



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2022 – 06:13 PM EDT

PDB ID : 7U39
Title : Structure of the apo form of Streptomyces venezuelae GlgX, the glycogen de-branching enzyme
Authors : Schumacher, M.A.
Deposited on : 2022-02-26
Resolution : 3.51 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

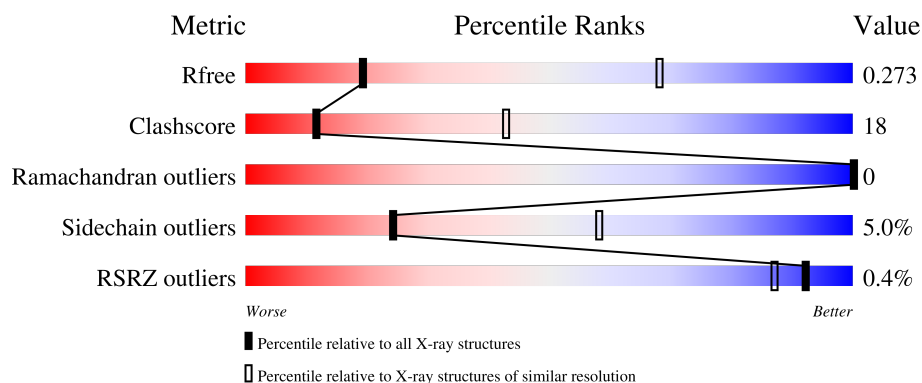
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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	709	 60% 37% ..
1	B	709	 59% 37% ..
1	C	709	 56% 41% ..
1	D	709	 60% 37% ..
1	E	709	 60% 36% ..

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Mol	Chain	Length	Quality of chain
1	F	709	<div><div><div>%</div><div><div></div><div>62%</div><div>34%</div><div></div></div><div>..</div></div></div>
1	G	709	<div><div><div>2%</div><div><div></div><div>60%</div><div>36%</div><div></div></div><div>..</div></div></div>
1	H	709	<div><div><div></div><div><div></div><div>60%</div><div>37%</div><div></div></div><div>..</div></div></div>
1	I	709	<div><div><div></div><div><div></div><div>59%</div><div>39%</div><div></div></div><div>..</div></div></div>
1	J	709	<div><div><div>%</div><div><div></div><div>58%</div><div>39%</div><div></div></div><div>..</div></div></div>
1	K	709	<div><div><div>%</div><div><div></div><div>60%</div><div>37%</div><div></div></div><div>..</div></div></div>
1	L	709	<div><div><div></div><div><div></div><div>58%</div><div>39%</div><div></div></div><div>..</div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 67324 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 Glycogen debranching enzyme GlgX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	703	Total	C	N	O	S	0	0	0
			5567	3499	1002	1042	24			
1	B	705	Total	C	N	O	S	0	0	0
			5595	3514	1013	1044	24			
1	C	699	Total	C	N	O	S	0	0	0
			5551	3487	1003	1037	24			
1	D	700	Total	C	N	O	S	0	0	0
			5566	3495	1007	1041	23			
1	E	700	Total	C	N	O	S	0	0	0
			5567	3497	1003	1044	23			
1	F	698	Total	C	N	O	S	0	0	0
			5549	3486	1003	1037	23			
1	G	698	Total	C	N	O	S	0	0	0
			5554	3490	1004	1037	23			
1	H	701	Total	C	N	O	S	0	0	0
			5570	3499	1009	1038	24			
1	I	701	Total	C	N	O	S	0	0	0
			5583	3506	1012	1042	23			
1	J	700	Total	C	N	O	S	0	0	0
			5557	3491	1001	1041	24			
1	K	701	Total	C	N	O	S	0	0	0
			5583	3506	1012	1042	23			
1	L	701	Total	C	N	O	S	0	0	0
			5564	3494	1004	1043	23			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A5P2ALW6
A	-1	SER	-	expression tag	UNP A0A5P2ALW6
A	0	HIS	-	expression tag	UNP A0A5P2ALW6
A	103	VAL	ILE	conflict	UNP A0A5P2ALW6
A	192	ARG	LYS	conflict	UNP A0A5P2ALW6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	296	ALA	SER	conflict	UNP A0A5P2ALW6
A	297	ASP	ASN	conflict	UNP A0A5P2ALW6
A	303	MET	THR	conflict	UNP A0A5P2ALW6
A	682	GLN	GLU	conflict	UNP A0A5P2ALW6
B	-2	GLY	-	expression tag	UNP A0A5P2ALW6
B	-1	SER	-	expression tag	UNP A0A5P2ALW6
B	0	HIS	-	expression tag	UNP A0A5P2ALW6
B	103	VAL	ILE	conflict	UNP A0A5P2ALW6
B	192	ARG	LYS	conflict	UNP A0A5P2ALW6
B	296	ALA	SER	conflict	UNP A0A5P2ALW6
B	297	ASP	ASN	conflict	UNP A0A5P2ALW6
B	303	MET	THR	conflict	UNP A0A5P2ALW6
B	682	GLN	GLU	conflict	UNP A0A5P2ALW6
C	-2	GLY	-	expression tag	UNP A0A5P2ALW6
C	-1	SER	-	expression tag	UNP A0A5P2ALW6
C	0	HIS	-	expression tag	UNP A0A5P2ALW6
C	103	VAL	ILE	conflict	UNP A0A5P2ALW6
C	192	ARG	LYS	conflict	UNP A0A5P2ALW6
C	296	ALA	SER	conflict	UNP A0A5P2ALW6
C	297	ASP	ASN	conflict	UNP A0A5P2ALW6
C	303	MET	THR	conflict	UNP A0A5P2ALW6
C	682	GLN	GLU	conflict	UNP A0A5P2ALW6
D	-2	GLY	-	expression tag	UNP A0A5P2ALW6
D	-1	SER	-	expression tag	UNP A0A5P2ALW6
D	0	HIS	-	expression tag	UNP A0A5P2ALW6
D	103	VAL	ILE	conflict	UNP A0A5P2ALW6
D	192	ARG	LYS	conflict	UNP A0A5P2ALW6
D	296	ALA	SER	conflict	UNP A0A5P2ALW6
D	297	ASP	ASN	conflict	UNP A0A5P2ALW6
D	303	MET	THR	conflict	UNP A0A5P2ALW6
D	682	GLN	GLU	conflict	UNP A0A5P2ALW6
E	-2	GLY	-	expression tag	UNP A0A5P2ALW6
E	-1	SER	-	expression tag	UNP A0A5P2ALW6
E	0	HIS	-	expression tag	UNP A0A5P2ALW6
E	103	VAL	ILE	conflict	UNP A0A5P2ALW6
E	192	ARG	LYS	conflict	UNP A0A5P2ALW6
E	296	ALA	SER	conflict	UNP A0A5P2ALW6
E	297	ASP	ASN	conflict	UNP A0A5P2ALW6
E	303	MET	THR	conflict	UNP A0A5P2ALW6
E	682	GLN	GLU	conflict	UNP A0A5P2ALW6
F	-2	GLY	-	expression tag	UNP A0A5P2ALW6
F	-1	SER	-	expression tag	UNP A0A5P2ALW6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP A0A5P2ALW6
F	103	VAL	ILE	conflict	UNP A0A5P2ALW6
F	192	ARG	LYS	conflict	UNP A0A5P2ALW6
F	296	ALA	SER	conflict	UNP A0A5P2ALW6
F	297	ASP	ASN	conflict	UNP A0A5P2ALW6
F	303	MET	THR	conflict	UNP A0A5P2ALW6
F	682	GLN	GLU	conflict	UNP A0A5P2ALW6
G	-2	GLY	-	expression tag	UNP A0A5P2ALW6
G	-1	SER	-	expression tag	UNP A0A5P2ALW6
G	0	HIS	-	expression tag	UNP A0A5P2ALW6
G	103	VAL	ILE	conflict	UNP A0A5P2ALW6
G	192	ARG	LYS	conflict	UNP A0A5P2ALW6
G	296	ALA	SER	conflict	UNP A0A5P2ALW6
G	297	ASP	ASN	conflict	UNP A0A5P2ALW6
G	303	MET	THR	conflict	UNP A0A5P2ALW6
G	682	GLN	GLU	conflict	UNP A0A5P2ALW6
H	-2	GLY	-	expression tag	UNP A0A5P2ALW6
H	-1	SER	-	expression tag	UNP A0A5P2ALW6
H	0	HIS	-	expression tag	UNP A0A5P2ALW6
H	103	VAL	ILE	conflict	UNP A0A5P2ALW6
H	192	ARG	LYS	conflict	UNP A0A5P2ALW6
H	296	ALA	SER	conflict	UNP A0A5P2ALW6
H	297	ASP	ASN	conflict	UNP A0A5P2ALW6
H	303	MET	THR	conflict	UNP A0A5P2ALW6
H	682	GLN	GLU	conflict	UNP A0A5P2ALW6
I	-2	GLY	-	expression tag	UNP A0A5P2ALW6
I	-1	SER	-	expression tag	UNP A0A5P2ALW6
I	0	HIS	-	expression tag	UNP A0A5P2ALW6
I	103	VAL	ILE	conflict	UNP A0A5P2ALW6
I	192	ARG	LYS	conflict	UNP A0A5P2ALW6
I	296	ALA	SER	conflict	UNP A0A5P2ALW6
I	297	ASP	ASN	conflict	UNP A0A5P2ALW6
I	303	MET	THR	conflict	UNP A0A5P2ALW6
I	682	GLN	GLU	conflict	UNP A0A5P2ALW6
J	-2	GLY	-	expression tag	UNP A0A5P2ALW6
J	-1	SER	-	expression tag	UNP A0A5P2ALW6
J	0	HIS	-	expression tag	UNP A0A5P2ALW6
J	103	VAL	ILE	conflict	UNP A0A5P2ALW6
J	192	ARG	LYS	conflict	UNP A0A5P2ALW6
J	296	ALA	SER	conflict	UNP A0A5P2ALW6
J	297	ASP	ASN	conflict	UNP A0A5P2ALW6
J	303	MET	THR	conflict	UNP A0A5P2ALW6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	682	GLN	GLU	conflict	UNP A0A5P2ALW6
K	-2	GLY	-	expression tag	UNP A0A5P2ALW6
K	-1	SER	-	expression tag	UNP A0A5P2ALW6
K	0	HIS	-	expression tag	UNP A0A5P2ALW6
K	103	VAL	ILE	conflict	UNP A0A5P2ALW6
K	192	ARG	LYS	conflict	UNP A0A5P2ALW6
K	296	ALA	SER	conflict	UNP A0A5P2ALW6
K	297	ASP	ASN	conflict	UNP A0A5P2ALW6
K	303	MET	THR	conflict	UNP A0A5P2ALW6
K	682	GLN	GLU	conflict	UNP A0A5P2ALW6
L	-2	GLY	-	expression tag	UNP A0A5P2ALW6
L	-1	SER	-	expression tag	UNP A0A5P2ALW6
L	0	HIS	-	expression tag	UNP A0A5P2ALW6
L	103	VAL	ILE	conflict	UNP A0A5P2ALW6
L	192	ARG	LYS	conflict	UNP A0A5P2ALW6
L	296	ALA	SER	conflict	UNP A0A5P2ALW6
L	297	ASP	ASN	conflict	UNP A0A5P2ALW6
L	303	MET	THR	conflict	UNP A0A5P2ALW6
L	682	GLN	GLU	conflict	UNP A0A5P2ALW6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	56	Total O 56 56	0	0
2	B	56	Total O 56 56	0	0
2	C	63	Total O 63 63	0	0
2	D	43	Total O 43 43	0	0
2	E	42	Total O 42 42	0	0
2	F	43	Total O 43 43	0	0
2	G	27	Total O 27 27	0	0
2	H	41	Total O 41 41	0	0
2	I	38	Total O 38 38	0	0
2	J	38	Total O 38 38	0	0

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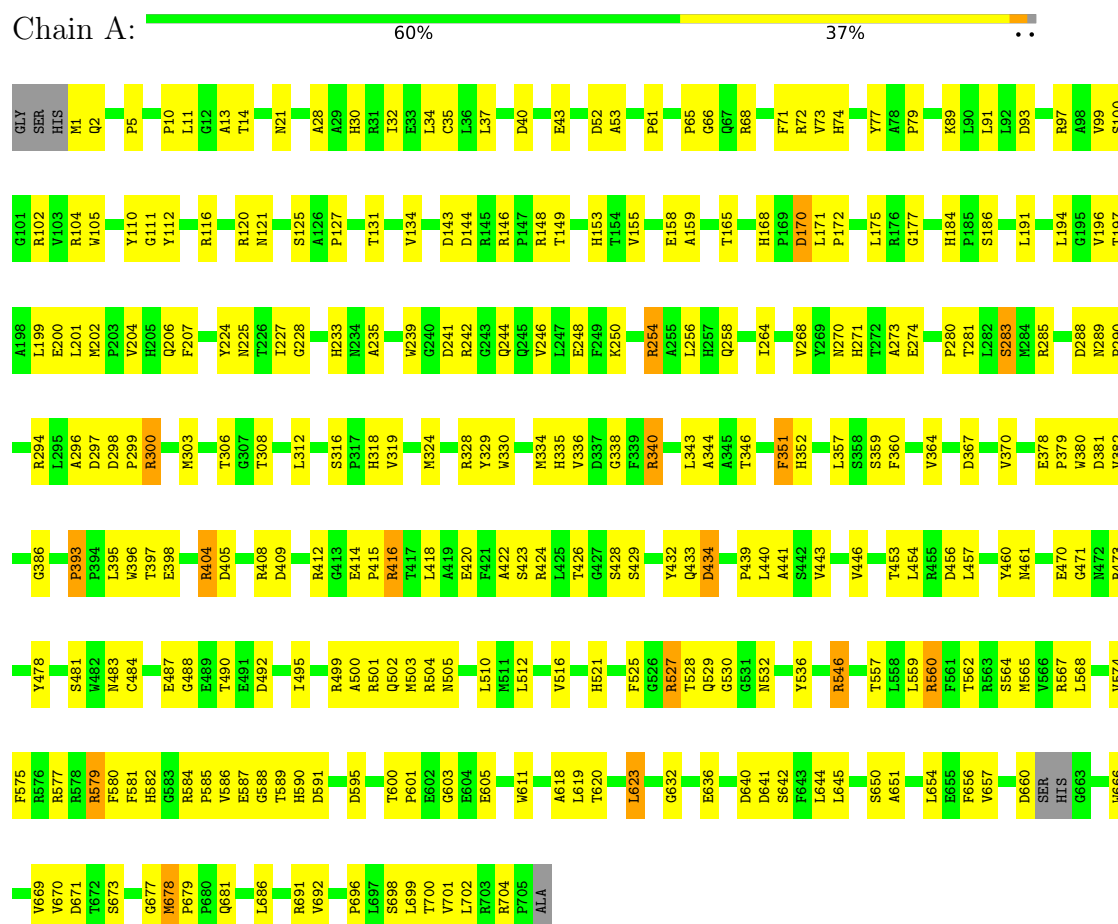
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	37	Total	O	0	0
			37	37		
2	L	34	Total	O	0	0
			34	34		

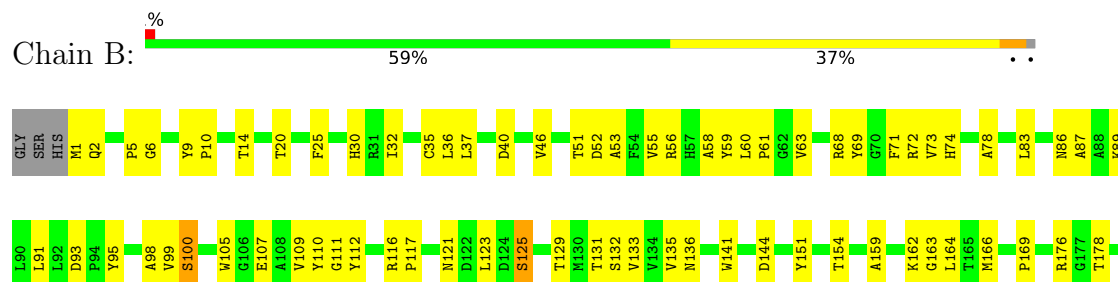
3 Residue-property plots [i](#)

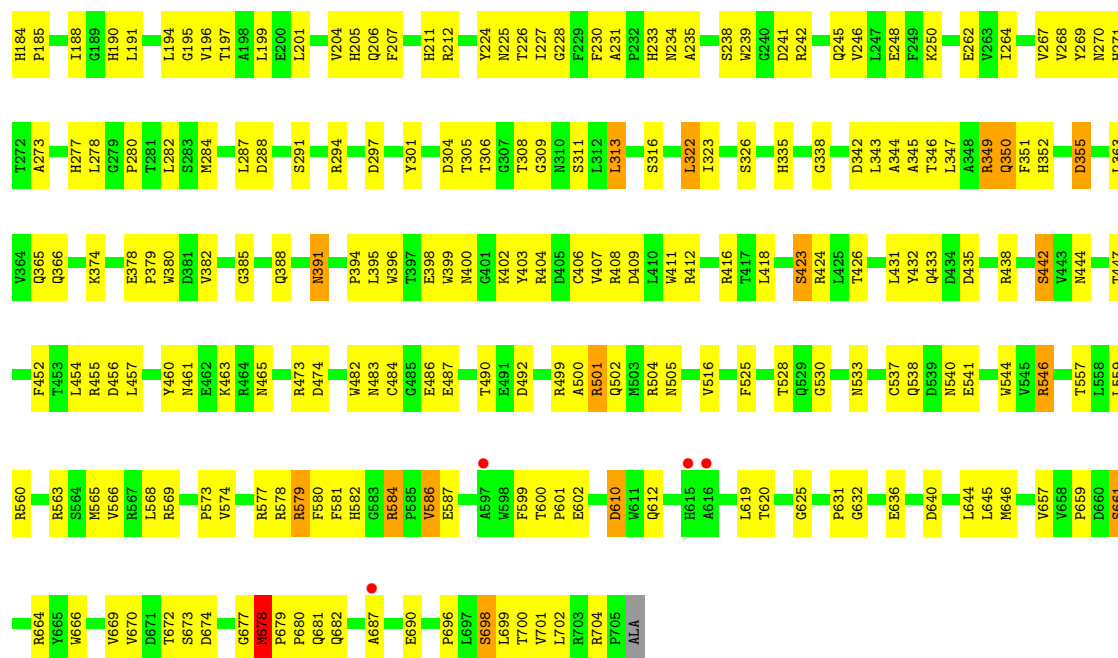
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Glycogen debranching enzyme GlgX



