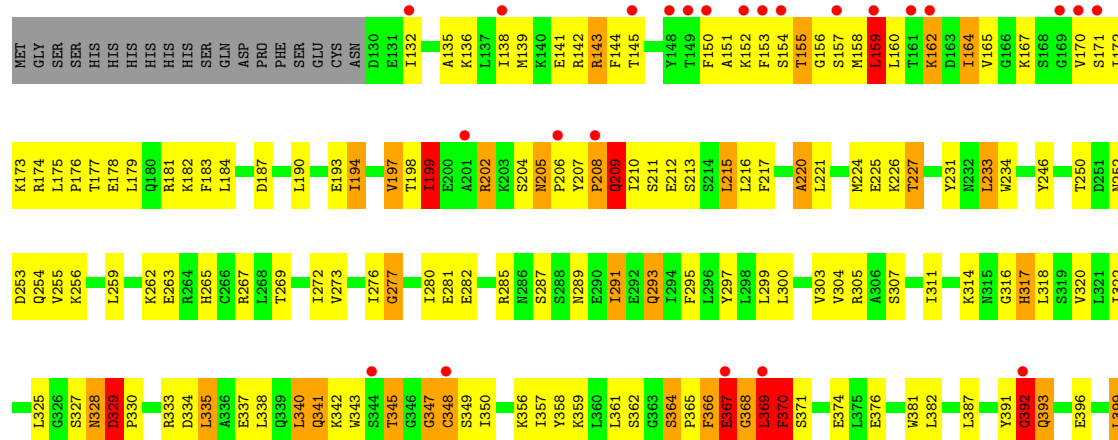




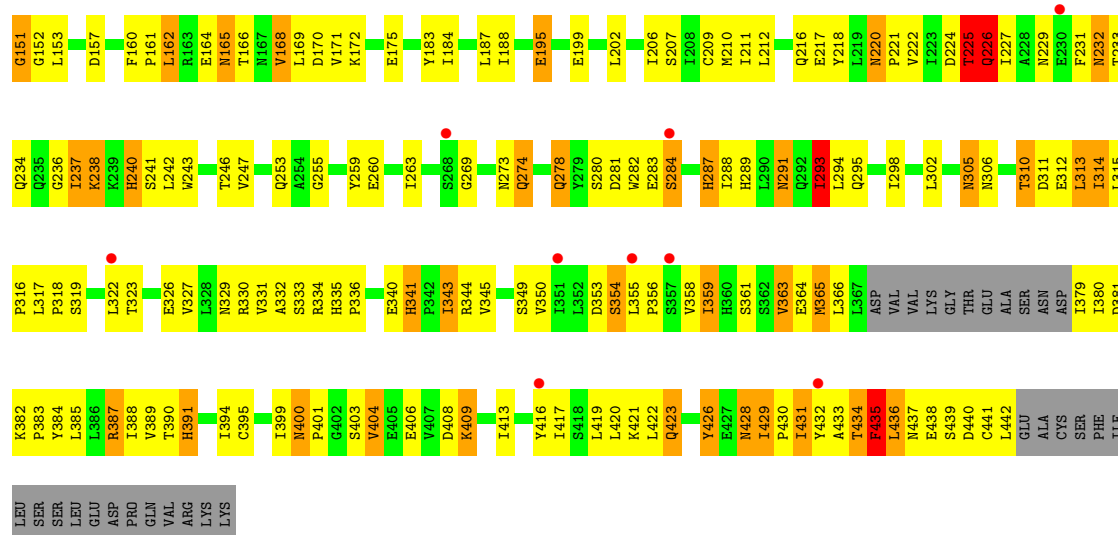
• Molecule 2: Nucleoporin NUP145C



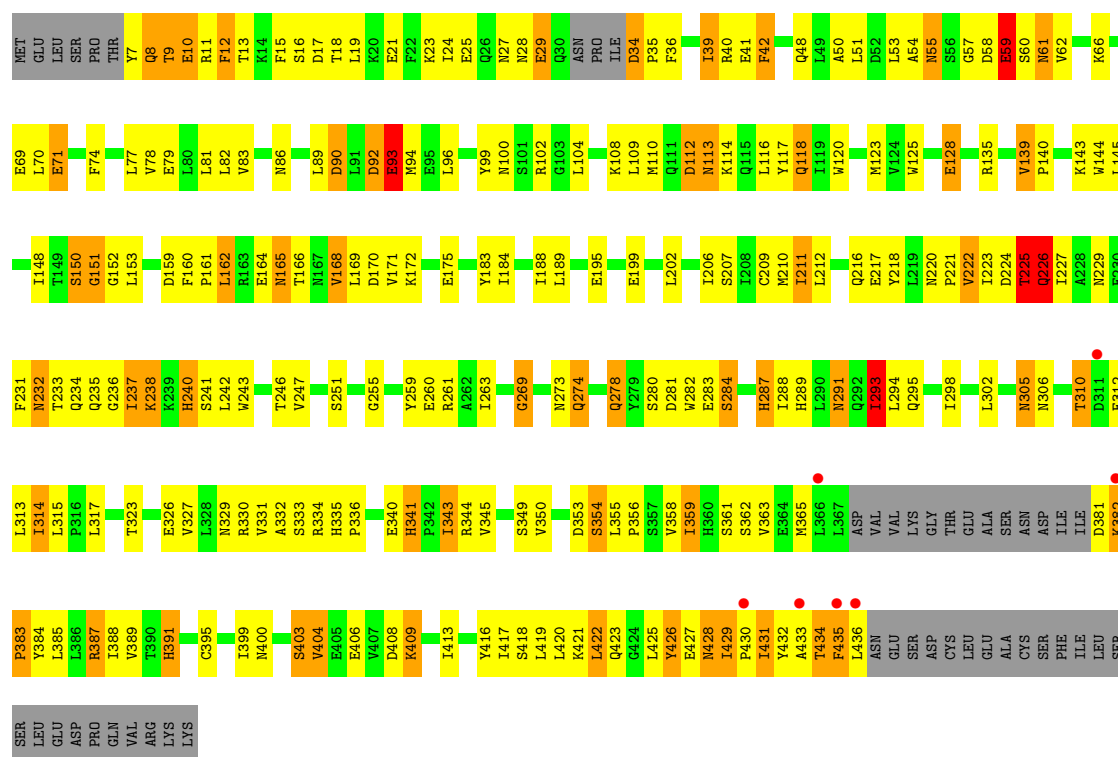
• Molecule 2: Nucleoporin NUP145C







• Molecule 3: Nucleoporin NUP84



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.40Å 194.05Å 327.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-3.20) 96.8 (50.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.273 0.243 , 0.246	Depositor DCC
R_{free} test set	5253 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 118.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27032	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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

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	0.66	7/2220 (0.3%)	1.00	14/3028 (0.5%)
1	D	0.64	7/2220 (0.3%)	0.99	14/3028 (0.5%)
1	G	0.64	9/2220 (0.4%)	0.99	14/3028 (0.5%)
2	B	0.71	12/3598 (0.3%)	1.15	29/4856 (0.6%)
2	E	0.73	14/3504 (0.4%)	1.17	32/4728 (0.7%)
2	H	0.73	14/3474 (0.4%)	1.17	29/4688 (0.6%)
3	C	0.83	16/3472 (0.5%)	1.25	50/4714 (1.1%)
3	F	0.83	15/3472 (0.4%)	1.25	56/4714 (1.2%)
3	I	0.82	14/3437 (0.4%)	1.21	48/4666 (1.0%)
All	All	0.75	108/27617 (0.4%)	1.15	286/37450 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	F	0	1
All	All	0	2

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	145	THR	CA-C	6.98	1.55	1.52
2	B	311	ILE	CA-CB	6.29	1.61	1.54
2	E	311	ILE	CA-CB	6.10	1.61	1.54
2	H	311	ILE	CA-CB	6.08	1.61	1.54
2	H	293	GLN	CD-OE1	5.63	1.34	1.23
2	E	341	GLN	CD-OE1	5.58	1.34	1.23
3	F	291	ASN	CG-ND2	-5.52	1.21	1.33
1	A	144	HIS	ND1-CE1	5.49	1.38	1.32
3	C	226	GLN	CD-OE1	5.47	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	293	GLN	CD-OE1	5.46	1.33	1.23
3	C	240	HIS	ND1-CE1	5.46	1.38	1.32
1	D	144	HIS	ND1-CE1	5.45	1.38	1.32
3	I	226	GLN	CD-OE1	5.45	1.33	1.23
2	E	525	HIS	ND1-CE1	5.44	1.38	1.32
2	B	341	GLN	CD-OE1	5.42	1.33	1.23
3	F	240	HIS	ND1-CE1	5.42	1.38	1.32
2	H	341	GLN	CD-OE1	5.42	1.33	1.23
2	H	525	HIS	ND1-CE1	5.42	1.38	1.32
2	B	317	HIS	ND1-CE1	5.40	1.38	1.32
2	E	317	HIS	ND1-CE1	5.40	1.38	1.32
2	H	423	GLN	CD-OE1	5.39	1.33	1.23
2	B	293	GLN	CD-OE1	5.38	1.33	1.23
3	F	226	GLN	CD-OE1	5.38	1.33	1.23
3	C	273	ASN	CG-ND2	-5.36	1.22	1.33
2	H	262	LYS	CG-CD	5.34	1.68	1.52
2	E	423	GLN	CD-OE1	5.33	1.33	1.23
1	A	43	HIS	ND1-CE1	5.33	1.37	1.32
2	B	262	LYS	CG-CD	5.32	1.68	1.52
2	B	423	GLN	CD-OE1	5.32	1.33	1.23
2	E	209	GLN	CD-OE1	5.32	1.33	1.23
1	D	43	HIS	ND1-CE1	5.31	1.37	1.32
2	H	317	HIS	ND1-CE1	5.31	1.37	1.32
3	I	100	ASN	CG-OD1	5.31	1.33	1.23
1	G	43	HIS	ND1-CE1	5.31	1.37	1.32
3	C	291	ASN	CG-ND2	-5.30	1.22	1.33
1	D	95	HIS	ND1-CE1	5.30	1.37	1.32
3	I	240	HIS	ND1-CE1	5.30	1.37	1.32
3	C	305	ASN	CG-ND2	-5.28	1.22	1.33
3	C	289	HIS	ND1-CE1	5.28	1.37	1.32
2	E	455	GLN	CD-OE1	5.28	1.33	1.23
3	I	273	ASN	CG-ND2	-5.28	1.22	1.33
3	I	305	ASN	CG-ND2	-5.28	1.22	1.33
3	C	391	HIS	ND1-CE1	5.27	1.37	1.32
2	E	329	ASP	C-N	-5.27	1.26	1.33
2	B	455	GLN	CD-OE1	5.26	1.33	1.23
2	H	455	GLN	CD-OE1	5.25	1.33	1.23
3	I	341	HIS	ND1-CE1	5.25	1.37	1.32
2	B	209	GLN	CD-OE1	5.25	1.33	1.23
3	F	113	ASN	CG-OD1	5.24	1.33	1.23
3	F	305	ASN	CG-ND2	-5.24	1.22	1.33
3	I	287	HIS	CD2-NE2	-5.24	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	262	LYS	CG-CD	5.24	1.68	1.52
3	F	341	HIS	ND1-CE1	5.23	1.37	1.32
3	C	287	HIS	ND1-CE1	5.23	1.37	1.32
1	G	240	GLN	CD-OE1	5.22	1.33	1.23
2	H	209	GLN	CD-OE1	5.21	1.33	1.23
2	B	525	HIS	ND1-CE1	5.21	1.37	1.32
3	F	391	HIS	ND1-CE1	5.21	1.37	1.32
1	G	238	ASN	CG-OD1	5.20	1.33	1.23
2	H	329	ASP	C-N	-5.20	1.26	1.33
1	D	238	ASN	CG-OD1	5.20	1.33	1.23
1	G	95	HIS	ND1-CE1	5.20	1.37	1.32
1	A	238	ASN	CG-OD1	5.19	1.33	1.23
1	A	240	GLN	CD-OE1	5.19	1.33	1.23
3	C	341	HIS	ND1-CE1	5.19	1.37	1.32
1	D	240	GLN	CD-OE1	5.19	1.33	1.23
3	I	118	GLN	CD-OE1	5.18	1.33	1.23
3	F	273	ASN	CG-ND2	-5.18	1.22	1.33
2	E	440	GLN	CD-OE1	5.18	1.33	1.23
3	F	287	HIS	ND1-CE1	5.18	1.37	1.32
1	D	227	GLN	CD-OE1	5.17	1.33	1.23
3	I	391	HIS	ND1-CE1	5.16	1.37	1.32
3	C	100	ASN	CG-OD1	5.16	1.33	1.23
2	B	535	GLN	CD-OE1	5.15	1.33	1.23
3	C	113	ASN	CG-OD1	5.15	1.33	1.23
2	H	498	ASN	CG-OD1	5.15	1.33	1.23
2	H	535	GLN	CD-OE1	5.15	1.33	1.23
3	I	287	HIS	ND1-CE1	5.15	1.37	1.32
3	F	118	GLN	CD-OE1	5.15	1.33	1.23
3	I	113	ASN	CG-OD1	5.15	1.33	1.23
2	H	460	ASN	CG-OD1	5.14	1.33	1.23
1	A	95	HIS	ND1-CE1	5.14	1.37	1.32
2	E	460	ASN	CG-OD1	5.13	1.33	1.23
1	G	227	GLN	CD-OE1	5.13	1.33	1.23
3	C	118	GLN	CD-OE1	5.13	1.33	1.23
1	G	180	ASN	CG-OD1	5.12	1.33	1.23
3	F	289	HIS	ND1-CE1	5.12	1.37	1.32
2	B	460	ASN	CG-OD1	5.12	1.33	1.23
1	D	180	ASN	CG-OD1	5.12	1.33	1.23
2	E	535	GLN	CD-OE1	5.11	1.33	1.23
3	C	61	ASN	CG-OD1	5.11	1.33	1.23
2	B	498	ASN	CG-OD1	5.10	1.33	1.23
1	G	144	HIS	ND1-CE1	5.10	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	240	HIS	CD2-NE2	-5.10	1.32	1.37
3	F	86	ASN	CG-OD1	5.09	1.33	1.23
3	F	100	ASN	CG-OD1	5.09	1.33	1.23
1	A	227	GLN	CD-OE1	5.09	1.33	1.23
2	E	498	ASN	CG-OD1	5.08	1.33	1.23
3	I	61	ASN	CG-OD1	5.08	1.33	1.23
3	C	26	GLN	CD-OE1	5.07	1.33	1.23
1	A	180	ASN	CG-OD1	5.07	1.33	1.23
3	F	61	ASN	CG-OD1	5.06	1.33	1.23
3	C	289	HIS	CD2-NE2	-5.05	1.32	1.37
1	G	95	HIS	CD2-NE2	-5.04	1.32	1.37
3	C	324	VAL	CA-CB	-5.04	1.48	1.54
1	G	144	HIS	CD2-NE2	-5.03	1.32	1.37
3	I	291	ASN	CG-ND2	-5.03	1.22	1.33
3	F	287	HIS	CD2-NE2	-5.01	1.32	1.37

All (286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	382	LYS	CA-C-N	12.94	136.01	119.84
3	C	382	LYS	C-N-CA	12.94	136.01	119.84
3	F	435	PHE	N-CA-C	12.18	126.41	109.11
3	F	436	LEU	CB-CA-C	-11.14	103.70	116.63
3	F	439	SER	N-CA-C	-10.49	100.42	113.01
3	F	436	LEU	N-CA-C	10.18	125.28	108.08
2	H	246	TYR	CA-C-N	9.67	129.78	119.05
2	H	246	TYR	C-N-CA	9.67	129.78	119.05
2	E	246	TYR	CA-C-N	9.64	129.75	119.05
2	E	246	TYR	C-N-CA	9.64	129.75	119.05
2	B	246	TYR	CA-C-N	9.62	129.73	119.05
2	B	246	TYR	C-N-CA	9.62	129.73	119.05
2	E	155	THR	N-CA-C	-9.43	100.95	111.14
2	H	155	THR	N-CA-C	-9.42	100.97	111.14
2	B	155	THR	N-CA-C	-9.41	100.98	111.14
3	I	435	PHE	N-CA-C	8.72	123.23	112.59
2	H	329	ASP	CA-C-N	8.69	129.55	119.47
2	H	329	ASP	C-N-CA	8.69	129.55	119.47
2	E	329	ASP	CA-C-N	8.44	129.26	119.47
2	E	329	ASP	C-N-CA	8.44	129.26	119.47
2	B	371	SER	N-CA-C	8.05	121.62	110.35
2	H	371	SER	N-CA-C	7.94	121.47	110.35
2	E	132	ILE	N-CA-C	-7.86	105.53	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	523	ASN	N-CA-C	-7.78	103.05	112.54
2	H	523	ASN	N-CA-C	-7.75	103.09	112.54
3	C	437	ASN	N-CA-C	-7.74	103.84	113.28
2	B	523	ASN	N-CA-C	-7.71	103.14	112.54
3	F	255	GLY	N-CA-C	-7.35	104.35	114.64
3	F	10	GLU	N-CA-C	-7.33	103.22	111.14
3	C	255	GLY	N-CA-C	-7.28	104.44	114.64
3	I	255	GLY	N-CA-C	-7.27	104.46	114.64
3	C	60	SER	N-CA-C	-7.25	104.69	113.97
3	F	59	GLU	N-CA-C	-7.22	104.35	113.01
1	G	43	HIS	CB-CG-CD2	-7.12	121.94	131.20
2	B	366	PHE	N-CA-C	-7.06	104.54	113.43
3	C	365	MET	N-CA-C	-7.05	104.76	113.15
2	E	366	PHE	N-CA-C	-7.03	104.57	113.43
2	H	366	PHE	N-CA-C	-7.03	104.58	113.43
1	D	43	HIS	CB-CG-CD2	-7.01	122.08	131.20
3	C	435	PHE	N-CA-C	7.00	123.34	114.31
1	A	43	HIS	CB-CG-CD2	-6.99	122.11	131.20
3	F	382	LYS	CA-C-N	6.99	128.57	119.84
3	F	382	LYS	C-N-CA	6.99	128.57	119.84
2	B	525	HIS	CB-CG-CD2	-6.79	122.37	131.20
2	E	525	HIS	CB-CG-CD2	-6.68	122.51	131.20
3	I	289	HIS	CB-CG-CD2	-6.67	122.52	131.20
2	H	525	HIS	CB-CG-CD2	-6.67	122.53	131.20
3	I	341	HIS	CB-CG-CD2	-6.67	122.52	131.20
2	H	317	HIS	CB-CG-CD2	-6.66	122.54	131.20
3	I	10	GLU	N-CA-C	-6.62	104.51	112.59
1	A	144	HIS	CB-CG-CD2	-6.61	122.60	131.20
3	F	341	HIS	CB-CG-CD2	-6.61	122.61	131.20
2	H	254	GLN	N-CA-C	-6.60	105.05	113.23
2	B	254	GLN	N-CA-C	-6.59	105.05	113.23
1	G	95	HIS	CB-CG-CD2	-6.59	122.63	131.20
3	C	240	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	A	95	HIS	CB-CG-CD2	-6.59	122.64	131.20
3	F	225	THR	N-CA-C	6.58	119.01	111.11
3	I	240	HIS	CB-CG-CD2	-6.57	122.65	131.20
3	I	359	ILE	N-CA-C	-6.57	103.92	110.30
2	E	317	HIS	CB-CG-CD2	-6.57	122.66	131.20
3	F	289	HIS	CB-CG-CD2	-6.57	122.66	131.20
3	C	341	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	G	144	HIS	CB-CG-CD2	-6.56	122.68	131.20
2	B	317	HIS	CB-CG-CD2	-6.55	122.68	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	240	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	D	95	HIS	CB-CG-CD2	-6.55	122.69	131.20
3	C	359	ILE	N-CA-C	-6.54	103.95	110.30
3	I	391	HIS	CB-CG-CD2	-6.54	122.70	131.20
2	E	254	GLN	N-CA-C	-6.54	105.12	113.23
2	H	524	ASP	N-CA-C	-6.53	105.47	113.50
3	I	409	LYS	N-CA-C	-6.53	103.85	110.97
1	D	144	HIS	CB-CG-CD2	-6.53	122.71	131.20
2	E	524	ASP	N-CA-C	-6.53	105.47	113.50
3	C	391	HIS	CB-CG-CD2	-6.52	122.72	131.20
3	F	359	ILE	N-CA-C	-6.52	103.98	110.30
2	B	524	ASP	N-CA-C	-6.52	105.48	113.50
3	F	168	VAL	N-CA-C	6.52	116.68	110.42
3	C	225	THR	N-CA-C	6.50	118.91	111.11
3	C	409	LYS	N-CA-C	-6.49	103.90	110.97
3	C	289	HIS	CB-CG-CD2	-6.47	122.79	131.20
3	F	391	HIS	CB-CG-CD2	-6.47	122.79	131.20
3	F	409	LYS	N-CA-C	-6.46	103.92	110.97
3	I	225	THR	N-CA-C	6.46	118.86	111.11
3	I	168	VAL	N-CA-C	6.44	116.60	110.42
3	F	112	ASP	N-CA-C	6.43	119.28	111.82
2	E	467	LYS	N-CA-C	-6.43	103.55	111.33
2	B	467	LYS	N-CA-C	-6.43	103.56	111.33
3	C	168	VAL	N-CA-C	6.41	116.57	110.42
3	C	112	ASP	N-CA-C	6.40	119.24	111.82
2	H	467	LYS	N-CA-C	-6.36	103.64	111.33
3	I	112	ASP	N-CA-C	6.34	119.18	111.82
3	F	240	HIS	N-CA-C	6.33	117.85	111.07
3	C	240	HIS	N-CA-C	6.32	117.83	111.07
3	I	240	HIS	N-CA-C	6.32	117.83	111.07
2	E	392	GLY	N-CA-C	6.29	128.08	113.18
2	H	392	GLY	N-CA-C	6.27	128.05	113.18
2	E	547	TYR	N-CA-C	-6.27	106.17	113.88
2	B	392	GLY	N-CA-C	6.26	128.01	113.18
3	C	289	HIS	N-CA-C	6.26	118.90	111.71
2	B	547	TYR	N-CA-C	-6.21	106.24	113.88
2	H	547	TYR	N-CA-C	-6.20	106.25	113.88
3	I	289	HIS	N-CA-C	6.18	118.81	111.71
3	F	289	HIS	N-CA-C	6.17	118.80	111.71
2	E	345	THR	N-CA-C	-6.12	102.97	110.61
2	B	364	SER	CA-C-N	6.10	126.22	119.87
2	B	364	SER	C-N-CA	6.10	126.22	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	364	SER	CA-C-N	6.10	126.21	119.87
2	E	364	SER	C-N-CA	6.10	126.21	119.87
1	D	43	HIS	CB-CG-ND1	6.09	131.83	122.70
3	C	287	HIS	CB-CG-CD2	-6.07	123.31	131.20
2	H	364	SER	CA-C-N	6.06	126.17	119.87
2	H	364	SER	C-N-CA	6.06	126.17	119.87
3	I	287	HIS	CB-CG-CD2	-6.05	123.33	131.20
3	C	220	ASN	CA-C-N	6.05	127.40	119.84
3	C	220	ASN	C-N-CA	6.05	127.40	119.84
3	C	222	VAL	N-CA-C	6.05	116.22	110.42
3	I	202	LEU	N-CA-C	6.02	118.64	111.71
2	H	345	THR	N-CA-C	-6.02	103.08	110.61
3	I	220	ASN	CA-C-N	6.01	127.35	119.84
3	I	220	ASN	C-N-CA	6.01	127.35	119.84
3	F	287	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	G	43	HIS	CB-CG-ND1	6.00	131.70	122.70
3	F	220	ASN	CA-C-N	6.00	127.34	119.84
3	F	220	ASN	C-N-CA	6.00	127.34	119.84
2	B	345	THR	N-CA-C	-5.99	103.12	110.61
1	G	177	GLY	N-CA-C	5.99	119.97	112.79
3	F	202	LEU	N-CA-C	5.99	118.59	111.71
1	A	43	HIS	CB-CG-ND1	5.98	131.67	122.70
3	F	222	VAL	N-CA-C	5.97	116.16	110.42
1	D	177	GLY	N-CA-C	5.97	119.95	112.79
1	D	276	ASN	N-CA-C	5.95	123.48	110.80
1	A	177	GLY	N-CA-C	5.94	119.92	112.79
3	C	202	LEU	N-CA-C	5.93	118.53	111.71
1	G	276	ASN	N-CA-C	5.92	123.42	110.80
3	F	341	HIS	CA-C-N	5.92	127.24	119.84
3	F	341	HIS	C-N-CA	5.92	127.24	119.84
1	A	276	ASN	N-CA-C	5.90	123.37	110.80
3	C	69	GLU	N-CA-C	-5.90	104.76	111.07
3	I	222	VAL	N-CA-C	5.89	116.08	110.42
3	I	341	HIS	CA-C-N	5.88	127.19	119.84
3	I	341	HIS	C-N-CA	5.88	127.19	119.84
3	F	69	GLU	N-CA-C	-5.87	104.79	111.07
3	C	341	HIS	CA-C-N	5.86	127.17	119.84
3	C	341	HIS	C-N-CA	5.86	127.17	119.84
3	C	420	LEU	N-CA-C	-5.85	105.63	112.89
3	F	232	ASN	N-CA-C	-5.85	107.13	114.56
1	G	144	HIS	CB-CG-ND1	5.85	131.47	122.70
3	I	69	GLU	N-CA-C	-5.84	104.82	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	317	HIS	CB-CG-ND1	5.83	131.45	122.70
2	E	544	LYS	N-CA-C	-5.82	106.13	113.18
2	H	256	LYS	N-CA-C	-5.82	104.62	110.97
3	C	238	LYS	N-CA-C	5.82	117.30	111.07
2	H	159	LEU	N-CA-C	5.82	119.05	109.85
2	E	159	LEU	N-CA-C	5.81	119.03	109.85
2	H	525	HIS	CB-CG-ND1	5.81	131.41	122.70
2	H	544	LYS	N-CA-C	-5.80	106.16	113.18
3	I	232	ASN	N-CA-C	-5.80	107.19	114.56
3	C	293	ILE	N-CA-C	-5.79	104.86	110.42
1	G	48	THR	N-CA-C	-5.79	98.83	108.32
3	I	340	GLU	N-CA-C	5.79	118.37	111.71
2	B	525	HIS	CB-CG-ND1	5.79	131.38	122.70
3	I	238	LYS	N-CA-C	5.79	117.26	111.07
3	C	340	GLU	N-CA-C	5.78	118.36	111.71
2	B	549	GLY	N-CA-C	5.78	124.58	114.76
3	C	341	HIS	CB-CG-ND1	5.78	131.37	122.70
3	I	293	ILE	N-CA-C	-5.78	104.87	110.42
3	F	238	LYS	N-CA-C	5.77	117.24	111.07
2	E	525	HIS	CB-CG-ND1	5.76	131.35	122.70
2	H	368	GLY	N-CA-C	5.76	122.66	111.66
2	B	159	LEU	N-CA-C	5.76	118.95	109.85
1	D	48	THR	N-CA-C	-5.75	98.89	108.32
2	B	544	LYS	N-CA-C	-5.75	106.22	113.18
3	F	340	GLU	N-CA-C	5.75	118.32	111.71
3	F	341	HIS	CB-CG-ND1	5.75	131.32	122.70
1	A	48	THR	N-CA-C	-5.74	98.91	108.32
2	H	317	HIS	CB-CG-ND1	5.74	131.31	122.70
3	F	60	SER	N-CA-C	-5.74	106.24	113.18
3	F	293	ILE	N-CA-C	-5.74	104.91	110.42
3	C	232	ASN	N-CA-C	-5.73	107.28	114.56
3	F	289	HIS	CB-CG-ND1	5.72	131.28	122.70
2	E	317	HIS	CB-CG-ND1	5.72	131.28	122.70
1	D	144	HIS	CB-CG-ND1	5.72	131.28	122.70
3	I	240	HIS	CB-CG-ND1	5.72	131.28	122.70
1	G	95	HIS	CB-CG-ND1	5.69	131.24	122.70
3	F	365	MET	N-CA-C	-5.67	106.33	113.20
3	I	341	HIS	CB-CG-ND1	5.66	131.19	122.70
3	C	240	HIS	CB-CG-ND1	5.66	131.19	122.70
2	B	416	ASP	CA-C-N	5.66	126.91	119.84
2	B	416	ASP	C-N-CA	5.66	126.91	119.84
3	I	60	SER	N-CA-C	-5.64	106.07	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	313	LEU	CA-C-N	5.62	128.40	120.42
3	C	313	LEU	C-N-CA	5.62	128.40	120.42
3	I	391	HIS	CB-CG-ND1	5.61	131.11	122.70
2	B	316	GLY	N-CA-C	5.60	119.26	112.49
1	A	95	HIS	CB-CG-ND1	5.59	131.09	122.70
2	E	416	ASP	CA-C-N	5.59	126.82	119.84
2	E	416	ASP	C-N-CA	5.59	126.82	119.84
3	F	313	LEU	CA-C-N	5.58	128.34	120.42
3	F	313	LEU	C-N-CA	5.58	128.34	120.42
2	H	416	ASP	CA-C-N	5.58	126.81	119.84
2	H	416	ASP	C-N-CA	5.58	126.81	119.84
2	B	125	PHE	N-CA-C	-5.57	105.80	112.59
1	A	144	HIS	CB-CG-ND1	5.56	131.04	122.70
3	I	289	HIS	CB-CG-ND1	5.55	131.03	122.70
2	E	316	GLY	N-CA-C	5.55	119.21	112.49
3	C	391	HIS	CB-CG-ND1	5.55	131.02	122.70
3	I	313	LEU	CA-C-N	5.53	128.28	120.42
3	I	313	LEU	C-N-CA	5.53	128.28	120.42
3	F	391	HIS	CB-CG-ND1	5.53	130.99	122.70
3	F	426	TYR	N-CA-C	-5.52	105.64	112.38
3	F	240	HIS	CB-CG-ND1	5.52	130.98	122.70
3	I	59	GLU	N-CA-C	5.48	122.47	110.80
3	I	426	TYR	N-CA-C	-5.47	105.71	112.38
1	D	95	HIS	CB-CG-ND1	5.46	130.88	122.70
3	F	150	SER	N-CA-C	-5.44	106.62	113.20
3	C	426	TYR	N-CA-C	-5.42	105.77	112.38
3	C	289	HIS	CB-CG-ND1	5.38	130.77	122.70
3	C	150	SER	N-CA-C	-5.38	106.69	113.20
3	I	287	HIS	CB-CG-ND1	5.37	130.75	122.70
3	C	195	GLU	N-CA-C	-5.35	105.45	111.28
2	E	256	LYS	N-CA-C	-5.35	104.49	111.02
2	E	199	ILE	N-CA-C	5.35	116.28	108.58
3	C	218	TYR	N-CA-C	5.32	117.95	109.96
3	I	150	SER	N-CA-C	-5.32	106.76	113.20
3	F	287	HIS	CB-CG-ND1	5.30	130.66	122.70
3	F	421	LYS	N-CA-C	-5.30	104.40	111.24
3	C	287	HIS	CB-CG-ND1	5.30	130.65	122.70
3	F	162	LEU	N-CA-C	-5.29	104.94	111.40
3	I	218	TYR	N-CA-C	5.29	117.90	109.96
3	I	162	LEU	N-CA-C	-5.29	104.95	111.40
2	H	316	GLY	N-CA-C	5.27	119.52	112.77
3	C	162	LEU	N-CA-C	-5.26	104.99	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	256	LYS	N-CA-C	-5.25	104.61	111.02
2	B	199	ILE	N-CA-C	5.24	116.13	108.58
2	H	199	ILE	N-CA-C	5.24	116.13	108.58
1	G	226	SER	N-CA-C	5.23	115.19	108.34
1	A	138	PRO	N-CA-C	5.22	119.39	111.19
3	C	216	GLN	N-CA-C	5.22	118.73	109.96
1	D	138	PRO	N-CA-C	5.22	119.39	111.19
3	I	195	GLU	N-CA-C	-5.22	105.59	111.28
3	I	428	ASN	N-CA-C	5.21	119.19	112.41
2	B	551	TYR	N-CA-C	5.21	118.71	109.96
3	F	218	TYR	N-CA-C	5.21	117.77	109.96
1	D	226	SER	N-CA-C	5.20	115.15	108.34
1	A	226	SER	N-CA-C	5.20	115.15	108.34
3	C	310	THR	N-CA-C	5.20	117.62	111.33
3	C	428	ASN	N-CA-C	5.20	119.16	112.41
1	G	138	PRO	N-CA-C	5.20	119.35	111.19
3	I	216	GLN	N-CA-C	5.19	118.68	109.96
3	F	310	THR	N-CA-C	5.19	117.61	111.33
1	D	92	ILE	N-CA-C	5.17	118.37	111.44
2	E	551	TYR	N-CA-C	5.16	118.63	109.96
3	F	195	GLU	N-CA-C	-5.16	105.65	111.28
3	F	216	GLN	N-CA-C	5.16	118.63	109.96
1	G	92	ILE	N-CA-C	5.14	118.33	111.44
3	C	260	GLU	N-CA-C	-5.14	105.59	111.14
3	F	139	VAL	CA-C-N	5.14	125.38	119.83
3	F	139	VAL	C-N-CA	5.14	125.38	119.83
3	I	139	VAL	CA-C-N	5.14	125.38	119.83
3	I	139	VAL	C-N-CA	5.14	125.38	119.83
1	A	92	ILE	N-CA-C	5.13	118.32	111.44
3	I	260	GLU	N-CA-C	-5.13	105.60	111.14
3	F	428	ASN	N-CA-C	5.12	119.07	112.41
3	I	420	LEU	N-CA-C	-5.12	105.78	112.23
1	D	22	LYS	N-CA-C	-5.11	108.07	114.56
2	E	370	PHE	N-CA-C	-5.11	99.93	110.80
2	E	369	LEU	N-CA-C	5.10	115.72	108.54
3	I	310	THR	N-CA-C	5.08	117.48	111.33
1	A	65	LYS	N-CA-C	-5.08	107.14	113.19
3	F	420	LEU	N-CA-C	-5.08	105.83	112.23
1	A	22	LYS	N-CA-C	-5.07	108.12	114.56
2	H	369	LEU	N-CA-C	5.07	116.31	109.11
3	C	139	VAL	CA-C-N	5.06	125.30	119.83
3	C	139	VAL	C-N-CA	5.06	125.30	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	65	LYS	N-CA-C	-5.06	107.17	113.19
2	E	404	GLN	N-CA-C	-5.06	105.66	111.07
1	G	22	LYS	N-CA-C	-5.04	108.16	114.56
2	E	182	LYS	N-CA-C	5.03	121.52	110.80
3	I	269	GLY	N-CA-C	-5.03	107.87	115.32
2	B	182	LYS	N-CA-C	5.03	121.51	110.80
3	C	269	GLY	N-CA-C	-5.02	107.88	115.32
3	F	260	GLU	N-CA-C	-5.02	105.72	111.14
3	F	439	SER	CA-C-N	5.02	127.93	120.31
3	F	439	SER	C-N-CA	5.02	127.93	120.31
1	D	65	LYS	N-CA-C	-5.00	107.24	113.19

