



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:21 PM UTC

PDB ID : 4LNF / pdb_00004lnf
Title : B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: structure of GS-Q
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.
Deposited on : 2013-07-11
Resolution : 2.95 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

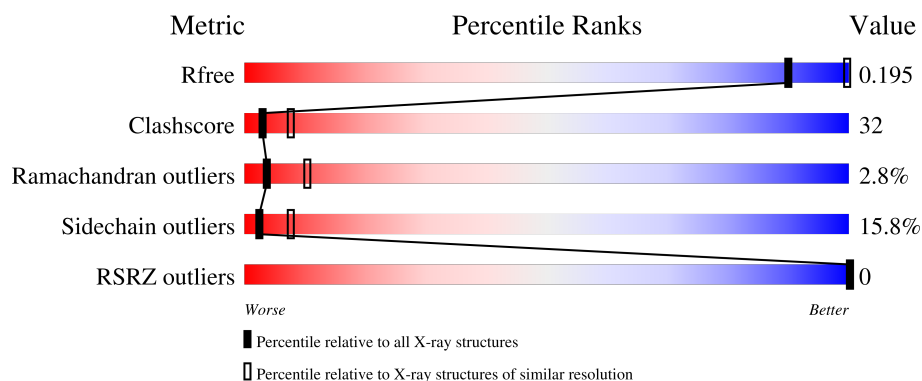
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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.



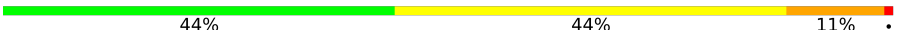
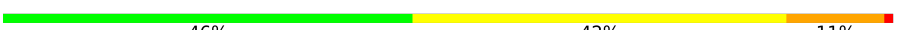
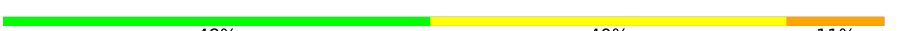
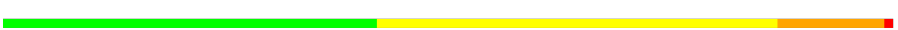
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	443	50% 40% 9%
1	B	443	45% 46% 8%
1	C	443	47% 44% 9%
1	D	443	48% 42% 9%
1	E	443	52% 40% 8%

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Mol	Chain	Length	Quality of chain
1	F	443	 44% 44% 11% .
1	G	443	 46% 42% 12% .
1	H	443	 45% 43% 12% .
1	I	443	 46% 42% 11% .
1	J	443	 48% 40% 11%
1	K	443	 42% 45% 12% .
1	L	443	 46% 43% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	A	504	-	-	X	-
4	PO4	C	504	-	-	X	-
4	PO4	G	504	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 42824 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 Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	B	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	C	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	D	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	E	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	F	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	G	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	H	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	I	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	J	441	Total	C	N	O	S	0	0	0
			3521	2250	587	668	16			
1	K	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	L	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

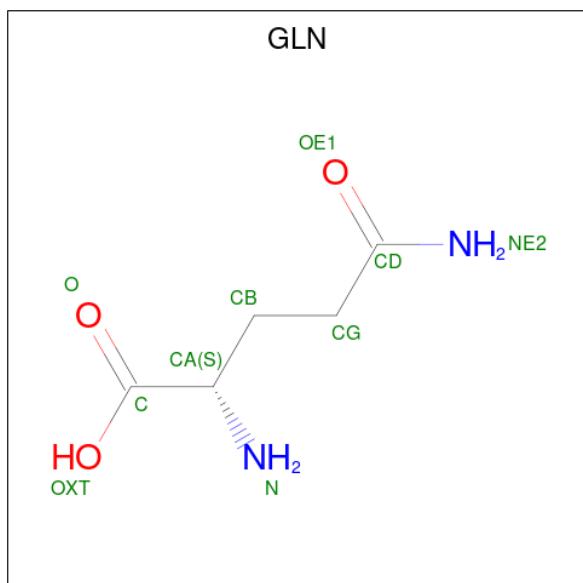
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mg	0	0
			3	3		
2	B	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	3	Total 3	Mg 3	0	0
2	D	3	Total 3	Mg 3	0	0
2	E	3	Total 3	Mg 3	0	0
2	F	3	Total 3	Mg 3	0	0
2	G	3	Total 3	Mg 3	0	0
2	H	3	Total 3	Mg 3	0	0
2	I	3	Total 3	Mg 3	0	0
2	J	3	Total 3	Mg 3	0	0
2	K	3	Total 3	Mg 3	0	0
2	L	3	Total 3	Mg 3	0	0

- Molecule 3 is GLUTAMINE (CCD ID: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 9	C 5	N 2	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			9	5	2	2		
3	C	1	Total	C	N	O	0	0
			9	5	2	2		
3	D	1	Total	C	N	O	0	0
			9	5	2	2		
3	E	1	Total	C	N	O	0	0
			9	5	2	2		
3	F	1	Total	C	N	O	0	0
			9	5	2	2		
3	G	1	Total	C	N	O	0	0
			9	5	2	2		
3	H	1	Total	C	N	O	0	0
			9	5	2	2		
3	I	1	Total	C	N	O	0	0
			9	5	2	2		
3	J	1	Total	C	N	O	0	0
			9	5	2	2		
3	K	1	Total	C	N	O	0	0
			9	5	2	2		
3	L	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	G	1	Total O P 5 4 1	0	0
4	H	1	Total O P 5 4 1	0	0

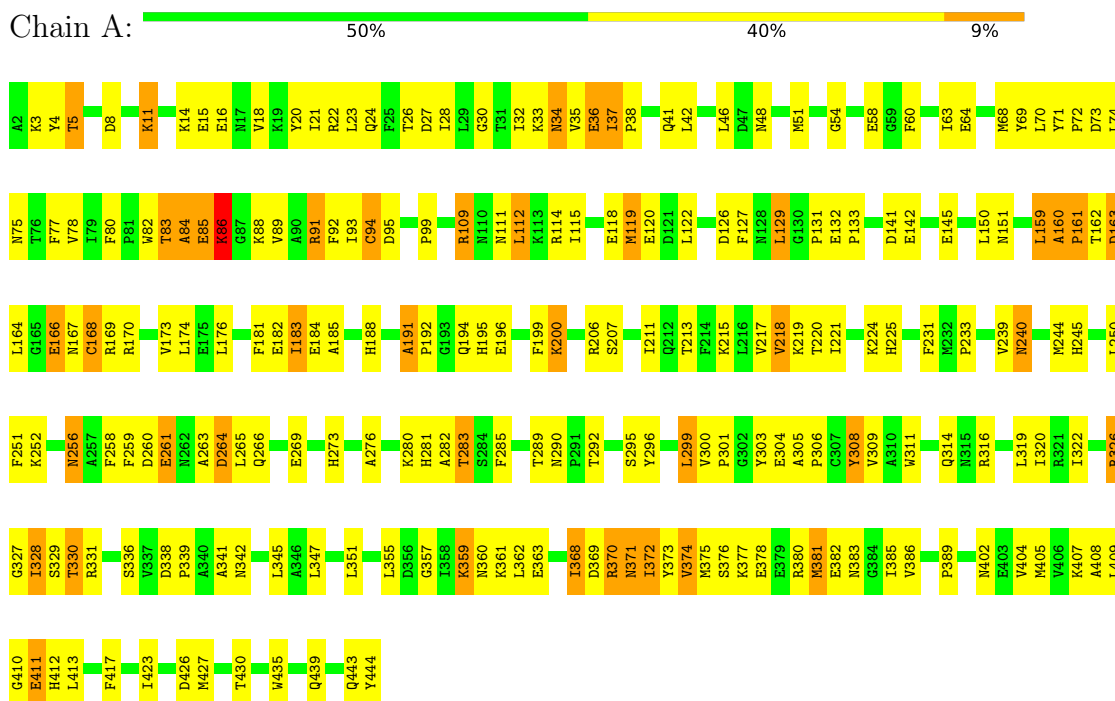
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	16	Total O 16 16	0	0
5	B	20	Total O 20 20	0	0
5	C	18	Total O 18 18	0	0
5	D	29	Total O 29 29	0	0
5	E	18	Total O 18 18	0	0
5	F	19	Total O 19 19	0	0
5	G	14	Total O 14 14	0	0
5	H	21	Total O 21 21	0	0
5	I	21	Total O 21 21	0	0
5	J	27	Total O 27 27	0	0
5	K	27	Total O 27 27	0	0
5	L	23	Total O 23 23	0	0

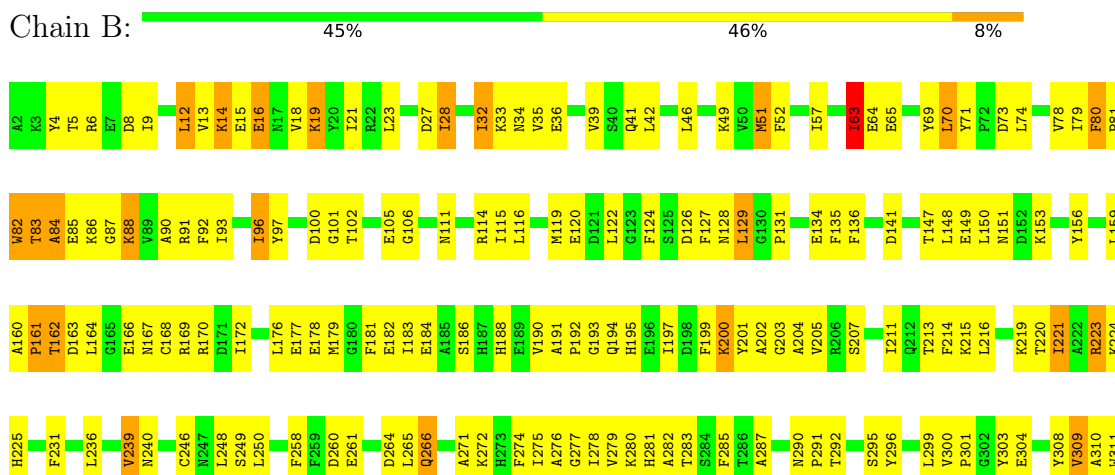
3 Residue-property plots

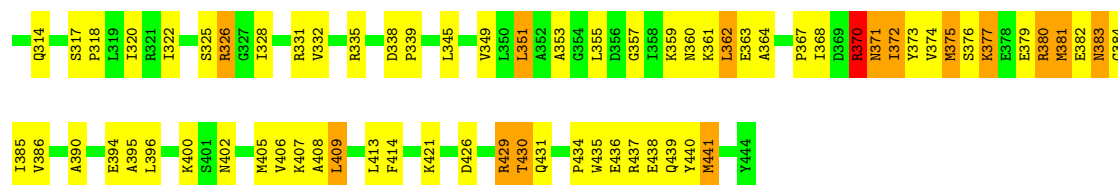
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Glutamine synthetase



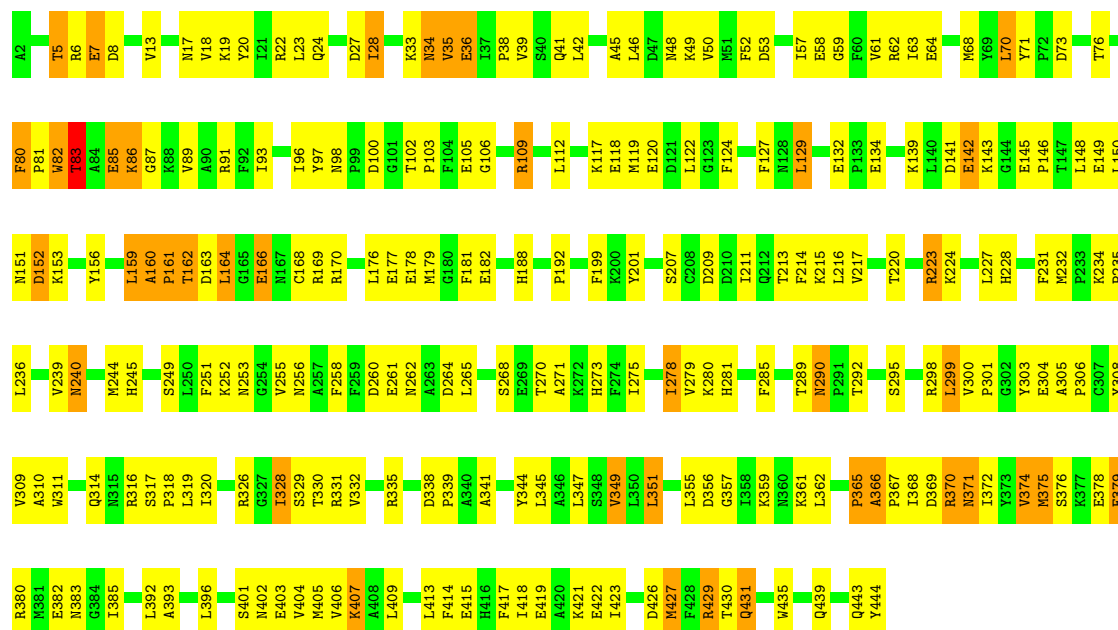
- Molecule 1: Glutamine synthetase





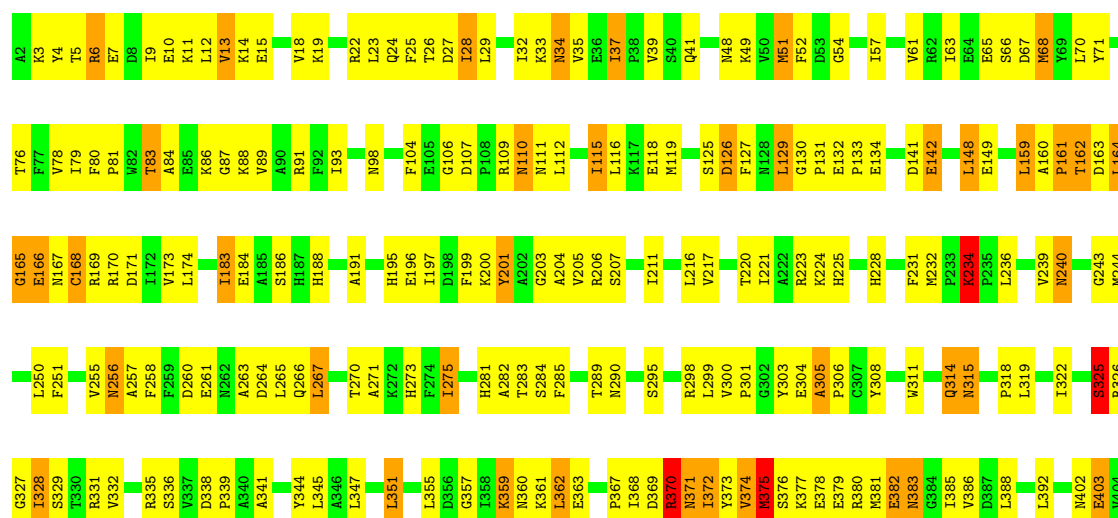
• Molecule 1: Glutamine synthetase

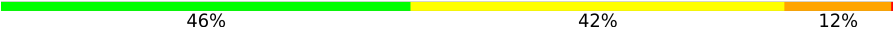
Chain C: 47% 44% 9%

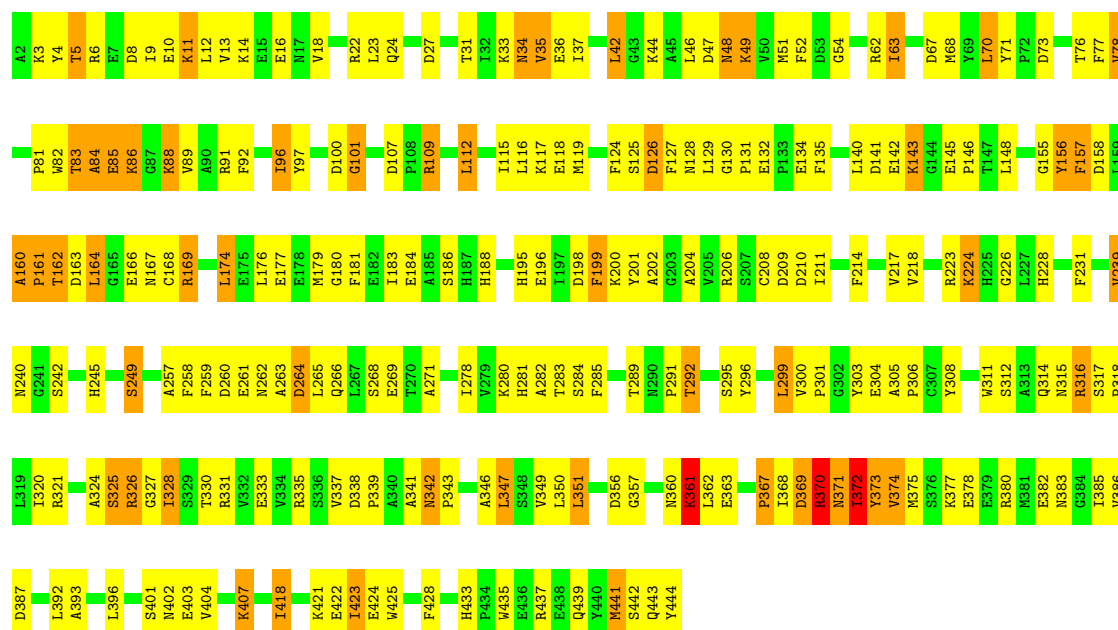


• Molecule 1: Glutamine synthetase

Chain D: 48% 42% 9%

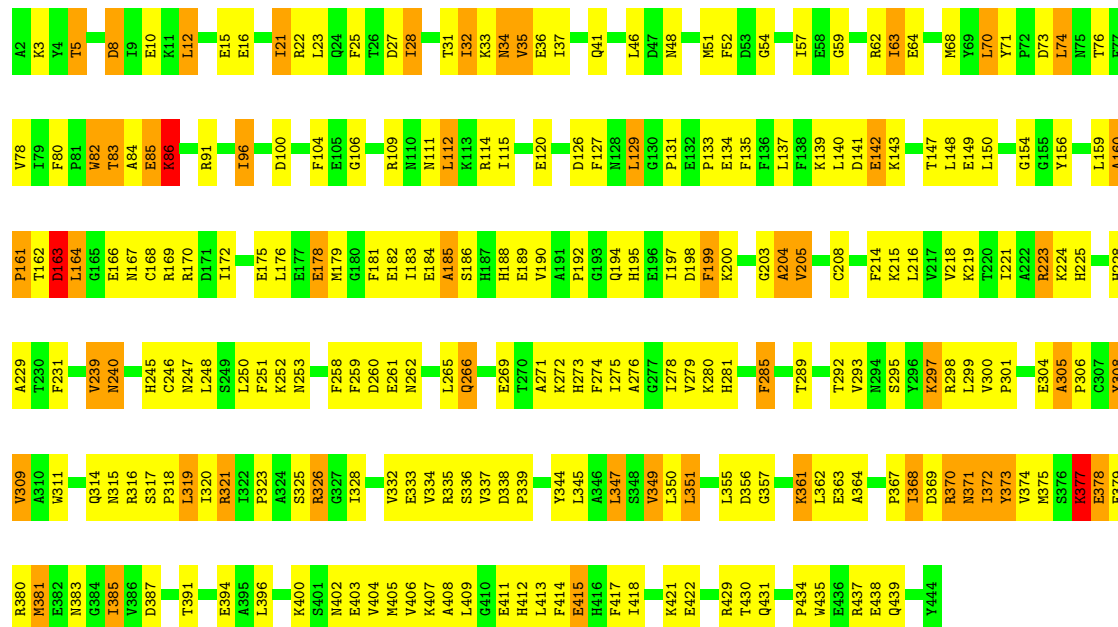


Chain G:  46% 42% 12%



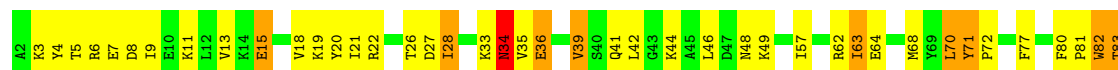
• Molecule 1: Glutamine synthetase

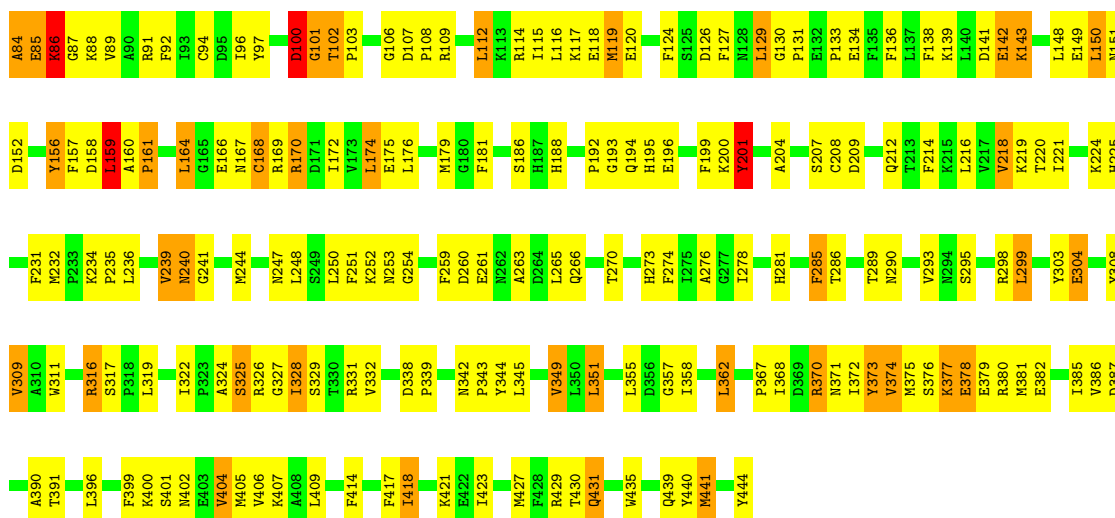
Chain H:  45% 43% 12%



• Molecule 1: Glutamine synthetase

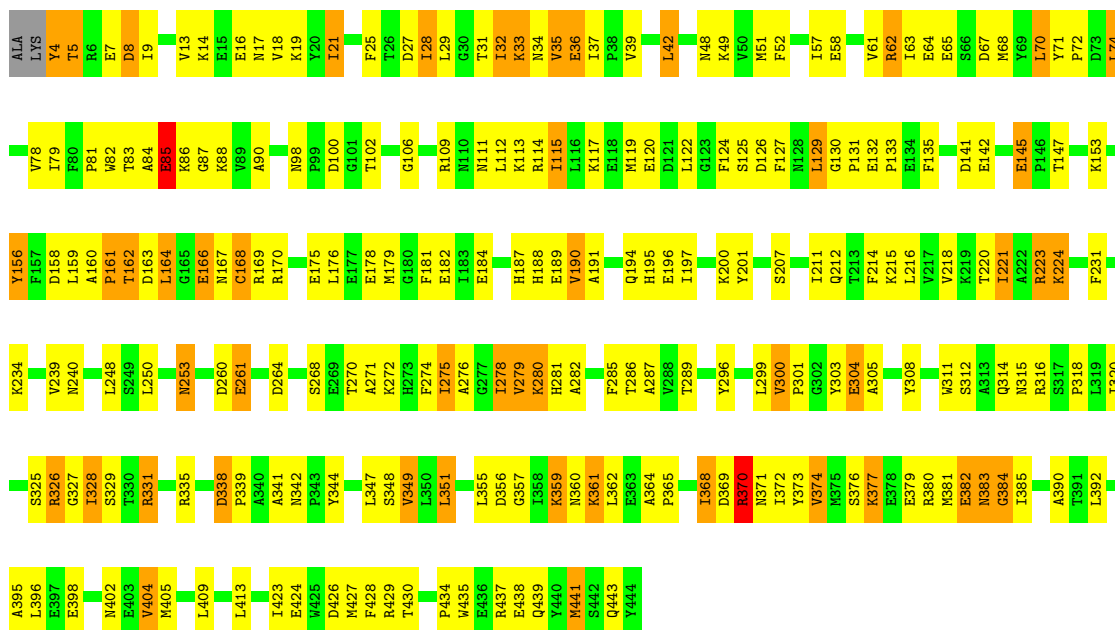
Chain I:  46% 42% 11%





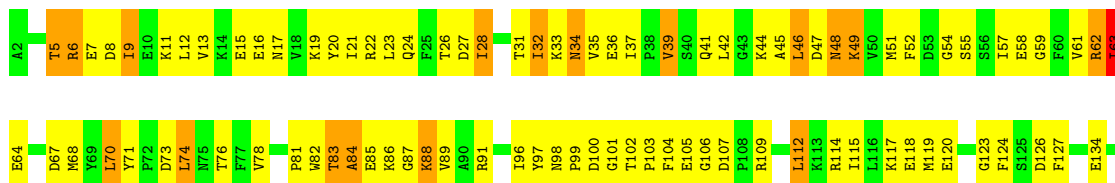
• Molecule 1: Glutamine synthetase

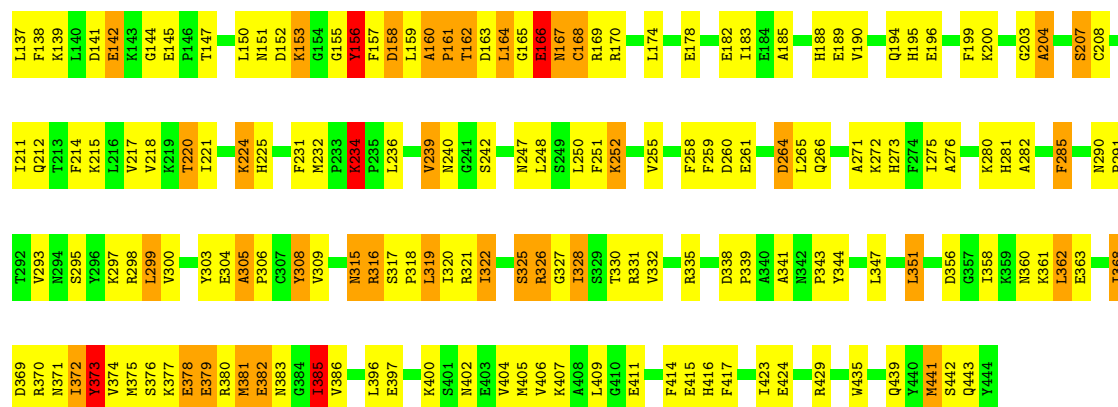
Chain J: 48% 40% 11%



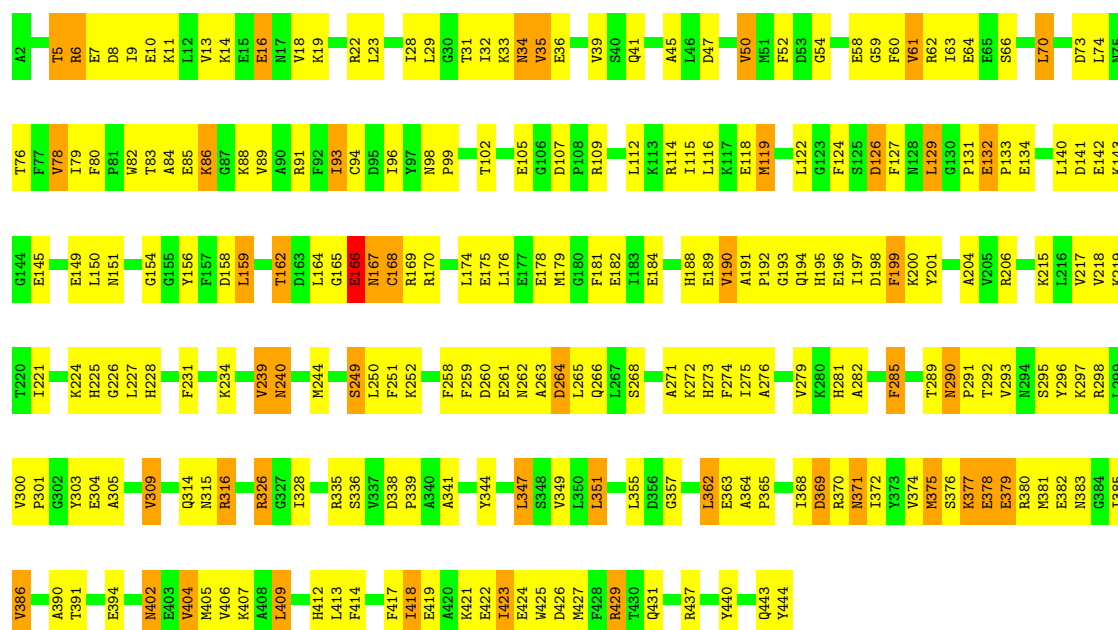
• Molecule 1: Glutamine synthetase

Chain K: 42% 45% 12%





• Molecule 1: Glutamine synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	112.00Å 137.50Å 137.70Å 119.80° 90.30° 93.40°	Depositor
Resolution (Å)	119.01 – 2.95 119.01 – 2.95	Depositor EDS
% Data completeness (in resolution range)	96.0 (119.01-2.95) 94.2 (119.01-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.194 , 0.259 0.188 , 0.195	Depositor DCC
R_{free} test set	11503 reflections (7.99%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.719	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.357 for -h,-k-l,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	42824	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG

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	0.51	0/3618	0.90	7/4895 (0.1%)
1	B	0.52	0/3618	0.91	7/4895 (0.1%)
1	C	0.52	0/3618	0.89	4/4895 (0.1%)
1	D	0.54	0/3618	0.92	14/4895 (0.3%)
1	E	0.53	0/3618	0.92	5/4895 (0.1%)
1	F	0.52	0/3618	0.89	3/4895 (0.1%)
1	G	0.52	0/3618	0.90	8/4895 (0.2%)
1	H	0.52	0/3618	0.90	4/4895 (0.1%)
1	I	0.53	0/3618	0.91	7/4895 (0.1%)
1	J	0.54	0/3604	0.91	7/4877 (0.1%)
1	K	0.54	0/3618	0.93	10/4895 (0.2%)
1	L	0.52	0/3618	0.92	7/4895 (0.1%)
All	All	0.53	0/43402	0.91	83/58722 (0.1%)

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	LYS	N-CA-C	-8.11	101.86	113.21
1	A	160	ALA	CA-C-N	7.95	129.77	119.84
1	A	160	ALA	C-N-CA	7.95	129.77	119.84
1	I	130	GLY	CA-C-N	7.70	127.46	119.76
1	I	130	GLY	C-N-CA	7.70	127.46	119.76
1	C	80	PHE	CA-C-N	7.69	127.87	119.87
1	C	80	PHE	C-N-CA	7.69	127.87	119.87
1	H	305	ALA	CA-C-N	7.56	127.99	119.83
1	H	305	ALA	C-N-CA	7.56	127.99	119.83
1	F	305	ALA	CA-C-N	7.38	127.14	119.76
1	F	305	ALA	C-N-CA	7.38	127.14	119.76
1	J	338	ASP	CA-C-N	7.28	126.95	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	338	ASP	C-N-CA	7.28	126.95	119.82
1	J	305	ALA	CA-C-N	7.22	127.20	119.76
1	J	305	ALA	C-N-CA	7.22	127.20	119.76
1	L	290	ASN	CA-C-N	7.21	126.92	119.64
1	L	290	ASN	C-N-CA	7.21	126.92	119.64
1	G	160	ALA	CA-C-N	7.00	128.59	119.84
1	G	160	ALA	C-N-CA	7.00	128.59	119.84
1	K	234	LYS	CA-C-N	6.95	126.43	118.85
1	K	234	LYS	C-N-CA	6.95	126.43	118.85
1	C	160	ALA	CA-C-N	6.70	128.22	119.84
1	C	160	ALA	C-N-CA	6.70	128.22	119.84
1	D	232	MET	CA-C-N	6.58	126.08	119.24
1	D	232	MET	C-N-CA	6.58	126.08	119.24
1	D	234	LYS	CA-C-N	6.49	125.72	118.97
1	D	234	LYS	C-N-CA	6.49	125.72	118.97
1	B	63	ILE	CB-CA-C	-6.35	105.40	111.05
1	K	160	ALA	CA-C-N	6.26	127.67	119.84
1	K	160	ALA	C-N-CA	6.26	127.67	119.84
1	D	305	ALA	CA-C-N	6.25	126.28	119.90
1	D	305	ALA	C-N-CA	6.25	126.28	119.90
1	E	433	HIS	CA-C-N	6.18	126.08	119.28
1	E	433	HIS	C-N-CA	6.18	126.08	119.28
1	K	86	LYS	N-CA-C	-6.00	106.12	113.50
1	B	191	ALA	CA-C-N	5.98	126.00	119.90
1	B	191	ALA	C-N-CA	5.98	126.00	119.90
1	K	305	ALA	CA-C-N	5.97	125.73	119.76
1	K	305	ALA	C-N-CA	5.97	125.73	119.76
1	D	86	LYS	N-CA-C	-5.94	105.21	112.88
1	D	322	ILE	CA-C-N	5.93	126.27	119.92
1	D	322	ILE	C-N-CA	5.93	126.27	119.92
1	B	122	LEU	N-CA-C	-5.91	104.93	114.09
1	G	305	ALA	CA-C-N	5.79	125.81	119.90
1	G	305	ALA	C-N-CA	5.79	125.81	119.90
1	G	433	HIS	CA-C-N	5.78	125.91	119.32
1	G	433	HIS	C-N-CA	5.78	125.91	119.32
1	J	130	GLY	CA-C-N	5.72	126.17	119.99
1	J	130	GLY	C-N-CA	5.72	126.17	119.99
1	A	322	ILE	CA-C-N	5.66	126.92	119.84
1	A	322	ILE	C-N-CA	5.66	126.92	119.84
1	G	257	ALA	CA-C-N	-5.61	115.05	122.85
1	G	257	ALA	C-N-CA	-5.61	115.05	122.85
1	H	160	ALA	CA-C-N	5.53	126.75	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	160	ALA	C-N-CA	5.53	126.75	119.84
1	B	190	VAL	N-CA-C	5.52	115.97	110.23
1	D	111	ASN	N-CA-C	-5.49	106.64	113.55
1	E	232	MET	CA-C-N	5.37	126.56	119.84
1	E	232	MET	C-N-CA	5.37	126.56	119.84
1	D	37	ILE	CA-C-N	5.36	125.82	120.14
1	D	37	ILE	C-N-CA	5.36	125.82	120.14
1	I	71	TYR	CA-C-N	5.36	125.28	119.76
1	I	71	TYR	C-N-CA	5.36	125.28	119.76
1	L	86	LYS	N-CA-C	-5.32	106.66	112.72
1	A	191	ALA	CA-C-N	5.31	125.56	119.83
1	A	191	ALA	C-N-CA	5.31	125.56	119.83
1	L	80	PHE	CA-C-N	5.25	124.75	119.19
1	L	80	PHE	C-N-CA	5.25	124.75	119.19
1	I	322	ILE	CA-C-N	5.25	125.53	119.92
1	I	322	ILE	C-N-CA	5.25	125.53	119.92
1	L	305	ALA	CA-C-N	5.24	125.98	120.11
1	L	305	ALA	C-N-CA	5.24	125.98	120.11
1	K	385	ILE	N-CA-C	5.20	114.09	106.55
1	D	24	GLN	N-CA-C	5.15	117.98	109.85
1	F	331	ARG	N-CA-C	5.14	117.19	109.23
1	D	32	ILE	N-CA-C	5.10	113.94	106.55
1	I	34	ASN	N-CA-C	5.07	116.01	108.60
1	B	80	PHE	CA-C-N	5.04	126.14	119.84
1	B	80	PHE	C-N-CA	5.04	126.14	119.84
1	K	107	ASP	CA-C-N	5.03	124.47	119.24
1	K	107	ASP	C-N-CA	5.03	124.47	119.24
1	J	275	ILE	N-CA-C	5.03	115.64	110.36
1	E	55	SER	N-CA-C	-5.01	107.23	113.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3535	0	3466	236	0
1	B	3535	0	3466	254	0
1	C	3535	0	3466	222	0
1	D	3535	0	3466	226	0
1	E	3535	0	3466	231	0
1	F	3535	0	3466	263	0
1	G	3535	0	3466	228	0
1	H	3535	0	3466	236	0
1	I	3535	0	3466	243	0
1	J	3521	0	3448	225	0
1	K	3535	0	3466	279	0
1	L	3535	0	3466	225	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	3	0	0	0	0
3	A	9	0	7	0	0
3	B	9	0	7	1	0
3	C	9	0	7	3	0
3	D	9	0	7	1	0
3	E	9	0	7	2	0
3	F	9	0	7	1	0
3	G	9	0	7	0	0
3	H	9	0	7	5	0
3	I	9	0	7	1	0
3	J	9	0	7	1	0
3	K	9	0	7	1	0
3	L	10	0	7	0	0
4	A	5	0	0	3	0
4	C	5	0	0	3	0
4	G	5	0	0	2	0
4	H	5	0	0	1	0
5	A	16	0	0	2	0
5	B	20	0	0	1	0
5	C	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	29	0	0	4	0
5	E	18	0	0	2	0
5	F	19	0	0	4	0
5	G	14	0	0	0	0
5	H	21	0	0	2	0
5	I	21	0	0	0	0
5	J	27	0	0	1	0
5	K	27	0	0	2	0
5	L	23	0	0	0	0
All	All	42824	0	41658	2693	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 32.