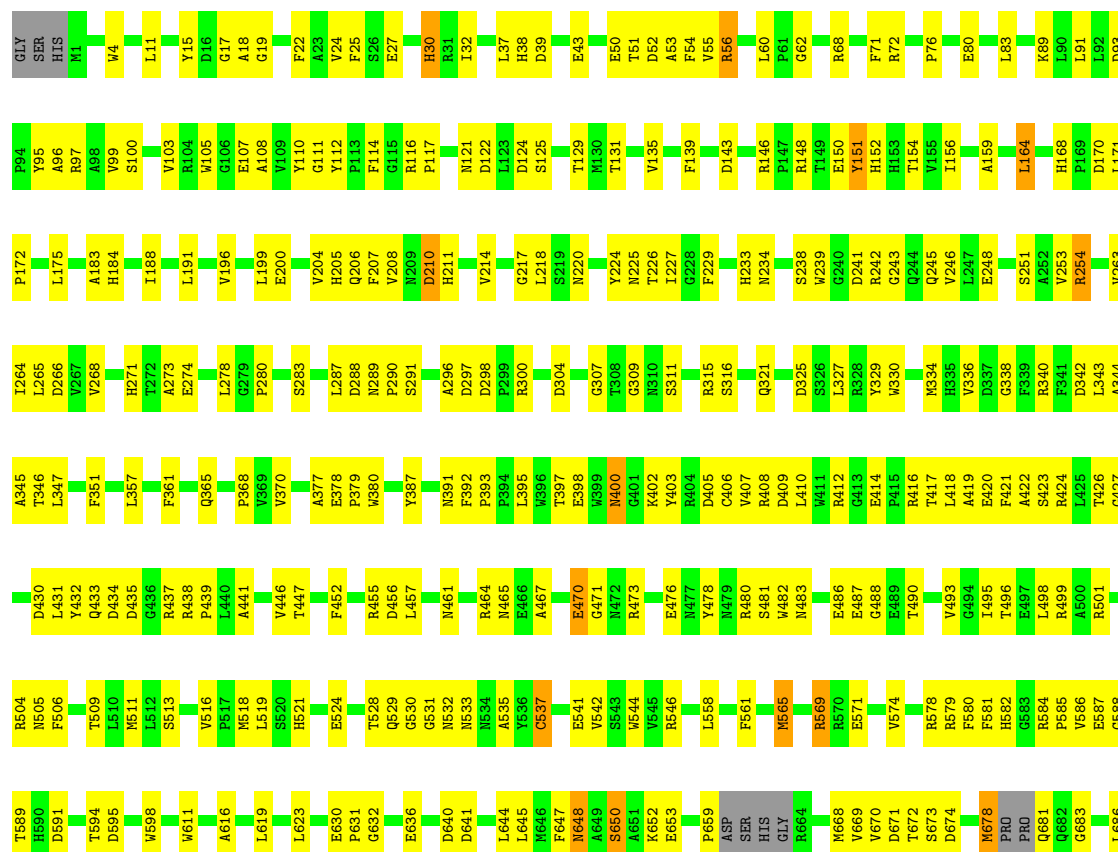
• Molecule 1: Glycogen debranching enzyme GlgX





• Molecule 1: Glycogen debranching enzyme GlgX

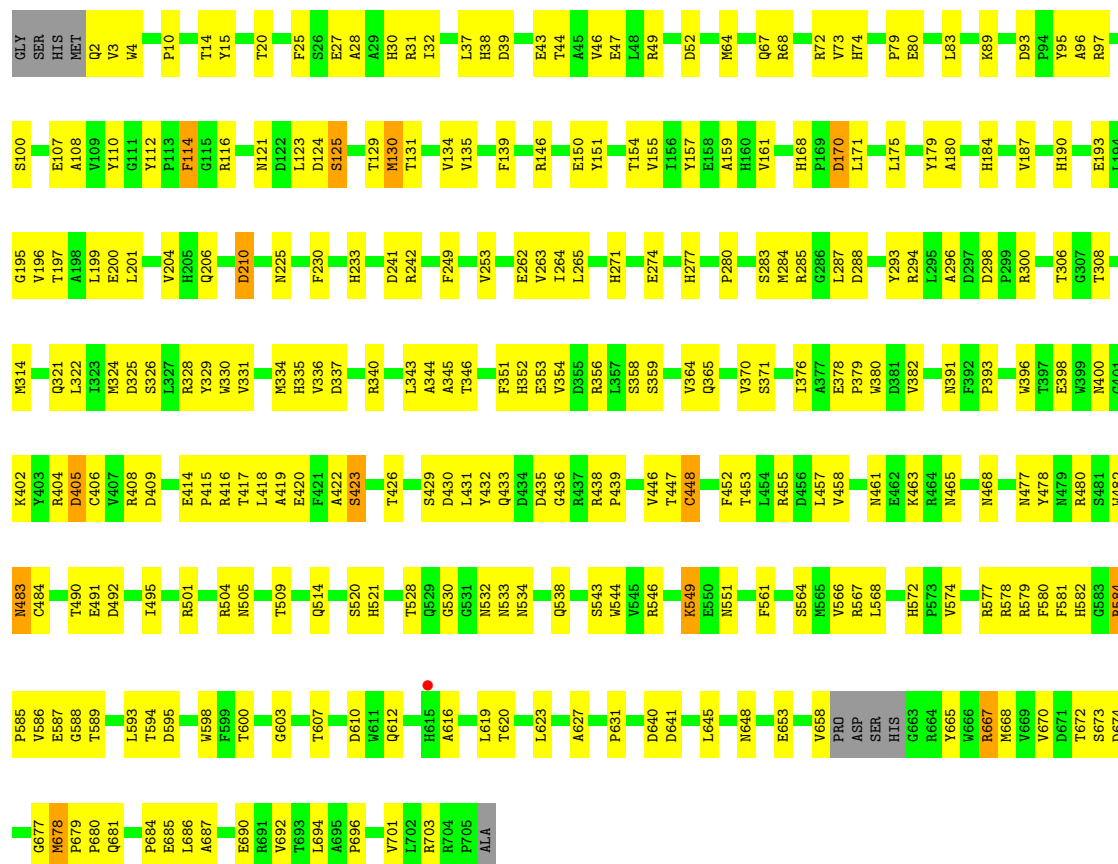
Chain C: 56% 41% ::





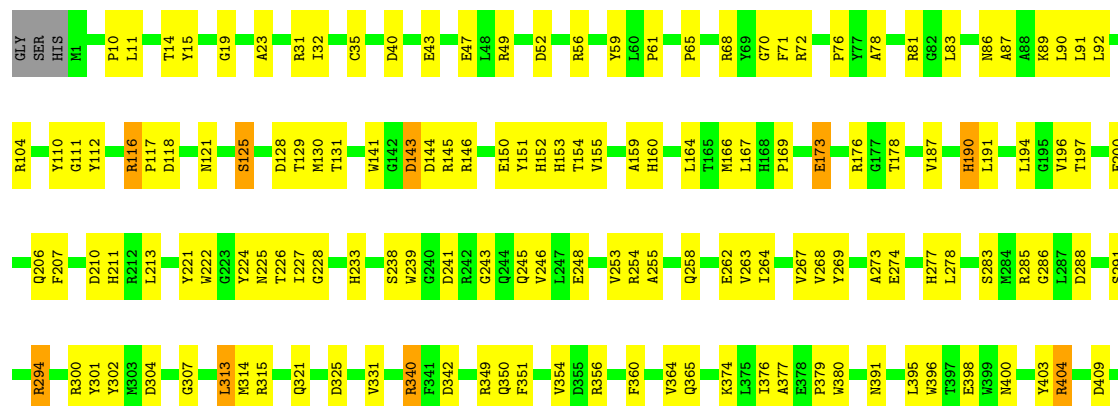
• Molecule 1: Glycogen debranching enzyme GlgX

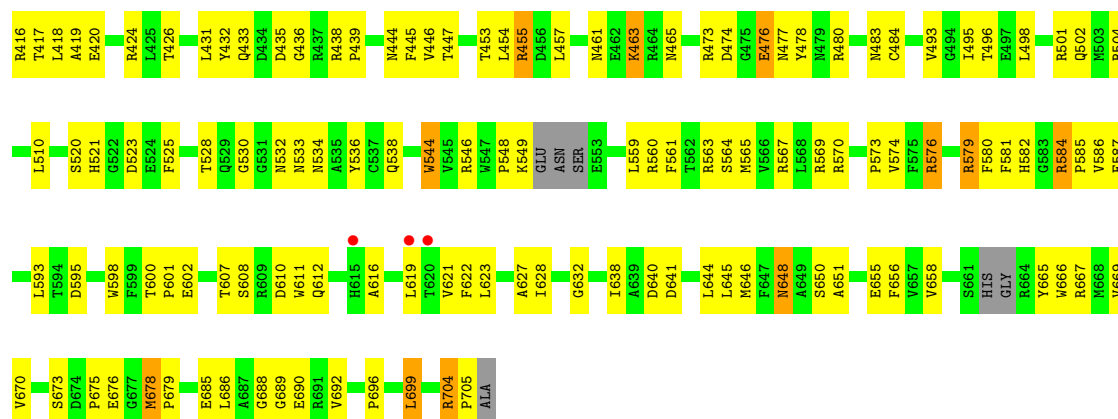
Chain D: 60% 37% ..



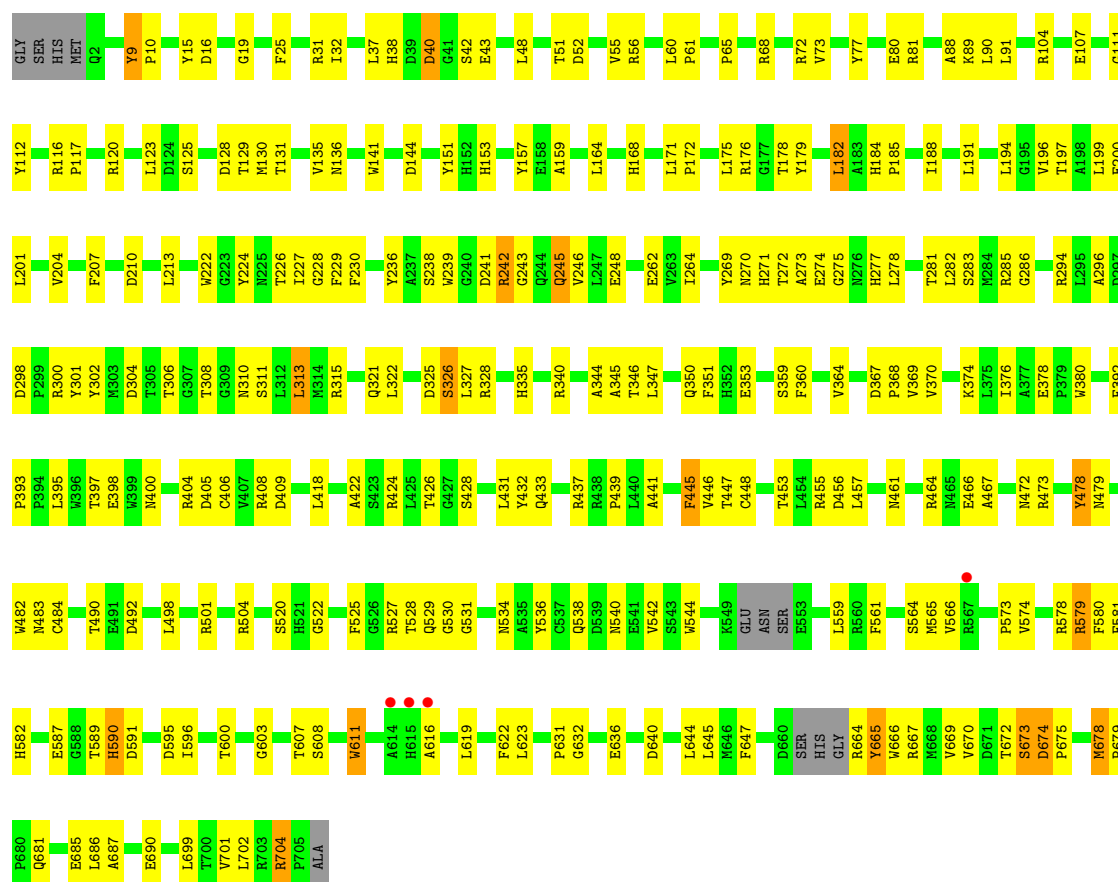
• Molecule 1: Glycogen debranching enzyme GlgX

Chain E: 60% 36% ..

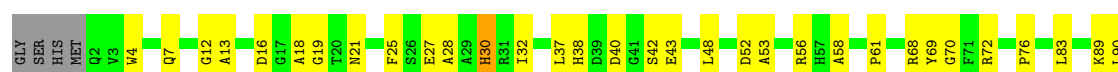




• Molecule 1: Glycogen debranching enzyme GlgX

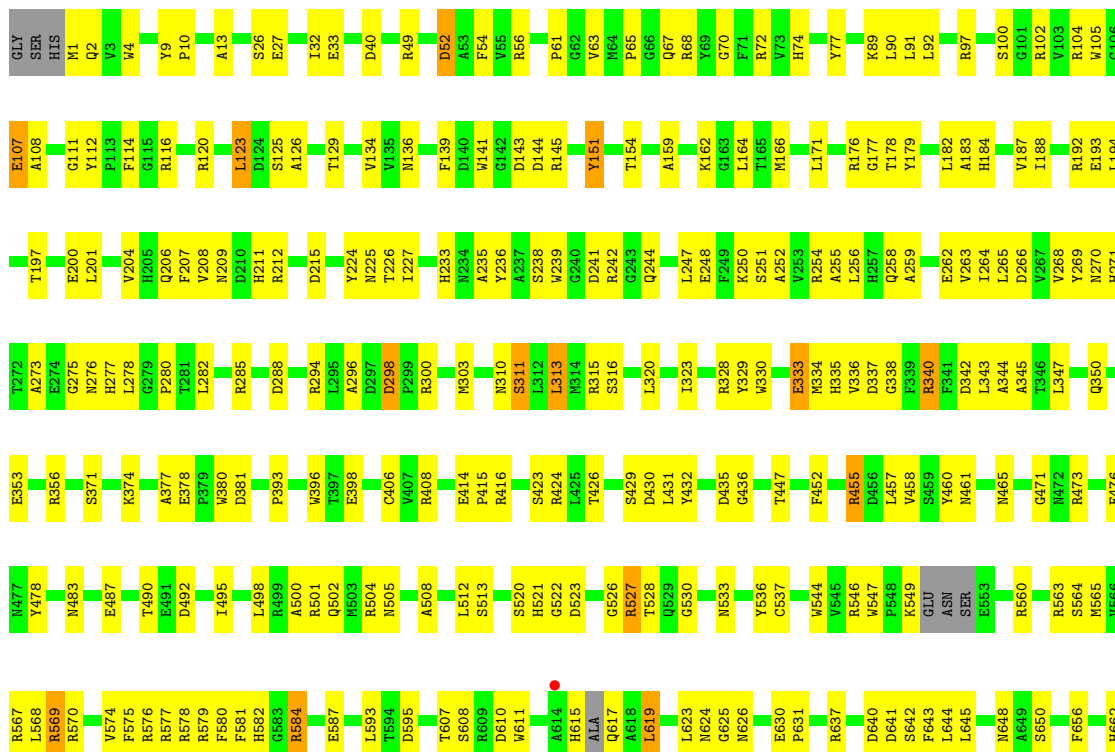


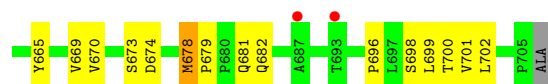
• Molecule 1: Glycogen debranching enzyme GlgX



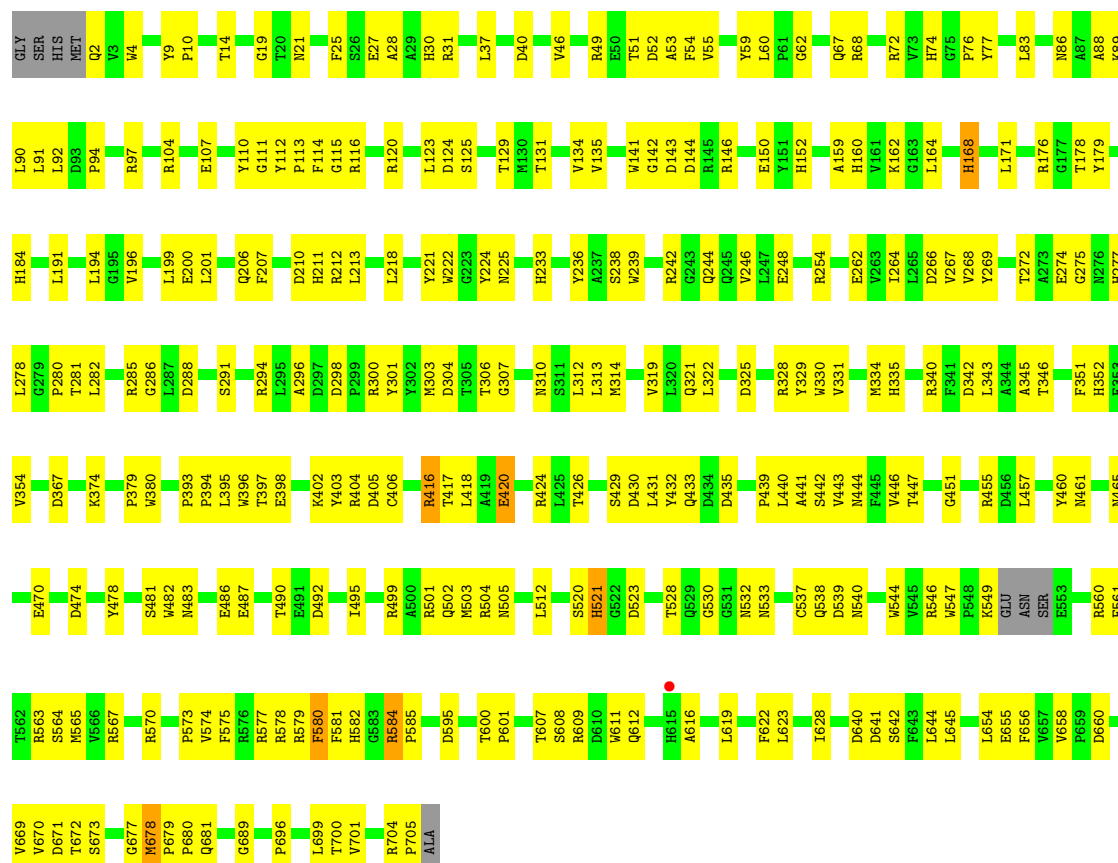


Chain H:  60% 37% .