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	435	PHE	Mainchain
3	F	435	PHE	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2160	0	2096	250	0
1	D	2160	0	2096	237	0
1	G	2160	0	2096	239	0
2	B	3528	0	3521	327	0
2	E	3438	0	3452	314	0
2	H	3409	0	3426	334	0
3	C	3404	0	3378	264	0
3	F	3404	0	3380	264	0
3	I	3369	0	3341	260	0
All	All	27032	0	26786	2305	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 43.

All (2305) 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:E:369:LEU:HG	2:E:369:LEU:O	1.36	1.13
2:E:208:PRO:HB3	2:E:531:LYS:HB2	1.32	1.10
1:A:131:LYS:HE3	1:A:137:SER:HB2	1.38	1.06
2:H:208:PRO:HB3	2:H:531:LYS:HB2	1.32	1.06
2:B:208:PRO:HB3	2:B:531:LYS:HB2	1.32	1.05
2:H:139:MET:HG2	2:H:144:PHE:O	1.56	1.05
1:A:126:SER:HB3	1:A:140:ILE:HG13	1.38	1.04
1:D:131:LYS:HE3	1:D:137:SER:HB2	1.38	1.04
3:C:70:LEU:HD22	3:C:343:ILE:HD11	1.35	1.03
1:G:131:LYS:HE3	1:G:137:SER:HB2	1.38	1.03
2:H:136:LYS:HA	2:H:139:MET:HB3	1.40	1.02
2:H:202:ARG:HG2	2:H:209:GLN:NE2	1.75	1.02
2:E:202:ARG:HG2	2:E:209:GLN:NE2	1.75	1.02
1:A:13:HIS:CE1	2:B:144:PHE:CZ	2.47	1.01
2:B:202:ARG:HG2	2:B:209:GLN:NE2	1.75	1.01
1:A:259:ARG:NH1	2:B:150:PHE:HB2	1.76	1.00
1:D:126:SER:HB3	1:D:140:ILE:HG13	1.38	1.00
1:G:126:SER:HB3	1:G:140:ILE:HG13	1.38	1.00
3:F:70:LEU:HD22	3:F:343:ILE:HD11	1.44	0.99
3:I:8:GLN:NE2	3:I:53:LEU:HG	1.77	0.99
3:F:13:THR:O	3:F:17:ASP:HB2	1.63	0.99
2:B:198:THR:HB	2:B:212:GLU:HB2	1.44	0.98
1:G:212:TRP:HA	1:G:222:LEU:CD2	1.94	0.98
1:G:229:ARG:HH11	1:G:229:ARG:HB2	1.29	0.98
1:D:212:TRP:HA	1:D:222:LEU:CD2	1.94	0.98
1:D:229:ARG:HH11	1:D:229:ARG:HB2	1.29	0.97
1:A:212:TRP:HA	1:A:222:LEU:CD2	1.94	0.97
2:H:320:VAL:HA	3:I:246:THR:HG21	1.45	0.97
2:H:198:THR:HB	2:H:212:GLU:HB2	1.44	0.96
1:A:229:ARG:HH11	1:A:229:ARG:HB2	1.29	0.96
2:E:198:THR:HB	2:E:212:GLU:HB2	1.45	0.96
3:I:384:TYR:HA	3:I:387:ARG:HH12	1.31	0.95
3:F:341:HIS:HE1	3:F:343:ILE:HG23	1.32	0.95
3:C:341:HIS:HE1	3:C:343:ILE:HG23	1.32	0.94
3:F:384:TYR:HA	3:F:387:ARG:HH12	1.31	0.94
3:I:341:HIS:HE1	3:I:343:ILE:HG23	1.32	0.94
1:G:227:GLN:HA	1:G:256:VAL:HG13	1.50	0.94
3:C:384:TYR:HA	3:C:387:ARG:HH12	1.30	0.93
2:B:524:ASP:HA	2:B:527:LEU:HD12	1.51	0.93
1:A:227:GLN:HA	1:A:256:VAL:HG13	1.50	0.93
1:D:229:ARG:HH12	1:D:252:LYS:HD3	1.34	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:89:LEU:HD22	3:I:114:LYS:HZ1	1.32	0.93
1:G:229:ARG:HH12	1:G:252:LYS:HD3	1.34	0.93
2:E:358:TYR:HE2	3:F:210:MET:HE1	1.32	0.93
1:D:227:GLN:HA	1:D:256:VAL:HG13	1.50	0.92
2:H:524:ASP:HA	2:H:527:LEU:HD12	1.51	0.92
2:E:524:ASP:HA	2:E:527:LEU:HD12	1.50	0.92
1:D:49:LEU:HB3	1:D:82:TRP:CZ3	2.05	0.92
1:G:64:PRO:HB2	2:H:543:LEU:HD11	1.50	0.92
2:E:320:VAL:HA	3:F:246:THR:HG21	1.52	0.92
1:A:49:LEU:HB3	1:A:82:TRP:CZ3	2.06	0.92
3:F:314:ILE:HG22	3:F:315:LEU:HG	1.52	0.91
3:I:8:GLN:HE22	3:I:53:LEU:HG	1.31	0.91
1:G:49:LEU:HB3	1:G:82:TRP:CZ3	2.05	0.91
1:A:261:SER:HB2	2:B:152:LYS:HG2	1.51	0.91
1:A:20:TYR:CE2	2:B:544:LYS:HD3	2.06	0.90
3:C:314:ILE:HG22	3:C:315:LEU:HG	1.51	0.90
2:H:155:THR:HG22	2:H:513:ARG:HG3	1.52	0.90
1:A:229:ARG:HB2	1:A:229:ARG:NH1	1.87	0.90
1:A:229:ARG:HH12	1:A:252:LYS:HD3	1.34	0.90
3:C:34:ASP:HB3	3:C:35:PRO:HD3	1.54	0.89
3:C:16:SER:HA	3:C:19:LEU:HD12	1.55	0.89
3:I:314:ILE:HG22	3:I:315:LEU:HG	1.51	0.89
1:G:229:ARG:HB2	1:G:229:ARG:NH1	1.87	0.89
1:D:229:ARG:HB2	1:D:229:ARG:NH1	1.87	0.89
3:I:34:ASP:HB3	3:I:35:PRO:HD3	1.54	0.88
2:E:181:ARG:HD2	2:E:448:GLN:OE1	1.74	0.88
3:F:280:SER:HB2	3:F:284:SER:HB3	1.56	0.88
3:F:34:ASP:HB3	3:F:35:PRO:HD3	1.55	0.88
1:D:229:ARG:NH1	1:D:252:LYS:HD3	1.88	0.87
1:A:229:ARG:NH1	1:A:252:LYS:HD3	1.88	0.87
3:C:280:SER:HB2	3:C:284:SER:HB3	1.56	0.87
1:G:229:ARG:NH1	1:G:252:LYS:HD3	1.88	0.87
2:H:181:ARG:HD2	2:H:448:GLN:OE1	1.74	0.87
3:I:8:GLN:C	3:I:10:GLU:H	1.82	0.87
3:I:70:LEU:HD22	3:I:343:ILE:HD11	1.56	0.87
1:D:17:LEU:HD12	2:E:154:SER:HA	1.54	0.87
1:G:232:ILE:HG12	1:G:247:LEU:HD23	1.56	0.87
2:H:291:ILE:H	2:H:291:ILE:HD12	1.40	0.87
2:B:524:ASP:O	2:B:527:LEU:HB2	1.75	0.86
2:E:524:ASP:O	2:E:527:LEU:HB2	1.75	0.86
3:I:341:HIS:CE1	3:I:343:ILE:HG23	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:HIS:CE1	2:B:144:PHE:CE1	2.63	0.86
3:F:341:HIS:CE1	3:F:343:ILE:HG23	2.10	0.86
1:D:232:ILE:HG12	1:D:247:LEU:HD23	1.56	0.86
2:H:524:ASP:O	2:H:527:LEU:HB2	1.75	0.86
2:B:181:ARG:HD2	2:B:448:GLN:OE1	1.75	0.85
1:A:64:PRO:HB3	2:B:547:TYR:HB2	1.57	0.85
3:F:437:ASN:O	3:F:440:ASP:HB2	1.77	0.85
3:I:280:SER:HB2	3:I:284:SER:HB3	1.56	0.85
3:I:237:ILE:C	3:I:237:ILE:HD12	2.02	0.85
1:A:20:TYR:HE2	2:B:544:LYS:HD3	1.35	0.85
3:C:341:HIS:CE1	3:C:343:ILE:HG23	2.10	0.85
1:A:261:SER:CB	2:B:152:LYS:HA	2.07	0.85
2:B:291:ILE:H	2:B:291:ILE:HD12	1.41	0.84
2:E:291:ILE:H	2:E:291:ILE:HD12	1.41	0.84
1:A:232:ILE:HG12	1:A:247:LEU:HD23	1.56	0.84
3:F:237:ILE:C	3:F:237:ILE:HD12	2.03	0.84
2:B:320:VAL:HA	3:C:246:THR:HG21	1.60	0.84
3:C:237:ILE:C	3:C:237:ILE:HD12	2.03	0.84
1:D:57:TRP:HE1	2:E:142:ARG:NH2	1.75	0.83
3:C:20:LYS:O	3:C:24:ILE:HG12	1.79	0.83
2:E:434:LEU:O	2:E:438:VAL:HG23	1.78	0.83
2:H:210:ILE:HD12	2:H:210:ILE:H	1.43	0.83
2:B:434:LEU:O	2:B:438:VAL:HG23	1.78	0.83
3:I:416:TYR:HE2	3:I:432:TYR:CE2	1.97	0.83
2:B:210:ILE:H	2:B:210:ILE:HD12	1.43	0.82
1:G:64:PRO:HB2	2:H:543:LEU:CD1	2.09	0.82
1:D:25:ALA:O	1:D:59:VAL:HG21	1.79	0.82
3:C:83:VAL:O	3:C:87:ALA:HB3	1.80	0.82
1:G:25:ALA:O	1:G:59:VAL:HG21	1.79	0.82
2:H:175:LEU:HD12	2:H:176:PRO:HD2	1.63	0.81
2:H:434:LEU:O	2:H:438:VAL:HG23	1.78	0.81
3:I:13:THR:HG22	3:I:17:ASP:OD2	1.81	0.81
2:E:512:MET:HG2	2:E:540:ALA:HB2	1.62	0.81
1:G:212:TRP:HA	1:G:222:LEU:HD23	1.62	0.81
1:A:78:LYS:HA	1:A:96:ALA:HB2	1.62	0.81
3:C:13:THR:O	3:C:17:ASP:HB2	1.78	0.81
1:D:78:LYS:HA	1:D:96:ALA:HB2	1.62	0.81
2:E:340:LEU:CD2	2:E:370:PHE:CD1	2.64	0.81
2:B:190:LEU:O	2:B:194:ILE:HG13	1.81	0.81
2:B:175:LEU:HD12	2:B:176:PRO:HD2	1.63	0.81
3:F:94:MET:HE2	3:F:108:LYS:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ALA:O	1:A:59:VAL:HG21	1.79	0.80
1:G:217:LEU:HD22	1:G:218:LEU:H	1.46	0.80
3:I:89:LEU:HD13	3:I:114:LYS:CE	2.11	0.80
1:D:217:LEU:HD22	1:D:218:LEU:H	1.47	0.80
1:G:19:TYR:HD2	1:G:20:TYR:CE1	1.99	0.80
3:I:8:GLN:HE22	3:I:53:LEU:CG	1.93	0.80
1:A:12:ILE:HD12	2:B:169:GLY:HA3	1.62	0.80
2:H:340:LEU:CD2	2:H:370:PHE:CD1	2.64	0.80
2:H:512:MET:HG2	2:H:540:ALA:HB2	1.61	0.80
1:A:19:TYR:HD2	1:A:20:TYR:CE1	1.98	0.80
2:B:442:THR:HG22	2:B:444:ALA:H	1.46	0.80
2:H:136:LYS:HA	2:H:139:MET:CB	2.11	0.80
1:G:78:LYS:HA	1:G:96:ALA:HB2	1.62	0.80
2:H:155:THR:O	2:H:513:ARG:HD2	1.80	0.80
2:H:442:THR:HG22	2:H:444:ALA:H	1.46	0.80
3:I:59:GLU:HA	3:I:62:VAL:HG23	1.62	0.80
1:D:19:TYR:HD2	1:D:20:TYR:CE1	1.99	0.80
2:E:175:LEU:HD12	2:E:176:PRO:HD2	1.63	0.79
2:E:210:ILE:HD12	2:E:210:ILE:H	1.43	0.79
2:B:512:MET:HG2	2:B:540:ALA:HB2	1.61	0.79
2:B:210:ILE:CD1	2:B:495:CYS:HB2	2.12	0.79
2:H:190:LEU:O	2:H:194:ILE:HG13	1.81	0.79
2:H:210:ILE:CD1	2:H:495:CYS:HB2	2.12	0.79
3:I:89:LEU:HD13	3:I:114:LYS:NZ	1.96	0.79
1:G:65:LYS:HA	2:H:546:ARG:NH2	1.97	0.79
2:E:210:ILE:CD1	2:E:495:CYS:HB2	2.12	0.79
2:E:442:THR:HG22	2:E:444:ALA:H	1.46	0.79
1:D:212:TRP:HA	1:D:222:LEU:HD23	1.62	0.79
2:H:265:HIS:HB2	2:H:399:LEU:HD21	1.64	0.79
1:G:278:VAL:HG21	2:H:151:ALA:HB3	1.64	0.78
3:I:416:TYR:CE2	3:I:432:TYR:CE2	2.71	0.78
2:E:190:LEU:O	2:E:194:ILE:HG13	1.81	0.78
2:E:265:HIS:HB2	2:E:399:LEU:HD21	1.65	0.78
3:F:416:TYR:CE2	3:F:432:TYR:CE2	2.71	0.78
3:I:419:LEU:HD23	3:I:422:LEU:HD12	1.65	0.78
3:C:20:LYS:HG2	3:C:431:ILE:CG1	2.14	0.78
2:E:320:VAL:HG22	3:F:246:THR:HG22	1.65	0.78
1:A:29:SER:HA	1:A:55:PRO:HB3	1.66	0.78
1:A:217:LEU:HD22	1:A:218:LEU:H	1.47	0.78
3:F:108:LYS:HE3	3:F:112:ASP:OD2	1.83	0.78
3:C:108:LYS:HE3	3:C:112:ASP:OD2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:358:TYR:CE2	3:F:210:MET:HE1	2.18	0.77
2:H:320:VAL:HG22	3:I:246:THR:HG22	1.64	0.77
1:G:29:SER:HA	1:G:55:PRO:HB3	1.66	0.77
2:B:265:HIS:HB2	2:B:399:LEU:HD21	1.64	0.77
1:D:29:SER:HA	1:D:55:PRO:HB3	1.66	0.77
1:A:63:HIS:HD2	1:A:65:LYS:HB2	1.50	0.77
3:C:74:PHE:O	3:C:78:VAL:HG23	1.85	0.77
2:H:524:ASP:HA	2:H:527:LEU:CD1	2.15	0.77
2:B:522:THR:HA	2:B:525:HIS:HB2	1.66	0.77
3:C:8:GLN:C	3:C:10:GLU:H	1.92	0.77
1:G:131:LYS:CE	1:G:137:SER:HB2	2.15	0.77
1:A:212:TRP:HA	1:A:222:LEU:HD23	1.62	0.77
2:B:524:ASP:HA	2:B:527:LEU:CD1	2.15	0.77
3:F:74:PHE:O	3:F:78:VAL:HG23	1.84	0.76
3:I:108:LYS:HE3	3:I:112:ASP:OD2	1.83	0.76
1:A:131:LYS:CE	1:A:137:SER:HB2	2.15	0.76
2:E:524:ASP:HA	2:E:527:LEU:CD1	2.15	0.76
3:F:416:TYR:HE2	3:F:432:TYR:CE2	2.02	0.76
2:H:522:THR:HA	2:H:525:HIS:HB2	1.66	0.76
2:E:522:THR:HA	2:E:525:HIS:HB2	1.66	0.76
3:I:74:PHE:O	3:I:78:VAL:HG23	1.85	0.76
1:A:225:VAL:HG13	1:A:257:LEU:HB2	1.67	0.75
3:C:116:LEU:HD21	3:C:294:LEU:HD11	1.69	0.75
1:A:208:ARG:NH2	2:B:143:ARG:HB2	2.01	0.75
1:D:131:LYS:CE	1:D:137:SER:HB2	2.15	0.75
3:C:18:THR:HG23	3:C:41:GLU:OE1	1.86	0.75
3:I:269:GLY:HA3	3:I:295:GLN:HG2	1.68	0.75
3:C:94:MET:HE2	3:C:108:LYS:HB2	1.69	0.74
3:C:269:GLY:HA3	3:C:295:GLN:HG2	1.68	0.74
1:D:275:ASP:O	1:D:276:ASN:HB2	1.86	0.74
1:G:259:ARG:HD2	2:H:152:LYS:HE3	1.69	0.74
2:B:165:VAL:HG12	2:B:165:VAL:O	1.84	0.74
3:F:269:GLY:HA3	3:F:295:GLN:HG2	1.69	0.74
2:B:155:THR:HG22	2:B:513:ARG:HD2	1.69	0.74
2:H:523:ASN:O	2:H:527:LEU:HG	1.87	0.74
3:I:116:LEU:HD21	3:I:294:LEU:HD11	1.69	0.74
2:E:340:LEU:HD22	2:E:370:PHE:CD1	2.23	0.74
1:D:225:VAL:HG13	1:D:257:LEU:HB2	1.67	0.74
1:G:10:GLU:O	1:G:11:LEU:HG	1.88	0.74
1:G:285:LEU:H	1:G:285:LEU:HD12	1.53	0.74
3:C:11:ARG:CG	3:C:12:PHE:N	2.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:LEU:CD2	2:E:170:VAL:HG21	2.18	0.74
2:E:207:TYR:CE1	2:E:504:GLU:HG3	2.23	0.74
2:E:369:LEU:O	2:E:369:LEU:CG	2.23	0.74
2:H:207:TYR:CE1	2:H:504:GLU:HG3	2.23	0.74
1:A:285:LEU:H	1:A:285:LEU:HD12	1.53	0.74
1:D:10:GLU:O	1:D:11:LEU:HG	1.88	0.74
2:E:523:ASN:O	2:E:527:LEU:HG	1.88	0.74
1:A:275:ASP:O	1:A:276:ASN:HB2	1.86	0.73
1:D:285:LEU:H	1:D:285:LEU:HD12	1.53	0.73
1:G:225:VAL:HG13	1:G:257:LEU:HB2	1.67	0.73
1:G:275:ASP:O	1:G:276:ASN:HB2	1.86	0.73
1:G:265:SER:HB2	2:H:509:ARG:HH22	1.52	0.73
3:I:293:ILE:HD11	3:I:327:VAL:HG21	1.70	0.73
1:D:57:TRP:NE1	2:E:142:ARG:NH2	2.35	0.73
2:B:512:MET:HA	2:B:540:ALA:HB1	1.69	0.73
3:C:384:TYR:HA	3:C:387:ARG:NH1	2.04	0.73
2:H:512:MET:HA	2:H:540:ALA:HB1	1.69	0.73
2:B:207:TYR:CE1	2:B:504:GLU:HG3	2.23	0.73
2:H:530:LEU:O	2:H:531:LYS:HG2	1.89	0.73
1:A:180:ASN:HA	1:A:207:VAL:HG23	1.71	0.73
3:F:116:LEU:HD21	3:F:294:LEU:HD11	1.68	0.73
3:F:227:ILE:C	3:F:229:ASN:H	1.96	0.73
1:G:17:LEU:HD12	2:H:154:SER:HA	1.70	0.73
2:H:340:LEU:HD23	2:H:370:PHE:CD1	2.24	0.73
2:B:442:THR:HG22	2:B:443:ASN:N	2.04	0.73
2:B:523:ASN:O	2:B:527:LEU:HG	1.88	0.73
3:C:227:ILE:C	3:C:229:ASN:H	1.96	0.73
3:F:293:ILE:HD11	3:F:327:VAL:HG21	1.70	0.73
1:G:180:ASN:HA	1:G:207:VAL:HG23	1.71	0.73
2:B:530:LEU:O	2:B:531:LYS:HG2	1.89	0.72
2:E:512:MET:HA	2:E:540:ALA:HB1	1.69	0.72
2:H:167:LYS:O	2:H:167:LYS:HD3	1.89	0.72
3:C:11:ARG:HG2	3:C:12:PHE:H	1.54	0.72
2:E:320:VAL:CA	3:F:246:THR:HG21	2.19	0.72
2:B:167:LYS:O	2:B:167:LYS:HD3	1.89	0.72
2:E:507:ILE:O	2:E:511:VAL:HG23	1.90	0.72
3:C:139:VAL:HG13	3:C:140:PRO:HD2	1.72	0.72
2:H:136:LYS:CA	2:H:139:MET:HB3	2.18	0.72
2:H:162:LYS:CE	2:H:164:ILE:HD11	2.20	0.72
1:A:103:ASN:OD1	2:B:142:ARG:NH2	2.22	0.72
2:E:162:LYS:CE	2:E:164:ILE:HD11	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:167:LYS:O	2:E:167:LYS:HD3	1.89	0.72
2:E:530:LEU:O	2:E:531:LYS:HG2	1.90	0.72
2:B:358:TYR:HE2	3:C:210:MET:HE1	1.55	0.72
1:G:138:PRO:HB2	1:G:140:ILE:HD11	1.72	0.72
1:A:261:SER:HB3	2:B:152:LYS:HA	1.72	0.72
3:C:20:LYS:HG2	3:C:431:ILE:HG12	1.70	0.72
3:C:293:ILE:HD11	3:C:327:VAL:HG21	1.71	0.72
2:E:442:THR:HG22	2:E:443:ASN:N	2.04	0.72
3:F:406:GLU:HA	3:F:409:LYS:HE3	1.72	0.72
2:B:187:ASP:HB3	2:B:523:ASN:ND2	2.05	0.71
3:C:8:GLN:O	3:C:10:GLU:N	2.23	0.71
3:I:384:TYR:HA	3:I:387:ARG:NH1	2.04	0.71
1:D:180:ASN:HA	1:D:207:VAL:HG23	1.71	0.71
2:E:494:SER:O	2:E:497:LEU:HD13	1.90	0.71
3:I:89:LEU:HD13	3:I:114:LYS:HE2	1.71	0.71
3:I:406:GLU:HA	3:I:409:LYS:HE3	1.72	0.71
3:F:7:TYR:O	3:F:9:THR:N	2.23	0.71
2:B:204:SER:O	2:B:205:ASN:HB3	1.91	0.71
2:B:507:ILE:O	2:B:511:VAL:HG23	1.90	0.71
3:C:20:LYS:NZ	3:C:428:ASN:OD1	2.23	0.71
2:E:187:ASP:HB3	2:E:523:ASN:ND2	2.05	0.71
3:I:227:ILE:C	3:I:229:ASN:H	1.96	0.71
3:C:8:GLN:HE22	3:C:53:LEU:HG	1.54	0.71
2:E:160:LEU:HD23	2:E:171:SER:O	1.91	0.71
3:F:139:VAL:HG13	3:F:140:PRO:HD2	1.72	0.71
3:F:384:TYR:HA	3:F:387:ARG:NH1	2.04	0.71
2:H:442:THR:HG22	2:H:443:ASN:N	2.04	0.71
2:H:507:ILE:O	2:H:511:VAL:HG23	1.90	0.71
3:I:139:VAL:HG13	3:I:140:PRO:HD2	1.72	0.71
3:I:385:LEU:O	3:I:389:VAL:HG23	1.91	0.71
3:F:350:VAL:HG22	3:F:355:LEU:HD22	1.73	0.71
2:H:187:ASP:HB3	2:H:523:ASN:ND2	2.05	0.71
1:A:259:ARG:HH12	2:B:150:PHE:HB2	1.55	0.71
3:C:93:GLU:HG3	3:C:94:MET:N	2.06	0.71
1:G:57:TRP:HE1	2:H:142:ARG:HH21	1.37	0.71
3:I:11:ARG:HG3	3:I:12:PHE:CD1	2.26	0.71
2:B:158:MET:HB2	2:B:173:LYS:O	1.91	0.71
2:E:159:LEU:HD13	2:E:160:LEU:H	1.56	0.71
3:C:350:VAL:HG22	3:C:355:LEU:HD22	1.73	0.70
1:D:138:PRO:HB2	1:D:140:ILE:HD11	1.72	0.70
1:G:126:SER:CB	1:G:140:ILE:HG13	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:204:SER:O	2:H:205:ASN:HB3	1.91	0.70
1:D:17:LEU:HD21	2:E:160:LEU:HD11	1.72	0.70
2:H:494:SER:O	2:H:497:LEU:HD13	1.91	0.70
3:I:409:LYS:O	3:I:413:ILE:HG13	1.91	0.70
1:A:83:LYS:HD3	1:A:92:ILE:HD12	1.73	0.70
2:B:494:SER:O	2:B:497:LEU:HD13	1.90	0.70
2:B:160:LEU:HD23	2:B:171:SER:O	1.91	0.70
1:D:217:LEU:HD13	1:D:218:LEU:N	2.07	0.70
3:I:350:VAL:HG22	3:I:355:LEU:HD22	1.73	0.70
1:A:138:PRO:HB2	1:A:140:ILE:HD11	1.72	0.70
2:E:521:SER:O	2:E:524:ASP:HB2	1.92	0.70
3:F:327:VAL:O	3:F:331:VAL:HG23	1.92	0.70
2:H:158:MET:HB2	2:H:173:LYS:O	1.91	0.70
3:I:293:ILE:HD11	3:I:327:VAL:CG2	2.21	0.70
2:B:521:SER:O	2:B:524:ASP:HB2	1.92	0.70
2:H:267:ARG:HH11	2:H:267:ARG:HG3	1.56	0.70
3:I:70:LEU:HD21	3:I:344:ARG:NH1	2.05	0.70
3:C:11:ARG:CG	3:C:12:PHE:H	2.04	0.70
3:C:406:GLU:HA	3:C:409:LYS:HE3	1.72	0.70
3:C:435:PHE:O	3:C:436:LEU:HD23	1.92	0.70
2:E:204:SER:O	2:E:205:ASN:HB3	1.91	0.70
3:C:385:LEU:O	3:C:389:VAL:HG23	1.91	0.70
2:E:327:SER:OG	3:F:238:LYS:HG3	1.91	0.70
2:E:391:TYR:O	2:E:393:GLN:N	2.25	0.70
1:G:217:LEU:HD13	1:G:218:LEU:N	2.07	0.70
3:I:434:THR:O	3:I:434:THR:HG22	1.91	0.70
1:A:126:SER:CB	1:A:140:ILE:HG13	2.21	0.70
2:B:159:LEU:HD13	2:B:160:LEU:H	1.56	0.70
3:C:409:LYS:O	3:C:413:ILE:HG13	1.91	0.70
2:H:533:PRO:O	2:H:537:ILE:HG13	1.92	0.70
3:I:327:VAL:O	3:I:331:VAL:HG23	1.92	0.70
2:E:267:ARG:HH11	2:E:267:ARG:HG3	1.56	0.69
2:E:299:LEU:HD23	2:E:387:LEU:HD21	1.74	0.69
2:E:544:LYS:O	2:E:548:GLU:HG3	1.92	0.69
3:F:293:ILE:HD11	3:F:327:VAL:CG2	2.22	0.69
2:H:521:SER:O	2:H:524:ASP:HB2	1.92	0.69
1:A:20:TYR:HD2	2:B:544:LYS:HZ2	1.38	0.69
1:A:217:LEU:HD13	1:A:218:LEU:N	2.07	0.69
2:B:533:PRO:O	2:B:537:ILE:HG13	1.92	0.69
3:C:382:LYS:HD3	3:C:384:TYR:OH	1.92	0.69
2:E:158:MET:HB2	2:E:173:LYS:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:409:LYS:O	3:F:413:ILE:HG13	1.91	0.69
3:F:385:LEU:O	3:F:389:VAL:HG23	1.91	0.69
2:H:159:LEU:HD13	2:H:160:LEU:H	1.56	0.69
2:H:544:LYS:O	2:H:548:GLU:HG3	1.92	0.69
1:A:12:ILE:HD13	2:B:168:SER:O	1.92	0.69
1:A:262:TRP:O	2:B:153:PHE:HB2	1.92	0.69
3:F:8:GLN:C	3:F:10:GLU:H	2.00	0.69
2:H:155:THR:HG22	2:H:513:ARG:CG	2.22	0.69
3:C:327:VAL:O	3:C:331:VAL:HG23	1.91	0.69
1:G:83:LYS:HD3	1:G:92:ILE:HD12	1.73	0.69
1:A:24:LEU:HD21	2:B:170:VAL:HG21	1.73	0.69
3:C:70:LEU:CD2	3:C:343:ILE:HD11	2.20	0.69
1:D:83:LYS:HD3	1:D:92:ILE:HD12	1.73	0.69
2:E:533:PRO:O	2:E:537:ILE:HG13	1.92	0.69
1:G:77:GLY:HA2	1:G:100:ALA:O	1.93	0.69
2:H:160:LEU:HD23	2:H:171:SER:O	1.91	0.69
3:I:23:LYS:NZ	3:I:434:THR:OG1	2.25	0.69
3:F:363:VAL:HG11	3:F:408:ASP:OD1	1.92	0.69
3:F:434:THR:O	3:F:434:THR:HG22	1.92	0.69
3:I:21:GLU:HB3	3:I:25:GLU:OE1	1.93	0.69
2:B:544:LYS:O	2:B:548:GLU:HG3	1.92	0.69
3:C:434:THR:O	3:C:434:THR:HG22	1.92	0.69
1:A:77:GLY:HA2	1:A:100:ALA:O	1.93	0.68
2:B:491:LEU:HD11	2:B:507:ILE:HG23	1.75	0.68
2:H:287:SER:OG	2:H:293:GLN:HG2	1.93	0.68
2:H:299:LEU:HD23	2:H:387:LEU:HD21	1.74	0.68
2:H:457:LEU:HD13	2:H:463:ARG:HB2	1.76	0.68
3:I:102:ARG:HD3	3:I:302:LEU:HD13	1.76	0.68
2:E:457:LEU:HD13	2:E:463:ARG:HB2	1.75	0.68
1:G:35:ILE:HB	1:G:47:ASP:HB2	1.75	0.68
2:H:391:TYR:O	2:H:393:GLN:N	2.26	0.68
3:I:435:PHE:O	3:I:436:LEU:HG	1.92	0.68
2:B:267:ARG:HH11	2:B:267:ARG:HG3	1.56	0.68
2:B:457:LEU:HD13	2:B:463:ARG:HB2	1.76	0.68
3:C:293:ILE:HD11	3:C:327:VAL:CG2	2.22	0.68
2:E:491:LEU:HD11	2:E:507:ILE:HG23	1.75	0.68
1:D:35:ILE:HB	1:D:47:ASP:HB2	1.75	0.68
1:D:77:GLY:HA2	1:D:100:ALA:O	1.93	0.68
2:E:329:ASP:OD2	3:F:236:GLY:N	2.25	0.68
3:F:319:SER:OG	2:H:337:GLU:HG2	1.94	0.68
3:F:438:GLU:C	3:F:440:ASP:H	2.00	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:SER:OG	2:B:293:GLN:HG2	1.93	0.68
2:B:314:LYS:HG2	3:C:162:LEU:O	1.94	0.68
1:G:20:TYR:CE2	2:H:544:LYS:HD3	2.29	0.68
2:B:391:TYR:O	2:B:393:GLN:N	2.26	0.67
2:H:418:ILE:H	2:H:418:ILE:HD13	1.59	0.67
3:C:8:GLN:NE2	3:C:53:LEU:HG	2.10	0.67
3:F:102:ARG:HD3	3:F:302:LEU:HD13	1.76	0.67
2:E:202:ARG:HG3	2:E:500:ASP:OD1	1.95	0.67
1:A:63:HIS:HD2	1:A:65:LYS:CB	2.08	0.67
2:B:299:LEU:HD23	2:B:387:LEU:HD21	1.75	0.67
2:B:418:ILE:HD13	2:B:418:ILE:H	1.60	0.67
2:E:287:SER:OG	2:E:293:GLN:HG2	1.93	0.67
3:F:438:GLU:OE1	3:F:438:GLU:HA	1.94	0.67
2:H:340:LEU:HD22	2:H:370:PHE:CD1	2.29	0.67
3:C:171:VAL:O	3:C:175:GLU:HG3	1.94	0.67
1:G:200:LEU:HD13	1:G:234:TRP:CE3	2.30	0.67
3:I:417:ILE:HG23	3:I:429:ILE:HG23	1.76	0.67
2:E:142:ARG:C	2:E:143:ARG:HG2	2.19	0.66
3:F:91:LEU:HG	3:F:92:ASP:H	1.60	0.66
2:H:320:VAL:CA	3:I:246:THR:HG21	2.23	0.66
1:A:35:ILE:HB	1:A:47:ASP:HB2	1.75	0.66
2:B:153:PHE:HA	2:B:159:LEU:HD22	1.77	0.66
2:B:320:VAL:HG22	3:C:246:THR:HG22	1.76	0.66
3:C:83:VAL:O	3:C:87:ALA:CB	2.43	0.66
1:D:200:LEU:HD13	1:D:234:TRP:CE3	2.30	0.66
2:E:354:ILE:HD13	3:F:157:ASP:CG	2.20	0.66
2:E:549:GLY:O	2:E:551:TYR:N	2.28	0.66
3:F:171:VAL:O	3:F:175:GLU:HG3	1.95	0.66
2:B:202:ARG:HG3	2:B:500:ASP:OD1	1.94	0.66
1:G:78:LYS:HA	1:G:96:ALA:CB	2.25	0.66
1:A:200:LEU:HD13	1:A:234:TRP:CE3	2.30	0.66
2:B:476:ALA:O	2:B:480:GLN:HG2	1.95	0.66
1:D:38:VAL:O	1:D:39:GLU:HG3	1.95	0.66
2:H:491:LEU:HD11	2:H:507:ILE:HG23	1.75	0.66
2:E:418:ILE:HD13	2:E:418:ILE:H	1.59	0.66
2:H:442:THR:HG22	2:H:443:ASN:H	1.60	0.66
2:H:476:ALA:O	2:H:480:GLN:HG2	1.95	0.66
3:I:77:LEU:HD12	3:I:125:TRP:CH2	2.31	0.66
1:G:217:LEU:HD13	1:G:218:LEU:H	1.61	0.66
1:A:217:LEU:HD13	1:A:218:LEU:H	1.61	0.66
2:B:178:GLU:HB2	2:B:480:GLN:OE1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:SER:O	2:B:329:ASP:N	2.29	0.66
2:B:416:ASP:O	2:B:420:VAL:HG23	1.95	0.66
2:H:202:ARG:HG3	2:H:500:ASP:OD1	1.95	0.66
2:H:347:GLY:O	2:H:349:SER:N	2.29	0.66
2:H:416:ASP:O	2:H:420:VAL:HG23	1.95	0.66
3:C:24:ILE:O	3:C:24:ILE:HG22	1.94	0.66
2:E:175:LEU:HD12	2:E:176:PRO:CD	2.26	0.66
2:E:327:SER:HA	3:F:238:LYS:HE3	1.76	0.66
3:F:34:ASP:HB3	3:F:35:PRO:CD	2.26	0.66
2:H:178:GLU:HB2	2:H:480:GLN:OE1	1.95	0.66
2:E:442:THR:HG22	2:E:443:ASN:H	1.61	0.66
1:G:38:VAL:O	1:G:39:GLU:HG3	1.95	0.66
2:H:155:THR:CG2	2:H:513:ARG:HG3	2.25	0.66
2:H:159:LEU:CD1	2:H:160:LEU:H	2.09	0.66
3:I:171:VAL:O	3:I:175:GLU:HG3	1.94	0.66
3:I:382:LYS:N	3:I:383:PRO:CD	2.58	0.66
1:A:83:LYS:HD3	1:A:92:ILE:CD1	2.26	0.65
3:C:102:ARG:HD3	3:C:302:LEU:HD13	1.77	0.65
1:G:284:ASN:OD1	1:G:286:GLU:HB2	1.96	0.65
2:H:136:LYS:HE3	2:H:139:MET:SD	2.36	0.65
2:H:162:LYS:HE2	2:H:164:ILE:HD11	1.78	0.65
3:I:89:LEU:HD13	3:I:114:LYS:HZ3	1.61	0.65
2:B:347:GLY:O	2:B:349:SER:N	2.29	0.65
2:E:314:LYS:HG3	3:F:162:LEU:HB3	1.78	0.65
2:E:347:GLY:O	2:E:349:SER:N	2.29	0.65
1:A:284:ASN:OD1	1:A:286:GLU:HB2	1.96	0.65
2:B:159:LEU:CD1	2:B:160:LEU:H	2.09	0.65
2:B:512:MET:O	2:B:514:GLU:N	2.29	0.65
1:D:57:TRP:HE1	2:E:142:ARG:HH21	1.43	0.65
1:D:78:LYS:HA	1:D:96:ALA:CB	2.25	0.65
2:E:178:GLU:HB2	2:E:480:GLN:OE1	1.95	0.65
1:G:229:ARG:HH12	1:G:252:LYS:CD	2.09	0.65
2:H:153:PHE:HA	2:H:159:LEU:HD22	1.77	0.65
3:I:34:ASP:HB3	3:I:35:PRO:CD	2.25	0.65
1:A:78:LYS:HA	1:A:96:ALA:CB	2.25	0.65
2:B:442:THR:HG22	2:B:443:ASN:H	1.61	0.65
2:E:476:ALA:O	2:E:480:GLN:HG2	1.95	0.65
1:A:38:VAL:O	1:A:39:GLU:HG3	1.95	0.65
1:G:20:TYR:HE2	2:H:544:LYS:HD3	1.62	0.65
1:D:284:ASN:OD1	1:D:286:GLU:HB2	1.96	0.65
1:G:265:SER:HB2	2:H:509:ARG:NH2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:512:MET:O	2:H:514:GLU:N	2.29	0.65
3:C:11:ARG:HG2	3:C:12:PHE:CD1	2.32	0.65
1:D:49:LEU:HD13	1:D:82:TRP:CE3	2.32	0.65
2:E:159:LEU:CD1	2:E:160:LEU:H	2.09	0.65
2:H:175:LEU:HD12	2:H:176:PRO:CD	2.26	0.65
1:D:83:LYS:HD3	1:D:92:ILE:CD1	2.26	0.65
1:G:19:TYR:OH	2:H:512:MET:HE3	1.97	0.65
1:G:49:LEU:HD13	1:G:82:TRP:CE3	2.32	0.65
1:A:205:ASP:HB3	1:A:227:GLN:HB3	1.79	0.65
1:D:229:ARG:HH12	1:D:252:LYS:CD	2.09	0.65
2:E:512:MET:O	2:E:514:GLU:N	2.29	0.64
1:G:83:LYS:HD3	1:G:92:ILE:CD1	2.27	0.64
2:H:392:GLY:O	2:H:393:GLN:CB	2.45	0.64
1:A:229:ARG:HH12	1:A:252:LYS:CD	2.10	0.64
2:B:177:THR:HG21	2:B:484:ALA:HB2	1.79	0.64
2:B:392:GLY:O	2:B:393:GLN:CB	2.46	0.64
1:D:24:LEU:HD21	2:E:170:VAL:HG21	1.77	0.64
3:F:416:TYR:CE2	3:F:432:TYR:HE2	2.15	0.64
3:C:429:ILE:N	3:C:430:PRO:CD	2.60	0.64
2:E:327:SER:O	2:E:329:ASP:N	2.29	0.64
2:E:416:ASP:O	2:E:420:VAL:HG23	1.96	0.64
3:I:58:ASP:HB3	3:I:61:ASN:OD1	1.97	0.64
3:I:429:ILE:N	3:I:430:PRO:CD	2.59	0.64
3:C:364:GLU:C	3:C:366:LEU:H	2.05	0.64
1:D:57:TRP:CZ2	2:E:142:ARG:HG2	2.32	0.64
1:D:217:LEU:HD22	1:D:218:LEU:N	2.12	0.64
2:E:153:PHE:HA	2:E:159:LEU:HD22	1.77	0.64
2:E:320:VAL:CG2	3:F:246:THR:HG22	2.26	0.64
3:F:429:ILE:N	3:F:430:PRO:CD	2.60	0.64
2:E:392:GLY:O	2:E:393:GLN:CB	2.46	0.64
3:F:20:LYS:HE2	3:F:431:ILE:HD11	1.79	0.64
1:A:140:ILE:HG22	1:A:141:ILE:N	2.13	0.64
2:B:175:LEU:HD12	2:B:176:PRO:CD	2.26	0.64
2:H:259:LEU:HD11	3:I:99:TYR:CD1	2.33	0.64
3:C:77:LEU:O	3:C:77:LEU:HD23	1.98	0.64
1:D:140:ILE:HG22	1:D:141:ILE:N	2.13	0.64
3:F:437:ASN:O	3:F:440:ASP:CB	2.45	0.64
1:A:229:ARG:HH11	1:A:229:ARG:CB	2.09	0.64
2:B:221:LEU:HD22	2:B:231:TYR:CE1	2.32	0.64
1:D:208:ARG:NH2	2:E:143:ARG:HG3	2.12	0.64
3:F:431:ILE:CD1	3:F:431:ILE:H	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:431:ILE:HD12	3:I:431:ILE:N	2.13	0.64
1:A:49:LEU:HD13	1:A:82:TRP:CE3	2.32	0.64
2:E:162:LYS:HE2	2:E:164:ILE:HD11	1.78	0.64
1:G:140:ILE:HG22	1:G:141:ILE:N	2.13	0.64
2:H:252:ASN:OD1	2:H:253:ASP:N	2.31	0.64
2:H:320:VAL:HA	3:I:246:THR:CG2	2.23	0.64
1:A:17:LEU:HD21	2:B:160:LEU:HD11	1.79	0.64
1:A:144:HIS:HB2	1:A:148:VAL:HG22	1.80	0.64
3:C:431:ILE:N	3:C:431:ILE:HD12	2.13	0.64
3:F:438:GLU:C	3:F:440:ASP:N	2.54	0.64
3:I:8:GLN:HE22	3:I:53:LEU:CD2	2.11	0.64
1:D:126:SER:CB	1:D:140:ILE:HG13	2.20	0.63
1:D:286:GLU:HG2	2:E:440:GLN:OE1	1.97	0.63
2:H:327:SER:O	2:H:329:ASP:N	2.29	0.63
2:E:210:ILE:HD11	2:E:495:CYS:HB2	1.79	0.63
2:E:221:LEU:HD22	2:E:231:TYR:CE1	2.33	0.63
2:H:202:ARG:HG2	2:H:209:GLN:HE22	1.63	0.63
1:D:205:ASP:HB3	1:D:227:GLN:HB3	1.79	0.63
3:C:20:LYS:HG2	3:C:431:ILE:HG13	1.79	0.63
1:D:227:GLN:OE1	1:D:256:VAL:HG11	1.99	0.63
3:F:77:LEU:O	3:F:77:LEU:HD23	1.98	0.63
1:G:65:LYS:HA	2:H:546:ARG:HH21	1.64	0.63
2:H:156:GLY:O	2:H:158:MET:HE2	1.99	0.63
3:I:62:VAL:HG12	3:I:66:LYS:HE3	1.80	0.63
2:E:252:ASN:OD1	2:E:253:ASP:N	2.31	0.63
1:G:105:VAL:HG13	1:G:105:VAL:O	1.99	0.63
1:G:205:ASP:HB3	1:G:227:GLN:HB3	1.79	0.63
3:I:431:ILE:CD1	3:I:431:ILE:H	2.11	0.63
3:C:62:VAL:HG12	3:C:66:LYS:HE3	1.80	0.63
2:E:521:SER:HB2	2:E:523:ASN:OD1	1.99	0.63
2:H:259:LEU:HD23	3:I:223:ILE:HD13	1.80	0.63
3:I:387:ARG:HB3	3:I:387:ARG:HH11	1.63	0.63
1:A:217:LEU:HD22	1:A:218:LEU:N	2.12	0.63
3:C:116:LEU:HD21	3:C:294:LEU:CD1	2.29	0.63
3:C:416:TYR:HE2	3:C:432:TYR:CE2	2.17	0.63
3:C:431:ILE:CD1	3:C:431:ILE:H	2.11	0.63
1:D:217:LEU:HD13	1:D:218:LEU:H	1.60	0.63
2:E:515:ILE:HD13	2:E:540:ALA:C	2.23	0.63
3:F:431:ILE:HD12	3:F:431:ILE:N	2.13	0.63
2:H:210:ILE:HD11	2:H:495:CYS:HB2	1.80	0.63
3:I:77:LEU:O	3:I:77:LEU:HD23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:416:TYR:CE2	3:I:432:TYR:HE2	2.16	0.63
2:E:202:ARG:HG2	2:E:209:GLN:HE22	1.63	0.63
3:F:387:ARG:HB3	3:F:387:ARG:HH11	1.64	0.63
1:G:55:PRO:HB2	1:G:57:TRP:CZ3	2.34	0.63
2:H:221:LEU:HD22	2:H:231:TYR:CE1	2.33	0.63
2:H:521:SER:HB2	2:H:523:ASN:OD1	1.99	0.63
2:B:515:ILE:HD13	2:B:540:ALA:C	2.23	0.63
3:C:20:LYS:HE2	3:C:431:ILE:CD1	2.29	0.63
1:D:105:VAL:HG13	1:D:105:VAL:O	1.99	0.63
1:A:55:PRO:HB2	1:A:57:TRP:CZ3	2.34	0.62
1:A:73:CYS:HB2	1:A:102:VAL:HG12	1.81	0.62
3:C:387:ARG:HB3	3:C:387:ARG:HH11	1.63	0.62
3:F:102:ARG:HD2	3:F:217:GLU:OE2	1.99	0.62
1:G:73:CYS:HB2	1:G:102:VAL:HG12	1.81	0.62
1:G:227:GLN:OE1	1:G:256:VAL:HG11	1.99	0.62
2:B:252:ASN:OD1	2:B:253:ASP:N	2.31	0.62
1:D:55:PRO:HB2	1:D:57:TRP:CZ3	2.34	0.62
2:E:156:GLY:O	2:E:158:MET:HE2	1.99	0.62
1:G:144:HIS:HB2	1:G:148:VAL:HG22	1.80	0.62
1:G:282:LYS:HE2	1:G:292:ALA:HB2	1.80	0.62
3:I:8:GLN:CD	3:I:53:LEU:HG	2.22	0.62
2:B:521:SER:HB2	2:B:523:ASN:OD1	1.99	0.62
1:G:64:PRO:CB	2:H:543:LEU:HD11	2.29	0.62
1:G:217:LEU:HD22	1:G:218:LEU:N	2.12	0.62
1:G:278:VAL:HG21	2:H:151:ALA:CB	2.29	0.62
2:H:515:ILE:HD13	2:H:540:ALA:C	2.24	0.62
1:A:259:ARG:NH1	2:B:150:PHE:CB	2.60	0.62
3:C:70:LEU:HB3	3:C:343:ILE:CD1	2.30	0.62
1:D:217:LEU:CD2	1:D:218:LEU:H	2.13	0.62
3:F:62:VAL:HG12	3:F:66:LYS:HE3	1.80	0.62
2:B:210:ILE:HD11	2:B:495:CYS:HB2	1.80	0.62