All (2693) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:ALA:HB2	1:G:88:LYS:HD3	1.30	1.10
1:K:160:ALA:HB1	1:K:161:PRO:HD2	1.20	1.10
1:H:357:GLY:HA2	1:H:362:LEU:HD23	1.21	1.09
1:K:316:ARG:HD3	1:K:316:ARG:N	1.66	1.09
1:A:357:GLY:HA2	1:A:362:LEU:HD12	1.11	1.08
1:C:22:ARG:HG2	1:C:34:ASN:HD22	1.17	1.08
1:C:357:GLY:HA2	1:C:362:LEU:HD12	1.35	1.08
1:J:357:GLY:HA2	1:J:362:LEU:HD12	1.25	1.08
1:A:163:ASP:HA	1:A:170:ARG:HH21	1.03	1.08
1:E:160:ALA:HB1	1:E:161:PRO:HD2	1.34	1.07
1:E:22:ARG:HH11	1:E:22:ARG:HG2	1.15	1.06
1:J:328:ILE:HD13	1:J:328:ILE:H	1.18	1.05
1:F:232:MET:HE1	1:L:437:ARG:HA	1.33	1.05
1:I:170:ARG:HG2	1:I:170:ARG:HH11	1.20	1.05
1:D:6:ARG:HH11	1:D:6:ARG:HG3	1.21	1.05
1:D:160:ALA:HB1	1:D:161:PRO:HD2	1.35	1.05
1:L:377:LYS:HG2	1:L:378:GLU:H	1.22	1.05
1:A:163:ASP:HB3	1:B:83:THR:HG21	1.37	1.04
1:E:357:GLY:HA2	1:E:362:LEU:HD12	1.38	1.04
1:F:160:ALA:HB1	1:F:161:PRO:HD2	1.36	1.03
1:I:261:GLU:HA	1:I:266:GLN:HG2	1.35	1.03
1:G:164:LEU:HD11	1:L:224:LYS:HD3	1.40	1.03
1:B:325:SER:HB2	1:B:331:ARG:HH22	1.21	1.00
1:G:258:PHE:HB2	1:G:271:ALA:HB2	1.39	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:GLU:OE1	1:J:145:GLU:HA	1.61	1.00
1:F:377:LYS:HG2	1:F:378:GLU:N	1.72	1.00
1:H:147:THR:HG22	1:H:149:GLU:H	1.25	0.99
1:D:370:ARG:HH11	1:D:370:ARG:HB2	1.23	0.99
1:H:160:ALA:HB1	1:H:161:PRO:HD2	1.44	0.99
1:H:261:GLU:HA	1:H:266:GLN:HG2	1.42	0.99
1:H:131:PRO:HG2	1:H:199:PHE:HE1	1.24	0.98
1:C:164:LEU:HD11	1:D:224:LYS:HG3	1.42	0.98
1:L:105:GLU:OE2	1:L:412:HIS:HB3	1.62	0.98
1:J:64:GLU:HG2	1:K:316:ARG:HD2	1.46	0.98
1:K:316:ARG:NH2	1:K:370:ARG:HA	1.79	0.98
1:C:13:VAL:HG13	1:C:18:VAL:HB	1.45	0.98
1:E:328:ILE:H	1:E:328:ILE:HD12	1.26	0.97
1:J:371:ASN:HD22	1:J:374:VAL:HG12	1.30	0.96
1:E:84:ALA:O	1:E:85:GLU:HB2	1.66	0.96
1:I:83:THR:HG21	1:I:89:VAL:HB	1.45	0.96
1:I:83:THR:O	1:I:85:GLU:HG3	1.67	0.95
1:B:281:HIS:HD2	1:B:402:ASN:HD21	0.96	0.95
1:B:371:ASN:HD22	1:B:374:VAL:HG13	1.32	0.95
1:J:383:ASN:HB2	1:J:385:ILE:HD13	1.49	0.95
1:I:85:GLU:O	1:I:86:LYS:HB3	1.66	0.94
1:A:261:GLU:HA	1:A:266:GLN:HG2	1.50	0.94
1:H:273:HIS:CD2	1:H:361:LYS:HA	2.03	0.94
1:C:371:ASN:HB3	1:C:374:VAL:HG12	1.48	0.93
1:G:164:LEU:HD13	1:L:224:LYS:HB2	1.49	0.93
1:E:85:GLU:HA	1:E:85:GLU:OE2	1.68	0.93
1:I:281:HIS:HD2	1:I:402:ASN:HD21	0.95	0.93
1:A:72:PRO:HA	1:A:94:CYS:HB3	1.51	0.92
1:I:150:LEU:HD13	1:I:192:PRO:HB2	1.50	0.92
1:C:371:ASN:HB3	1:C:374:VAL:CG1	1.99	0.92
1:H:285:PHE:HB2	1:H:349:VAL:HG11	1.52	0.92
1:H:223:ARG:HH22	1:H:228:HIS:HD2	1.09	0.92
1:I:404:VAL:HG22	1:I:405:MET:HE2	1.51	0.91
1:H:131:PRO:HG2	1:H:199:PHE:CE1	2.03	0.91
1:A:281:HIS:HD2	1:A:402:ASN:HD21	1.14	0.91
1:D:160:ALA:HB3	1:D:169:ARG:HH12	1.35	0.91
1:F:377:LYS:HG2	1:F:378:GLU:H	1.31	0.91
1:C:22:ARG:HG2	1:C:34:ASN:ND2	1.85	0.91
1:I:160:ALA:HB1	1:I:161:PRO:HD2	1.53	0.91
1:K:280:LYS:HD3	1:K:281:HIS:CE1	2.05	0.91
1:K:115:ILE:HG22	1:K:351:LEU:HD12	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLU:OE2	4:A:504:PO4:O1	1.89	0.90
1:K:372:ILE:O	1:K:373:TYR:HB2	1.70	0.90
1:C:160:ALA:HB3	1:C:169:ARG:NH2	1.86	0.90
1:F:357:GLY:HA2	1:F:362:LEU:HD22	1.53	0.90
1:I:371:ASN:HB2	1:I:374:VAL:CG2	2.01	0.90
1:B:357:GLY:HA2	1:B:362:LEU:HD23	1.53	0.89
1:E:281:HIS:HD2	1:E:402:ASN:HD21	1.20	0.89
1:F:160:ALA:HB2	1:F:188:HIS:CD2	2.07	0.89
1:A:119:MET:HE3	1:A:127:PHE:HB2	1.55	0.89
1:H:208:CYS:SG	1:H:347:LEU:HD23	2.12	0.89
1:E:83:THR:HG21	1:E:89:VAL:HB	1.53	0.89
1:I:281:HIS:CD2	1:I:402:ASN:HD21	1.88	0.89
1:J:74:LEU:H	1:J:74:LEU:HD22	1.37	0.89
1:J:368:ILE:HG21	1:J:372:ILE:HD11	1.52	0.88
1:A:163:ASP:HA	1:A:170:ARG:NH2	1.87	0.88
1:F:160:ALA:HB3	1:F:169:ARG:NH2	1.87	0.88
1:I:370:ARG:HB2	1:I:371:ASN:OD1	1.73	0.88
1:B:160:ALA:HB3	1:B:169:ARG:HH12	1.38	0.87
1:G:258:PHE:CB	1:G:271:ALA:HB2	2.05	0.87
1:A:163:ASP:HB3	1:B:83:THR:CG2	2.03	0.87
1:D:261:GLU:HA	1:D:266:GLN:HG2	1.55	0.86
1:G:184:GLU:HG2	1:G:200:LYS:HD3	1.54	0.86
1:L:261:GLU:HA	1:L:266:GLN:HE21	1.39	0.86
1:A:261:GLU:H	1:A:261:GLU:CD	1.79	0.86
1:H:273:HIS:HD2	1:H:361:LYS:HA	1.36	0.86
1:K:156:TYR:O	1:K:158:ASP:N	2.06	0.86
1:I:86:LYS:HG3	1:I:86:LYS:O	1.76	0.86
1:J:100:ASP:OD1	1:J:102:THR:HG22	1.76	0.86
1:H:223:ARG:HH22	1:H:228:HIS:CD2	1.93	0.86
1:B:281:HIS:CD2	1:B:402:ASN:HD21	1.89	0.85
1:G:160:ALA:HB1	1:G:161:PRO:HD2	1.54	0.85
1:L:402:ASN:HD21	1:L:404:VAL:HG13	1.41	0.85
1:E:316:ARG:HB2	1:E:370:ARG:HH12	1.39	0.85
1:F:285:PHE:HB2	1:F:349:VAL:CG1	2.07	0.85
1:F:375:MET:HB3	1:F:379:GLU:HB2	1.56	0.85
1:C:160:ALA:HB3	1:C:169:ARG:HH22	1.36	0.85
1:E:375:MET:HE2	1:E:379:GLU:HB3	1.59	0.85
1:C:380:ARG:HB3	1:C:385:ILE:HB	1.59	0.85
1:H:160:ALA:HB3	1:H:169:ARG:HH12	1.42	0.85
1:I:160:ALA:HB3	1:I:169:ARG:HH12	1.41	0.84
1:D:170:ARG:HH12	1:E:85:GLU:HG2	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:382:GLU:C	1:F:383:ASN:HD22	1.84	0.84
1:J:231:PHE:HB3	1:J:339:PRO:HB2	1.58	0.84
1:K:100:ASP:OD1	1:K:102:THR:HG22	1.77	0.84
1:F:342:ASN:C	1:F:342:ASN:HD22	1.85	0.84
1:L:182:GLU:HG2	1:L:200:LYS:HD2	1.60	0.84
1:B:437:ARG:HD3	1:H:148:LEU:HD21	1.59	0.84
1:K:316:ARG:HH21	1:K:370:ARG:HD2	1.42	0.84
1:I:83:THR:CG2	1:I:89:VAL:HB	2.08	0.83
1:H:285:PHE:HB2	1:H:349:VAL:CG1	2.08	0.83
1:B:357:GLY:HA2	1:B:362:LEU:CD2	2.08	0.83
1:D:129:LEU:HG	1:D:347:LEU:HD11	1.60	0.83
1:F:371:ASN:O	1:F:374:VAL:HG22	1.79	0.83
1:D:325:SER:O	1:D:326:ARG:HD3	1.79	0.83
1:B:115:ILE:HG22	1:B:351:LEU:HD13	1.58	0.83
1:G:316:ARG:HH11	1:G:373:TYR:HB2	1.43	0.83
1:H:231:PHE:HB3	1:H:339:PRO:HB2	1.60	0.83
1:E:164:LEU:HD11	1:F:224:LYS:HG3	1.59	0.83
1:K:22:ARG:HG2	1:K:22:ARG:HH11	1.42	0.83
1:L:316:ARG:HD2	1:L:316:ARG:C	2.03	0.83
1:B:371:ASN:O	1:B:374:VAL:HG22	1.79	0.82
1:L:402:ASN:C	1:L:402:ASN:HD22	1.87	0.82
1:B:370:ARG:HD3	1:B:371:ASN:N	1.94	0.82
1:E:328:ILE:HD12	1:E:328:ILE:N	1.94	0.82
1:L:119:MET:CE	1:L:127:PHE:HB2	2.10	0.82
1:E:314:GLN:HE21	1:F:64:GLU:HB3	1.45	0.82
1:G:370:ARG:HD3	1:G:370:ARG:H	1.44	0.82
1:I:357:GLY:HA2	1:I:362:LEU:HD22	1.62	0.82
1:L:357:GLY:HA2	1:L:362:LEU:HD22	1.61	0.82
1:E:164:LEU:HD12	1:F:224:LYS:HB2	1.60	0.81
1:A:224:LYS:HB2	1:F:164:LEU:CD1	2.11	0.81
1:C:375:MET:HG2	1:C:379:GLU:HB3	1.61	0.81
1:H:281:HIS:HD2	1:H:402:ASN:HD21	1.28	0.81
1:D:315:ASN:C	1:E:64:GLU:HG2	2.05	0.81
1:G:78:VAL:HG13	1:G:91:ARG:HG3	1.62	0.81
1:A:63:ILE:HG22	1:A:64:GLU:HG3	1.62	0.81
1:I:377:LYS:HD3	1:I:378:GLU:OE2	1.79	0.81
1:A:359:LYS:HB3	1:A:359:LYS:HZ3	1.46	0.81
1:K:20:TYR:OH	1:K:36:GLU:HG3	1.80	0.81
1:H:357:GLY:CA	1:H:362:LEU:HD23	2.08	0.81
1:K:160:ALA:CB	1:K:161:PRO:HD2	2.05	0.81
1:I:371:ASN:ND2	1:I:375:MET:HE3	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ILE:HG22	1:C:320:ILE:HD11	1.64	0.80
1:F:338:ASP:HB2	1:F:339:PRO:HD2	1.61	0.80
1:H:35:VAL:HG11	1:H:70:LEU:HD21	1.64	0.80
1:L:63:ILE:HG22	1:L:64:GLU:HG3	1.64	0.80
1:K:11:LYS:HE2	1:K:15:GLU:HG2	1.62	0.80
1:D:28:ILE:O	1:D:28:ILE:HG12	1.82	0.80
1:I:63:ILE:O	1:J:316:ARG:HD3	1.80	0.79
1:K:19:LYS:HD2	1:K:87:GLY:HA3	1.64	0.79
1:A:48:ASN:HB3	1:A:71:TYR:CD1	2.18	0.79
1:G:357:GLY:HA2	1:G:362:LEU:HD12	1.63	0.79
1:H:224:LYS:HG3	1:I:164:LEU:HD21	1.63	0.79
1:C:415:GLU:OE1	1:C:415:GLU:HA	1.81	0.79
1:E:176:LEU:O	1:E:181:PHE:HB2	1.82	0.79
1:B:127:PHE:CZ	1:B:248:LEU:HD22	2.17	0.79
1:L:231:PHE:HB3	1:L:339:PRO:HB2	1.65	0.79
1:C:232:MET:HE2	1:I:441:MET:HA	1.63	0.79
1:F:371:ASN:HD22	1:F:374:VAL:HG13	1.48	0.79
1:H:32:ILE:HD11	1:I:159:LEU:HD23	1.64	0.79
1:H:63:ILE:HG22	1:H:64:GLU:HG3	1.62	0.79
1:A:163:ASP:CA	1:A:170:ARG:HH21	1.93	0.79
1:G:54:GLY:HA3	1:G:68:MET:HG3	1.65	0.79
1:A:164:LEU:HD11	1:B:224:LYS:HB2	1.65	0.79
1:G:115:ILE:HG22	1:G:351:LEU:HD13	1.65	0.78
1:K:33:LYS:HA	1:L:158:ASP:HA	1.64	0.78
1:L:423:ILE:O	1:L:427:MET:HG3	1.83	0.78
1:I:240:ASN:HD22	1:I:303:TYR:HD1	1.29	0.78
1:A:308:TYR:CE1	1:A:372:ILE:HD11	2.18	0.78
1:G:224:LYS:HB2	1:H:164:LEU:HD22	1.65	0.78
1:H:371:ASN:O	1:H:374:VAL:HG22	1.82	0.78
1:H:133:PRO:HD2	1:H:197:ILE:O	1.83	0.78
1:B:21:ILE:HD13	1:B:42:LEU:HD13	1.64	0.78
1:E:328:ILE:H	1:E:328:ILE:CD1	1.97	0.78
1:J:160:ALA:HB1	1:J:161:PRO:HD2	1.64	0.78
1:B:300:VAL:HG13	1:B:301:PRO:HD2	1.62	0.78
1:C:132:GLU:OE2	4:C:504:PO4:O2	2.00	0.78
1:I:371:ASN:HB2	1:I:374:VAL:HG21	1.63	0.78
1:G:82:TRP:CD1	1:G:83:THR:H	2.00	0.77
1:I:64:GLU:HB3	1:J:314:GLN:NE2	1.99	0.77
1:A:119:MET:CE	1:A:127:PHE:HB2	2.13	0.77
1:C:100:ASP:OD1	1:C:102:THR:HG22	1.84	0.77
1:G:285:PHE:HB2	1:G:349:VAL:HG21	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:404:VAL:HG22	1:L:405:MET:HE2	1.64	0.77
1:J:98:ASN:HD22	1:J:102:THR:HG23	1.49	0.77
1:K:160:ALA:HB3	1:K:169:ARG:HH12	1.50	0.77
1:K:315:ASN:ND2	1:K:370:ARG:H	1.83	0.77
1:I:63:ILE:HG22	1:I:64:GLU:HG3	1.66	0.77
1:G:249:SER:HA	1:G:258:PHE:CZ	2.20	0.77
1:D:68:MET:HE1	1:D:104:PHE:HB2	1.67	0.77
1:D:256:ASN:HD22	1:D:258:PHE:H	1.33	0.77
1:E:169:ARG:HH11	1:E:195:HIS:CD2	2.02	0.77
1:A:261:GLU:CD	1:A:261:GLU:N	2.42	0.76
1:C:160:ALA:HB1	1:C:161:PRO:HD2	1.65	0.76
1:G:132:GLU:OE1	4:G:504:PO4:O1	2.02	0.76
1:K:383:ASN:HB2	1:K:385:ILE:HD13	1.64	0.76
1:G:311:TRP:CZ2	1:G:367:PRO:HG3	2.20	0.76
1:E:51:MET:CE	1:E:67:ASP:HB3	2.16	0.76
1:C:280:LYS:HD3	1:C:281:HIS:CE1	2.20	0.76
1:E:22:ARG:HH11	1:E:22:ARG:CG	1.98	0.76
1:A:405:MET:HE2	1:A:405:MET:HA	1.66	0.76
1:D:256:ASN:ND2	1:D:258:PHE:H	1.83	0.76
1:A:41:GLN:HE22	1:F:200:LYS:NZ	1.83	0.76
1:E:357:GLY:HA2	1:E:362:LEU:CD1	2.16	0.76
1:H:28:ILE:HD12	1:H:413:LEU:HD23	1.66	0.76
1:D:160:ALA:HB2	1:D:188:HIS:CD2	2.20	0.76
1:K:163:ASP:HA	1:K:170:ARG:HH21	1.49	0.75
1:E:22:ARG:HG2	1:E:22:ARG:NH1	1.94	0.75
1:H:371:ASN:HB3	1:H:374:VAL:HG13	1.66	0.75
1:B:150:LEU:HD13	1:B:192:PRO:HB2	1.66	0.75
1:D:6:ARG:HG3	1:D:6:ARG:NH1	1.97	0.75
1:J:83:THR:HG22	1:K:163:ASP:HB3	1.69	0.75
1:K:316:ARG:HD3	1:K:316:ARG:H	1.47	0.75
1:E:129:LEU:HD23	1:E:248:LEU:HD23	1.69	0.75
1:E:157:PHE:O	1:F:33:LYS:HB3	1.87	0.75
1:I:20:TYR:HB3	1:I:89:VAL:HG22	1.68	0.75
1:K:11:LYS:HG3	1:K:15:GLU:OE2	1.87	0.75
1:J:115:ILE:HG22	1:J:351:LEU:HD13	1.69	0.74
1:J:223:ARG:HH11	1:J:223:ARG:CG	2.00	0.74
1:K:63:ILE:O	1:L:316:ARG:HD3	1.87	0.74
1:I:169:ARG:HD2	1:I:186:SER:HB2	1.70	0.74
1:B:82:TRP:HE3	1:B:82:TRP:H	1.34	0.74
1:G:342:ASN:HD22	1:G:342:ASN:C	1.94	0.74
1:I:261:GLU:HA	1:I:266:GLN:CG	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:328:ILE:H	1:J:328:ILE:CD1	1.98	0.74
1:C:164:LEU:HD11	1:D:224:LYS:CG	2.15	0.74
1:F:28:ILE:HD11	1:F:417:PHE:HB2	1.70	0.74
1:G:316:ARG:NH1	1:G:373:TYR:HB2	2.03	0.74
1:I:281:HIS:HD2	1:I:402:ASN:ND2	1.79	0.74
1:G:338:ASP:HB2	1:G:339:PRO:HD2	1.70	0.74
1:G:6:ARG:O	1:G:10:GLU:HG3	1.88	0.74
1:D:165:GLY:O	5:D:617:HOH:O	2.05	0.74
1:J:328:ILE:HD13	1:J:328:ILE:N	1.99	0.74
1:A:281:HIS:CD2	1:A:402:ASN:HD21	2.04	0.74
1:D:234:LYS:HE3	1:D:239:VAL:O	1.87	0.74
1:I:170:ARG:HG2	1:I:170:ARG:NH1	2.00	0.74
1:K:9:ILE:HD13	1:K:74:LEU:HD12	1.70	0.73
1:A:3:LYS:HB3	1:A:75:ASN:OD1	1.87	0.73
1:J:224:LYS:HB2	1:K:164:LEU:HD21	1.70	0.73
1:F:285:PHE:HB2	1:F:349:VAL:HG11	1.69	0.73
1:F:85:GLU:O	1:F:86:LYS:HB2	1.86	0.73
1:L:119:MET:HE1	1:L:127:PHE:HB2	1.69	0.73
1:A:30:GLY:HA2	1:A:342:ASN:ND2	2.02	0.73
1:E:140:LEU:HD12	1:E:226:GLY:C	2.12	0.73
1:I:6:ARG:HG3	1:I:46:LEU:HD13	1.69	0.73
1:B:377:LYS:O	1:B:381:MET:HG2	1.88	0.73
1:E:208:CYS:SG	1:E:347:LEU:HD12	2.27	0.73
1:H:131:PRO:CG	1:H:199:PHE:HE1	2.01	0.73
1:F:370:ARG:HG2	1:F:371:ASN:N	2.02	0.73
1:H:357:GLY:HA2	1:H:362:LEU:CD2	2.10	0.73
1:H:378:GLU:O	1:H:381:MET:HG3	1.87	0.73
1:D:370:ARG:HB2	1:D:370:ARG:NH1	2.03	0.73
1:I:81:PRO:HD3	1:I:179:MET:HE3	1.71	0.73
1:K:11:LYS:O	1:K:15:GLU:HG3	1.88	0.73
1:K:315:ASN:HD21	1:K:370:ARG:H	1.37	0.73
1:D:406:VAL:HG22	1:D:414:PHE:CE1	2.24	0.73
1:J:371:ASN:ND2	1:J:374:VAL:H	1.87	0.73
1:J:398:GLU:OE2	5:J:614:HOH:O	2.06	0.73
1:H:300:VAL:HG13	1:H:301:PRO:HD2	1.69	0.72
1:J:63:ILE:HG22	1:K:316:ARG:HD2	1.71	0.72
1:B:223:ARG:HH11	1:B:223:ARG:HG3	1.55	0.72
1:G:403:GLU:O	1:G:407:LYS:HG2	1.87	0.72
1:H:5:THR:HG23	1:H:8:ASP:OD1	1.88	0.72
1:J:9:ILE:O	1:J:13:VAL:HG23	1.90	0.72
1:J:160:ALA:HB2	1:J:188:HIS:CD2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LYS:HB2	1:F:164:LEU:HD12	1.71	0.72
1:H:402:ASN:OD1	1:H:404:VAL:HG12	1.88	0.72
1:A:159:LEU:HG	1:B:34:ASN:OD1	1.88	0.72
1:E:160:ALA:CB	1:E:161:PRO:HD2	2.17	0.72
1:C:98:ASN:HD22	1:C:102:THR:HG23	1.55	0.72
1:F:97:TYR:HE2	1:F:103:PRO:HG3	1.54	0.72
1:F:232:MET:CE	1:L:437:ARG:HA	2.18	0.72
1:D:418:ILE:O	1:D:422:GLU:HG3	1.88	0.72
1:E:265:LEU:O	1:E:326:ARG:NH1	2.22	0.72
1:B:4:TYR:HB3	1:B:9:ILE:HD11	1.72	0.72
1:H:214:PHE:O	1:H:218:VAL:HG23	1.88	0.72
1:C:403:GLU:O	1:C:407:LYS:HG3	1.90	0.72
1:E:311:TRP:CZ2	1:E:367:PRO:HG3	2.25	0.72
1:G:142:GLU:H	1:G:142:GLU:CD	1.97	0.72
1:L:316:ARG:HD2	1:L:316:ARG:O	1.89	0.71
1:G:167:ASN:HD21	1:L:22:ARG:HH22	1.39	0.71
1:A:300:VAL:CG1	1:A:301:PRO:HD2	2.20	0.71
1:C:311:TRP:CZ2	1:C:367:PRO:HD3	2.25	0.71
1:G:155:GLY:O	1:G:156:TYR:O	2.08	0.71
1:J:129:LEU:HD13	1:J:131:PRO:HG3	1.73	0.71
1:B:309:VAL:HG23	1:B:386:VAL:O	1.90	0.71
1:G:82:TRP:CD1	1:G:83:THR:N	2.58	0.71
1:A:162:THR:HG22	1:A:163:ASP:N	2.06	0.71
1:F:419:GLU:O	1:F:423:ILE:HG23	1.90	0.71
1:B:82:TRP:HE1	1:B:220:THR:HG21	1.54	0.71
1:J:4:TYR:CD2	1:J:4:TYR:N	2.58	0.71
1:A:326:ARG:HD3	1:A:330:THR:OG1	1.89	0.71
1:F:376:SER:N	1:F:379:GLU:HG3	2.06	0.71
1:J:260:ASP:HB2	1:J:268:SER:HA	1.73	0.71
1:L:217:VAL:O	1:L:221:ILE:HG12	1.91	0.71
1:C:162:THR:HG21	1:D:220:THR:OG1	1.91	0.70
1:J:224:LYS:CB	1:K:164:LEU:HD21	2.21	0.70
1:K:51:MET:CE	1:K:67:ASP:HB3	2.21	0.70
1:K:160:ALA:HB2	1:K:188:HIS:HB2	1.73	0.70
1:B:182:GLU:O	1:B:200:LYS:HG3	1.91	0.70
1:B:281:HIS:HD2	1:B:402:ASN:ND2	1.81	0.70
1:G:156:TYR:O	1:G:158:ASP:N	2.24	0.70
1:G:328:ILE:N	1:G:328:ILE:HD12	2.06	0.70
1:G:383:ASN:HB2	1:G:385:ILE:HD12	1.73	0.70
1:B:236:LEU:HB2	1:B:239:VAL:CG2	2.22	0.70
1:C:176:LEU:O	1:C:181:PHE:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:48:ASN:HB3	1:K:71:TYR:CD1	2.27	0.70
1:H:166:GLU:O	1:H:166:GLU:CD	2.35	0.70
1:G:86:LYS:HG3	1:G:86:LYS:O	1.90	0.70
1:G:160:ALA:CB	1:G:188:HIS:CD2	2.74	0.70
1:J:279:VAL:HG11	1:J:365:PRO:HG2	1.74	0.70
1:E:160:ALA:HB3	1:E:169:ARG:HH12	1.57	0.70
1:D:311:TRP:CZ2	1:D:367:PRO:HG3	2.27	0.70
1:G:160:ALA:HB2	1:G:188:HIS:CD2	2.26	0.70
1:H:371:ASN:HB3	1:H:374:VAL:CG1	2.21	0.70
1:L:390:ALA:HB3	1:L:394:GLU:OE1	1.91	0.70
1:L:418:ILE:O	1:L:422:GLU:HG3	1.92	0.70
1:B:129:LEU:HD23	1:B:248:LEU:HD23	1.73	0.69
1:E:100:ASP:OD2	1:E:101:GLY:N	2.22	0.69
1:C:22:ARG:CG	1:C:34:ASN:ND2	2.55	0.69
1:C:435:TRP:O	1:C:439:GLN:HG2	1.91	0.69
1:E:28:ILE:HG22	1:E:57:ILE:O	1.92	0.69
1:H:321:ARG:HG2	1:H:335:ARG:HD2	1.73	0.69
1:B:84:ALA:HA	1:B:87:GLY:O	1.93	0.69
1:F:259:PHE:CD2	1:F:327:GLY:HA2	2.27	0.69
1:F:261:GLU:HA	1:F:266:GLN:NE2	2.07	0.69
1:H:223:ARG:NH2	1:H:228:HIS:HD2	1.85	0.69
1:I:142:GLU:H	1:I:142:GLU:CD	1.98	0.69
1:E:316:ARG:HB2	1:E:370:ARG:NH1	2.07	0.69
1:E:381:MET:C	1:E:383:ASN:H	1.98	0.69
1:F:28:ILE:HG22	1:F:57:ILE:O	1.91	0.69
1:J:98:ASN:HB2	1:J:102:THR:O	1.93	0.69
1:J:435:TRP:O	1:J:439:GLN:HG2	1.92	0.69
1:A:359:LYS:HB3	1:A:359:LYS:NZ	2.08	0.69
1:D:160:ALA:CB	1:D:188:HIS:HD2	2.06	0.69
1:I:380:ARG:HA	1:I:385:ILE:HD12	1.74	0.69
1:A:375:MET:HE1	1:A:383:ASN:ND2	2.07	0.69
1:E:285:PHE:HB2	1:E:349:VAL:HG11	1.74	0.69
1:F:160:ALA:CB	1:F:188:HIS:CD2	2.76	0.69
1:J:48:ASN:HB3	1:J:71:TYR:CE1	2.28	0.69
1:C:160:ALA:HB2	1:C:188:HIS:CD2	2.27	0.69
1:F:160:ALA:CB	1:F:188:HIS:HD2	2.04	0.69
1:F:368:ILE:HG21	1:F:372:ILE:HD11	1.74	0.69
1:H:54:GLY:HA3	1:H:68:MET:HE3	1.74	0.69
1:J:4:TYR:N	1:J:4:TYR:HD2	1.89	0.69
1:J:189:GLU:OE1	3:J:503:GLN:OE1	2.11	0.69
1:B:13:VAL:HG13	1:B:18:VAL:HB	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:191:ALA:HB3	1:L:194:GLN:HE21	1.57	0.69
1:E:51:MET:HE3	1:E:67:ASP:HB3	1.75	0.69
1:K:63:ILE:HG22	1:K:64:GLU:HG3	1.73	0.69
1:C:83:THR:HG22	1:C:85:GLU:OE2	1.92	0.68
1:C:281:HIS:HD2	1:C:402:ASN:HD21	1.39	0.68
1:H:142:GLU:CD	1:H:142:GLU:H	1.99	0.68
1:K:375:MET:HG3	1:K:380:ARG:HG3	1.75	0.68
1:E:169:ARG:HH11	1:E:195:HIS:HD2	1.38	0.68
1:I:371:ASN:HD21	1:I:375:MET:HE3	1.57	0.68
1:K:315:ASN:HB3	1:K:318:PRO:HG3	1.75	0.68
1:B:223:ARG:HG3	1:B:223:ARG:NH1	2.09	0.68
1:D:236:LEU:HB2	1:D:239:VAL:HG22	1.75	0.68
1:F:97:TYR:CE2	1:F:103:PRO:HG3	2.29	0.68
1:G:164:LEU:CD1	1:L:224:LYS:HB2	2.23	0.68
1:B:394:GLU:OE1	5:B:605:HOH:O	2.11	0.68
1:D:159:LEU:HD23	1:E:32:ILE:HD11	1.76	0.68
1:G:4:TYR:HB3	1:G:9:ILE:CD1	2.24	0.68
1:G:377:LYS:HZ2	1:G:380:ARG:HH22	1.41	0.68
1:H:147:THR:HG22	1:H:149:GLU:N	2.03	0.68
1:A:206:ARG:HG2	1:A:206:ARG:HH11	1.59	0.68
1:A:308:TYR:HE1	1:A:372:ILE:HD11	1.57	0.68
1:B:211:ILE:O	1:B:215:LYS:HG3	1.94	0.68
1:G:27:ASP:HB3	1:G:33:LYS:HE3	1.75	0.68
1:K:309:VAL:HA	1:K:319:LEU:HD23	1.76	0.68
1:K:405:MET:HA	1:K:405:MET:HE2	1.75	0.68
1:A:282:ALA:HA	1:A:285:PHE:CZ	2.29	0.68
1:H:375:MET:HE2	1:H:379:GLU:HG2	1.74	0.68
1:F:148:LEU:HD11	1:L:437:ARG:HD3	1.75	0.68
1:J:224:LYS:CG	1:K:164:LEU:HD21	2.24	0.68
1:B:81:PRO:HD2	1:B:82:TRP:CZ3	2.29	0.67
1:C:199:PHE:HZ	1:C:214:PHE:CD1	2.13	0.67
1:E:160:ALA:O	1:E:161:PRO:O	2.12	0.67
1:E:189:GLU:OE1	3:E:501:GLN:OE1	2.12	0.67
1:K:182:GLU:HB3	1:K:200:LYS:HD2	1.76	0.67
1:A:435:TRP:O	1:A:439:GLN:HG2	1.94	0.67
1:F:24:GLN:NE2	1:F:91:ARG:HH11	1.92	0.67
1:G:81:PRO:HD3	1:G:179:MET:HE3	1.75	0.67
1:J:85:GLU:O	1:J:86:LYS:HB2	1.93	0.67
1:D:236:LEU:HB2	1:D:239:VAL:CG2	2.25	0.67
1:F:160:ALA:HB3	1:F:169:ARG:HH21	1.59	0.67
1:A:142:GLU:H	1:A:142:GLU:CD	1.99	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:CD1	1:B:224:LYS:HB2	2.25	0.67
1:C:231:PHE:O	1:C:339:PRO:HG2	1.95	0.67
1:C:378:GLU:CD	1:C:378:GLU:H	2.02	0.67
1:E:285:PHE:HB2	1:E:349:VAL:CG1	2.25	0.67
1:F:300:VAL:HG13	1:F:301:PRO:HD2	1.74	0.67
1:A:435:TRP:HB2	5:A:602:HOH:O	1.95	0.67
1:D:131:PRO:HG2	1:D:199:PHE:CD1	2.30	0.67
1:E:5:THR:HG23	1:E:8:ASP:OD1	1.95	0.67
1:E:48:ASN:HB3	1:E:71:TYR:CD1	2.30	0.67
1:E:160:ALA:HB2	1:E:188:HIS:CD2	2.29	0.67
1:E:314:GLN:NE2	1:F:64:GLU:HB3	2.08	0.67
1:L:234:LYS:HD2	1:L:298:ARG:HA	1.76	0.67
1:C:45:ALA:HA	1:C:50:VAL:HG23	1.75	0.67
1:H:280:LYS:HD3	1:H:281:HIS:CE1	2.28	0.67
1:B:96:ILE:HD12	1:B:96:ILE:N	2.10	0.67
1:D:281:HIS:HD2	1:D:402:ASN:HD21	1.41	0.67
1:E:316:ARG:CB	1:E:370:ARG:HH12	2.07	0.67
1:E:351:LEU:HD22	1:E:355:LEU:HG	1.77	0.67
1:J:64:GLU:HG2	1:K:316:ARG:CD	2.22	0.67
1:K:281:HIS:HD2	1:K:402:ASN:HD21	1.41	0.67
1:D:83:THR:HG21	1:D:89:VAL:HB	1.75	0.67
1:H:315:ASN:ND2	1:H:373:TYR:OH	2.27	0.67
1:A:182:GLU:HB3	1:A:200:LYS:HG3	1.76	0.66
1:H:319:LEU:HD12	1:H:336:SER:HB3	1.77	0.66
1:I:150:LEU:CD1	1:I:192:PRO:HB2	2.24	0.66
1:K:13:VAL:HG21	1:K:42:LEU:CD2	2.25	0.66
1:K:308:TYR:CD1	1:K:372:ILE:HG13	2.29	0.66
1:L:377:LYS:HG2	1:L:378:GLU:N	1.98	0.66
1:A:83:THR:HG21	1:A:89:VAL:H	1.58	0.66
1:D:134:GLU:OE2	3:D:503:GLN:OE1	2.12	0.66
1:I:281:HIS:CG	1:I:405:MET:HE3	2.29	0.66
1:H:285:PHE:HD1	1:H:285:PHE:C	2.04	0.66
1:K:127:PHE:CZ	1:K:248:LEU:HD22	2.30	0.66
1:B:151:ASN:OD1	1:B:193:GLY:HA2	1.96	0.66
1:D:19:LYS:HG3	1:D:87:GLY:HA3	1.77	0.66
1:E:371:ASN:HA	1:E:374:VAL:CG2	2.26	0.66
1:A:169:ARG:NH2	1:A:195:HIS:ND1	2.43	0.66
1:F:285:PHE:HB2	1:F:349:VAL:HG13	1.76	0.66
1:I:308:TYR:CD1	1:I:372:ILE:HG22	2.30	0.66
1:J:27:ASP:OD1	1:J:31:THR:HB	1.95	0.66
1:K:298:ARG:NH2	1:K:338:ASP:HB3	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ASP:N	1:A:264:ASP:OD1	2.29	0.66
1:C:48:ASN:HB3	1:C:71:TYR:CD1	2.31	0.66
1:G:200:LYS:HE2	1:L:41:GLN:OE1	1.95	0.66
1:G:371:ASN:OD1	1:G:371:ASN:N	2.27	0.66
1:I:27:ASP:HB3	1:I:33:LYS:HD2	1.78	0.66
1:L:371:ASN:OD1	1:L:374:VAL:HB	1.96	0.66
1:J:359:LYS:NZ	1:J:359:LYS:HB3	2.10	0.66
1:L:191:ALA:HB3	1:L:194:GLN:NE2	2.10	0.66
1:A:20:TYR:HB3	1:A:89:VAL:HG13	1.78	0.66
1:A:316:ARG:HD3	1:B:63:ILE:O	1.96	0.66
1:B:81:PRO:HD2	1:B:82:TRP:HZ3	1.61	0.66
1:C:236:LEU:HB2	1:C:239:VAL:CG2	2.26	0.66
1:D:260:ASP:O	1:D:266:GLN:HA	1.96	0.66
1:F:22:ARG:HG2	1:F:22:ARG:HH11	1.60	0.66
1:F:57:ILE:HD11	1:F:96:ILE:HG13	1.77	0.66
1:G:308:TYR:OH	1:G:372:ILE:HG23	1.96	0.66
1:J:371:ASN:ND2	1:J:374:VAL:HG12	2.08	0.66
1:K:13:VAL:HG21	1:K:42:LEU:HD21	1.78	0.66
1:K:142:GLU:CD	1:K:142:GLU:H	2.04	0.66
1:L:83:THR:HA	1:L:85:GLU:OE2	1.96	0.66
1:L:316:ARG:HB2	1:L:370:ARG:HH12	1.59	0.65
1:L:419:GLU:O	1:L:423:ILE:HG23	1.96	0.65
1:I:34:ASN:HD22	1:I:34:ASN:C	2.03	0.65
1:I:338:ASP:HB2	1:I:339:PRO:HD2	1.77	0.65
1:K:156:TYR:C	1:K:158:ASP:H	2.04	0.65
1:B:371:ASN:ND2	1:B:374:VAL:HG13	2.08	0.65
1:A:160:ALA:HB1	1:A:161:PRO:HD2	1.78	0.65
1:C:338:ASP:HB2	1:C:339:PRO:HD2	1.78	0.65
1:D:372:ILE:HG13	1:D:373:TYR:H	1.60	0.65
1:H:63:ILE:HG22	1:H:64:GLU:CG	2.26	0.65
1:A:34:ASN:HD22	1:A:34:ASN:C	2.05	0.65
1:A:36:GLU:OE2	1:F:169:ARG:NH1	2.30	0.65
1:C:371:ASN:O	1:C:374:VAL:HG13	1.97	0.65
1:C:357:GLY:CA	1:C:362:LEU:HD12	2.20	0.65
1:F:176:LEU:O	1:F:181:PHE:HB2	1.97	0.65
1:G:156:TYR:C	1:G:158:ASP:H	2.04	0.65
1:A:34:ASN:C	1:A:34:ASN:ND2	2.52	0.65
1:L:70:LEU:HD12	1:L:94:CYS:HB3	1.77	0.65
1:L:391:THR:OG1	1:L:394:GLU:HG3	1.97	0.65
1:C:443:GLN:HG2	1:C:444:TYR:CE2	2.32	0.65
1:D:11:LYS:O	1:D:15:GLU:HG3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:TYR:HB2	1:F:190:VAL:HG12	1.79	0.65
1:F:380:ARG:HG2	1:F:385:ILE:HG21	1.79	0.65
1:H:261:GLU:HA	1:H:266:GLN:CG	2.23	0.65
1:I:81:PRO:CD	1:I:179:MET:HE3	2.27	0.65
1:L:402:ASN:ND2	1:L:405:MET:H	1.95	0.65
1:J:281:HIS:HD2	1:J:402:ASN:HD21	1.45	0.65
1:B:134:GLU:OE2	3:B:503:GLN:HB2	1.97	0.64
1:B:406:VAL:HG22	1:B:414:PHE:CE1	2.31	0.64
1:F:292:THR:O	1:F:295:SER:HB2	1.96	0.64
1:J:359:LYS:HB3	1:J:359:LYS:HZ3	1.62	0.64
1:K:51:MET:HE1	1:K:67:ASP:HB3	1.78	0.64
1:K:316:ARG:HH22	1:K:370:ARG:HA	1.62	0.64
1:D:170:ARG:NH1	1:E:85:GLU:HG2	2.09	0.64
1:G:67:ASP:O	1:G:68:MET:HG2	1.96	0.64
1:H:304:GLU:HG2	1:H:335:ARG:HH12	1.62	0.64
1:A:159:LEU:HD13	1:B:32:ILE:HD11	1.79	0.64
1:B:338:ASP:HB2	1:B:339:PRO:HD2	1.79	0.64
1:G:134:GLU:O	1:G:242:SER:HB3	1.98	0.64
1:L:273:HIS:O	1:L:276:ALA:HB3	1.98	0.64
1:B:381:MET:O	1:B:383:ASN:N	2.30	0.64
1:I:240:ASN:ND2	1:I:303:TYR:HD1	1.96	0.64
1:J:52:PHE:CE1	1:J:70:LEU:HD13	2.32	0.64
1:J:441:MET:HG3	1:J:441:MET:O	1.96	0.64
1:L:142:GLU:H	1:L:142:GLU:CD	2.04	0.64
1:A:30:GLY:HA2	1:A:342:ASN:HD22	1.63	0.64
1:G:377:LYS:NZ	1:G:380:ARG:HH22	1.94	0.64
1:H:259:PHE:CZ	1:H:261:GLU:HB3	2.33	0.64
1:K:385:ILE:HD12	1:K:385:ILE:N	2.12	0.64
1:D:206:ARG:HH11	1:D:206:ARG:HG3	1.62	0.64
1:E:131:PRO:HG2	1:E:199:PHE:HD1	1.63	0.64
1:G:23:LEU:HB3	1:G:70:LEU:CD2	2.28	0.64
1:J:32:ILE:HD11	1:J:216:LEU:HD12	1.77	0.64
1:E:205:VAL:HG13	1:E:206:ARG:N	2.13	0.64
1:F:368:ILE:HG21	1:F:372:ILE:CD1	2.27	0.64
1:G:23:LEU:HB3	1:G:70:LEU:HD21	1.80	0.64
1:H:215:LYS:O	1:H:219:LYS:HG3	1.97	0.64
1:H:316:ARG:HB3	1:H:373:TYR:CE1	2.33	0.64
1:A:162:THR:CG2	1:A:163:ASP:H	2.11	0.64
1:C:278:ILE:CG2	1:C:320:ILE:HD11	2.28	0.64
1:D:28:ILE:HD11	1:D:417:PHE:HB2	1.79	0.64
1:D:234:LYS:HG3	1:D:298:ARG:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:ASN:HD22	1:D:257:ALA:N	1.96	0.64
1:G:245:HIS:ND1	4:G:504:PO4:O1	2.31	0.64
1:J:175:GLU:HG3	1:J:221:ILE:HD11	1.80	0.64
1:K:160:ALA:HB1	1:K:161:PRO:CD	2.12	0.64
1:B:407:LYS:HB3	1:B:407:LYS:NZ	2.13	0.64
1:E:231:PHE:HB3	1:E:339:PRO:HB2	1.79	0.64
1:H:317:SER:N	1:H:373:TYR:OH	2.31	0.64
1:L:83:THR:HG21	1:L:89:VAL:HB	1.79	0.64
1:D:160:ALA:CB	1:D:161:PRO:HD2	2.17	0.63
1:D:243:GLY:CA	1:D:298:ARG:NH1	2.61	0.63
1:E:316:ARG:H	1:E:370:ARG:NH1	1.96	0.63
1:H:224:LYS:HG3	1:I:164:LEU:CD2	2.28	0.63
1:A:314:GLN:NE2	5:A:614:HOH:O	2.30	0.63
1:C:109:ARG:HD2	1:C:344:TYR:CE2	2.33	0.63
1:H:405:MET:HA	1:H:405:MET:HE2	1.81	0.63
1:L:224:LYS:HG2	1:L:225:HIS:CD2	2.34	0.63
1:L:231:PHE:HB3	1:L:339:PRO:CB	2.27	0.63
1:B:231:PHE:HB3	1:B:339:PRO:HB2	1.78	0.63
1:B:248:LEU:HB2	1:B:332:VAL:HG23	1.79	0.63
1:C:91:ARG:C	1:C:91:ARG:HD2	2.23	0.63
1:C:375:MET:HA	1:C:379:GLU:OE1	1.98	0.63
1:I:57:ILE:HD11	1:I:96:ILE:HG12	1.79	0.63
1:B:32:ILE:HD11	1:B:216:LEU:HD22	1.81	0.63
1:C:231:PHE:HB3	1:C:339:PRO:HB2	1.81	0.63
1:D:162:THR:HG21	1:E:220:THR:OG1	1.97	0.63
1:F:402:ASN:O	1:F:406:VAL:HG23	1.97	0.63
1:I:231:PHE:HB3	1:I:339:PRO:HB2	1.80	0.63
1:I:236:LEU:HB2	1:I:239:VAL:HG13	1.79	0.63
1:L:303:TYR:O	1:L:304:GLU:HB2	1.98	0.63
1:A:119:MET:HE1	1:A:127:PHE:N	2.13	0.63
1:E:357:GLY:CA	1:E:362:LEU:HD12	2.23	0.63
1:E:372:ILE:HG13	1:E:373:TYR:H	1.64	0.63
1:F:253:ASN:ND2	1:F:253:ASN:O	2.31	0.63
1:F:293:VAL:HB	1:L:440:TYR:OH	1.99	0.63
1:H:285:PHE:C	1:H:285:PHE:CD1	2.77	0.63
1:C:24:GLN:NE2	1:C:91:ARG:HH11	1.96	0.63
1:C:151:ASN:O	1:C:152:ASP:HB3	1.99	0.63
1:E:316:ARG:H	1:E:370:ARG:HH12	1.46	0.63
1:I:371:ASN:HB2	1:I:374:VAL:HG22	1.80	0.63
1:I:376:SER:HB2	1:I:377:LYS:NZ	2.13	0.63
1:J:189:GLU:OE2	1:J:190:VAL:HG12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:SER:O	1:E:62:ARG:HG2	1.99	0.63
1:G:96:ILE:HG12	1:G:107:ASP:CG	2.23	0.63
1:H:292:THR:O	1:H:295:SER:HB2	1.99	0.63
1:A:281:HIS:HD2	1:A:402:ASN:ND2	1.93	0.63
1:E:164:LEU:CD1	1:F:224:LYS:HG3	2.29	0.63
1:F:160:ALA:O	1:F:161:PRO:O	2.17	0.63
1:G:368:ILE:O	1:G:369:ASP:HB2	1.98	0.63
1:H:35:VAL:HG11	1:H:70:LEU:CD2	2.29	0.63
1:I:166:GLU:O	1:I:168:CYS:N	2.32	0.63
1:D:166:GLU:HG2	1:D:168:CYS:H	1.64	0.62
1:E:201:TYR:O	1:E:201:TYR:CD2	2.52	0.62
1:B:150:LEU:CD1	1:B:192:PRO:HB2	2.29	0.62
1:B:296:TYR:HB3	1:B:390:ALA:O	1.99	0.62
1:F:441:MET:O	1:L:228:HIS:HE1	1.82	0.62
1:I:316:ARG:HD2	1:I:316:ARG:O	2.00	0.62
1:L:300:VAL:HG13	1:L:301:PRO:HD2	1.79	0.62
1:B:381:MET:HE2	1:B:381:MET:HA	1.81	0.62
1:D:115:ILE:HG22	1:D:351:LEU:HD12	1.82	0.62
1:L:402:ASN:C	1:L:402:ASN:ND2	2.55	0.62
1:F:281:HIS:HE1	1:F:356:ASP:OD2	1.82	0.62
1:G:5:THR:HG23	1:G:8:ASP:CG	2.23	0.62
1:I:170:ARG:HH11	1:I:170:ARG:CG	2.05	0.62
1:J:160:ALA:HB2	1:J:188:HIS:HD2	1.64	0.62
1:J:300:VAL:HG13	1:J:301:PRO:HD2	1.81	0.62
1:K:261:GLU:HA	1:K:266:GLN:NE2	2.14	0.62
1:A:30:GLY:CA	1:A:342:ASN:HD22	2.11	0.62
1:B:51:MET:HE2	1:B:69:TYR:CZ	2.34	0.62
1:F:24:GLN:HE21	1:F:91:ARG:HD3	1.64	0.62
1:H:265:LEU:O	1:H:326:ARG:NH1	2.32	0.62
1:I:440:TYR:HD1	1:I:444:TYR:HE2	1.48	0.62
1:L:170:ARG:HG2	1:L:170:ARG:HH11	1.65	0.62
1:G:83:THR:HG21	1:G:89:VAL:HB	1.82	0.62
1:H:380:ARG:O	1:H:385:ILE:HB	2.00	0.62
1:L:406:VAL:HG22	1:L:414:PHE:CE1	2.34	0.62
1:F:383:ASN:HD22	1:F:383:ASN:N	1.95	0.62
1:G:16:GLU:OE1	1:G:16:GLU:HA	1.98	0.62
1:K:220:THR:OG1	1:L:162:THR:HG21	1.98	0.62
1:E:51:MET:HE1	1:E:67:ASP:HB3	1.81	0.62
1:E:77:PHE:HD1	1:E:92:PHE:CZ	2.18	0.62
1:F:132:GLU:OE2	1:F:245:HIS:ND1	2.33	0.62
1:I:80:PHE:CD1	1:I:89:VAL:HG12	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:142:GLU:H	1:J:142:GLU:CD	2.07	0.62
1:J:357:GLY:CA	1:J:362:LEU:HD12	2.16	0.62
1:J:359:LYS:NZ	1:J:359:LYS:CB	2.63	0.62
1:K:160:ALA:O	1:K:162:THR:N	2.33	0.62
1:L:133:PRO:HD2	1:L:197:ILE:O	1.99	0.62
1:B:300:VAL:CG1	1:B:301:PRO:HD2	2.28	0.61
1:E:150:LEU:HD13	1:E:192:PRO:O	2.01	0.61
1:H:378:GLU:HA	1:H:381:MET:HG2	1.83	0.61
1:L:175:GLU:O	1:L:179:MET:HB2	2.00	0.61
1:A:355:LEU:O	1:A:359:LYS:HG2	1.99	0.61
1:E:23:LEU:HB3	1:E:70:LEU:HD23	1.80	0.61
1:G:312:SER:HB2	1:G:368:ILE:HG13	1.82	0.61
1:J:132:GLU:HB3	1:J:196:GLU:OE1	2.01	0.61
1:B:57:ILE:HD11	1:B:96:ILE:HG12	1.81	0.61
1:C:355:LEU:O	1:C:359:LYS:HG2	2.00	0.61
1:D:357:GLY:HA2	1:D:362:LEU:HD22	1.82	0.61
1:H:54:GLY:O	1:H:57:ILE:HD12	2.00	0.61
1:I:378:GLU:O	1:I:382:GLU:HB2	2.00	0.61
1:K:370:ARG:HH22	1:K:374:VAL:HG13	1.64	0.61
1:F:435:TRP:CD1	1:L:431:GLN:HG2	2.36	0.61
1:H:109:ARG:HG3	1:H:344:TYR:CE2	2.35	0.61
1:H:139:LYS:O	1:H:147:THR:HB	1.99	0.61
1:K:273:HIS:O	1:K:276:ALA:HB3	2.00	0.61
1:C:370:ARG:O	1:C:371:ASN:HB2	2.00	0.61
1:E:268:SER:O	1:E:272:LYS:HD2	2.00	0.61
1:E:371:ASN:HA	1:E:374:VAL:HG23	1.80	0.61
1:I:308:TYR:CD1	1:I:372:ILE:CG2	2.84	0.61
1:J:404:VAL:HG22	1:J:405:MET:HE2	1.81	0.61
1:K:9:ILE:CD1	1:K:74:LEU:HD12	2.30	0.61
1:A:359:LYS:NZ	1:A:359:LYS:CB	2.62	0.61
1:B:21:ILE:CD1	1:B:42:LEU:HD13	2.30	0.61
1:B:147:THR:HG22	1:B:148:LEU:N	2.15	0.61
1:F:54:GLY:O	1:F:57:ILE:HG13	2.01	0.61
1:G:224:LYS:HB2	1:H:164:LEU:CD2	2.31	0.61
1:I:199:PHE:HZ	1:I:214:PHE:CG	2.17	0.61
1:I:260:ASP:OD2	1:I:263:ALA:HB2	2.01	0.61
1:A:368:ILE:HD11	1:A:385:ILE:HD11	1.83	0.61
1:C:71:TYR:CG	1:C:97:TYR:HD1	2.18	0.61
1:C:357:GLY:HA2	1:C:362:LEU:CD1	2.22	0.61
1:D:163:ASP:HB2	1:E:82:TRP:HE1	1.66	0.61
1:G:125:SER:C	1:G:126:ASP:OD2	2.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:48:ASN:HB3	1:H:71:TYR:CD1	2.35	0.61
1:H:351:LEU:HD22	1:H:355:LEU:HG	1.83	0.61
1:C:163:ASP:HB3	1:D:83:THR:HG22	1.83	0.61
1:D:160:ALA:O	1:D:161:PRO:O	2.18	0.61
1:E:430:THR:HG22	1:K:300:VAL:HG11	1.82	0.61
1:G:249:SER:HA	1:G:258:PHE:CE1	2.36	0.61
1:H:396:LEU:HD22	1:H:418:ILE:HD13	1.82	0.61
1:C:71:TYR:CG	1:C:97:TYR:CD1	2.89	0.61
1:D:76:THR:O	1:D:78:VAL:HG23	2.01	0.61
1:D:160:ALA:CB	1:D:188:HIS:CD2	2.83	0.61
1:D:290:ASN:HB3	1:D:295:SER:HB3	1.83	0.61
1:E:129:LEU:HD13	1:E:131:PRO:HD3	1.81	0.61
1:K:22:ARG:HG2	1:K:22:ARG:NH1	2.14	0.61
1:B:160:ALA:HB2	1:B:188:HIS:CD2	2.36	0.61
1:F:78:VAL:HG11	1:F:179:MET:HE3	1.83	0.61
1:B:381:MET:C	1:B:383:ASN:H	2.09	0.60
1:D:383:ASN:C	1:D:385:ILE:H	2.06	0.60
1:J:115:ILE:HG22	1:J:351:LEU:CD1	2.30	0.60
1:L:351:LEU:HD22	1:L:355:LEU:HG	1.81	0.60
1:A:290:ASN:HB3	1:A:295:SER:HB3	1.81	0.60
1:B:376:SER:HB2	1:B:379:GLU:HG3	1.83	0.60
1:D:26:THR:HG22	1:D:27:ASP:O	2.00	0.60
1:F:232:MET:CE	1:L:440:TYR:HB2	2.32	0.60
1:H:435:TRP:O	1:H:439:GLN:HG2	2.01	0.60
1:J:338:ASP:HB2	1:J:339:PRO:CD	2.31	0.60
1:J:74:LEU:HD22	1:J:74:LEU:N	2.14	0.60
1:L:309:VAL:HG23	1:L:386:VAL:O	2.02	0.60
1:A:114:ARG:NH1	1:A:115:ILE:HD11	2.16	0.60
1:D:377:LYS:O	1:D:381:MET:HB2	2.01	0.60