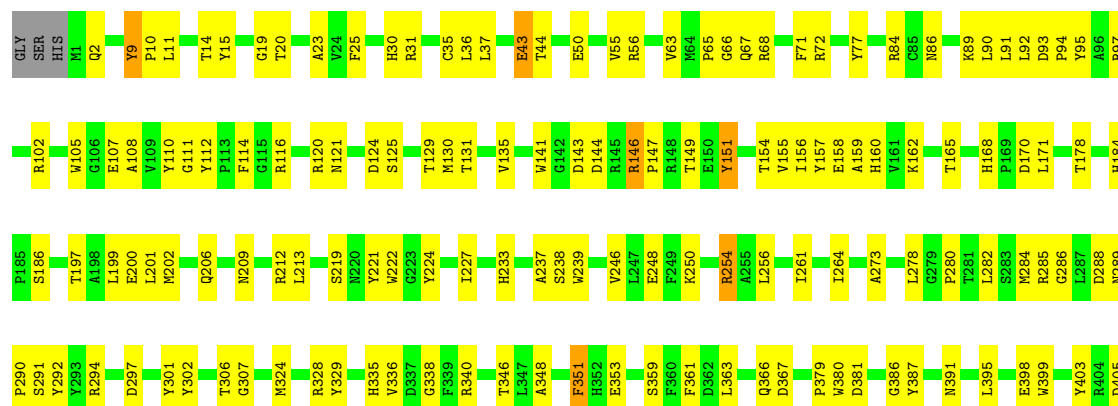


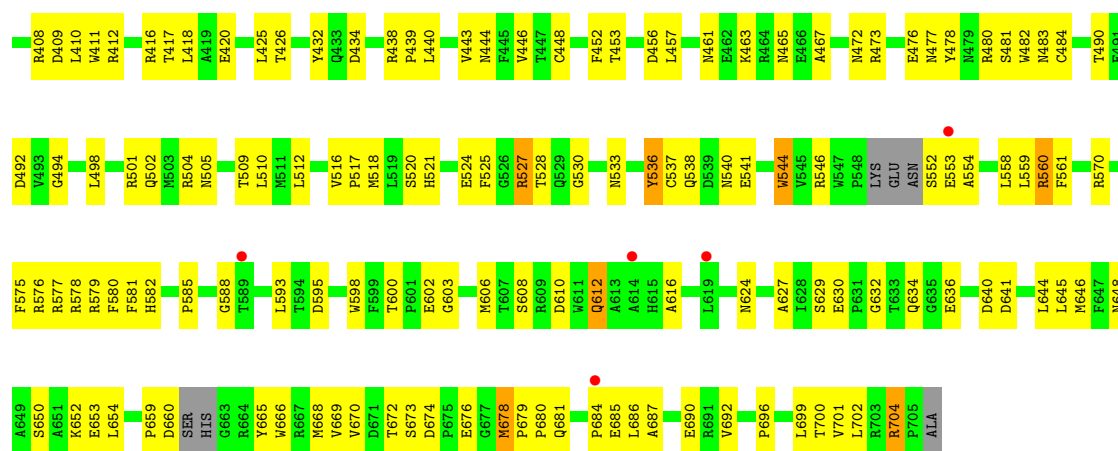


- Molecule 1: Glycogen debranching enzyme GlgX

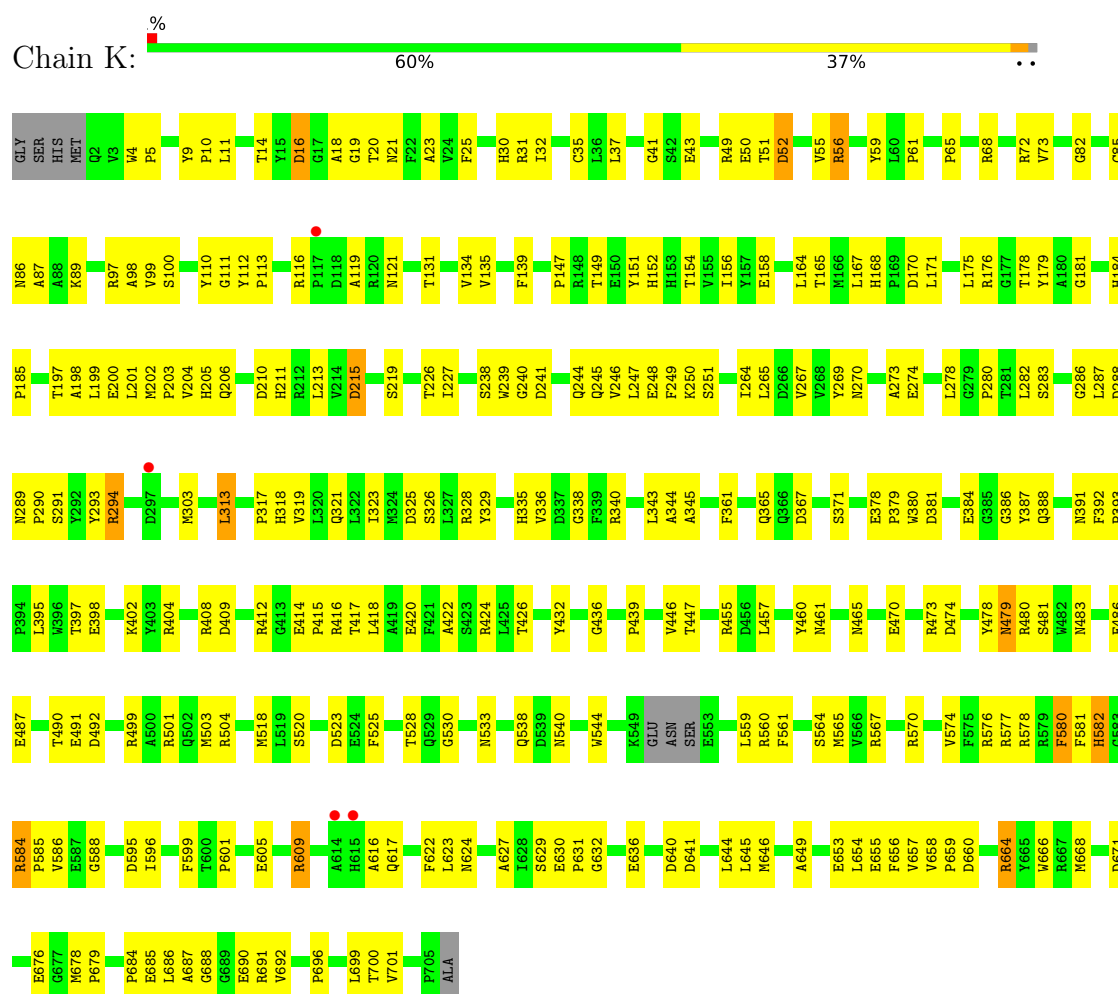


- Molecule 1: Glycogen debranching enzyme GlgX

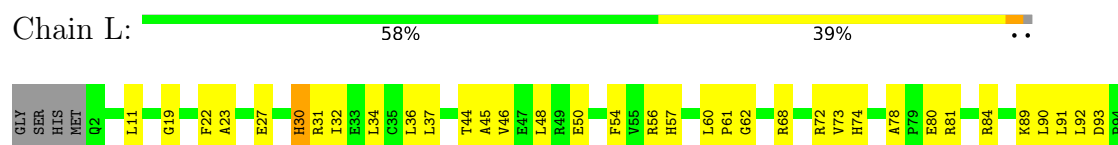




• Molecule 1: Glycogen debranching enzyme GlgX



• Molecule 1: Glycogen debranching enzyme GlgX





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	181.50Å 204.86Å 195.72Å 90.00° 90.43° 90.00°	Depositor
Resolution (Å)	67.92 – 3.51 67.92 – 3.66	Depositor EDS
% Data completeness (in resolution range)	83.5 (67.92-3.51) 83.5 (67.92-3.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.211 , 0.276 0.209 , 0.273	Depositor DCC
R_{free} test set	1920 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.912	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 20.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.037 for -h,-l,-k 0.035 for -h,l,k 0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	67324	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/5720	0.58	4/7785 (0.1%)
1	B	0.30	0/5750	0.56	5/7825 (0.1%)
1	C	0.31	0/5700	0.54	0/7752
1	D	0.30	0/5718	0.55	1/7779 (0.0%)
1	E	0.31	0/5719	0.56	0/7781
1	F	0.30	0/5701	0.54	2/7757 (0.0%)
1	G	0.30	0/5706	0.53	0/7763
1	H	0.31	0/5723	0.54	0/7785
1	I	0.29	0/5737	0.54	0/7805
1	J	0.31	0/5709	0.56	2/7768 (0.0%)
1	K	0.30	0/5737	0.56	0/7805
1	L	0.30	0/5715	0.54	3/7776 (0.0%)
All	All	0.30	0/68635	0.55	17/93381 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	L	0	1
All	All	0	11

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	ASP	N-CA-C	-8.64	87.67	111.00
1	J	673	SER	C-N-CA	-7.04	104.10	121.70
1	A	298	ASP	CB-CA-C	6.68	123.76	110.40
1	A	546	ARG	C-N-CA	-6.09	106.48	121.70
1	B	673	SER	C-N-CA	-6.05	106.57	121.70
1	L	673	SER	C-N-CA	-5.87	107.02	121.70
1	F	673	SER	C-N-CA	-5.47	108.01	121.70
1	F	182	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	299	PRO	N-CA-CB	-5.26	96.82	102.60
1	B	351	PHE	N-CA-C	5.22	125.11	111.00
1	D	436	GLY	N-CA-C	-5.22	100.04	113.10
1	B	355	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	342	ASP	CB-CG-OD2	5.14	122.93	118.30
1	L	431	LEU	CA-CB-CG	5.07	126.96	115.30
1	B	350	GLN	N-CA-C	5.06	124.67	111.00
1	J	593	LEU	CA-CB-CG	5.05	126.91	115.30
1	L	699	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	586	VAL	Peptide
1	B	661	SER	Peptide
1	B	678	MET	Peptide
1	D	678	MET	Peptide
1	E	678	MET	Peptide
1	F	678	MET	Peptide
1	G	678	MET	Peptide
1	H	678	MET	Peptide
1	I	678	MET	Peptide
1	J	678	MET	Peptide
1	L	678	MET	Peptide

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	5567	0	5245	200	0
1	B	5595	0	5282	204	0
1	C	5551	0	5244	228	0
1	D	5566	0	5256	179	0
1	E	5567	0	5253	194	0
1	F	5549	0	5234	173	0
1	G	5554	0	5246	186	0
1	H	5570	0	5254	178	0
1	I	5583	0	5274	192	0
1	J	5557	0	5240	199	0
1	K	5583	0	5274	192	0
1	L	5564	0	5244	201	0
2	A	56	0	0	1	0
2	B	56	0	0	0	0
2	C	63	0	0	0	0
2	D	43	0	0	1	0
2	E	42	0	0	2	0
2	F	43	0	0	0	0
2	G	27	0	0	0	0
2	H	41	0	0	1	0
2	I	38	0	0	4	0
2	J	38	0	0	1	0
2	K	37	0	0	0	0
2	L	34	0	0	2	0
All	All	67324	0	63046	2278	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 18.