3:F:116:LEU:HD21	3:F:294:LEU:CD1	2.29	0.62
1:G:229:ARG:HH11	1:G:229:ARG:CB	2.09	0.62
3:I:363:VAL:HG11	3:I:408:ASP:OD1	1.99	0.62
1:A:8:HIS:O	1:A:9:ASN:HB2	1.97	0.62
2:B:314:LYS:HG3	3:C:162:LEU:HB3	1.80	0.62
3:C:102:ARG:HD2	3:C:217:GLU:OE2	1.99	0.62
3:F:93:GLU:HG2	3:F:94:MET:H	1.65	0.62
3:I:10:GLU:O	3:I:13:THR:HB	1.99	0.62
3:I:426:TYR:HA	3:I:429:ILE:HG13	1.81	0.62
3:C:20:LYS:HE2	3:C:431:ILE:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:HIS:NE2	2:B:144:PHE:CE1	2.68	0.62
1:A:227:GLN:OE1	1:A:256:VAL:HG11	1.99	0.62
1:D:73:CYS:HB2	1:D:102:VAL:HG12	1.81	0.62
1:D:229:ARG:HH11	1:D:229:ARG:CB	2.09	0.62
1:A:217:LEU:CD2	1:A:218:LEU:H	2.13	0.62
1:A:282:LYS:HE2	1:A:292:ALA:HB2	1.80	0.62
2:B:156:GLY:O	2:B:158:MET:HE2	1.98	0.62
3:C:426:TYR:HA	3:C:429:ILE:HG13	1.81	0.62
3:F:8:GLN:O	3:F:10:GLU:N	2.32	0.62
3:F:11:ARG:HB2	3:F:12:PHE:CD1	2.35	0.62
3:F:12:PHE:CD1	3:F:12:PHE:N	2.63	0.62
3:I:102:ARG:HD2	3:I:217:GLU:OE2	1.99	0.62
1:A:13:HIS:HE1	2:B:144:PHE:CE2	2.18	0.62
2:B:179:LEU:HD11	2:B:477:PHE:HE1	1.65	0.62
2:B:202:ARG:HG2	2:B:209:GLN:HE22	1.62	0.62
3:I:79:GLU:O	3:I:83:VAL:HG23	2.00	0.62
3:C:22:PHE:C	3:C:24:ILE:H	2.08	0.61
1:D:144:HIS:HB2	1:D:148:VAL:HG22	1.80	0.61
3:F:426:TYR:HA	3:F:429:ILE:HG13	1.81	0.61
3:C:11:ARG:HG3	3:C:12:PHE:N	2.15	0.61
2:E:340:LEU:HD23	2:E:370:PHE:CD1	2.35	0.61
1:A:105:VAL:O	1:A:105:VAL:HG13	1.98	0.61
2:H:179:LEU:HD21	2:H:184:LEU:HD13	1.82	0.61
2:H:179:LEU:HD11	2:H:477:PHE:HE1	1.65	0.61
3:I:116:LEU:HD21	3:I:294:LEU:CD1	2.30	0.61
2:B:267:ARG:HG3	2:B:267:ARG:NH1	2.15	0.61
3:C:34:ASP:HB3	3:C:35:PRO:CD	2.25	0.61
2:H:325:LEU:CD2	2:H:361:LEU:HD23	2.30	0.61
3:F:21:GLU:O	3:F:25:GLU:HG3	2.01	0.61
3:I:417:ILE:HG23	3:I:429:ILE:CG2	2.30	0.61
2:B:512:MET:C	2:B:514:GLU:H	2.09	0.61
2:E:325:LEU:CD2	2:E:361:LEU:HD23	2.29	0.61
2:H:547:TYR:CE2	2:H:548:GLU:HG2	2.36	0.61
3:F:16:SER:HA	3:F:19:LEU:HD12	1.83	0.61
3:I:94:MET:HE3	3:I:104:LEU:HD22	1.83	0.61
2:B:226:LYS:HA	2:B:231:TYR:CD2	2.36	0.61
3:C:79:GLU:O	3:C:83:VAL:HG23	2.00	0.61
1:G:227:GLN:HA	1:G:256:VAL:CG1	2.28	0.61
3:C:310:THR:HG23	3:C:311:ASP:N	2.15	0.61
1:G:96:ALA:C	1:G:98:HIS:H	2.09	0.61
3:C:11:ARG:C	3:C:13:THR:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:226:LYS:HA	2:H:231:TYR:CD2	2.36	0.60
1:D:96:ALA:C	1:D:98:HIS:H	2.09	0.60
2:E:226:LYS:HA	2:E:231:TYR:CD2	2.36	0.60
1:G:19:TYR:O	2:H:155:THR:HG21	2.01	0.60
3:I:387:ARG:NH1	3:I:387:ARG:HB3	2.17	0.60
2:H:512:MET:C	2:H:514:GLU:H	2.09	0.60
3:C:431:ILE:HD12	3:C:431:ILE:H	1.66	0.60
1:D:282:LYS:HE2	1:D:292:ALA:HB2	1.80	0.60
1:G:264:LEU:HD22	2:H:509:ARG:HD2	1.83	0.60
2:H:210:ILE:HD12	2:H:495:CYS:HB2	1.84	0.60
3:I:421:LYS:C	3:I:423:GLN:H	2.09	0.60
3:C:387:ARG:NH1	3:C:387:ARG:HB3	2.17	0.60
2:E:280:ILE:HG21	2:E:300:LEU:HG	1.83	0.60
1:G:282:LYS:CE	1:G:292:ALA:HB2	2.32	0.60
3:I:431:ILE:HD12	3:I:431:ILE:H	1.66	0.60
1:A:79:VAL:HG22	1:A:102:VAL:HG11	1.82	0.60
3:C:341:HIS:O	3:C:345:VAL:HG23	2.02	0.60
2:E:179:LEU:HD11	2:E:477:PHE:HE1	1.65	0.60
2:E:512:MET:C	2:E:514:GLU:H	2.09	0.60
3:F:77:LEU:HD12	3:F:125:TRP:CH2	2.37	0.60
3:F:431:ILE:H	3:F:431:ILE:HD12	1.66	0.60
3:I:341:HIS:O	3:I:345:VAL:HG23	2.02	0.60
1:D:285:LEU:HD12	1:D:285:LEU:N	2.17	0.60
2:H:267:ARG:HG3	2:H:267:ARG:NH1	2.15	0.60
2:E:142:ARG:HH11	2:E:142:ARG:HG3	1.67	0.60
3:I:34:ASP:CB	3:I:35:PRO:HD3	2.29	0.60
1:A:146:ILE:O	1:A:146:ILE:HG22	2.02	0.60
3:C:20:LYS:HZ3	3:C:428:ASN:CG	2.09	0.60
1:D:140:ILE:H	1:D:140:ILE:HD12	1.67	0.60
3:F:79:GLU:O	3:F:83:VAL:HG23	2.00	0.60
3:F:341:HIS:O	3:F:345:VAL:HG23	2.02	0.60
1:G:217:LEU:CD2	1:G:218:LEU:H	2.13	0.60
2:B:314:LYS:HE3	3:C:162:LEU:HB3	1.84	0.60
1:D:282:LYS:CE	1:D:292:ALA:HB2	2.32	0.60
2:E:402:LEU:O	2:E:405:SER:HB3	2.02	0.60
1:G:79:VAL:HG22	1:G:102:VAL:HG11	1.82	0.60
1:A:96:ALA:C	1:A:98:HIS:H	2.09	0.59
1:A:140:ILE:H	1:A:140:ILE:HD12	1.67	0.59
1:A:264:LEU:HD12	2:B:155:THR:O	2.01	0.59
1:A:285:LEU:HD12	1:A:285:LEU:N	2.17	0.59
2:B:179:LEU:HD21	2:B:184:LEU:HD13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:ILE:HG21	2:B:300:LEU:HG	1.84	0.59
3:C:8:GLN:C	3:C:10:GLU:N	2.60	0.59
3:C:34:ASP:CB	3:C:35:PRO:HD3	2.29	0.59
1:D:259:ARG:HD2	2:E:152:LYS:HE3	1.84	0.59
2:E:466:SER:HB2	2:E:469:THR:H	1.67	0.59
2:H:402:LEU:O	2:H:405:SER:HB3	2.02	0.59
3:I:70:LEU:HB3	3:I:343:ILE:CD1	2.32	0.59
1:A:227:GLN:HA	1:A:256:VAL:CG1	2.28	0.59
3:F:387:ARG:NH1	3:F:387:ARG:HB3	2.17	0.59
3:I:15:PHE:CD1	3:I:387:ARG:HD3	2.36	0.59
1:A:282:LYS:CE	1:A:292:ALA:HB2	2.32	0.59
1:D:79:VAL:HG22	1:D:102:VAL:HG11	1.83	0.59
1:A:259:ARG:HH11	2:B:150:PHE:HB2	1.61	0.59
3:C:11:ARG:C	3:C:13:THR:N	2.55	0.59
3:C:349:SER:OG	3:C:358:VAL:HG21	2.02	0.59
2:E:179:LEU:HD21	2:E:184:LEU:HD13	1.83	0.59
3:I:11:ARG:HG3	3:I:12:PHE:CE1	2.37	0.59
1:D:57:TRP:HE1	2:E:142:ARG:CZ	2.14	0.59
3:C:417:ILE:HG23	3:C:429:ILE:HD13	1.84	0.59
1:G:146:ILE:HG22	1:G:146:ILE:O	2.02	0.59
3:I:349:SER:OG	3:I:358:VAL:HG21	2.02	0.59
2:B:466:SER:HB2	2:B:469:THR:H	1.67	0.59
3:C:319:SER:OG	2:E:337:GLU:HG2	2.03	0.59
1:D:227:GLN:NE2	2:E:143:ARG:HH12	2.01	0.59
2:B:402:LEU:O	2:B:405:SER:HB3	2.02	0.59
1:D:146:ILE:O	1:D:146:ILE:HG22	2.02	0.59
1:D:212:TRP:CG	1:D:222:LEU:HD21	2.37	0.59
2:E:210:ILE:HD12	2:E:495:CYS:HB2	1.84	0.59
1:D:15:ALA:HB2	1:D:26:THR:HG22	1.84	0.59
2:H:138:ILE:HA	2:H:141:GLU:HG2	1.84	0.59
2:H:466:SER:HB2	2:H:469:THR:H	1.67	0.59
1:A:63:HIS:CD2	1:A:65:LYS:HB2	2.36	0.59
1:A:200:LEU:HD11	1:A:243:TRP:CD1	2.38	0.59
1:A:212:TRP:CG	1:A:222:LEU:HD21	2.38	0.59
3:C:11:ARG:O	3:C:13:THR:N	2.36	0.59
1:D:200:LEU:HD11	1:D:243:TRP:CD1	2.38	0.58
3:F:349:SER:OG	3:F:358:VAL:HG21	2.02	0.58
1:D:17:LEU:HD12	2:E:154:SER:CA	2.32	0.58
1:A:272:SER:OG	2:B:151:ALA:HB3	2.03	0.58
1:G:247:LEU:O	1:G:248:LEU:C	2.46	0.58
2:H:177:THR:HG21	2:H:484:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:304:VAL:HG13	3:I:314:ILE:HD11	1.83	0.58
3:I:406:GLU:HG2	3:I:409:LYS:NZ	2.18	0.58
3:C:227:ILE:C	3:C:229:ASN:N	2.61	0.58
3:I:227:ILE:C	3:I:229:ASN:N	2.61	0.58
3:F:366:LEU:HB2	3:F:379:ILE:HG21	1.85	0.58
1:G:15:ALA:HB2	1:G:26:THR:HG22	1.84	0.58
2:H:280:ILE:HG21	2:H:300:LEU:HG	1.84	0.58
3:C:406:GLU:HG2	3:C:409:LYS:NZ	2.18	0.58
2:E:269:THR:O	2:E:273:VAL:HG23	2.04	0.58
1:G:157:THR:HG21	2:H:501:LYS:NZ	2.19	0.58
1:G:200:LEU:HD11	1:G:243:TRP:CD1	2.38	0.58
1:A:15:ALA:HB2	1:A:26:THR:HG22	1.84	0.58
1:A:20:TYR:HD2	2:B:544:LYS:NZ	2.01	0.58
1:A:247:LEU:O	1:A:248:LEU:C	2.46	0.58
3:F:359:ILE:HG21	3:F:404:VAL:HG11	1.85	0.58
1:G:138:PRO:C	1:G:139:ILE:HD12	2.29	0.58
2:H:285:ARG:HG3	2:H:285:ARG:HH11	1.68	0.58
1:A:37:GLU:HG2	1:A:46:ILE:HD12	1.86	0.58
2:B:269:THR:O	2:B:273:VAL:HG23	2.04	0.58
3:C:20:LYS:NZ	3:C:428:ASN:CG	2.62	0.58
1:D:9:ASN:HD22	1:D:9:ASN:H	1.52	0.58
1:A:138:PRO:C	1:A:139:ILE:HD12	2.29	0.58
1:D:138:PRO:C	1:D:139:ILE:HD12	2.29	0.58
1:G:140:ILE:HD12	1:G:140:ILE:H	1.67	0.58
1:A:258:TRP:NE1	2:B:148:TYR:HA	2.18	0.58
2:B:213:SER:HB3	2:B:459:PHE:CG	2.39	0.58
2:B:250:THR:HG21	2:B:255:VAL:HB	1.86	0.58
2:E:425:TYR:O	2:E:463:ARG:NH2	2.37	0.58
1:G:212:TRP:CG	1:G:222:LEU:HD21	2.38	0.58
1:A:12:ILE:CD1	2:B:168:SER:O	2.52	0.57
2:B:285:ARG:HH11	2:B:285:ARG:HG3	1.68	0.57
2:E:285:ARG:HH11	2:E:285:ARG:HG3	1.69	0.57
1:G:285:LEU:HD12	1:G:285:LEU:N	2.17	0.57
2:H:340:LEU:CD2	2:H:370:PHE:CG	2.87	0.57
2:H:538:PHE:CD1	2:H:538:PHE:C	2.82	0.57
1:D:43:HIS:CD2	2:E:168:SER:HB3	2.39	0.57
1:D:181:LEU:HD22	1:D:199:THR:HG22	1.87	0.57
3:F:34:ASP:CB	3:F:35:PRO:HD3	2.30	0.57
3:F:91:LEU:CG	3:F:92:ASP:H	2.17	0.57
3:F:428:ASN:C	3:F:430:PRO:HD2	2.29	0.57
2:H:250:THR:HG21	2:H:255:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:425:TYR:O	2:H:463:ARG:NH2	2.38	0.57
1:D:37:GLU:HG2	1:D:46:ILE:HD12	1.86	0.57
2:E:267:ARG:HG3	2:E:267:ARG:NH1	2.15	0.57
3:F:406:GLU:HG2	3:F:409:LYS:NZ	2.18	0.57
2:H:259:LEU:CD2	3:I:223:ILE:HD13	2.34	0.57
3:I:23:LYS:HZ3	3:I:431:ILE:HA	1.69	0.57
1:A:181:LEU:HD22	1:A:199:THR:CG2	2.35	0.57
1:A:191:ALA:C	1:A:193:THR:H	2.13	0.57
2:B:538:PHE:C	2:B:538:PHE:CD1	2.82	0.57
1:D:29:SER:C	1:D:31:LYS:H	2.13	0.57
2:E:538:PHE:CD1	2:E:538:PHE:C	2.82	0.57
3:F:86:ASN:C	3:F:88:ASP:H	2.13	0.57
2:H:291:ILE:H	2:H:291:ILE:CD1	2.16	0.57
1:A:13:HIS:CE1	2:B:144:PHE:CE2	2.90	0.57
1:A:29:SER:C	1:A:31:LYS:H	2.13	0.57
2:B:198:THR:CB	2:B:212:GLU:HB2	2.29	0.57
1:D:191:ALA:C	1:D:193:THR:H	2.13	0.57
2:H:213:SER:HB3	2:H:459:PHE:CG	2.39	0.57
1:A:20:TYR:CE2	2:B:544:LYS:CD	2.84	0.57
2:B:165:VAL:O	2:B:165:VAL:CG1	2.52	0.57
1:D:73:CYS:HB2	1:D:102:VAL:CG1	2.35	0.57
1:G:29:SER:C	1:G:31:LYS:H	2.13	0.57
2:B:202:ARG:CG	2:B:209:GLN:NE2	2.60	0.57
2:B:210:ILE:HD12	2:B:495:CYS:HB2	1.84	0.57
2:B:425:TYR:O	2:B:463:ARG:NH2	2.37	0.57
3:I:418:SER:O	3:I:422:LEU:HG	2.03	0.57
2:E:133:ASP:O	2:E:137:LEU:HG	2.05	0.57
1:G:191:ALA:C	1:G:193:THR:H	2.13	0.57
1:D:181:LEU:HD22	1:D:199:THR:CG2	2.35	0.57
2:H:202:ARG:CG	2:H:209:GLN:NE2	2.60	0.57
2:H:269:THR:O	2:H:273:VAL:HG23	2.04	0.57
1:A:16:VAL:HG21	1:A:59:VAL:O	2.05	0.57
1:A:73:CYS:HB2	1:A:102:VAL:CG1	2.35	0.57
2:B:160:LEU:HA	2:B:171:SER:O	2.05	0.57
2:B:358:TYR:CE2	3:C:210:MET:HE1	2.38	0.57
3:C:428:ASN:C	3:C:430:PRO:HD2	2.30	0.57
1:D:247:LEU:O	1:D:248:LEU:C	2.46	0.57
2:E:205:ASN:OD1	2:E:207:TYR:HB2	2.05	0.57
2:E:213:SER:HB3	2:E:459:PHE:CG	2.40	0.57
3:F:50:ALA:HB1	3:F:69:GLU:HG2	1.86	0.57
1:G:227:GLN:O	1:G:256:VAL:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:TYR:HA	1:D:171:ARG:NH2	2.19	0.56
2:E:198:THR:CB	2:E:212:GLU:HB2	2.29	0.56
3:F:116:LEU:CD2	3:F:294:LEU:HD11	2.35	0.56
3:I:160:PHE:CE2	3:I:168:VAL:HG11	2.40	0.56
1:D:227:GLN:O	1:D:256:VAL:HG22	2.05	0.56
3:I:416:TYR:HE2	3:I:432:TYR:HE2	1.47	0.56
1:A:141:ILE:HD12	1:A:185:TRP:CE3	2.40	0.56
2:B:327:SER:C	2:B:329:ASP:H	2.13	0.56
2:B:525:HIS:C	2:B:527:LEU:N	2.62	0.56
1:D:16:VAL:HG21	1:D:59:VAL:O	2.05	0.56
3:F:379:ILE:HG13	3:F:385:LEU:HG	1.87	0.56
2:H:369:LEU:O	2:H:370:PHE:HB2	2.05	0.56
3:C:116:LEU:CD2	3:C:294:LEU:HD11	2.35	0.56
1:D:10:GLU:O	1:D:11:LEU:CG	2.54	0.56
3:F:326:GLU:O	3:F:330:ARG:HG3	2.06	0.56
1:G:181:LEU:HD22	1:G:199:THR:HG22	1.86	0.56
2:H:320:VAL:CG2	3:I:246:THR:HG22	2.35	0.56
2:H:340:LEU:HD22	2:H:370:PHE:CG	2.40	0.56
3:I:428:ASN:C	3:I:430:PRO:HD2	2.30	0.56
1:A:227:GLN:O	1:A:256:VAL:HG22	2.05	0.56
1:A:261:SER:CB	2:B:152:LYS:HG2	2.32	0.56
1:D:227:GLN:HA	1:D:256:VAL:CG1	2.28	0.56
2:E:325:LEU:HD23	2:E:361:LEU:HD23	1.88	0.56
1:G:16:VAL:HG21	1:G:59:VAL:O	2.05	0.56
1:G:37:GLU:HG2	1:G:46:ILE:HD12	1.86	0.56
2:H:138:ILE:HA	2:H:141:GLU:CG	2.35	0.56
2:E:324:TYR:CE2	3:F:237:ILE:HG21	2.39	0.56
1:G:20:TYR:CE2	2:H:544:LYS:HA	2.41	0.56
1:G:181:LEU:HD22	1:G:199:THR:CG2	2.35	0.56
3:I:70:LEU:HB3	3:I:343:ILE:HD11	1.87	0.56
1:A:181:LEU:HD22	1:A:199:THR:HG22	1.87	0.56
2:B:205:ASN:OD1	2:B:207:TYR:HB2	2.05	0.56
2:B:291:ILE:H	2:B:291:ILE:CD1	2.16	0.56
3:C:387:ARG:HG2	3:C:391:HIS:CE1	2.41	0.56
2:E:225:GLU:C	2:E:227:THR:H	2.14	0.56
3:F:160:PHE:CE2	3:F:168:VAL:HG11	2.40	0.56
3:F:387:ARG:HG2	3:F:391:HIS:CE1	2.41	0.56
3:F:441:CYS:O	3:F:442:LEU:HG	2.06	0.56
1:G:237:ASP:OD1	1:G:244:LYS:HE3	2.06	0.56
2:H:205:ASN:OD1	2:H:207:TYR:HB2	2.05	0.56
1:A:12:ILE:CD1	2:B:169:GLY:HA3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:23:LYS:O	3:F:26:GLN:HB2	2.06	0.56
3:F:226:GLN:CD	3:F:226:GLN:H	2.13	0.56
1:A:13:HIS:ND1	2:B:148:TYR:CE2	2.74	0.56
3:C:50:ALA:HB1	3:C:69:GLU:HG2	1.87	0.56
3:C:160:PHE:CE2	3:C:168:VAL:HG11	2.40	0.56
3:C:326:GLU:O	3:C:330:ARG:HG3	2.06	0.56
2:E:162:LYS:HE3	2:E:164:ILE:HD11	1.88	0.56
2:E:314:LYS:HZ1	3:F:253:GLN:HB3	1.71	0.56
1:G:233:ILE:HD11	1:G:248:LEU:HD13	1.88	0.56
3:I:116:LEU:CD2	3:I:294:LEU:HD11	2.35	0.56
2:B:225:GLU:C	2:B:227:THR:H	2.14	0.55
2:E:202:ARG:NE	2:E:202:ARG:HA	2.21	0.55
2:E:250:THR:HG21	2:E:255:VAL:HB	1.86	0.55
2:H:325:LEU:HD23	2:H:361:LEU:HD23	1.89	0.55
1:A:63:HIS:C	1:A:65:LYS:H	2.15	0.55
1:D:138:PRO:HB2	1:D:140:ILE:CD1	2.37	0.55
1:D:209:ASP:OD1	1:D:259:ARG:HD3	2.06	0.55
1:D:221:TYR:O	1:D:222:LEU:HD23	2.06	0.55
2:E:202:ARG:CG	2:E:209:GLN:NE2	2.61	0.55
1:G:209:ASP:OD1	1:G:259:ARG:HD3	2.06	0.55
1:G:221:TYR:O	1:G:222:LEU:HD23	2.06	0.55
3:I:326:GLU:O	3:I:330:ARG:HG3	2.07	0.55
3:I:387:ARG:HG2	3:I:391:HIS:CE1	2.41	0.55
3:C:226:GLN:CD	3:C:226:GLN:H	2.14	0.55
1:D:9:ASN:ND2	1:D:9:ASN:N	2.54	0.55
1:D:19:TYR:O	2:E:155:THR:HG21	2.06	0.55
1:D:63:HIS:C	1:D:65:LYS:H	2.14	0.55
3:F:94:MET:CE	3:F:108:LYS:HB2	2.35	0.55
1:G:105:VAL:HA	1:G:117:LEU:O	2.07	0.55
1:G:109:PRO:HD2	1:G:112:TYR:CD1	2.42	0.55
2:H:160:LEU:HA	2:H:171:SER:O	2.05	0.55
1:G:73:CYS:HB2	1:G:102:VAL:CG1	2.35	0.55
2:H:327:SER:C	2:H:329:ASP:H	2.13	0.55
2:H:453:LEU:HD23	2:H:453:LEU:C	2.32	0.55
3:I:110:MET:SD	3:I:116:LEU:HD22	2.47	0.55
2:E:160:LEU:HA	2:E:171:SER:O	2.05	0.55
2:H:162:LYS:HE3	2:H:164:ILE:HD11	1.88	0.55
1:A:109:PRO:HD2	1:A:112:TYR:CD1	2.42	0.55
1:A:117:LEU:HB2	1:A:153:TRP:HE1	1.72	0.55
1:A:127:VAL:HG21	1:A:194:TYR:CE1	2.41	0.55
2:B:155:THR:HG22	2:B:513:ARG:CD	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:TYR:HE2	2:B:536:LEU:HD22	1.72	0.55
2:B:320:VAL:CA	3:C:246:THR:HG21	2.35	0.55
2:E:453:LEU:HD23	2:E:453:LEU:C	2.32	0.55
1:G:10:GLU:O	1:G:11:LEU:CG	2.54	0.55
1:D:57:TRP:NE1	2:E:142:ARG:CZ	2.70	0.55
1:D:139:ILE:O	1:D:139:ILE:HG22	2.07	0.55
2:E:303:VAL:HG13	2:E:322:ILE:HG22	1.89	0.55
2:E:369:LEU:O	2:E:370:PHE:HB2	2.07	0.55
3:F:16:SER:O	3:F:19:LEU:HB2	2.07	0.55
1:A:112:TYR:HA	1:A:171:ARG:NH2	2.22	0.55
1:A:209:ASP:OD1	1:A:259:ARG:HD3	2.06	0.55
1:A:237:ASP:OD1	1:A:244:LYS:HE3	2.06	0.55
2:B:150:PHE:CE2	2:B:162:LYS:HB2	2.41	0.55
2:E:291:ILE:H	2:E:291:ILE:CD1	2.17	0.55
3:F:143:LYS:HE3	3:F:144:TRP:NE1	2.22	0.55
1:G:138:PRO:HB2	1:G:140:ILE:CD1	2.37	0.55
2:H:207:TYR:HE2	2:H:536:LEU:HD22	1.72	0.55
3:I:143:LYS:HE3	3:I:144:TRP:NE1	2.22	0.55
1:A:139:ILE:O	1:A:139:ILE:HG22	2.07	0.55
1:D:105:VAL:HA	1:D:117:LEU:O	2.07	0.55
1:D:109:PRO:HD2	1:D:112:TYR:CD1	2.42	0.55
2:E:339:GLN:HB2	3:F:206:ILE:HG21	1.89	0.55
3:I:7:TYR:HB3	3:I:10:GLU:OE1	2.06	0.55
1:A:138:PRO:HB2	1:A:140:ILE:CD1	2.37	0.55
1:A:233:ILE:HD11	1:A:248:LEU:HD13	1.88	0.55
2:B:202:ARG:NE	2:B:202:ARG:HA	2.21	0.55
2:B:303:VAL:HG13	2:B:322:ILE:HG22	1.89	0.55
2:B:453:LEU:HD23	2:B:453:LEU:C	2.32	0.55
3:C:110:MET:SD	3:C:116:LEU:HD22	2.47	0.55
3:C:184:ILE:O	3:C:188:ILE:HG13	2.07	0.55
1:D:19:TYR:CD2	1:D:20:TYR:CE1	2.88	0.55
1:D:117:LEU:HB2	1:D:153:TRP:HE1	1.72	0.55
1:D:237:ASP:OD1	1:D:244:LYS:HE3	2.06	0.55
3:F:16:SER:HA	3:F:19:LEU:CD1	2.36	0.55
1:G:63:HIS:C	1:G:65:LYS:H	2.14	0.55
1:A:221:TYR:O	1:A:222:LEU:HD23	2.06	0.54
1:D:271:LEU:C	1:D:278:VAL:HG13	2.32	0.54
2:E:207:TYR:HE2	2:E:536:LEU:HD22	1.72	0.54
3:F:20:LYS:O	3:F:23:LYS:N	2.40	0.54
1:G:19:TYR:CD2	1:G:20:TYR:CE1	2.89	0.54
2:H:202:ARG:HA	2:H:202:ARG:NE	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:474:THR:HG21	2:H:497:LEU:HD12	1.89	0.54
1:G:217:LEU:HG	2:H:475:PHE:CE1	2.42	0.54
1:G:140:ILE:HD12	1:G:140:ILE:N	2.23	0.54
3:I:206:ILE:O	3:I:209:CYS:HB3	2.08	0.54
2:B:354:ILE:HD13	3:C:157:ASP:CG	2.32	0.54
1:G:117:LEU:HB2	1:G:153:TRP:HE1	1.72	0.54
2:H:225:GLU:C	2:H:227:THR:H	2.14	0.54
3:I:184:ILE:O	3:I:188:ILE:HG13	2.08	0.54
3:C:143:LYS:HE3	3:C:144:TRP:NE1	2.22	0.54
3:C:206:ILE:O	3:C:209:CYS:HB3	2.07	0.54
1:D:233:ILE:HD11	1:D:248:LEU:HD13	1.88	0.54
3:F:110:MET:SD	3:F:116:LEU:HD22	2.47	0.54
1:G:279:THR:CB	1:G:281:TRP:HE1	2.21	0.54
2:B:221:LEU:HB3	2:B:231:TYR:HE1	1.73	0.54
2:E:327:SER:C	2:E:329:ASP:H	2.13	0.54
2:E:342:LYS:HD2	3:F:206:ILE:HD11	1.90	0.54
3:F:416:TYR:CD2	3:F:432:TYR:CE2	2.95	0.54
2:H:303:VAL:HG13	2:H:322:ILE:HG22	1.89	0.54
1:A:105:VAL:HA	1:A:117:LEU:O	2.07	0.54
1:A:140:ILE:HD12	1:A:140:ILE:N	2.23	0.54
2:B:484:ALA:O	2:B:485:GLN:HB2	2.08	0.54
3:F:8:GLN:C	3:F:10:GLU:N	2.65	0.54
1:G:139:ILE:O	1:G:139:ILE:HG22	2.07	0.54
1:D:279:THR:HB	1:D:281:TRP:HE1	1.73	0.54
2:E:509:ARG:HH11	2:E:509:ARG:HG2	1.72	0.54
1:G:31:LYS:HG2	1:G:54:GLY:O	2.08	0.54
1:G:109:PRO:HD2	1:G:112:TYR:CE1	2.43	0.54
1:G:271:LEU:C	1:G:278:VAL:HG13	2.32	0.54
3:I:70:LEU:HD11	3:I:344:ARG:NH2	2.23	0.54
1:A:271:LEU:C	1:A:278:VAL:HG13	2.32	0.54
1:D:9:ASN:HD22	1:D:9:ASN:N	2.05	0.54
1:D:140:ILE:HD12	1:D:140:ILE:N	2.23	0.54
1:D:279:THR:CB	1:D:281:TRP:HE1	2.21	0.54
3:F:23:LYS:HA	3:F:26:GLN:OE1	2.07	0.54
2:H:509:ARG:HG2	2:H:509:ARG:HH11	1.72	0.54
3:I:160:PHE:HE2	3:I:168:VAL:HG11	1.73	0.54
1:A:279:THR:HB	1:A:281:TRP:HE1	1.73	0.54
2:B:474:THR:HG21	2:B:497:LEU:HD12	1.90	0.54
2:B:512:MET:C	2:B:514:GLU:N	2.66	0.54
3:C:384:TYR:CD1	3:C:385:LEU:N	2.76	0.54
1:A:31:LYS:HG2	1:A:54:GLY:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:LEU:HD21	2:B:421:ILE:HD11	1.90	0.53
1:D:61:TRP:CD1	1:D:61:TRP:H	2.26	0.53
2:E:546:ARG:HB2	2:E:551:TYR:CE1	2.42	0.53
1:G:61:TRP:CD1	1:G:61:TRP:H	2.26	0.53
2:H:233:LEU:HD21	2:H:421:ILE:HD11	1.90	0.53
3:I:92:ASP:O	3:I:93:GLU:C	2.51	0.53
3:I:226:GLN:CD	3:I:226:GLN:H	2.14	0.53
1:D:95:HIS:CE1	1:D:97:VAL:HG22	2.43	0.53
1:A:225:VAL:CG2	1:A:271:LEU:HD22	2.38	0.53
2:B:145:THR:HG22	2:B:147:SER:H	1.72	0.53
2:B:442:THR:CG2	2:B:443:ASN:N	2.72	0.53
2:B:449:PHE:CE2	2:B:453:LEU:HD12	2.43	0.53
1:D:109:PRO:HD2	1:D:112:TYR:CE1	2.43	0.53
1:G:95:HIS:CE1	1:G:97:VAL:HG22	2.43	0.53
1:G:225:VAL:HG21	1:G:271:LEU:HD22	1.91	0.53
2:H:207:TYR:CE2	2:H:536:LEU:HD22	2.44	0.53
3:I:102:ARG:NH2	3:I:241:SER:H	2.06	0.53
1:D:31:LYS:HG2	1:D:54:GLY:O	2.08	0.53
1:D:262:TRP:CZ3	1:D:269:LEU:HB2	2.44	0.53
2:E:150:PHE:CE2	2:E:162:LYS:HB2	2.44	0.53
2:E:207:TYR:CE2	2:E:536:LEU:HD22	2.43	0.53
2:E:484:ALA:O	2:E:485:GLN:HB2	2.09	0.53
3:F:160:PHE:HE2	3:F:168:VAL:HG11	1.74	0.53
3:F:184:ILE:O	3:F:188:ILE:HG13	2.08	0.53
3:I:148:ILE:CD1	3:I:153:LEU:HD12	2.39	0.53
1:A:95:HIS:CE1	1:A:97:VAL:HG22	2.43	0.53
1:A:103:ASN:HD21	2:B:142:ARG:HH22	1.57	0.53
3:C:77:LEU:CD2	3:C:81:LEU:HD12	2.39	0.53
1:G:112:TYR:HA	1:G:171:ARG:NH2	2.23	0.53
2:H:449:PHE:CE2	2:H:453:LEU:HD12	2.43	0.53
2:H:515:ILE:CD1	2:H:544:LYS:HB2	2.38	0.53
3:I:77:LEU:CD2	3:I:81:LEU:HD12	2.39	0.53
1:A:181:LEU:HD23	1:A:201:GLU:HG2	1.91	0.53
2:E:221:LEU:HB3	2:E:231:TYR:HE1	1.73	0.53
2:E:474:THR:HG21	2:E:497:LEU:HD12	1.90	0.53
3:F:227:ILE:C	3:F:229:ASN:N	2.61	0.53
3:F:384:TYR:CD1	3:F:385:LEU:N	2.76	0.53
1:G:225:VAL:CG2	1:G:271:LEU:HD22	2.38	0.53
3:I:23:LYS:HA	3:I:27:ASN:OD1	2.09	0.53
3:C:148:ILE:CD1	3:C:153:LEU:HD12	2.39	0.53
3:C:160:PHE:HE2	3:C:168:VAL:HG11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:VAL:CG2	1:D:271:LEU:HD22	2.38	0.53
3:F:70:LEU:HB3	3:F:343:ILE:CD1	2.38	0.53
3:F:83:VAL:O	3:F:87:ALA:HB3	2.09	0.53
3:F:117:TYR:O	3:F:120:TRP:HB3	2.09	0.53
1:A:225:VAL:HG21	1:A:271:LEU:HD22	1.91	0.53
1:A:279:THR:CB	1:A:281:TRP:HE1	2.21	0.53
2:B:509:ARG:HG2	2:B:509:ARG:HH11	1.72	0.53
3:C:35:PRO:HB2	3:C:399:ILE:HG12	1.90	0.53
1:G:262:TRP:CZ3	1:G:269:LEU:HB2	2.44	0.53
2:H:221:LEU:HB3	2:H:231:TYR:HE1	1.73	0.53
2:H:297:TYR:CE2	2:H:305:ARG:HD2	2.44	0.53
1:A:262:TRP:CZ3	1:A:269:LEU:HB2	2.44	0.53
1:A:265:SER:O	2:B:483:PHE:CE2	2.62	0.53
3:C:7:TYR:CD1	3:C:7:TYR:C	2.87	0.53
3:C:365:MET:HB3	3:C:379:ILE:CG2	2.39	0.53
1:D:181:LEU:HD23	1:D:201:GLU:HG2	1.91	0.53
2:E:515:ILE:CD1	2:E:544:LYS:HB2	2.39	0.53
3:F:77:LEU:CD2	3:F:81:LEU:HD12	2.38	0.53
2:H:484:ALA:O	2:H:485:GLN:HB2	2.08	0.53
1:A:121:SER:O	1:A:147:GLY:HA2	2.09	0.53
1:A:261:SER:HB2	2:B:152:LYS:CG	2.33	0.53
2:B:138:ILE:O	2:B:141:GLU:HG2	2.09	0.53
2:B:174:ARG:O	2:B:175:LEU:C	2.52	0.53
3:C:102:ARG:NH2	3:C:241:SER:H	2.06	0.53
1:D:27:CYS:HB2	1:D:56:VAL:HB	1.91	0.53
1:D:225:VAL:HG13	1:D:257:LEU:CB	2.39	0.53
1:D:225:VAL:HG21	1:D:271:LEU:HD22	1.91	0.53
2:H:415:ASP:HA	2:H:442:THR:HG21	1.91	0.53
2:H:512:MET:C	2:H:514:GLU:N	2.66	0.53
2:H:525:HIS:C	2:H:527:LEU:N	2.62	0.53
3:I:421:LYS:C	3:I:423:GLN:N	2.66	0.53
1:D:217:LEU:CD1	1:D:218:LEU:H	2.22	0.52
2:E:297:TYR:CE2	2:E:305:ARG:HD2	2.44	0.52
2:E:415:ASP:HA	2:E:442:THR:HG21	1.91	0.52
2:E:442:THR:CG2	2:E:443:ASN:N	2.72	0.52
2:E:525:HIS:C	2:E:527:LEU:N	2.62	0.52
3:F:102:ARG:NH2	3:F:241:SER:H	2.07	0.52
3:I:86:ASN:O	3:I:86:ASN:ND2	2.42	0.52
2:B:207:TYR:CE2	2:B:536:LEU:HD22	2.43	0.52
2:E:233:LEU:HD21	2:E:421:ILE:HD11	1.90	0.52
2:E:551:TYR:CD2	2:E:552:LEU:HG	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:206:ILE:O	3:F:209:CYS:HB3	2.07	0.52
1:G:181:LEU:HD23	1:G:201:GLU:HG2	1.91	0.52
3:I:160:PHE:HB3	3:I:161:PRO:HD3	1.92	0.52
1:A:61:TRP:CD1	1:A:61:TRP:H	2.27	0.52
1:A:259:ARG:HB2	1:A:272:SER:HB2	1.92	0.52
1:A:273:GLY:C	1:A:275:ASP:H	2.17	0.52
3:C:416:TYR:CE2	3:C:432:TYR:CE2	2.98	0.52
1:D:9:ASN:OD1	1:D:12:ILE:HD11	2.10	0.52
1:D:273:GLY:C	1:D:275:ASP:H	2.17	0.52
2:H:335:LEU:HD12	3:I:206:ILE:HG23	1.92	0.52
2:H:442:THR:CG2	2:H:443:ASN:N	2.72	0.52
3:I:117:TYR:O	3:I:120:TRP:HB3	2.10	0.52
3:I:243:TRP:O	3:I:247:VAL:HG23	2.09	0.52
3:C:117:TYR:O	3:C:120:TRP:HB3	2.10	0.52
3:C:431:ILE:N	3:C:431:ILE:CD1	2.72	0.52
1:D:243:TRP:CD1	1:D:243:TRP:H	2.27	0.52
2:E:449:PHE:CE2	2:E:453:LEU:HD12	2.44	0.52
2:H:150:PHE:CE2	2:H:162:LYS:HB2	2.44	0.52
3:C:143:LYS:HG3	3:C:144:TRP:N	2.25	0.52
3:C:342:PRO:HG2	3:C:382:LYS:CD	2.39	0.52
1:D:40:GLY:O	2:E:172:ILE:HD13	2.09	0.52
2:E:448:GLN:HG3	2:E:477:PHE:CZ	2.45	0.52
3:F:113:ASN:C	3:F:113:ASN:OD1	2.52	0.52
3:C:20:LYS:HE2	3:C:431:ILE:CG1	2.39	0.52
1:D:259:ARG:HB2	1:D:272:SER:HB2	1.91	0.52
2:E:320:VAL:HA	3:F:246:THR:CG2	2.34	0.52
1:A:109:PRO:HD2	1:A:112:TYR:CE1	2.43	0.52
2:B:369:LEU:O	2:B:370:PHE:HB2	2.10	0.52
2:B:415:ASP:HA	2:B:442:THR:HG21	1.91	0.52
2:B:551:TYR:CD2	2:B:552:LEU:HG	2.44	0.52
1:D:121:SER:O	1:D:147:GLY:HA2	2.09	0.52
3:F:10:GLU:O	3:F:11:ARG:C	2.52	0.52
2:B:515:ILE:CD1	2:B:544:LYS:HB2	2.39	0.52
1:D:118:VAL:O	1:D:125:VAL:HA	2.10	0.52
2:E:142:ARG:HB3	2:E:144:PHE:CD1	2.44	0.52
2:E:442:THR:HG22	2:E:444:ALA:N	2.21	0.52
3:F:148:ILE:CD1	3:F:153:LEU:HD12	2.39	0.52
2:H:527:LEU:HA	2:H:530:LEU:HD13	1.92	0.52
1:A:118:VAL:O	1:A:125:VAL:HA	2.10	0.52
2:B:442:THR:HG22	2:B:444:ALA:N	2.21	0.52
3:C:77:LEU:HD12	3:C:125:TRP:CH2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:GLY:C	1:G:275:ASP:H	2.17	0.52
2:H:448:GLN:HG3	2:H:477:PHE:CZ	2.45	0.52
3:I:113:ASN:C	3:I:113:ASN:OD1	2.53	0.52
1:A:243:TRP:CD1	1:A:243:TRP:H	2.27	0.52
2:B:297:TYR:CE2	2:B:305:ARG:HD2	2.44	0.52
2:B:448:GLN:HG3	2:B:477:PHE:CZ	2.45	0.52
3:C:243:TRP:O	3:C:247:VAL:HG23	2.10	0.52
1:D:283:GLU:HB2	1:D:289:TRP:CZ3	2.45	0.52
3:F:243:TRP:O	3:F:247:VAL:HG23	2.09	0.52
3:I:35:PRO:HB2	3:I:399:ILE:HG12	1.92	0.52
1:A:19:TYR:CD2	1:A:20:TYR:CE1	2.88	0.51
2:E:341:GLN:O	2:E:342:LYS:C	2.53	0.51
2:E:512:MET:C	2:E:514:GLU:N	2.66	0.51
1:G:27:CYS:HB2	1:G:56:VAL:HB	1.91	0.51
1:G:121:SER:O	1:G:147:GLY:HA2	2.10	0.51
1:G:279:THR:HB	1:G:281:TRP:HE1	1.73	0.51
2:H:442:THR:HG22	2:H:444:ALA:N	2.21	0.51
3:I:77:LEU:HB2	3:I:125:TRP:CE2	2.45	0.51
1:A:24:LEU:HD21	2:B:170:VAL:CG2	2.38	0.51
1:A:283:GLU:HB2	1:A:289:TRP:CZ3	2.46	0.51
2:B:289:ASN:O	2:B:293:GLN:HG3	2.11	0.51
3:C:20:LYS:CG	3:C:431:ILE:HG12	2.39	0.51
3:C:70:LEU:HB3	3:C:343:ILE:HD11	1.91	0.51
2:E:320:VAL:HG22	3:F:246:THR:CG2	2.38	0.51
1:A:15:ALA:CB	2:B:170:VAL:HG11	2.41	0.51
3:C:113:ASN:OD1	3:C:113:ASN:C	2.53	0.51
3:C:363:VAL:HG11	3:C:408:ASP:OD1	2.09	0.51
1:G:62:ALA:HB2	1:G:107:TRP:CE2	2.45	0.51
1:G:217:LEU:CD1	1:G:218:LEU:H	2.22	0.51
1:G:268:VAL:HG12	1:G:269:LEU:N	2.25	0.51
2:H:174:ARG:O	2:H:175:LEU:C	2.52	0.51
3:I:166:THR:O	3:I:166:THR:HG22	2.10	0.51
3:I:384:TYR:CD1	3:I:385:LEU:N	2.78	0.51
1:A:151:ALA:HB2	1:A:175:THR:HG22	1.91	0.51
2:B:511:VAL:HG21	2:B:536:LEU:HD21	1.93	0.51
3:C:160:PHE:HB3	3:C:161:PRO:HD3	1.92	0.51
1:D:217:LEU:HG	2:E:475:PHE:CE1	2.45	0.51
2:E:152:LYS:O	2:E:159:LEU:HD13	2.11	0.51
1:G:57:TRP:HE1	2:H:142:ARG:NH2	2.07	0.51
2:H:141:GLU:HG3	2:H:142:ARG:N	2.26	0.51
1:A:103:ASN:HD21	2:B:142:ARG:NH2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:HD2	1:A:253:PHE:O	2.11	0.51
2:B:152:LYS:N	2:B:159:LEU:HD11	2.26	0.51
1:D:229:ARG:HD2	1:D:253:PHE:O	2.11	0.51
1:D:268:VAL:HG12	1:D:269:LEU:N	2.25	0.51
2:E:174:ARG:O	2:E:175:LEU:C	2.53	0.51
3:F:143:LYS:HG3	3:F:144:TRP:N	2.25	0.51
3:F:160:PHE:HB3	3:F:161:PRO:HD3	1.93	0.51
1:G:118:VAL:O	1:G:125:VAL:HA	2.10	0.51
1:G:225:VAL:HG13	1:G:257:LEU:CB	2.39	0.51
3:I:18:THR:HG23	3:I:41:GLU:OE1	2.10	0.51
3:I:359:ILE:HG21	3:I:404:VAL:CG1	2.40	0.51
2:B:202:ARG:NH2	2:B:209:GLN:O	2.44	0.51
1:D:54:GLY:HA3	1:D:75:TYR:HB3	1.93	0.51
2:E:511:VAL:HG21	2:E:536:LEU:HD21	1.93	0.51
1:G:54:GLY:HA3	1:G:75:TYR:HB3	1.93	0.51
1:G:229:ARG:HD2	1:G:253:PHE:O	2.11	0.51
2:H:512:MET:HA	2:H:540:ALA:CB	2.41	0.51
3:I:294:LEU:O	3:I:298:ILE:CD1	2.58	0.51
3:F:384:TYR:CA	3:F:387:ARG:HH12	2.15	0.51
1:G:180:ASN:ND2	1:G:205:ASP:N	2.59	0.51
1:G:283:GLU:HB2	1:G:289:TRP:CZ3	2.46	0.51
2:H:152:LYS:N	2:H:159:LEU:HD11	2.26	0.51
2:H:255:VAL:HG22	3:I:222:VAL:O	2.11	0.51
1:A:54:GLY:HA3	1:A:75:TYR:HB3	1.93	0.51
2:E:152:LYS:N	2:E:159:LEU:HD11	2.26	0.51
2:E:314:LYS:NZ	3:F:253:GLN:HB3	2.26	0.51
3:F:71:GLU:O	3:F:74:PHE:HB3	2.11	0.51
1:G:8:HIS:O	1:G:9:ASN:ND2	2.43	0.51
2:H:198:THR:CB	2:H:212:GLU:HB2	2.29	0.51
2:H:547:TYR:CD2	2:H:548:GLU:HG2	2.46	0.51
3:I:359:ILE:HG21	3:I:404:VAL:HG11	1.92	0.51
3:I:400:ASN:HB2	3:I:403:SER:OG	2.10	0.51
3:I:431:ILE:N	3:I:431:ILE:CD1	2.72	0.51
2:E:272:ILE:HG23	2:E:382:LEU:HG	1.93	0.51
3:F:417:ILE:HG23	3:F:429:ILE:HG23	1.93	0.51
1:A:27:CYS:HB2	1:A:56:VAL:HB	1.91	0.51
1:D:180:ASN:ND2	1:D:205:ASP:N	2.59	0.51