1:H:168:CYS:O	1:H:172:ILE:HG13	2.00	0.60
1:I:325:SER:O	1:I:326:ARG:HD3	2.02	0.60
1:A:132:GLU:CD	4:A:504:PO4:O1	2.45	0.60
1:F:24:GLN:NE2	1:F:91:ARG:HD3	2.16	0.60
1:F:160:ALA:HB3	1:F:169:ARG:HH22	1.66	0.60
1:K:54:GLY:HA3	1:K:68:MET:SD	2.42	0.60
1:A:127:PHE:CE2	1:A:351:LEU:HB2	2.37	0.60
1:C:316:ARG:HD3	1:D:63:ILE:O	2.01	0.60
1:I:80:PHE:HD1	1:I:89:VAL:HG12	1.67	0.60
1:D:51:MET:HE1	1:D:67:ASP:HB3	1.82	0.60
1:D:84:ALA:HA	1:D:87:GLY:O	2.02	0.60
1:D:133:PRO:HG3	1:D:199:PHE:HE1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:LYS:O	1:D:201:TYR:O	2.20	0.60
1:D:405:MET:HE2	1:D:405:MET:HA	1.83	0.60
1:A:273:HIS:O	1:A:276:ALA:HB3	2.01	0.60
1:A:338:ASP:C	1:A:338:ASP:OD2	2.45	0.60
1:C:299:LEU:HD12	1:C:306:PRO:O	2.02	0.60
1:H:23:LEU:HB2	1:H:35:VAL:HG13	1.84	0.60
1:I:371:ASN:O	1:I:375:MET:HG2	2.02	0.60
1:J:74:LEU:H	1:J:74:LEU:CD2	2.12	0.60
1:F:187:HIS:HD2	1:F:188:HIS:O	1.85	0.60
1:I:234:LYS:HE3	1:I:239:VAL:O	2.02	0.60
1:A:162:THR:CG2	1:A:163:ASP:N	2.64	0.59
1:C:300:VAL:HG13	1:C:301:PRO:HD2	1.82	0.59
1:D:264:ASP:O	1:D:265:LEU:HB2	2.02	0.59
1:E:129:LEU:HD23	1:E:248:LEU:CD2	2.31	0.59
1:H:63:ILE:O	1:I:316:ARG:HD3	2.01	0.59
1:K:37:ILE:HD12	1:K:41:GLN:HB2	1.83	0.59
1:K:381:MET:C	1:K:383:ASN:H	2.10	0.59
1:A:164:LEU:HD11	1:B:224:LYS:CB	2.31	0.59
1:A:375:MET:HE1	1:A:383:ASN:HD21	1.67	0.59
1:G:371:ASN:O	1:G:374:VAL:HG13	2.02	0.59
1:G:374:VAL:HG22	1:G:375:MET:N	2.17	0.59
1:K:83:THR:O	1:K:84:ALA:HB3	2.02	0.59
1:K:328:ILE:O	1:K:328:ILE:HG13	2.02	0.59
1:L:300:VAL:CG1	1:L:301:PRO:HD2	2.32	0.59
1:A:207:SER:O	1:A:211:ILE:HG13	2.02	0.59
1:C:160:ALA:CB	1:C:188:HIS:CD2	2.85	0.59
1:D:383:ASN:HB2	1:D:385:ILE:HG12	1.84	0.59
1:F:342:ASN:HD22	1:F:343:PRO:N	2.01	0.59
1:H:12:LEU:O	1:H:16:GLU:HB2	2.02	0.59
1:I:109:ARG:NH1	1:I:209:ASP:OD1	2.35	0.59
1:I:368:ILE:HD13	1:I:370:ARG:NH2	2.16	0.59
1:J:129:LEU:CD1	1:J:131:PRO:HG3	2.32	0.59
1:J:370:ARG:HG2	1:J:370:ARG:HH11	1.67	0.59
1:K:28:ILE:HD11	1:K:417:PHE:HB2	1.85	0.59
1:K:363:GLU:HA	1:K:363:GLU:OE2	2.00	0.59
1:A:264:ASP:O	1:A:265:LEU:HB2	2.01	0.59
1:C:328:ILE:H	1:C:328:ILE:HD13	1.68	0.59
1:D:228:HIS:HE1	1:J:441:MET:O	1.86	0.59
1:G:116:LEU:HD23	1:G:351:LEU:HD11	1.83	0.59
1:L:119:MET:HG2	1:L:124:PHE:HB2	1.84	0.59
1:A:164:LEU:HD11	1:B:224:LYS:CG	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:THR:O	1:B:84:ALA:HB2	2.02	0.59
1:E:201:TYR:CD2	1:E:201:TYR:C	2.79	0.59
1:E:224:LYS:O	1:E:224:LYS:HD2	2.01	0.59
1:F:22:ARG:HD2	1:F:80:PHE:HE1	1.67	0.59
1:G:224:LYS:HD2	1:H:164:LEU:HD21	1.84	0.59
1:E:316:ARG:N	1:E:370:ARG:HH12	2.01	0.59
1:B:160:ALA:HB1	1:B:161:PRO:HD2	1.85	0.59
1:E:77:PHE:HB2	1:E:92:PHE:CE2	2.38	0.59
1:F:368:ILE:HG21	1:F:372:ILE:CG1	2.32	0.59
1:G:52:PHE:CE1	1:G:70:LEU:HD12	2.38	0.59
1:G:357:GLY:HA2	1:G:362:LEU:CD1	2.30	0.59
1:A:20:TYR:OH	1:A:36:GLU:HG3	2.02	0.59
1:D:275:ILE:H	1:D:275:ILE:HD13	1.68	0.59
1:D:303:TYR:O	1:D:304:GLU:HB2	2.01	0.59
1:E:4:TYR:HB3	1:E:9:ILE:CD1	2.33	0.59
1:F:244:MET:HE2	1:F:339:PRO:HA	1.85	0.59
1:H:272:LYS:HZ2	1:H:364:ALA:HB3	1.67	0.59
1:H:319:LEU:CD1	1:H:336:SER:HB3	2.32	0.59
1:I:80:PHE:HD2	1:I:179:MET:CE	2.15	0.59
1:L:28:ILE:CD1	1:L:58:GLU:HA	2.33	0.59
1:B:282:ALA:HA	1:B:285:PHE:CZ	2.38	0.59
1:C:141:ASP:OD1	1:C:145:GLU:HB2	2.03	0.59
1:D:131:PRO:HG2	1:D:199:PHE:HD1	1.68	0.59
1:E:311:TRP:CH2	1:E:367:PRO:HG3	2.38	0.59
1:H:5:THR:HG23	1:H:8:ASP:CG	2.28	0.59
1:J:338:ASP:HB2	1:J:339:PRO:HD2	1.85	0.59
1:C:52:PHE:CE1	1:C:70:LEU:HD13	2.38	0.59
1:G:82:TRP:HD1	1:G:83:THR:N	2.01	0.59
1:K:371:ASN:HB3	1:K:375:MET:HE3	1.85	0.59
1:L:119:MET:HE3	1:L:127:PHE:HB2	1.81	0.59
1:L:417:PHE:O	1:L:421:LYS:HG2	2.03	0.59
1:B:318:PRO:O	1:B:335:ARG:HD3	2.03	0.58
1:C:134:GLU:OE1	3:C:502:GLN:N	2.37	0.58
1:C:351:LEU:HD22	1:C:355:LEU:HG	1.84	0.58
1:D:224:LYS:HE2	1:D:225:HIS:CE1	2.38	0.58
1:D:243:GLY:HA2	1:D:298:ARG:NH1	2.18	0.58
1:F:440:TYR:OH	1:L:293:VAL:HB	2.03	0.58
1:G:129:LEU:CD1	1:G:347:LEU:HD21	2.33	0.58
1:G:164:LEU:CD1	1:L:224:LYS:HD3	2.26	0.58
1:K:231:PHE:HB3	1:K:339:PRO:HB2	1.83	0.58
1:A:22:ARG:HH22	1:F:167:ASN:HD21	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HD12	1:A:336:SER:HB3	1.84	0.58
1:C:365:PRO:O	1:C:366:ALA:HB2	2.01	0.58
1:F:27:ASP:HB3	1:F:33:LYS:HD2	1.85	0.58
1:F:298:ARG:NH1	3:F:503:GLN:O	2.36	0.58
1:F:328:ILE:H	1:F:328:ILE:HD12	1.68	0.58
1:F:368:ILE:HG21	1:F:372:ILE:HG13	1.85	0.58
1:G:281:HIS:HE1	1:G:356:ASP:OD2	1.86	0.58
1:K:17:ASN:HD22	1:K:87:GLY:HA2	1.67	0.58
1:E:163:ASP:HB3	1:F:83:THR:HG22	1.85	0.58
1:I:126:ASP:HB2	1:I:251:PHE:HB2	1.84	0.58
1:I:329:SER:O	1:I:331:ARG:HD2	2.02	0.58
1:K:338:ASP:HB2	1:K:339:PRO:HD2	1.85	0.58
1:L:261:GLU:HA	1:L:266:GLN:NE2	2.13	0.58
1:L:264:ASP:N	1:L:264:ASP:OD1	2.36	0.58
1:A:160:ALA:HB3	1:A:169:ARG:HH12	1.69	0.58
1:E:208:CYS:SG	1:E:347:LEU:CD1	2.91	0.58
1:H:281:HIS:NE2	1:H:404:VAL:HG11	2.18	0.58
1:D:250:LEU:C	1:D:251:PHE:HD1	2.10	0.58
1:D:275:ILE:HD13	1:D:275:ILE:N	2.19	0.58
1:D:282:ALA:HA	1:D:285:PHE:CZ	2.39	0.58
1:J:380:ARG:O	1:J:385:ILE:HB	2.03	0.58
1:L:109:ARG:HG3	1:L:344:TYR:CE2	2.38	0.58
1:B:16:GLU:HA	1:B:16:GLU:OE2	2.03	0.58
1:E:252:LYS:O	1:E:253:ASN:HB2	2.03	0.58
1:F:342:ASN:C	1:F:342:ASN:ND2	2.57	0.58
1:I:308:TYR:HD1	1:I:372:ILE:CG2	2.17	0.58
1:K:280:LYS:HD2	1:K:362:LEU:HD21	1.84	0.58
1:B:32:ILE:O	1:B:32:ILE:HG12	1.99	0.58
1:C:27:ASP:HB3	1:C:33:LYS:HE3	1.86	0.58
1:C:371:ASN:HB3	1:C:374:VAL:HG11	1.85	0.58
1:D:265:LEU:O	1:D:326:ARG:NH1	2.34	0.58
1:E:134:GLU:OE2	3:E:501:GLN:HB2	2.03	0.58
1:I:316:ARG:HD2	1:I:316:ARG:C	2.29	0.58
1:J:129:LEU:HB3	1:J:207:SER:OG	2.03	0.58
1:A:289:THR:O	1:A:341:ALA:HB2	2.02	0.58
1:K:27:ASP:OD1	1:K:31:THR:HB	2.04	0.58
1:A:217:VAL:O	1:A:221:ILE:HG12	2.04	0.58
1:B:437:ARG:O	1:B:441:MET:HB3	2.04	0.58
1:I:285:PHE:HB2	1:I:349:VAL:HG11	1.86	0.58
1:D:217:VAL:O	1:D:221:ILE:HG12	2.03	0.58
1:E:318:PRO:O	1:E:335:ARG:HD3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:252:LYS:O	1:F:255:VAL:HG23	2.04	0.58
1:I:160:ALA:HB2	1:I:188:HIS:HB2	1.86	0.58
1:I:231:PHE:O	1:I:339:PRO:HG2	2.03	0.58
1:J:223:ARG:HH11	1:J:223:ARG:HG3	1.68	0.58
1:A:28:ILE:HD11	1:A:417:PHE:HB2	1.86	0.57
1:B:375:MET:HE2	1:B:379:GLU:HB3	1.85	0.57
1:C:146:PRO:HG3	1:C:228:HIS:CD2	2.39	0.57
1:C:431:GLN:HG2	1:I:435:TRP:CD1	2.39	0.57
1:I:19:LYS:HA	1:I:39:VAL:HB	1.85	0.57
1:L:423:ILE:HG13	1:L:424:GLU:N	2.19	0.57
1:A:22:ARG:NH2	1:F:167:ASN:HD21	2.02	0.57
1:B:169:ARG:NH2	1:B:195:HIS:ND1	2.52	0.57
1:C:109:ARG:HG2	1:C:109:ARG:HH21	1.69	0.57
1:G:5:THR:H	1:G:8:ASP:HB2	1.69	0.57
1:G:318:PRO:O	1:G:335:ARG:HD3	2.03	0.57
1:A:160:ALA:O	1:A:161:PRO:O	2.21	0.57
1:A:357:GLY:HA2	1:A:362:LEU:CD1	2.06	0.57
1:B:18:VAL:HG21	1:B:79:ILE:HD12	1.84	0.57
1:C:290:ASN:HB3	1:C:295:SER:HB3	1.87	0.57
1:D:166:GLU:HG2	1:D:168:CYS:N	2.18	0.57
1:D:207:SER:O	1:D:211:ILE:HG13	2.05	0.57
1:E:311:TRP:CB	1:E:320:ILE:HB	2.34	0.57
1:B:23:LEU:HB3	1:B:70:LEU:HD23	1.86	0.57
1:D:28:ILE:HD11	1:D:417:PHE:CA	2.34	0.57
1:E:91:ARG:HD2	1:E:91:ARG:C	2.30	0.57
1:E:437:ARG:HG3	1:K:232:MET:HE1	1.87	0.57
1:J:282:ALA:HA	1:J:285:PHE:CE2	2.40	0.57
1:K:370:ARG:C	1:K:370:ARG:HE	2.13	0.57
1:B:160:ALA:HB1	1:B:161:PRO:CD	2.34	0.57
1:E:13:VAL:HG13	1:E:18:VAL:HB	1.86	0.57
1:G:383:ASN:HB2	1:G:385:ILE:CD1	2.34	0.57
1:H:22:ARG:NH1	1:H:36:GLU:OE1	2.37	0.57
1:I:440:TYR:HD1	1:I:444:TYR:CE2	2.22	0.57
1:J:70:LEU:O	1:J:72:PRO:HD3	2.05	0.57
1:J:384:GLY:C	1:J:385:ILE:HD12	2.29	0.57
1:B:325:SER:HB2	1:B:331:ARG:NH2	2.05	0.57
1:B:409:LEU:O	1:B:413:LEU:HD12	2.03	0.57
1:F:232:MET:HE1	1:L:437:ARG:CA	2.22	0.57
1:G:342:ASN:C	1:G:342:ASN:ND2	2.63	0.57
1:G:377:LYS:HD2	1:G:387:ASP:OD1	2.04	0.57
1:I:86:LYS:HE2	1:J:178:GLU:OE1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:32:ILE:CD1	1:J:216:LEU:HD12	2.34	0.57
1:J:182:GLU:HB3	1:J:200:LYS:HD3	1.86	0.57
1:H:129:LEU:CD1	1:H:347:LEU:HD21	2.34	0.57
1:I:64:GLU:HB3	1:J:314:GLN:HE21	1.68	0.57
1:L:285:PHE:CD1	1:L:285:PHE:C	2.83	0.57
1:A:300:VAL:HG12	1:A:301:PRO:HD2	1.86	0.57
1:B:18:VAL:HG21	1:B:79:ILE:CD1	2.35	0.57
1:B:162:THR:HG22	1:B:163:ASP:H	1.68	0.57
1:B:280:LYS:HD3	1:B:281:HIS:CE1	2.40	0.57
1:B:314:GLN:HG3	1:B:314:GLN:O	2.05	0.57
1:C:311:TRP:O	1:C:367:PRO:HA	2.04	0.57
1:E:435:TRP:O	1:E:439:GLN:HG2	2.03	0.57
1:F:380:ARG:HG2	1:F:385:ILE:CG2	2.35	0.57
1:H:385:ILE:HD13	1:H:385:ILE:N	2.19	0.57
1:J:371:ASN:HD21	1:J:373:TYR:HB2	1.69	0.57
1:K:335:ARG:NH2	5:K:607:HOH:O	2.37	0.57
1:B:435:TRP:O	1:B:439:GLN:HG2	2.05	0.57
1:C:414:PHE:O	1:C:418:ILE:HD13	2.04	0.57
1:F:34:ASN:ND2	1:F:34:ASN:C	2.63	0.57
1:F:376:SER:H	1:F:379:GLU:HG3	1.68	0.57
1:G:22:ARG:NH1	1:G:36:GLU:HG2	2.19	0.57
1:G:129:LEU:HD11	1:G:347:LEU:HD21	1.86	0.57
1:G:282:ALA:HA	1:G:285:PHE:CE2	2.39	0.57
1:L:182:GLU:HG2	1:L:200:LYS:CD	2.34	0.57
1:J:28:ILE:HG13	1:J:57:ILE:O	2.05	0.57
1:K:85:GLU:CD	1:K:85:GLU:N	2.63	0.57
1:K:212:GLN:HE22	1:K:215:LYS:NZ	2.02	0.57
1:A:162:THR:HG22	1:A:163:ASP:H	1.65	0.56
1:G:378:GLU:HA	1:G:378:GLU:OE2	2.04	0.56
1:K:78:VAL:HG21	1:K:91:ARG:NH2	2.20	0.56
1:A:215:LYS:HG2	1:A:231:PHE:CE2	2.40	0.56
1:A:443:GLN:HE21	1:A:444:TYR:HE2	1.51	0.56
1:H:377:LYS:HA	1:H:380:ARG:NH2	2.20	0.56
1:K:316:ARG:NH2	1:K:370:ARG:HD2	2.17	0.56
1:A:309:VAL:HG13	1:A:319:LEU:HD22	1.87	0.56
1:A:330:THR:O	1:A:330:THR:HG22	2.04	0.56
1:A:378:GLU:H	1:A:378:GLU:CD	2.14	0.56
1:B:311:TRP:CE2	1:B:367:PRO:HB3	2.40	0.56
1:B:311:TRP:CZ2	1:B:367:PRO:HB3	2.39	0.56
1:C:298:ARG:NH1	3:C:502:GLN:O	2.39	0.56
1:E:84:ALA:O	1:E:85:GLU:CB	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:PHE:CD2	1:E:351:LEU:HG	2.40	0.56
1:E:240:ASN:O	5:E:602:HOH:O	2.18	0.56
1:F:131:PRO:C	1:F:133:PRO:HD3	2.31	0.56
1:F:160:ALA:HB1	1:F:161:PRO:CD	2.24	0.56
1:F:434:PRO:O	1:F:438:GLU:HG3	2.05	0.56
1:F:435:TRP:HB2	5:F:613:HOH:O	2.04	0.56
1:G:285:PHE:HB2	1:G:349:VAL:CG2	2.32	0.56
1:H:34:ASN:HB3	1:I:159:LEU:HD22	1.87	0.56
1:I:11:LYS:O	1:I:15:GLU:HB2	2.05	0.56
1:I:345:LEU:HD22	1:I:409:LEU:CD2	2.35	0.56
1:J:426:ASP:O	1:J:430:THR:HG23	2.05	0.56
1:K:32:ILE:HD11	1:L:159:LEU:HD23	1.88	0.56
1:K:406:VAL:HG22	1:K:414:PHE:CE1	2.40	0.56
1:L:260:ASP:O	1:L:266:GLN:HA	2.05	0.56
1:L:292:THR:O	1:L:295:SER:HB2	2.05	0.56
1:B:164:LEU:HD12	1:C:220:THR:HG22	1.86	0.56
1:C:234:LYS:HE3	1:C:239:VAL:O	2.05	0.56
1:F:377:LYS:CG	1:F:378:GLU:N	2.57	0.56
1:I:399:PHE:HZ	1:I:409:LEU:HD12	1.70	0.56
1:K:104:PHE:CZ	1:K:106:GLY:HA3	2.40	0.56
1:K:371:ASN:O	1:K:374:VAL:HG22	2.05	0.56
1:L:29:LEU:C	1:L:31:THR:H	2.12	0.56
1:A:338:ASP:HB2	1:A:339:PRO:HD2	1.88	0.56
1:C:213:THR:O	1:C:216:LEU:HB3	2.06	0.56
1:C:329:SER:O	1:C:331:ARG:HD3	2.06	0.56
1:E:300:VAL:HG13	1:E:301:PRO:HD2	1.88	0.56
1:G:374:VAL:CG2	1:G:375:MET:N	2.67	0.56
1:K:236:LEU:HB2	1:K:239:VAL:HG23	1.88	0.56
1:G:42:LEU:HD12	1:G:42:LEU:O	2.05	0.56
1:G:162:THR:HG22	1:G:163:ASP:H	1.70	0.56
1:I:417:PHE:O	1:I:421:LYS:HG2	2.05	0.56
1:K:208:CYS:SG	1:K:343:PRO:HB2	2.45	0.56
1:K:370:ARG:NH2	1:K:374:VAL:HG22	2.19	0.56
1:A:160:ALA:HB2	1:A:188:HIS:CD2	2.41	0.56
1:F:206:ARG:O	1:F:206:ARG:HD3	2.06	0.56
1:C:349:VAL:HG22	1:C:405:MET:SD	2.45	0.56
1:H:338:ASP:C	1:H:338:ASP:OD2	2.49	0.56
1:K:281:HIS:HE1	1:K:356:ASP:OD1	1.88	0.56
1:A:95:ASP:OD1	1:A:109:ARG:HD2	2.05	0.56
1:B:80:PHE:HB3	1:B:82:TRP:CZ3	2.41	0.56
1:E:160:ALA:CB	1:E:169:ARG:HH12	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:383:ASN:N	1:F:383:ASN:ND2	2.52	0.56
1:I:285:PHE:HB2	1:I:349:VAL:CG1	2.36	0.56
1:J:325:SER:O	1:J:326:ARG:HD3	2.06	0.56
1:K:37:ILE:CD1	1:K:45:ALA:HB2	2.35	0.56
1:K:155:GLY:O	1:K:156:TYR:O	2.24	0.56
1:K:250:LEU:HB2	1:K:258:PHE:CE2	2.41	0.56
1:L:166:GLU:HG3	1:L:167:ASN:H	1.71	0.56
1:A:405:MET:O	1:A:408:ALA:HB3	2.06	0.56
1:C:164:LEU:HD11	1:D:224:LYS:CB	2.36	0.56
1:D:363:GLU:OE1	1:D:363:GLU:HA	2.04	0.56
1:E:3:LYS:HE2	1:E:4:TYR:CE1	2.41	0.56
1:F:116:LEU:O	1:F:119:MET:HE2	2.06	0.56
1:H:378:GLU:HA	1:H:381:MET:CG	2.36	0.56
3:H:503:GLN:N	5:H:601:HOH:O	2.38	0.56
1:J:106:GLY:O	1:J:413:LEU:HD21	2.06	0.56
1:B:129:LEU:HD21	1:B:246:CYS:HB3	1.87	0.55
1:D:107:ASP:HB3	1:D:110:ASN:HB2	1.87	0.55
1:D:385:ILE:HD13	1:D:385:ILE:N	2.21	0.55
1:G:78:VAL:HG13	1:G:91:ARG:CG	2.35	0.55
1:J:160:ALA:CB	1:J:188:HIS:HD2	2.18	0.55
1:J:223:ARG:HG3	1:J:223:ARG:NH1	2.21	0.55
1:K:152:ASP:O	1:K:153:LYS:HE3	2.06	0.55
1:L:19:LYS:HA	1:L:39:VAL:HB	1.87	0.55
1:L:176:LEU:O	1:L:181:PHE:HB2	2.06	0.55
1:C:97:TYR:CD2	1:C:103:PRO:HA	2.41	0.55
1:D:275:ILE:N	1:D:275:ILE:CD1	2.69	0.55
1:E:164:LEU:CD1	1:F:224:LYS:HB2	2.34	0.55
1:E:169:ARG:NH1	1:E:195:HIS:HD2	2.03	0.55
1:E:402:ASN:O	1:E:406:VAL:HG23	2.06	0.55
1:H:112:LEU:HD11	1:H:204:ALA:HB1	1.88	0.55
1:H:166:GLU:O	1:H:166:GLU:CG	2.54	0.55
1:H:189:GLU:OE1	3:H:503:GLN:OE1	2.23	0.55
1:K:82:TRP:HZ3	1:K:221:ILE:HD11	1.72	0.55
1:L:105:GLU:OE2	1:L:412:HIS:CB	2.46	0.55
1:A:376:SER:O	1:A:380:ARG:N	2.37	0.55
1:B:375:MET:HE2	1:B:379:GLU:CB	2.36	0.55
1:F:201:TYR:CD1	1:F:201:TYR:C	2.84	0.55
1:H:115:ILE:HG22	1:H:351:LEU:HD13	1.87	0.55
1:J:285:PHE:CD1	1:J:285:PHE:C	2.83	0.55
1:K:370:ARG:NH2	1:K:374:VAL:HG13	2.22	0.55
1:A:260:ASP:O	1:A:263:ALA:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ILE:HD13	1:B:90:ALA:HB2	1.87	0.55
1:D:318:PRO:O	1:D:335:ARG:HD2	2.06	0.55
1:E:22:ARG:CG	1:E:22:ARG:NH1	2.63	0.55
1:F:156:TYR:CG	1:F:190:VAL:HG13	2.42	0.55
1:G:85:GLU:N	1:G:85:GLU:CD	2.64	0.55
1:G:160:ALA:CB	1:G:188:HIS:HD2	2.18	0.55
1:I:224:LYS:HB2	1:J:164:LEU:CD2	2.36	0.55
1:K:44:LYS:O	1:K:46:LEU:O	2.24	0.55
1:K:141:ASP:C	1:K:141:ASP:OD2	2.50	0.55
1:L:119:MET:HE1	1:L:127:PHE:N	2.22	0.55
1:D:6:ARG:O	1:D:10:GLU:HG3	2.06	0.55
1:D:169:ARG:NH2	1:D:195:HIS:ND1	2.55	0.55
1:K:21:ILE:HD13	1:K:39:VAL:HA	1.89	0.55
1:L:119:MET:HE2	1:L:250:LEU:CD2	2.37	0.55
1:L:150:LEU:HD13	1:L:192:PRO:O	2.06	0.55
1:I:152:ASP:CG	1:I:188:HIS:HE2	2.14	0.55
1:K:5:THR:HG23	1:K:8:ASP:OD2	2.06	0.55
1:A:372:ILE:C	1:A:372:ILE:HD12	2.31	0.55
1:E:4:TYR:HB3	1:E:9:ILE:HD11	1.87	0.55
1:E:163:ASP:CB	1:F:83:THR:HG22	2.37	0.55
1:G:82:TRP:HH2	1:G:217:VAL:HG22	1.71	0.55
1:K:291:PRO:HG3	1:K:341:ALA:HA	1.89	0.55
1:L:96:ILE:N	1:L:96:ILE:HD12	2.22	0.55
1:B:277:GLY:HA3	1:B:353:ALA:O	2.06	0.55
1:H:175:GLU:O	1:H:179:MET:HG3	2.06	0.55
1:K:380:ARG:O	1:K:385:ILE:HB	2.06	0.55
1:L:52:PHE:CD1	1:L:70:LEU:HD22	2.41	0.55
1:L:112:LEU:HD21	1:L:204:ALA:HB1	1.87	0.55
1:E:11:LYS:O	1:E:15:GLU:HG3	2.07	0.55
1:G:13:VAL:HG21	1:G:42:LEU:CD2	2.37	0.55
1:G:132:GLU:HB3	1:G:196:GLU:OE1	2.06	0.55
1:G:300:VAL:HG13	1:G:301:PRO:HD2	1.88	0.55
1:H:104:PHE:CZ	1:H:106:GLY:HA3	2.41	0.55
1:H:260:ASP:O	1:H:266:GLN:HA	2.07	0.55
1:J:48:ASN:HB3	1:J:71:TYR:CD1	2.42	0.55
1:J:58:GLU:O	1:J:61:VAL:HG22	2.07	0.55
1:J:160:ALA:O	1:J:161:PRO:C	2.50	0.55
1:J:423:ILE:HG22	1:J:427:MET:HE2	1.89	0.55
1:L:285:PHE:C	1:L:285:PHE:HD1	2.15	0.55
1:C:316:ARG:HD2	1:C:316:ARG:O	2.07	0.55
1:E:77:PHE:CD1	1:E:92:PHE:CZ	2.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:TRP:HB2	1:E:320:ILE:HB	1.89	0.55
1:J:100:ASP:OD1	1:J:100:ASP:C	2.49	0.55
1:L:224:LYS:HG3	1:L:224:LYS:O	2.06	0.55
1:A:296:TYR:N	1:A:296:TYR:CD1	2.71	0.54
1:B:381:MET:C	1:B:383:ASN:N	2.66	0.54
1:F:11:LYS:O	1:F:15:GLU:HG3	2.07	0.54
1:F:231:PHE:HB3	1:F:339:PRO:HB2	1.89	0.54
1:H:16:GLU:OE1	1:H:16:GLU:HA	2.06	0.54
1:I:304:GLU:O	1:I:317:SER:HB2	2.07	0.54
1:I:435:TRP:O	1:I:439:GLN:HG2	2.06	0.54
1:L:34:ASN:C	1:L:34:ASN:ND2	2.65	0.54
1:L:265:LEU:O	1:L:326:ARG:NH1	2.40	0.54
1:B:141:ASP:OD2	1:B:141:ASP:C	2.49	0.54
1:E:184:GLU:CD	1:E:200:LYS:HG3	2.32	0.54
1:E:370:ARG:HD2	1:F:64:GLU:OE2	2.07	0.54
1:I:377:LYS:HD2	1:I:377:LYS:N	2.22	0.54
1:J:191:ALA:H	1:J:194:GLN:NE2	2.05	0.54
1:E:82:TRP:CD1	1:E:83:THR:N	2.74	0.54
1:F:168:CYS:O	1:F:172:ILE:HG12	2.08	0.54
1:F:265:LEU:O	1:F:326:ARG:NH1	2.41	0.54
1:F:338:ASP:HB2	1:F:339:PRO:CD	2.34	0.54
1:H:309:VAL:HG13	1:H:319:LEU:CD2	2.38	0.54
1:I:77:PHE:HB2	1:I:92:PHE:CE2	2.42	0.54
1:K:11:LYS:HE2	1:K:15:GLU:CG	2.35	0.54
1:L:70:LEU:HD12	1:L:94:CYS:CB	2.37	0.54
1:B:160:ALA:HB2	1:B:188:HIS:HB2	1.90	0.54
1:C:82:TRP:O	1:C:83:THR:OG1	2.20	0.54
1:G:129:LEU:HD23	1:G:130:GLY:N	2.22	0.54
1:I:5:THR:HG22	1:I:8:ASP:CG	2.32	0.54
1:I:80:PHE:CZ	1:I:91:ARG:HB3	2.43	0.54
1:I:114:ARG:O	1:I:117:LYS:HB3	2.08	0.54
1:J:129:LEU:HD23	1:J:248:LEU:HD23	1.89	0.54
1:C:160:ALA:O	1:C:161:PRO:O	2.25	0.54
1:G:208:CYS:SG	1:G:347:LEU:HD23	2.48	0.54
1:I:5:THR:HG22	1:I:8:ASP:OD2	2.07	0.54
1:J:287:ALA:HB2	1:J:395:ALA:HB1	1.89	0.54
1:A:191:ALA:H	1:A:194:GLN:NE2	2.06	0.54
1:C:345:LEU:HD22	1:C:409:LEU:HD22	1.89	0.54
1:E:160:ALA:CB	1:E:188:HIS:CD2	2.90	0.54
1:F:259:PHE:CE2	1:F:327:GLY:HA2	2.41	0.54
1:G:418:ILE:O	1:G:422:GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:223:ARG:NH2	1:H:228:HIS:CD2	2.66	0.54
1:I:380:ARG:C	1:I:382:GLU:H	2.15	0.54
1:A:72:PRO:CA	1:A:94:CYS:HB3	2.31	0.54
1:A:141:ASP:OD1	1:A:145:GLU:HB2	2.08	0.54
1:B:207:SER:O	1:B:211:ILE:HG13	2.08	0.54
1:B:224:LYS:O	1:B:224:LYS:HG2	2.06	0.54
1:C:142:GLU:CD	1:C:142:GLU:H	2.16	0.54
1:E:162:THR:HG21	1:F:220:THR:OG1	2.08	0.54
1:I:100:ASP:HB2	1:I:102:THR:HG23	1.90	0.54
1:I:376:SER:HB2	1:I:377:LYS:HZ3	1.72	0.54
1:J:98:ASN:ND2	1:J:102:THR:HG23	2.21	0.54
1:K:51:MET:HE2	1:K:67:ASP:HB3	1.90	0.54
1:A:359:LYS:HG3	1:A:360:ASN:HD22	1.72	0.54
1:F:5:THR:HG23	1:F:8:ASP:OD2	2.07	0.54
1:H:308:TYR:CE1	1:H:372:ILE:HG13	2.42	0.54
1:K:46:LEU:C	1:K:48:ASN:H	2.14	0.54
1:F:24:GLN:HG3	1:F:93:ILE:HD13	1.89	0.54
1:F:27:ASP:C	1:F:27:ASP:OD2	2.50	0.54
1:F:48:ASN:HB3	1:F:71:TYR:CE1	2.42	0.54
1:G:85:GLU:O	1:G:86:LYS:CB	2.56	0.54
1:H:224:LYS:HE2	1:H:225:HIS:CD2	2.42	0.54
1:K:298:ARG:HG3	1:K:298:ARG:O	2.08	0.54
1:A:328:ILE:HD12	1:A:329:SER:N	2.23	0.54
1:A:357:GLY:CA	1:A:362:LEU:HD12	2.07	0.54
1:B:78:VAL:HG11	1:B:179:MET:CE	2.38	0.54
1:E:80:PHE:HB2	1:E:83:THR:CG2	2.38	0.54
1:H:160:ALA:HB2	1:H:188:HIS:HB2	1.90	0.54
1:L:380:ARG:HG2	1:L:385:ILE:CG2	2.38	0.54
1:A:250:LEU:C	1:A:251:PHE:HD1	2.16	0.53
1:A:260:ASP:O	1:A:266:GLN:HA	2.08	0.53
1:B:129:LEU:O	1:B:201:TYR:HA	2.08	0.53
1:B:261:GLU:HA	1:B:266:GLN:HG2	1.91	0.53
1:I:377:LYS:H	1:I:377:LYS:CD	2.19	0.53
1:K:236:LEU:HB2	1:K:239:VAL:CG2	2.38	0.53
1:L:23:LEU:HB2	1:L:35:VAL:HG22	1.90	0.53
1:C:316:ARG:CD	1:D:63:ILE:O	2.55	0.53
1:F:104:PHE:CZ	1:F:106:GLY:HA3	2.43	0.53
1:F:117:LYS:HB2	1:F:117:LYS:NZ	2.24	0.53
1:I:131:PRO:HD2	1:I:199:PHE:HB2	1.89	0.53
1:B:18:VAL:CG2	1:B:79:ILE:HD12	2.39	0.53
1:D:260:ASP:OD1	1:D:263:ALA:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:LYS:HA	1:F:192:PRO:HB3	1.90	0.53
1:H:21:ILE:HD11	1:H:37:ILE:HD11	1.89	0.53
1:I:220:THR:HG23	1:J:162:THR:HB	1.91	0.53
1:A:86:LYS:HZ1	1:F:175:GLU:CD	2.16	0.53
1:A:300:VAL:HG13	1:A:301:PRO:HD2	1.89	0.53
1:A:426:ASP:O	1:A:430:THR:HG23	2.08	0.53
1:B:96:ILE:N	1:B:96:ILE:CD1	2.71	0.53
3:C:502:GLN:NE2	4:C:504:PO4:O3	2.41	0.53
1:D:13:VAL:HG12	1:D:14:LYS:N	2.24	0.53
1:D:200:LYS:O	1:D:201:TYR:C	2.52	0.53
1:D:243:GLY:HA3	1:D:298:ARG:NH1	2.23	0.53
1:H:418:ILE:O	1:H:422:GLU:HG3	2.09	0.53
1:I:239:VAL:CG2	1:I:240:ASN:N	2.70	0.53
1:J:17:ASN:ND2	1:J:87:GLY:HA2	2.23	0.53
1:J:21:ILE:HD12	1:J:39:VAL:HA	1.91	0.53
1:J:187:HIS:HD2	1:J:188:HIS:O	1.91	0.53
1:J:325:SER:HB2	1:J:331:ARG:HH11	1.72	0.53
1:C:264:ASP:O	1:C:265:LEU:HB2	2.09	0.53
1:D:54:GLY:HA3	1:D:68:MET:HG3	1.90	0.53
1:D:319:LEU:CD1	1:D:336:SER:HB3	2.37	0.53
1:F:52:PHE:CE1	1:F:70:LEU:HD13	2.43	0.53
1:I:34:ASN:C	1:I:34:ASN:ND2	2.65	0.53
1:I:311:TRP:CZ2	1:I:367:PRO:HD3	2.43	0.53
1:J:369:ASP:CG	1:J:370:ARG:H	2.16	0.53
1:B:265:LEU:O	1:B:326:ARG:NH1	2.42	0.53
1:C:19:LYS:HB2	1:C:87:GLY:HA3	1.89	0.53
1:E:308:TYR:CE1	1:E:372:ILE:HB	2.44	0.53
1:F:11:LYS:HG2	1:F:15:GLU:OE1	2.09	0.53
1:F:283:THR:O	1:F:398:GLU:HG2	2.08	0.53
1:H:160:ALA:HB2	1:H:188:HIS:CD2	2.43	0.53
1:K:27:ASP:CG	1:K:31:THR:HB	2.34	0.53
1:K:138:PHE:CE2	1:K:150:LEU:HD23	2.44	0.53
1:K:152:ASP:C	1:K:153:LYS:HE3	2.34	0.53
1:K:160:ALA:HB3	1:K:169:ARG:NH1	2.21	0.53
1:A:83:THR:O	1:A:85:GLU:HG3	2.09	0.53
1:C:426:ASP:O	1:C:430:THR:HG23	2.09	0.53
1:E:96:ILE:HD12	1:E:96:ILE:N	2.24	0.53
1:G:23:LEU:HB2	1:G:35:VAL:O	2.09	0.53
1:G:169:ARG:HG3	1:G:195:HIS:ND1	2.23	0.53
1:G:299:LEU:HD12	1:G:306:PRO:O	2.08	0.53
1:H:275:ILE:O	1:H:279:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:411:GLU:O	1:H:415:GLU:HB2	2.09	0.53
1:H:434:PRO:O	1:H:438:GLU:HG3	2.09	0.53
1:A:91:ARG:NH2	1:A:213:THR:OG1	2.42	0.53
1:A:239:VAL:HG12	1:A:240:ASN:N	2.23	0.53
1:D:54:GLY:HA3	1:D:68:MET:SD	2.48	0.53
1:E:228:HIS:HE1	1:K:441:MET:O	1.91	0.53
1:E:281:HIS:HD2	1:E:402:ASN:ND2	1.98	0.53
1:E:372:ILE:HG13	1:E:373:TYR:N	2.23	0.53
1:F:160:ALA:CB	1:F:161:PRO:HD2	2.20	0.53
1:G:129:LEU:HD23	1:G:129:LEU:C	2.33	0.53
1:G:372:ILE:HG22	1:G:373:TYR:N	2.24	0.53
1:I:119:MET:HG3	1:I:124:PHE:HB2	1.90	0.53
1:J:18:VAL:HA	1:J:88:LYS:HB2	1.91	0.53
1:J:176:LEU:O	1:J:181:PHE:HB2	2.08	0.53
1:J:224:LYS:HB2	1:K:164:LEU:CD2	2.39	0.53
1:A:259:PHE:CZ	1:A:261:GLU:HG3	2.43	0.53
1:D:166:GLU:HG2	1:D:167:ASN:N	2.23	0.53
1:H:437:ARG:NH1	5:H:614:HOH:O	2.41	0.53
1:I:70:LEU:O	1:I:72:PRO:HD3	2.09	0.53
1:K:115:ILE:HA	1:K:118:GLU:HG3	1.91	0.53
1:K:411:GLU:O	1:K:415:GLU:HG2	2.09	0.53
1:L:199:PHE:N	1:L:199:PHE:CD1	2.74	0.53
1:B:176:LEU:O	1:B:181:PHE:HB2	2.08	0.53
1:B:308:TYR:CE2	1:B:380:ARG:NH1	2.77	0.53
1:H:51:MET:HE1	1:I:324:ALA:HB3	1.91	0.53
1:I:28:ILE:HD11	1:I:417:PHE:HB2	1.91	0.53
1:A:164:LEU:HD11	1:B:224:LYS:HG3	1.89	0.52
1:B:183:ILE:N	1:B:183:ILE:HD12	2.23	0.52
1:D:205:VAL:HG23	1:D:206:ARG:N	2.24	0.52
1:D:338:ASP:HB2	1:D:339:PRO:HD2	1.91	0.52
1:F:83:THR:HG21	1:F:89:VAL:HB	1.91	0.52
1:I:351:LEU:HD22	1:I:355:LEU:HG	1.90	0.52
1:B:8:ASP:O	1:B:12:LEU:HD12	2.09	0.52
1:C:426:ASP:HA	1:C:429:ARG:HG2	1.92	0.52
1:I:390:ALA:C	1:I:391:THR:HG23	2.34	0.52
1:L:159:LEU:C	1:L:159:LEU:HD12	2.33	0.52
1:B:223:ARG:HH11	1:B:223:ARG:CG	2.19	0.52
1:D:160:ALA:HB1	1:D:161:PRO:CD	2.25	0.52
1:D:301:PRO:HA	1:D:373:TYR:HE2	1.74	0.52
1:E:27:ASP:OD1	1:E:31:THR:HB	2.08	0.52
1:E:259:PHE:CD1	1:E:327:GLY:HA2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:ILE:HD13	1:G:96:ILE:N	2.24	0.52
1:H:417:PHE:O	1:H:421:LYS:HG2	2.10	0.52
1:J:398:GLU:OE2	1:J:398:GLU:HA	2.09	0.52
1:B:357:GLY:HA2	1:B:362:LEU:HD22	1.90	0.52
1:D:186:SER:OG	1:E:36:GLU:HG3	2.09	0.52
1:D:360:ASN:O	1:D:361:LYS:C	2.51	0.52
1:G:392:LEU:HD12	1:G:392:LEU:O	2.09	0.52
1:I:250:LEU:C	1:I:251:PHE:HD1	2.17	0.52
1:J:316:ARG:O	1:J:316:ARG:HD2	2.09	0.52
1:K:46:LEU:C	1:K:48:ASN:N	2.66	0.52
1:K:370:ARG:C	1:K:370:ARG:NE	2.67	0.52
1:A:22:ARG:HD3	1:A:34:ASN:OD1	2.09	0.52
1:A:345:LEU:HD21	1:A:413:LEU:HD13	1.91	0.52
1:B:160:ALA:HB2	1:B:188:HIS:HD2	1.74	0.52
1:D:369:ASP:OD2	1:D:371:ASN:HB3	2.08	0.52
1:D:370:ARG:O	1:D:371:ASN:HB2	2.09	0.52
1:G:160:ALA:O	1:G:161:PRO:O	2.27	0.52
1:G:259:PHE:CE1	1:G:327:GLY:HA2	2.44	0.52
1:K:52:PHE:CZ	1:K:54:GLY:HA2	2.44	0.52
1:K:285:PHE:C	1:K:285:PHE:CD1	2.87	0.52
1:L:28:ILE:HD12	1:L:58:GLU:HA	1.91	0.52
1:A:360:ASN:O	1:A:361:LYS:C	2.52	0.52
1:C:162:THR:HG22	1:C:163:ASP:H	1.72	0.52
1:C:252:LYS:O	1:C:253:ASN:HB2	2.09	0.52
1:D:206:ARG:HG3	1:D:206:ARG:NH1	2.25	0.52
1:F:325:SER:O	1:F:326:ARG:HD3	2.09	0.52
1:H:25:PHE:CZ	1:H:52:PHE:CE2	2.98	0.52
1:J:28:ILE:HD12	1:J:29:LEU:HG	1.91	0.52
1:J:357:GLY:HA2	1:J:362:LEU:CD1	2.18	0.52
1:L:281:HIS:HD2	1:L:402:ASN:OD1	1.93	0.52
1:A:41:GLN:HE22	1:F:200:LYS:HZ1	1.54	0.52
1:A:163:ASP:CB	1:B:83:THR:HG21	2.25	0.52
1:B:106:GLY:O	1:B:413:LEU:HD21	2.09	0.52
1:C:444:TYR:OXT	1:I:231:PHE:N	2.40	0.52
1:G:109:ARG:NH1	1:G:209:ASP:OD1	2.41	0.52
1:G:308:TYR:CE1	1:G:372:ILE:HD12	2.45	0.52
1:J:13:VAL:HG13	1:J:18:VAL:HB	1.92	0.52
1:K:5:THR:O	1:K:8:ASP:N	2.42	0.52
1:K:100:ASP:OD1	1:K:100:ASP:C	2.51	0.52
1:K:316:ARG:NH2	1:K:370:ARG:CZ	2.72	0.52
1:B:371:ASN:HB3	1:B:374:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ASP:OD2	1:C:338:ASP:C	2.52	0.52
1:D:68:MET:HE1	1:D:104:PHE:CB	2.37	0.52
1:G:119:MET:HG2	1:G:124:PHE:HB2	1.91	0.52
1:G:346:ALA:O	1:G:350:LEU:HG	2.09	0.52
1:H:162:THR:C	1:H:164:LEU:H	2.18	0.52
1:J:67:ASP:O	1:J:68:MET:HG3	2.09	0.52
1:J:360:ASN:O	1:J:361:LYS:C	2.52	0.52
1:K:119:MET:HG2	1:K:124:PHE:HB2	1.90	0.52
1:K:378:GLU:CD	1:K:378:GLU:N	2.68	0.52
1:L:215:LYS:O	1:L:219:LYS:HG2	2.10	0.52
1:A:290:ASN:ND2	1:A:299:LEU:HD21	2.24	0.52
1:F:260:ASP:O	1:F:266:GLN:HA	2.10	0.52
1:I:13:VAL:HG13	1:I:18:VAL:HB	1.91	0.52
1:K:16:GLU:HB3	1:K:88:LYS:NZ	2.25	0.52
1:K:315:ASN:HD21	1:K:370:ARG:N	2.07	0.52
1:E:35:VAL:HG13	1:E:70:LEU:HD21	1.90	0.52
1:E:129:LEU:HD13	1:E:129:LEU:C	2.34	0.52
1:E:169:ARG:HE	1:E:195:HIS:HD2	1.58	0.52
1:H:317:SER:OG	1:H:373:TYR:HE2	1.93	0.52
1:H:319:LEU:O	1:H:319:LEU:HG	2.10	0.52
1:I:377:LYS:HD2	1:I:377:LYS:H	1.75	0.52
1:K:78:VAL:HG21	1:K:91:ARG:HH21	1.75	0.52
1:L:201:TYR:CD1	1:L:201:TYR:C	2.87	0.52
1:A:77:PHE:HB2	1:A:92:PHE:CE2	2.45	0.51
1:C:61:VAL:HG11	1:C:419:GLU:HG2	1.91	0.51
1:F:232:MET:HE2	1:L:440:TYR:HB2	1.91	0.51
1:F:368:ILE:HG22	1:F:369:ASP:N	2.25	0.51
1:H:147:THR:CG2	1:H:148:LEU:N	2.73	0.51
1:H:372:ILE:O	1:H:380:ARG:HD3	2.11	0.51
1:H:396:LEU:O	1:H:400:LYS:HG2	2.10	0.51
1:I:402:ASN:C	1:I:402:ASN:OD1	2.54	0.51
1:K:123:GLY:O	1:K:252:LYS:HD3	2.10	0.51
1:K:194:GLN:C	1:K:195:HIS:CD2	2.88	0.51
1:K:258:PHE:HA	1:K:271:ALA:HB2	1.92	0.51
1:L:377:LYS:CG	1:L:378:GLU:N	2.71	0.51
1:C:260:ASP:HB2	1:C:268:SER:HB3	1.92	0.51
1:G:47:ASP:O	1:G:49:LYS:HG2	2.10	0.51
1:G:231:PHE:O	1:G:339:PRO:HG2	2.10	0.51
1:H:169:ARG:NH2	1:H:195:HIS:ND1	2.58	0.51
1:I:100:ASP:OD1	1:I:100:ASP:N	2.32	0.51
1:I:170:ARG:HG3	1:I:174:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:404:VAL:CG2	1:I:405:MET:HE2	2.33	0.51
1:J:349:VAL:HG22	1:J:405:MET:SD	2.50	0.51
1:K:317:SER:HA	1:K:335:ARG:NH1	2.25	0.51
1:L:134:GLU:HG2	1:L:196:GLU:HB2	1.92	0.51
1:L:141:ASP:OD1	1:L:145:GLU:HB2	2.11	0.51
1:L:165:GLY:O	1:L:166:GLU:C	2.53	0.51
1:L:165:GLY:O	1:L:167:ASN:N	2.43	0.51
1:L:260:ASP:OD2	1:L:260:ASP:C	2.53	0.51
1:B:52:PHE:CE1	1:B:70:LEU:HD13	2.45	0.51
1:B:160:ALA:O	1:B:161:PRO:O	2.28	0.51
1:E:160:ALA:CB	1:E:188:HIS:HD2	2.24	0.51
1:E:280:LYS:HD3	1:E:281:HIS:CE1	2.44	0.51
1:G:206:ARG:NH1	1:G:210:ASP:OD1	2.44	0.51
1:I:274:PHE:O	1:I:278:ILE:HG12	2.10	0.51
1:K:76:THR:O	1:K:78:VAL:HG23	2.11	0.51
1:L:73:ASP:C	1:L:73:ASP:OD1	2.54	0.51
1:L:114:ARG:NH2	1:L:407:LYS:O	2.43	0.51
1:A:82:TRP:O	1:A:83:THR:C	2.54	0.51
1:B:167:ASN:HD22	1:B:170:ARG:NH1	2.08	0.51
1:D:256:ASN:HD22	1:D:256:ASN:C	2.18	0.51
1:F:199:PHE:HZ	1:F:214:PHE:CD1	2.28	0.51
1:I:91:ARG:HD2	1:I:91:ARG:C	2.35	0.51
1:I:261:GLU:OE1	1:I:261:GLU:N	2.37	0.51
1:L:105:GLU:C	1:L:105:GLU:CD	2.78	0.51
1:B:147:THR:HG22	1:B:148:LEU:H	1.75	0.51
1:B:407:LYS:HB3	1:B:407:LYS:HZ2	1.76	0.51
1:C:281:HIS:CD2	1:C:402:ASN:HD21	2.26	0.51
1:D:23:LEU:HD13	1:D:70:LEU:HD23	1.92	0.51
1:E:48:ASN:HB3	1:E:71:TYR:CE1	2.44	0.51
1:E:175:GLU:OE1	1:F:86:LYS:HE2	2.10	0.51
1:E:259:PHE:CZ	1:E:261:GLU:HB2	2.46	0.51
1:G:6:ARG:HD2	1:G:46:LEU:HD13	1.92	0.51
1:H:147:THR:HG22	1:H:148:LEU:N	2.24	0.51
1:K:383:ASN:C	1:K:385:ILE:H	2.17	0.51
1:A:370:ARG:O	1:A:371:ASN:HB3	2.11	0.51
1:D:13:VAL:HG22	1:D:18:VAL:HB	1.93	0.51
1:E:21:ILE:HD13	1:E:39:VAL:HA	1.93	0.51
1:G:371:ASN:C	1:G:374:VAL:HG13	2.35	0.51
1:H:383:ASN:C	1:H:385:ILE:H	2.18	0.51
1:K:134:GLU:OE2	3:K:503:GLN:NE2	2.43	0.51
1:K:224:LYS:HD2	1:K:225:HIS:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:282:ALA:HA	1:K:285:PHE:CZ	2.46	0.51
1:L:5:THR:O	1:L:6:ARG:C	2.53	0.51
1:F:150:LEU:HD22	1:F:192:PRO:O	2.11	0.51
1:F:264:ASP:O	1:F:265:LEU:HB2	2.11	0.51
1:F:328:ILE:H	1:F:328:ILE:CD1	2.22	0.51
1:I:176:LEU:O	1:I:181:PHE:HB2	2.11	0.51
1:I:239:VAL:HG23	1:I:240:ASN:N	2.26	0.51
1:J:231:PHE:HB3	1:J:339:PRO:CB	2.37	0.51
1:J:383:ASN:N	1:J:383:ASN:OD1	2.43	0.51
1:K:161:PRO:O	1:K:162:THR:HG23	2.10	0.51
1:K:260:ASP:O	1:K:266:GLN:HA	2.10	0.51
1:A:41:GLN:HE22	1:F:200:LYS:HZ2	1.54	0.51
1:B:119:MET:HG2	1:B:124:PHE:HB2	1.92	0.51
1:D:141:ASP:HB2	1:D:142:GLU:OE2	2.11	0.51
1:D:159:LEU:HD22	1:E:34:ASN:HB3	1.93	0.51
1:D:338:ASP:C	1:D:338:ASP:OD2	2.53	0.51
1:E:208:CYS:HB2	1:E:344:TYR:CE2	2.45	0.51
1:I:112:LEU:HD11	1:I:204:ALA:HB1	1.93	0.51
1:K:82:TRP:CZ3	1:K:221:ILE:HD11	2.46	0.51
1:K:264:ASP:O	1:K:265:LEU:HB2	2.10	0.51
1:L:151:ASN:OD1	1:L:193:GLY:HA2	2.10	0.51
1:A:111:ASN:OD1	1:A:114:ARG:HD3	2.11	0.51
1:A:206:ARG:HG2	1:A:206:ARG:NH1	2.26	0.51
1:B:197:ILE:HD12	1:B:214:PHE:HE1	1.76	0.51
1:E:381:MET:C	1:E:383:ASN:N	2.66	0.51
1:E:381:MET:O	1:E:383:ASN:N	2.43	0.51
1:H:27:ASP:HB3	1:H:33:LYS:HE3	1.92	0.51
1:J:28:ILE:HD12	1:J:29:LEU:N	2.26	0.51
1:K:435:TRP:O	1:K:439:GLN:HG2	2.11	0.51
1:B:345:LEU:HD22	1:B:409:LEU:HD22	1.92	0.51
1:F:32:ILE:HD11	1:F:216:LEU:HD22	1.92	0.51
1:F:261:GLU:HA	1:F:266:GLN:HE21	1.75	0.51
1:F:371:ASN:ND2	1:F:373:TYR:HB2	2.26	0.51
1:G:48:ASN:HB3	1:G:71:TYR:CD1	2.46	0.51
1:G:435:TRP:O	1:G:439:GLN:HG2	2.11	0.51
1:K:165:GLY:O	1:K:167:ASN:N	2.44	0.51
1:K:316:ARG:HH21	1:K:370:ARG:CD	2.19	0.51
1:L:426:ASP:O	1:L:429:ARG:HG2	2.11	0.51
1:B:164:LEU:HD11	1:C:82:TRP:CD1	2.46	0.50
1:C:48:ASN:HB3	1:C:71:TYR:CE1	2.46	0.50
1:F:6:ARG:HG3	1:F:46:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:THR:O	5:F:601:HOH:O	2.18	0.50
1:G:140:LEU:HD12	1:G:226:GLY:HA2	1.93	0.50
1:J:61:VAL:O	1:J:62:ARG:C	2.55	0.50
1:J:129:LEU:HD12	1:J:207:SER:OG	2.11	0.50
1:J:280:LYS:HG2	1:J:281:HIS:CE1	2.47	0.50
1:J:376:SER:OG	1:J:379:GLU:HG3	2.11	0.50
1:K:46:LEU:O	1:K:47:ASP:HB2	2.12	0.50
1:L:59:GLY:O	1:L:62:ARG:HB2	2.11	0.50
1:L:260:ASP:OD1	1:L:263:ALA:HB2	2.11	0.50
1:B:370:ARG:HB2	1:B:370:ARG:HH11	1.76	0.50
1:C:106:GLY:O	1:C:413:LEU:HD21	2.10	0.50