All (2278) 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:H:102:ARG:HH12	1:H:208:VAL:HA	1.32	0.94
1:B:294:ARG:HH22	1:B:305:THR:HG23	1.32	0.94
1:C:493:VAL:HA	1:C:496:THR:HB	1.54	0.90
1:J:391:ASN:HD21	1:K:317:PRO:HG3	1.36	0.90
1:B:501:ARG:NH2	1:B:696:PRO:O	2.05	0.89
1:L:501:ARG:NH2	1:L:696:PRO:O	2.06	0.88
1:A:227:ILE:HD12	1:A:228:GLY:H	1.39	0.86
1:A:254:ARG:NH1	1:A:258:GLN:OE1	2.09	0.85
1:F:32:ILE:HG12	1:F:73:VAL:HG22	1.56	0.85
1:C:653:GLU:HG3	1:C:696:PRO:HD3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:239:TRP:O	1:H:244:GLN:NE2	2.11	0.83
1:G:513:SER:O	1:G:569:ARG:NH2	2.10	0.83
1:H:227:ILE:HG23	1:H:273:ALA:HB3	1.60	0.83
1:J:227:ILE:HG23	1:J:273:ALA:HB3	1.60	0.83
1:A:225:ASN:HD22	1:A:271:HIS:HE1	1.25	0.83
1:B:599:PHE:HB2	1:B:620:THR:HB	1.58	0.83
1:F:501:ARG:HG3	1:F:672:THR:HG22	1.59	0.82
1:H:584:ARG:NH1	1:H:630:GLU:OE2	2.12	0.82
1:A:206:GLN:HG2	1:A:227:ILE:HD11	1.59	0.82
1:D:429:SER:HB3	1:D:581:PHE:O	1.80	0.82
1:I:239:TRP:O	1:I:244:GLN:NE2	2.11	0.82
1:K:409:ASP:OD1	1:K:412:ARG:NH1	2.13	0.82
1:E:528:THR:HG22	1:E:530:GLY:H	1.45	0.82
1:I:460:TYR:HA	1:I:487:GLU:HG3	1.62	0.82
1:E:206:GLN:HG3	1:E:233:HIS:HA	1.60	0.81
1:C:671:ASP:H	1:C:678:MET:HB3	1.46	0.81
1:B:89:LYS:HE3	1:B:111:GLY:HA2	1.61	0.81
1:C:501:ARG:NH2	1:C:696:PRO:O	2.14	0.81
1:K:32:ILE:HD12	1:K:56:ARG:HG3	1.59	0.81
1:J:461:ASN:OD1	1:J:483:ASN:ND2	2.14	0.81
1:L:102:ARG:HD3	1:L:102:ARG:H	1.47	0.80
1:E:658:VAL:O	1:E:689:GLY:N	2.14	0.80
1:G:528:THR:HG22	1:G:530:GLY:H	1.47	0.80
1:J:608:SER:O	1:J:612:GLN:NE2	2.14	0.80
1:A:529:GLN:NE2	1:A:532:ASN:O	2.14	0.80
1:C:579:ARG:NH2	1:I:51:THR:O	2.15	0.80
1:A:52:ASP:OD1	1:E:579:ARG:NH2	2.15	0.80
1:A:426:THR:HG21	1:A:586:VAL:HG12	1.63	0.80
1:D:206:GLN:HG3	1:D:233:HIS:HA	1.63	0.80
1:F:199:LEU:HD22	1:F:201:LEU:HD12	1.63	0.79
1:L:227:ILE:HG23	1:L:273:ALA:HB3	1.63	0.79
1:B:461:ASN:OD1	1:B:483:ASN:ND2	2.14	0.79
1:K:416:ARG:HD2	1:K:420:GLU:HG2	1.65	0.79
1:A:306:THR:HA	1:A:346:THR:HG21	1.65	0.79
1:G:199:LEU:HD22	1:G:201:LEU:HD12	1.65	0.79
1:F:528:THR:HG22	1:F:530:GLY:H	1.48	0.79
1:G:501:ARG:NH2	1:G:696:PRO:O	2.16	0.79
1:I:567:ARG:HG3	1:I:570:ARG:HH21	1.48	0.78
1:D:89:LYS:NZ	1:D:108:ALA:O	2.17	0.78
1:I:574:VAL:HG22	1:I:628:ILE:HD11	1.64	0.78
1:F:501:ARG:HD2	1:F:673:SER:HA	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:484:CYS:HB3	1:G:498:LEU:HD22	1.66	0.77
1:L:426:THR:HG23	1:L:581:PHE:HB2	1.66	0.77
1:I:528:THR:HG22	1:I:530:GLY:H	1.47	0.77
1:J:143:ASP:H	1:J:254:ARG:HH21	1.30	0.77
1:C:504:ARG:HB2	1:C:672:THR:HG23	1.67	0.77
1:A:43:GLU:OE2	1:A:72:ARG:NH1	2.17	0.77
1:I:178:THR:HG21	1:I:238:SER:HB3	1.67	0.77
1:E:648:ASN:ND2	1:E:650:SER:O	2.18	0.77
1:G:504:ARG:HB2	1:G:672:THR:HG23	1.65	0.76
1:I:199:LEU:HD22	1:I:201:LEU:HD12	1.68	0.76
1:K:361:PHE:HD1	1:K:393:PRO:HD3	1.50	0.76
1:H:143:ASP:O	1:H:145:ARG:N	2.19	0.76
1:L:32:ILE:HD12	1:L:56:ARG:HG3	1.67	0.76
1:B:269:TYR:HB2	1:B:347:LEU:HD11	1.67	0.76
1:G:597:ALA:HB3	1:G:622:PHE:HB3	1.66	0.76
1:D:461:ASN:HD21	1:D:483:ASN:HD22	1.31	0.75
1:D:667:ARG:HD3	1:D:685:GLU:HG2	1.68	0.75
1:I:501:ARG:NH2	1:I:696:PRO:O	2.20	0.75
1:K:199:LEU:HD22	1:K:201:LEU:HD12	1.69	0.75
1:H:298:ASP:OD1	1:H:300:ARG:NH1	2.20	0.75
1:C:644:LEU:HD21	1:C:659:PRO:HD2	1.67	0.75
1:D:93:ASP:HB3	1:D:96:ALA:HB2	1.67	0.75
1:I:206:GLN:HG3	1:I:233:HIS:HA	1.67	0.75
1:B:178:THR:HG21	1:B:238:SER:HB3	1.67	0.75
1:C:156:ILE:HB	1:C:518:MET:HG3	1.69	0.75
1:F:422:ALA:O	1:F:426:THR:OG1	2.05	0.75
1:J:306:THR:HG23	1:J:346:THR:HG21	1.69	0.75
1:B:159:ALA:HB1	1:B:164:LEU:HG	1.68	0.75
1:I:490:THR:HG22	1:I:492:ASP:H	1.50	0.75
1:I:2:GLN:N	2:I:802:HOH:O	2.20	0.74
1:J:501:ARG:NH2	1:J:696:PRO:O	2.20	0.74
1:I:402:LYS:HD2	1:I:431:LEU:HD11	1.69	0.74
1:E:669:VAL:HG13	1:E:670:VAL:HG23	1.68	0.74
1:F:644:LEU:HD23	1:F:702:LEU:HD12	1.67	0.74
1:I:86:ASN:HA	1:I:120:ARG:HH21	1.50	0.74
1:K:227:ILE:HG23	1:K:273:ALA:HB3	1.67	0.74
1:L:161:VAL:HG22	1:L:201:LEU:HD23	1.67	0.74
1:A:300:ARG:HG3	1:A:300:ARG:HH11	1.52	0.74
1:E:178:THR:HG21	1:E:238:SER:HB3	1.68	0.74
1:L:151:TYR:HE1	1:L:397:THR:HG21	1.52	0.74
1:A:671:ASP:HB3	1:A:678:MET:HG3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:VAL:HG13	1:B:670:VAL:HG23	1.68	0.74
1:E:89:LYS:HA	1:E:125:SER:HB3	1.68	0.74
1:J:89:LYS:HE3	1:J:111:GLY:HA2	1.69	0.74
1:K:486:GLU:O	1:K:499:ARG:NH2	2.21	0.74
1:J:72:ARG:NH2	1:J:124:ASP:OD1	2.20	0.74
1:E:253:VAL:HG22	1:E:263:VAL:HG21	1.70	0.73
1:H:580:PHE:O	1:H:584:ARG:NH2	2.21	0.73
1:A:89:LYS:HE3	1:A:111:GLY:HA2	1.70	0.73
1:B:581:PHE:HD1	1:B:584:ARG:HD3	1.52	0.73
1:C:397:THR:HG22	1:C:441:ALA:HB3	1.68	0.73
1:G:28:ALA:N	1:G:288:ASP:OD1	2.22	0.73
1:J:465:ASN:ND2	1:J:533:ASN:OD1	2.18	0.73
1:C:365:GLN:OE1	1:C:391:ASN:ND2	2.21	0.73
1:C:423:SER:HA	1:C:426:THR:HB	1.68	0.73
1:E:574:VAL:HG22	1:E:628:ILE:HD11	1.70	0.73
1:G:38:HIS:O	1:G:68:ARG:NH2	2.21	0.73
1:C:409:ASP:OD2	1:C:416:ARG:NH1	2.22	0.73
1:D:574:VAL:HG11	1:D:623:LEU:HB3	1.71	0.73
1:K:99:VAL:HB	1:K:206:GLN:HE22	1.54	0.73
1:C:135:VAL:HG13	1:C:246:VAL:HG11	1.70	0.73
1:G:155:VAL:HG13	1:G:517:PRO:HG2	1.69	0.73
1:C:206:GLN:HG3	1:C:233:HIS:HA	1.70	0.73
1:C:585:PRO:HG2	1:C:588:GLY:H	1.54	0.72
1:E:141:TRP:HB3	1:E:144:ASP:HB2	1.70	0.72
1:F:89:LYS:HE3	1:F:111:GLY:HA2	1.70	0.72
1:K:156:ILE:HB	1:K:518:MET:HG3	1.71	0.72
1:F:40:ASP:OD1	1:F:42:SER:OG	2.06	0.72
1:G:89:LYS:HE3	1:G:111:GLY:HA2	1.70	0.72
1:C:225:ASN:HD22	1:C:271:HIS:CE1	2.06	0.72
1:G:433:GLN:HG2	1:G:438:ARG:HB2	1.69	0.72
1:E:43:GLU:HG2	1:E:72:ARG:HH12	1.54	0.72
1:D:2:GLN:N	2:D:801:HOH:O	2.21	0.72
1:D:199:LEU:HD22	1:D:201:LEU:HD12	1.70	0.72
1:E:365:GLN:OE1	1:E:391:ASN:ND2	2.22	0.72
1:H:501:ARG:HD2	1:H:673:SER:HA	1.70	0.72
1:L:274:GLU:OE1	1:L:293:TYR:OH	2.07	0.72
1:G:269:TYR:HB2	1:G:347:LEU:HD11	1.69	0.71
1:G:660:ASP:OD2	1:G:666:TRP:NE1	2.23	0.71
1:I:110:TYR:HA	1:I:280:PRO:HA	1.70	0.71
1:A:579:ARG:NH2	1:E:52:ASP:OD1	2.23	0.71
1:J:490:THR:HG22	1:J:492:ASP:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:THR:HG23	1:A:308:THR:H	1.55	0.71
1:A:381:ASP:HA	1:A:386:GLY:HA2	1.73	0.71
1:C:288:ASP:OD2	1:C:291:SER:OG	2.06	0.71
1:J:585:PRO:HG2	1:J:588:GLY:H	1.55	0.71
1:A:640:ASP:OD2	1:A:641:ASP:N	2.23	0.71
1:C:32:ILE:HD12	1:C:56:ARG:HG3	1.71	0.71
1:D:314:MET:HB2	1:D:354:VAL:HG21	1.71	0.71
1:G:644:LEU:HB3	1:G:702:LEU:HB2	1.71	0.71
1:L:89:LYS:HE3	1:L:111:GLY:HA2	1.71	0.71
1:A:227:ILE:HG23	1:A:273:ALA:HB3	1.73	0.71
1:D:15:TYR:HE1	1:D:64:MET:HA	1.54	0.71
1:B:306:THR:HB	1:B:346:THR:HG21	1.71	0.70
1:G:404:ARG:NH1	1:G:405:ASP:OD1	2.24	0.70
1:F:144:ASP:OD2	1:F:335:HIS:ND1	2.23	0.70
1:H:89:LYS:HE3	1:H:111:GLY:HA2	1.74	0.70
1:E:89:LYS:HE3	1:E:111:GLY:HA2	1.72	0.70
1:J:90:LEU:H	1:J:125:SER:HB3	1.55	0.70
1:J:686:LEU:HD13	1:J:692:VAL:HG21	1.74	0.70
1:L:528:THR:HG22	1:L:530:GLY:H	1.56	0.70
1:F:446:VAL:HG23	1:F:447:THR:HG22	1.74	0.70
1:H:426:THR:HG23	1:H:581:PHE:HB2	1.74	0.70
1:C:225:ASN:HD22	1:C:271:HIS:HE1	1.39	0.70
1:F:227:ILE:HG23	1:F:273:ALA:HB3	1.74	0.70
1:D:468:ASN:ND2	1:D:534:ASN:O	2.25	0.69
1:I:396:TRP:O	2:I:801:HOH:O	2.10	0.69
1:K:461:ASN:HD21	1:K:483:ASN:HD22	1.40	0.69
1:C:159:ALA:HA	1:C:521:HIS:ND1	2.07	0.69
1:E:116:ARG:NH2	2:E:801:HOH:O	2.25	0.69
1:L:584:ARG:NH2	1:L:630:GLU:OE2	2.25	0.69
1:A:227:ILE:HD12	1:A:228:GLY:N	2.08	0.69
1:A:660:ASP:HB3	1:A:666:TRP:HE1	1.56	0.69
1:B:661:SER:HB3	1:B:664:ARG:HE	1.57	0.69
1:D:426:THR:HG22	1:D:581:PHE:HB2	1.73	0.69
1:G:393:PRO:HG2	1:G:396:TRP:HB2	1.75	0.69
1:E:600:THR:HG22	1:E:602:GLU:H	1.58	0.69
1:L:151:TYR:HD2	1:L:374:LYS:HZ2	1.39	0.69
1:E:10:PRO:HG2	1:E:14:THR:HG21	1.75	0.69
1:H:294:ARG:NH2	1:H:353:GLU:OE2	2.26	0.69
1:D:10:PRO:HG2	1:D:14:THR:HG21	1.75	0.69
1:F:426:THR:HG22	1:F:581:PHE:HB2	1.75	0.69
1:A:585:PRO:HG2	1:A:588:GLY:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:541:GLU:HA	1:C:544:TRP:CD1	2.27	0.69
1:J:453:THR:OG1	1:J:456:ASP:OD1	2.11	0.69
1:J:669:VAL:HG13	1:J:670:VAL:HG23	1.75	0.69
1:K:465:ASN:ND2	1:K:533:ASN:OD1	2.26	0.69
1:K:538:GLN:HG3	1:K:540:ASN:HD21	1.56	0.69
1:C:51:THR:O	1:I:579:ARG:NH2	2.26	0.69
1:D:225:ASN:HA	1:D:271:HIS:CE1	2.28	0.69
1:D:418:LEU:HD13	1:D:616:ALA:HB1	1.74	0.69
1:J:36:LEU:HB2	1:J:44:THR:HB	1.73	0.69
1:L:669:VAL:HG13	1:L:670:VAL:HG23	1.73	0.68
1:C:172:PRO:HG2	1:C:175:LEU:HG	1.74	0.68
1:C:501:ARG:O	1:C:505:ASN:ND2	2.26	0.68
1:D:32:ILE:HG12	1:D:73:VAL:HG22	1.76	0.68
1:E:560:ARG:O	1:E:564:SER:OG	2.11	0.68
1:D:686:LEU:HD13	1:D:692:VAL:HG21	1.75	0.68
1:G:664:ARG:HB3	1:G:704:ARG:HE	1.59	0.68
1:A:155:VAL:N	1:A:197:THR:OG1	2.17	0.68
1:D:37:LEU:HB2	1:D:68:ARG:HB2	1.74	0.68
1:B:288:ASP:OD2	1:B:291:SER:OG	2.11	0.68
1:B:645:LEU:HD22	1:B:701:VAL:HG22	1.75	0.68
1:G:340:ARG:NH2	1:G:378:GLU:OE1	2.27	0.68
1:H:648:ASN:HD21	1:H:696:PRO:HA	1.59	0.68
1:I:10:PRO:HG2	1:I:14:THR:HG21	1.76	0.68
1:E:81:ARG:NH1	2:E:802:HOH:O	2.27	0.68
1:I:224:TYR:HA	1:I:268:VAL:HG21	1.76	0.68
1:J:457:LEU:HD12	1:J:481:SER:HB3	1.76	0.68
1:L:151:TYR:CE1	1:L:397:THR:HG21	2.29	0.68
1:L:224:TYR:HA	1:L:268:VAL:HG21	1.75	0.68
1:L:490:THR:HG22	1:L:492:ASP:H	1.57	0.68
1:A:300:ARG:HH11	1:A:300:ARG:CG	2.07	0.68
1:A:429:SER:HB3	1:A:581:PHE:O	1.93	0.68
1:I:426:THR:HG23	1:I:581:PHE:HB2	1.76	0.68
1:J:381:ASP:HA	1:J:386:GLY:HA2	1.74	0.68
1:A:632:GLY:HA3	1:A:636:GLU:HG2	1.76	0.68
1:H:501:ARG:NH2	1:H:696:PRO:O	2.27	0.68
1:K:384:GLU:O	1:K:388:GLN:NE2	2.27	0.68
1:F:207:PHE:HA	1:F:226:THR:HA	1.76	0.67
1:H:579:ARG:HB3	1:H:584:ARG:HH22	1.58	0.67
1:L:158:GLU:HA	1:L:200:GLU:HB3	1.75	0.67
1:B:490:THR:HG22	1:B:492:ASP:H	1.57	0.67
1:C:578:ARG:HH21	1:C:631:PRO:HD2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:345:ALA:HA	1:G:380:TRP:HB3	1.74	0.67
1:C:241:ASP:OD1	1:C:242:ARG:NH1	2.26	0.67
1:F:448:CYS:HA	1:F:520:SER:HB3	1.76	0.67
1:J:294:ARG:HH12	1:J:353:GLU:HG3	1.58	0.67
1:L:417:THR:HB	1:L:420:GLU:H	1.59	0.67
1:C:640:ASP:OD2	1:C:641:ASP:N	2.28	0.67
1:E:658:VAL:HB	1:E:688:GLY:HA2	1.77	0.67
1:C:668:MET:HG2	1:C:678:MET:HE2	1.77	0.67
1:E:446:VAL:HG23	1:E:447:THR:HG22	1.77	0.67
1:H:224:TYR:HA	1:H:268:VAL:HG21	1.76	0.67
1:H:565:MET:HG2	1:H:679:PRO:HG3	1.77	0.67
1:I:461:ASN:OD1	1:I:483:ASN:ND2	2.28	0.67
1:B:199:LEU:HD22	1:B:201:LEU:HD12	1.77	0.67
1:B:201:LEU:HD23	1:B:204:VAL:HG11	1.77	0.67
1:B:294:ARG:NH1	1:B:350:GLN:HG2	2.10	0.67
1:B:46:VAL:HG11	1:B:60:LEU:HD21	1.76	0.67
1:D:294:ARG:NH2	1:D:353:GLU:OE2	2.27	0.67
1:C:125:SER:O	1:C:129:THR:OG1	2.13	0.67
1:E:210:ASP:HB2	1:E:213:LEU:HB2	1.76	0.67
1:C:89:LYS:NZ	1:C:108:ALA:O	2.24	0.66
1:E:404:ARG:HB2	1:E:445:PHE:O	1.95	0.66
1:G:294:ARG:HB2	1:G:313:LEU:HG	1.76	0.66
1:D:253:VAL:HG22	1:D:263:VAL:HG21	1.77	0.66
1:G:110:TYR:HH	1:G:211:HIS:HD1	1.41	0.66
1:K:501:ARG:NH2	1:K:696:PRO:O	2.26	0.66
1:F:461:ASN:HD21	1:F:483:ASN:HD22	1.41	0.66
1:I:608:SER:HA	1:I:611:TRP:HB2	1.76	0.66
1:B:227:ILE:HG23	1:B:273:ALA:HB3	1.77	0.66
1:E:438:ARG:HG3	1:E:439:PRO:HD2	1.78	0.66
1:G:288:ASP:OD2	1:G:291:SER:OG	2.12	0.66
1:L:171:LEU:HD22	1:L:184:HIS:CG	2.30	0.66
1:G:509:THR:O	1:G:513:SER:OG	2.13	0.66
1:I:416:ARG:HG2	1:I:420:GLU:HG2	1.78	0.66
1:A:300:ARG:HG3	1:A:300:ARG:NH1	2.08	0.66
1:K:446:VAL:HG23	1:K:447:THR:HG22	1.78	0.66
1:F:328:ARG:NH1	1:F:367:ASP:OD1	2.28	0.66