2:E:289:ASN:O	2:E:293:GLN:HG3	2.11	0.51
2:B:522:THR:HA	2:B:525:HIS:CB	2.39	0.50
2:B:527:LEU:HA	2:B:530:LEU:HD13	1.92	0.50
1:D:62:ALA:HB2	1:D:107:TRP:CE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:138:ILE:HG22	2:E:138:ILE:O	2.11	0.50
1:G:259:ARG:HB2	1:G:272:SER:HB2	1.92	0.50
2:H:202:ARG:NH2	2:H:209:GLN:O	2.44	0.50
3:I:54:ALA:O	3:I:55:ASN:C	2.53	0.50
3:I:71:GLU:O	3:I:74:PHE:HB3	2.11	0.50
3:I:235:GLN:HG2	3:I:236:GLY:N	2.25	0.50
1:A:180:ASN:ND2	1:A:205:ASP:N	2.59	0.50
2:B:152:LYS:O	2:B:159:LEU:HD13	2.11	0.50
2:B:272:ILE:HG23	2:B:382:LEU:HG	1.93	0.50
2:E:142:ARG:HG2	2:E:144:PHE:HE1	1.77	0.50
2:E:172:ILE:N	2:E:172:ILE:HD12	2.27	0.50
3:F:166:THR:O	3:F:166:THR:HG22	2.10	0.50
2:H:289:ASN:O	2:H:293:GLN:HG3	2.11	0.50
1:A:62:ALA:HB2	1:A:107:TRP:CE2	2.45	0.50
1:A:236:GLN:HB2	1:A:243:TRP:CE3	2.46	0.50
3:C:342:PRO:HG2	3:C:382:LYS:HD2	1.92	0.50
3:C:439:SER:C	3:C:441:CYS:H	2.18	0.50
3:F:70:LEU:CD2	3:F:343:ILE:HD11	2.30	0.50
3:F:294:LEU:O	3:F:298:ILE:CD1	2.59	0.50
1:A:217:LEU:CD1	1:A:218:LEU:H	2.23	0.50
1:A:225:VAL:HG13	1:A:257:LEU:CB	2.39	0.50
1:A:268:VAL:HG12	1:A:269:LEU:N	2.25	0.50
3:C:24:ILE:O	3:C:24:ILE:CG2	2.60	0.50
2:E:427:ALA:O	2:E:429:GLU:N	2.45	0.50
2:E:460:ASN:C	2:E:462:THR:H	2.19	0.50
3:F:77:LEU:HD23	3:F:77:LEU:C	2.36	0.50
3:C:25:GLU:HG2	3:C:25:GLU:O	2.12	0.50
3:C:54:ALA:O	3:C:55:ASN:C	2.55	0.50
2:E:202:ARG:NH2	2:E:209:GLN:O	2.44	0.50
2:E:527:LEU:HA	2:E:530:LEU:HD13	1.92	0.50
1:G:53:GLU:HB2	1:G:76:ASP:CB	2.42	0.50
1:G:57:TRP:NE1	2:H:142:ARG:HH21	2.04	0.50
2:H:142:ARG:O	2:H:143:ARG:HB2	2.12	0.50
2:H:460:ASN:C	2:H:462:THR:H	2.19	0.50
2:H:546:ARG:O	2:H:546:ARG:CG	2.60	0.50
3:I:23:LYS:NZ	3:I:431:ILE:HA	2.26	0.50
1:A:263:SER:HB3	2:B:153:PHE:CE1	2.47	0.50
2:B:142:ARG:HA	2:B:142:ARG:HH11	1.77	0.50
1:D:236:GLN:HB2	1:D:243:TRP:CE3	2.46	0.50
1:A:249:LYS:HE2	1:A:253:PHE:CE2	2.47	0.50
2:B:427:ALA:O	2:B:429:GLU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:TYR:CE2	2:B:454:ILE:HD11	2.47	0.50
1:G:154:ALA:HB2	1:G:212:TRP:CE3	2.46	0.50
2:H:442:THR:CG2	2:H:443:ASN:H	2.25	0.50
3:I:143:LYS:HG3	3:I:144:TRP:N	2.25	0.50
3:I:237:ILE:HD12	3:I:237:ILE:O	2.12	0.50
3:I:382:LYS:N	3:I:383:PRO:HD2	2.26	0.50
1:A:140:ILE:HG22	1:A:141:ILE:H	1.77	0.50
2:B:304:VAL:HG13	3:C:314:ILE:HD11	1.94	0.50
2:B:512:MET:HA	2:B:540:ALA:CB	2.41	0.50
3:C:166:THR:O	3:C:166:THR:HG22	2.10	0.50
3:F:9:THR:O	3:F:9:THR:HG22	2.11	0.50
3:F:380:ILE:O	3:F:380:ILE:HG22	2.12	0.50
1:G:236:GLN:HB2	1:G:243:TRP:CE3	2.47	0.50
1:G:249:LYS:HE2	1:G:253:PHE:CE2	2.47	0.50
2:H:152:LYS:O	2:H:159:LEU:HD13	2.11	0.50
2:H:272:ILE:HG23	2:H:382:LEU:HG	1.93	0.50
2:B:172:ILE:N	2:B:172:ILE:HD12	2.27	0.50
2:B:529:ARG:O	2:B:530:LEU:C	2.55	0.50
3:C:20:LYS:HE2	3:C:431:ILE:HD11	1.94	0.50
3:C:71:GLU:O	3:C:74:PHE:HB3	2.11	0.50
2:E:165:VAL:HG12	2:E:165:VAL:O	2.11	0.50
2:E:320:VAL:N	3:F:246:THR:HG21	2.26	0.50
2:E:512:MET:HA	2:E:540:ALA:CB	2.41	0.50
1:G:243:TRP:CD1	1:G:243:TRP:H	2.27	0.50
2:H:511:VAL:HG21	2:H:536:LEU:HD21	1.93	0.50
2:B:460:ASN:C	2:B:462:THR:H	2.19	0.49
3:C:227:ILE:C	3:C:227:ILE:HD12	2.37	0.49
1:D:53:GLU:HB2	1:D:76:ASP:CB	2.42	0.49
1:D:249:LYS:HE2	1:D:253:PHE:CE2	2.47	0.49
2:E:435:TYR:CE2	2:E:454:ILE:HD11	2.47	0.49
2:H:165:VAL:O	2:H:165:VAL:HG12	2.11	0.49
2:H:427:ALA:O	2:H:429:GLU:N	2.45	0.49
3:C:93:GLU:HG3	3:C:94:MET:H	1.76	0.49
2:E:442:THR:CG2	2:E:443:ASN:H	2.25	0.49
3:F:431:ILE:CD1	3:F:431:ILE:N	2.72	0.49
1:A:14:ASP:HB3	1:A:58:ARG:HA	1.95	0.49
3:C:58:ASP:C	3:C:60:SER:H	2.20	0.49
3:C:294:LEU:O	3:C:298:ILE:CD1	2.59	0.49
2:E:159:LEU:O	2:E:173:LYS:HB2	2.12	0.49
2:E:526:ILE:C	2:E:529:ARG:HB2	2.37	0.49
3:F:54:ALA:O	3:F:55:ASN:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:GLU:HG2	1:G:130:PHE:N	2.27	0.49
2:H:419:GLY:O	2:H:423:GLN:HG3	2.12	0.49
3:I:350:VAL:HG22	3:I:355:LEU:CD2	2.41	0.49
2:B:320:VAL:HA	3:C:246:THR:CG2	2.38	0.49
2:B:327:SER:OG	3:C:238:LYS:HG3	2.13	0.49
3:C:237:ILE:HD12	3:C:237:ILE:O	2.12	0.49
2:E:546:ARG:CG	2:E:546:ARG:O	2.59	0.49
3:I:77:LEU:HD23	3:I:77:LEU:C	2.36	0.49
3:I:227:ILE:C	3:I:227:ILE:HD12	2.37	0.49
2:B:159:LEU:O	2:B:173:LYS:HB2	2.12	0.49
2:B:466:SER:HB3	2:B:468:GLU:HG2	1.94	0.49
1:D:154:ALA:HB2	1:D:212:TRP:CE3	2.48	0.49
2:E:529:ARG:O	2:E:530:LEU:C	2.55	0.49
2:E:530:LEU:O	2:E:531:LYS:CG	2.59	0.49
3:F:58:ASP:C	3:F:60:SER:H	2.20	0.49
3:F:387:ARG:HG2	3:F:391:HIS:ND1	2.27	0.49
1:G:140:ILE:HG22	1:G:141:ILE:H	1.77	0.49
2:H:466:SER:HB3	2:H:468:GLU:HG2	1.95	0.49
3:I:384:TYR:O	3:I:388:ILE:HG13	2.13	0.49
3:I:387:ARG:HG2	3:I:391:HIS:ND1	2.28	0.49
2:B:419:GLY:O	2:B:423:GLN:HG3	2.13	0.49
2:B:546:ARG:CG	2:B:546:ARG:O	2.60	0.49
3:C:22:PHE:C	3:C:24:ILE:N	2.69	0.49
3:C:77:LEU:HD23	3:C:77:LEU:C	2.37	0.49
3:F:353:ASP:O	3:F:355:LEU:N	2.43	0.49
2:H:341:GLN:O	2:H:342:LYS:C	2.52	0.49
2:H:526:ILE:C	2:H:529:ARG:HB2	2.37	0.49
2:H:529:ARG:O	2:H:530:LEU:C	2.55	0.49
3:I:381:ASP:N	3:I:383:PRO:HD2	2.27	0.49
1:A:53:GLU:HB2	1:A:76:ASP:CB	2.42	0.49
3:C:282:TRP:HE3	3:C:283:GLU:OE2	1.96	0.49
3:F:237:ILE:HD12	3:F:237:ILE:O	2.12	0.49
2:H:435:TYR:CE2	2:H:454:ILE:HD11	2.47	0.49
3:I:11:ARG:C	3:I:13:THR:N	2.71	0.49
1:A:48:THR:O	1:A:49:LEU:HD23	2.13	0.49
2:B:442:THR:CG2	2:B:443:ASN:H	2.25	0.49
3:C:77:LEU:HD21	3:C:81:LEU:HD12	1.95	0.49
2:H:172:ILE:HD12	2:H:172:ILE:N	2.27	0.49
2:H:304:VAL:CG1	3:I:314:ILE:HD11	2.43	0.49
3:I:353:ASP:O	3:I:355:LEU:N	2.44	0.49
2:B:197:VAL:HG12	2:B:210:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:387:ARG:HG2	3:C:391:HIS:ND1	2.28	0.49
3:C:410:SER:HA	3:C:436:LEU:HD11	1.94	0.49
1:D:112:TYR:CZ	1:D:171:ARG:HG2	2.48	0.49
1:D:259:ARG:HH11	1:D:259:ARG:HG3	1.78	0.49
3:F:227:ILE:C	3:F:227:ILE:HD12	2.37	0.49
1:G:31:LYS:HD3	1:G:52:HIS:O	2.13	0.49
2:H:522:THR:HA	2:H:525:HIS:CB	2.39	0.49
1:A:57:TRP:HA	1:A:57:TRP:HE3	1.78	0.49
1:A:259:ARG:HH11	1:A:259:ARG:HG3	1.78	0.49
2:B:530:LEU:O	2:B:531:LYS:CG	2.59	0.49
2:E:197:VAL:HG12	2:E:210:ILE:HG23	1.94	0.49
3:F:50:ALA:HB1	3:F:69:GLU:CG	2.42	0.49
1:G:11:LEU:HD23	2:H:162:LYS:NZ	2.28	0.49
1:G:259:ARG:HG3	1:G:259:ARG:HH11	1.78	0.49
2:H:524:ASP:CA	2:H:527:LEU:HD12	2.35	0.49
3:I:12:PHE:H	3:I:12:PHE:HD1	1.49	0.49
3:I:207:SER:HA	3:I:210:MET:HE3	1.95	0.49
3:C:433:ALA:O	3:C:435:PHE:N	2.46	0.48
3:C:434:THR:O	3:C:434:THR:CG2	2.61	0.48
1:D:48:THR:O	1:D:49:LEU:HD23	2.13	0.48
2:E:419:GLY:O	2:E:423:GLN:HG3	2.13	0.48
2:H:155:THR:HG22	2:H:513:ARG:CD	2.43	0.48
2:H:159:LEU:O	2:H:173:LYS:HB2	2.12	0.48
3:I:237:ILE:HD11	3:I:240:HIS:HA	1.95	0.48
2:B:526:ILE:C	2:B:529:ARG:HB2	2.37	0.48
3:C:384:TYR:CA	3:C:387:ARG:HH12	2.15	0.48
1:D:205:ASP:CB	1:D:227:GLN:HB3	2.44	0.48
2:E:508:LYS:HG2	2:E:509:ARG:N	2.28	0.48
2:B:145:THR:O	2:B:147:SER:N	2.46	0.48
3:C:365:MET:HB3	3:C:379:ILE:HG22	1.94	0.48
2:E:160:LEU:HD23	2:E:172:ILE:HA	1.96	0.48
3:F:148:ILE:HD13	3:F:153:LEU:HD12	1.95	0.48
2:H:530:LEU:O	2:H:531:LYS:CG	2.59	0.48
1:D:202:GLY:HA2	1:D:245:LYS:NZ	2.29	0.48
1:A:129:GLU:HG2	1:A:130:PHE:N	2.27	0.48
3:C:148:ILE:HD13	3:C:153:LEU:HD12	1.95	0.48
3:C:350:VAL:HG22	3:C:355:LEU:CD2	2.41	0.48
1:D:129:GLU:HG2	1:D:130:PHE:N	2.27	0.48
1:D:140:ILE:HG22	1:D:141:ILE:H	1.77	0.48
2:E:399:LEU:HB3	2:E:425:TYR:OH	2.14	0.48
3:F:77:LEU:HD21	3:F:81:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:TRP:HA	1:G:57:TRP:HE3	1.78	0.48
2:H:197:VAL:HG12	2:H:210:ILE:HG23	1.94	0.48
3:I:282:TRP:HE3	3:I:283:GLU:OE2	1.97	0.48
2:B:145:THR:C	2:B:147:SER:H	2.22	0.48
2:B:172:ILE:HD12	2:B:172:ILE:H	1.79	0.48
3:C:11:ARG:HG2	3:C:12:PHE:HD1	1.78	0.48
1:D:270:ALA:HB2	2:E:153:PHE:CE1	2.49	0.48
2:E:154:SER:HB3	2:E:158:MET:H	1.79	0.48
2:E:449:PHE:HE2	2:E:453:LEU:HD12	1.79	0.48
2:E:466:SER:HB3	2:E:468:GLU:HG2	1.94	0.48
3:F:58:ASP:C	3:F:60:SER:N	2.69	0.48
3:F:282:TRP:HE3	3:F:283:GLU:OE2	1.96	0.48
3:F:305:ASN:O	3:F:306:ASN:C	2.56	0.48
3:F:416:TYR:HE2	3:F:432:TYR:CZ	2.32	0.48
2:H:449:PHE:HE2	2:H:453:LEU:HD12	1.78	0.48
3:I:433:ALA:O	3:I:435:PHE:N	2.46	0.48
1:A:31:LYS:HD3	1:A:52:HIS:O	2.13	0.48
2:B:341:GLN:O	2:B:342:LYS:C	2.52	0.48
3:C:355:LEU:N	3:C:356:PRO:HD2	2.29	0.48
2:E:491:LEU:HD12	2:E:507:ILE:HD13	1.95	0.48
2:E:522:THR:HA	2:E:525:HIS:CB	2.39	0.48
3:F:207:SER:HA	3:F:210:MET:HE3	1.95	0.48
1:G:227:GLN:C	1:G:229:ARG:H	2.22	0.48
2:H:527:LEU:C	2:H:529:ARG:N	2.71	0.48
2:B:135:ALA:O	2:B:138:ILE:N	2.46	0.48
2:B:508:LYS:HG2	2:B:509:ARG:N	2.29	0.48
3:C:237:ILE:HD11	3:C:240:HIS:HA	1.95	0.48
2:E:327:SER:OG	3:F:238:LYS:CG	2.62	0.48
3:F:237:ILE:HD11	3:F:240:HIS:HA	1.95	0.48
3:F:355:LEU:N	3:F:356:PRO:HD2	2.29	0.48
1:G:20:TYR:CE2	2:H:544:LYS:CD	2.97	0.48
1:G:52:HIS:CE1	1:G:80:LEU:HD12	2.49	0.48
1:G:117:LEU:HB2	1:G:153:TRP:NE1	2.29	0.48
1:G:157:THR:HG21	2:H:501:LYS:HZ2	1.79	0.48
2:H:314:LYS:HE3	3:I:162:LEU:HB3	1.95	0.48
3:I:189:LEU:HD23	3:I:189:LEU:HA	1.71	0.48
1:A:280:LEU:HB2	1:A:292:ALA:O	2.14	0.48
1:D:31:LYS:HD3	1:D:52:HIS:O	2.13	0.48
2:E:392:GLY:O	2:E:393:GLN:HB2	2.14	0.48
3:F:406:GLU:HG2	3:F:409:LYS:HZ1	1.78	0.48
1:G:48:THR:O	1:G:49:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:94:MET:HE2	3:I:108:LYS:HB2	1.95	0.48
1:A:171:ARG:O	1:A:172:LYS:HG3	2.14	0.48
3:C:207:SER:HA	3:C:210:MET:HE3	1.96	0.48
3:C:364:GLU:C	3:C:366:LEU:N	2.69	0.48
3:F:355:LEU:H	3:F:356:PRO:HD2	1.79	0.48
3:F:433:ALA:O	3:F:435:PHE:N	2.45	0.48
1:G:171:ARG:O	1:G:172:LYS:HG3	2.14	0.48
2:H:392:GLY:O	2:H:393:GLN:HB2	2.14	0.48
3:I:86:ASN:OD1	3:I:399:ILE:HG22	2.14	0.48
3:I:305:ASN:O	3:I:306:ASN:C	2.56	0.48
1:A:121:SER:C	1:A:123:GLY:H	2.22	0.47
1:A:205:ASP:CB	1:A:227:GLN:HB3	2.43	0.47
1:A:227:GLN:C	1:A:229:ARG:H	2.22	0.47
2:B:508:LYS:HA	2:B:536:LEU:HD11	1.96	0.47
3:C:428:ASN:C	3:C:430:PRO:CD	2.87	0.47
2:E:515:ILE:HD12	2:E:544:LYS:HB2	1.95	0.47
2:H:172:ILE:HD12	2:H:172:ILE:H	1.79	0.47
3:I:104:LEU:CD1	3:I:224:ASP:HB3	2.44	0.47
3:F:428:ASN:C	3:F:430:PRO:CD	2.87	0.47
1:G:127:VAL:HG21	1:G:194:TYR:CE1	2.49	0.47
1:G:253:PHE:O	1:G:255:ASP:N	2.48	0.47
1:A:290:GLU:HG3	1:A:291:PRO:HD2	1.96	0.47
3:C:170:ASP:OD1	3:C:172:LYS:N	2.47	0.47
3:C:355:LEU:H	3:C:356:PRO:HD2	1.79	0.47
1:D:121:SER:C	1:D:123:GLY:H	2.22	0.47
3:F:437:ASN:O	3:F:437:ASN:OD1	2.33	0.47
1:G:280:LEU:HB2	1:G:292:ALA:O	2.14	0.47
2:H:358:TYR:HE2	3:I:210:MET:HE1	1.79	0.47
2:H:508:LYS:HG2	2:H:509:ARG:N	2.29	0.47
3:I:148:ILE:HD13	3:I:153:LEU:HD12	1.96	0.47
3:I:428:ASN:C	3:I:430:PRO:CD	2.87	0.47
2:B:154:SER:HB3	2:B:158:MET:H	1.79	0.47
2:B:515:ILE:O	2:B:519:ARG:HG3	2.15	0.47
1:D:57:TRP:HA	1:D:57:TRP:HE3	1.78	0.47
1:D:253:PHE:O	1:D:255:ASP:N	2.48	0.47
3:F:242:LEU:HB2	3:F:312:GLU:HG2	1.96	0.47
3:F:341:HIS:CE1	3:F:343:ILE:HD12	2.50	0.47
2:H:160:LEU:HD23	2:H:172:ILE:HA	1.96	0.47
3:I:77:LEU:HD21	3:I:81:LEU:HD12	1.95	0.47
3:I:355:LEU:N	3:I:356:PRO:HD2	2.30	0.47
1:A:202:GLY:HA2	1:A:245:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:PHE:O	1:A:255:ASP:N	2.48	0.47
2:B:160:LEU:HD23	2:B:172:ILE:HA	1.95	0.47
2:B:491:LEU:HD12	2:B:507:ILE:HD13	1.95	0.47
1:D:117:LEU:HB2	1:D:153:TRP:NE1	2.29	0.47
3:F:350:VAL:HG22	3:F:355:LEU:CD2	2.41	0.47
1:G:57:TRP:HA	1:G:57:TRP:CE3	2.49	0.47
2:H:210:ILE:H	2:H:210:ILE:CD1	2.21	0.47
2:H:515:ILE:HD12	2:H:544:LYS:HB2	1.94	0.47
3:I:355:LEU:H	3:I:356:PRO:HD2	1.80	0.47
3:I:434:THR:O	3:I:434:THR:CG2	2.61	0.47
2:B:515:ILE:HD12	2:B:544:LYS:HB2	1.95	0.47
1:D:14:ASP:HB3	1:D:58:ARG:HA	1.95	0.47
1:D:227:GLN:C	1:D:229:ARG:H	2.22	0.47
2:E:324:TYR:CD2	3:F:237:ILE:HG21	2.48	0.47
1:G:202:GLY:HA2	1:G:245:LYS:NZ	2.29	0.47
2:H:221:LEU:HD22	2:H:231:TYR:CD1	2.49	0.47
2:H:495:CYS:C	2:H:497:LEU:H	2.23	0.47
2:H:522:THR:O	2:H:526:ILE:HG13	2.15	0.47
1:A:206:TRP:H	1:A:206:TRP:CD1	2.33	0.47
1:A:215:THR:HG23	1:A:215:THR:O	2.15	0.47
2:B:366:PHE:O	2:B:368:GLY:N	2.43	0.47
2:B:392:GLY:O	2:B:393:GLN:HB2	2.14	0.47
2:B:449:PHE:HE2	2:B:453:LEU:HD12	1.78	0.47
2:B:522:THR:O	2:B:526:ILE:HG13	2.15	0.47
3:C:104:LEU:CD1	3:C:224:ASP:HB3	2.44	0.47
3:C:235:GLN:HG2	3:C:236:GLY:N	2.30	0.47
1:D:52:HIS:CE1	1:D:80:LEU:HD12	2.49	0.47
1:D:57:TRP:HA	1:D:57:TRP:CE3	2.49	0.47
1:D:140:ILE:CG2	1:D:141:ILE:N	2.78	0.47
1:D:280:LEU:HB2	1:D:292:ALA:O	2.14	0.47
1:D:290:GLU:HG3	1:D:291:PRO:HD2	1.97	0.47
3:F:94:MET:HE2	3:F:108:LYS:CB	2.42	0.47
3:F:104:LEU:CD1	3:F:224:ASP:HB3	2.44	0.47
1:G:14:ASP:HB3	1:G:58:ARG:HA	1.95	0.47
2:H:154:SER:HB3	2:H:158:MET:H	1.79	0.47
2:H:250:THR:HG23	3:I:99:TYR:OH	2.13	0.47
2:H:399:LEU:HB3	2:H:425:TYR:OH	2.14	0.47
2:H:491:LEU:HD12	2:H:507:ILE:HD13	1.96	0.47
3:I:24:ILE:HG22	3:I:25:GLU:N	2.28	0.47
3:I:317:LEU:HA	3:I:317:LEU:HD23	1.59	0.47
3:C:16:SER:HB2	3:C:432:TYR:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:313:LEU:HD13	2:E:341:GLN:HB3	1.97	0.47
1:D:11:LEU:HD23	2:E:162:LYS:NZ	2.29	0.47
1:D:208:ARG:HH21	2:E:143:ARG:HG3	1.80	0.47
1:D:217:LEU:CG	1:D:218:LEU:H	2.28	0.47
2:E:495:CYS:C	2:E:497:LEU:H	2.23	0.47
2:E:508:LYS:HA	2:E:536:LEU:HD11	1.97	0.47
1:G:57:TRP:NE1	2:H:142:ARG:NH2	2.62	0.47
1:G:74:SER:HB3	1:G:76:ASP:OD1	2.15	0.47
1:G:205:ASP:CB	1:G:227:GLN:HB3	2.44	0.47
3:I:242:LEU:HB2	3:I:312:GLU:HG2	1.96	0.47
1:A:52:HIS:CE1	1:A:80:LEU:HD12	2.49	0.47
3:C:11:ARG:CG	3:C:12:PHE:CD1	2.97	0.47
3:C:305:ASN:O	3:C:306:ASN:C	2.56	0.47
1:D:215:THR:HG23	1:D:215:THR:O	2.15	0.47
3:F:364:GLU:C	3:F:366:LEU:H	2.23	0.47
1:G:43:HIS:ND1	1:G:43:HIS:N	2.63	0.47
1:G:102:VAL:HG13	1:G:118:VAL:HG13	1.97	0.47
1:G:121:SER:C	1:G:123:GLY:H	2.22	0.47
1:G:141:ILE:HD12	1:G:185:TRP:CE3	2.50	0.47
2:H:435:TYR:OH	2:H:450:CYS:HB3	2.15	0.47
3:I:7:TYR:O	3:I:9:THR:N	2.47	0.47
1:A:57:TRP:HA	1:A:57:TRP:CE3	2.49	0.47
1:A:117:LEU:HB2	1:A:153:TRP:NE1	2.29	0.47
1:A:217:LEU:CG	1:A:218:LEU:H	2.28	0.47
2:B:399:LEU:HB3	2:B:425:TYR:OH	2.14	0.47
2:E:172:ILE:HD12	2:E:172:ILE:H	1.79	0.47
2:H:364:SER:HB3	2:H:367:GLU:HB2	1.97	0.47
2:H:515:ILE:O	2:H:519:ARG:HG3	2.14	0.47
3:I:89:LEU:HD22	3:I:114:LYS:NZ	2.17	0.47
3:C:274:GLN:O	3:C:278:GLN:HB3	2.15	0.46
3:C:284:SER:O	3:C:287:HIS:HB3	2.15	0.46
3:C:341:HIS:CE1	3:C:343:ILE:HD12	2.50	0.46
1:D:171:ARG:O	1:D:172:LYS:HG3	2.14	0.46
2:E:142:ARG:O	2:E:143:ARG:HG2	2.14	0.46
2:E:276:ILE:O	2:E:277:GLY:C	2.58	0.46
2:E:333:ARG:HG2	2:E:362:SER:O	2.15	0.46
1:G:11:LEU:HD23	2:H:162:LYS:HZ1	1.80	0.46
1:G:206:TRP:CD1	1:G:206:TRP:H	2.33	0.46
1:A:43:HIS:ND1	1:A:43:HIS:N	2.63	0.46
1:A:205:ASP:CG	1:A:227:GLN:HB3	2.40	0.46
3:C:139:VAL:CG1	3:C:140:PRO:HD2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:310:THR:CG2	3:C:311:ASP:N	2.78	0.46
2:E:206:PRO:O	2:E:533:PRO:HG3	2.15	0.46
2:E:515:ILE:O	2:E:519:ARG:HG3	2.15	0.46
2:E:522:THR:O	2:E:526:ILE:HG13	2.15	0.46
3:F:274:GLN:O	3:F:278:GLN:HB3	2.15	0.46
1:D:63:HIS:C	1:D:65:LYS:N	2.74	0.46
1:D:205:ASP:CG	1:D:227:GLN:HB3	2.40	0.46
2:E:221:LEU:HD22	2:E:231:TYR:CD1	2.50	0.46
3:F:379:ILE:C	3:F:381:ASP:H	2.23	0.46
3:I:170:ASP:OD1	3:I:172:LYS:N	2.48	0.46
3:I:341:HIS:CE1	3:I:343:ILE:HD12	2.50	0.46
2:B:134:ASN:O	2:B:138:ILE:HG13	2.15	0.46
2:B:221:LEU:HD22	2:B:231:TYR:CD1	2.49	0.46
2:B:276:ILE:O	2:B:277:GLY:C	2.59	0.46
3:C:439:SER:C	3:C:441:CYS:N	2.73	0.46
1:D:63:HIS:O	1:D:65:LYS:N	2.49	0.46
2:E:340:LEU:HD22	2:E:370:PHE:CG	2.50	0.46
3:F:170:ASP:OD1	3:F:172:LYS:N	2.48	0.46
1:G:65:LYS:CA	2:H:546:ARG:NH2	2.73	0.46
1:G:205:ASP:CG	1:G:227:GLN:HB3	2.40	0.46
1:G:215:THR:HG23	1:G:215:THR:O	2.15	0.46
2:H:508:LYS:HA	2:H:536:LEU:HD11	1.96	0.46
3:I:274:GLN:O	3:I:278:GLN:HB3	2.15	0.46
1:A:63:HIS:C	1:A:65:LYS:N	2.74	0.46
2:B:206:PRO:O	2:B:533:PRO:HG3	2.15	0.46
2:B:435:TYR:OH	2:B:450:CYS:HB3	2.15	0.46
1:D:206:TRP:H	1:D:206:TRP:CD1	2.33	0.46
3:F:313:LEU:HB3	2:H:338:LEU:HD11	1.98	0.46
1:G:37:GLU:CG	1:G:46:ILE:HD12	2.45	0.46
1:G:53:GLU:HB2	1:G:76:ASP:HB3	1.98	0.46
2:H:155:THR:C	2:H:513:ARG:HD2	2.38	0.46
2:H:333:ARG:HG2	2:H:362:SER:O	2.15	0.46
1:A:53:GLU:HB2	1:A:76:ASP:HB3	1.98	0.46
1:A:61:TRP:O	1:A:107:TRP:CD1	2.69	0.46
1:A:151:ALA:CB	1:A:175:THR:HG22	2.46	0.46
2:B:526:ILE:O	2:B:529:ARG:HB2	2.16	0.46
1:D:229:ARG:HH11	1:D:252:LYS:HB3	1.81	0.46
2:E:250:THR:CG2	2:E:255:VAL:HB	2.45	0.46
2:E:546:ARG:O	2:E:546:ARG:HG2	2.15	0.46
1:G:290:GLU:HG3	1:G:291:PRO:HD2	1.97	0.46
2:H:206:PRO:O	2:H:533:PRO:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:546:ARG:O	2:H:546:ARG:HG2	2.15	0.46
3:I:281:ASP:O	3:I:282:TRP:C	2.59	0.46
1:A:37:GLU:CG	1:A:46:ILE:HD12	2.45	0.46
2:B:327:SER:HA	3:C:238:LYS:HE3	1.98	0.46
1:D:37:GLU:CG	1:D:46:ILE:HD12	2.45	0.46
2:E:514:GLU:O	2:E:516:THR:N	2.49	0.46
3:F:7:TYR:CD1	3:F:7:TYR:N	2.84	0.46
3:F:59:GLU:HA	3:F:62:VAL:HG23	1.98	0.46
2:H:259:LEU:HD11	3:I:99:TYR:CG	2.50	0.46
2:H:348:CYS:O	2:H:349:SER:OG	2.30	0.46
3:I:36:PHE:HB3	3:I:40:ARG:HH21	1.81	0.46
1:A:63:HIS:O	1:A:65:LYS:N	2.49	0.46
1:A:78:LYS:CA	1:A:96:ALA:HB2	2.41	0.46
1:A:253:PHE:C	1:A:255:ASP:H	2.24	0.46
2:B:452:TYR:HD2	2:B:452:TYR:O	1.98	0.46
3:C:104:LEU:HA	3:C:104:LEU:HD23	1.72	0.46
2:E:142:ARG:HG3	2:E:142:ARG:NH1	2.31	0.46
2:E:527:LEU:C	2:E:529:ARG:N	2.71	0.46
3:F:10:GLU:HG3	3:F:11:ARG:N	2.31	0.46
3:F:36:PHE:HB3	3:F:40:ARG:HH21	1.80	0.46
3:F:434:THR:O	3:F:434:THR:CG2	2.61	0.46
1:G:63:HIS:C	1:G:65:LYS:N	2.74	0.46
1:G:229:ARG:HH11	1:G:252:LYS:HB3	1.80	0.46
3:I:21:GLU:HB3	3:I:25:GLU:CD	2.40	0.46
3:I:237:ILE:C	3:I:237:ILE:CD1	2.75	0.46
1:A:261:SER:HB2	2:B:152:LYS:HA	1.91	0.46
2:B:417:PRO:HG2	2:B:418:ILE:HD13	1.98	0.46
1:D:57:TRP:CH2	2:E:144:PHE:CE1	3.04	0.46
2:E:234:TRP:CH2	2:E:452:TYR:CD1	3.04	0.46
2:E:435:TYR:OH	2:E:450:CYS:HB3	2.15	0.46
3:F:68:TRP:CH2	3:F:387:ARG:NH2	2.84	0.46
2:H:452:TYR:O	2:H:452:TYR:HD2	1.99	0.46
2:H:526:ILE:O	2:H:529:ARG:HB2	2.16	0.46
2:B:164:ILE:HG13	2:B:164:ILE:O	2.15	0.46
3:C:406:GLU:HA	3:C:409:LYS:CE	2.45	0.46
2:E:210:ILE:HD12	2:E:495:CYS:CB	2.46	0.46
2:E:318:LEU:HD23	2:E:318:LEU:O	2.16	0.46
3:F:13:THR:O	3:F:17:ASP:CB	2.51	0.46
3:F:441:CYS:O	3:F:441:CYS:SG	2.74	0.46
2:H:250:THR:CG2	2:H:255:VAL:HB	2.45	0.46
2:H:338:LEU:O	2:H:342:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:417:PRO:HG2	2:H:418:ILE:HD13	1.98	0.46
1:A:102:VAL:HG13	1:A:118:VAL:HG13	1.98	0.45
1:A:140:ILE:CG2	1:A:141:ILE:N	2.78	0.45
2:B:250:THR:CG2	2:B:255:VAL:HB	2.45	0.45
2:B:333:ARG:HG2	2:B:362:SER:O	2.16	0.45
2:B:338:LEU:O	2:B:342:LYS:HG3	2.16	0.45
2:B:420:VAL:CG1	2:B:438:VAL:HG11	2.46	0.45
3:C:242:LEU:HB2	3:C:312:GLU:HG2	1.97	0.45
1:D:10:GLU:OE1	1:D:10:GLU:N	2.45	0.45
2:E:225:GLU:C	2:E:227:THR:N	2.73	0.45
3:F:139:VAL:CG1	3:F:140:PRO:HD2	2.43	0.45
1:G:140:ILE:CG2	1:G:141:ILE:N	2.78	0.45
2:H:234:TRP:CH2	2:H:452:TYR:CD1	3.04	0.45
3:I:139:VAL:CG1	3:I:140:PRO:HD2	2.42	0.45
3:I:284:SER:O	3:I:287:HIS:HB3	2.16	0.45
1:A:8:HIS:O	1:A:9:ASN:CB	2.65	0.45
1:A:151:ALA:HA	1:A:174:VAL:O	2.16	0.45
1:D:61:TRP:O	1:D:107:TRP:CD1	2.69	0.45
1:D:102:VAL:HG13	1:D:118:VAL:HG13	1.97	0.45
2:E:338:LEU:O	2:E:342:LYS:HG3	2.16	0.45
2:E:342:LYS:HD2	3:F:206:ILE:CD1	2.47	0.45
3:F:284:SER:O	3:F:287:HIS:HB3	2.16	0.45
1:G:217:LEU:CG	1:G:218:LEU:H	2.28	0.45
2:H:318:LEU:HD23	2:H:318:LEU:O	2.16	0.45
3:I:8:GLN:C	3:I:10:GLU:N	2.53	0.45
3:I:294:LEU:O	3:I:298:ILE:HD12	2.17	0.45
3:C:36:PHE:HB3	3:C:40:ARG:HH21	1.81	0.45
3:C:269:GLY:HA3	3:C:295:GLN:CG	2.42	0.45
3:C:281:ASP:O	3:C:282:TRP:C	2.60	0.45
1:D:253:PHE:C	1:D:255:ASP:H	2.24	0.45
1:G:61:TRP:O	1:G:107:TRP:CD1	2.69	0.45
2:H:225:GLU:O	2:H:231:TYR:HB2	2.15	0.45
2:H:343:TRP:C	2:H:345:THR:H	2.24	0.45
3:I:413:ILE:O	3:I:417:ILE:HG13	2.17	0.45
2:B:210:ILE:HD12	2:B:495:CYS:CB	2.46	0.45
2:B:495:CYS:C	2:B:497:LEU:H	2.23	0.45
3:C:23:LYS:O	3:C:26:GLN:OE1	2.34	0.45
3:C:144:TRP:O	3:C:148:ILE:HG12	2.17	0.45
3:C:413:ILE:O	3:C:417:ILE:HG13	2.17	0.45
2:E:225:GLU:O	2:E:231:TYR:HB2	2.16	0.45
2:E:366:PHE:O	2:E:368:GLY:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:417:PRO:HG2	2:E:418:ILE:HD13	1.98	0.45
3:F:233:THR:HG22	3:F:234:GLN:O	2.17	0.45
3:F:406:GLU:HA	3:F:409:LYS:CE	2.45	0.45
2:H:276:ILE:O	2:H:277:GLY:C	2.59	0.45
3:I:406:GLU:HG2	3:I:409:LYS:HZ1	1.80	0.45
2:B:246:TYR:HA	2:B:247:PRO:HD2	1.76	0.45
3:C:183:TYR:CE2	3:C:199:GLU:HG3	2.52	0.45
1:G:253:PHE:C	1:G:255:ASP:H	2.24	0.45
2:B:210:ILE:H	2:B:210:ILE:CD1	2.22	0.45
2:B:364:SER:HB3	2:B:367:GLU:HB2	1.98	0.45
3:C:18:THR:O	3:C:19:LEU:C	2.59	0.45
3:C:406:GLU:HG2	3:C:409:LYS:HZ1	1.81	0.45
2:E:265:HIS:HB2	2:E:399:LEU:CD2	2.42	0.45
2:E:526:ILE:O	2:E:529:ARG:HB2	2.16	0.45
3:F:294:LEU:O	3:F:298:ILE:HD12	2.17	0.45
2:H:210:ILE:HD12	2:H:495:CYS:CB	2.46	0.45
1:A:126:SER:HB3	1:A:140:ILE:CG1	2.28	0.45
3:C:189:LEU:HD23	3:C:189:LEU:HA	1.70	0.45
1:D:43:HIS:ND1	1:D:43:HIS:N	2.63	0.45
1:D:74:SER:HB3	1:D:76:ASP:OD1	2.16	0.45
1:D:205:ASP:O	1:D:206:TRP:C	2.60	0.45
3:F:42:PHE:CZ	3:F:391:HIS:HB3	2.52	0.45
3:F:144:TRP:O	3:F:148:ILE:HG12	2.17	0.45
1:G:63:HIS:O	1:G:65:LYS:N	2.49	0.45
1:G:205:ASP:O	1:G:206:TRP:C	2.60	0.45
2:H:215:LEU:HB3	2:H:452:TYR:CE2	2.52	0.45
1:A:74:SER:HB3	1:A:76:ASP:OD1	2.15	0.45
2:B:215:LEU:HB3	2:B:452:TYR:CE2	2.52	0.45
3:C:206:ILE:H	3:C:206:ILE:HD12	1.82	0.45
3:C:353:ASP:O	3:C:355:LEU:N	2.44	0.45
1:D:232:ILE:HG12	1:D:247:LEU:CD2	2.38	0.45
2:E:340:LEU:CD2	2:E:370:PHE:CG	2.99	0.45
2:E:420:VAL:CG1	2:E:438:VAL:HG11	2.46	0.45
2:H:420:VAL:CG1	2:H:438:VAL:HG11	2.46	0.45
3:I:102:ARG:NH2	3:I:241:SER:OG	2.45	0.45
3:I:144:TRP:O	3:I:148:ILE:HG12	2.17	0.45
1:A:229:ARG:HH11	1:A:252:LYS:HB3	1.81	0.45
2:B:234:TRP:CH2	2:B:452:TYR:CD1	3.04	0.45
2:B:514:GLU:O	2:B:516:THR:N	2.50	0.45
3:C:135:ARG:HG3	3:C:183:TYR:CE2	2.52	0.45
3:C:313:LEU:O	2:E:342:LYS:HE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:LEU:HD13	1:D:218:LEU:HB2	1.99	0.45
2:E:197:VAL:HG11	2:E:210:ILE:CG1	2.47	0.45
2:E:215:LEU:HB3	2:E:452:TYR:CE2	2.52	0.45
2:E:343:TRP:C	2:E:345:THR:H	2.25	0.45
2:E:452:TYR:HD2	2:E:452:TYR:O	1.98	0.45
3:F:319:SER:CB	2:H:337:GLU:HG2	2.47	0.45
1:G:151:ALA:HB2	1:G:175:THR:HG22	1.99	0.45
2:H:142:ARG:O	2:H:143:ARG:CB	2.65	0.45
1:A:205:ASP:O	1:A:206:TRP:C	2.60	0.45
2:B:327:SER:OG	3:C:238:LYS:N	2.33	0.45
1:D:127:VAL:HG21	1:D:194:TYR:CE1	2.52	0.45
2:E:233:LEU:HD21	2:E:421:ILE:CD1	2.47	0.45
3:F:48:GLN:HA	3:F:51:LEU:HD12	1.99	0.45
3:F:281:ASP:O	3:F:282:TRP:C	2.59	0.45
3:F:413:ILE:O	3:F:417:ILE:HG13	2.17	0.45
1:G:9:ASN:HD21	1:G:34:LYS:HE3	1.81	0.45
1:G:10:GLU:OE1	1:G:10:GLU:N	2.45	0.45
2:B:348:CYS:O	2:B:349:SER:OG	2.30	0.44
2:B:374:GLU:C	2:B:376:GLU:H	2.25	0.44
2:B:546:ARG:O	2:B:546:ARG:HG2	2.15	0.44
1:D:17:LEU:HD21	2:E:160:LEU:CD1	2.43	0.44
1:D:53:GLU:HB2	1:D:76:ASP:HB3	1.98	0.44
3:F:70:LEU:HB3	3:F:343:ILE:HD11	1.99	0.44
3:F:77:LEU:HD12	3:F:125:TRP:CZ2	2.52	0.44
3:F:183:TYR:CE2	3:F:199:GLU:HG3	2.52	0.44
3:F:329:ASN:O	3:F:332:ALA:HB3	2.17	0.44
1:G:58:ARG:NH2	1:G:259:ARG:HE	2.14	0.44
2:H:525:HIS:C	2:H:529:ARG:HD2	2.42	0.44
1:A:76:ASP:C	1:A:78:LYS:H	2.25	0.44
1:A:217:LEU:HD13	1:A:218:LEU:HB2	1.99	0.44
2:B:155:THR:HG22	2:B:513:ARG:CG	2.48	0.44
2:B:318:LEU:O	2:B:318:LEU:HD23	2.16	0.44
3:C:12:PHE:H	3:C:12:PHE:HD1	1.61	0.44
2:E:327:SER:C	2:E:329:ASP:N	2.75	0.44
3:F:135:ARG:HG3	3:F:183:TYR:CE2	2.52	0.44
2:H:153:PHE:HA	2:H:159:LEU:CD2	2.46	0.44
2:H:366:PHE:O	2:H:368:GLY:N	2.47	0.44
2:H:514:GLU:O	2:H:516:THR:N	2.50	0.44
2:H:538:PHE:O	2:H:541:GLN:HB3	2.17	0.44
3:I:183:TYR:CE2	3:I:199:GLU:HG3	2.52	0.44
3:I:329:ASN:O	3:I:332:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:VAL:HG11	2:B:210:ILE:CG1	2.47	0.44
2:B:225:GLU:O	2:B:231:TYR:HB2	2.16	0.44
2:B:525:HIS:C	2:B:529:ARG:HD2	2.42	0.44
1:D:151:ALA:HB2	1:D:175:THR:HG22	1.99	0.44
1:D:208:ARG:HD3	1:D:208:ARG:HA	1.81	0.44
2:E:538:PHE:O	2:E:541:GLN:HB3	2.18	0.44
1:G:19:TYR:CD2	2:H:543:LEU:HD21	2.52	0.44
1:G:76:ASP:C	1:G:78:LYS:H	2.25	0.44
1:G:96:ALA:C	1:G:98:HIS:N	2.76	0.44
2:H:184:LEU:HD23	2:H:184:LEU:HA	1.85	0.44
2:H:233:LEU:HD21	2:H:421:ILE:CD1	2.48	0.44
1:A:232:ILE:HG12	1:A:247:LEU:CD2	2.38	0.44
1:A:262:TRP:C	2:B:153:PHE:CD1	2.95	0.44
2:B:142:ARG:HG3	2:B:142:ARG:NH1	2.33	0.44
2:B:175:LEU:CD1	2:B:176:PRO:HD2	2.42	0.44
2:B:327:SER:C	2:B:329:ASP:N	2.75	0.44
3:C:39:ILE:HD11	3:C:399:ILE:HD11	1.99	0.44
3:C:225:THR:HG22	3:C:226:GLN:N	2.32	0.44
1:G:126:SER:HB3	1:G:140:ILE:CG1	2.28	0.44
1:G:281:TRP:CD1	1:G:281:TRP:N	2.86	0.44
2:H:136:LYS:C	2:H:139:MET:HB3	2.43	0.44
3:C:34:ASP:CB	3:C:35:PRO:CD	2.93	0.44
3:C:358:VAL:O	3:C:361:SER:HB3	2.18	0.44
1:D:76:ASP:C	1:D:78:LYS:H	2.25	0.44
1:D:273:GLY:O	1:D:275:ASP:N	2.46	0.44
2:E:374:GLU:C	2:E:376:GLU:H	2.26	0.44
3:F:317:LEU:HD23	3:F:317:LEU:HA	1.58	0.44
2:H:174:ARG:HA	2:H:174:ARG:HE	1.82	0.44
2:H:255:VAL:HG13	3:I:223:ILE:HA	1.99	0.44
2:H:263:GLU:OE1	2:H:263:GLU:HA	2.18	0.44
3:I:23:LYS:CE	3:I:434:THR:OG1	2.65	0.44
3:I:384:TYR:CA	3:I:387:ARG:HH12	2.15	0.44
1:A:66:PHE:CZ	1:A:113:GLY:O	2.71	0.44
3:C:233:THR:HG22	3:C:234:GLN:O	2.17	0.44
2:E:159:LEU:CD1	2:E:160:LEU:N	2.79	0.44
2:E:304:VAL:HG21	3:F:311:ASP:HB3	1.99	0.44
1:G:78:LYS:CA	1:G:96:ALA:HB2	2.41	0.44
2:H:225:GLU:C	2:H:227:THR:N	2.73	0.44
2:H:265:HIS:CB	2:H:399:LEU:HD21	2.42	0.44
3:I:77:LEU:HD12	3:I:125:TRP:CZ3	2.52	0.44
3:I:135:ARG:HG3	3:I:183:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PRO:O	1:A:111:GLU:N	2.51	0.44
1:A:279:THR:HB	1:A:281:TRP:NE1	2.33	0.44
2:B:343:TRP:C	2:B:345:THR:H	2.25	0.44
2:B:516:THR:OG1	2:B:544:LYS:HE2	2.18	0.44
3:C:7:TYR:O	3:C:10:GLU:HB2	2.18	0.44
3:C:382:LYS:HA	3:C:383:PRO:HD3	1.47	0.44
2:E:299:LEU:CD2	2:E:387:LEU:HD21	2.46	0.44
1:G:95:HIS:ND1	1:G:128:VAL:HG21	2.33	0.44
1:A:9:ASN:HD22	1:A:9:ASN:HA	1.49	0.44