1:D:68:MET:HE1	1:D:104:PHE:CG	2.46	0.50
1:D:256:ASN:HD21	1:D:258:PHE:HB2	1.76	0.50
1:E:163:ASP:HA	1:E:170:ARG:HH21	1.75	0.50
1:I:33:LYS:NZ	1:J:158:ASP:OD1	2.45	0.50
1:I:48:ASN:HB3	1:I:71:TYR:CD1	2.47	0.50
1:I:259:PHE:CD2	1:I:327:GLY:HA2	2.46	0.50
1:K:48:ASN:N	1:K:48:ASN:OD1	2.40	0.50
1:C:57:ILE:HD11	1:C:96:ILE:HG12	1.94	0.50
1:C:244:MET:HG2	1:C:244:MET:O	2.11	0.50
1:C:417:PHE:O	1:C:421:LYS:HG2	2.11	0.50
1:E:27:ASP:CG	1:E:31:THR:HB	2.36	0.50
1:E:114:ARG:HD3	5:E:612:HOH:O	2.12	0.50
1:G:278:ILE:CG2	1:G:320:ILE:HD11	2.41	0.50
1:I:82:TRP:O	1:I:83:THR:C	2.54	0.50
1:K:73:ASP:CG	1:K:76:THR:HG23	2.36	0.50
1:K:83:THR:HG21	1:K:89:VAL:HB	1.92	0.50
1:K:308:TYR:HD1	1:K:372:ILE:CD1	2.23	0.50
1:B:160:ALA:HB3	1:B:169:ARG:NH1	2.19	0.50
1:C:251:PHE:CD1	1:C:256:ASN:HA	2.47	0.50
1:D:289:THR:O	1:D:341:ALA:HB2	2.11	0.50
1:H:308:TYR:CD2	1:H:387:ASP:OD1	2.65	0.50
1:I:160:ALA:HB2	1:I:188:HIS:CD2	2.46	0.50
1:J:278:ILE:HG22	1:J:320:ILE:HD11	1.92	0.50
1:K:48:ASN:HB3	1:K:71:TYR:CE1	2.46	0.50
1:K:62:ARG:HD2	1:L:156:TYR:HD2	1.76	0.50
1:K:381:MET:C	1:K:383:ASN:N	2.69	0.50
1:A:69:TYR:CE1	1:A:99:PRO:HA	2.46	0.50
1:C:378:GLU:CD	1:C:378:GLU:N	2.68	0.50
1:H:54:GLY:HA3	1:H:68:MET:CE	2.40	0.50
1:I:127:PHE:CD2	1:I:351:LEU:HG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:134:GLU:OE2	3:I:503:GLN:HB2	2.10	0.50
1:J:303:TYR:O	1:J:304:GLU:HB2	2.12	0.50
1:J:381:MET:O	1:J:383:ASN:O	2.29	0.50
1:A:30:GLY:N	1:A:342:ASN:HD22	2.09	0.50
1:B:163:ASP:HA	1:B:170:ARG:HH12	1.77	0.50
1:D:109:ARG:HG3	1:D:344:TYR:CE2	2.47	0.50
1:D:160:ALA:HB1	1:D:188:HIS:HD2	1.73	0.50
1:E:13:VAL:HG21	1:E:42:LEU:CD2	2.42	0.50
1:F:308:TYR:HB3	1:F:387:ASP:HA	1.94	0.50
1:G:11:LYS:NZ	1:G:11:LYS:HB3	2.26	0.50
1:H:154:GLY:C	1:H:188:HIS:CE1	2.90	0.50
1:H:160:ALA:O	1:H:161:PRO:O	2.30	0.50
1:J:119:MET:HG2	1:J:124:PHE:HB2	1.94	0.50
1:K:259:PHE:CD2	1:K:327:GLY:HA2	2.47	0.50
1:L:381:MET:C	1:L:383:ASN:H	2.20	0.50
1:A:191:ALA:H	1:A:194:GLN:HE21	1.60	0.50
1:A:311:TRP:CB	1:A:320:ILE:HB	2.42	0.50
1:B:308:TYR:CD1	1:B:372:ILE:CG2	2.94	0.50
1:C:318:PRO:O	1:C:335:ARG:HD3	2.12	0.50
1:D:5:THR:O	1:D:6:ARG:C	2.55	0.50
1:D:171:ASP:OD2	1:E:85:GLU:HG3	2.12	0.50
1:E:281:HIS:CD2	1:E:402:ASN:HD21	2.12	0.50
1:F:309:VAL:O	1:F:310:ALA:HB2	2.12	0.50
1:G:141:ASP:OD1	1:G:145:GLU:HB2	2.11	0.50
1:G:281:HIS:HD2	1:G:402:ASN:HD21	1.59	0.50
1:G:311:TRP:CH2	1:G:367:PRO:HG3	2.46	0.50
1:H:35:VAL:CG1	1:H:70:LEU:HD21	2.40	0.50
1:H:289:THR:HB	1:H:337:VAL:HG13	1.94	0.50
1:I:112:LEU:HD22	1:I:116:LEU:HG	1.93	0.50
1:K:285:PHE:C	1:K:285:PHE:HD1	2.20	0.50
1:K:397:GLU:OE1	1:K:397:GLU:HA	2.11	0.50
1:L:140:LEU:HD12	1:L:226:GLY:HA2	1.93	0.50
1:L:224:LYS:HG2	1:L:225:HIS:HD2	1.75	0.50
1:D:231:PHE:HB3	1:D:339:PRO:HB2	1.94	0.50
1:H:362:LEU:HD22	1:H:362:LEU:N	2.26	0.50
1:J:377:LYS:O	1:J:381:MET:HG2	2.12	0.50
1:K:321:ARG:HG2	1:K:322:ILE:N	2.26	0.50
1:B:5:THR:O	1:B:6:ARG:C	2.55	0.50
1:B:160:ALA:CB	1:B:188:HIS:HD2	2.25	0.50
1:C:5:THR:O	1:C:8:ASP:N	2.44	0.50
1:D:282:ALA:HA	1:D:285:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:ILE:O	1:D:380:ARG:HD3	2.12	0.50
1:D:381:MET:C	1:D:383:ASN:H	2.20	0.50
1:E:131:PRO:HG2	1:E:199:PHE:CD1	2.45	0.50
1:F:34:ASN:C	1:F:34:ASN:HD22	2.20	0.50
1:J:160:ALA:O	1:J:161:PRO:O	2.29	0.50
1:J:370:ARG:HG2	1:J:370:ARG:NH1	2.27	0.50
1:K:259:PHE:CG	1:K:327:GLY:HA2	2.47	0.50
1:L:304:GLU:O	1:L:335:ARG:NH2	2.42	0.50
1:A:5:THR:H	1:A:8:ASP:HB2	1.77	0.49
1:A:220:THR:HG23	1:F:162:THR:HB	1.94	0.49
1:C:6:ARG:HD2	1:C:46:LEU:HD13	1.93	0.49
1:C:392:LEU:O	1:C:396:LEU:HG	2.12	0.49
1:D:327:GLY:C	1:D:329:SER:H	2.19	0.49
1:F:368:ILE:HG13	1:F:372:ILE:HD11	1.94	0.49
1:G:71:TYR:CG	1:G:97:TYR:CD1	3.00	0.49
1:G:183:ILE:HA	1:G:199:PHE:HA	1.92	0.49
1:B:28:ILE:HD12	1:B:413:LEU:HD22	1.93	0.49
1:C:59:GLY:O	1:C:62:ARG:HG3	2.11	0.49
1:D:142:GLU:H	1:D:142:GLU:CD	2.19	0.49
1:E:13:VAL:HG21	1:E:42:LEU:HD21	1.93	0.49
1:F:22:ARG:HG2	1:F:22:ARG:NH1	2.27	0.49
1:K:317:SER:N	1:K:318:PRO:HD3	2.27	0.49
1:C:162:THR:HG23	1:D:216:LEU:HD11	1.94	0.49
1:D:13:VAL:CG1	1:D:14:LYS:N	2.75	0.49
1:H:203:GLY:O	1:H:204:ALA:C	2.55	0.49
1:I:152:ASP:OD1	1:I:193:GLY:HA2	2.12	0.49
1:I:380:ARG:O	1:I:385:ILE:HB	2.12	0.49
1:B:164:LEU:HD21	1:C:82:TRP:HB3	1.95	0.49
1:C:376:SER:O	1:C:379:GLU:HB2	2.12	0.49
1:D:380:ARG:O	1:D:385:ILE:HB	2.12	0.49
1:E:52:PHE:CE1	1:E:70:LEU:CD1	2.95	0.49
1:G:402:ASN:O	1:G:403:GLU:C	2.55	0.49
1:H:48:ASN:HB3	1:H:71:TYR:CE1	2.47	0.49
1:H:129:LEU:HD21	1:H:246:CYS:HB3	1.94	0.49
1:J:122:LEU:HD21	1:J:359:LYS:HZ1	1.77	0.49
1:K:48:ASN:ND2	1:K:71:TYR:CD2	2.80	0.49
1:K:115:ILE:CG2	1:K:351:LEU:HD12	2.31	0.49
1:E:261:GLU:O	1:E:262:ASN:CG	2.54	0.49
1:F:131:PRO:O	1:F:133:PRO:HD3	2.12	0.49
1:H:406:VAL:HG13	1:H:414:PHE:CD1	2.47	0.49
1:K:319:LEU:HG	1:K:320:ILE:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:116:LEU:O	1:L:119:MET:HB3	2.12	0.49
1:A:200:LYS:NZ	1:B:41:GLN:OE1	2.44	0.49
1:A:282:ALA:HA	1:A:285:PHE:CE2	2.47	0.49
1:B:12:LEU:O	1:B:16:GLU:HB2	2.12	0.49
1:B:351:LEU:HD22	1:B:355:LEU:HG	1.95	0.49
1:C:139:LYS:HD2	1:C:149:GLU:HB3	1.95	0.49
1:D:223:ARG:NH2	5:D:614:HOH:O	2.45	0.49
1:E:3:LYS:HG2	1:E:4:TYR:N	2.27	0.49
1:F:73:ASP:CG	1:F:76:THR:HG23	2.37	0.49
1:F:215:LYS:O	1:F:219:LYS:HD3	2.11	0.49
1:H:273:HIS:O	1:H:276:ALA:HB3	2.13	0.49
1:I:3:LYS:HE2	1:I:4:TYR:CE1	2.47	0.49
1:I:152:ASP:OD2	1:I:188:HIS:NE2	2.39	0.49
1:I:376:SER:OG	1:I:379:GLU:HG3	2.12	0.49
1:K:377:LYS:O	1:K:381:MET:HB2	2.12	0.49
1:C:309:VAL:HG13	1:C:319:LEU:CD2	2.43	0.49
1:F:232:MET:SD	1:F:235:PRO:HA	2.52	0.49
1:F:418:ILE:O	1:F:422:GLU:HG3	2.13	0.49
1:H:176:LEU:O	1:H:181:PHE:HB2	2.11	0.49
1:H:391:THR:OG1	1:H:394:GLU:HG3	2.13	0.49
1:I:4:TYR:HB3	1:I:9:ILE:HD11	1.95	0.49
1:I:83:THR:O	1:I:84:ALA:C	2.55	0.49
1:L:443:GLN:NE2	1:L:444:TYR:CE2	2.81	0.49
1:B:276:ALA:HB2	1:B:364:ALA:HA	1.94	0.49
1:E:22:ARG:HH12	1:E:36:GLU:CD	2.21	0.49
1:F:125:SER:N	1:F:251:PHE:O	2.45	0.49
1:G:83:THR:O	1:G:85:GLU:HG3	2.13	0.49
1:G:156:TYR:C	1:G:158:ASP:N	2.69	0.49
1:H:106:GLY:O	1:H:413:LEU:HD21	2.12	0.49
1:I:224:LYS:HB2	1:J:164:LEU:HD21	1.95	0.49
1:L:275:ILE:O	1:L:279:VAL:HG23	2.12	0.49
1:A:3:LYS:HE2	1:A:4:TYR:CE1	2.48	0.49
1:A:34:ASN:ND2	1:A:34:ASN:O	2.41	0.49
1:B:162:THR:HB	1:C:220:THR:HG23	1.95	0.49
1:C:285:PHE:C	1:C:285:PHE:CD1	2.90	0.49
1:F:325:SER:HB2	1:F:329:SER:HB3	1.95	0.49
1:G:292:THR:O	1:G:295:SER:HB2	2.13	0.49
1:G:325:SER:HB2	1:G:331:ARG:HH22	1.78	0.49
1:J:383:ASN:O	1:J:385:ILE:N	2.37	0.49
1:K:368:ILE:HG12	1:K:372:ILE:HG22	1.94	0.49
1:A:308:TYR:CE1	1:A:372:ILE:CD1	2.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:TRP:O	1:B:83:THR:HG23	2.13	0.49
1:B:431:GLN:O	1:H:297:LYS:NZ	2.46	0.49
1:C:24:GLN:HG3	1:C:93:ILE:HG12	1.94	0.49
1:D:402:ASN:C	1:D:402:ASN:OD1	2.56	0.49
1:E:289:THR:O	1:E:341:ALA:HB2	2.13	0.49
1:G:261:GLU:O	1:G:266:GLN:NE2	2.46	0.49
1:G:291:PRO:HG3	1:G:341:ALA:HA	1.94	0.49
1:I:106:GLY:O	1:I:108:PRO:HD3	2.13	0.49
1:K:380:ARG:HG2	1:K:385:ILE:HG21	1.95	0.49
1:A:16:GLU:OE2	1:A:16:GLU:HA	2.12	0.48
1:A:22:ARG:NH1	1:A:36:GLU:CD	2.71	0.48
1:A:402:ASN:C	1:A:402:ASN:OD1	2.56	0.48
1:B:287:ALA:HB2	1:B:395:ALA:O	2.12	0.48
1:E:129:LEU:CD1	1:E:131:PRO:HD3	2.44	0.48
1:F:156:TYR:CD1	1:F:190:VAL:HG13	2.48	0.48
1:F:182:GLU:O	1:F:200:LYS:HG3	2.13	0.48
1:J:35:VAL:HG13	1:J:70:LEU:HD21	1.95	0.48
1:J:383:ASN:HB2	1:J:385:ILE:CD1	2.33	0.48
1:K:139:LYS:O	1:K:147:THR:HG23	2.13	0.48
1:A:37:ILE:HD12	1:A:38:PRO:O	2.13	0.48
1:A:250:LEU:O	1:A:251:PHE:HD1	1.95	0.48
1:B:23:LEU:HB3	1:B:70:LEU:CD2	2.42	0.48
1:B:166:GLU:HG2	1:B:168:CYS:H	1.79	0.48
1:C:300:VAL:HG21	1:I:430:THR:HG22	1.94	0.48
1:E:207:SER:O	1:E:211:ILE:HG13	2.13	0.48
1:F:57:ILE:HD12	1:F:104:PHE:CE2	2.47	0.48
1:G:201:TYR:CD1	1:G:201:TYR:C	2.91	0.48
1:G:249:SER:HA	1:G:258:PHE:HZ	1.74	0.48
1:H:134:GLU:OE2	3:H:503:GLN:OE1	2.29	0.48
1:I:96:ILE:N	1:I:96:ILE:HD12	2.28	0.48
1:I:396:LEU:O	1:I:400:LYS:HG3	2.13	0.48
1:K:248:LEU:N	1:K:332:VAL:O	2.42	0.48
1:L:170:ARG:HG2	1:L:170:ARG:NH1	2.28	0.48
1:C:234:LYS:HD3	1:C:298:ARG:HA	1.95	0.48
1:D:119:MET:HE1	1:D:126:ASP:HA	1.96	0.48
1:D:132:GLU:HB3	1:D:196:GLU:OE1	2.13	0.48
1:F:274:PHE:O	1:F:278:ILE:HG12	2.14	0.48
1:G:338:ASP:C	1:G:338:ASP:OD2	2.56	0.48
1:G:370:ARG:H	1:G:370:ARG:CD	2.19	0.48
1:H:129:LEU:HD11	1:H:347:LEU:HD21	1.95	0.48
1:J:5:THR:HG23	1:J:8:ASP:CG	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:46:LEU:HB3	5:K:614:HOH:O	2.13	0.48
1:K:360:ASN:O	1:K:361:LYS:C	2.56	0.48
1:K:371:ASN:HB3	1:K:375:MET:CE	2.42	0.48
1:L:5:THR:HG23	1:L:8:ASP:CG	2.39	0.48
1:L:129:LEU:O	1:L:201:TYR:HA	2.13	0.48
1:L:268:SER:O	1:L:271:ALA:HB3	2.13	0.48
1:A:115:ILE:HA	1:A:118:GLU:HG3	1.96	0.48
1:C:82:TRP:C	1:C:83:THR:OG1	2.57	0.48
1:D:28:ILE:HD11	1:D:417:PHE:CB	2.41	0.48
1:D:351:LEU:O	1:D:355:LEU:HG	2.13	0.48
1:D:374:VAL:HG22	1:D:375:MET:N	2.29	0.48
1:D:376:SER:O	1:D:380:ARG:HG3	2.14	0.48
1:D:383:ASN:C	1:D:385:ILE:N	2.72	0.48
1:E:240:ASN:HD22	1:E:303:TYR:HD1	1.61	0.48
1:E:345:LEU:HD22	1:E:409:LEU:CD2	2.43	0.48
1:F:371:ASN:HD21	1:F:373:TYR:HB2	1.78	0.48
1:I:44:LYS:HE2	1:J:184:GLU:OE2	2.14	0.48
1:I:208:CYS:HB3	1:I:344:TYR:CE2	2.47	0.48
1:I:270:THR:HG23	1:I:358:ILE:HD13	1.96	0.48
1:I:368:ILE:HB	1:I:372:ILE:HD11	1.95	0.48
1:K:78:VAL:HG23	1:K:91:ARG:HE	1.76	0.48
1:K:203:GLY:O	1:K:204:ALA:C	2.57	0.48
1:K:240:ASN:ND2	1:K:303:TYR:HD2	2.10	0.48
1:B:127:PHE:HZ	1:B:248:LEU:HD22	1.72	0.48
1:E:131:PRO:HD2	1:E:199:PHE:HB2	1.95	0.48
1:F:133:PRO:HD2	1:F:197:ILE:O	2.13	0.48
1:F:162:THR:C	1:F:164:LEU:H	2.21	0.48
1:F:260:ASP:HB2	1:F:268:SER:HB3	1.96	0.48
1:H:141:ASP:OD2	1:H:143:LYS:N	2.47	0.48
1:K:19:LYS:HA	1:K:39:VAL:HB	1.95	0.48
1:L:249:SER:HA	1:L:258:PHE:CE1	2.48	0.48
1:A:54:GLY:HA3	1:A:68:MET:SD	2.53	0.48
1:C:118:GLU:O	1:C:122:LEU:HD23	2.13	0.48
1:C:371:ASN:CB	1:C:374:VAL:HG12	2.31	0.48
1:D:170:ARG:HG3	1:D:174:LEU:HD11	1.96	0.48
1:F:129:LEU:HD22	1:F:131:PRO:HD3	1.95	0.48
1:G:157:PHE:C	1:L:33:LYS:HD2	2.38	0.48
1:H:127:PHE:CZ	1:H:248:LEU:HD22	2.47	0.48
1:I:48:ASN:HB3	1:I:71:TYR:CE1	2.47	0.48
1:J:86:LYS:HE3	1:K:178:GLU:OE1	2.12	0.48
1:K:309:VAL:HA	1:K:319:LEU:CD2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:THR:C	1:A:164:LEU:H	2.21	0.48
1:A:258:PHE:HB2	1:A:330:THR:HG22	1.95	0.48
1:D:372:ILE:HG13	1:D:373:TYR:N	2.27	0.48
1:E:431:GLN:HG2	1:K:435:TRP:CD1	2.49	0.48
1:F:308:TYR:CE1	1:F:372:ILE:HG21	2.48	0.48
1:F:402:ASN:C	1:F:402:ASN:OD1	2.57	0.48
1:H:204:ALA:O	1:H:205:VAL:C	2.55	0.48
1:J:162:THR:HG22	1:J:163:ASP:H	1.79	0.48
1:J:369:ASP:CG	1:J:370:ARG:N	2.71	0.48
1:K:402:ASN:O	1:K:406:VAL:HG23	2.14	0.48
1:L:129:LEU:HD12	1:L:347:LEU:HD11	1.94	0.48
1:B:310:ALA:HB1	1:B:368:ILE:HG12	1.95	0.48
1:B:429:ARG:HD3	1:B:430:THR:HG23	1.95	0.48
1:C:156:TYR:O	1:D:33:LYS:NZ	2.37	0.48
1:D:129:LEU:HD13	1:D:131:PRO:HD3	1.96	0.48
1:F:24:GLN:HE22	1:F:91:ARG:HH11	1.61	0.48
1:F:45:ALA:HA	1:F:50:VAL:HG23	1.96	0.48
1:F:281:HIS:O	1:F:282:ALA:C	2.56	0.48
1:I:160:ALA:O	1:I:161:PRO:O	2.32	0.48
1:I:285:PHE:CD1	1:I:285:PHE:C	2.92	0.48
1:J:271:ALA:O	1:J:275:ILE:HG13	2.14	0.48
1:K:32:ILE:O	1:K:32:ILE:HG13	2.12	0.48
1:K:247:ASN:HB3	1:K:331:ARG:HG3	1.95	0.48
1:L:368:ILE:HG21	1:L:372:ILE:HG23	1.96	0.48
1:A:129:LEU:HD13	1:A:131:PRO:HG3	1.94	0.48
1:A:221:ILE:O	1:A:224:LYS:HB3	2.14	0.48
1:C:24:GLN:NE2	1:C:91:ARG:NH1	2.60	0.48
1:I:316:ARG:HB3	1:I:373:TYR:CE1	2.49	0.48
1:C:23:LEU:HD12	1:C:35:VAL:HG22	1.95	0.48
1:D:160:ALA:HB2	1:D:188:HIS:HB2	1.95	0.48
1:D:380:ARG:HB3	1:D:385:ILE:HG21	1.96	0.48
1:D:403:GLU:O	1:D:407:LYS:HG3	2.14	0.48
1:F:52:PHE:CE2	1:F:54:GLY:HA2	2.49	0.48
1:G:82:TRP:O	1:G:83:THR:C	2.57	0.48
1:J:281:HIS:HE1	1:J:356:ASP:OD1	1.96	0.48
1:L:169:ARG:NH2	1:L:195:HIS:ND1	2.58	0.48
1:L:218:VAL:O	1:L:219:LYS:C	2.56	0.48
1:B:100:ASP:OD1	1:B:101:GLY:N	2.47	0.47
1:B:314:GLN:NE2	1:C:64:GLU:HB2	2.29	0.47
1:D:315:ASN:O	1:E:64:GLU:HG2	2.14	0.47
1:E:83:THR:CG2	1:E:89:VAL:HB	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:342:ASN:HD22	1:G:343:PRO:N	2.12	0.47
1:H:80:PHE:CZ	1:H:91:ARG:HB3	2.49	0.47
1:H:351:LEU:CD2	1:H:355:LEU:HG	2.44	0.47
1:I:84:ALA:HB2	1:I:88:LYS:HG2	1.96	0.47
1:J:109:ARG:HG3	1:J:344:TYR:CE2	2.49	0.47
1:K:166:GLU:O	1:K:168:CYS:N	2.47	0.47
1:B:32:ILE:CD1	1:B:216:LEU:HD22	2.43	0.47
1:F:55:SER:O	1:F:62:ARG:HG3	2.14	0.47
1:H:48:ASN:N	1:H:48:ASN:OD1	2.47	0.47
1:I:247:ASN:HB3	1:I:331:ARG:HG3	1.96	0.47
1:J:78:VAL:HG11	1:J:179:MET:HE3	1.97	0.47
1:K:109:ARG:HG3	1:K:344:TYR:CE2	2.49	0.47
1:K:385:ILE:N	1:K:385:ILE:CD1	2.75	0.47
1:A:22:ARG:NH1	1:A:36:GLU:OE1	2.47	0.47
1:B:82:TRP:O	1:B:82:TRP:CG	2.67	0.47
1:C:369:ASP:O	1:C:370:ARG:C	2.56	0.47
1:D:273:HIS:CE1	1:D:361:LYS:HA	2.49	0.47
1:F:232:MET:HE3	1:L:440:TYR:HB2	1.96	0.47
1:F:250:LEU:HD23	1:F:250:LEU:HA	1.72	0.47
1:G:5:THR:HG23	1:G:8:ASP:OD1	2.14	0.47
1:G:86:LYS:HD2	1:H:178:GLU:OE1	2.15	0.47
1:I:326:ARG:HD3	1:I:326:ARG:HA	1.53	0.47
1:J:371:ASN:HD22	1:J:374:VAL:CG1	2.14	0.47
1:K:119:MET:CE	1:K:120:GLU:HG3	2.44	0.47
1:L:381:MET:O	1:L:383:ASN:N	2.47	0.47
1:L:425:TRP:CZ3	1:L:429:ARG:HD2	2.49	0.47
1:A:259:PHE:CE2	1:A:261:GLU:HG3	2.50	0.47
1:B:178:GLU:OE2	1:C:86:LYS:HG3	2.15	0.47
1:C:365:PRO:O	1:C:366:ALA:CB	2.63	0.47
1:C:379:GLU:O	1:C:382:GLU:HB3	2.15	0.47
1:D:7:GLU:H	1:D:7:GLU:CD	2.22	0.47
1:D:27:ASP:C	1:D:29:LEU:H	2.22	0.47
1:D:243:GLY:CA	1:D:298:ARG:HH12	2.27	0.47
1:E:376:SER:H	1:E:379:GLU:HB2	1.79	0.47
1:H:82:TRP:HE1	1:H:221:ILE:HD11	1.80	0.47
1:H:163:ASP:OD1	1:H:170:ARG:NE	2.48	0.47
1:H:184:GLU:O	1:H:185:ALA:HB2	2.13	0.47
1:J:78:VAL:HG12	1:J:79:ILE:N	2.28	0.47
1:J:141:ASP:HB3	1:J:147:THR:HG22	1.95	0.47
1:K:290:ASN:HB3	1:K:295:SER:HB3	1.96	0.47
1:L:381:MET:C	1:L:383:ASN:N	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:THR:O	1:C:6:ARG:C	2.57	0.47
1:C:73:ASP:CG	1:C:76:THR:HG23	2.39	0.47
1:D:173:VAL:HG22	1:D:183:ILE:HD13	1.94	0.47
1:H:83:THR:C	1:H:85:GLU:OE2	2.58	0.47
1:J:17:ASN:HD21	1:J:87:GLY:HA2	1.79	0.47
1:J:28:ILE:CD1	1:J:29:LEU:HG	2.44	0.47
1:J:163:ASP:HA	1:J:170:ARG:NH1	2.29	0.47
1:K:27:ASP:OD2	1:K:27:ASP:C	2.58	0.47
1:L:404:VAL:HG22	1:L:405:MET:CE	2.42	0.47
1:B:182:GLU:HB3	1:B:200:LYS:HE2	1.96	0.47
1:B:271:ALA:O	1:B:275:ILE:HD12	2.15	0.47
1:D:170:ARG:O	1:D:174:LEU:HD12	2.15	0.47
1:D:381:MET:C	1:D:383:ASN:N	2.72	0.47
1:F:201:TYR:C	1:F:201:TYR:HD1	2.23	0.47
1:F:285:PHE:CD1	1:F:285:PHE:C	2.93	0.47
1:F:303:TYR:CD2	1:F:303:TYR:N	2.83	0.47
1:F:309:VAL:HG13	1:F:319:LEU:HD23	1.96	0.47
1:K:199:PHE:HZ	1:K:214:PHE:CG	2.32	0.47
1:A:46:LEU:C	1:A:48:ASN:H	2.23	0.47
1:A:319:LEU:CD1	1:A:336:SER:HB3	2.45	0.47
1:B:23:LEU:HD13	1:B:70:LEU:HD23	1.97	0.47
1:B:136:PHE:CE2	1:B:194:GLN:HB2	2.49	0.47
1:B:224:LYS:HE2	1:B:225:HIS:CD2	2.49	0.47
1:C:28:ILE:HD11	1:C:413:LEU:HD23	1.95	0.47
1:D:377:LYS:O	1:D:381:MET:N	2.32	0.47
1:E:26:THR:OG1	1:E:212:GLN:NE2	2.48	0.47
1:E:160:ALA:HB1	1:E:161:PRO:CD	2.25	0.47
1:F:111:ASN:O	1:F:114:ARG:HB3	2.15	0.47
1:F:156:TYR:HB2	1:F:190:VAL:CG1	2.42	0.47
1:G:312:SER:O	1:G:321:ARG:HA	2.15	0.47
1:G:320:ILE:HA	1:G:333:GLU:O	2.15	0.47
1:I:22:ARG:NH1	1:I:36:GLU:OE1	2.48	0.47
1:I:35:VAL:CG1	1:I:70:LEU:HD21	2.45	0.47
1:I:97:TYR:CE2	1:I:103:PRO:HG3	2.50	0.47
1:I:170:ARG:NH1	1:I:170:ARG:CG	2.70	0.47
1:I:224:LYS:HE3	1:I:225:HIS:NE2	2.28	0.47
1:J:127:PHE:CD2	1:J:351:LEU:HG	2.48	0.47
1:J:312:SER:OG	1:J:315:ASN:HB2	2.14	0.47
1:J:371:ASN:HD22	1:J:374:VAL:H	1.60	0.47
1:J:385:ILE:HD12	1:J:385:ILE:N	2.30	0.47
1:K:5:THR:O	1:K:6:ARG:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:376:SER:O	1:L:377:LYS:C	2.58	0.47
1:A:184:GLU:O	1:A:185:ALA:HB2	2.15	0.47
1:A:347:LEU:HD13	1:A:347:LEU:HA	1.80	0.47
1:D:148:LEU:N	1:D:148:LEU:HD23	2.30	0.47
1:D:164:LEU:O	1:D:165:GLY:O	2.33	0.47
1:E:396:LEU:HD23	1:E:396:LEU:HA	1.78	0.47
1:F:241:GLY:HA3	1:F:298:ARG:HG2	1.96	0.47
1:G:71:TYR:CD1	1:G:97:TYR:CD1	3.03	0.47
1:H:73:ASP:C	1:H:73:ASP:OD1	2.57	0.47
1:H:129:LEU:HD12	1:H:347:LEU:HD21	1.97	0.47
1:J:141:ASP:OD2	1:J:141:ASP:C	2.58	0.47
1:L:28:ILE:HD11	1:L:58:GLU:HA	1.97	0.47
1:A:184:GLU:OE1	1:A:200:LYS:HE3	2.15	0.47
1:A:314:GLN:HG3	1:A:314:GLN:O	2.15	0.47
1:B:164:LEU:HB2	1:C:220:THR:HG22	1.95	0.47
1:C:153:LYS:HA	1:C:192:PRO:HB3	1.96	0.47
1:G:100:ASP:CG	1:G:101:GLY:H	2.23	0.47
1:G:260:ASP:CG	1:G:263:ALA:HB2	2.39	0.47
1:I:241:GLY:HA3	1:I:298:ARG:HG3	1.97	0.47
1:J:223:ARG:HH11	1:J:223:ARG:HG2	1.76	0.47
1:J:281:HIS:CD2	1:J:402:ASN:HD21	2.30	0.47
1:K:378:GLU:HB2	1:K:379:GLU:OE1	2.15	0.47
1:L:70:LEU:HD13	1:L:70:LEU:HA	1.60	0.47
1:A:245:HIS:ND1	4:A:504:PO4:O1	2.48	0.47
1:B:115:ILE:CG2	1:B:351:LEU:HD13	2.38	0.47
1:C:159:LEU:HD22	1:D:34:ASN:CB	2.44	0.47
1:C:289:THR:O	1:C:341:ALA:HB2	2.15	0.47
1:D:359:LYS:CB	1:D:359:LYS:NZ	2.78	0.47
1:E:129:LEU:HD12	1:E:207:SER:HB3	1.96	0.47
1:F:382:GLU:C	1:F:383:ASN:ND2	2.63	0.47
1:H:28:ILE:HD12	1:H:413:LEU:CD2	2.40	0.47
1:K:234:LYS:HE2	1:K:298:ARG:HA	1.97	0.47
1:E:109:ARG:NH1	1:E:209:ASP:OD1	2.43	0.46
1:E:393:ALA:HB2	1:E:425:TRP:CE2	2.50	0.46
1:F:164:LEU:HD23	1:F:164:LEU:HA	1.81	0.46
1:H:59:GLY:O	1:H:62:ARG:HG3	2.14	0.46
1:I:274:PHE:C	1:I:274:PHE:CD2	2.93	0.46
1:J:109:ARG:O	1:J:113:LYS:HG3	2.15	0.46
1:J:285:PHE:C	1:J:285:PHE:HD1	2.23	0.46
1:K:22:ARG:HH11	1:K:22:ARG:CG	2.20	0.46
1:K:217:VAL:O	1:K:221:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:11:LYS:HB3	1:L:11:LYS:HE2	1.44	0.46
1:A:176:LEU:O	1:A:181:PHE:HB2	2.15	0.46
1:B:176:LEU:HD11	1:B:214:PHE:HD1	1.80	0.46
1:B:396:LEU:O	1:B:400:LYS:HG3	2.14	0.46
1:C:127:PHE:CD2	1:C:351:LEU:HG	2.50	0.46
1:C:370:ARG:HH21	1:C:374:VAL:CG2	2.28	0.46
1:E:119:MET:HG2	1:E:124:PHE:HB2	1.95	0.46
1:G:315:ASN:CG	1:G:316:ARG:H	2.23	0.46
1:H:10:GLU:OE1	1:H:10:GLU:HA	2.14	0.46
1:H:251:PHE:N	1:H:251:PHE:HD1	2.13	0.46
1:H:258:PHE:HA	1:H:271:ALA:HB2	1.98	0.46
1:I:160:ALA:O	1:I:161:PRO:C	2.57	0.46
1:K:212:GLN:HE22	1:K:215:LYS:HZ1	1.63	0.46
1:B:91:ARG:HD2	1:B:91:ARG:C	2.39	0.46
1:B:186:SER:O	1:C:36:GLU:HG2	2.15	0.46
1:D:133:PRO:HD2	1:D:197:ILE:O	2.15	0.46
1:E:322:ILE:HD11	1:E:332:VAL:HG22	1.97	0.46
1:E:371:ASN:HA	1:E:374:VAL:HG21	1.95	0.46
1:H:135:PHE:HB3	1:H:231:PHE:CE1	2.51	0.46
1:I:252:LYS:HZ2	1:I:252:LYS:HB3	1.79	0.46
1:J:27:ASP:CG	1:J:31:THR:HB	2.41	0.46
1:J:282:ALA:HA	1:J:285:PHE:CZ	2.50	0.46
1:K:376:SER:O	1:K:379:GLU:HG2	2.15	0.46
1:L:260:ASP:CG	1:L:263:ALA:HB2	2.41	0.46
1:L:274:PHE:C	1:L:274:PHE:CD2	2.92	0.46
1:L:369:ASP:CG	1:L:370:ARG:H	2.23	0.46
1:B:85:GLU:O	1:B:86:LYS:CB	2.63	0.46
1:B:276:ALA:HB2	1:B:364:ALA:CA	2.46	0.46
1:C:36:GLU:HG2	1:C:36:GLU:H	1.55	0.46
1:C:310:ALA:HB1	1:C:368:ILE:HG12	1.98	0.46
1:E:132:GLU:HG2	1:E:198:ASP:OD1	2.16	0.46
1:F:48:ASN:HB3	1:F:71:TYR:CD1	2.49	0.46
1:F:224:LYS:HD2	1:F:225:HIS:CD2	2.50	0.46
1:G:375:MET:HG3	1:G:380:ARG:HG3	1.96	0.46
1:H:34:ASN:ND2	1:H:34:ASN:C	2.74	0.46
1:H:46:LEU:HD22	1:H:74:LEU:HD11	1.97	0.46
1:H:70:LEU:C	1:H:71:TYR:HD1	2.23	0.46
1:I:127:PHE:CZ	1:I:248:LEU:HD22	2.51	0.46
1:J:326:ARG:HD3	1:J:326:ARG:HA	1.38	0.46
1:J:402:ASN:OD1	1:J:404:VAL:HG13	2.16	0.46
1:K:308:TYR:CE1	1:K:372:ILE:HG13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:326:ARG:HD2	1:K:330:THR:HG23	1.97	0.46
1:L:351:LEU:CD2	1:L:355:LEU:HG	2.46	0.46
1:A:48:ASN:HB3	1:A:71:TYR:CE1	2.50	0.46
1:D:376:SER:H	1:D:379:GLU:HB2	1.80	0.46
1:E:32:ILE:HD11	1:E:216:LEU:HD12	1.97	0.46
1:E:167:ASN:HD21	1:F:22:ARG:NH2	2.14	0.46
1:E:290:ASN:HB3	1:E:295:SER:HB3	1.97	0.46
1:E:393:ALA:HB2	1:E:425:TRP:CD2	2.51	0.46
1:F:299:LEU:HD12	1:F:306:PRO:O	2.16	0.46
1:H:182:GLU:O	1:H:200:LYS:HG2	2.15	0.46
1:I:201:TYR:C	1:I:201:TYR:CD2	2.94	0.46
1:J:163:ASP:HA	1:J:170:ARG:HH12	1.79	0.46
1:J:211:ILE:O	1:J:215:LYS:HG3	2.16	0.46
1:K:97:TYR:HD2	1:K:101:GLY:O	1.97	0.46
1:L:33:LYS:O	1:L:34:ASN:HB3	2.14	0.46
1:A:14:LYS:HE2	1:A:14:LYS:HB2	1.81	0.46
1:A:381:MET:C	1:A:383:ASN:N	2.74	0.46
1:A:423:ILE:O	1:A:427:MET:HG3	2.15	0.46
1:C:326:ARG:HA	1:C:326:ARG:HD3	1.72	0.46
1:E:316:ARG:HD2	1:E:316:ARG:C	2.40	0.46
1:G:77:PHE:CD1	1:G:92:PHE:CZ	3.03	0.46
1:I:169:ARG:NH2	1:I:195:HIS:ND1	2.63	0.46
1:I:212:GLN:OE1	1:I:343:PRO:HG3	2.16	0.46
1:I:380:ARG:C	1:I:385:ILE:HB	2.41	0.46
1:J:308:TYR:CZ	1:J:372:ILE:HB	2.51	0.46
1:A:290:ASN:HD22	1:A:299:LEU:HD21	1.80	0.46
1:B:260:ASP:C	1:B:260:ASP:OD1	2.59	0.46
1:B:430:THR:HG22	1:H:300:VAL:HG21	1.97	0.46
1:C:20:TYR:HB3	1:C:89:VAL:HG22	1.98	0.46
1:C:369:ASP:CG	1:C:370:ARG:H	2.23	0.46
1:C:379:GLU:O	1:C:383:ASN:ND2	2.48	0.46
1:C:414:PHE:CE1	1:C:418:ILE:HD11	2.50	0.46
1:E:164:LEU:HB2	1:F:220:THR:CG2	2.46	0.46
1:E:308:TYR:OH	1:E:373:TYR:HD1	1.98	0.46
1:E:326:ARG:HA	1:E:326:ARG:HD3	1.49	0.46
1:F:14:LYS:HB2	1:F:14:LYS:NZ	2.30	0.46
1:H:251:PHE:N	1:H:251:PHE:CD1	2.84	0.46
1:H:278:ILE:CG2	1:H:320:ILE:HD11	2.46	0.46
1:I:139:LYS:HD3	1:I:149:GLU:CD	2.41	0.46
1:J:318:PRO:O	1:J:335:ARG:HD3	2.15	0.46
1:K:5:THR:HG23	1:K:8:ASP:CG	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASN:ND2	1:A:36:GLU:OE1	2.45	0.46
1:B:405:MET:HE2	1:B:405:MET:HA	1.96	0.46
1:D:345:LEU:HD22	1:D:409:LEU:HD22	1.98	0.46
1:E:239:VAL:HG23	1:E:240:ASN:N	2.30	0.46
1:E:308:TYR:OH	1:E:373:TYR:CD1	2.69	0.46
1:E:325:SER:HB2	1:E:331:ARG:HH22	1.80	0.46
1:F:172:ILE:CD1	1:F:218:VAL:HA	2.46	0.46
1:H:85:GLU:CD	1:H:85:GLU:N	2.74	0.46
1:H:308:TYR:HD2	1:H:387:ASP:OD1	1.97	0.46
1:L:417:PHE:HD2	1:L:418:ILE:HD13	1.80	0.46
1:A:119:MET:HE1	1:A:126:ASP:C	2.41	0.46
1:B:435:TRP:CD1	1:H:431:GLN:HG2	2.50	0.46
1:D:106:GLY:O	1:D:413:LEU:HD21	2.16	0.46
1:H:141:ASP:OD2	1:H:141:ASP:C	2.59	0.46
1:J:37:ILE:HG22	1:K:185:ALA:HB2	1.98	0.46
1:J:145:GLU:OE1	1:J:145:GLU:CA	2.44	0.46
1:L:6:ARG:NH1	1:L:10:GLU:OE2	2.43	0.46
1:L:126:ASP:OD2	1:L:126:ASP:N	2.49	0.46
1:L:281:HIS:O	1:L:282:ALA:C	2.59	0.46
1:L:383:ASN:O	1:L:385:ILE:HD12	2.16	0.46
1:A:22:ARG:HH12	1:A:36:GLU:CD	2.24	0.46
1:A:83:THR:OG1	1:A:84:ALA:N	2.49	0.46
1:A:111:ASN:O	1:A:115:ILE:HG12	2.16	0.46
1:A:261:GLU:C	1:A:263:ALA:H	2.23	0.46
1:D:116:LEU:O	1:D:119:MET:HG2	2.15	0.46
1:D:380:ARG:HB3	1:D:385:ILE:CG2	2.45	0.46
1:E:80:PHE:HB2	1:E:83:THR:HG21	1.99	0.46
1:E:205:VAL:HG13	1:E:206:ARG:H	1.82	0.46
1:F:211:ILE:O	1:F:214:PHE:HB3	2.15	0.46
1:F:285:PHE:CB	1:F:349:VAL:HG13	2.46	0.46
1:I:168:CYS:O	1:I:169:ARG:C	2.59	0.46
1:L:52:PHE:CE2	1:L:54:GLY:HA2	2.51	0.46
1:L:296:TYR:N	1:L:296:TYR:CD1	2.84	0.46
1:A:20:TYR:O	1:A:21:ILE:HD13	2.16	0.45
1:B:236:LEU:HB2	1:B:239:VAL:HG23	1.99	0.45
1:B:275:ILE:O	1:B:279:VAL:HG23	2.16	0.45
1:B:371:ASN:HB3	1:B:374:VAL:CG1	2.46	0.45
1:C:35:VAL:HG13	1:C:70:LEU:HD21	1.98	0.45
1:C:97:TYR:CD2	1:C:103:PRO:CA	2.99	0.45
1:C:129:LEU:HB3	1:C:207:SER:OG	2.15	0.45
1:C:211:ILE:O	1:C:215:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ASN:N	1:C:290:ASN:ND2	2.64	0.45
1:D:3:LYS:HE2	1:D:4:TYR:CE1	2.51	0.45
1:D:91:ARG:HD2	1:D:91:ARG:C	2.41	0.45
1:E:34:ASN:ND2	1:E:34:ASN:C	2.74	0.45
1:J:224:LYS:HG3	1:K:164:LEU:HD21	1.97	0.45
1:K:370:ARG:O	1:K:371:ASN:ND2	2.49	0.45
1:B:85:GLU:O	1:B:85:GLU:HG3	2.17	0.45
1:C:7:GLU:CD	1:C:7:GLU:H	2.24	0.45
1:C:370:ARG:NH1	1:C:375:MET:HE3	2.30	0.45
1:D:383:ASN:N	1:D:383:ASN:OD1	2.47	0.45
1:F:260:ASP:CG	1:F:263:ALA:HB2	2.41	0.45
1:F:391:THR:OG1	1:F:394:GLU:HG3	2.17	0.45
1:G:91:ARG:HD2	1:G:91:ARG:C	2.41	0.45
1:H:370:ARG:HD2	1:H:371:ASN:H	1.81	0.45
1:K:19:LYS:HD2	1:K:87:GLY:CA	2.40	0.45
1:L:166:GLU:O	1:L:167:ASN:C	2.58	0.45
1:A:300:VAL:HG12	1:A:301:PRO:CD	2.47	0.45
1:A:410:GLY:O	1:A:411:GLU:C	2.58	0.45
1:B:215:LYS:O	1:B:219:LYS:HB2	2.17	0.45
1:C:298:ARG:NH1	1:C:305:ALA:HB2	2.30	0.45
1:D:315:ASN:HD21	1:D:372:ILE:HG12	1.82	0.45
1:E:273:HIS:O	1:E:276:ALA:HB3	2.16	0.45
1:F:304:GLU:O	1:F:317:SER:HB2	2.15	0.45
1:G:361:LYS:HE2	1:G:361:LYS:HB3	1.71	0.45
1:J:437:ARG:HG2	1:J:441:MET:HE2	1.98	0.45
1:K:26:THR:HG22	1:K:27:ASP:O	2.16	0.45
1:K:282:ALA:HA	1:K:285:PHE:CE1	2.50	0.45
1:L:6:ARG:NH2	1:L:47:ASP:OD1	2.48	0.45
1:A:218:VAL:O	1:A:219:LYS:C	2.60	0.45
1:B:42:LEU:O	1:B:46:LEU:HG	2.16	0.45
1:B:156:TYR:HD2	1:C:62:ARG:HD2	1.81	0.45
1:B:303:TYR:O	1:B:304:GLU:HB2	2.16	0.45
1:B:326:ARG:HD3	1:B:326:ARG:HA	1.49	0.45
1:B:426:ASP:OD1	1:B:429:ARG:HD2	2.16	0.45
1:C:160:ALA:HB2	1:C:188:HIS:CG	2.51	0.45
1:C:199:PHE:CZ	1:C:214:PHE:CD1	2.99	0.45
1:D:243:GLY:HA2	1:D:298:ARG:HH12	1.81	0.45
1:E:32:ILE:CD1	1:E:216:LEU:HD12	2.46	0.45
1:E:266:GLN:OE1	1:E:326:ARG:HG3	2.16	0.45
1:E:370:ARG:C	1:E:371:ASN:HD22	2.24	0.45
1:F:248:LEU:HD11	1:F:334:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:ARG:HD2	1:H:156:TYR:HD2	1.81	0.45
1:G:67:ASP:C	1:G:68:MET:HG2	2.41	0.45
1:G:308:TYR:CZ	1:G:372:ILE:HD12	2.52	0.45
1:G:423:ILE:O	1:G:424:GLU:C	2.59	0.45
1:H:298:ARG:NH1	3:H:503:GLN:O	2.49	0.45
1:J:81:PRO:HG2	1:J:82:TRP:H	1.81	0.45
1:J:220:THR:HG22	1:K:164:LEU:HD13	1.98	0.45
1:K:234:LYS:HE3	1:K:297:LYS:O	2.16	0.45
1:A:150:LEU:HD13	1:A:192:PRO:O	2.16	0.45
1:B:162:THR:C	1:B:164:LEU:H	2.24	0.45
1:C:427:MET:HE2	1:C:427:MET:HB3	1.75	0.45
1:F:6:ARG:NH1	1:F:47:ASP:OD1	2.50	0.45
1:G:82:TRP:CG	1:H:164:LEU:HD12	2.51	0.45
1:H:402:ASN:OD1	1:H:402:ASN:C	2.59	0.45
1:K:22:ARG:NH1	1:K:22:ARG:CG	2.80	0.45
1:A:122:LEU:HD21	1:A:359:LYS:HZ3	1.80	0.45
1:B:27:ASP:OD1	1:B:33:LYS:HE3	2.17	0.45
1:B:78:VAL:HG11	1:B:179:MET:HE2	1.98	0.45
1:B:170:ARG:HG3	1:C:20:TYR:CE2	2.52	0.45
1:B:434:PRO:HA	1:B:437:ARG:NH1	2.31	0.45
1:C:39:VAL:C	1:C:41:GLN:H	2.23	0.45
1:C:109:ARG:HG2	1:C:109:ARG:NH2	2.30	0.45
1:G:143:LYS:HE2	1:G:143:LYS:HB2	1.66	0.45
1:G:184:GLU:CG	1:G:200:LYS:HD3	2.36	0.45
1:G:314:GLN:O	1:G:369:ASP:OD2	2.34	0.45
1:I:156:TYR:O	1:I:158:ASP:N	2.50	0.45
1:I:224:LYS:CB	1:J:164:LEU:HD21	2.46	0.45
1:I:281:HIS:CD2	1:I:405:MET:HE3	2.52	0.45
1:I:396:LEU:HD11	1:I:421:LYS:HB3	1.99	0.45
1:J:81:PRO:HG2	1:J:82:TRP:CE3	2.52	0.45
1:K:207:SER:O	1:K:211:ILE:HG13	2.16	0.45
1:K:396:LEU:O	1:K:400:LYS:HD3	2.16	0.45
1:L:115:ILE:O	1:L:118:GLU:HB3	2.17	0.45
1:L:279:VAL:HG11	1:L:365:PRO:HG3	1.99	0.45
1:L:374:VAL:O	1:L:376:SER:N	2.49	0.45
1:C:393:ALA:O	1:C:396:LEU:N	2.49	0.45
1:D:125:SER:C	1:D:126:ASP:OD1	2.59	0.45
1:E:205:VAL:CG1	1:E:206:ARG:N	2.79	0.45
1:E:431:GLN:O	1:K:297:LYS:NZ	2.40	0.45
1:F:21:ILE:HG12	1:F:42:LEU:HD13	1.99	0.45
1:F:167:ASN:HB3	1:F:170:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:PRO:HG3	1:F:341:ALA:HA	1.99	0.45
1:H:21:ILE:HD11	1:H:23:LEU:HD21	1.99	0.45
1:J:368:ILE:HD12	1:J:368:ILE:HA	1.67	0.45
1:L:76:THR:HB	1:L:93:ILE:HG13	1.99	0.45
1:L:347:LEU:HD23	1:L:347:LEU:HA	1.48	0.45
1:B:376:SER:O	1:B:380:ARG:HB2	2.16	0.45
1:C:232:MET:HE3	1:C:235:PRO:HB3	1.99	0.45
1:D:271:ALA:O	1:D:275:ILE:HD13	2.17	0.45
1:E:360:ASN:O	1:E:361:LYS:C	2.60	0.45
1:E:423:ILE:O	1:E:424:GLU:C	2.58	0.45
1:F:116:LEU:O	1:F:119:MET:HB3	2.17	0.45
1:G:239:VAL:HG23	1:G:240:ASN:N	2.32	0.45
1:H:86:LYS:HB2	1:H:86:LYS:NZ	2.32	0.45
1:I:273:HIS:O	1:I:276:ALA:HB3	2.16	0.45
1:J:115:ILE:N	1:J:115:ILE:CD1	2.80	0.45
1:L:371:ASN:O	1:L:375:MET:HE2	2.16	0.45
1:A:244:MET:HE2	1:A:244:MET:HB3	1.73	0.45
1:A:412:HIS:O	1:A:413:LEU:C	2.58	0.45
1:B:405:MET:O	1:B:408:ALA:HB3	2.17	0.45
1:C:407:LYS:NZ	1:C:407:LYS:HB3	2.32	0.45
1:E:80:PHE:HB2	1:E:83:THR:HG23	1.99	0.45
1:F:252:LYS:O	1:F:253:ASN:OD1	2.35	0.45
1:F:281:HIS:O	1:F:284:SER:N	2.48	0.45
1:H:304:GLU:HG2	1:H:335:ARG:NH1	2.28	0.45
1:I:129:LEU:O	1:I:201:TYR:HA	2.17	0.45
1:I:295:SER:O	1:I:299:LEU:HD22	2.17	0.45
1:J:36:GLU:H	1:J:36:GLU:HG2	1.63	0.45
1:J:260:ASP:HB2	1:J:268:SER:CA	2.46	0.45
1:K:250:LEU:C	1:K:251:PHE:HD1	2.25	0.45
1:K:368:ILE:HG12	1:K:372:ILE:CG2	2.47	0.45
1:L:105:GLU:C	1:L:107:ASP:H	2.25	0.45
1:B:5:THR:O	1:B:8:ASP:N	2.50	0.45
1:B:88:LYS:HE2	1:B:88:LYS:HB2	1.60	0.45
1:C:402:ASN:O	1:C:406:VAL:HG23	2.17	0.45
1:D:54:GLY:O	1:D:57:ILE:HD13	2.17	0.45
1:E:272:LYS:HA	1:E:275:ILE:HD12	1.99	0.45
1:G:115:ILE:O	1:G:118:GLU:HB2	2.17	0.45
1:G:264:ASP:O	1:G:265:LEU:HB2	2.17	0.45
1:I:124:PHE:HD2	1:I:252:LYS:HG3	1.82	0.45
1:I:239:VAL:HG23	1:I:240:ASN:H	1.81	0.45
1:K:16:GLU:HB3	1:K:88:LYS:HZ3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:119:MET:HE2	1:K:119:MET:HB3	1.77	0.45
1:L:402:ASN:ND2	1:L:404:VAL:H	2.15	0.45
1:C:311:TRP:CB	1:C:320:ILE:HB	2.47	0.44
1:D:265:LEU:O	1:D:267:LEU:HD22	2.17	0.44
1:G:73:ASP:CG	1:G:76:THR:HG23	2.43	0.44
1:G:141:ASP:OD2	1:G:141:ASP:C	2.60	0.44
1:G:303:TYR:O	1:G:304:GLU:HB2	2.16	0.44
1:G:326:ARG:HD3	1:G:330:THR:OG1	2.16	0.44
1:H:28:ILE:CD1	1:H:413:LEU:HD23	2.43	0.44
1:I:224:LYS:HB2	1:J:164:LEU:HD22	1.99	0.44
1:J:62:ARG:HD2	1:K:156:TYR:CD1	2.53	0.44
1:L:114:ARG:NH2	1:L:115:ILE:HD11	2.33	0.44
1:L:370:ARG:HD2	1:L:370:ARG:HA	1.78	0.44
1:A:435:TRP:CE3	1:G:428:PHE:HD1	2.36	0.44
1:B:285:PHE:CD1	1:B:285:PHE:C	2.95	0.44
1:B:351:LEU:CD2	1:B:355:LEU:HG	2.47	0.44
1:C:163:ASP:HA	1:C:170:ARG:NH1	2.32	0.44
1:D:39:VAL:O	1:D:39:VAL:HG22	2.17	0.44
1:H:137:LEU:HD23	1:H:229:ALA:HA	1.99	0.44
1:H:316:ARG:HD2	1:H:316:ARG:O	2.17	0.44
1:I:26:THR:HG22	1:I:27:ASP:O	2.18	0.44
1:I:35:VAL:HG11	1:I:70:LEU:CD2	2.46	0.44
1:I:252:LYS:O	1:I:253:ASN:HB2	2.17	0.44
1:J:338:ASP:C	1:J:338:ASP:OD2	2.60	0.44
1:J:423:ILE:CG2	1:J:427:MET:HE2	2.46	0.44
1:A:159:LEU:CD1	1:B:32:ILE:HD11	2.47	0.44
1:A:280:LYS:HD3	1:A:281:HIS:CE1	2.53	0.44
1:A:283:THR:HG22	1:A:389:PRO:HD3	1.99	0.44
1:B:177:GLU:HG3	1:C:38:PRO:HB3	1.99	0.44
1:B:261:GLU:HA	1:B:266:GLN:CG	2.47	0.44
1:D:25:PHE:N	1:D:25:PHE:CD2	2.84	0.44
1:D:308:TYR:CE1	1:D:373:TYR:CE1	3.05	0.44
1:E:285:PHE:HB2	1:E:349:VAL:HG13	1.99	0.44
1:E:316:ARG:HD3	1:F:63:ILE:O	2.17	0.44
1:E:369:ASP:O	1:E:370:ARG:HB2	2.17	0.44
1:F:326:ARG:HD3	1:F:326:ARG:HA	1.62	0.44
1:H:308:TYR:HD1	1:H:372:ILE:HD12	1.83	0.44