1:I:294:ARG:HE	1:I:303:MET:HB2	1.60	0.66
1:I:403:TYR:HD1	1:I:424:ARG:HB3	1.61	0.66
1:A:432:TYR:O	1:A:582:HIS:NE2	2.28	0.66
1:B:51:THR:HG23	1:B:56:ARG:HG2	1.77	0.66
1:D:15:TYR:CE1	1:D:64:MET:HA	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:GLU:OE1	1:E:374:LYS:NZ	2.26	0.66
1:E:418:LEU:HD11	1:E:619:LEU:HD11	1.78	0.66
1:H:608:SER:HA	1:H:611:TRP:HD1	1.61	0.66
1:K:99:VAL:HB	1:K:206:GLN:NE2	2.10	0.66
1:L:365:GLN:OE1	1:L:391:ASN:ND2	2.29	0.66
1:E:587:GLU:HG2	1:E:611:TRP:HE1	1.61	0.66
1:A:461:ASN:OD1	1:A:483:ASN:ND2	2.29	0.65
1:D:204:VAL:HG21	1:D:265:LEU:HD22	1.77	0.65
1:E:227:ILE:HG23	1:E:273:ALA:HB3	1.78	0.65
1:B:246:VAL:HG22	1:B:250:LYS:HE3	1.78	0.65
1:E:91:LEU:HD11	1:E:286:GLY:HA3	1.77	0.65
1:C:105:TRP:CE3	1:C:211:HIS:HB2	2.32	0.65
1:F:632:GLY:N	1:F:636:GLU:O	2.27	0.65
1:L:19:GLY:HA3	1:L:61:PRO:HA	1.76	0.65
1:L:624:ASN:N	2:L:801:HOH:O	2.29	0.65
1:A:644:LEU:HD23	1:A:702:LEU:HD12	1.77	0.65
1:E:621:VAL:HB	1:E:645:LEU:HD12	1.77	0.65
1:B:30:HIS:HB2	1:B:74:HIS:O	1.96	0.65
1:G:560:ARG:NH2	1:G:676:GLU:O	2.30	0.65
1:A:225:ASN:HD22	1:A:271:HIS:CE1	2.12	0.65
1:C:43:GLU:OE2	1:C:72:ARG:NH1	2.29	0.65
1:C:379:PRO:HD3	1:C:398:GLU:HB3	1.79	0.65
1:C:632:GLY:HA3	1:C:636:GLU:HG3	1.77	0.65
1:G:446:VAL:HG23	1:G:447:THR:HG22	1.79	0.65
1:E:173:GLU:HA	1:E:176:ARG:HG3	1.79	0.65
1:L:37:LEU:HD11	1:L:90:LEU:HD21	1.77	0.65
1:A:68:ARG:HB3	1:A:131:THR:HG21	1.78	0.64
1:K:19:GLY:HA3	1:K:61:PRO:HA	1.78	0.64
1:K:567:ARG:HG3	1:K:570:ARG:HH21	1.61	0.64
1:A:53:ALA:HA	1:E:436:GLY:HA3	1.77	0.64
1:J:155:VAL:HG13	1:J:517:PRO:HG2	1.79	0.64
1:D:72:ARG:NH2	1:D:124:ASP:OD1	2.30	0.64
1:I:210:ASP:HB2	1:I:213:LEU:HD13	1.79	0.64
1:A:168:HIS:CE1	1:A:170:ASP:HB2	2.33	0.64
1:J:463:LYS:HE2	1:J:477:ASN:HA	1.79	0.64
1:B:195:GLY:HA3	1:B:566:VAL:HG11	1.80	0.64
1:B:600:THR:HG22	1:B:602:GLU:H	1.63	0.64
1:D:344:ALA:HB3	1:D:378:GLU:HB3	1.79	0.64
1:D:501:ARG:HA	1:D:504:ARG:HD2	1.80	0.64
1:G:657:VAL:HG12	1:G:690:GLU:O	1.97	0.64
1:I:72:ARG:NH2	1:I:124:ASP:OD1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:LEU:HG	1:A:503:MET:HG2	1.80	0.64
1:C:39:ASP:HB2	1:J:66:GLY:HA3	1.79	0.64
1:E:501:ARG:NH2	1:E:696:PRO:O	2.24	0.64
1:A:201:LEU:HD23	1:A:204:VAL:HG11	1.79	0.64
1:C:200:GLU:HA	1:C:264:ILE:O	1.98	0.64
1:G:669:VAL:HG13	1:G:670:VAL:HG23	1.80	0.64
1:L:73:VAL:HG21	1:L:287:LEU:HA	1.80	0.64
1:A:110:TYR:HA	1:A:280:PRO:HA	1.80	0.64
1:G:344:ALA:HB3	1:G:378:GLU:H	1.63	0.64
1:G:409:ASP:OD2	1:G:480:ARG:NH1	2.31	0.64
1:E:504:ARG:NH2	1:E:675:PRO:O	2.31	0.63
1:C:476:GLU:H	1:C:533:ASN:HD21	1.45	0.63
1:I:262:GLU:OE2	1:I:374:LYS:NZ	2.26	0.63
1:J:666:TRP:O	1:J:685:GLU:HB2	1.98	0.63
1:K:89:LYS:HE3	1:K:111:GLY:HA2	1.80	0.63
1:H:490:THR:HG22	1:H:492:ASP:H	1.63	0.63
1:I:275:GLY:O	1:I:310:ASN:ND2	2.29	0.63
1:J:640:ASP:OD2	1:J:641:ASP:N	2.31	0.63
1:G:43:GLU:HG2	1:G:72:ARG:HH12	1.63	0.63
1:G:205:HIS:HB2	1:G:226:THR:HG21	1.80	0.63
1:G:664:ARG:HB3	1:G:704:ARG:NE	2.14	0.63
1:I:501:ARG:HA	1:I:504:ARG:HD2	1.81	0.63
1:H:578:ARG:HH22	1:H:631:PRO:HD2	1.64	0.63
1:B:224:TYR:HA	1:B:268:VAL:HG21	1.81	0.63
1:D:365:GLN:OE1	1:D:391:ASN:ND2	2.32	0.63
1:F:191:LEU:HB3	1:F:196:VAL:HG22	1.81	0.63
1:F:664:ARG:HG2	1:F:704:ARG:HH21	1.64	0.63
1:G:315:ARG:HH11	1:G:354:VAL:HG12	1.64	0.62
1:I:46:VAL:HG11	1:I:60:LEU:HD21	1.81	0.62
1:E:548:PRO:O	1:E:549:LYS:HD2	1.99	0.62
1:G:105:TRP:CE3	1:G:211:HIS:HB2	2.34	0.62
1:H:102:ARG:NH1	1:H:208:VAL:HA	2.10	0.62
1:B:473:ARG:NH1	1:C:307:GLY:HA2	2.15	0.62
1:C:253:VAL:HG22	1:C:263:VAL:HG21	1.81	0.62
1:E:651:ALA:O	1:E:696:PRO:HB3	1.99	0.62
1:F:129:THR:HG23	1:F:282:LEU:HD22	1.81	0.62
1:I:37:LEU:O	1:I:67:GLN:NE2	2.31	0.62
1:K:97:ARG:HB2	1:K:135:VAL:HG21	1.82	0.62
1:L:313:LEU:CD2	1:L:315:ARG:HG2	2.28	0.62
1:B:644:LEU:HD23	1:B:702:LEU:HD12	1.81	0.62
1:F:327:LEU:HD13	1:F:370:VAL:HG11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:TYR:HD1	1:C:424:ARG:HB3	1.62	0.62
1:A:446:VAL:HG13	1:A:510:LEU:HD22	1.81	0.62
1:C:342:ASP:OD1	1:C:343:LEU:N	2.32	0.62
1:I:25:PHE:HB2	1:I:55:VAL:HG22	1.80	0.62
1:F:418:LEU:HD13	1:F:616:ALA:HB1	1.80	0.62
1:G:422:ALA:O	1:G:426:THR:OG1	2.12	0.62
1:G:644:LEU:O	1:G:702:LEU:N	2.29	0.62
1:H:280:PRO:HB2	1:H:282:LEU:HG	1.80	0.62
1:I:417:THR:HB	1:I:420:GLU:H	1.64	0.62
1:K:345:ALA:HA	1:K:380:TRP:HB3	1.81	0.62
1:A:409:ASP:OD1	1:A:412:ARG:NH1	2.33	0.61
1:I:288:ASP:OD2	1:I:291:SER:OG	2.18	0.61
1:A:207:PHE:H	1:A:233:HIS:HD2	1.48	0.61
1:D:43:GLU:CD	1:D:72:ARG:HH12	2.04	0.61
1:E:167:LEU:HD13	1:E:544:TRP:HB3	1.82	0.61
1:E:418:LEU:HD13	1:E:616:ALA:HB1	1.82	0.61
1:I:446:VAL:HG23	1:I:447:THR:HG22	1.82	0.61
1:J:448:CYS:HA	1:J:520:SER:HB3	1.82	0.61
1:B:538:GLN:HG3	1:B:540:ASN:HD21	1.66	0.61
1:F:573:PRO:HD2	1:F:640:ASP:HB2	1.82	0.61
1:F:589:THR:O	1:F:591:ASP:N	2.34	0.61
1:I:97:ARG:HB2	1:I:135:VAL:HG21	1.80	0.61
1:I:146:ARG:HH22	1:I:331:VAL:HG13	1.65	0.61
1:G:501:ARG:HH21	1:G:698:SER:HB2	1.65	0.61
1:I:418:LEU:HD13	1:I:616:ALA:HB1	1.83	0.61
1:K:110:TYR:HA	1:K:280:PRO:HA	1.83	0.61
1:L:644:LEU:HD21	1:L:659:PRO:HD2	1.83	0.61
1:A:577:ARG:HH12	1:A:595:ASP:HB2	1.65	0.61
1:B:502:GLN:HA	1:B:505:ASN:HD22	1.66	0.61
1:C:151:TYR:HE1	1:C:395:LEU:HD22	1.64	0.61
1:I:274:GLU:O	1:I:285:ARG:NH2	2.33	0.61
1:A:528:THR:HG22	1:A:530:GLY:H	1.66	0.61
1:K:418:LEU:HD13	1:K:616:ALA:HB1	1.83	0.61
1:D:490:THR:HG22	1:D:492:ASP:H	1.65	0.61
1:E:194:LEU:HD12	1:E:563:ARG:HG3	1.81	0.61
1:E:418:LEU:HD21	1:E:619:LEU:HD21	1.83	0.61
1:F:579:ARG:NH2	1:H:52:ASP:OD1	2.33	0.61
1:G:451:GLY:HA2	1:G:533:ASN:HB2	1.83	0.61
1:J:288:ASP:OD2	1:J:291:SER:OG	2.19	0.61
1:L:168:HIS:HD2	1:L:187:VAL:HG22	1.65	0.61
1:B:460:TYR:HA	1:B:487:GLU:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:151:TYR:HE1	1:K:397:THR:HG21	1.66	0.61
1:D:465:ASN:ND2	1:D:533:ASN:OD1	2.26	0.60
1:E:463:LYS:HE2	1:E:477:ASN:HA	1.83	0.60
1:J:644:LEU:HD21	1:J:659:PRO:HD2	1.83	0.60
1:K:65:PRO:HA	1:K:134:VAL:HG12	1.82	0.60
1:K:664:ARG:HG3	1:K:664:ARG:O	2.01	0.60
1:D:274:GLU:OE1	1:D:293:TYR:OH	2.14	0.60
1:H:89:LYS:HA	1:H:125:SER:HB2	1.83	0.60
1:H:207:PHE:HA	1:H:226:THR:HA	1.83	0.60
1:A:99:VAL:HB	1:A:206:GLN:NE2	2.16	0.60
1:E:418:LEU:HG	1:E:611:TRP:CZ3	2.36	0.60
1:G:644:LEU:HD23	1:G:702:LEU:HD12	1.83	0.60
1:G:646:MET:N	1:G:700:THR:O	2.29	0.60
1:J:184:HIS:ND1	1:J:186:SER:OG	2.29	0.60
1:B:105:TRP:HB3	1:B:211:HIS:CD2	2.36	0.60
1:D:31:ARG:NH1	1:D:47:GLU:OE1	2.35	0.60
1:G:243:GLY:O	1:G:246:VAL:HG12	2.00	0.60
1:G:461:ASN:OD1	1:G:483:ASN:ND2	2.33	0.60
1:I:160:HIS:NE2	1:I:236:TYR:OH	2.32	0.60
1:K:577:ARG:NH2	1:K:629:SER:H	1.98	0.60
1:A:580:PHE:HD1	1:A:582:HIS:CE1	2.20	0.60
1:G:541:GLU:HA	1:G:544:TRP:CD1	2.37	0.60
1:H:595:ASP:HA	1:H:624:ASN:HB3	1.83	0.60
1:I:501:ARG:O	1:I:505:ASN:ND2	2.33	0.60
1:G:548:PRO:O	1:G:549:LYS:HD2	2.02	0.60
1:I:441:ALA:N	2:I:801:HOH:O	2.34	0.60
1:K:644:LEU:HB2	1:K:666:TRP:CZ3	2.37	0.60
1:I:89:LYS:HE3	1:I:111:GLY:HA2	1.83	0.60
1:K:426:THR:HG22	1:K:581:PHE:HB2	1.83	0.60
1:L:429:SER:HB3	1:L:581:PHE:O	2.01	0.60
1:C:327:LEU:HD13	1:C:370:VAL:HG11	1.83	0.60
1:I:144:ASP:OD2	1:I:335:HIS:ND1	2.35	0.60
1:E:150:GLU:OE1	1:E:152:HIS:NE2	2.35	0.60
1:J:206:GLN:HG3	1:J:233:HIS:HA	1.84	0.60
1:J:525:PHE:HE2	1:J:559:LEU:HD22	1.67	0.60
1:K:85:CYS:HA	1:K:286:GLY:HA2	1.83	0.60
1:C:446:VAL:HG23	1:C:447:THR:HG22	1.84	0.59
1:E:573:PRO:HD2	1:E:640:ASP:HB2	1.84	0.59
1:B:227:ILE:HD12	1:B:228:GLY:N	2.17	0.59
1:E:461:ASN:OD1	1:E:483:ASN:ND2	2.35	0.59
1:B:311:SER:HB2	1:B:350:GLN:NE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:461:ASN:HD21	1:C:483:ASN:HD22	1.49	0.59
1:H:238:SER:N	1:H:248:GLU:OE2	2.35	0.59
1:I:560:ARG:HA	1:I:563:ARG:HB2	1.83	0.59
1:K:461:ASN:ND2	1:K:483:ASN:HD22	2.00	0.59
1:L:408:ARG:HH21	1:L:479:ASN:HB3	1.67	0.59
1:A:352:HIS:HB2	1:A:357:LEU:HD22	1.85	0.59
1:K:577:ARG:HH22	1:K:629:SER:H	1.50	0.59
1:B:402:LYS:HD2	1:B:431:LEU:HD21	1.84	0.59
1:I:129:THR:HG23	1:I:282:LEU:HD22	1.85	0.59
1:I:430:ASP:N	1:I:430:ASP:OD1	2.32	0.59
1:A:13:ALA:HB1	1:A:134:VAL:HG22	1.84	0.59
1:A:502:GLN:HA	1:A:505:ASN:HD22	1.67	0.59
1:B:433:GLN:HG3	1:B:435:ASP:HB2	1.84	0.59
1:D:129:THR:HG22	1:D:130:MET:H	1.66	0.59
1:J:294:ARG:HH12	1:J:353:GLU:CG	2.16	0.59
1:K:171:LEU:HD22	1:K:184:HIS:CG	2.38	0.59
1:L:632:GLY:HA3	1:L:636:GLU:HG3	1.84	0.59
1:B:322:LEU:O	1:B:326:SER:N	2.33	0.59
1:C:430:ASP:N	1:C:430:ASP:OD1	2.36	0.59
1:C:671:ASP:OD1	1:C:673:SER:OG	2.13	0.59
1:L:194:LEU:HD12	1:L:563:ARG:HG3	1.83	0.59
1:J:280:PRO:O	1:J:285:ARG:NH2	2.34	0.59
1:K:288:ASP:OD2	1:K:291:SER:OG	2.11	0.59
1:K:490:THR:HG22	1:K:491:GLU:H	1.67	0.59
1:B:664:ARG:HG2	1:B:704:ARG:HH21	1.68	0.59
1:I:86:ASN:HA	1:I:120:ARG:NH2	2.16	0.59
1:J:162:LYS:HE2	1:J:544:TRP:HH2	1.68	0.59
1:H:643:PHE:HE2	1:H:669:VAL:HG11	1.67	0.58
1:D:95:TYR:HA	1:D:230:PHE:CD1	2.38	0.58
1:J:159:ALA:HA	1:J:521:HIS:ND1	2.18	0.58
1:D:484:CYS:O	1:D:495:ILE:HD12	2.02	0.58
1:E:580:PHE:HB2	1:E:582:HIS:CD2	2.38	0.58
1:F:262:GLU:OE2	1:F:374:LYS:NZ	2.36	0.58
1:C:408:ARG:HA	1:C:506:PHE:HZ	1.67	0.58
1:L:405:ASP:O	1:L:416:ARG:NH1	2.37	0.58
1:E:155:VAL:HG12	1:E:196:VAL:HG12	1.85	0.58
1:K:269:TYR:HH	1:K:326:SER:HG	1.51	0.58
1:K:596:ILE:HG13	1:K:623:LEU:HD23	1.85	0.58
1:D:97:ARG:HD3	1:D:329:TYR:CE1	2.39	0.58
1:I:89:LYS:HA	1:I:125:SER:HB2	1.85	0.58
1:I:560:ARG:O	1:I:564:SER:OG	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:379:PRO:HD3	1:K:398:GLU:HB3	1.86	0.58
1:C:501:ARG:HA	1:C:504:ARG:HG3	1.85	0.58
1:E:409:ASP:OD2	1:E:416:ARG:NH2	2.37	0.58
1:F:77:TYR:CD2	1:F:120:ARG:HB2	2.39	0.58
1:F:275:GLY:O	1:F:310:ASN:ND2	2.37	0.58
1:E:520:SER:OG	1:E:523:ASP:OD2	2.21	0.58
1:B:105:TRP:HB3	1:B:211:HIS:HD2	1.67	0.58
1:E:595:ASP:HA	1:E:627:ALA:HB3	1.85	0.58
1:K:25:PHE:HB2	1:K:55:VAL:HG22	1.86	0.58
1:B:270:ASN:OD1	1:B:271:HIS:HD2	1.87	0.58
1:C:225:ASN:HD21	1:C:273:ALA:HA	1.68	0.58
1:F:608:SER:HA	1:F:611:TRP:HB2	1.84	0.58
1:J:157:TYR:HE1	1:J:524:GLU:OE1	1.86	0.58
1:L:157:TYR:O	1:L:200:GLU:N	2.33	0.58
1:A:184:HIS:ND1	1:A:186:SER:OG	2.28	0.57
1:A:318:HIS:ND1	1:A:318:HIS:O	2.37	0.57
1:B:465:ASN:ND2	1:B:533:ASN:OD1	2.35	0.57
1:D:345:ALA:HA	1:D:380:TRP:HB3	1.86	0.57
1:G:468:ASN:OD1	1:G:532:ASN:ND2	2.33	0.57
1:H:33:GLU:OE2	1:H:74:HIS:NE2	2.37	0.57
1:L:508:ALA:O	1:L:512:LEU:HG	2.04	0.57
1:A:155:VAL:H	1:A:197:THR:HG1	1.50	0.57
1:B:365:GLN:OE1	1:B:391:ASN:ND2	2.36	0.57
1:E:11:LEU:HA	1:E:23:ALA:HB3	1.85	0.57
1:I:306:THR:HA	1:I:346:THR:HG21	1.86	0.57
1:I:672:THR:HB	1:I:699:LEU:H	1.69	0.57
1:J:129:THR:HG23	1:J:282:LEU:HD22	1.86	0.57
1:L:640:ASP:OD2	1:L:641:ASP:N	2.37	0.57
1:A:364:VAL:HG13	1:A:370:VAL:HG12	1.86	0.57
1:A:686:LEU:HD13	1:A:692:VAL:HG21	1.85	0.57
1:C:68:ARG:HB3	1:C:131:THR:HG21	1.85	0.57
1:C:225:ASN:HA	1:C:271:HIS:CE1	2.39	0.57
1:I:580:PHE:HD1	1:I:582:HIS:NE2	2.02	0.57
1:J:452:PHE:HB3	1:J:456:ASP:HB2	1.86	0.57
1:H:9:TYR:CD2	1:H:10:PRO:HA	2.39	0.57
1:I:4:TRP:HB2	1:I:59:TYR:O	2.03	0.57
1:E:420:GLU:O	1:E:424:ARG:HG2	2.04	0.57
1:G:68:ARG:HD3	1:G:242:ARG:NH1	2.20	0.57
1:D:298:ASP:OD1	1:D:300:ARG:NH1	2.38	0.57
1:D:658:VAL:O	1:D:658:VAL:HG12	2.03	0.57
1:E:380:TRP:HZ3	1:E:396:TRP:CH2	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:484:CYS:HB3	1:E:498:LEU:HD23	1.87	0.57
1:F:37:LEU:HD11	1:F:90:LEU:HD21	1.86	0.57