1:A:10:GLU:OE1	1:A:10:GLU:HA	2.18	0.44
1:A:95:HIS:ND1	1:A:128:VAL:HG21	2.33	0.44
2:B:265:HIS:CB	2:B:399:LEU:HD21	2.42	0.44
2:B:381:TRP:CD2	2:B:412:LEU:HD22	2.52	0.44
2:B:527:LEU:C	2:B:529:ARG:N	2.72	0.44
3:C:16:SER:O	3:C:19:LEU:HB2	2.18	0.44
3:C:116:LEU:CD2	3:C:294:LEU:CD1	2.95	0.44
1:D:58:ARG:NH2	1:D:259:ARG:HE	2.16	0.44
1:D:66:PHE:CZ	1:D:113:GLY:O	2.71	0.44
2:E:427:ALA:O	2:E:428:ASN:C	2.61	0.44
3:F:269:GLY:HA3	3:F:295:GLN:CG	2.42	0.44
3:F:298:ILE:HD12	3:F:298:ILE:N	2.33	0.44
1:G:217:LEU:HD13	1:G:218:LEU:HB2	1.99	0.44
2:H:381:TRP:CD2	2:H:412:LEU:HD22	2.53	0.44
2:H:399:LEU:O	2:H:403:VAL:HG23	2.18	0.44
3:I:48:GLN:HA	3:I:51:LEU:HD12	1.99	0.44
3:I:144:TRP:CZ2	3:I:169:LEU:HD11	2.53	0.44
1:A:154:ALA:HB2	1:A:212:TRP:CE3	2.53	0.44
2:B:263:GLU:HA	2:B:263:GLU:OE1	2.17	0.44
3:C:164:GLU:O	3:C:165:ASN:O	2.36	0.44
3:C:294:LEU:HG	3:C:298:ILE:HD11	1.99	0.44
3:C:329:ASN:O	3:C:332:ALA:HB3	2.18	0.44
1:D:236:GLN:HG3	1:D:241:GLY:O	2.18	0.44
2:E:153:PHE:HA	2:E:159:LEU:CD2	2.46	0.44
2:E:193:GLU:HG3	2:E:215:LEU:HD11	2.00	0.44
3:F:358:VAL:O	3:F:361:SER:HB3	2.18	0.44
1:G:38:VAL:HG12	1:G:39:GLU:N	2.33	0.44
2:H:197:VAL:HG11	2:H:210:ILE:CG1	2.47	0.44
3:I:416:TYR:CD2	3:I:432:TYR:CE2	3.06	0.44
1:A:12:ILE:HG21	1:A:26:THR:HB	2.00	0.43
1:A:31:LYS:HG2	1:A:54:GLY:C	2.43	0.43
1:A:38:VAL:HG12	1:A:39:GLU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLY:O	1:A:275:ASP:N	2.47	0.43
2:B:193:GLU:HG3	2:B:215:LEU:HD11	2.00	0.43
1:D:95:HIS:ND1	1:D:128:VAL:HG21	2.33	0.43
2:E:263:GLU:HA	2:E:263:GLU:OE1	2.17	0.43
3:F:144:TRP:CZ2	3:F:169:LEU:HD11	2.53	0.43
3:F:212:LEU:HD23	3:F:212:LEU:HA	1.74	0.43
3:F:436:LEU:HB3	3:F:437:ASN:H	1.46	0.43
1:G:57:TRP:CH2	2:H:144:PHE:CE1	3.05	0.43
2:H:340:LEU:HD23	2:H:370:PHE:CE1	2.53	0.43
2:H:340:LEU:HD22	2:H:370:PHE:CB	2.48	0.43
2:H:427:ALA:O	2:H:428:ASN:C	2.61	0.43
3:I:164:GLU:O	3:I:165:ASN:O	2.36	0.43
3:I:419:LEU:O	3:I:423:GLN:HB2	2.18	0.43
2:B:525:HIS:O	2:B:526:ILE:C	2.62	0.43
3:C:9:THR:HG22	3:C:9:THR:O	2.17	0.43
2:E:174:ARG:HA	2:E:174:ARG:HE	1.82	0.43
2:E:393:GLN:HG2	2:E:396:GLU:HB2	2.00	0.43
1:G:20:TYR:CD1	1:G:20:TYR:N	2.86	0.43
1:G:112:TYR:CZ	1:G:171:ARG:HG2	2.54	0.43
1:G:170:SER:HA	1:G:186:LYS:HE3	2.00	0.43
1:G:233:ILE:HD11	1:G:248:LEU:CD1	2.48	0.43
2:H:135:ALA:O	2:H:139:MET:HB2	2.18	0.43
2:H:150:PHE:CZ	2:H:170:VAL:HG12	2.53	0.43
2:H:150:PHE:HZ	2:H:170:VAL:HG12	1.83	0.43
3:I:104:LEU:HD23	3:I:104:LEU:HA	1.72	0.43
3:I:294:LEU:HG	3:I:298:ILE:HD11	1.99	0.43
3:I:425:LEU:C	3:I:427:GLU:N	2.76	0.43
1:A:20:TYR:N	1:A:20:TYR:CD1	2.87	0.43
1:A:219:ARG:HB2	1:A:236:GLN:O	2.19	0.43
2:B:174:ARG:HE	2:B:174:ARG:HA	1.82	0.43
2:B:495:CYS:C	2:B:497:LEU:N	2.76	0.43
3:C:316:PRO:HB3	2:E:338:LEU:HB2	1.99	0.43
3:C:317:LEU:HA	3:C:317:LEU:HD23	1.58	0.43
3:C:354:SER:O	3:C:358:VAL:HG23	2.19	0.43
1:D:38:VAL:HG12	1:D:39:GLU:N	2.33	0.43
2:E:150:PHE:HZ	2:E:170:VAL:HG12	1.83	0.43
2:E:381:TRP:CD2	2:E:412:LEU:HD22	2.53	0.43
3:F:298:ILE:HD12	3:F:298:ILE:H	1.83	0.43
3:F:384:TYR:O	3:F:388:ILE:HG13	2.18	0.43
1:G:219:ARG:HB2	1:G:236:GLN:O	2.19	0.43
2:H:393:GLN:HG2	2:H:396:GLU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:206:ILE:H	3:I:206:ILE:HD12	1.84	0.43
3:I:354:SER:O	3:I:358:VAL:HG23	2.19	0.43
1:A:274:GLY:O	2:B:147:SER:HB2	2.19	0.43
2:B:135:ALA:C	2:B:137:LEU:N	2.73	0.43
2:B:265:HIS:HB2	2:B:399:LEU:CD2	2.42	0.43
2:B:538:PHE:O	2:B:541:GLN:HB3	2.18	0.43
3:C:144:TRP:CZ2	3:C:169:LEU:HD11	2.54	0.43
3:C:294:LEU:O	3:C:298:ILE:HD13	2.18	0.43
1:D:233:ILE:HD11	1:D:248:LEU:CD1	2.48	0.43
3:F:24:ILE:HD13	3:F:24:ILE:N	2.34	0.43
3:F:343:ILE:HD13	3:F:344:ARG:N	2.34	0.43
2:H:330:PRO:HA	2:H:333:ARG:HB2	2.00	0.43
2:H:467:LYS:HD2	2:H:498:ASN:HB3	2.01	0.43
2:H:516:THR:OG1	2:H:544:LYS:HE2	2.18	0.43
3:I:233:THR:HG22	3:I:234:GLN:O	2.17	0.43
1:A:185:TRP:CE2	1:A:196:LEU:HD13	2.54	0.43
1:A:281:TRP:CD1	1:A:281:TRP:N	2.86	0.43
1:D:31:LYS:HG2	1:D:54:GLY:C	2.43	0.43
1:D:170:SER:HA	1:D:186:LYS:HE3	2.00	0.43
1:D:232:ILE:HG21	1:D:234:TRP:CZ2	2.53	0.43
2:E:495:CYS:C	2:E:497:LEU:N	2.77	0.43
2:E:525:HIS:C	2:E:529:ARG:HD2	2.43	0.43
2:E:525:HIS:O	2:E:526:ILE:C	2.62	0.43
3:F:102:ARG:NH2	3:F:241:SER:OG	2.45	0.43
3:F:294:LEU:HD12	3:F:294:LEU:HA	1.81	0.43
1:G:66:PHE:CZ	1:G:113:GLY:O	2.71	0.43
2:H:314:LYS:HG2	3:I:162:LEU:O	2.19	0.43
3:I:225:THR:HG22	3:I:226:GLN:N	2.33	0.43
3:I:298:ILE:HD12	3:I:298:ILE:N	2.33	0.43
3:I:343:ILE:HD13	3:I:344:ARG:N	2.34	0.43
3:I:421:LYS:O	3:I:423:GLN:N	2.52	0.43
2:B:202:ARG:HE	2:B:209:GLN:HB2	1.84	0.43
3:C:298:ILE:HD12	3:C:298:ILE:N	2.34	0.43
3:C:384:TYR:O	3:C:388:ILE:HG13	2.19	0.43
3:C:425:LEU:C	3:C:427:GLU:N	2.76	0.43
1:D:185:TRP:CE2	1:D:196:LEU:HD13	2.54	0.43
1:D:208:ARG:HE	1:D:258:TRP:HZ3	1.67	0.43
1:D:264:LEU:HD12	2:E:155:THR:O	2.19	0.43
2:E:297:TYR:HE2	2:E:305:ARG:HH11	1.67	0.43
2:E:399:LEU:O	2:E:403:VAL:HG23	2.19	0.43
3:F:104:LEU:HD23	3:F:104:LEU:HA	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:THR:HB	1:G:281:TRP:NE1	2.33	0.43
1:G:289:TRP:CD1	1:G:289:TRP:N	2.87	0.43
2:H:193:GLU:HG3	2:H:215:LEU:HD11	2.00	0.43
2:H:318:LEU:HD11	2:H:357:ILE:HD12	2.00	0.43
1:A:103:ASN:CG	2:B:142:ARG:NH2	2.76	0.43
1:A:103:ASN:ND2	2:B:142:ARG:NH2	2.66	0.43
3:C:16:SER:HB3	3:C:432:TYR:OH	2.17	0.43
3:C:77:LEU:CD2	3:C:77:LEU:C	2.92	0.43
3:C:212:LEU:HA	3:C:212:LEU:HD23	1.75	0.43
2:E:150:PHE:CZ	2:E:170:VAL:HG12	2.53	0.43
2:E:246:TYR:HA	2:E:247:PRO:HD2	1.76	0.43
2:E:468:GLU:OE1	2:E:468:GLU:N	2.47	0.43
3:F:206:ILE:H	3:F:206:ILE:HD12	1.83	0.43
3:F:294:LEU:HG	3:F:298:ILE:HD11	2.00	0.43
1:G:232:ILE:HG21	1:G:234:TRP:CZ2	2.54	0.43
3:I:77:LEU:CD2	3:I:77:LEU:C	2.92	0.43
3:I:143:LYS:HE3	3:I:144:TRP:CD1	2.54	0.43
3:I:435:PHE:O	3:I:436:LEU:CG	2.65	0.43
1:A:102:VAL:CG1	1:A:118:VAL:HG13	2.49	0.43
1:A:208:ARG:HA	1:A:208:ARG:HD3	1.81	0.43
2:B:142:ARG:O	2:B:143:ARG:CB	2.66	0.43
2:B:150:PHE:HZ	2:B:170:VAL:HG12	1.83	0.43
2:B:225:GLU:C	2:B:227:THR:N	2.73	0.43
2:B:325:LEU:CD2	2:B:361:LEU:HD23	2.49	0.43
2:B:340:LEU:HD12	2:B:340:LEU:HA	1.80	0.43
2:B:427:ALA:O	2:B:428:ASN:C	2.60	0.43
2:B:467:LYS:HD2	2:B:498:ASN:HB3	2.01	0.43
3:C:143:LYS:HE3	3:C:144:TRP:CD1	2.54	0.43
3:F:34:ASP:CB	3:F:35:PRO:CD	2.93	0.43
3:F:164:GLU:O	3:F:165:ASN:O	2.36	0.43
3:F:225:THR:HG22	3:F:226:GLN:N	2.32	0.43
1:G:31:LYS:HG2	1:G:54:GLY:C	2.43	0.43
2:H:285:ARG:HG3	2:H:285:ARG:NH1	2.33	0.43
3:I:116:LEU:CD2	3:I:294:LEU:CD1	2.96	0.43
2:B:233:LEU:HD21	2:B:421:ILE:CD1	2.47	0.43
2:B:318:LEU:HD11	2:B:357:ILE:HD12	2.01	0.43
1:G:236:GLN:HG3	1:G:241:GLY:O	2.18	0.43
1:G:273:GLY:O	1:G:275:ASP:N	2.46	0.43
2:H:327:SER:OG	3:I:238:LYS:HG3	2.19	0.43
3:I:24:ILE:O	3:I:25:GLU:C	2.62	0.43
3:I:294:LEU:O	3:I:298:ILE:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:LEU:CD1	2:B:160:LEU:N	2.79	0.43
2:B:314:LYS:HE3	3:C:162:LEU:CB	2.47	0.43
2:B:393:GLN:HG2	2:B:396:GLU:HB2	2.00	0.43
3:C:48:GLN:HA	3:C:51:LEU:HD12	1.99	0.43
1:D:102:VAL:CG1	1:D:118:VAL:HG13	2.49	0.43
1:D:219:ARG:HB2	1:D:236:GLN:O	2.19	0.43
1:D:279:THR:HB	1:D:281:TRP:NE1	2.33	0.43
1:D:281:TRP:CD1	1:D:281:TRP:N	2.86	0.43
2:E:524:ASP:CA	2:E:527:LEU:HD12	2.35	0.43
1:G:102:VAL:CG1	1:G:118:VAL:HG13	2.49	0.43
1:G:108:ALA:HB1	1:G:112:TYR:HD1	1.84	0.43
1:G:264:LEU:HB3	2:H:509:ARG:NH1	2.33	0.43
2:H:138:ILE:HG23	2:H:141:GLU:OE2	2.18	0.43
3:C:294:LEU:O	3:C:298:ILE:HD12	2.18	0.42
1:D:29:SER:C	1:D:31:LYS:N	2.76	0.42
1:D:108:ALA:HB1	1:D:112:TYR:HD1	1.84	0.42
1:D:229:ARG:NH1	1:D:252:LYS:HB3	2.34	0.42
2:E:197:VAL:HG11	2:E:210:ILE:HG12	2.01	0.42
2:E:516:THR:OG1	2:E:544:LYS:HE2	2.18	0.42
1:G:208:ARG:HE	1:G:258:TRP:HZ3	1.67	0.42
1:G:229:ARG:NH1	1:G:252:LYS:HB3	2.34	0.42
2:H:297:TYR:HE2	2:H:305:ARG:HH11	1.67	0.42
2:H:347:GLY:C	2:H:349:SER:N	2.77	0.42
2:H:359:LYS:HG3	2:H:365:PRO:HA	2.01	0.42
2:B:177:THR:CG2	2:B:484:ALA:HB2	2.45	0.42
2:B:366:PHE:C	2:B:368:GLY:H	2.28	0.42
2:B:396:GLU:OE1	2:B:396:GLU:N	2.51	0.42
3:C:11:ARG:HD2	3:C:12:PHE:CE1	2.54	0.42
3:C:343:ILE:HD13	3:C:344:ARG:N	2.34	0.42
1:D:57:TRP:CH2	2:E:144:PHE:HE1	2.37	0.42
3:F:77:LEU:CD2	3:F:77:LEU:C	2.92	0.42
3:F:316:PRO:HB2	2:H:334:ASP:HB3	2.00	0.42
1:G:12:ILE:HG21	1:G:26:THR:HB	2.01	0.42
1:G:185:TRP:CE2	1:G:196:LEU:HD13	2.53	0.42
2:H:374:GLU:C	2:H:376:GLU:H	2.25	0.42
2:H:495:CYS:C	2:H:497:LEU:N	2.77	0.42
3:I:21:GLU:HG2	3:I:25:GLU:OE2	2.18	0.42
3:I:59:GLU:HA	3:I:62:VAL:CG2	2.42	0.42
3:I:269:GLY:HA3	3:I:295:GLN:CG	2.42	0.42
3:I:358:VAL:O	3:I:361:SER:HB3	2.18	0.42
1:A:108:ALA:HB1	1:A:112:TYR:HD1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:NH1	1:A:252:LYS:HB3	2.34	0.42
2:B:153:PHE:HA	2:B:159:LEU:CD2	2.46	0.42
2:B:198:THR:O	2:B:211:SER:HB3	2.19	0.42
2:B:330:PRO:HA	2:B:333:ARG:HB2	2.02	0.42
2:B:399:LEU:O	2:B:403:VAL:HG23	2.19	0.42
3:C:42:PHE:CZ	3:C:391:HIS:HB3	2.55	0.42
3:C:283:GLU:H	3:C:283:GLU:CD	2.28	0.42
1:D:96:ALA:C	1:D:98:HIS:N	2.76	0.42
1:D:217:LEU:CD2	2:E:475:PHE:HE1	2.31	0.42
2:E:202:ARG:HE	2:E:209:GLN:HB2	1.84	0.42
2:H:136:LYS:HE2	2:H:136:LYS:HB3	1.82	0.42
2:H:295:PHE:CE1	2:H:356:LYS:HB3	2.55	0.42
2:H:320:VAL:HG11	3:I:211:ILE:HD13	2.02	0.42
3:I:16:SER:O	3:I:19:LEU:HB2	2.20	0.42
1:A:100:ALA:CB	1:A:121:SER:HB2	2.50	0.42
1:A:180:ASN:ND2	1:A:204:SER:C	2.78	0.42
1:A:233:ILE:HD11	1:A:248:LEU:CD1	2.48	0.42
1:A:236:GLN:HG3	1:A:241:GLY:O	2.18	0.42
2:B:142:ARG:O	2:B:143:ARG:HB2	2.19	0.42
2:B:150:PHE:CZ	2:B:170:VAL:HG12	2.54	0.42
2:B:314:LYS:HE3	3:C:162:LEU:HD22	2.01	0.42
2:B:347:GLY:C	2:B:349:SER:N	2.77	0.42
3:C:332:ALA:C	3:C:334:ARG:H	2.28	0.42
1:D:180:ASN:ND2	1:D:204:SER:C	2.78	0.42
3:F:10:GLU:O	3:F:12:PHE:N	2.52	0.42
3:F:150:SER:O	3:F:151:GLY:O	2.37	0.42
3:F:294:LEU:O	3:F:298:ILE:HD13	2.20	0.42
3:F:354:SER:O	3:F:358:VAL:HG23	2.19	0.42
1:G:100:ALA:CB	1:G:121:SER:HB2	2.49	0.42
1:G:109:PRO:O	1:G:111:GLU:N	2.52	0.42
2:H:525:HIS:O	2:H:526:ILE:C	2.61	0.42
3:I:28:ASN:O	3:I:29:GLU:O	2.38	0.42
3:I:53:LEU:O	3:I:61:ASN:HB3	2.20	0.42
2:B:295:PHE:CE1	2:B:356:LYS:HB3	2.54	0.42
3:C:220:ASN:HA	3:C:221:PRO:HD3	1.88	0.42
1:D:212:TRP:HA	1:D:222:LEU:HD22	1.92	0.42
2:E:330:PRO:HA	2:E:333:ARG:HB2	2.01	0.42
3:F:93:GLU:CG	3:F:94:MET:H	2.31	0.42
3:F:221:PRO:HG3	3:F:231:PHE:HB2	2.01	0.42
1:G:240:GLN:O	1:G:241:GLY:C	2.63	0.42
2:H:250:THR:HG23	3:I:99:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:396:GLU:OE1	2:H:396:GLU:N	2.52	0.42
2:H:522:THR:C	2:H:525:HIS:H	2.28	0.42
1:A:232:ILE:HG21	1:A:234:TRP:CZ2	2.53	0.42
2:B:527:LEU:O	2:B:530:LEU:HB2	2.20	0.42
3:C:227:ILE:O	3:C:229:ASN:N	2.53	0.42
3:C:298:ILE:HD12	3:C:298:ILE:H	1.85	0.42
1:D:15:ALA:CB	1:D:26:THR:HG22	2.49	0.42
1:D:61:TRP:CD1	1:D:61:TRP:N	2.87	0.42
1:D:109:PRO:O	1:D:111:GLU:N	2.52	0.42
1:D:141:ILE:HD12	1:D:185:TRP:CE3	2.54	0.42
1:G:15:ALA:CB	1:G:26:THR:HG22	2.49	0.42
2:H:175:LEU:CD1	2:H:176:PRO:HD2	2.42	0.42
2:H:197:VAL:HG21	2:H:492:PHE:CZ	2.55	0.42
3:I:8:GLN:O	3:I:10:GLU:N	2.52	0.42
3:I:9:THR:HG22	3:I:423:GLN:OE1	2.20	0.42
3:I:82:LEU:HD23	3:I:82:LEU:HA	1.80	0.42
3:I:355:LEU:HD12	3:I:355:LEU:HA	1.84	0.42
1:A:289:TRP:CD1	1:A:289:TRP:N	2.87	0.42
2:B:208:PRO:HB3	2:B:531:LYS:CB	2.24	0.42
2:B:491:LEU:O	2:B:494:SER:HB2	2.19	0.42
3:C:7:TYR:CD1	3:C:7:TYR:O	2.72	0.42
3:C:355:LEU:HD12	3:C:355:LEU:HA	1.83	0.42
1:D:12:ILE:HG21	1:D:26:THR:HB	2.01	0.42
1:D:100:ALA:CB	1:D:121:SER:HB2	2.49	0.42
2:E:234:TRP:CZ3	2:E:452:TYR:CD1	3.08	0.42
2:E:348:CYS:O	2:E:349:SER:OG	2.30	0.42
2:E:467:LYS:HD2	2:E:498:ASN:HB3	2.01	0.42
1:G:61:TRP:CD1	1:G:61:TRP:N	2.87	0.42
1:G:229:ARG:CG	1:G:256:VAL:HA	2.50	0.42
1:A:170:SER:HA	1:A:186:LYS:HE3	2.00	0.42
2:B:202:ARG:CG	2:B:500:ASP:OD1	2.67	0.42
3:C:206:ILE:HD12	3:C:206:ILE:N	2.35	0.42
1:D:20:TYR:CD1	1:D:20:TYR:N	2.87	0.42
1:D:240:GLN:O	1:D:241:GLY:C	2.63	0.42
1:D:289:TRP:CD1	1:D:289:TRP:N	2.87	0.42
2:E:175:LEU:CD1	2:E:176:PRO:HD2	2.42	0.42
2:E:197:VAL:HG21	2:E:492:PHE:CZ	2.55	0.42
2:E:265:HIS:CB	2:E:399:LEU:HD21	2.42	0.42
3:F:35:PRO:HB2	3:F:399:ILE:HG12	2.00	0.42
3:I:150:SER:O	3:I:151:GLY:O	2.37	0.42
1:A:141:ILE:HD12	1:A:185:TRP:CZ3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:VAL:HG11	2:B:210:ILE:HG12	2.02	0.42
3:C:221:PRO:HG3	3:C:231:PHE:HB2	2.01	0.42
2:E:318:LEU:HD11	2:E:357:ILE:HD12	2.01	0.42
2:E:359:LYS:HG3	2:E:365:PRO:HA	2.01	0.42
1:G:29:SER:C	1:G:31:LYS:N	2.76	0.42
1:G:79:VAL:CG2	1:G:102:VAL:HG11	2.49	0.42
1:G:282:LYS:NZ	2:H:178:GLU:OE2	2.53	0.42
3:I:11:ARG:C	3:I:13:THR:H	2.27	0.42
1:A:112:TYR:CZ	1:A:171:ARG:HG2	2.54	0.42
1:A:202:GLY:HA3	1:A:245:LYS:HE3	2.02	0.42
1:A:240:GLN:O	1:A:241:GLY:C	2.63	0.42
1:A:277:LYS:HG3	1:A:278:VAL:N	2.35	0.42
1:A:282:LYS:CD	1:A:292:ALA:HB2	2.50	0.42
1:A:285:LEU:H	1:A:285:LEU:CD1	2.27	0.42
2:B:128:CYS:O	2:B:132:ILE:HG13	2.20	0.42
2:B:299:LEU:HD23	2:B:299:LEU:HA	1.79	0.42
3:C:42:PHE:HD2	3:C:42:PHE:HA	1.76	0.42
3:C:421:LYS:C	3:C:423:GLN:N	2.77	0.42
1:D:55:PRO:HD3	2:E:138:ILE:HD13	2.00	0.42
1:D:229:ARG:CG	1:D:256:VAL:HA	2.50	0.42
2:E:347:GLY:C	2:E:349:SER:N	2.77	0.42
3:F:11:ARG:C	3:F:13:THR:N	2.77	0.42
3:F:17:ASP:O	3:F:20:LYS:HB2	2.20	0.42
3:F:20:LYS:O	3:F:24:ILE:HG12	2.20	0.42
3:F:116:LEU:CD2	3:F:294:LEU:CD1	2.95	0.42
3:F:125:TRP:O	3:F:128:GLU:HB3	2.20	0.42
3:F:195:GLU:OE2	3:F:195:GLU:N	2.44	0.42
3:F:419:LEU:HA	3:F:422:LEU:HB2	2.00	0.42
1:G:216:VAL:HG23	2:H:505:ASP:OD2	2.20	0.42
1:G:285:LEU:H	1:G:285:LEU:CD1	2.27	0.42
2:H:202:ARG:HE	2:H:209:GLN:HB2	1.84	0.42
2:H:317:HIS:ND1	3:I:159:ASP:OD1	2.53	0.42
3:I:123:MET:HE2	3:I:123:MET:HB3	1.86	0.42
2:B:197:VAL:HG21	2:B:492:PHE:CZ	2.55	0.41
2:B:297:TYR:HE2	2:B:305:ARG:HH11	1.67	0.41
3:C:11:ARG:O	3:C:12:PHE:C	2.62	0.41
3:C:102:ARG:HH22	3:C:241:SER:H	1.68	0.41
3:C:187:LEU:HD23	3:C:187:LEU:HA	1.93	0.41
3:C:378:ASP:HB3	3:C:381:ASP:OD2	2.19	0.41
2:E:198:THR:O	2:E:211:SER:HB3	2.19	0.41
2:E:216:LEU:O	2:E:217:PHE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:295:PHE:CE1	2:E:356:LYS:HB3	2.55	0.41
3:F:259:TYR:O	3:F:263:ILE:HG13	2.20	0.41
2:H:291:ILE:HD12	2:H:291:ILE:N	2.20	0.41
2:H:491:LEU:O	2:H:494:SER:HB2	2.20	0.41
2:H:527:LEU:O	2:H:530:LEU:HB2	2.20	0.41
3:I:8:GLN:O	3:I:11:ARG:HG2	2.21	0.41
3:I:235:GLN:HG2	3:I:236:GLY:H	1.85	0.41
1:A:200:LEU:HD11	1:A:243:TRP:CG	2.55	0.41
1:A:229:ARG:CG	1:A:256:VAL:HA	2.50	0.41
2:B:142:ARG:HH11	2:B:142:ARG:HG3	1.84	0.41
2:B:187:ASP:HB3	2:B:523:ASN:HD22	1.82	0.41
2:B:359:LYS:HG3	2:B:365:PRO:HA	2.01	0.41
3:C:125:TRP:O	3:C:128:GLU:HB3	2.20	0.41
3:C:150:SER:O	3:C:151:GLY:O	2.37	0.41
3:C:323:THR:O	3:C:327:VAL:HG23	2.20	0.41
3:C:341:HIS:HA	3:C:342:PRO:HD3	1.90	0.41
3:C:359:ILE:HG21	3:C:404:VAL:HG11	2.03	0.41
1:D:282:LYS:CD	1:D:292:ALA:HB2	2.50	0.41
2:E:527:LEU:O	2:E:530:LEU:HB2	2.19	0.41
3:F:288:ILE:O	3:F:291:ASN:HB3	2.21	0.41
1:G:200:LEU:HD11	1:G:243:TRP:CG	2.55	0.41
2:H:198:THR:O	2:H:211:SER:HB3	2.19	0.41
2:H:216:LEU:O	2:H:217:PHE:C	2.63	0.41
3:I:227:ILE:O	3:I:229:ASN:N	2.53	0.41
1:A:140:ILE:CG2	1:A:141:ILE:H	2.33	0.41
2:B:252:ASN:OD1	2:B:252:ASN:C	2.63	0.41
2:B:359:LYS:HA	2:B:359:LYS:HD2	1.80	0.41
2:B:466:SER:O	2:B:467:LYS:C	2.63	0.41
2:B:468:GLU:OE1	2:B:468:GLU:N	2.47	0.41
2:B:504:GLU:O	2:B:505:ASP:C	2.63	0.41
3:C:39:ILE:HA	3:C:42:PHE:HB2	2.02	0.41
1:D:233:ILE:HG22	1:D:235:THR:HG23	2.03	0.41
3:F:39:ILE:HA	3:F:42:PHE:HB2	2.02	0.41
3:F:322:LEU:HD23	3:F:322:LEU:HA	1.77	0.41
3:F:332:ALA:C	3:F:334:ARG:H	2.28	0.41
3:F:433:ALA:C	3:F:435:PHE:H	2.27	0.41
1:G:151:ALA:HA	1:G:174:VAL:O	2.20	0.41
1:G:277:LYS:HG3	1:G:278:VAL:N	2.35	0.41
2:H:139:MET:CG	2:H:144:PHE:O	2.47	0.41
2:H:252:ASN:OD1	2:H:252:ASN:C	2.63	0.41
2:H:479:ALA:C	2:H:481:LEU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:12:PHE:CD1	3:I:12:PHE:N	2.70	0.41
3:I:39:ILE:HA	3:I:42:PHE:HB2	2.02	0.41
3:I:125:TRP:O	3:I:128:GLU:HB3	2.20	0.41
3:I:298:ILE:HD12	3:I:298:ILE:H	1.84	0.41
2:B:291:ILE:HD12	2:B:291:ILE:N	2.21	0.41
2:B:347:GLY:O	2:B:348:CYS:C	2.63	0.41
2:B:512:MET:O	2:B:515:ILE:HG12	2.20	0.41
2:B:522:THR:C	2:B:525:HIS:H	2.28	0.41
2:B:525:HIS:C	2:B:527:LEU:H	2.28	0.41
3:C:50:ALA:HB1	3:C:69:GLU:CG	2.49	0.41
3:C:68:TRP:CH2	3:C:387:ARG:NH2	2.89	0.41
1:D:79:VAL:CG2	1:D:102:VAL:HG11	2.49	0.41
1:D:277:LYS:HG3	1:D:278:VAL:N	2.35	0.41
2:E:197:VAL:CG1	2:E:210:ILE:HG23	2.51	0.41
2:E:319:SER:C	3:F:246:THR:HG21	2.45	0.41
1:G:180:ASN:ND2	1:G:204:SER:C	2.78	0.41
2:H:159:LEU:CD1	2:H:160:LEU:N	2.79	0.41
2:H:208:PRO:HB3	2:H:531:LYS:CB	2.25	0.41
2:H:208:PRO:O	2:H:209:GLN:CB	2.68	0.41
2:H:347:GLY:O	2:H:348:CYS:C	2.63	0.41
1:A:208:ARG:HE	1:A:258:TRP:HZ3	1.67	0.41
1:A:283:GLU:HB2	1:A:289:TRP:CH2	2.56	0.41
2:B:145:THR:C	2:B:147:SER:N	2.77	0.41
3:C:288:ILE:O	3:C:291:ASN:HB3	2.21	0.41
3:C:421:LYS:O	3:C:424:GLY:N	2.44	0.41
3:C:433:ALA:C	3:C:435:PHE:H	2.28	0.41
1:D:200:LEU:HD11	1:D:243:TRP:CG	2.55	0.41
1:D:283:GLU:HB2	1:D:289:TRP:CH2	2.56	0.41
2:E:291:ILE:HD12	2:E:291:ILE:N	2.21	0.41
3:F:143:LYS:HE3	3:F:144:TRP:CD1	2.54	0.41
3:F:323:THR:O	3:F:327:VAL:HG23	2.20	0.41
3:F:432:TYR:O	3:F:435:PHE:HD1	2.04	0.41
1:G:212:TRP:HA	1:G:222:LEU:HD22	1.92	0.41
1:G:233:ILE:HG22	1:G:235:THR:HG23	2.03	0.41
2:H:198:THR:O	2:H:198:THR:HG22	2.20	0.41
2:H:359:LYS:HD2	2:H:359:LYS:HA	1.80	0.41
3:I:102:ARG:HH22	3:I:241:SER:H	1.68	0.41
3:I:259:TYR:O	3:I:263:ILE:HG13	2.20	0.41
3:I:283:GLU:H	3:I:283:GLU:CD	2.28	0.41
1:A:262:TRP:C	2:B:153:PHE:HD1	2.28	0.41
2:B:320:VAL:CG2	3:C:246:THR:HG22	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:ASP:OD1	2:B:331:ARG:HB2	2.20	0.41
2:B:545:ASP:O	2:B:549:GLY:N	2.49	0.41
3:C:15:PHE:H	3:C:15:PHE:HD1	1.68	0.41
1:D:191:ALA:C	1:D:193:THR:N	2.79	0.41
1:D:202:GLY:HA3	1:D:245:LYS:HE3	2.02	0.41
2:E:202:ARG:CG	2:E:500:ASP:OD1	2.67	0.41
2:E:248:TYR:CD2	2:E:248:TYR:N	2.88	0.41
2:E:252:ASN:OD1	2:E:252:ASN:C	2.63	0.41
2:E:319:SER:OG	3:F:246:THR:HG23	2.21	0.41
2:E:492:PHE:CD2	2:E:492:PHE:C	2.98	0.41
3:F:227:ILE:O	3:F:229:ASN:N	2.53	0.41
3:F:237:ILE:C	3:F:237:ILE:CD1	2.76	0.41
3:F:363:VAL:HG12	3:F:364:GLU:N	2.35	0.41
1:G:19:TYR:CD2	2:H:543:LEU:CD2	3.03	0.41
1:G:202:GLY:HA3	1:G:245:LYS:HE3	2.02	0.41
2:H:197:VAL:HG11	2:H:210:ILE:HG12	2.02	0.41
2:H:406:HIS:CE1	2:H:410:PHE:CE1	3.09	0.41
3:I:21:GLU:HA	3:I:25:GLU:HG3	2.02	0.41
3:I:433:ALA:C	3:I:435:PHE:H	2.28	0.41
2:B:197:VAL:CG1	2:B:210:ILE:HG23	2.51	0.41
3:C:50:ALA:O	3:C:54:ALA:HB2	2.21	0.41
3:C:108:LYS:O	3:C:109:LEU:C	2.64	0.41
3:C:259:TYR:O	3:C:263:ILE:HG13	2.20	0.41
3:C:432:TYR:O	3:C:435:PHE:HD1	2.03	0.41
2:E:364:SER:HB3	2:E:367:GLU:HB2	2.02	0.41
2:E:491:LEU:O	2:E:494:SER:HB2	2.19	0.41
2:E:522:THR:C	2:E:525:HIS:H	2.28	0.41
3:F:50:ALA:O	3:F:54:ALA:HB2	2.21	0.41
3:F:283:GLU:H	3:F:283:GLU:CD	2.28	0.41
3:F:317:LEU:HA	3:F:318:PRO:HD2	1.90	0.41
1:G:31:LYS:HA	1:G:56:VAL:HG23	2.03	0.41
1:G:282:LYS:CD	1:G:292:ALA:HB2	2.50	0.41
2:H:197:VAL:CG1	2:H:210:ILE:HG23	2.51	0.41
2:H:234:TRP:CZ3	2:H:452:TYR:CD1	3.08	0.41
2:H:468:GLU:OE1	2:H:468:GLU:N	2.46	0.41
2:H:513:ARG:O	2:H:513:ARG:HG2	2.21	0.41
3:I:50:ALA:O	3:I:54:ALA:HB2	2.21	0.41
3:I:221:PRO:HG3	3:I:231:PHE:HB2	2.01	0.41
2:B:160:LEU:CD2	2:B:172:ILE:HA	2.50	0.41
2:B:406:HIS:CE1	2:B:410:PHE:CE1	3.09	0.41
2:B:468:GLU:H	2:B:468:GLU:CD	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:VAL:O	1:D:125:VAL:HG13	2.21	0.41
2:E:525:HIS:C	2:E:527:LEU:H	2.28	0.41
2:H:160:LEU:CD2	2:H:172:ILE:HA	2.50	0.41
2:H:187:ASP:HB3	2:H:523:ASN:HD22	1.82	0.41
1:A:9:ASN:OD1	1:A:12:ILE:HD11	2.21	0.41
1:A:96:ALA:O	1:A:98:HIS:N	2.52	0.41
1:A:118:VAL:O	1:A:125:VAL:HG13	2.21	0.41
1:A:233:ILE:HG22	1:A:235:THR:HG23	2.03	0.41
1:A:265:SER:O	2:B:483:PHE:CZ	2.74	0.41
2:B:198:THR:O	2:B:198:THR:HG22	2.20	0.41
2:B:216:LEU:O	2:B:217:PHE:C	2.63	0.41
2:B:495:CYS:O	2:B:497:LEU:N	2.54	0.41
2:B:518:LEU:C	2:B:519:ARG:HG2	2.45	0.41
3:C:145:LEU:HD12	3:C:145:LEU:HA	1.75	0.41
3:C:280:SER:CB	3:C:284:SER:HB3	2.41	0.41
3:C:441:CYS:C	3:C:442:LEU:HG	2.45	0.41
1:D:31:LYS:HA	1:D:56:VAL:HG23	2.03	0.41
1:D:77:GLY:CA	1:D:100:ALA:O	2.67	0.41
1:D:78:LYS:CA	1:D:96:ALA:HB2	2.42	0.41
1:D:271:LEU:O	1:D:278:VAL:HG13	2.21	0.41
2:E:198:THR:O	2:E:198:THR:HG22	2.20	0.41
2:E:199:ILE:HG22	2:E:209:GLN:H	1.86	0.41
2:E:208:PRO:O	2:E:209:GLN:CB	2.68	0.41
2:E:342:LYS:CD	3:F:206:ILE:HD11	2.51	0.41
2:E:479:ALA:C	2:E:481:LEU:N	2.78	0.41
2:E:495:CYS:O	2:E:497:LEU:N	2.54	0.41
2:E:512:MET:O	2:E:515:ILE:HG12	2.21	0.41
2:E:513:ARG:HG2	2:E:513:ARG:O	2.21	0.41
3:F:14:LYS:O	3:F:17:ASP:HB3	2.21	0.41
3:F:187:LEU:HD23	3:F:187:LEU:HA	1.92	0.41
3:F:220:ASN:HA	3:F:221:PRO:HD3	1.87	0.41
3:F:335:HIS:O	3:F:336:PRO:C	2.64	0.41
3:F:400:ASN:O	3:F:401:PRO:C	2.64	0.41
1:G:270:ALA:HB2	2:H:153:PHE:CE1	2.55	0.41
1:G:283:GLU:HB2	1:G:289:TRP:CH2	2.55	0.41
2:H:250:THR:HG21	2:H:255:VAL:CB	2.50	0.41
2:H:265:HIS:HB2	2:H:399:LEU:CD2	2.42	0.41
2:H:299:LEU:CD2	2:H:387:LEU:HD21	2.46	0.41
2:H:512:MET:O	2:H:515:ILE:HG12	2.20	0.41
3:I:108:LYS:O	3:I:109:LEU:C	2.64	0.41
3:I:145:LEU:HD12	3:I:145:LEU:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:323:THR:O	3:I:327:VAL:HG23	2.20	0.41
1:A:61:TRP:CD1	1:A:61:TRP:N	2.87	0.41
2:B:162:LYS:HE2	2:B:164:ILE:CG2	2.51	0.41
2:B:234:TRP:CZ3	2:B:452:TYR:CD1	3.08	0.41
2:B:250:THR:HG21	2:B:255:VAL:CB	2.50	0.41
2:B:392:GLY:O	2:B:393:GLN:HB3	2.19	0.41
2:B:513:ARG:HG2	2:B:513:ARG:O	2.21	0.41
3:C:220:ASN:OD1	3:C:220:ASN:C	2.64	0.41
2:E:314:LYS:HG2	3:F:162:LEU:O	2.21	0.41
2:E:518:LEU:C	2:E:519:ARG:HG2	2.45	0.41
3:F:7:TYR:O	3:F:8:GLN:C	2.64	0.41
3:F:58:ASP:HB2	3:F:60:SER:H	1.85	0.41
3:F:355:LEU:HD12	3:F:355:LEU:HA	1.84	0.41
3:F:419:LEU:O	3:F:423:GLN:HB2	2.21	0.41
1:G:60:ASP:H	1:G:70:LEU:CD1	2.34	0.41
2:H:199:ILE:HG22	2:H:209:GLN:H	1.86	0.41
2:H:504:GLU:O	2:H:505:ASP:C	2.63	0.41
3:I:288:ILE:O	3:I:291:ASN:HB3	2.21	0.41
3:I:332:ALA:C	3:I:334:ARG:H	2.28	0.41
3:I:362:SER:O	3:I:365:MET:HB3	2.21	0.41
1:A:79:VAL:CG2	1:A:102:VAL:HG11	2.49	0.40
2:B:199:ILE:HG22	2:B:209:GLN:H	1.86	0.40
2:B:389:LEU:HD23	2:B:389:LEU:HA	1.86	0.40
3:C:48:GLN:O	3:C:51:LEU:HB2	2.21	0.40
1:D:151:ALA:HA	1:D:174:VAL:O	2.20	0.40
2:E:347:GLY:O	2:E:348:CYS:C	2.63	0.40
2:E:525:HIS:O	2:E:527:LEU:N	2.54	0.40
3:F:88:ASP:O	3:F:90:ASP:N	2.54	0.40
3:F:108:LYS:O	3:F:109:LEU:C	2.64	0.40
2:H:153:PHE:HE2	2:H:175:LEU:HD22	1.86	0.40
3:I:355:LEU:O	3:I:356:PRO:C	2.63	0.40
3:I:432:TYR:O	3:I:435:PHE:HD1	2.04	0.40
1:A:71:ALA:HB2	1:A:107:TRP:CZ2	2.57	0.40
2:B:208:PRO:O	2:B:209:GLN:CB	2.69	0.40
3:C:164:GLU:O	3:C:165:ASN:C	2.64	0.40
1:D:95:HIS:CG	1:D:128:VAL:HG21	2.57	0.40
1:D:151:ALA:CB	1:D:175:THR:HG22	2.51	0.40
1:D:285:LEU:H	1:D:285:LEU:CD1	2.27	0.40
2:E:142:ARG:HG2	2:E:144:PHE:CE1	2.54	0.40
2:E:202:ARG:HD2	2:E:500:ASP:OD1	2.21	0.40
2:E:517:LEU:HD12	2:E:517:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:ALA:HB2	1:G:107:TRP:CZ2	2.56	0.40
1:G:155:PRO:HG3	1:G:214:PRO:HA	2.02	0.40
1:G:273:GLY:C	1:G:275:ASP:N	2.79	0.40
2:H:138:ILE:O	2:H:142:ARG:HB2	2.20	0.40
2:H:495:CYS:O	2:H:497:LEU:N	2.54	0.40
3:I:23:LYS:O	3:I:27:ASN:HB2	2.21	0.40
3:I:335:HIS:O	3:I:336:PRO:C	2.64	0.40
2:B:202:ARG:HD2	2:B:500:ASP:OD1	2.21	0.40
1:D:80:LEU:O	1:D:82:TRP:CD1	2.75	0.40
2:E:160:LEU:CD2	2:E:172:ILE:HA	2.50	0.40
2:E:285:ARG:HG3	2:E:285:ARG:NH1	2.33	0.40
2:E:392:GLY:O	2:E:393:GLN:HB3	2.19	0.40
2:E:504:GLU:O	2:E:505:ASP:C	2.63	0.40
3:F:332:ALA:C	3:F:334:ARG:N	2.79	0.40
1:G:264:LEU:HB3	2:H:509:ARG:CZ	2.51	0.40
2:H:190:LEU:CD1	2:H:492:PHE:HD1	2.35	0.40
2:H:220:ALA:O	2:H:224:MET:HG3	2.22	0.40
2:H:515:ILE:HD11	2:H:544:LYS:HB2	2.04	0.40
3:I:10:GLU:O	3:I:10:GLU:HG3	2.22	0.40
3:I:94:MET:HE3	3:I:96:LEU:HD21	2.04	0.40
3:I:164:GLU:O	3:I:165:ASN:C	2.65	0.40
2:B:325:LEU:HD23	2:B:361:LEU:HD23	2.03	0.40
2:B:517:LEU:N	2:B:517:LEU:HD12	2.37	0.40
3:C:41:GLU:O	3:C:42:PHE:C	2.64	0.40
3:C:81:LEU:CD2	3:C:118:GLN:HG2	2.51	0.40
1:D:71:ALA:HB2	1:D:107:TRP:CZ2	2.56	0.40
1:D:81:ILE:HG12	1:D:130:PHE:HZ	1.86	0.40
3:F:220:ASN:OD1	3:F:220:ASN:C	2.64	0.40
3:F:390:THR:O	3:F:394:ILE:HG12	2.22	0.40
1:G:236:GLN:O	1:G:237:ASP:C	2.64	0.40
2:H:518:LEU:C	2:H:519:ARG:HG2	2.45	0.40
3:I:41:GLU:O	3:I:42:PHE:C	2.65	0.40
3:I:90:ASP:OD1	3:I:90:ASP:N	2.54	0.40
3:I:251:SER:O	3:I:261:ARG:HD2	2.21	0.40
1:A:29:SER:C	1:A:31:LYS:N	2.77	0.40
1:A:81:ILE:HG12	1:A:130:PHE:HZ	1.86	0.40
1:A:271:LEU:O	1:A:278:VAL:HG13	2.21	0.40
2:B:525:HIS:O	2:B:527:LEU:N	2.54	0.40
1:D:57:TRP:HD1	1:D:102:VAL:O	2.05	0.40
2:E:153:PHE:HE2	2:E:175:LEU:HD22	1.86	0.40
3:F:52:ASP:C	3:F:54:ALA:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:102:ARG:HH22	3:F:241:SER:H	1.68	0.40
3:F:206:ILE:HD12	3:F:206:ILE:N	2.36	0.40
3:F:355:LEU:O	3:F:356:PRO:C	2.63	0.40
1:G:81:ILE:HG12	1:G:130:PHE:HZ	1.86	0.40
1:G:118:VAL:O	1:G:125:VAL:HG13	2.21	0.40
2:H:517:LEU:N	2:H:517:LEU:HD12	2.37	0.40
2:H:525:HIS:C	2:H:527:LEU:H	2.28	0.40
2:H:545:ASP:C	2:H:547:TYR:H	2.29	0.40
3:I:212:LEU:HA	3:I:212:LEU:HD23	1.76	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	270/297 (91%)	199 (74%)	51 (19%)	20 (7%)	1	6
1	D	270/297 (91%)	200 (74%)	51 (19%)	19 (7%)	1	6
1	G	270/297 (91%)	200 (74%)	50 (18%)	20 (7%)	1	6
2	B	432/442 (98%)	346 (80%)	55 (13%)	31 (7%)	1	6
2	E	421/442 (95%)	343 (82%)	48 (11%)	30 (7%)	1	6
2	H	418/442 (95%)	339 (81%)	49 (12%)	30 (7%)	1	6
3	C	413/460 (90%)	341 (83%)	55 (13%)	17 (4%)	2	17
3	F	413/460 (90%)	343 (83%)	53 (13%)	17 (4%)	2	17
3	I	408/460 (89%)	334 (82%)	56 (14%)	18 (4%)	2	15
All	All	3315/3597 (92%)	2645 (80%)	468 (14%)	202 (6%)	1	9