1:J:371:ASN:ND2	1:J:373:TYR:HB2	2.32	0.44
1:A:224:LYS:NZ	1:A:225:HIS:CE1	2.85	0.44
1:A:327:GLY:O	1:A:330:THR:HB	2.18	0.44
1:B:119:MET:HE2	1:B:120:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ASN:O	1:B:361:LYS:C	2.60	0.44
1:C:96:ILE:HD12	1:C:96:ILE:N	2.32	0.44
1:F:305:ALA:HA	1:F:306:PRO:HD3	1.72	0.44
1:I:338:ASP:OD2	1:I:338:ASP:C	2.59	0.44
1:L:58:GLU:O	1:L:61:VAL:HG23	2.17	0.44
1:L:78:VAL:HG13	1:L:91:ARG:HE	1.81	0.44
1:L:261:GLU:C	1:L:263:ALA:H	2.26	0.44
1:L:338:ASP:C	1:L:338:ASP:OD2	2.60	0.44
1:A:23:LEU:HD13	1:A:70:LEU:HD23	1.99	0.44
1:B:85:GLU:O	1:B:86:LYS:HB2	2.18	0.44
1:B:128:ASN:HA	1:B:202:ALA:O	2.18	0.44
1:C:163:ASP:HA	1:C:170:ARG:HH12	1.82	0.44
1:C:177:GLU:HG2	5:D:624:HOH:O	2.16	0.44
1:E:259:PHE:CE1	1:E:327:GLY:HA2	2.53	0.44
1:F:148:LEU:HD12	1:F:236:LEU:HD23	2.00	0.44
1:H:96:ILE:HD13	1:H:96:ILE:N	2.32	0.44
1:I:20:TYR:OH	1:I:36:GLU:HG3	2.17	0.44
1:I:286:THR:HA	1:I:289:THR:OG1	2.18	0.44
1:I:390:ALA:O	1:I:391:THR:CG2	2.64	0.44
1:J:13:VAL:HG21	1:J:42:LEU:HD21	1.99	0.44
1:J:423:ILE:O	1:J:424:GLU:C	2.60	0.44
1:K:49:LYS:HD3	1:K:49:LYS:HA	1.75	0.44
1:K:416:HIS:O	1:K:417:PHE:C	2.60	0.44
1:L:326:ARG:HA	1:L:326:ARG:HD3	1.67	0.44
1:L:423:ILE:HG13	1:L:424:GLU:H	1.83	0.44
1:A:372:ILE:HG13	1:A:373:TYR:N	2.32	0.44
1:B:201:TYR:C	1:B:201:TYR:CD1	2.95	0.44
1:C:80:PHE:HA	1:C:81:PRO:HD3	1.67	0.44
1:C:162:THR:HB	1:D:220:THR:HG23	1.99	0.44
1:C:258:PHE:HA	1:C:271:ALA:HB2	1.99	0.44
1:D:84:ALA:HA	1:D:87:GLY:C	2.42	0.44
1:D:372:ILE:HD12	1:D:373:TYR:CE1	2.52	0.44
1:E:274:PHE:O	1:E:278:ILE:HG12	2.17	0.44
1:E:314:GLN:NE2	1:F:64:GLU:CB	2.80	0.44
1:F:5:THR:O	1:F:7:GLU:N	2.51	0.44
1:F:71:TYR:CG	1:F:97:TYR:CD1	3.05	0.44
1:F:112:LEU:HA	1:F:112:LEU:HD23	1.70	0.44
1:G:328:ILE:HD12	1:G:328:ILE:H	1.82	0.44
1:G:374:VAL:HG22	1:G:375:MET:H	1.81	0.44
1:H:134:GLU:OE2	3:H:503:GLN:HB2	2.18	0.44
1:H:274:PHE:C	1:H:274:PHE:CD2	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:ASN:OD1	1:I:72:PRO:HD2	2.17	0.44
1:I:63:ILE:HD13	1:I:63:ILE:HA	1.79	0.44
1:K:293:VAL:HG23	1:K:424:GLU:HG2	1.99	0.44
1:L:132:GLU:HB3	1:L:198:ASP:OD1	2.18	0.44
1:C:314:GLN:HE22	1:D:66:SER:HB2	1.82	0.44
1:E:5:THR:O	1:E:6:ARG:C	2.59	0.44
1:E:23:LEU:CB	1:E:70:LEU:HD23	2.47	0.44
1:E:282:ALA:HA	1:E:285:PHE:CZ	2.52	0.44
1:F:80:PHE:HA	1:F:81:PRO:HD3	1.77	0.44
1:F:109:ARG:HD2	1:F:344:TYR:CE2	2.53	0.44
1:F:175:GLU:OE1	1:F:175:GLU:HA	2.17	0.44
1:G:169:ARG:NH2	1:G:195:HIS:ND1	2.65	0.44
1:I:240:ASN:ND2	1:I:303:TYR:CD1	2.83	0.44
1:I:265:LEU:O	1:I:326:ARG:NH1	2.51	0.44
1:I:380:ARG:HB3	1:I:385:ILE:HB	2.00	0.44
1:J:250:LEU:HA	1:J:250:LEU:HD23	1.86	0.44
1:K:236:LEU:CB	1:K:239:VAL:HG23	2.47	0.44
1:K:242:SER:O	1:K:339:PRO:HD2	2.17	0.44
1:L:272:LYS:O	1:L:364:ALA:HB2	2.17	0.44
1:A:372:ILE:C	1:A:374:VAL:H	2.26	0.44
1:C:151:ASN:ND2	1:C:166:GLU:OE2	2.51	0.44
1:C:418:ILE:HD12	1:C:418:ILE:N	2.32	0.44
1:G:78:VAL:CG1	1:G:91:ARG:NE	2.80	0.44
1:G:82:TRP:CH2	1:G:217:VAL:HG22	2.53	0.44
1:I:166:GLU:O	1:I:166:GLU:OE2	2.36	0.44
1:K:214:PHE:O	1:K:218:VAL:HG23	2.17	0.44
1:K:316:ARG:HH21	1:K:370:ARG:HA	1.75	0.44
1:C:53:ASP:OD2	1:C:53:ASP:C	2.61	0.44
1:C:102:THR:OG1	1:C:103:PRO:HD2	2.17	0.44
1:D:6:ARG:NH1	1:D:6:ARG:CG	2.72	0.44
1:E:25:PHE:HE2	1:E:35:VAL:HG12	1.82	0.44
1:F:353:ALA:N	1:F:405:MET:HE1	2.33	0.44
1:G:83:THR:O	1:G:84:ALA:C	2.60	0.44
1:J:435:TRP:CH2	1:J:439:GLN:HG3	2.53	0.44
1:K:220:THR:HG23	1:L:162:THR:HB	1.99	0.44
1:K:308:TYR:CE2	1:K:380:ARG:NH1	2.86	0.44
1:L:84:ALA:HB2	1:L:88:LYS:HD3	1.99	0.44
1:L:234:LYS:HD3	1:L:297:LYS:O	2.17	0.44
1:C:41:GLN:O	1:C:42:LEU:C	2.61	0.43
1:C:162:THR:C	1:C:164:LEU:H	2.25	0.43
1:C:443:GLN:HG3	1:C:443:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:ASN:HD21	1:D:104:PHE:HA	1.83	0.43
1:E:32:ILE:HD11	1:E:216:LEU:CD1	2.48	0.43
1:E:54:GLY:O	1:E:57:ILE:HD12	2.18	0.43
1:E:261:GLU:O	1:E:262:ASN:CB	2.66	0.43
1:F:84:ALA:O	1:F:85:GLU:O	2.35	0.43
1:G:5:THR:O	1:G:6:ARG:C	2.61	0.43
1:G:44:LYS:HE2	1:H:184:GLU:OE1	2.17	0.43
1:G:259:PHE:CD1	1:G:327:GLY:HA2	2.53	0.43
1:H:111:ASN:OD1	1:H:114:ARG:NH1	2.50	0.43
1:H:281:HIS:HE1	1:H:356:ASP:OD2	2.00	0.43
1:H:316:ARG:HB3	1:H:373:TYR:CZ	2.53	0.43
1:H:405:MET:O	1:H:408:ALA:HB3	2.18	0.43
1:I:134:GLU:HG2	1:I:196:GLU:OE1	2.18	0.43
1:I:141:ASP:HB2	1:I:142:GLU:OE1	2.17	0.43
1:I:440:TYR:CD1	1:I:444:TYR:HE2	2.32	0.43
1:K:142:GLU:C	1:K:144:GLY:H	2.26	0.43
1:L:289:THR:OG1	1:L:290:ASN:ND2	2.51	0.43
1:A:64:GLU:HG2	1:F:316:ARG:HA	2.00	0.43
1:A:309:VAL:HG13	1:A:319:LEU:CD2	2.46	0.43
1:C:71:TYR:CD2	1:C:97:TYR:CD1	3.06	0.43
1:D:25:PHE:CZ	1:D:52:PHE:CE2	3.06	0.43
1:F:402:ASN:OD1	1:F:404:VAL:HG13	2.18	0.43
1:G:86:LYS:O	1:G:86:LYS:CG	2.63	0.43
1:H:403:GLU:O	1:H:403:GLU:OE2	2.35	0.43
1:I:68:MET:HB3	1:I:68:MET:HE2	1.66	0.43
1:I:285:PHE:C	1:I:285:PHE:HD1	2.26	0.43
1:I:367:PRO:O	1:I:370:ARG:NH1	2.50	0.43
1:K:84:ALA:N	1:K:85:GLU:OE2	2.52	0.43
1:K:189:GLU:OE2	1:K:190:VAL:HG23	2.18	0.43
1:L:96:ILE:N	1:L:96:ILE:CD1	2.81	0.43
1:L:380:ARG:HG2	1:L:385:ILE:HG21	1.99	0.43
1:A:220:THR:OG1	1:F:162:THR:HG21	2.19	0.43
1:A:443:GLN:HG2	1:A:444:TYR:CD2	2.53	0.43
1:B:311:TRP:HB3	1:B:320:ILE:HB	2.00	0.43
1:F:148:LEU:HD11	1:L:437:ARG:CD	2.45	0.43
1:G:377:LYS:HD3	1:G:380:ARG:CZ	2.49	0.43
1:H:86:LYS:HE2	1:I:175:GLU:OE1	2.19	0.43
1:I:136:PHE:CE2	1:I:194:GLN:HB2	2.53	0.43
1:J:214:PHE:CZ	1:J:218:VAL:HG21	2.53	0.43
1:J:327:GLY:C	1:J:329:SER:N	2.74	0.43
1:K:5:THR:O	1:K:7:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:64:GLU:HB3	1:L:314:GLN:HE21	1.83	0.43
1:C:176:LEU:HD22	1:C:181:PHE:CE1	2.53	0.43
1:C:304:GLU:O	1:C:317:SER:HB2	2.17	0.43
1:C:402:ASN:C	1:C:402:ASN:OD1	2.61	0.43
1:E:412:HIS:CE1	1:E:416:HIS:CE1	3.06	0.43
1:F:357:GLY:HA2	1:F:362:LEU:CD2	2.37	0.43
1:F:359:LYS:HG3	1:F:360:ASN:ND2	2.33	0.43
1:F:417:PHE:O	1:F:421:LYS:HG2	2.17	0.43
1:H:21:ILE:HG12	1:H:37:ILE:CG1	2.49	0.43
1:H:396:LEU:HD11	1:H:421:LYS:HB3	2.00	0.43
1:I:308:TYR:HD1	1:I:372:ILE:HG21	1.84	0.43
1:J:133:PRO:HD2	1:J:197:ILE:O	2.18	0.43
1:K:59:GLY:O	1:K:62:ARG:HG3	2.18	0.43
1:L:377:LYS:O	1:L:381:MET:HG2	2.17	0.43
1:A:27:ASP:C	1:A:27:ASP:OD2	2.61	0.43
1:A:122:LEU:HD12	1:A:355:LEU:HD13	2.01	0.43
1:B:167:ASN:HD21	1:C:22:ARG:HH22	1.66	0.43
1:C:223:ARG:O	1:C:224:LYS:C	2.61	0.43
1:F:221:ILE:O	1:F:224:LYS:HB3	2.19	0.43
1:F:371:ASN:OD1	1:F:373:TYR:HB2	2.19	0.43
1:H:305:ALA:HA	1:H:306:PRO:HD3	1.80	0.43
1:J:160:ALA:HB2	1:J:188:HIS:HB2	1.99	0.43
1:J:216:LEU:HD23	1:J:216:LEU:C	2.43	0.43
1:J:342:ASN:C	1:J:342:ASN:OD1	2.61	0.43
1:K:23:LEU:HB3	1:K:70:LEU:HD22	2.01	0.43
1:B:135:PHE:CZ	1:B:195:HIS:HB2	2.53	0.43
1:B:166:GLU:HG2	1:B:168:CYS:N	2.32	0.43
1:C:73:ASP:C	1:C:73:ASP:OD1	2.61	0.43
1:D:370:ARG:HH11	1:D:370:ARG:CB	2.12	0.43
1:K:98:ASN:HB3	1:K:99:PRO:HD2	2.00	0.43
1:K:305:ALA:HA	1:K:306:PRO:HD3	1.74	0.43
1:A:345:LEU:HD22	1:A:409:LEU:HD22	2.01	0.43
1:C:85:GLU:O	1:C:86:LYS:HB2	2.18	0.43
1:C:201:TYR:CD1	1:C:201:TYR:C	2.97	0.43
1:D:371:ASN:HD21	1:D:374:VAL:HG22	1.84	0.43
1:F:197:ILE:HD12	1:F:214:PHE:CE1	2.54	0.43
1:F:213:THR:O	1:F:216:LEU:HB3	2.19	0.43
1:G:308:TYR:CD2	1:G:380:ARG:NH1	2.87	0.43
1:H:269:GLU:HA	1:H:269:GLU:OE2	2.19	0.43
1:J:289:THR:O	1:J:341:ALA:HB2	2.19	0.43
1:J:359:LYS:CB	1:J:359:LYS:HZ2	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:134:GLU:HG2	1:K:196:GLU:HB2	2.01	0.43
1:L:176:LEU:C	1:L:181:PHE:HB2	2.43	0.43
1:A:11:LYS:HE2	1:A:15:GLU:OE1	2.19	0.43
1:A:383:ASN:C	1:A:385:ILE:H	2.26	0.43
1:E:51:MET:HE3	1:E:51:MET:HB3	1.77	0.43
1:E:85:GLU:OE2	1:E:85:GLU:CA	2.52	0.43
1:G:296:TYR:CD1	1:G:296:TYR:N	2.86	0.43
1:G:324:ALA:O	1:G:325:SER:C	2.62	0.43
1:G:396:LEU:HD11	1:G:421:LYS:HB3	2.00	0.43
1:H:239:VAL:HG23	1:H:240:ASN:N	2.34	0.43
1:H:280:LYS:HD3	1:H:281:HIS:NE2	2.33	0.43
1:H:326:ARG:HA	1:H:326:ARG:HD3	1.38	0.43
1:H:368:ILE:HD13	1:H:368:ILE:N	2.33	0.43
1:H:380:ARG:HD2	1:H:385:ILE:HG21	2.01	0.43
1:H:396:LEU:HD22	1:H:418:ILE:CD1	2.48	0.43
1:I:107:ASP:OD1	1:I:107:ASP:C	2.61	0.43
1:I:380:ARG:NH1	1:I:387:ASP:OD1	2.52	0.43
1:K:112:LEU:HD23	1:K:112:LEU:HA	1.72	0.43
1:K:372:ILE:O	1:K:372:ILE:HG12	2.18	0.43
1:L:409:LEU:HD12	1:L:413:LEU:HB3	2.00	0.43
1:A:80:PHE:HB3	1:A:82:TRP:CE3	2.54	0.43
1:A:231:PHE:O	1:A:339:PRO:HG2	2.18	0.43
1:B:27:ASP:C	1:B:27:ASP:OD2	2.62	0.43
1:D:48:ASN:HB3	1:D:71:TYR:CE1	2.53	0.43
1:D:78:VAL:HG12	1:D:79:ILE:N	2.33	0.43
1:D:191:ALA:HB2	1:D:240:ASN:HB2	2.00	0.43
1:F:140:LEU:HD12	1:F:226:GLY:C	2.44	0.43
1:G:62:ARG:C	1:G:63:ILE:HG12	2.44	0.43
1:G:167:ASN:ND2	1:L:22:ARG:HH22	2.11	0.43
1:I:62:ARG:NE	1:J:156:TYR:CE2	2.87	0.43
1:I:82:TRP:HB2	1:I:83:THR:H	1.48	0.43
1:I:317:SER:O	1:I:373:TYR:OH	2.36	0.43
1:I:402:ASN:O	1:I:406:VAL:HG23	2.19	0.43
1:K:83:THR:O	1:K:84:ALA:CB	2.65	0.43
1:D:347:LEU:HD23	1:D:347:LEU:HA	1.66	0.43
1:E:127:PHE:CE2	1:E:351:LEU:HG	2.53	0.43
1:F:409:LEU:HA	1:F:409:LEU:HD23	1.61	0.43
1:G:48:ASN:OD1	1:G:48:ASN:N	2.52	0.43
1:H:63:ILE:HA	1:H:63:ILE:HD13	1.77	0.43
1:H:73:ASP:O	1:H:76:THR:OG1	2.33	0.43
1:H:281:HIS:CE1	1:H:356:ASP:OD2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:315:ASN:CG	1:H:316:ARG:N	2.77	0.43
1:J:338:ASP:CB	1:J:339:PRO:CD	2.96	0.43
1:K:28:ILE:HD11	1:K:417:PHE:CB	2.49	0.43
1:K:37:ILE:HD12	1:K:41:GLN:CB	2.47	0.43
1:K:57:ILE:HD11	1:K:96:ILE:HG13	2.00	0.43
1:K:62:ARG:HD2	1:L:156:TYR:CD2	2.54	0.43
1:A:265:LEU:O	1:A:326:ARG:NH1	2.51	0.42
1:D:308:TYR:HE1	1:D:373:TYR:CD1	2.37	0.42
1:F:310:ALA:HB1	1:F:368:ILE:HG12	2.01	0.42
1:G:317:SER:N	1:G:318:PRO:CD	2.81	0.42
1:G:421:LYS:HA	1:G:421:LYS:HD3	1.81	0.42
1:H:150:LEU:HD13	1:H:192:PRO:O	2.18	0.42
1:I:85:GLU:O	1:I:86:LYS:CB	2.48	0.42
1:I:232:MET:HE2	1:I:235:PRO:HA	2.00	0.42
1:J:191:ALA:H	1:J:194:GLN:HE21	1.67	0.42
1:J:370:ARG:HB3	1:J:371:ASN:H	1.55	0.42
1:L:291:PRO:HG3	1:L:341:ALA:HA	2.00	0.42
1:A:251:PHE:CD1	1:A:256:ASN:HA	2.54	0.42
1:B:51:MET:HE2	1:B:69:TYR:CE1	2.55	0.42
1:B:317:SER:OG	1:B:373:TYR:CZ	2.72	0.42
1:D:68:MET:HE2	1:D:68:MET:HB3	1.71	0.42
1:D:375:MET:HB2	1:D:379:GLU:HB3	2.00	0.42
1:E:160:ALA:O	1:E:161:PRO:C	2.62	0.42
1:E:297:LYS:HA	1:E:297:LYS:HD3	1.81	0.42
1:E:396:LEU:HD11	1:E:421:LYS:HB3	2.01	0.42
1:F:300:VAL:CG1	1:F:301:PRO:HD2	2.47	0.42
1:F:377:LYS:O	1:F:378:GLU:C	2.62	0.42
1:F:423:ILE:HG13	1:F:424:GLU:N	2.33	0.42
1:H:221:ILE:O	1:H:224:LYS:HB3	2.20	0.42
1:H:345:LEU:HD22	1:H:409:LEU:HD22	2.01	0.42
1:I:124:PHE:HB3	1:I:250:LEU:HD22	2.00	0.42
1:J:437:ARG:O	1:J:441:MET:HB3	2.19	0.42
1:A:376:SER:O	1:A:377:LYS:C	2.62	0.42
1:B:73:ASP:C	1:B:73:ASP:OD2	2.62	0.42
1:C:71:TYR:CD1	1:C:97:TYR:HD1	2.37	0.42
1:C:109:ARG:HD2	1:C:344:TYR:CZ	2.53	0.42
1:D:51:MET:HE3	1:D:51:MET:HB3	1.58	0.42
1:G:12:LEU:HA	1:G:12:LEU:HD23	1.66	0.42
1:G:85:GLU:O	1:G:86:LYS:HB2	2.19	0.42
1:G:131:PRO:HG2	1:G:199:PHE:HE1	1.83	0.42
1:G:258:PHE:HB3	1:G:271:ALA:HB2	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:311:TRP:CZ2	1:H:367:PRO:HD3	2.55	0.42
1:H:385:ILE:N	1:H:385:ILE:CD1	2.81	0.42
1:K:42:LEU:O	1:K:45:ALA:HB3	2.19	0.42
1:L:16:GLU:HG2	1:L:79:ILE:HD13	2.01	0.42
1:A:305:ALA:HA	1:A:306:PRO:HD3	1.91	0.42
1:B:28:ILE:O	1:B:28:ILE:HG13	2.18	0.42
1:B:162:THR:CG2	1:C:216:LEU:HD11	2.49	0.42
1:B:183:ILE:N	1:B:183:ILE:CD1	2.82	0.42
1:B:291:PRO:C	1:B:421:LYS:HZ2	2.27	0.42
1:B:291:PRO:HB2	1:B:421:LYS:NZ	2.34	0.42
1:B:426:ASP:HA	1:B:429:ARG:HG3	2.01	0.42
1:B:436:GLU:OE2	1:H:297:LYS:HD3	2.20	0.42
1:C:275:ILE:O	1:C:279:VAL:HG23	2.20	0.42
1:C:371:ASN:ND2	5:D:621:HOH:O	2.45	0.42
1:D:129:LEU:O	1:D:201:TYR:HA	2.20	0.42
1:D:169:ARG:HD2	1:D:186:SER:HB2	2.01	0.42
1:F:29:LEU:HD21	1:F:421:LYS:NZ	2.33	0.42
1:G:34:ASN:ND2	1:G:34:ASN:C	2.78	0.42
1:G:129:LEU:C	1:G:129:LEU:CD2	2.92	0.42
1:G:258:PHE:HA	1:G:268:SER:OG	2.19	0.42
1:H:167:ASN:HB3	1:H:170:ARG:NH2	2.34	0.42
1:H:245:HIS:CE1	4:H:504:PO4:O3	2.73	0.42
1:H:308:TYR:CD1	1:H:372:ILE:HG13	2.54	0.42
1:I:342:ASN:O	1:I:343:PRO:C	2.62	0.42
1:K:183:ILE:N	1:K:183:ILE:HD13	2.35	0.42
1:K:299:LEU:HD12	1:K:299:LEU:HA	1.93	0.42
1:L:168:CYS:SG	1:L:227:LEU:HD12	2.60	0.42
1:A:70:LEU:HG	1:A:94:CYS:SG	2.60	0.42
1:A:119:MET:HE1	1:A:127:PHE:HB2	1.99	0.42
1:A:231:PHE:HB2	1:G:444:TYR:OXT	2.20	0.42
1:A:371:ASN:OD1	1:A:371:ASN:O	2.37	0.42
1:C:153:LYS:H	1:C:153:LYS:HG2	1.63	0.42
1:C:374:VAL:HG22	1:C:375:MET:N	2.34	0.42
1:D:129:LEU:HD22	1:D:130:GLY:N	2.34	0.42
1:D:376:SER:O	1:D:377:LYS:C	2.62	0.42
1:G:129:LEU:HD23	1:G:130:GLY:C	2.45	0.42
1:G:328:ILE:H	1:G:328:ILE:CD1	2.33	0.42
1:J:351:LEU:HD22	1:J:355:LEU:HG	2.00	0.42
1:K:380:ARG:CG	1:K:385:ILE:HG21	2.49	0.42
1:L:239:VAL:HG23	1:L:240:ASN:N	2.34	0.42
1:A:24:GLN:HB3	1:A:93:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PHE:CD1	1:A:60:PHE:C	2.97	0.42
1:A:119:MET:HB2	1:A:355:LEU:HD11	2.02	0.42
1:A:164:LEU:HB3	1:B:220:THR:HG23	2.02	0.42
1:B:129:LEU:HD13	1:B:131:PRO:HD3	2.01	0.42
1:B:163:ASP:HA	1:B:170:ARG:NH1	2.34	0.42
1:B:203:GLY:O	1:B:204:ALA:C	2.62	0.42
1:B:213:THR:O	1:B:216:LEU:HB3	2.18	0.42
1:B:236:LEU:HD12	1:B:239:VAL:HG21	2.02	0.42
1:C:240:ASN:ND2	1:C:303:TYR:HD1	2.17	0.42
1:D:12:LEU:HA	1:D:12:LEU:HD23	1.84	0.42
1:D:80:PHE:CZ	1:D:91:ARG:HB3	2.54	0.42
1:E:200:LYS:O	1:E:201:TYR:C	2.62	0.42
1:F:399:PHE:HZ	1:F:409:LEU:HD12	1.84	0.42
1:I:119:MET:HG2	1:I:120:GLU:N	2.33	0.42
1:I:224:LYS:HE3	1:I:225:HIS:CD2	2.55	0.42
1:J:260:ASP:O	1:J:261:GLU:C	2.62	0.42
1:J:370:ARG:HD3	1:J:370:ARG:HA	1.72	0.42
1:K:97:TYR:CE2	1:K:103:PRO:HG3	2.55	0.42
1:A:33:LYS:HE2	1:F:158:ASP:OD2	2.19	0.42
1:C:216:LEU:O	1:C:217:VAL:C	2.62	0.42
1:C:251:PHE:HE1	1:C:256:ASN:ND2	2.18	0.42
1:F:234:LYS:HE3	1:F:239:VAL:O	2.19	0.42
1:F:412:HIS:CE1	1:F:416:HIS:CE1	3.07	0.42
1:G:186:SER:O	1:L:36:GLU:HG2	2.19	0.42
1:G:338:ASP:HB2	1:G:339:PRO:CD	2.45	0.42
1:G:368:ILE:O	1:G:369:ASP:CB	2.67	0.42
1:H:176:LEU:HD22	1:H:181:PHE:CD1	2.54	0.42
1:J:311:TRP:HB3	1:J:320:ILE:HB	2.01	0.42
1:J:380:ARG:HG2	1:J:385:ILE:HG21	2.00	0.42
1:K:45:ALA:C	1:K:46:LEU:O	2.58	0.42
1:K:168:CYS:O	1:K:169:ARG:C	2.63	0.42
1:K:316:ARG:NH2	1:K:370:ARG:NH1	2.68	0.42
1:B:162:THR:HG22	1:B:163:ASP:N	2.34	0.42
1:B:199:PHE:HZ	1:B:214:PHE:CD1	2.37	0.42
1:B:258:PHE:HZ	1:B:274:PHE:CD1	2.38	0.42
1:C:17:ASN:ND2	1:C:87:GLY:HA2	2.35	0.42
1:D:160:ALA:CB	1:D:161:PRO:CD	2.94	0.42
1:D:423:ILE:O	1:D:427:MET:HG3	2.19	0.42
1:E:21:ILE:N	1:E:21:ILE:HD12	2.34	0.42
1:E:25:PHE:CD2	1:E:25:PHE:N	2.88	0.42
1:F:282:ALA:HA	1:F:285:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:TRP:CD1	1:H:164:LEU:HD12	2.54	0.42
1:H:100:ASP:C	1:H:100:ASP:OD1	2.62	0.42
1:H:250:LEU:C	1:H:251:PHE:HD1	2.27	0.42
1:J:201:TYR:C	1:J:201:TYR:CD2	2.96	0.42
1:K:27:ASP:HB3	1:K:33:LYS:HE3	2.01	0.42
1:K:33:LYS:O	1:K:34:ASN:HB3	2.19	0.42
1:L:60:PHE:HE1	1:L:423:ILE:HG12	1.85	0.42
1:L:116:LEU:HD23	1:L:116:LEU:HA	1.85	0.42
1:B:379:GLU:O	1:B:383:ASN:ND2	2.53	0.42
1:D:98:ASN:ND2	1:D:104:PHE:HA	2.34	0.42
1:D:435:TRP:CH2	1:J:428:PHE:HB2	2.55	0.42
1:E:274:PHE:C	1:E:274:PHE:CD2	2.97	0.42
1:F:98:ASN:HB2	1:F:102:THR:HG23	2.02	0.42
1:G:377:LYS:NZ	1:G:380:ARG:NH2	2.65	0.42
1:J:25:PHE:CE1	1:J:33:LYS:HB2	2.55	0.42
1:J:285:PHE:HB2	1:J:349:VAL:CG1	2.50	0.42
1:J:300:VAL:HG13	1:J:301:PRO:CD	2.50	0.42
1:K:161:PRO:O	1:K:162:THR:OG1	2.36	0.42
1:K:261:GLU:HA	1:K:266:GLN:HE21	1.82	0.42
1:L:418:ILE:HD13	1:L:418:ILE:N	2.34	0.42
1:A:413:LEU:HD23	1:A:413:LEU:HA	1.78	0.42
1:B:115:ILE:N	1:B:115:ILE:HD12	2.35	0.42
1:D:305:ALA:HA	1:D:306:PRO:HD3	1.90	0.42
1:F:311:TRP:CB	1:F:320:ILE:HB	2.50	0.42
1:I:28:ILE:O	1:I:28:ILE:HD13	2.19	0.42
1:I:138:PHE:CE2	1:I:150:LEU:HD23	2.55	0.42
1:J:85:GLU:C	1:J:85:GLU:OE1	2.63	0.42
1:L:250:LEU:C	1:L:251:PHE:HD1	2.28	0.42
1:L:421:LYS:HA	1:L:421:LYS:HD3	1.86	0.42
1:B:14:LYS:HE3	1:B:14:LYS:HB2	1.70	0.41
1:B:186:SER:OG	1:C:36:GLU:HG3	2.20	0.41
1:B:338:ASP:OD2	1:B:338:ASP:C	2.63	0.41
1:B:440:TYR:OH	1:H:293:VAL:HB	2.19	0.41
1:C:58:GLU:O	1:C:61:VAL:HG22	2.20	0.41
1:E:142:GLU:CD	1:E:142:GLU:H	2.27	0.41
1:E:370:ARG:C	1:E:371:ASN:ND2	2.78	0.41
1:F:231:PHE:HA	5:F:601:HOH:O	2.20	0.41
1:F:372:ILE:CG2	1:F:380:ARG:HD2	2.50	0.41
1:G:13:VAL:HG21	1:G:42:LEU:HD21	2.02	0.41
1:G:36:GLU:OE1	1:H:186:SER:OG	2.35	0.41
1:G:112:LEU:HD11	1:G:204:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:PHE:HZ	1:H:412:HIS:CE1	2.37	0.41
1:H:245:HIS:CD2	1:H:335:ARG:HA	2.55	0.41
1:H:252:LYS:O	1:H:253:ASN:HB2	2.20	0.41
1:H:315:ASN:CG	1:H:316:ARG:H	2.28	0.41
1:H:403:GLU:HG3	1:H:407:LYS:HE3	2.01	0.41
1:I:160:ALA:HB1	1:I:161:PRO:CD	2.39	0.41
1:J:16:GLU:O	1:J:88:LYS:HG3	2.20	0.41
1:J:28:ILE:HD12	1:J:29:LEU:H	1.85	0.41
1:J:62:ARG:HD2	1:K:156:TYR:HD1	1.84	0.41
1:J:274:PHE:CE2	1:J:278:ILE:CD1	3.03	0.41
1:K:51:MET:HE2	1:K:51:MET:HB3	1.93	0.41
1:K:114:ARG:NH2	1:K:407:LYS:O	2.43	0.41
1:K:370:ARG:NH2	1:K:371:ASN:O	2.53	0.41
1:L:98:ASN:HB3	1:L:99:PRO:HD2	2.02	0.41
1:L:182:GLU:CG	1:L:200:LYS:HD2	2.41	0.41
1:L:189:GLU:O	1:L:190:VAL:C	2.63	0.41
1:L:244:MET:HE2	1:L:244:MET:HB3	1.84	0.41
1:L:379:GLU:O	1:L:383:ASN:OD1	2.38	0.41
1:L:418:ILE:HD12	1:L:418:ILE:HA	1.84	0.41
1:B:83:THR:O	1:B:84:ALA:CB	2.67	0.41
1:B:215:LYS:O	1:B:219:LYS:HD3	2.21	0.41
1:B:380:ARG:HG3	1:B:385:ILE:HB	2.02	0.41
1:B:381:MET:HE1	1:B:386:VAL:HA	2.01	0.41
1:C:285:PHE:C	1:C:285:PHE:HD1	2.28	0.41
1:D:127:PHE:CD2	1:D:351:LEU:HG	2.55	0.41
1:D:435:TRP:O	1:D:439:GLN:HG2	2.20	0.41
1:F:116:LEU:HD23	1:F:116:LEU:HA	1.83	0.41
1:I:328:ILE:H	1:I:328:ILE:HG13	1.40	0.41
1:J:392:LEU:O	1:J:396:LEU:HG	2.20	0.41
1:L:34:ASN:C	1:L:34:ASN:HD22	2.26	0.41
1:A:162:THR:O	1:A:164:LEU:N	2.54	0.41
1:A:328:ILE:H	1:A:328:ILE:HG13	1.61	0.41
1:C:46:LEU:HD23	1:C:46:LEU:HA	1.88	0.41
1:C:177:GLU:C	1:C:179:MET:H	2.27	0.41
1:D:281:HIS:CD2	1:D:402:ASN:HD21	2.30	0.41
1:E:162:THR:C	1:E:164:LEU:H	2.28	0.41
1:E:203:GLY:O	1:E:204:ALA:C	2.63	0.41
1:F:133:PRO:HG2	1:F:199:PHE:HE1	1.84	0.41
1:G:214:PHE:CZ	1:G:218:VAL:HG21	2.55	0.41
1:G:260:ASP:OD1	1:G:260:ASP:C	2.63	0.41
1:H:381:MET:C	1:H:383:ASN:N	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:78:VAL:CG1	1:J:79:ILE:N	2.83	0.41
1:K:145:GLU:HA	1:K:145:GLU:OE2	2.20	0.41
1:K:272:LYS:HA	1:K:275:ILE:HD12	2.02	0.41
1:K:304:GLU:O	1:K:335:ARG:NH1	2.53	0.41
1:K:382:GLU:C	1:K:383:ASN:OD1	2.64	0.41
1:A:381:MET:C	1:A:383:ASN:H	2.29	0.41
1:B:129:LEU:CD2	1:B:248:LEU:HD23	2.46	0.41
1:B:184:GLU:OE2	1:B:200:LYS:HD2	2.19	0.41
1:B:381:MET:O	1:B:384:GLY:N	2.35	0.41
1:C:209:ASP:OD2	1:C:344:TYR:OH	2.35	0.41
1:D:314:GLN:NE2	1:E:64:GLU:HB3	2.35	0.41
1:E:25:PHE:CE1	1:E:33:LYS:HB2	2.55	0.41
1:G:145:GLU:HA	1:G:146:PRO:HD3	1.91	0.41
1:G:162:THR:C	1:G:164:LEU:H	2.27	0.41
1:G:289:THR:HB	1:G:337:VAL:HG22	2.01	0.41
1:H:350:LEU:HD23	1:H:350:LEU:HA	1.92	0.41
1:L:115:ILE:HG22	1:L:351:LEU:HD13	2.02	0.41
1:L:154:GLY:C	1:L:188:HIS:CE1	2.99	0.41
1:A:162:THR:C	1:A:164:LEU:N	2.79	0.41
1:A:368:ILE:HD12	1:A:368:ILE:HA	1.60	0.41
1:B:91:ARG:HD2	1:B:92:PHE:N	2.35	0.41
1:B:129:LEU:CD1	1:B:131:PRO:HD3	2.50	0.41
1:B:258:PHE:HA	1:B:271:ALA:HB2	2.03	0.41
1:B:309:VAL:CG2	1:B:386:VAL:HG13	2.51	0.41
1:B:372:ILE:HD12	1:B:372:ILE:HA	1.76	0.41
1:C:97:TYR:CE2	1:C:103:PRO:HB3	2.54	0.41
1:C:119:MET:HG2	1:C:124:PHE:HB2	2.01	0.41
1:C:418:ILE:O	1:C:422:GLU:HG3	2.20	0.41
1:F:252:LYS:O	1:F:253:ASN:CG	2.64	0.41
1:H:160:ALA:CB	1:H:161:PRO:HD2	2.24	0.41
1:I:124:PHE:CB	1:I:250:LEU:HD22	2.50	0.41
1:J:135:PHE:CZ	1:J:195:HIS:HB2	2.56	0.41
1:L:402:ASN:ND2	1:L:404:VAL:N	2.69	0.41
1:B:71:TYR:CD1	1:B:97:TYR:CD1	3.08	0.41
1:C:273:HIS:CE1	1:C:361:LYS:HA	2.56	0.41
1:C:281:HIS:CE1	1:C:356:ASP:OD2	2.73	0.41
1:D:244:MET:O	1:D:244:MET:HG2	2.20	0.41
1:E:11:LYS:O	1:E:15:GLU:CG	2.68	0.41
1:E:164:LEU:HD23	1:E:164:LEU:HA	1.82	0.41
1:F:89:VAL:HG12	1:F:90:ALA:N	2.35	0.41
1:F:139:LYS:HD2	1:F:149:GLU:CD	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:SER:O	1:F:187:HIS:HB3	2.21	0.41
1:F:265:LEU:HD23	1:F:265:LEU:HA	1.85	0.41
1:G:174:LEU:HD12	1:G:174:LEU:HA	1.70	0.41
1:G:176:LEU:O	1:G:181:PHE:HB2	2.20	0.41
1:G:258:PHE:CB	1:G:271:ALA:CB	2.90	0.41
1:G:393:ALA:HB2	1:G:425:TRP:CE2	2.55	0.41
1:H:135:PHE:CZ	1:H:195:HIS:HB2	2.55	0.41
1:H:370:ARG:HD2	1:H:371:ASN:O	2.20	0.41
1:I:175:GLU:HG3	1:I:221:ILE:HD11	2.02	0.41
1:K:120:GLU:HA	1:K:124:PHE:O	2.20	0.41
1:K:363:GLU:OE2	1:K:363:GLU:CA	2.69	0.41
1:L:107:ASP:OD1	1:L:107:ASP:C	2.63	0.41
1:L:368:ILE:HG21	1:L:372:ILE:CG2	2.51	0.41
1:A:119:MET:HA	1:A:355:LEU:HD11	2.03	0.41
1:A:303:TYR:O	1:A:304:GLU:HB2	2.21	0.41
1:A:370:ARG:HD2	1:B:64:GLU:OE2	2.21	0.41
1:B:290:ASN:HB3	1:B:295:SER:HB3	2.03	0.41
1:E:274:PHE:CE2	1:E:278:ILE:HD11	2.55	0.41
1:F:26:THR:HG22	1:F:27:ASP:O	2.19	0.41
1:F:111:ASN:O	1:F:112:LEU:C	2.61	0.41
1:F:260:ASP:OD1	1:F:260:ASP:C	2.64	0.41
1:G:48:ASN:ND2	1:G:71:TYR:CD2	2.89	0.41
1:G:315:ASN:CG	1:G:316:ARG:N	2.79	0.41
1:H:23:LEU:HD11	1:H:37:ILE:HD13	2.01	0.41
1:I:21:ILE:HG12	1:I:42:LEU:HD13	2.02	0.41
1:I:390:ALA:C	1:I:391:THR:CG2	2.94	0.41
1:K:58:GLU:O	1:K:61:VAL:HG22	2.20	0.41
1:L:166:GLU:HG3	1:L:167:ASN:N	2.34	0.41
1:L:225:HIS:O	1:L:227:LEU:HG	2.21	0.41
1:L:315:ASN:CG	1:L:316:ARG:N	2.78	0.41
1:A:120:GLU:C	1:A:122:LEU:H	2.29	0.41
1:B:111:ASN:OD1	1:B:114:ARG:NH1	2.54	0.41
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.92	0.41
1:B:274:PHE:CE2	1:B:278:ILE:HD11	2.56	0.41
1:D:388:LEU:HD23	1:D:388:LEU:HA	1.93	0.41
1:E:82:TRP:O	1:E:83:THR:C	2.64	0.41
1:F:82:TRP:CD1	1:F:83:THR:H	2.38	0.41
1:F:97:TYR:CD2	1:F:103:PRO:HA	2.56	0.41
1:F:443:GLN:NE2	5:F:606:HOH:O	2.34	0.41
1:G:51:MET:CE	1:G:67:ASP:HB3	2.51	0.41
1:G:265:LEU:O	1:G:326:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:443:GLN:HB3	1:G:444:TYR:CD2	2.55	0.41
1:H:140:LEU:HD23	1:H:140:LEU:HA	1.81	0.41
1:I:151:ASN:HD22	1:I:166:GLU:CD	2.27	0.41
1:I:351:LEU:O	1:I:355:LEU:HG	2.20	0.41
1:I:414:PHE:O	1:I:418:ILE:HG13	2.21	0.41
1:J:111:ASN:OD1	1:J:114:ARG:NH1	2.54	0.41
1:J:214:PHE:O	1:J:215:LYS:C	2.63	0.41
1:J:272:LYS:HB3	1:J:272:LYS:HE2	1.77	0.41
1:K:55:SER:O	1:K:62:ARG:HG2	2.20	0.41
1:K:70:LEU:C	1:K:71:TYR:HD1	2.29	0.41
1:K:194:GLN:C	1:K:195:HIS:CG	2.99	0.41
1:L:7:GLU:H	1:L:7:GLU:CD	2.28	0.41
1:A:73:ASP:OD1	1:A:73:ASP:C	2.64	0.41
1:A:83:THR:HA	1:A:85:GLU:OE2	2.21	0.41
1:A:133:PRO:CA	1:A:244:MET:HG3	2.51	0.41
1:A:160:ALA:CB	1:A:188:HIS:CD2	3.03	0.41
1:A:251:PHE:CE1	1:A:256:ASN:HA	2.56	0.41
1:A:369:ASP:O	1:A:371:ASN:N	2.54	0.41
1:B:100:ASP:OD1	1:B:100:ASP:C	2.64	0.41
1:B:160:ALA:O	1:B:161:PRO:C	2.63	0.41
1:B:164:LEU:CD2	1:C:82:TRP:HB3	2.50	0.41
1:B:172:ILE:HG13	1:B:221:ILE:HG21	2.02	0.41
1:B:278:ILE:HG23	1:B:285:PHE:CZ	2.56	0.41
1:C:163:ASP:CG	1:D:22:ARG:HH21	2.29	0.41
1:C:326:ARG:HA	1:C:330:THR:OG1	2.20	0.41
1:C:435:TRP:CD1	1:I:431:GLN:HG2	2.56	0.41
1:D:205:VAL:HG23	1:D:206:ARG:H	1.83	0.41
1:D:329:SER:O	1:D:331:ARG:NH2	2.46	0.41
1:E:28:ILE:HD11	1:E:417:PHE:HB2	2.02	0.41
1:E:91:ARG:HD2	1:E:92:PHE:N	2.35	0.41
1:E:169:ARG:NE	1:E:195:HIS:HD2	2.19	0.41
1:F:5:THR:C	1:F:7:GLU:N	2.79	0.41
1:F:168:CYS:O	1:F:172:ILE:CG1	2.68	0.41
1:F:184:GLU:O	1:F:185:ALA:HB2	2.20	0.41
1:F:197:ILE:HD12	1:F:214:PHE:HE1	1.86	0.41
1:F:231:PHE:O	1:F:339:PRO:HG2	2.21	0.41
1:F:375:MET:HA	1:F:379:GLU:HG3	2.03	0.41
1:G:23:LEU:HD13	1:G:70:LEU:HD23	2.03	0.41
1:G:127:PHE:HE2	1:G:347:LEU:HD12	1.86	0.41
1:G:146:PRO:HG3	1:G:228:HIS:CD2	2.56	0.41
1:H:27:ASP:OD2	1:H:31:THR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:245:HIS:HA	1:H:334:VAL:O	2.21	0.41
1:H:247:ASN:OD1	1:H:333:GLU:HB2	2.21	0.41
1:I:115:ILE:O	1:I:118:GLU:HB2	2.21	0.41
1:I:141:ASP:OD2	1:I:143:LYS:N	2.54	0.41
1:I:172:ILE:O	1:I:176:LEU:HG	2.20	0.41
1:I:218:VAL:O	1:I:219:LYS:C	2.64	0.41
1:I:289:THR:OG1	1:I:290:ASN:ND2	2.54	0.41
1:I:351:LEU:HD22	1:I:351:LEU:O	2.21	0.41
1:J:79:ILE:HG12	1:J:90:ALA:HB2	2.02	0.41
1:J:168:CYS:O	1:J:169:ARG:C	2.64	0.41
1:J:296:TYR:HB3	1:J:390:ALA:O	2.21	0.41
1:K:8:ASP:O	1:K:12:LEU:HB2	2.21	0.41
1:K:32:ILE:C	1:K:32:ILE:HD12	2.45	0.41
1:K:316:ARG:HH22	1:K:370:ARG:CZ	2.33	0.41
1:L:13:VAL:HG13	1:L:18:VAL:HB	2.01	0.41
1:L:29:LEU:C	1:L:31:THR:N	2.76	0.41
1:L:129:LEU:HD22	1:L:131:PRO:HD3	2.02	0.41
1:L:374:VAL:O	1:L:375:MET:C	2.64	0.41
1:A:252:LYS:NZ	1:A:252:LYS:HB2	2.36	0.41
1:B:52:PHE:CE1	1:B:70:LEU:CD1	3.03	0.41
1:D:160:ALA:HB2	1:D:188:HIS:CG	2.53	0.41
1:E:316:ARG:N	1:E:370:ARG:NH1	2.64	0.41
1:F:127:PHE:CZ	1:F:248:LEU:HD22	2.56	0.41
1:G:88:LYS:HZ3	1:G:88:LYS:HG3	1.72	0.41
1:G:360:ASN:O	1:G:361:LYS:C	2.64	0.41
1:H:421:LYS:HA	1:H:421:LYS:HD3	1.75	0.41
1:I:33:LYS:HE3	1:J:156:TYR:O	2.21	0.41
1:I:100:ASP:HB2	1:I:101:GLY:H	1.72	0.41
1:I:133:PRO:CA	1:I:244:MET:HG3	2.50	0.41
1:I:309:VAL:HG13	1:I:319:LEU:HD22	2.03	0.41
1:K:37:ILE:HD11	1:K:45:ALA:HB2	2.03	0.41
1:K:73:ASP:OD1	1:K:73:ASP:C	2.64	0.41
1:K:316:ARG:NH2	1:K:370:ARG:CD	2.82	0.41
1:K:375:MET:HE2	1:K:375:MET:HB3	1.92	0.41
1:L:119:MET:HA	1:L:355:LEU:CD1	2.51	0.41
1:L:380:ARG:O	1:L:385:ILE:HB	2.21	0.41
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.86	0.40
1:A:132:GLU:HB3	1:A:196:GLU:OE2	2.20	0.40
1:D:54:GLY:HA3	1:D:68:MET:CG	2.50	0.40
1:D:115:ILE:CG2	1:D:351:LEU:HD12	2.49	0.40
1:D:382:GLU:C	1:D:383:ASN:OD1	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ASN:O	1:D:385:ILE:N	2.54	0.40
1:D:392:LEU:O	1:D:392:LEU:HD12	2.21	0.40
1:D:417:PHE:O	1:D:421:LYS:HG2	2.21	0.40
1:E:160:ALA:CB	1:E:161:PRO:CD	2.94	0.40
1:F:124:PHE:CD2	1:F:252:LYS:HG3	2.56	0.40
1:F:374:VAL:HG23	1:F:375:MET:N	2.36	0.40
1:F:421:LYS:HD3	1:F:421:LYS:HA	1.82	0.40
1:G:9:ILE:HG22	1:G:10:GLU:N	2.35	0.40
1:G:27:ASP:OD2	1:G:31:THR:N	2.53	0.40
1:H:318:PRO:O	1:H:335:ARG:HD3	2.21	0.40
1:J:351:LEU:O	1:J:355:LEU:HG	2.21	0.40
1:A:120:GLU:C	1:A:122:LEU:N	2.79	0.40
1:B:434:PRO:O	1:B:438:GLU:HG3	2.21	0.40
1:C:227:LEU:HD23	1:C:227:LEU:HA	1.82	0.40
1:D:115:ILE:HA	1:D:118:GLU:HG3	2.03	0.40
1:D:327:GLY:C	1:D:329:SER:N	2.79	0.40
1:E:375:MET:HE3	1:E:375:MET:HB3	1.82	0.40
1:F:281:HIS:CD2	1:F:402:ASN:HD21	2.40	0.40
1:F:281:HIS:CE1	1:F:356:ASP:OD2	2.69	0.40
1:G:326:ARG:HD3	1:G:326:ARG:HA	1.54	0.40
1:H:189:GLU:HB3	1:H:194:GLN:NE2	2.36	0.40
1:I:80:PHE:HA	1:I:179:MET:HE3	2.03	0.40
1:I:85:GLU:OE2	1:I:87:GLY:O	2.39	0.40
1:J:51:MET:HE2	1:K:325:SER:OG	2.21	0.40
1:J:434:PRO:O	1:J:438:GLU:HG3	2.20	0.40
1:K:73:ASP:OD1	1:K:76:THR:HG23	2.21	0.40
1:L:259:PHE:CD1	1:L:260:ASP:N	2.88	0.40
1:A:168:CYS:O	1:A:169:ARG:C	2.64	0.40
1:B:81:PRO:HG2	1:B:82:TRP:HE3	1.86	0.40
1:C:245:HIS:ND1	4:C:504:PO4:O2	2.54	0.40
1:D:160:ALA:HB3	1:D:169:ARG:NH1	2.18	0.40
1:E:85:GLU:HB3	1:E:86:LYS:H	1.74	0.40
1:E:380:ARG:NH1	1:E:387:ASP:OD2	2.54	0.40
1:F:100:ASP:O	1:F:100:ASP:CG	2.63	0.40
1:G:282:ALA:C	1:G:284:SER:N	2.79	0.40
1:I:423:ILE:O	1:I:427:MET:HG3	2.22	0.40
1:J:122:LEU:HD21	1:J:359:LYS:NZ	2.36	0.40
1:J:125:SER:HB2	1:J:253:ASN:N	2.36	0.40
1:L:119:MET:HB2	1:L:355:LEU:HD11	2.03	0.40
1:L:338:ASP:HB2	1:L:339:PRO:CD	2.51	0.40
1:L:409:LEU:HA	1:L:409:LEU:HD22	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD12	1:A:42:LEU:O	2.21	0.40
1:A:173:VAL:HG13	1:A:183:ILE:HD12	2.04	0.40
1:B:272:LYS:HB2	1:B:272:LYS:HE2	1.93	0.40
1:B:309:VAL:HG21	1:B:386:VAL:HG13	2.03	0.40
1:C:24:GLN:O	1:C:93:ILE:HA	2.22	0.40
1:D:163:ASP:HA	1:D:167:ASN:HD22	1.87	0.40
1:D:351:LEU:HD23	1:D:351:LEU:HA	1.91	0.40
1:D:371:ASN:ND2	1:D:374:VAL:HG22	2.36	0.40
1:E:169:ARG:HE	1:E:195:HIS:CD2	2.36	0.40
1:F:134:GLU:OE2	1:F:196:GLU:OE2	2.39	0.40
1:F:360:ASN:O	1:F:361:LYS:C	2.64	0.40
1:G:42:LEU:HD12	1:G:46:LEU:HG	2.02	0.40
1:G:135:PHE:CD1	1:G:135:PHE:N	2.90	0.40
1:I:124:PHE:CD2	1:I:252:LYS:HG3	2.56	0.40
1:I:244:MET:HE2	1:I:244:MET:HB3	1.91	0.40
1:J:276:ALA:HB2	1:J:364:ALA:HA	2.02	0.40
1:K:160:ALA:CB	1:K:169:ARG:HH22	2.34	0.40
1:K:165:GLY:C	1:K:167:ASN:H	2.28	0.40
1:L:298:ARG:O	1:L:298:ARG:HG3	2.21	0.40
1:A:91:ARG:O	1:A:91:ARG:HG3	2.20	0.40
1:A:224:LYS:HD2	1:F:164:LEU:HD11	2.03	0.40
1:A:239:VAL:CG1	1:A:240:ASN:N	2.84	0.40
1:A:258:PHE:CB	1:A:330:THR:CG2	2.99	0.40
1:A:258:PHE:HB3	1:A:330:THR:CG2	2.51	0.40
1:B:19:LYS:HA	1:B:39:VAL:HB	2.03	0.40
1:B:100:ASP:OD1	1:B:102:THR:HG23	2.22	0.40
1:B:278:ILE:HG23	1:B:285:PHE:HZ	1.87	0.40
1:C:42:LEU:HD12	1:C:42:LEU:HA	1.92	0.40
1:C:100:ASP:OD1	1:C:100:ASP:C	2.64	0.40
1:D:80:PHE:HA	1:D:81:PRO:HD3	1.79	0.40
1:D:203:GLY:O	1:D:204:ALA:C	2.64	0.40
1:E:140:LEU:HD22	1:E:144:GLY:O	2.22	0.40
1:E:282:ALA:HA	1:E:285:PHE:CE2	2.57	0.40
1:E:377:LYS:HA	1:E:380:ARG:NH1	2.36	0.40
1:G:128:ASN:HD22	1:G:202:ALA:C	2.29	0.40
1:G:181:PHE:HD2	1:G:199:PHE:CD2	2.39	0.40
1:G:437:ARG:O	1:G:441:MET:HB3	2.22	0.40
1:H:183:ILE:HA	1:H:199:PHE:HB3	2.03	0.40
1:I:374:VAL:CG2	1:I:375:MET:N	2.84	0.40
1:K:137:LEU:HA	1:K:137:LEU:HD23	1.81	0.40
1:K:161:PRO:O	1:K:162:THR:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:347:LEU:HD13	1:K:347:LEU:HA	1.97	0.40
1:K:373:TYR:HD2	1:K:373:TYR:HA	1.71	0.40
1:L:45:ALA:HA	1:L:50:VAL:HG22	2.03	0.40
1:L:409:LEU:CD1	1:L:413:LEU:HB3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/443 (100%)	383 (87%)	46 (10%)	12 (3%)	4	11
1	B	441/443 (100%)	390 (88%)	46 (10%)	5 (1%)	11	29
1	C	441/443 (100%)	392 (89%)	38 (9%)	11 (2%)	4	12
1	D	441/443 (100%)	391 (89%)	38 (9%)	12 (3%)	4	11
1	E	441/443 (100%)	385 (87%)	42 (10%)	14 (3%)	3	8
1	F	441/443 (100%)	385 (87%)	44 (10%)	12 (3%)	4	11
1	G	441/443 (100%)	372 (84%)	52 (12%)	17 (4%)	2	5
1	H	441/443 (100%)	395 (90%)	33 (8%)	13 (3%)	3	9
1	I	441/443 (100%)	385 (87%)	40 (9%)	16 (4%)	2	6
1	J	439/443 (99%)	392 (89%)	36 (8%)	11 (2%)	4	12
1	K	441/443 (100%)	381 (86%)	43 (10%)	17 (4%)	2	5
1	L	441/443 (100%)	382 (87%)	50 (11%)	9 (2%)	6	17
All	All	5290/5316 (100%)	4633 (88%)	508 (10%)	149 (3%)	4	10