1:J:146:ARG:HH21	1:J:335:HIS:HA	1.70	0.57
1:K:432:TYR:HB3	1:K:439:PRO:O	2.05	0.57
1:L:175:LEU:HD22	1:L:180:ALA:HB3	1.86	0.57
1:L:443:VAL:HA	1:L:516:VAL:HB	1.85	0.57
1:A:158:GLU:HA	1:A:200:GLU:HB3	1.87	0.57
1:A:296:ALA:HB3	1:A:303:MET:HG2	1.86	0.57
1:C:103:VAL:HG21	1:C:208:VAL:HG13	1.87	0.57
1:I:669:VAL:HG13	1:I:670:VAL:HG23	1.87	0.57
1:K:644:LEU:HD21	1:K:659:PRO:HD2	1.86	0.57
1:L:125:SER:O	1:L:125:SER:OG	2.22	0.57
1:B:541:GLU:OE2	1:B:546:ARG:NH2	2.38	0.57
1:E:398:GLU:OE1	1:E:432:TYR:HE1	1.87	0.57
1:H:429:SER:HB3	1:H:581:PHE:O	2.04	0.57
1:I:502:GLN:HA	1:I:505:ASN:HD22	1.70	0.57
1:L:405:ASP:OD2	1:L:480:ARG:NE	2.38	0.57
1:D:157:TYR:HD1	1:D:196:VAL:HG11	1.70	0.57
1:D:422:ALA:O	1:D:426:THR:OG1	2.22	0.57
1:F:490:THR:HG22	1:F:492:ASP:H	1.70	0.57
1:H:587:GLU:HG2	1:H:611:TRP:HZ2	1.70	0.57
1:H:670:VAL:HG13	1:H:679:PRO:HD3	1.86	0.57
1:J:561:PHE:HD2	1:J:679:PRO:HG3	1.69	0.57
1:K:490:THR:HG22	1:K:492:ASP:H	1.70	0.57
1:A:330:TRP:CE3	1:A:334:MET:HG3	2.40	0.57
1:D:379:PRO:HD3	1:D:398:GLU:HB3	1.85	0.57
1:F:239:TRP:CE3	1:F:248:GLU:HG2	2.40	0.57
1:G:595:ASP:HA	1:G:624:ASN:HB3	1.86	0.57
1:G:660:ASP:CG	1:G:666:TRP:HE1	2.08	0.57
1:A:89:LYS:O	1:A:91:LEU:HD22	2.05	0.56
1:K:528:THR:HG22	1:K:530:GLY:H	1.70	0.56
1:A:159:ALA:HB3	1:A:199:LEU:HD21	1.87	0.56
1:G:32:ILE:HD12	1:G:56:ARG:HG3	1.85	0.56
1:H:90:LEU:H	1:H:125:SER:HB3	1.69	0.56
1:A:501:ARG:HH21	1:A:698:SER:HB2	1.70	0.56
1:D:432:TYR:HD1	1:D:439:PRO:HB2	1.69	0.56
1:E:433:GLN:HG3	1:E:435:ASP:HB2	1.87	0.56
1:E:463:LYS:NZ	1:E:474:ASP:O	2.35	0.56
1:G:468:ASN:ND2	1:G:534:ASN:O	2.39	0.56
1:I:501:ARG:HG3	1:I:672:THR:HG22	1.88	0.56
1:C:243:GLY:O	1:C:246:VAL:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:LEU:HD22	1:C:611:TRP:CZ3	2.41	0.56
1:D:68:ARG:HB3	1:D:131:THR:HG21	1.88	0.56
1:E:154:THR:HA	1:E:197:THR:OG1	2.05	0.56
1:E:169:PRO:HA	1:E:176:ARG:HH21	1.70	0.56
1:A:416:ARG:HD2	1:A:420:GLU:HG2	1.87	0.56
1:A:501:ARG:O	1:A:505:ASN:ND2	2.38	0.56
1:A:645:LEU:HD22	1:A:701:VAL:HG22	1.88	0.56
1:B:117:PRO:HD3	1:C:217:GLY:HA3	1.86	0.56
1:E:351:PHE:HE1	1:E:360:PHE:CG	2.22	0.56
1:E:418:LEU:HG	1:E:611:TRP:HZ3	1.70	0.56
1:I:9:TYR:CD2	1:I:10:PRO:HA	2.40	0.56
1:K:11:LEU:HA	1:K:23:ALA:HB3	1.86	0.56
1:K:654:LEU:HD12	1:K:655:GLU:H	1.69	0.56
1:L:19:GLY:HA2	1:L:62:GLY:H	1.70	0.56
1:L:580:PHE:HD1	1:L:582:HIS:CE1	2.22	0.56
1:L:612:GLN:NE2	2:L:802:HOH:O	2.30	0.56
1:D:112:TYR:C	1:D:121:ASN:HB2	2.26	0.56
1:D:501:ARG:HA	1:D:504:ARG:HH11	1.71	0.56
1:E:160:HIS:O	1:E:164:LEU:HB2	2.06	0.56
1:F:678:MET:HG3	1:F:681:GLN:HG2	1.88	0.56
1:G:135:VAL:HG11	1:G:246:VAL:HG11	1.86	0.56
1:H:239:TRP:N	1:H:248:GLU:OE2	2.38	0.56
1:L:158:GLU:OE2	1:L:449:HIS:ND1	2.34	0.56
1:L:561:PHE:HA	1:L:679:PRO:HG2	1.88	0.56
1:A:281:THR:HG23	1:A:285:ARG:HB3	1.87	0.56
1:D:283:SER:O	1:D:287:LEU:HG	2.05	0.56
1:E:380:TRP:HZ3	1:E:396:TRP:HH2	1.53	0.56
1:F:408:ARG:HE	1:F:457:LEU:CD1	2.18	0.56
1:J:632:GLY:HA3	1:J:636:GLU:HG3	1.88	0.56
1:K:361:PHE:CD1	1:K:393:PRO:HD3	2.38	0.56
1:L:486:GLU:O	1:L:499:ARG:NH2	2.38	0.56
1:L:559:LEU:HG	1:L:563:ARG:HD3	1.86	0.56
1:C:38:HIS:ND1	1:J:65:PRO:HD2	2.21	0.56
1:C:265:LEU:HG	1:C:336:VAL:HG11	1.88	0.56
1:A:89:LYS:NZ	1:A:121:ASN:OD1	2.32	0.56
1:C:107:GLU:HG3	1:C:114:PHE:CD1	2.40	0.56
1:C:150:GLU:O	1:C:154:THR:OG1	2.23	0.56
1:D:433:GLN:HG2	1:D:438:ARG:HB2	1.87	0.56
1:H:423:SER:HA	1:H:426:THR:HB	1.88	0.56
1:H:569:ARG:NH2	1:H:575:PHE:O	2.38	0.56
1:J:391:ASN:HD21	1:K:317:PRO:CG	2.15	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:483:ASN:H	1:L:483:ASN:HD22	1.52	0.56
1:B:6:GLY:HA2	1:B:59:TYR:HB2	1.88	0.56
1:B:25:PHE:HB2	1:B:55:VAL:HG22	1.87	0.56
1:H:239:TRP:CE3	1:H:248:GLU:HG2	2.40	0.56
1:H:406:CYS:SG	1:H:416:ARG:NH1	2.79	0.56
1:H:625:GLY:N	1:H:642:SER:OG	2.34	0.56
1:K:239:TRP:CD2	1:K:248:GLU:HG3	2.41	0.56
1:K:678:MET:N	1:K:679:PRO:HD2	2.20	0.56
1:D:30:HIS:HB2	1:D:74:HIS:O	2.06	0.55
1:D:528:THR:HG22	1:D:530:GLY:H	1.71	0.55
1:F:578:ARG:HH22	1:F:631:PRO:HD2	1.70	0.55
1:G:89:LYS:HA	1:G:125:SER:HB3	1.87	0.55
1:I:191:LEU:HB3	1:I:196:VAL:HG22	1.88	0.55
1:L:470:GLU:O	1:L:473:ARG:NE	2.30	0.55
1:A:239:TRP:CD2	1:A:248:GLU:HG2	2.41	0.55
1:A:525:PHE:HE2	1:A:559:LEU:HD22	1.71	0.55
1:D:155:VAL:N	1:D:197:THR:OG1	2.26	0.55
1:G:408:ARG:O	1:G:412:ARG:HB2	2.06	0.55
1:I:345:ALA:HA	1:I:380:TRP:HB3	1.87	0.55
1:A:104:ARG:NH2	1:A:127:PRO:O	2.40	0.55
1:B:46:VAL:HG21	1:B:60:LEU:HD11	1.89	0.55
1:B:109:VAL:HA	1:B:125:SER:HB2	1.87	0.55
1:C:505:ASN:O	1:C:509:THR:OG1	2.15	0.55
1:E:565:MET:HE2	1:E:565:MET:HA	1.88	0.55
1:E:593:LEU:O	1:E:627:ALA:HB2	2.06	0.55
1:F:179:TYR:O	1:F:182:LEU:HB3	2.06	0.55
1:H:560:ARG:O	1:H:564:SER:OG	2.24	0.55
1:I:179:TYR:HB2	1:I:248:GLU:OE1	2.06	0.55
1:I:658:VAL:HB	1:I:689:GLY:H	1.72	0.55
1:F:467:ALA:HA	1:J:301:TYR:CZ	2.42	0.55
1:F:525:PHE:HE2	1:F:559:LEU:HD22	1.70	0.55
1:K:560:ARG:NH2	1:K:676:GLU:O	2.40	0.55
1:A:574:VAL:HG12	1:A:623:LEU:HD22	1.88	0.55
1:C:529:GLN:HG2	1:C:542:VAL:HG12	1.88	0.55
1:D:468:ASN:OD1	1:D:532:ASN:ND2	2.33	0.55
1:E:584:ARG:HB2	1:E:585:PRO:HD2	1.89	0.55
1:J:157:TYR:CE2	1:J:159:ALA:HB2	2.40	0.55
1:A:408:ARG:HE	1:A:457:LEU:HD13	1.71	0.55
1:B:557:THR:HA	1:B:560:ARG:HG2	1.87	0.55
1:C:264:ILE:HG12	1:C:338:GLY:HA3	1.86	0.55
1:G:108:ALA:HA	1:G:123:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:488:GLY:O	1:G:499:ARG:NH2	2.36	0.55
1:H:27:GLU:N	1:H:288:ASP:OD1	2.39	0.55
1:J:43:GLU:OE2	1:J:72:ARG:NH1	2.29	0.55
1:K:418:LEU:O	1:K:422:ALA:N	2.34	0.55
1:A:344:ALA:H	1:A:378:GLU:HG3	1.72	0.55
1:D:306:THR:HG21	1:D:346:THR:HG23	1.89	0.55
1:D:417:THR:HG22	1:D:419:ALA:H	1.72	0.55
1:D:564:SER:HA	1:D:567:ARG:HB2	1.89	0.55
1:D:585:PRO:HB2	1:D:587:GLU:HG2	1.88	0.55
1:E:239:TRP:CE3	1:E:248:GLU:HG2	2.42	0.55
1:H:640:ASP:OD2	1:H:641:ASP:N	2.40	0.55
1:J:159:ALA:O	1:J:202:MET:HG3	2.06	0.55
1:K:86:ASN:ND2	1:K:121:ASN:O	2.40	0.55
1:K:460:TYR:HA	1:K:487:GLU:HG3	1.88	0.55
1:L:346:THR:HG22	1:L:350:GLN:HE22	1.72	0.55
1:C:632:GLY:N	1:C:636:GLU:O	2.39	0.55
1:G:52:ASP:CG	1:L:579:ARG:HH22	2.09	0.55
1:I:607:THR:O	1:I:611:TRP:N	2.39	0.55
1:B:678:MET:HG3	1:B:681:GLN:HG2	1.89	0.55
1:C:227:ILE:HG23	1:C:273:ALA:HB3	1.89	0.55
1:E:71:PHE:O	1:E:91:LEU:N	2.38	0.55
1:G:201:LEU:N	1:G:264:ILE:O	2.32	0.55
1:I:162:LYS:NZ	1:I:539:ASP:OD1	2.38	0.55
1:J:644:LEU:HD23	1:J:702:LEU:HD12	1.89	0.55
1:A:461:ASN:HD21	1:A:483:ASN:H	1.54	0.54
1:G:664:ARG:HD3	1:G:664:ARG:N	2.22	0.54
1:H:200:GLU:HA	1:H:264:ILE:O	2.07	0.54
1:B:169:PRO:HA	1:B:176:ARG:HH21	1.71	0.54
1:B:311:SER:CB	1:B:350:GLN:NE2	2.70	0.54
1:C:191:LEU:HB3	1:C:196:VAL:HG22	1.89	0.54
1:C:283:SER:O	1:C:287:LEU:HG	2.07	0.54
1:K:561:PHE:CE1	1:K:565:MET:HG3	2.42	0.54
1:K:686:LEU:HD11	1:K:692:VAL:CG2	2.37	0.54
1:L:632:GLY:HA2	1:L:638:ILE:HD11	1.90	0.54
1:A:172:PRO:HG2	1:A:175:LEU:HG	1.88	0.54
1:A:460:TYR:HA	1:A:487:GLU:HG3	1.89	0.54
1:C:330:TRP:HA	1:C:334:MET:HB2	1.88	0.54
1:D:607:THR:OG1	1:D:610:ASP:HB2	2.07	0.54
1:E:194:LEU:HA	1:E:563:ARG:HG2	1.88	0.54
1:H:105:TRP:CD2	1:H:211:HIS:HB2	2.42	0.54
1:K:202:MET:HB3	1:K:203:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:344:ALA:HB3	1:L:378:GLU:H	1.72	0.54
1:A:159:ALA:O	1:A:202:MET:HG3	2.07	0.54
1:C:408:ARG:HA	1:C:506:PHE:CZ	2.42	0.54
1:E:431:LEU:HD22	1:E:432:TYR:CE1	2.42	0.54
1:F:112:TYR:CZ	1:F:278:LEU:HA	2.42	0.54
1:J:156:ILE:HB	1:J:518:MET:HG3	1.89	0.54
1:A:396:TRP:CE3	1:A:439:PRO:HG3	2.42	0.54
1:C:19:GLY:HA2	1:C:62:GLY:H	1.72	0.54
1:C:408:ARG:HG2	1:C:457:LEU:HD21	1.89	0.54
1:C:584:ARG:NH2	1:C:630:GLU:OE2	2.40	0.54
1:D:588:GLY:HA3	1:D:594:THR:OG1	2.08	0.54
1:E:379:PRO:HD3	1:E:398:GLU:HB3	1.88	0.54
1:G:393:PRO:O	1:G:395:LEU:N	2.39	0.54
1:H:460:TYR:HA	1:H:487:GLU:HG3	1.89	0.54
1:K:86:ASN:OD1	1:K:87:ALA:N	2.41	0.54
1:K:660:ASP:O	1:K:664:ARG:NH2	2.26	0.54
1:A:102:ARG:HH12	1:A:104:ARG:HH11	1.55	0.54
1:B:581:PHE:CD1	1:B:584:ARG:HD3	2.39	0.54
1:F:665:TYR:O	1:F:704:ARG:HG3	2.08	0.54
1:G:431:LEU:HB2	1:G:432:TYR:CE2	2.42	0.54
1:I:379:PRO:HD3	1:I:398:GLU:HB3	1.89	0.54
1:J:15:TYR:HD1	1:J:19:GLY:O	1.91	0.54
1:B:379:PRO:HD3	1:B:398:GLU:HB3	1.88	0.54
1:B:426:THR:HG23	1:B:581:PHE:HB2	1.89	0.54
1:C:619:LEU:HB2	1:C:647:PHE:HB2	1.90	0.54
1:E:110:TYR:OH	1:E:211:HIS:ND1	2.40	0.54
1:H:206:GLN:HG3	1:H:233:HIS:HA	1.89	0.54
1:C:476:GLU:HB2	1:C:533:ASN:ND2	2.22	0.54
1:J:645:LEU:HD22	1:J:701:VAL:HG22	1.89	0.54
1:K:653:GLU:HB3	1:K:696:PRO:HD3	1.89	0.54
1:L:476:GLU:N	1:L:533:ASN:HD21	2.06	0.54
1:E:207:PHE:HA	1:E:226:THR:HA	1.88	0.54
1:G:224:TYR:HA	1:G:268:VAL:HG21	1.88	0.54
1:H:393:PRO:HG2	1:H:396:TRP:HB2	1.90	0.54
1:L:361:PHE:HD1	1:L:393:PRO:HD2	1.72	0.54
1:L:505:ASN:ND2	1:L:697:LEU:O	2.39	0.54
1:A:5:PRO:HG2	1:E:632:GLY:O	2.08	0.54
1:A:194:LEU:HD11	1:A:562:THR:HG22	1.90	0.54
1:B:110:TYR:HA	1:B:280:PRO:HA	1.90	0.54
1:I:146:ARG:NH2	1:I:331:VAL:HG13	2.23	0.54
1:J:71:PHE:HE1	1:J:93:ASP:HB2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:35:CYS:HB3	1:K:43:GLU:HG2	1.89	0.54
1:L:584:ARG:HB2	1:L:585:PRO:HD2	1.90	0.54
1:A:414:GLU:HG3	1:A:415:PRO:HD3	1.90	0.53
1:C:171:LEU:HD22	1:C:184:HIS:CG	2.43	0.53
1:D:97:ARG:HB2	1:D:135:VAL:HG21	1.89	0.53
1:E:340:ARG:HA	1:E:376:ILE:O	2.08	0.53
1:E:565:MET:HG2	1:E:679:PRO:HG3	1.90	0.53
1:E:704:ARG:NH1	1:E:705:PRO:O	2.41	0.53
1:G:429:SER:HB3	1:G:581:PHE:O	2.08	0.53
1:I:658:VAL:HB	1:I:689:GLY:N	2.23	0.53
1:B:463:LYS:NZ	1:B:474:ASP:O	2.38	0.53
1:C:486:GLU:O	1:C:499:ARG:NH2	2.41	0.53
1:J:89:LYS:HA	1:J:125:SER:HB3	1.90	0.53
1:K:391:ASN:HA	1:K:436:GLY:O	2.08	0.53
1:B:294:ARG:HA	1:B:313:LEU:HG	1.90	0.53
1:C:205:HIS:HB2	1:C:226:THR:HG21	1.90	0.53
1:D:549:LYS:C	1:D:551:ASN:H	2.12	0.53
1:E:561:PHE:CE1	1:E:565:MET:HG3	2.43	0.53
1:F:269:TYR:HB2	1:F:347:LEU:HD11	1.90	0.53
1:F:306:THR:HA	1:F:346:THR:HG21	1.89	0.53
1:J:157:TYR:HE2	1:J:159:ALA:HB2	1.73	0.53
1:B:5:PRO:O	1:B:58:ALA:HA	2.09	0.53
1:C:671:ASP:N	1:C:678:MET:HB3	2.19	0.53
1:E:68:ARG:HB3	1:E:131:THR:HG21	1.90	0.53
1:E:455:ARG:HD2	1:E:528:THR:OG1	2.08	0.53
1:H:212:ARG:NH2	1:H:536:TYR:OH	2.41	0.53
1:H:574:VAL:HG11	1:H:623:LEU:HB3	1.90	0.53
1:C:589:THR:O	1:C:591:ASP:N	2.42	0.53
1:E:304:ASP:CG	1:E:307:GLY:H	2.11	0.53
1:F:200:GLU:HA	1:F:264:ILE:O	2.08	0.53
1:G:448:CYS:HA	1:G:520:SER:HB3	1.89	0.53
1:I:654:LEU:HD23	1:I:655:GLU:H	1.74	0.53
1:J:678:MET:HG3	1:J:681:GLN:HG3	1.91	0.53
1:K:16:ASP:HB2	1:K:59:TYR:HE1	1.72	0.53
1:K:426:THR:HG21	1:K:586:VAL:HG13	1.91	0.53
1:A:274:GLU:OE2	1:A:283:SER:N	2.40	0.53
1:C:351:PHE:HB3	1:C:357:LEU:HA	1.91	0.53
1:C:402:LYS:HD2	1:C:431:LEU:HD11	1.90	0.53
1:G:156:ILE:HB	1:G:518:MET:HG3	1.90	0.53
1:I:97:ARG:HD3	1:I:329:TYR:CZ	2.43	0.53
1:K:97:ARG:HD3	1:K:329:TYR:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:521:HIS:CD2	1:L:527:ARG:HH12	2.26	0.53
1:A:207:PHE:H	1:A:233:HIS:CD2	2.27	0.53
1:B:225:ASN:HA	1:B:271:HIS:CE1	2.44	0.53
1:C:452:PHE:HB3	1:C:456:ASP:HB2	1.91	0.53
1:C:678:MET:HE3	1:C:683:GLY:HA3	1.89	0.53
1:E:35:CYS:HB3	1:E:43:GLU:HG3	1.90	0.53
1:F:9:TYR:CD2	1:F:10:PRO:HA	2.43	0.53
1:F:619:LEU:HB2	1:F:647:PHE:HB2	1.89	0.53
1:K:210:ASP:HB2	1:K:213:LEU:HD13	1.90	0.53
1:K:525:PHE:HE2	1:K:559:LEU:HD22	1.74	0.53
1:B:10:PRO:HD2	1:B:14:THR:HG21	1.91	0.53