All (202) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	254	PRO
2	B	209	GLN
2	B	348	CYS
2	B	367	GLU
2	B	370	PHE
2	B	392	GLY
2	B	393	GLN
2	B	428	ASN
2	B	513	ARG
3	C	9	THR
3	C	11	ARG
3	C	55	ASN
3	C	90	ASP
3	C	165	ASN
3	C	434	THR
1	D	254	PRO
2	E	209	GLN
2	E	348	CYS
2	E	367	GLU
2	E	370	PHE
2	E	392	GLY
2	E	393	GLN
2	E	428	ASN
2	E	513	ARG
2	E	550	ASN
3	F	8	GLN
3	F	9	THR
3	F	11	ARG
3	F	55	ASN
3	F	165	ASN
3	F	434	THR
1	G	254	PRO
2	H	209	GLN
2	H	348	CYS
2	H	367	GLU
2	H	370	PHE
2	H	392	GLY
2	H	393	GLN
2	H	428	ASN
2	H	513	ARG
3	I	8	GLN
3	I	29	GLU

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Mol	Chain	Res	Type
3	I	165	ASN
3	I	434	THR
1	A	97	VAL
1	A	110	HIS
1	A	248	LEU
2	B	139	MET
2	B	146	ALA
2	B	157	SER
2	B	182	LYS
2	B	183	PHE
2	B	205	ASN
2	B	220	ALA
2	B	277	GLY
2	B	328	ASN
2	B	347	GLY
2	B	515	ILE
2	B	531	LYS
2	B	535	GLN
3	C	151	GLY
3	C	226	GLN
1	D	97	VAL
1	D	110	HIS
1	D	248	LEU
2	E	157	SER
2	E	182	LYS
2	E	183	PHE
2	E	205	ASN
2	E	220	ALA
2	E	277	GLY
2	E	328	ASN
2	E	347	GLY
2	E	515	ILE
2	E	531	LYS
2	E	535	GLN
3	F	90	ASP
3	F	151	GLY
3	F	226	GLN
1	G	97	VAL
1	G	110	HIS
1	G	248	LEU
2	H	143	ARG
2	H	157	SER