All (149) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	THR
1	A	161	PRO
1	A	166	GLU
1	A	371	ASN
1	A	411	GLU
1	B	84	ALA
1	B	161	PRO
1	C	83	THR
1	C	86	LYS
1	C	161	PRO
1	C	366	ALA
1	C	370	ARG
1	D	83	THR
1	D	161	PRO
1	D	165	GLY
1	D	201	TYR
1	D	315	ASN
1	E	83	THR
1	E	85	GLU
1	E	143	LYS
1	E	161	PRO
1	E	262	ASN
1	F	85	GLU
1	F	161	PRO
1	G	83	THR
1	G	86	LYS
1	G	156	TYR
1	G	161	PRO
1	G	166	GLU
1	G	369	ASP
1	G	370	ARG
1	H	82	TRP
1	H	161	PRO
1	H	204	ALA
1	H	370	ARG
1	I	84	ALA
1	I	86	LYS
1	I	157	PHE
1	I	161	PRO
1	I	167	ASN
1	J	62	ARG
1	J	85	GLU
1	J	161	PRO

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Mol	Chain	Res	Type
1	J	370	ARG
1	K	6	ARG
1	K	83	THR
1	K	156	TYR
1	K	157	PHE
1	K	161	PRO
1	L	82	TRP
1	L	166	GLU
1	L	375	MET
1	A	218	VAL
1	A	370	ARG
1	B	370	ARG
1	B	375	MET
1	B	382	GLU
1	C	166	GLU
1	D	328	ILE
1	D	370	ARG
1	D	371	ASN
1	E	201	TYR
1	E	370	ARG
1	E	382	GLU
1	E	411	GLU
1	F	6	ARG
1	F	166	GLU
1	F	190	VAL
1	F	261	GLU
1	G	84	ALA
1	G	157	PHE
1	G	224	LYS
1	H	86	LYS
1	H	377	LYS
1	I	83	THR
1	I	100	ASP
1	J	261	GLU
1	K	46	LEU
1	K	166	GLU
1	K	167	ASN
1	K	373	TYR
1	L	6	ARG
1	L	369	ASP
1	L	371	ASN
1	L	382	GLU