1:B:528:THR:HG22	1:B:530:GLY:H	1.73	0.53
1:H:644:LEU:HD23	1:H:702:LEU:HD12	1.90	0.53
1:I:107:GLU:HG2	1:I:114:PHE:CE2	2.44	0.53
1:B:144:ASP:OD2	1:B:335:HIS:ND1	2.42	0.53
1:C:417:THR:HG22	1:C:419:ALA:H	1.74	0.53
1:D:265:LEU:HD21	1:D:336:VAL:HG21	1.91	0.53
1:F:270:ASN:HA	1:F:350:GLN:HE22	1.74	0.53
1:I:429:SER:HB3	1:I:581:PHE:O	2.09	0.53
1:B:185:PRO:HA	1:B:188:ILE:HB	1.90	0.53
1:E:360:PHE:O	1:E:364:VAL:HG23	2.09	0.53
1:E:586:VAL:O	1:E:598:TRP:NE1	2.33	0.53
1:H:192:ARG:HD2	1:H:259:ALA:HB1	1.91	0.53
1:I:37:LEU:HD12	1:I:131:THR:HG21	1.91	0.53
1:I:600:THR:HG22	1:I:601:PRO:HD2	1.90	0.53
1:J:528:THR:HG22	1:J:530:GLY:H	1.74	0.53
1:K:294:ARG:HA	1:K:313:LEU:HG	1.90	0.53
1:C:476:GLU:N	1:C:533:ASN:HD21	2.07	0.52
1:D:168:HIS:CE1	1:D:170:ASP:HB2	2.43	0.52
1:E:31:ARG:NH1	1:E:47:GLU:OE2	2.36	0.52
1:G:13:ALA:HB1	1:G:134:VAL:HG22	1.90	0.52
1:I:679:PRO:HG2	1:I:680:PRO:HD3	1.90	0.52
1:B:311:SER:OG	1:B:350:GLN:NE2	2.42	0.52
1:D:274:GLU:OE2	1:D:283:SER:N	2.38	0.52
1:F:534:ASN:OD1	1:F:536:TYR:HD2	1.91	0.52
1:G:207:PHE:HB2	1:G:225:ASN:O	2.09	0.52
1:G:464:ARG:N	1:G:531:GLY:O	2.42	0.52
1:H:580:PHE:O	1:H:582:HIS:N	2.35	0.52
1:I:267:VAL:HB	1:I:269:TYR:CE1	2.44	0.52
1:J:143:ASP:H	1:J:254:ARG:NH2	2.05	0.52
1:J:158:GLU:HA	1:J:200:GLU:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:399:TRP:HA	1:J:443:VAL:HG23	1.90	0.52
1:K:640:ASP:OD2	1:K:641:ASP:N	2.42	0.52
1:A:11:LEU:HD13	1:A:318:HIS:NE2	2.24	0.52
1:A:144:ASP:OD2	1:A:335:HIS:ND1	2.35	0.52
1:C:50:GLU:OE2	1:I:578:ARG:NH2	2.41	0.52
1:F:210:ASP:HB2	1:F:213:LEU:HB2	1.90	0.52
1:J:20:THR:OG1	1:J:63:VAL:O	2.25	0.52
1:J:502:GLN:HA	1:J:505:ASN:HD22	1.73	0.52
1:L:246:VAL:HG22	1:L:250:LYS:HE3	1.91	0.52
1:A:670:VAL:HG13	1:A:679:PRO:HD3	1.92	0.52
1:B:36:LEU:HD11	1:B:60:LEU:HD12	1.91	0.52
1:F:504:ARG:HB3	1:F:561:PHE:CZ	2.45	0.52
1:G:458:VAL:HG11	1:G:502:GLN:HB3	1.91	0.52
1:K:617:GLN:HB2	1:K:649:ALA:HB3	1.92	0.52
1:L:351:PHE:HB3	1:L:357:LEU:HA	1.91	0.52
1:L:433:GLN:NE2	1:L:435:ASP:OD2	2.43	0.52
1:B:565:MET:HE1	1:B:568:LEU:HD22	1.91	0.52
1:D:402:LYS:O	1:D:406:CYS:HB2	2.08	0.52
1:D:404:ARG:O	1:D:408:ARG:HB2	2.10	0.52
1:D:584:ARG:H	1:D:584:ARG:HE	1.56	0.52
1:F:25:PHE:HB2	1:F:55:VAL:HG22	1.91	0.52
1:G:68:ARG:HD3	1:G:242:ARG:CZ	2.40	0.52
1:H:159:ALA:HA	1:H:521:HIS:ND1	2.24	0.52
1:A:393:PRO:HG2	1:A:396:TRP:CD1	2.45	0.52
1:E:632:GLY:HA2	1:E:638:ILE:HD11	1.92	0.52
1:H:1:MET:HG3	1:H:2:GLN:H	1.75	0.52
1:H:129:THR:HG23	1:H:282:LEU:HD22	1.91	0.52
1:J:418:LEU:HD21	1:J:606:MET:SD	2.50	0.52
1:K:200:GLU:HA	1:K:264:ILE:O	2.09	0.52
1:K:393:PRO:O	1:K:395:LEU:N	2.41	0.52
1:L:580:PHE:HB2	1:L:582:HIS:CE1	2.44	0.52
1:A:589:THR:O	1:A:591:ASP:N	2.43	0.52
1:C:524:GLU:O	1:C:558:LEU:HG	2.09	0.52
1:D:340:ARG:HA	1:D:376:ILE:O	2.10	0.52
1:D:483:ASN:HD22	1:D:483:ASN:H	1.58	0.52
1:F:484:CYS:HB3	1:F:498:LEU:HD22	1.91	0.52
1:F:600:THR:O	1:F:603:GLY:N	2.43	0.52
1:J:9:TYR:CD2	1:J:10:PRO:HA	2.45	0.52
1:J:97:ARG:HD3	1:J:329:TYR:CE1	2.44	0.52
1:J:162:LYS:HE2	1:J:544:TRP:CH2	2.45	0.52
1:K:601:PRO:HA	1:K:656:PHE:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:657:VAL:CG2	1:K:691:ARG:HE	2.22	0.52
1:C:99:VAL:HB	1:C:206:GLN:NE2	2.25	0.52
1:E:190:HIS:O	1:E:190:HIS:ND1	2.43	0.52
1:H:336:VAL:HG12	1:H:338:GLY:H	1.75	0.52
1:H:669:VAL:HG13	1:H:670:VAL:HG23	1.91	0.52
1:J:366:GLN:OE1	1:K:328:ARG:NH2	2.40	0.52
1:J:577:ARG:HH12	1:J:595:ASP:HB2	1.74	0.52
1:A:171:LEU:HD23	1:A:184:HIS:CD2	2.45	0.52
1:B:239:TRP:CD2	1:B:248:GLU:HG2	2.44	0.52
1:C:686:LEU:HD13	1:C:692:VAL:HG21	1.91	0.52
1:E:640:ASP:OD2	1:E:641:ASP:N	2.42	0.52
1:G:574:VAL:HG22	1:G:628:ILE:HD11	1.91	0.52
1:I:89:LYS:HG3	1:I:281:THR:HB	1.92	0.52
1:I:91:LEU:HD11	1:I:286:GLY:HA3	1.92	0.52
1:A:393:PRO:O	1:A:395:LEU:N	2.41	0.52
1:C:344:ALA:HB3	1:C:378:GLU:HG2	1.92	0.52
1:D:321:GLN:HG2	1:D:325:ASP:OD1	2.10	0.52
1:G:404:ARG:O	1:G:408:ARG:HB2	2.08	0.52
1:B:580:PHE:O	1:B:582:HIS:N	2.39	0.51
1:C:18:ALA:HB1	1:J:2:GLN:OE1	2.09	0.51
1:C:426:THR:HG23	1:C:581:PHE:CB	2.41	0.51
1:D:190:HIS:HA	1:D:193:GLU:HG2	1.92	0.51
1:D:271:HIS:HB3	1:D:308:THR:HB	1.92	0.51
1:D:505:ASN:O	1:D:509:THR:OG1	2.27	0.51
1:D:580:PHE:O	1:D:582:HIS:N	2.43	0.51
1:D:670:VAL:HB	1:D:701:VAL:HB	1.90	0.51
1:F:104:ARG:NH1	1:F:128:ASP:OD1	2.42	0.51
1:F:281:THR:HG23	1:F:285:ARG:HB3	1.92	0.51
1:H:112:TYR:CE2	1:H:278:LEU:HA	2.45	0.51
1:H:178:THR:HG21	1:H:238:SER:HB3	1.92	0.51
1:I:239:TRP:HB2	1:I:248:GLU:HG3	1.92	0.51
1:J:408:ARG:HG2	1:J:457:LEU:HD11	1.92	0.51
1:A:404:ARG:HG2	1:A:405:ASP:N	2.25	0.51
1:A:657:VAL:HG12	1:A:691:ARG:HG2	1.93	0.51
1:B:136:ASN:HD22	1:G:42:SER:HB2	1.75	0.51
1:C:80:GLU:HG3	1:C:300:ARG:HH21	1.74	0.51
1:C:591:ASP:OD1	1:C:594:THR:HG23	2.09	0.51
1:E:118:ASP:OD1	1:E:300:ARG:HD3	2.10	0.51
1:E:227:ILE:HD12	1:E:228:GLY:N	2.25	0.51
1:I:654:LEU:HD23	1:I:655:GLU:N	2.25	0.51
1:J:580:PHE:HB2	1:J:582:HIS:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:227:ILE:HD12	1:L:228:GLY:N	2.25	0.51
1:A:428:SER:HB3	1:A:432:TYR:HD2	1.75	0.51
1:B:277:HIS:CD2	1:B:278:LEU:HG	2.45	0.51
1:D:280:PRO:O	1:D:285:ARG:NH2	2.41	0.51
1:H:648:ASN:O	1:H:648:ASN:ND2	2.44	0.51
1:I:654:LEU:HB3	1:I:656:PHE:HE1	1.75	0.51
1:B:129:THR:HG23	1:B:282:LEU:HD22	1.93	0.51
1:D:352:HIS:CG	1:D:382:VAL:HG11	2.46	0.51
1:D:620:THR:HA	1:D:645:LEU:O	2.10	0.51
1:E:191:LEU:HB3	1:E:196:VAL:CG2	2.40	0.51
1:F:112:TYR:CD1	1:F:117:PRO:HA	2.45	0.51
1:L:595:ASP:OD1	1:L:595:ASP:N	2.40	0.51
1:L:596:ILE:HA	1:L:622:PHE:O	2.10	0.51
1:A:557:THR:HA	1:A:560:ARG:HG2	1.92	0.51
1:C:93:ASP:HB3	1:C:96:ALA:HB2	1.91	0.51
1:C:206:GLN:NE2	1:C:234:ASN:HB3	2.24	0.51
1:G:573:PRO:HA	1:G:576:ARG:HG3	1.91	0.51
1:J:687:ALA:H	1:J:690:GLU:HG2	1.75	0.51
1:A:600:THR:HB	1:A:603:GLY:H	1.75	0.51
1:C:670:VAL:HB	1:C:701:VAL:HB	1.93	0.51
1:C:207:PHE:HB2	1:C:225:ASN:O	2.11	0.51
1:D:653:GLU:HG3	1:D:696:PRO:HD3	1.93	0.51
1:G:366:GLN:NE2	1:L:363:LEU:HD21	2.26	0.51
1:L:11:LEU:HB2	1:L:95:TYR:CE2	2.45	0.51
1:A:453:THR:OG1	1:A:456:ASP:OD1	2.15	0.51
1:B:294:ARG:HD3	1:B:311:SER:HB3	1.92	0.51
1:E:104:ARG:NH1	1:E:128:ASP:OD1	2.43	0.51
1:E:239:TRP:CD2	1:E:248:GLU:HG2	2.46	0.51
1:J:504:ARG:HA	1:J:561:PHE:HE1	1.76	0.51
1:J:561:PHE:HD2	1:J:679:PRO:CG	2.23	0.51
1:K:567:ARG:HG3	1:K:570:ARG:NH2	2.25	0.51
1:A:79:PRO:O	1:A:300:ARG:HG2	2.10	0.51
1:B:573:PRO:HD2	1:B:640:ASP:HB2	1.93	0.51
1:B:699:LEU:HD23	1:B:700:THR:H	1.76	0.51
1:C:584:ARG:HD3	1:C:595:ASP:OD2	2.11	0.51
1:D:146:ARG:HH22	1:D:331:VAL:CG1	2.24	0.51
1:G:283:SER:O	1:G:287:LEU:HG	2.10	0.51
1:H:162:LYS:HA	1:H:177:GLY:HA2	1.91	0.51
1:H:678:MET:HG2	1:H:681:GLN:O	2.10	0.51
1:I:200:GLU:HA	1:I:264:ILE:O	2.10	0.51
1:B:163:GLY:HA2	1:B:544:TRP:CE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:SER:HA	1:B:426:THR:HB	1.93	0.51
1:B:426:THR:HG23	1:B:581:PHE:HD2	1.75	0.51
1:C:143:ASP:H	1:C:254:ARG:NH2	2.09	0.51
1:F:574:VAL:HG11	1:F:623:LEU:HB3	1.93	0.51
1:F:595:ASP:N	1:F:595:ASP:OD1	2.44	0.51
1:F:669:VAL:HG13	1:F:670:VAL:HG23	1.92	0.51
1:I:171:LEU:HD12	1:I:176:ARG:HA	1.93	0.51
1:L:206:GLN:HG3	1:L:233:HIS:HA	1.93	0.51
1:L:257:HIS:NE2	1:L:337:ASP:OD2	2.44	0.51
1:B:2:GLN:O	1:B:61:PRO:HD2	2.10	0.50
1:D:409:ASP:OD2	1:D:416:ARG:NH2	2.44	0.50
1:D:461:ASN:HD21	1:D:483:ASN:ND2	2.06	0.50
1:G:172:PRO:O	1:G:176:ARG:HG3	2.11	0.50
1:I:330:TRP:CE3	1:I:334:MET:HG3	2.46	0.50
1:I:678:MET:HG3	1:I:681:GLN:HG3	1.93	0.50
1:K:687:ALA:HB3	1:K:690:GLU:HB3	1.93	0.50
1:L:306:THR:HA	1:L:346:THR:HG21	1.93	0.50
1:L:397:THR:HG22	1:L:441:ALA:HB3	1.92	0.50
1:B:363:LEU:O	1:B:366:GLN:HG3	2.11	0.50
1:B:385:GLY:HA3	1:B:388:GLN:HG3	1.92	0.50
1:C:225:ASN:ND2	1:C:273:ALA:HA	2.25	0.50
1:D:79:PRO:HB2	1:D:300:ARG:HG2	1.93	0.50
1:D:501:ARG:HE	1:D:673:SER:HA	1.77	0.50
1:F:135:VAL:HG11	1:F:246:VAL:HG11	1.92	0.50
1:F:172:PRO:HG2	1:F:175:LEU:HG	1.93	0.50
1:G:168:HIS:CE1	1:G:170:ASP:HB2	2.46	0.50
1:G:201:LEU:HD23	1:G:204:VAL:HG11	1.93	0.50
1:J:147:PRO:O	1:J:149:THR:N	2.43	0.50
1:L:72:ARG:NH2	1:L:124:ASP:OD1	2.42	0.50
1:A:601:PRO:HB3	1:A:656:PHE:CE1	2.46	0.50
1:B:227:ILE:HD12	1:B:228:GLY:H	1.76	0.50
1:B:398:GLU:HB2	1:B:432:TYR:CE1	2.46	0.50
1:C:110:TYR:HA	1:C:280:PRO:HA	1.92	0.50
1:D:284:MET:HB2	1:D:293:TYR:OH	2.12	0.50
1:F:674:ASP:OD2	1:F:678:MET:HB2	2.11	0.50
1:L:184:HIS:CG	1:L:185:PRO:HD2	2.46	0.50
1:C:100:SER:HA	1:C:241:ASP:HB2	1.94	0.50
1:C:421:PHE:HE1	1:C:619:LEU:HD12	1.76	0.50
1:E:300:ARG:HH11	1:E:301:TYR:HE1	1.58	0.50
1:E:670:VAL:HA	1:E:678:MET:O	2.12	0.50
1:F:15:TYR:HD1	1:F:19:GLY:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:ILE:HG21	1:F:376:ILE:HD12	1.94	0.50
1:F:304:ASP:OD2	1:J:473:ARG:NH1	2.44	0.50
1:I:37:LEU:HB2	1:I:68:ARG:HB2	1.93	0.50
1:I:89:LYS:HD3	1:I:125:SER:HB2	1.94	0.50
1:J:125:SER:O	1:J:129:THR:OG1	2.23	0.50
1:K:211:HIS:HD2	1:K:215:ASP:HB2	1.75	0.50
1:L:476:GLU:H	1:L:533:ASN:HD21	1.59	0.50
1:A:492:ASP:HB3	1:A:495:ILE:HD12	1.93	0.50
1:C:464:ARG:HB2	1:C:531:GLY:HA3	1.94	0.50
1:E:125:SER:O	1:E:129:THR:OG1	2.24	0.50
1:E:380:TRP:CZ3	1:E:396:TRP:CH2	3.00	0.50
1:F:294:ARG:NH2	1:F:353:GLU:OE2	2.44	0.50
1:J:538:GLN:HG3	1:J:540:ASN:HD21	1.77	0.50
1:C:97:ARG:HB2	1:C:135:VAL:HG21	1.93	0.50
1:E:567:ARG:HG2	1:E:570:ARG:HH21	1.75	0.50
1:F:238:SER:N	1:F:248:GLU:OE2	2.44	0.50
1:F:473:ARG:NH1	1:J:307:GLY:HA2	2.27	0.50
1:G:27:GLU:N	1:G:288:ASP:OD1	2.44	0.50
1:I:194:LEU:HA	1:I:563:ARG:HG2	1.94	0.50
1:A:397:THR:HG22	1:A:441:ALA:HB3	1.94	0.50
1:C:343:LEU:HB3	1:C:346:THR:HB	1.92	0.50
1:C:471:GLY:O	1:C:473:ARG:HG3	2.11	0.50
1:D:414:GLU:HG2	1:D:415:PRO:HD2	1.94	0.50
1:E:68:ARG:HB3	1:E:131:THR:CG2	2.42	0.50
1:F:51:THR:O	1:H:579:ARG:NH2	2.33	0.50
1:F:461:ASN:ND2	1:F:483:ASN:HD22	2.09	0.50
1:G:211:HIS:O	1:G:215:ASP:HB2	2.12	0.50
1:G:408:ARG:HG3	1:G:506:PHE:CE2	2.47	0.50
1:G:447:THR:OG1	1:G:452:PHE:O	2.27	0.50
1:H:4:TRP:CE2	1:H:61:PRO:HG3	2.47	0.50
1:H:151:TYR:CE2	1:H:374:LYS:HD3	2.47	0.50
1:H:193:GLU:OE1	1:H:563:ARG:NH1	2.45	0.50
1:K:470:GLU:O	1:K:473:ARG:NE	2.32	0.50
1:B:194:LEU:HA	1:B:563:ARG:HG2	1.93	0.50
1:B:486:GLU:O	1:B:499:ARG:NH2	2.45	0.50
1:C:11:LEU:HD12	1:C:95:TYR:CE1	2.47	0.50
1:D:393:PRO:HG2	1:D:396:TRP:CD1	2.47	0.50
1:D:648:ASN:HB2	1:D:694:LEU:HD23	1.94	0.50
1:E:525:PHE:CE2	1:E:559:LEU:HD13	2.47	0.50
1:F:184:HIS:CD2	1:F:185:PRO:HD2	2.47	0.50
1:G:426:THR:HG22	1:G:581:PHE:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:ASP:OD2	1:H:335:HIS:ND1	2.44	0.50
1:K:318:HIS:HA	1:K:321:GLN:HB2	1.94	0.50
1:K:520:SER:OG	1:K:523:ASP:OD2	2.26	0.50
1:L:153:HIS:O	1:L:197:THR:HG21	2.12	0.50
1:A:644:LEU:HB2	1:A:666:TRP:CZ3	2.47	0.50
1:B:352:HIS:HB3	1:B:382:VAL:HG11	1.92	0.50
1:C:457:LEU:HD12	1:C:481:SER:HB3	1.94	0.50
1:D:168:HIS:HB3	1:D:171:LEU:HG	1.94	0.50
1:E:19:GLY:HA3	1:E:59:TYR:OH	2.12	0.50
1:H:26:SER:O	1:H:54:PHE:HB3	2.12	0.50
1:I:451:GLY:HA2	1:I:533:ASN:HB2	1.94	0.50
1:I:457:LEU:HD12	1:I:481:SER:HB3	1.94	0.50
1:K:32:ILE:HG12	1:K:73:VAL:HG22	1.94	0.50
1:A:671:ASP:O	1:A:678:MET:HB2	2.11	0.49
1:C:151:TYR:HD2	1:C:516:VAL:HG21	1.77	0.49
1:C:668:MET:HG2	1:C:678:MET:CE	2.41	0.49
1:D:504:ARG:HB2	1:D:672:THR:HG23	1.93	0.49
1:F:277:HIS:HB3	1:F:302:TYR:HE2	1.77	0.49
1:G:97:ARG:HD3	1:G:329:TYR:CE1	2.46	0.49
1:K:112:TYR:CZ	1:K:278:LEU:HA	2.46	0.49
1:C:400:ASN:C	1:C:400:ASN:HD22	2.15	0.49