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Mol	Chain	Res	Type
2	H	182	LYS
2	H	183	PHE
2	H	205	ASN
2	H	220	ALA
2	H	277	GLY
2	H	328	ASN
2	H	347	GLY
2	H	515	ILE
2	H	531	LYS
2	H	535	GLN
3	I	55	ASN
3	I	59	GLU
3	I	151	GLY
3	I	226	GLN
1	A	19	TYR
1	A	51	GLY
1	A	105	VAL
1	A	115	LEU
1	A	202	GLY
1	A	206	TRP
1	A	207	VAL
1	A	208	ARG
2	B	162	LYS
2	B	530	LEU
2	B	536	LEU
3	C	12	PHE
3	C	19	LEU
1	D	19	TYR
1	D	51	GLY
1	D	105	VAL
1	D	115	LEU
1	D	202	GLY
1	D	206	TRP
1	D	207	VAL
1	D	208	ARG
2	E	162	LYS
2	E	530	LEU
2	E	536	LEU
3	F	21	GLU
3	F	87	ALA
1	G	19	TYR
1	G	51	GLY

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Mol	Chain	Res	Type
1	G	105	VAL
1	G	115	LEU
1	G	202	GLY
1	G	206	TRP
1	G	207	VAL
1	G	208	ARG
2	H	162	LYS
2	H	530	LEU
2	H	536	LEU
3	I	57	GLY
3	I	93	GLU
3	I	383	PRO
2	B	144	PHE
2	B	164	ILE
2	B	496	PHE
2	B	508	LYS
2	B	516	THR
2	B	527	LEU
3	C	21	GLU
3	C	59	GLU
3	C	403	SER
1	D	11	LEU
2	E	164	ILE
2	E	496	PHE
2	E	508	LYS
2	E	516	THR
2	E	527	LEU
3	F	403	SER
1	G	11	LEU
2	H	164	ILE
2	H	496	PHE
2	H	508	LYS
2	H	516	THR
2	H	527	LEU
3	I	92	ASP
3	I	403	SER
1	A	114	PRO
3	C	152	GLY
3	C	354	SER
1	D	114	PRO
3	F	20	LYS
3	F	152	GLY