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Mol	Chain	Res	Type
1	A	84	ALA
1	A	163	ASP
1	A	256	ASN
1	C	365	PRO
1	C	371	ASN
1	D	375	MET
1	E	62	ARG
1	E	166	GLU
1	F	83	THR
1	F	163	ASP
1	F	310	ALA
1	G	3	LYS
1	G	367	PRO
1	H	83	THR
1	I	82	TRP
1	I	159	LEU
1	I	201	TYR
1	I	254	GLY
1	I	325	SER
1	J	166	GLU
1	J	361	LYS
1	J	382	GLU
1	K	62	ARG
1	K	84	ALA
1	K	158	ASP
1	K	162	THR
1	K	204	ALA
1	K	382	GLU
1	A	382	GLU
1	C	379	GLU
1	D	325	SER
1	E	144	GLY
1	F	224	LYS
1	F	255	VAL
1	G	101	GLY
1	G	180	GLY
1	H	84	ALA
1	H	163	ASP
1	H	185	ALA
1	H	262	ASN
1	I	381	MET
1	J	84	ALA

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Mol	Chain	Res	Type
1	J	304	GLU
1	C	261	GLU
1	G	325	SER
1	G	361	LYS
1	H	361	LYS
1	I	101	GLY
1	C	152	ASP
1	G	372	ILE
1	I	304	GLU
1	L	167	ASN
1	D	61	VAL
1	E	101	GLY
1	F	101	GLY
1	L	190	VAL
1	A	233	PRO
1	H	323	PRO
1	K	81	PRO
1	D	372	ILE
1	I	218	VAL
1	K	63	ILE
1	E	291	PRO
1	J	384	GLY