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Mol	Chain	Res	Type
3	F	354	SER
1	G	114	PRO
3	I	152	GLY
3	I	354	SER
3	I	422	LEU
1	A	64	PRO
1	A	83	LYS
1	A	192	GLN
1	A	243	TRP
1	A	276	ASN
3	C	333	SER
1	D	64	PRO
1	D	83	LYS
1	D	243	TRP
1	D	276	ASN
3	F	333	SER
1	G	64	PRO
1	G	83	LYS
1	G	192	GLN
1	G	243	TRP
1	G	276	ASN
3	I	333	SER
1	A	216	VAL
1	D	216	VAL
3	F	383	PRO
1	G	216	VAL
2	B	208	PRO
2	E	208	PRO
2	H	208	PRO
2	E	329	ASP
2	H	329	ASP
3	C	383	PRO
3	I	382	LYS

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	233/252 (92%)	221 (95%)	12 (5%)	21	54
1	D	233/252 (92%)	222 (95%)	11 (5%)	23	57
1	G	233/252 (92%)	223 (96%)	10 (4%)	26	59
2	B	397/404 (98%)	359 (90%)	38 (10%)	8	32
2	E	386/404 (96%)	349 (90%)	37 (10%)	8	32
2	H	383/404 (95%)	348 (91%)	35 (9%)	9	34
3	C	387/425 (91%)	356 (92%)	31 (8%)	11	40
3	F	387/425 (91%)	354 (92%)	33 (8%)	10	37
3	I	382/425 (90%)	355 (93%)	27 (7%)	13	44
All	All	3021/3243 (93%)	2787 (92%)	234 (8%)	12	41

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	13	HIS
1	A	20	TYR
1	A	30	ASP
1	A	43	HIS
1	A	46	ILE
1	A	57	TRP
1	A	70	LEU
1	A	217	LEU
1	A	225	VAL
1	A	237	ASP
1	A	275	ASP
2	B	142	ARG
2	B	143	ARG
2	B	144	PHE
2	B	159	LEU
2	B	177	THR
2	B	194	ILE
2	B	197	VAL
2	B	199	ILE
2	B	202	ARG
2	B	209	GLN
2	B	215	LEU
2	B	227	THR
2	B	233	LEU
2	B	281	GLU

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Mol	Chain	Res	Type
2	B	282	GLU
2	B	291	ILE
2	B	307	SER
2	B	328	ASN
2	B	335	LEU
2	B	340	LEU
2	B	350	ILE
2	B	367	GLU
2	B	369	LEU
2	B	399	LEU
2	B	407	LEU
2	B	414	TYR
2	B	418	ILE
2	B	430	ASN
2	B	437	GLU
2	B	439	ARG
2	B	447	VAL
2	B	455	GLN
2	B	457	LEU
2	B	468	GLU
2	B	490	SER
2	B	515	ILE
2	B	547	TYR
2	B	550	ASN
3	C	18	THR
3	C	26	GLN
3	C	34	ASP
3	C	39	ILE
3	C	42	PHE
3	C	58	ASP
3	C	71	GLU
3	C	86	ASN
3	C	92	ASP
3	C	118	GLN
3	C	128	GLU
3	C	211	ILE
3	C	225	THR
3	C	226	GLN
3	C	232	ASN
3	C	237	ILE
3	C	274	GLN
3	C	278	GLN

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Mol	Chain	Res	Type
3	C	284	SER
3	C	293	ILE
3	C	314	ILE
3	C	343	ILE
3	C	363	VAL
3	C	365	MET
3	C	379	ILE
3	C	387	ARG
3	C	395	CYS
3	C	404	VAL
3	C	422	LEU
3	C	429	ILE
3	C	431	ILE
1	D	9	ASN
1	D	20	TYR
1	D	30	ASP
1	D	43	HIS
1	D	46	ILE
1	D	57	TRP
1	D	70	LEU
1	D	217	LEU
1	D	225	VAL
1	D	237	ASP
1	D	275	ASP
2	E	142	ARG
2	E	143	ARG
2	E	145	THR
2	E	159	LEU
2	E	194	ILE
2	E	197	VAL
2	E	199	ILE
2	E	202	ARG
2	E	209	GLN
2	E	215	LEU
2	E	227	THR
2	E	233	LEU
2	E	281	GLU
2	E	282	GLU
2	E	291	ILE
2	E	307	SER
2	E	328	ASN
2	E	335	LEU

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Mol	Chain	Res	Type
2	E	340	LEU
2	E	350	ILE
2	E	367	GLU
2	E	369	LEU
2	E	370	PHE
2	E	399	LEU
2	E	407	LEU
2	E	414	TYR
2	E	418	ILE
2	E	430	ASN
2	E	437	GLU
2	E	439	ARG
2	E	447	VAL
2	E	455	GLN
2	E	457	LEU
2	E	468	GLU
2	E	490	SER
2	E	515	ILE
2	E	550	ASN
3	F	7	TYR
3	F	12	PHE
3	F	19	LEU
3	F	24	ILE
3	F	34	ASP
3	F	39	ILE
3	F	42	PHE
3	F	58	ASP
3	F	71	GLU
3	F	86	ASN
3	F	118	GLN
3	F	128	GLU
3	F	211	ILE
3	F	225	THR
3	F	226	GLN
3	F	232	ASN
3	F	237	ILE
3	F	274	GLN
3	F	278	GLN
3	F	284	SER
3	F	293	ILE
3	F	310	THR
3	F	314	ILE

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Mol	Chain	Res	Type
3	F	343	ILE
3	F	363	VAL
3	F	365	MET
3	F	387	ARG
3	F	395	CYS
3	F	400	ASN
3	F	404	VAL
3	F	423	GLN
3	F	429	ILE
3	F	431	ILE
1	G	20	TYR
1	G	30	ASP
1	G	43	HIS
1	G	46	ILE
1	G	57	TRP
1	G	70	LEU
1	G	217	LEU
1	G	225	VAL
1	G	237	ASP
1	G	275	ASP
2	H	132	ILE
2	H	159	LEU
2	H	194	ILE
2	H	197	VAL
2	H	199	ILE
2	H	202	ARG
2	H	209	GLN
2	H	215	LEU
2	H	227	THR
2	H	233	LEU
2	H	281	GLU
2	H	282	GLU
2	H	291	ILE
2	H	307	SER
2	H	328	ASN
2	H	335	LEU
2	H	340	LEU
2	H	350	ILE
2	H	367	GLU
2	H	369	LEU
2	H	370	PHE
2	H	399	LEU

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Mol	Chain	Res	Type
2	H	407	LEU
2	H	414	TYR
2	H	418	ILE
2	H	430	ASN
2	H	437	GLU
2	H	439	ARG
2	H	447	VAL
2	H	455	GLN
2	H	457	LEU
2	H	468	GLU
2	H	490	SER
2	H	515	ILE
2	H	547	TYR
3	I	9	THR
3	I	12	PHE
3	I	34	ASP
3	I	39	ILE
3	I	42	PHE
3	I	71	GLU
3	I	90	ASP
3	I	93	GLU
3	I	118	GLN
3	I	128	GLU
3	I	211	ILE
3	I	225	THR
3	I	226	GLN
3	I	232	ASN
3	I	237	ILE
3	I	274	GLN
3	I	278	GLN
3	I	284	SER
3	I	293	ILE
3	I	310	THR
3	I	314	ILE
3	I	343	ILE
3	I	387	ARG
3	I	395	CYS
3	I	404	VAL
3	I	429	ILE
3	I	431	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	63	HIS
1	A	95	HIS
1	A	98	HIS
1	A	276	ASN
2	B	209	GLN
2	B	328	ASN
2	B	455	GLN
2	B	523	ASN
3	C	216	GLN
3	C	235	GLN
3	C	273	ASN
1	D	9	ASN
1	D	276	ASN
2	E	209	GLN
2	E	455	GLN
2	E	523	ASN
3	F	27	ASN
3	F	229	ASN
3	F	273	ASN
1	G	9	ASN
1	G	276	ASN
2	H	209	GLN
2	H	455	GLN
2	H	498	ASN
2	H	523	ASN
3	I	229	ASN
3	I	273	ASN
3	I	400	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	274/297 (92%)	0.79	28 (10%) 12 8	103, 167, 201, 202	0
1	D	274/297 (92%)	1.06	45 (16%) 4 3	101, 185, 202, 202	0
1	G	274/297 (92%)	1.06	44 (16%) 4 3	127, 193, 202, 202	0
2	B	434/442 (98%)	0.23	24 (5%) 30 19	36, 101, 181, 202	2 (0%)
2	E	423/442 (95%)	0.28	31 (7%) 21 13	41, 93, 192, 202	2 (0%)
2	H	420/442 (95%)	0.42	32 (7%) 20 13	46, 121, 200, 202	2 (0%)
3	C	419/460 (91%)	0.18	17 (4%) 41 25	5, 95, 175, 202	19 (4%)
3	F	419/460 (91%)	0.19	18 (4%) 40 24	6, 96, 178, 201	19 (4%)
3	I	414/460 (90%)	-0.08	7 (1%) 69 49	48, 95, 181, 202	0
All	All	3351/3597 (93%)	0.39	246 (7%) 21 13	5, 123, 201, 202	44 (1%)

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	ALA	6.8
1	D	223	ALA	5.7
1	A	260	ALA	5.4
2	E	367	GLU	5.2
2	B	392	GLY	5.2
2	H	543	LEU	5.1
1	A	43	HIS	5.0
1	G	266	GLY	5.0
2	E	138	ILE	4.9
3	F	60	SER	4.8
2	B	145	THR	4.8
2	B	367	GLU	4.5
1	D	265	SER	4.5
2	B	144	PHE	4.4
2	H	392	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	146	ILE	4.2
1	D	114	PRO	4.2
2	H	547	TYR	4.2
2	H	348	CYS	4.1
1	G	12	ILE	4.0
1	G	95	HIS	4.0
2	H	367	GLU	4.0
1	A	15	ALA	3.9
2	H	537	ILE	3.9
2	E	392	GLY	3.9
2	B	527	LEU	3.9
3	I	436	LEU	3.9
2	E	135	ALA	3.8
2	B	547	TYR	3.8
1	G	17	LEU	3.7
1	A	17	LEU	3.7
2	H	169	GLY	3.7
1	A	270	ALA	3.7
3	I	366	LEU	3.7
1	D	15	ALA	3.7
2	B	172	ILE	3.7
2	E	134	ASN	3.7
2	E	150	PHE	3.6
1	D	11	LEU	3.6
1	D	72	SER	3.5
2	H	369	LEU	3.5
3	C	114	LYS	3.5
1	D	12	ILE	3.5
3	C	60	SER	3.5
3	C	283	GLU	3.4
2	E	139	MET	3.4
1	D	224	SER	3.4
1	A	11	LEU	3.4
1	D	273	GLY	3.4
3	F	59	GLU	3.4
1	D	247	LEU	3.4
1	G	118	VAL	3.4
2	E	148	TYR	3.4
3	F	432	TYR	3.4
1	D	9	ASN	3.3
2	H	149	THR	3.3
1	G	247	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
3	I	430	PRO	3.3
1	D	73	CYS	3.3
1	G	260	ALA	3.3
1	D	272	SER	3.2
1	G	9	ASN	3.2
1	A	278	VAL	3.2
1	G	184	ILE	3.2
2	E	151	ALA	3.2
2	E	144	PHE	3.2
1	G	63	HIS	3.2
2	H	484	ALA	3.2
1	A	70	LEU	3.1
1	G	148	VAL	3.1
1	A	95	HIS	3.1
2	B	179	LEU	3.1
2	H	170	VAL	3.1
1	G	15	ALA	3.0
2	B	131	GLU	3.0
2	H	132	ILE	3.0
2	E	513	ARG	3.0
2	E	133	ASP	3.0
1	A	194	TYR	3.0
1	D	293	GLY	3.0
1	G	72	SER	2.9
1	G	272	SER	2.9
2	H	344	SER	2.9
2	E	348	CYS	2.9
3	F	114	LYS	2.9
2	E	168	SER	2.9
2	B	550	ASN	2.9
1	G	128	VAL	2.9
3	C	15	PHE	2.9
1	D	110	HIS	2.8
1	G	170	SER	2.8
3	C	284	SER	2.8
1	D	157	THR	2.8
2	H	150	PHE	2.8
2	H	549	GLY	2.8
1	D	143	ALA	2.8
1	D	279	THR	2.8
1	G	11	LEU	2.8
2	E	145	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	161	THR	2.8
1	A	71	ALA	2.8
1	G	81	ILE	2.8
1	G	253	PHE	2.7
3	C	380	ILE	2.8
1	D	128	VAL	2.7
1	D	17	LEU	2.7
1	D	271	LEU	2.7
2	B	168	SER	2.7
3	F	15	PHE	2.7
1	D	136	THR	2.7
3	C	253	GLN	2.7
3	F	115	GLN	2.7
1	D	218	LEU	2.7
3	C	268	SER	2.7
2	B	369	LEU	2.7
1	A	272	SER	2.7
2	B	162	LYS	2.7
1	A	209	ASP	2.7
3	I	311	ASP	2.7
1	A	13	HIS	2.7
2	B	513	ARG	2.7
3	F	268	SER	2.7
1	D	117	LEU	2.6
2	H	157	SER	2.6
1	G	218	LEU	2.6
2	H	201	ALA	2.6
3	C	355	LEU	2.6
3	F	351	ILE	2.6
1	G	73	CYS	2.6
1	A	265	SER	2.6
1	D	66	PHE	2.6
1	G	265	SER	2.6
2	E	538	PHE	2.6
2	H	154	SER	2.6
3	I	435	PHE	2.5
1	G	273	GLY	2.5
1	D	267	ASN	2.5
3	F	40	ARG	2.5
2	H	148	TYR	2.5
2	E	137	LEU	2.5
3	F	322	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	210	VAL	2.5
3	C	440	ASP	2.5
2	E	457	LEU	2.5
1	A	152	SER	2.5
1	G	258	TRP	2.5
3	F	355	LEU	2.5
1	A	139	ILE	2.5
1	D	118	VAL	2.5
1	D	71	ALA	2.4
1	G	136	THR	2.4
3	C	115	GLN	2.4
3	I	433	ALA	2.4
3	C	322	LEU	2.4
1	A	19	TYR	2.4
1	A	92	ILE	2.4
2	E	162	LYS	2.4
1	G	110	HIS	2.4
2	E	347	GLY	2.4
1	D	146	ILE	2.4
1	G	222	LEU	2.4
3	F	284	SER	2.4
1	D	69	ILE	2.4
1	G	145	ALA	2.4
2	E	509	ARG	2.4
2	E	483	PHE	2.4
2	H	153	PHE	2.4
1	A	261	SER	2.4
3	F	142	SER	2.4
1	D	210	VAL	2.4
1	G	79	VAL	2.4
2	B	128	CYS	2.4
2	H	206	PRO	2.4
1	D	134	GLY	2.3
2	H	208	PRO	2.3
1	D	63	HIS	2.3
2	E	512	MET	2.3
2	E	518	LEU	2.3
3	F	230	GLU	2.3
2	E	526	ILE	2.3
1	A	33	ILE	2.3
2	B	526	ILE	2.3
1	D	209	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	128	VAL	2.3
2	H	533	PRO	2.3
2	H	159	LEU	2.3
1	D	225	VAL	2.3
1	D	95	HIS	2.2
1	D	193	THR	2.2
2	B	149	THR	2.2
2	B	127	GLU	2.2
1	D	92	ILE	2.2
2	H	138	ILE	2.2
3	C	39	ILE	2.2
2	E	530	LEU	2.2
1	G	90	SER	2.2
1	D	139	ILE	2.2
3	C	398	ILE	2.2
3	C	40	ARG	2.2
1	G	144	HIS	2.2
2	E	155	THR	2.2
2	B	403	VAL	2.2
1	D	184	ILE	2.2
1	G	92	ILE	2.2
1	G	143	ALA	2.2
2	B	447	VAL	2.2
3	F	416	TYR	2.2
1	G	261	SER	2.2
2	H	171	SER	2.2
2	H	536	LEU	2.2
1	G	93	ALA	2.2
2	B	146	ALA	2.2
1	A	155	PRO	2.2
1	D	130	PHE	2.2
1	G	179	ASP	2.2
2	H	152	LYS	2.1
2	H	162	LYS	2.1
3	I	382	LYS	2.1
2	H	145	THR	2.1
2	B	182	LYS	2.1
1	A	106	GLN	2.1
1	G	16	VAL	2.1
1	G	112	TYR	2.1
2	H	481	LEU	2.1
2	B	158	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	113	GLY	2.1
1	G	155	PRO	2.1
3	F	357	SER	2.1
1	D	80	LEU	2.1
2	E	527	LEU	2.1
1	A	136	THR	2.1
1	G	139	ILE	2.1
3	C	420	LEU	2.1
3	F	39	ILE	2.1
2	B	516	THR	2.1
2	E	169	GLY	2.1
3	F	8	GLN	2.1
1	G	138	PRO	2.1
1	D	137	SER	2.0
1	D	26	THR	2.0
2	E	186	ASP	2.0
1	A	134	GLY	2.0
2	E	170	VAL	2.0
1	G	217	LEU	2.0
1	G	230	THR	2.0
3	C	416	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.