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	382/382 (100%)	330 (86%)	52 (14%)	3	10
1	B	382/382 (100%)	322 (84%)	60 (16%)	2	8
1	C	382/382 (100%)	327 (86%)	55 (14%)	3	8
1	D	382/382 (100%)	325 (85%)	57 (15%)	3	8
1	E	382/382 (100%)	330 (86%)	52 (14%)	3	10
1	F	382/382 (100%)	318 (83%)	64 (17%)	2	6
1	G	382/382 (100%)	318 (83%)	64 (17%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	382/382 (100%)	318 (83%)	64 (17%)	2	6
1	I	382/382 (100%)	325 (85%)	57 (15%)	3	8
1	J	381/382 (100%)	311 (82%)	70 (18%)	1	4
1	K	382/382 (100%)	318 (83%)	64 (17%)	2	6
1	L	382/382 (100%)	322 (84%)	60 (16%)	2	8
All	All	4583/4584 (100%)	3864 (84%)	719 (16%)	2	8

All (719) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	11	LYS
1	A	18	VAL
1	A	26	THR
1	A	32	ILE
1	A	34	ASN
1	A	35	VAL
1	A	36	GLU
1	A	37	ILE
1	A	51	MET
1	A	58	GLU
1	A	74	LEU
1	A	78	VAL
1	A	85	GLU
1	A	86	LYS
1	A	88	LYS
1	A	91	ARG
1	A	94	CYS
1	A	109	ARG
1	A	112	LEU
1	A	119	MET
1	A	129	LEU
1	A	151	ASN
1	A	159	LEU
1	A	166	GLU
1	A	167	ASN
1	A	168	CYS
1	A	174	LEU
1	A	183	ILE
1	A	199	PHE

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Mol	Chain	Res	Type
1	A	200	LYS
1	A	240	ASN
1	A	261	GLU
1	A	264	ASP
1	A	269	GLU
1	A	283	THR
1	A	292	THR
1	A	299	LEU
1	A	308	TYR
1	A	326	ARG
1	A	328	ILE
1	A	330	THR
1	A	331	ARG
1	A	359	LYS
1	A	363	GLU
1	A	368	ILE
1	A	372	ILE
1	A	374	VAL
1	A	381	MET
1	A	386	VAL
1	A	404	VAL
1	A	407	LYS
1	B	12	LEU
1	B	14	LYS
1	B	15	GLU
1	B	16	GLU
1	B	19	LYS
1	B	28	ILE
1	B	32	ILE
1	B	35	VAL
1	B	36	GLU
1	B	49	LYS
1	B	51	MET
1	B	63	ILE
1	B	65	GLU
1	B	70	LEU
1	B	74	LEU
1	B	82	TRP
1	B	83	THR
1	B	88	LYS
1	B	93	ILE
1	B	96	ILE

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Mol	Chain	Res	Type
1	B	105	GLU
1	B	116	LEU
1	B	126	ASP
1	B	129	LEU
1	B	149	GLU
1	B	153	LYS
1	B	159	LEU
1	B	162	THR
1	B	200	LYS
1	B	205	VAL
1	B	221	ILE
1	B	223	ARG
1	B	239	VAL
1	B	240	ASN
1	B	249	SER
1	B	264	ASP
1	B	266	GLN
1	B	283	THR
1	B	292	THR
1	B	299	LEU
1	B	309	VAL
1	B	322	ILE
1	B	326	ARG
1	B	328	ILE
1	B	349	VAL
1	B	351	LEU
1	B	359	LYS
1	B	362	LEU
1	B	363	GLU
1	B	370	ARG
1	B	371	ASN
1	B	372	ILE
1	B	377	LYS
1	B	380	ARG
1	B	381	MET
1	B	383	ASN
1	B	409	LEU
1	B	429	ARG
1	B	430	THR
1	B	441	MET
1	C	5	THR
1	C	7	GLU

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Mol	Chain	Res	Type
1	C	28	ILE
1	C	34	ASN
1	C	35	VAL
1	C	36	GLU
1	C	49	LYS
1	C	63	ILE
1	C	68	MET
1	C	70	LEU
1	C	82	TRP
1	C	83	THR
1	C	85	GLU
1	C	105	GLU
1	C	109	ARG
1	C	112	LEU
1	C	117	LYS
1	C	120	GLU
1	C	129	LEU
1	C	142	GLU
1	C	143	LYS
1	C	148	LEU
1	C	150	LEU
1	C	159	LEU
1	C	162	THR
1	C	164	LEU
1	C	168	CYS
1	C	178	GLU
1	C	182	GLU
1	C	223	ARG
1	C	240	ASN
1	C	249	SER
1	C	255	VAL
1	C	262	ASN
1	C	270	THR
1	C	278	ILE
1	C	290	ASN
1	C	292	THR
1	C	299	LEU
1	C	308	TYR
1	C	328	ILE
1	C	332	VAL
1	C	347	LEU
1	C	349	VAL

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Mol	Chain	Res	Type
1	C	351	LEU
1	C	372	ILE
1	C	374	VAL
1	C	375	MET
1	C	401	SER
1	C	404	VAL
1	C	407	LYS
1	C	423	ILE
1	C	427	MET
1	C	429	ARG
1	C	431	GLN
1	D	6	ARG
1	D	9	ILE
1	D	13	VAL
1	D	28	ILE
1	D	34	ASN
1	D	35	VAL
1	D	37	ILE
1	D	41	GLN
1	D	49	LYS
1	D	51	MET
1	D	65	GLU
1	D	68	MET
1	D	88	LYS
1	D	93	ILE
1	D	110	ASN
1	D	112	LEU
1	D	115	ILE
1	D	126	ASP
1	D	129	LEU
1	D	142	GLU
1	D	148	LEU
1	D	149	GLU
1	D	159	LEU
1	D	162	THR
1	D	164	LEU
1	D	166	GLU
1	D	168	CYS
1	D	183	ILE
1	D	184	GLU
1	D	234	LYS
1	D	240	ASN

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Mol	Chain	Res	Type
1	D	255	VAL
1	D	256	ASN
1	D	267	LEU
1	D	270	THR
1	D	275	ILE
1	D	283	THR
1	D	284	SER
1	D	299	LEU
1	D	300	VAL
1	D	314	GLN
1	D	325	SER
1	D	328	ILE
1	D	332	VAL
1	D	351	LEU
1	D	359	LYS
1	D	362	LEU
1	D	368	ILE
1	D	370	ARG
1	D	374	VAL
1	D	375	MET
1	D	378	GLU
1	D	382	GLU
1	D	383	ASN
1	D	386	VAL
1	D	403	GLU
1	D	411	GLU
1	E	5	THR
1	E	9	ILE
1	E	11	LYS
1	E	15	GLU
1	E	19	LYS
1	E	22	ARG
1	E	24	GLN
1	E	28	ILE
1	E	32	ILE
1	E	34	ASN
1	E	35	VAL
1	E	40	SER
1	E	63	ILE
1	E	75	ASN
1	E	85	GLU
1	E	117	LYS

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Mol	Chain	Res	Type
1	E	148	LEU
1	E	159	LEU
1	E	162	THR
1	E	164	LEU
1	E	166	GLU
1	E	168	CYS
1	E	179	MET
1	E	200	LYS
1	E	201	TYR
1	E	219	LYS
1	E	221	ILE
1	E	223	ARG
1	E	239	VAL
1	E	240	ASN
1	E	249	SER
1	E	255	VAL
1	E	262	ASN
1	E	284	SER
1	E	290	ASN
1	E	299	LEU
1	E	316	ARG
1	E	325	SER
1	E	326	ARG
1	E	328	ILE
1	E	333	GLU
1	E	349	VAL
1	E	351	LEU
1	E	359	LYS
1	E	361	LYS
1	E	363	GLU
1	E	369	ASP
1	E	371	ASN
1	E	374	VAL
1	E	375	MET
1	E	400	LYS
1	E	404	VAL
1	F	5	THR
1	F	9	ILE
1	F	14	LYS
1	F	15	GLU
1	F	29	LEU
1	F	32	ILE

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Mol	Chain	Res	Type
1	F	33	LYS
1	F	34	ASN
1	F	35	VAL
1	F	36	GLU
1	F	37	ILE
1	F	41	GLN
1	F	62	ARG
1	F	85	GLU
1	F	112	LEU
1	F	117	LYS
1	F	129	LEU
1	F	142	GLU
1	F	162	THR
1	F	164	LEU
1	F	166	GLU
1	F	168	CYS
1	F	172	ILE
1	F	190	VAL
1	F	201	TYR
1	F	205	VAL
1	F	207	SER
1	F	221	ILE
1	F	224	LYS
1	F	234	LYS
1	F	236	LEU
1	F	239	VAL
1	F	240	ASN
1	F	253	ASN
1	F	255	VAL
1	F	261	GLU
1	F	262	ASN
1	F	266	GLN
1	F	269	GLU
1	F	286	THR
1	F	292	THR
1	F	299	LEU
1	F	312	SER
1	F	314	GLN
1	F	325	SER
1	F	328	ILE
1	F	334	VAL
1	F	342	ASN

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Mol	Chain	Res	Type
1	F	349	VAL
1	F	351	LEU
1	F	361	LYS
1	F	362	LEU
1	F	370	ARG
1	F	375	MET
1	F	377	LYS
1	F	379	GLU
1	F	380	ARG
1	F	382	GLU
1	F	383	ASN
1	F	385	ILE
1	F	400	LYS
1	F	404	VAL
1	F	423	ILE
1	F	441	MET
1	G	5	THR
1	G	11	LYS
1	G	14	LYS
1	G	18	VAL
1	G	24	GLN
1	G	34	ASN
1	G	35	VAL
1	G	37	ILE
1	G	42	LEU
1	G	48	ASN
1	G	49	LYS
1	G	63	ILE
1	G	70	LEU
1	G	78	VAL
1	G	85	GLU
1	G	88	LYS
1	G	96	ILE
1	G	109	ARG
1	G	112	LEU
1	G	117	LYS
1	G	126	ASP
1	G	143	LYS
1	G	148	LEU
1	G	162	THR
1	G	164	LEU
1	G	168	CYS

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Mol	Chain	Res	Type
1	G	169	ARG
1	G	174	LEU
1	G	177	GLU
1	G	198	ASP
1	G	199	PHE
1	G	211	ILE
1	G	223	ARG
1	G	239	VAL
1	G	249	SER
1	G	262	ASN
1	G	264	ASP
1	G	269	GLU
1	G	280	LYS
1	G	283	THR
1	G	292	THR
1	G	299	LEU
1	G	316	ARG
1	G	326	ARG
1	G	328	ILE
1	G	342	ASN
1	G	347	LEU
1	G	351	LEU
1	G	361	LYS
1	G	363	GLU
1	G	370	ARG
1	G	371	ASN
1	G	372	ILE
1	G	373	TYR
1	G	374	VAL
1	G	382	GLU
1	G	386	VAL
1	G	401	SER
1	G	404	VAL
1	G	407	LYS
1	G	418	ILE
1	G	423	ILE
1	G	441	MET
1	G	442	SER
1	H	3	LYS
1	H	5	THR
1	H	8	ASP
1	H	12	LEU

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Mol	Chain	Res	Type
1	H	15	GLU
1	H	21	ILE
1	H	28	ILE
1	H	32	ILE
1	H	34	ASN
1	H	35	VAL
1	H	41	GLN
1	H	63	ILE
1	H	70	LEU
1	H	74	LEU
1	H	78	VAL
1	H	85	GLU
1	H	86	LYS
1	H	96	ILE
1	H	112	LEU
1	H	120	GLU
1	H	126	ASP
1	H	129	LEU
1	H	142	GLU
1	H	159	LEU
1	H	163	ASP
1	H	164	LEU
1	H	178	GLU
1	H	190	VAL
1	H	198	ASP
1	H	199	PHE
1	H	205	VAL
1	H	216	LEU
1	H	223	ARG
1	H	239	VAL
1	H	240	ASN
1	H	266	GLN
1	H	285	PHE
1	H	297	LYS
1	H	299	LEU
1	H	308	TYR
1	H	309	VAL
1	H	314	GLN
1	H	319	LEU
1	H	321	ARG
1	H	325	SER
1	H	326	ARG

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Mol	Chain	Res	Type
1	H	328	ILE
1	H	332	VAL
1	H	347	LEU
1	H	349	VAL
1	H	351	LEU
1	H	363	GLU
1	H	368	ILE
1	H	369	ASP
1	H	371	ASN
1	H	372	ILE
1	H	373	TYR
1	H	377	LYS
1	H	378	GLU
1	H	381	MET
1	H	385	ILE
1	H	415	GLU
1	H	429	ARG
1	H	430	THR
1	I	7	GLU
1	I	15	GLU
1	I	28	ILE
1	I	34	ASN
1	I	36	GLU
1	I	39	VAL
1	I	41	GLN
1	I	49	LYS
1	I	63	ILE
1	I	70	LEU
1	I	85	GLU
1	I	86	LYS
1	I	94	CYS
1	I	100	ASP
1	I	102	THR
1	I	112	LEU
1	I	119	MET
1	I	129	LEU
1	I	142	GLU
1	I	143	LYS
1	I	148	LEU
1	I	150	LEU
1	I	156	TYR
1	I	159	LEU

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Mol	Chain	Res	Type
1	I	164	LEU
1	I	168	CYS
1	I	170	ARG
1	I	174	LEU
1	I	200	LYS
1	I	201	TYR
1	I	207	SER
1	I	216	LEU
1	I	239	VAL
1	I	240	ASN
1	I	285	PHE
1	I	293	VAL
1	I	299	LEU
1	I	309	VAL
1	I	316	ARG
1	I	328	ILE
1	I	332	VAL
1	I	349	VAL
1	I	351	LEU
1	I	362	LEU
1	I	370	ARG
1	I	373	TYR
1	I	374	VAL
1	I	377	LYS
1	I	378	GLU
1	I	386	VAL
1	I	401	SER
1	I	404	VAL
1	I	407	LYS
1	I	418	ILE
1	I	429	ARG
1	I	431	GLN
1	I	441	MET
1	J	4	TYR
1	J	5	THR
1	J	7	GLU
1	J	8	ASP
1	J	14	LYS
1	J	19	LYS
1	J	21	ILE
1	J	28	ILE
1	J	32	ILE

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Mol	Chain	Res	Type
1	J	33	LYS
1	J	34	ASN
1	J	35	VAL
1	J	36	GLU
1	J	42	LEU
1	J	49	LYS
1	J	65	GLU
1	J	70	LEU
1	J	74	LEU
1	J	85	GLU
1	J	112	LEU
1	J	115	ILE
1	J	117	LYS
1	J	120	GLU
1	J	126	ASP
1	J	129	LEU
1	J	145	GLU
1	J	153	LYS
1	J	156	TYR
1	J	159	LEU
1	J	162	THR
1	J	164	LEU
1	J	166	GLU
1	J	167	ASN
1	J	168	CYS
1	J	190	VAL
1	J	212	GLN
1	J	221	ILE
1	J	223	ARG
1	J	224	LYS
1	J	234	LYS
1	J	239	VAL
1	J	240	ASN
1	J	253	ASN
1	J	264	ASP
1	J	270	THR
1	J	278	ILE
1	J	279	VAL
1	J	280	LYS
1	J	286	THR
1	J	299	LEU
1	J	300	VAL

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Mol	Chain	Res	Type
1	J	326	ARG
1	J	328	ILE
1	J	331	ARG
1	J	347	LEU
1	J	348	SER
1	J	349	VAL
1	J	351	LEU
1	J	359	LYS
1	J	368	ILE
1	J	370	ARG
1	J	374	VAL
1	J	377	LYS
1	J	382	GLU
1	J	383	ASN
1	J	404	VAL
1	J	409	LEU
1	J	429	ARG
1	J	441	MET
1	J	443	GLN
1	K	5	THR
1	K	9	ILE
1	K	24	GLN
1	K	28	ILE
1	K	32	ILE
1	K	34	ASN
1	K	35	VAL
1	K	39	VAL
1	K	48	ASN
1	K	49	LYS
1	K	63	ILE
1	K	70	LEU
1	K	74	LEU
1	K	88	LYS
1	K	105	GLU
1	K	112	LEU
1	K	117	LYS
1	K	126	ASP
1	K	142	GLU
1	K	151	ASN
1	K	153	LYS
1	K	156	TYR
1	K	159	LEU

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Mol	Chain	Res	Type
1	K	164	LEU
1	K	166	GLU
1	K	168	CYS
1	K	174	LEU
1	K	207	SER
1	K	220	THR
1	K	224	LYS
1	K	234	LYS
1	K	239	VAL
1	K	252	LYS
1	K	255	VAL
1	K	264	ASP
1	K	285	PHE
1	K	299	LEU
1	K	308	TYR
1	K	315	ASN
1	K	316	ARG
1	K	319	LEU
1	K	322	ILE
1	K	325	SER
1	K	326	ARG
1	K	328	ILE
1	K	351	LEU
1	K	358	ILE
1	K	362	LEU
1	K	368	ILE
1	K	369	ASP
1	K	372	ILE
1	K	373	TYR
1	K	378	GLU
1	K	379	GLU
1	K	381	MET
1	K	385	ILE
1	K	386	VAL
1	K	404	VAL
1	K	409	LEU
1	K	423	ILE
1	K	429	ARG
1	K	441	MET
1	K	442	SER
1	K	443	GLN
1	L	5	THR

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Mol	Chain	Res	Type
1	L	9	ILE
1	L	14	LYS
1	L	16	GLU
1	L	32	ILE
1	L	34	ASN
1	L	35	VAL
1	L	50	VAL
1	L	61	VAL
1	L	66	SER
1	L	70	LEU
1	L	74	LEU
1	L	78	VAL
1	L	86	LYS
1	L	93	ILE
1	L	102	THR
1	L	119	MET
1	L	122	LEU
1	L	126	ASP
1	L	129	LEU
1	L	132	GLU
1	L	143	LYS
1	L	149	GLU
1	L	159	LEU
1	L	162	THR
1	L	164	LEU
1	L	166	GLU
1	L	168	CYS
1	L	174	LEU
1	L	178	GLU
1	L	184	GLU
1	L	199	PHE
1	L	206	ARG
1	L	239	VAL
1	L	240	ASN
1	L	249	SER
1	L	252	LYS
1	L	262	ASN
1	L	264	ASP
1	L	285	PHE
1	L	309	VAL
1	L	316	ARG
1	L	326	ARG

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Mol	Chain	Res	Type
1	L	328	ILE
1	L	336	SER
1	L	347	LEU
1	L	349	VAL
1	L	351	LEU
1	L	362	LEU
1	L	363	GLU
1	L	377	LYS
1	L	378	GLU
1	L	379	GLU
1	L	386	VAL
1	L	402	ASN
1	L	404	VAL
1	L	409	LEU
1	L	418	ILE
1	L	423	ILE
1	L	429	ARG

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

Mol	Chain	Res	Type
1	A	17	ASN
1	A	41	GLN
1	A	98	ASN
1	A	110	ASN
1	A	187	HIS
1	A	194	GLN
1	A	225	HIS
1	A	281	HIS
1	A	342	ASN
1	A	360	ASN
1	A	383	ASN
1	A	431	GLN
1	A	443	GLN
1	B	17	ASN
1	B	110	ASN
1	B	128	ASN
1	B	167	ASN
1	B	194	GLN
1	B	240	ASN
1	B	281	HIS
1	B	314	GLN

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Mol	Chain	Res	Type
1	B	360	ASN
1	B	371	ASN
1	B	383	ASN
1	C	17	ASN
1	C	24	GLN
1	C	34	ASN
1	C	98	ASN
1	C	128	ASN
1	C	151	ASN
1	C	194	GLN
1	C	225	HIS
1	C	228	HIS
1	C	240	ASN
1	C	281	HIS
1	C	290	ASN
1	C	360	ASN
1	C	431	GLN
1	C	443	GLN
1	D	34	ASN
1	D	98	ASN
1	D	110	ASN
1	D	194	GLN
1	D	212	GLN
1	D	228	HIS
1	D	256	ASN
1	D	281	HIS
1	D	290	ASN
1	D	314	GLN
1	D	371	ASN
1	E	111	ASN
1	E	167	ASN
1	E	187	HIS
1	E	188	HIS
1	E	195	HIS
1	E	212	GLN
1	E	228	HIS
1	E	240	ASN
1	E	253	ASN
1	E	262	ASN
1	E	281	HIS
1	E	290	ASN
1	E	314	GLN

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Mol	Chain	Res	Type
1	E	371	ASN
1	E	412	HIS
1	E	443	GLN
1	F	17	ASN
1	F	24	GLN
1	F	41	GLN
1	F	167	ASN
1	F	187	HIS
1	F	188	HIS
1	F	225	HIS
1	F	266	GLN
1	F	281	HIS
1	F	314	GLN
1	F	342	ASN
1	F	360	ASN
1	F	371	ASN
1	F	383	ASN
1	F	412	HIS
1	F	433	HIS
1	G	75	ASN
1	G	98	ASN
1	G	110	ASN
1	G	128	ASN
1	G	167	ASN
1	G	187	HIS
1	G	194	GLN
1	G	225	HIS
1	G	228	HIS
1	G	240	ASN
1	G	247	ASN
1	G	281	HIS
1	G	342	ASN
1	G	383	ASN
1	G	416	HIS
1	G	443	GLN
1	H	17	ASN
1	H	41	GLN
1	H	110	ASN
1	H	128	ASN
1	H	187	HIS
1	H	194	GLN
1	H	212	GLN

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Mol	Chain	Res	Type
1	H	225	HIS
1	H	228	HIS
1	H	281	HIS
1	H	290	ASN
1	H	315	ASN
1	I	41	GLN
1	I	110	ASN
1	I	128	ASN
1	I	151	ASN
1	I	240	ASN
1	I	245	HIS
1	I	281	HIS
1	I	290	ASN
1	I	360	ASN
1	I	443	GLN
1	J	17	ASN
1	J	34	ASN
1	J	98	ASN
1	J	110	ASN
1	J	187	HIS
1	J	194	GLN
1	J	228	HIS
1	J	245	HIS
1	J	247	ASN
1	J	253	ASN
1	J	281	HIS
1	J	290	ASN
1	J	371	ASN
1	J	412	HIS
1	K	17	ASN
1	K	128	ASN
1	K	194	GLN
1	K	212	GLN
1	K	225	HIS
1	K	240	ASN
1	K	266	GLN
1	K	281	HIS
1	K	290	ASN
1	K	314	GLN
1	K	315	ASN
1	K	371	ASN
1	K	439	GLN

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Mol	Chain	Res	Type
1	L	110	ASN
1	L	128	ASN
1	L	187	HIS
1	L	194	GLN
1	L	212	GLN
1	L	225	HIS
1	L	228	HIS
1	L	240	ASN
1	L	247	ASN
1	L	266	GLN
1	L	281	HIS
1	L	290	ASN
1	L	360	ASN
1	L	402	ASN
1	L	416	HIS
1	L	443	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 36 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLN	A	503	2	7,8,9	0.42	0	4,9,11	0.02	0
4	PO4	C	504	2	4,4,4	0.94	0	6,6,6	0.65	0
3	GLN	G	503	2	7,8,9	0.55	0	4,9,11	0.03	0
3	GLN	D	503	2	7,8,9	0.48	0	4,9,11	0.45	0
3	GLN	B	503	2	7,8,9	0.78	0	4,9,11	0.31	0
3	GLN	C	502	2	7,8,9	0.54	0	4,9,11	0.13	0
3	GLN	F	503	-	7,8,9	0.49	0	4,9,11	0.10	0
3	GLN	L	503	2	8,9,9	0.71	0	8,11,11	1.09	1 (12%)
4	PO4	G	504	2	4,4,4	0.88	0	6,6,6	0.73	0
4	PO4	H	504	2	4,4,4	0.97	0	6,6,6	0.70	0
4	PO4	A	504	2	4,4,4	0.82	0	6,6,6	0.97	0
3	GLN	E	501	2	7,8,9	0.88	0	4,9,11	0.26	0
3	GLN	H	503	2	7,8,9	0.56	0	4,9,11	0.09	0
3	GLN	K	503	-	7,8,9	0.45	0	4,9,11	0.24	0
3	GLN	I	503	-	7,8,9	0.67	0	4,9,11	0.14	0
3	GLN	J	503	2	7,8,9	0.50	0	4,9,11	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLN	A	503	2	-	1/6/7/9	-
3	GLN	G	503	2	-	3/6/7/9	-
3	GLN	D	503	2	-	2/6/7/9	-
3	GLN	B	503	2	-	2/6/7/9	-
3	GLN	C	502	2	-	3/6/7/9	-
3	GLN	F	503	-	-	2/6/7/9	-
3	GLN	L	503	2	-	4/9/9/9	-
3	GLN	E	501	2	-	3/6/7/9	-
3	GLN	H	503	2	-	4/6/7/9	-
3	GLN	K	503	-	-	2/6/7/9	-
3	GLN	I	503	-	-	4/6/7/9	-
3	GLN	J	503	2	-	3/6/7/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	503	GLN	OXT-C-O	-2.79	117.74	124.08

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	GLN	N-CA-CB-CG
3	B	503	GLN	C-CA-CB-CG
3	C	502	GLN	N-CA-CB-CG
3	E	501	GLN	N-CA-CB-CG
3	E	501	GLN	C-CA-CB-CG
3	G	503	GLN	N-CA-CB-CG
3	G	503	GLN	C-CA-CB-CG
3	H	503	GLN	O-C-CA-CB
3	H	503	GLN	N-CA-CB-CG
3	H	503	GLN	C-CA-CB-CG
3	I	503	GLN	O-C-CA-CB
3	I	503	GLN	N-CA-CB-CG
3	I	503	GLN	C-CA-CB-CG
3	J	503	GLN	N-CA-CB-CG
3	J	503	GLN	C-CA-CB-CG
3	K	503	GLN	O-C-CA-CB
3	L	503	GLN	N-CA-CB-CG
3	E	501	GLN	CA-CB-CG-CD
3	J	503	GLN	CA-CB-CG-CD
3	D	503	GLN	CA-CB-CG-CD
3	H	503	GLN	CA-CB-CG-CD
3	I	503	GLN	CA-CB-CG-CD
3	F	503	GLN	CA-CB-CG-CD
3	L	503	GLN	C-CA-CB-CG
3	L	503	GLN	OXT-C-CA-CB
3	C	502	GLN	C-CA-CB-CG
3	F	503	GLN	N-CA-CB-CG
3	L	503	GLN	O-C-CA-CB
3	C	502	GLN	NE2-CD-CG-CB
3	A	503	GLN	C-CA-CB-CG
3	D	503	GLN	C-CA-CB-CG
3	G	503	GLN	CA-CB-CG-CD
3	K	503	GLN	N-CA-CB-CG

There are no ring outliers.

13 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	504	PO4	3	0
3	D	503	GLN	1	0
3	B	503	GLN	1	0
3	C	502	GLN	3	0
3	F	503	GLN	1	0
4	G	504	PO4	2	0
4	H	504	PO4	1	0
4	A	504	PO4	3	0
3	E	501	GLN	2	0
3	H	503	GLN	5	0
3	K	503	GLN	1	0
3	I	503	GLN	1	0
3	J	503	GLN	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	443/443 (100%)	-1.65	0 100 100	24, 38, 70, 96	0
1	B	443/443 (100%)	-1.67	0 100 100	24, 37, 71, 98	0
1	C	443/443 (100%)	-1.66	0 100 100	20, 36, 65, 98	0
1	D	443/443 (100%)	-1.65	0 100 100	22, 34, 68, 92	0
1	E	443/443 (100%)	-1.63	0 100 100	21, 35, 69, 99	0
1	F	443/443 (100%)	-1.64	0 100 100	20, 36, 70, 102	0
1	G	443/443 (100%)	-1.65	0 100 100	24, 37, 68, 100	0
1	H	443/443 (100%)	-1.64	0 100 100	24, 36, 68, 104	0
1	I	443/443 (100%)	-1.66	0 100 100	20, 35, 67, 97	0
1	J	441/443 (99%)	-1.66	0 100 100	21, 34, 67, 98	0
1	K	443/443 (100%)	-1.62	0 100 100	22, 36, 70, 106	0
1	L	443/443 (100%)	-1.66	0 100 100	23, 36, 68, 101	0
All	All	5314/5316 (99%)	-1.65	0 100 100	20, 36, 70, 106	0

There are no RSRZ outliers to report.

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	E	504	1/1	0.98	0.03	30,30,30,30	0
4	PO4	H	504	5/5	0.98	0.06	91,92,112,116	0
2	MG	D	501	1/1	0.99	0.06	23,23,23,23	0
2	MG	D	502	1/1	0.99	0.05	35,35,35,35	0
2	MG	E	502	1/1	0.99	0.06	28,28,28,28	0
2	MG	A	505	1/1	0.99	0.03	31,31,31,31	0
2	MG	F	501	1/1	0.99	0.04	34,34,34,34	0
2	MG	F	502	1/1	0.99	0.02	29,29,29,29	0
2	MG	F	504	1/1	0.99	0.04	25,25,25,25	0
2	MG	G	502	1/1	0.99	0.03	35,35,35,35	0
2	MG	G	505	1/1	0.99	0.05	31,31,31,31	0
2	MG	I	501	1/1	0.99	0.04	19,19,19,19	0
2	MG	I	502	1/1	0.99	0.03	28,28,28,28	0
2	MG	I	504	1/1	0.99	0.04	28,28,28,28	0
2	MG	J	501	1/1	0.99	0.04	28,28,28,28	0
2	MG	J	504	1/1	0.99	0.03	21,21,21,21	0
2	MG	K	502	1/1	0.99	0.05	30,30,30,30	0
2	MG	K	504	1/1	0.99	0.03	21,21,21,21	0
2	MG	L	504	1/1	0.99	0.05	28,28,28,28	0
3	GLN	A	503	9/10	0.99	0.04	37,41,50,57	0
3	GLN	B	503	9/10	0.99	0.05	28,34,37,38	0
3	GLN	D	503	9/10	0.99	0.06	23,29,33,35	0
3	GLN	E	501	9/10	0.99	0.06	22,26,33,36	0
3	GLN	G	503	9/10	0.99	0.05	35,39,44,45	0
3	GLN	H	503	9/10	0.99	0.04	32,37,47,47	0
3	GLN	J	503	9/10	0.99	0.05	25,32,37,41	0
3	GLN	K	503	9/10	0.99	0.05	26,33,39,40	0
4	PO4	A	504	5/5	0.99	0.04	80,81,89,94	0
4	PO4	C	504	5/5	0.99	0.03	35,44,67,68	0
4	PO4	G	504	5/5	0.99	0.04	81,82,94,97	0
2	MG	C	505	1/1	0.99	0.07	32,32,32,32	0
2	MG	C	503	1/1	1.00	0.04	33,33,33,33	0
2	MG	A	502	1/1	1.00	0.02	45,45,45,45	0
2	MG	L	501	1/1	1.00	0.03	22,22,22,22	0
2	MG	L	502	1/1	1.00	0.02	26,26,26,26	0
2	MG	G	501	1/1	1.00	0.02	45,45,45,45	0
2	MG	A	501	1/1	1.00	0.01	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	501	1/1	1.00	0.04	24,24,24,24	0
3	GLN	C	502	9/10	1.00	0.03	31,34,37,39	0
2	MG	H	501	1/1	1.00	0.01	32,32,32,32	0
2	MG	H	502	1/1	1.00	0.02	50,50,50,50	0
3	GLN	F	503	9/10	1.00	0.03	29,32,35,36	0
2	MG	H	505	1/1	1.00	0.02	21,21,21,21	0
2	MG	D	504	1/1	1.00	0.01	20,20,20,20	0
3	GLN	I	503	9/10	1.00	0.03	26,29,34,35	0
2	MG	B	502	1/1	1.00	0.04	29,29,29,29	0
2	MG	E	503	1/1	1.00	0.01	25,25,25,25	0
3	GLN	L	503	10/10	1.00	0.03	31,33,41,44	0
2	MG	B	504	1/1	1.00	0.03	39,39,39,39	0
2	MG	J	502	1/1	1.00	0.06	23,23,23,23	0
2	MG	C	501	1/1	1.00	0.02	29,29,29,29	0
2	MG	K	501	1/1	1.00	0.04	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.