1:E:112:TYR:CA	1:E:121:ASN:HB2	2.42	0.49
1:E:560:ARG:NH2	1:E:676:GLU:O	2.45	0.49
1:F:184:HIS:CG	1:F:185:PRO:HD2	2.47	0.49
1:G:590:HIS:ND1	1:G:605:GLU:OE2	2.43	0.49
1:J:482:TRP:CH2	1:J:484:CYS:HA	2.46	0.49
1:L:46:VAL:HG11	1:L:60:LEU:HD21	1.94	0.49
1:C:435:ASP:O	1:I:53:ALA:HA	2.12	0.49
1:E:274:GLU:HB3	1:E:285:ARG:NH2	2.27	0.49
1:F:424:ARG:HD3	1:F:428:SER:HB3	1.94	0.49
1:F:687:ALA:HB3	1:F:690:GLU:HB2	1.95	0.49
1:H:294:ARG:HA	1:H:313:LEU:HG	1.94	0.49
1:J:35:CYS:SG	1:J:43:GLU:HG2	2.52	0.49
1:J:84:ARG:HD2	1:J:302:TYR:OH	2.12	0.49
1:J:552:SER:OG	1:J:553:GLU:N	2.44	0.49
1:K:175:LEU:O	1:K:181:GLY:HA3	2.13	0.49
1:C:669:VAL:HG13	1:C:670:VAL:HG23	1.94	0.49
1:D:157:TYR:CD1	1:D:196:VAL:HG11	2.47	0.49
1:G:475:GLY:HA2	1:G:534:ASN:HB2	1.95	0.49
1:I:670:VAL:HA	1:I:678:MET:O	2.12	0.49
1:A:199:LEU:HD22	1:A:201:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:MET:O	1:A:328:ARG:HG2	2.13	0.49
1:A:699:LEU:HD23	1:A:700:THR:N	2.28	0.49
1:B:162:LYS:O	1:B:166:MET:HB2	2.12	0.49
1:D:324:MET:HB3	1:D:328:ARG:HH12	1.78	0.49
1:E:686:LEU:HD13	1:E:690:GLU:OE1	2.12	0.49
1:H:139:PHE:HB3	1:H:141:TRP:NE1	2.27	0.49
1:J:151:TYR:CE1	1:J:395:LEU:HD22	2.47	0.49
1:K:21:ASN:HA	1:K:59:TYR:HA	1.95	0.49
1:K:490:THR:HG22	1:K:491:GLU:N	2.27	0.49
1:K:685:GLU:H	1:K:685:GLU:CD	2.16	0.49
1:L:99:VAL:HB	1:L:206:GLN:NE2	2.26	0.49
1:B:32:ILE:HG12	1:B:73:VAL:HG22	1.93	0.49
1:B:207:PHE:HB2	1:B:225:ASN:O	2.13	0.49
1:B:586:VAL:O	1:B:587:GLU:HG3	2.12	0.49
1:C:100:SER:HB2	1:C:241:ASP:OD1	2.13	0.49
1:C:112:TYR:C	1:C:121:ASN:HB2	2.33	0.49
1:E:493:VAL:HA	1:E:496:THR:HG22	1.94	0.49
1:F:179:TYR:CE1	1:F:236:TYR:HB2	2.47	0.49
1:G:377:ALA:O	1:G:398:GLU:HA	2.13	0.49
1:H:250:LYS:HE2	1:H:333:GLU:O	2.13	0.49
1:I:207:PHE:HB2	1:I:225:ASN:O	2.13	0.49
1:A:657:VAL:CG1	1:A:691:ARG:HG2	2.43	0.49
1:B:234:ASN:HD22	1:B:234:ASN:H	1.59	0.49
1:C:15:TYR:CZ	1:C:17:GLY:HA2	2.47	0.49
1:E:76:PRO:HB2	1:E:83:LEU:HD13	1.94	0.49
1:I:152:HIS:CD2	1:I:578:ARG:HG2	2.48	0.49
1:J:679:PRO:HG2	1:J:680:PRO:HD3	1.95	0.49
1:A:10:PRO:HG2	1:A:14:THR:HG21	1.94	0.49
1:B:99:VAL:HB	1:B:206:GLN:NE2	2.26	0.49
1:B:394:PRO:O	1:B:395:LEU:HD23	2.13	0.49
1:B:646:MET:HB2	1:B:700:THR:HB	1.93	0.49
1:F:453:THR:H	1:F:456:ASP:HB2	1.77	0.49
1:G:227:ILE:HD11	1:G:283:SER:HB3	1.94	0.49
1:K:139:PHE:HZ	1:K:251:SER:HB3	1.78	0.49
1:L:168:HIS:CD2	1:L:187:VAL:HG22	2.47	0.49
1:A:2:GLN:N	2:A:801:HOH:O	2.44	0.49
1:A:149:THR:HG22	1:A:153:HIS:HB2	1.95	0.49
1:B:20:THR:OG1	1:B:63:VAL:O	2.29	0.49
1:E:187:VAL:O	1:E:191:LEU:HD12	2.13	0.49
1:F:227:ILE:HD12	1:F:228:GLY:N	2.28	0.49
1:H:179:TYR:CZ	1:H:236:TYR:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:442:SER:O	1:I:444:ASN:ND2	2.45	0.49
1:J:25:PHE:HB2	1:J:55:VAL:HG22	1.95	0.49
1:J:84:ARG:HD2	1:J:302:TYR:HH	1.76	0.49
1:A:294:ARG:NH1	1:A:296:ALA:HB2	2.28	0.49
1:A:580:PHE:O	1:A:584:ARG:NH2	2.46	0.49
1:D:100:SER:HB2	1:D:241:ASP:OD1	2.13	0.49
1:E:173:GLU:HG3	1:E:176:ARG:HH11	1.76	0.49
1:E:417:THR:HG22	1:E:419:ALA:H	1.77	0.49
1:E:426:THR:CG2	1:E:581:PHE:HB2	2.43	0.49
1:F:453:THR:OG1	1:F:456:ASP:OD1	2.25	0.49
1:F:464:ARG:HB2	1:F:531:GLY:HA3	1.95	0.49
1:F:561:PHE:CE1	1:F:565:MET:HG3	2.48	0.49
1:G:483:ASN:OD1	1:G:486:GLU:N	2.46	0.49
1:K:499:ARG:O	1:K:503:MET:HG3	2.12	0.49
1:A:306:THR:HA	1:A:346:THR:CG2	2.40	0.48
1:B:95:TYR:HA	1:B:230:PHE:CD1	2.47	0.48
1:B:355:ASP:OD1	1:B:355:ASP:O	2.30	0.48
1:C:171:LEU:HD22	1:C:184:HIS:CD2	2.48	0.48
1:C:412:ARG:NH1	1:C:414:GLU:OE1	2.46	0.48
1:D:405:ASP:OD1	1:D:480:ARG:NH2	2.46	0.48
1:D:600:THR:O	1:D:603:GLY:N	2.43	0.48
1:G:230:PHE:CE1	1:G:326:SER:HB2	2.48	0.48
1:I:90:LEU:H	1:I:125:SER:HB3	1.77	0.48
1:I:433:GLN:O	1:I:440:LEU:HA	2.13	0.48
1:K:283:SER:O	1:K:287:LEU:HG	2.13	0.48
1:L:19:GLY:CA	1:L:62:GLY:H	2.26	0.48
1:A:590:HIS:HB3	1:A:605:GLU:OE2	2.12	0.48
1:B:565:MET:HE2	1:B:565:MET:HA	1.96	0.48
1:C:139:PHE:HZ	1:C:251:SER:HB3	1.78	0.48
1:D:150:GLU:O	1:D:154:THR:OG1	2.30	0.48
1:E:112:TYR:CE2	1:E:278:LEU:HA	2.48	0.48
1:E:243:GLY:O	1:E:246:VAL:HG12	2.13	0.48
1:F:157:TYR:HE2	1:F:159:ALA:HB2	1.79	0.48
1:F:222:TRP:CD2	1:F:536:TYR:HA	2.49	0.48
1:G:112:TYR:CZ	1:G:278:LEU:HA	2.47	0.48
1:G:361:PHE:HZ	1:G:380:TRP:HH2	1.61	0.48
1:G:365:GLN:OE1	1:G:391:ASN:ND2	2.46	0.48
1:K:152:HIS:H	1:K:152:HIS:CD2	2.31	0.48
1:D:204:VAL:CG2	1:D:265:LEU:HD22	2.42	0.48
1:F:596:ILE:HG13	1:F:623:LEU:HD23	1.94	0.48
1:I:19:GLY:HA2	1:I:62:GLY:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:418:LEU:HD11	1:I:619:LEU:HD21	1.95	0.48
1:L:313:LEU:HD22	1:L:315:ARG:HG2	1.95	0.48
1:C:121:ASN:OD1	1:C:122:ASP:N	2.46	0.48
1:C:465:ASN:OD1	1:C:532:ASN:HA	2.14	0.48
1:F:408:ARG:HE	1:F:457:LEU:HD13	1.78	0.48
1:F:644:LEU:HB2	1:F:666:TRP:CZ3	2.47	0.48
1:G:581:PHE:HA	1:G:584:ARG:NH1	2.28	0.48
1:K:164:LEU:HB3	1:K:165:THR:HG23	1.95	0.48
1:K:501:ARG:HA	1:K:504:ARG:HH11	1.79	0.48
1:L:200:GLU:HA	1:L:264:ILE:O	2.14	0.48
1:L:269:TYR:HB2	1:L:347:LEU:HD11	1.96	0.48
1:A:246:VAL:HG22	1:A:250:LYS:HE3	1.94	0.48
1:B:699:LEU:HD23	1:B:700:THR:N	2.29	0.48
1:C:528:THR:HG22	1:C:530:GLY:H	1.77	0.48
1:E:150:GLU:O	1:E:154:THR:OG1	2.23	0.48
1:G:160:HIS:HA	1:G:202:MET:HB2	1.94	0.48
1:G:686:LEU:HD13	1:G:692:VAL:HG21	1.95	0.48
1:H:377:ALA:O	1:H:398:GLU:HA	2.13	0.48
1:H:513:SER:O	1:H:569:ARG:NH2	2.43	0.48
1:I:499:ARG:O	1:I:503:MET:HG3	2.13	0.48
1:J:105:TRP:HH2	1:J:280:PRO:HG3	1.78	0.48
1:J:135:VAL:HG13	1:J:246:VAL:HG11	1.95	0.48
1:L:315:ARG:HB3	1:L:354:VAL:HB	1.96	0.48
1:B:206:GLN:HB3	1:B:227:ILE:HD11	1.95	0.48
1:C:112:TYR:CZ	1:C:278:LEU:HA	2.48	0.48
1:E:593:LEU:O	1:E:593:LEU:HD13	2.14	0.48
1:G:599:PHE:HB2	1:G:620:THR:HB	1.96	0.48
1:H:432:TYR:O	1:H:582:HIS:NE2	2.46	0.48
1:I:212:ARG:HG3	1:I:213:LEU:HD12	1.96	0.48
1:I:218:LEU:HD13	1:I:537:CYS:HB2	1.95	0.48
1:J:306:THR:CG2	1:J:346:THR:HG21	2.39	0.48
1:J:363:LEU:O	1:J:366:GLN:HG3	2.13	0.48
1:A:398:GLU:O	1:A:443:VAL:HB	2.14	0.48
1:A:470:GLU:OE2	1:A:536:TYR:OH	2.31	0.48
1:B:154:THR:HB	1:B:516:VAL:HG13	1.95	0.48
1:B:207:PHE:HA	1:B:226:THR:HA	1.94	0.48
1:C:146:ARG:O	1:C:148:ARG:N	2.46	0.48
1:D:324:MET:HB3	1:D:328:ARG:NH1	2.29	0.48
1:F:88:ALA:HB1	1:F:123:LEU:O	2.13	0.48
1:H:435:ASP:OD1	1:H:436:GLY:N	2.41	0.48
1:I:465:ASN:OD1	1:I:532:ASN:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:158:GLU:HA	1:K:200:GLU:HB3	1.94	0.48
1:L:188:ILE:HG12	1:L:256:LEU:HD23	1.96	0.48
1:A:105:TRP:HH2	1:A:280:PRO:HG3	1.79	0.48
1:C:393:PRO:O	1:C:395:LEU:N	2.41	0.48
1:E:525:PHE:HE2	1:E:559:LEU:HD13	1.78	0.48
1:G:76:PRO:HG2	1:G:83:LEU:HD13	1.96	0.48
1:H:320:LEU:HA	1:H:323:ILE:HD12	1.94	0.48
1:I:520:SER:OG	1:I:523:ASP:OD2	2.29	0.48
1:J:209:ASN:ND2	1:J:219:SER:HB2	2.27	0.48
1:K:574:VAL:HG23	1:K:640:ASP:OD1	2.13	0.48
1:L:84:ARG:HD2	1:L:285:ARG:HD2	1.96	0.48
1:A:250:LYS:O	1:A:254:ARG:HB2	2.14	0.48
1:C:678:MET:CE	1:C:683:GLY:HA3	2.44	0.48
1:E:15:TYR:CE1	1:E:65:PRO:HD3	2.48	0.48
1:E:70:GLY:HA3	1:E:90:LEU:HD11	1.96	0.48
1:I:611:TRP:O	1:I:612:GLN:NE2	2.47	0.48
1:K:538:GLN:HG3	1:K:540:ASN:ND2	2.26	0.48
1:A:521:HIS:O	1:A:527:ARG:NH2	2.47	0.48
1:C:227:ILE:CG2	1:C:273:ALA:HB3	2.44	0.48
1:D:73:VAL:HG21	1:D:287:LEU:HA	1.96	0.48
1:D:538:GLN:O	1:D:543:SER:OG	2.32	0.48
1:E:92:LEU:HB2	1:E:283:SER:HB2	1.96	0.48
1:E:426:THR:HG21	1:E:586:VAL:HG12	1.96	0.48
1:F:340:ARG:NH2	1:F:378:GLU:OE1	2.47	0.48
1:G:501:ARG:HG3	1:G:672:THR:HG22	1.96	0.48
1:H:193:GLU:O	1:H:563:ARG:HG2	2.14	0.48
1:H:643:PHE:CE2	1:H:669:VAL:HG11	2.49	0.48
1:K:328:ARG:NH1	1:K:367:ASP:OD1	2.47	0.48
1:K:595:ASP:N	1:K:595:ASP:OD1	2.46	0.48
1:L:209:ASN:ND2	1:L:219:SER:HB2	2.29	0.48
1:L:380:TRP:CD1	1:L:382:VAL:HG23	2.49	0.48
1:A:654:LEU:HD23	1:A:654:LEU:HA	1.69	0.47
1:F:68:ARG:HD3	1:F:242:ARG:NH1	2.29	0.47
1:H:1:MET:HG3	1:H:2:GLN:N	2.29	0.47
1:H:570:ARG:O	1:H:576:ARG:NH2	2.47	0.47
1:J:199:LEU:HD22	1:J:201:LEU:HD12	1.95	0.47
1:K:668:MET:HB3	1:K:684:PRO:O	2.14	0.47
1:L:272:THR:HG22	1:L:274:GLU:H	1.79	0.47
1:A:68:ARG:HB3	1:A:131:THR:CG2	2.44	0.47
1:B:304:ASP:HB2	1:B:309:GLY:O	2.14	0.47
1:B:581:PHE:HA	1:B:584:ARG:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ARG:HG3	1:C:316:SER:N	2.28	0.47
1:D:200:GLU:HA	1:D:264:ILE:O	2.14	0.47
1:D:453:THR:O	1:D:457:LEU:HB2	2.14	0.47
1:L:172:PRO:O	1:L:176:ARG:HG3	2.14	0.47
1:B:500:ALA:O	1:B:504:ARG:NH1	2.47	0.47
1:E:379:PRO:HB3	1:E:398:GLU:OE1	2.15	0.47
1:E:644:LEU:HB2	1:E:666:TRP:CZ3	2.50	0.47
1:F:272:THR:HG22	1:F:274:GLU:H	1.79	0.47
1:G:426:THR:HG22	1:G:581:PHE:CB	2.44	0.47
1:H:100:SER:HB2	1:H:241:ASP:OD1	2.14	0.47
1:K:645:LEU:HD23	1:K:701:VAL:HG13	1.97	0.47
1:L:453:THR:HG21	1:L:527:ARG:HE	1.79	0.47
1:A:37:LEU:HD22	1:A:43:GLU:HG2	1.96	0.47
1:A:165:THR:O	1:A:177:GLY:N	2.46	0.47
1:C:89:LYS:HD3	1:C:125:SER:HB2	1.96	0.47
1:C:433:GLN:HG2	1:C:438:ARG:HB2	1.96	0.47
1:C:574:VAL:HG23	1:C:640:ASP:OD1	2.14	0.47
1:D:39:ASP:OD1	1:D:242:ARG:NH2	2.47	0.47
1:E:146:ARG:HH22	1:E:331:VAL:HG13	1.80	0.47
1:G:191:LEU:HD22	1:G:196:VAL:HG21	1.97	0.47
1:H:648:ASN:ND2	1:H:696:PRO:HA	2.26	0.47
1:I:272:THR:HG22	1:I:274:GLU:H	1.79	0.47
1:I:567:ARG:HG3	1:I:570:ARG:NH2	2.25	0.47
1:J:629:SER:O	1:J:630:GLU:HG3	2.13	0.47
1:B:112:TYR:HD1	1:B:117:PRO:HA	1.79	0.47
1:C:24:VAL:O	1:C:55:VAL:HG13	2.15	0.47
1:C:210:ASP:OD1	1:C:210:ASP:N	2.47	0.47
1:D:578:ARG:NE	1:D:631:PRO:O	2.45	0.47
1:F:43:GLU:HG2	1:F:72:ARG:HH12	1.79	0.47
1:F:406:CYS:HA	1:F:409:ASP:HB2	1.97	0.47
1:G:460:TYR:HA	1:G:487:GLU:HG3	1.95	0.47
1:H:105:TRP:CE3	1:H:211:HIS:HB2	2.49	0.47
1:J:678:MET:HG2	1:J:681:GLN:O	2.15	0.47
1:K:461:ASN:OD1	1:K:483:ASN:ND2	2.47	0.47
1:K:577:ARG:HH21	1:K:630:GLU:CD	2.18	0.47
1:L:175:LEU:HB3	1:L:181:GLY:CA	2.44	0.47
1:L:446:VAL:HG11	1:L:506:PHE:HB3	1.95	0.47
1:A:77:TYR:HB2	1:A:120:ARG:CZ	2.45	0.47
1:A:344:ALA:HB3	1:A:378:GLU:H	1.78	0.47
1:B:398:GLU:HB2	1:B:432:TYR:HE1	1.78	0.47
1:C:152:HIS:CE1	1:C:578:ARG:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:GLN:HG2	1:C:325:ASP:OD1	2.15	0.47
1:F:239:TRP:CD2	1:F:248:GLU:HG2	2.49	0.47
1:G:256:LEU:HD12	1:G:263:VAL:HG22	1.95	0.47
1:G:394:PRO:O	1:G:395:LEU:HD23	2.15	0.47
1:J:112:TYR:CZ	1:J:278:LEU:HA	2.50	0.47
1:L:224:TYR:HD2	1:L:268:VAL:HG22	1.80	0.47
1:L:455:ARG:HD2	1:L:528:THR:OG1	2.14	0.47
1:A:71:PHE:HE1	1:A:93:ASP:HB2	1.80	0.47
1:A:191:LEU:HD22	1:A:196:VAL:HG21	1.95	0.47
1:A:579:ARG:HH22	1:E:52:ASP:CG	2.15	0.47
1:B:71:PHE:CE1	1:B:93:ASP:HB2	2.50	0.47
1:C:38:HIS:CE1	1:J:65:PRO:HD2	2.49	0.47
1:D:463:LYS:HE2	1:D:477:ASN:HA	1.97	0.47
1:E:166:MET:HB3	1:E:167:LEU:HD12	1.97	0.47
1:E:207:PHE:H	1:E:233:HIS:CE1	2.32	0.47
1:E:403:TYR:HD1	1:E:424:ARG:HB3	1.79	0.47
1:E:607:THR:H	1:E:610:ASP:HB3	1.80	0.47
1:F:141:TRP:HB3	1:F:144:ASP:HB2	1.96	0.47
1:F:230:PHE:CE1	1:F:326:SER:HB2	2.49	0.47
1:F:345:ALA:HA	1:F:380:TRP:HB3	1.97	0.47
1:G:405:ASP:O	1:G:409:ASP:HB2	2.15	0.47
1:G:624:ASN:HB3	1:G:627:ALA:HB3	1.95	0.47
1:H:68:ARG:HD3	1:H:242:ARG:NH1	2.30	0.47
1:H:107:GLU:OE2	1:H:114:PHE:HB2	2.15	0.47
1:H:415:PRO:CB	1:H:615:HIS:HA	2.45	0.47
1:I:49:ARG:HA	1:I:49:ARG:HD2	1.76	0.47
1:I:294:ARG:HE	1:I:303:MET:CB	2.27	0.47
1:I:465:ASN:ND2	1:I:533:ASN:OD1	2.45	0.47
1:J:504:ARG:HB2	1:J:672:THR:HG23	1.96	0.47
1:K:578:ARG:HH22	1:K:631:PRO:HD2	1.79	0.47
1:L:110:TYR:HA	1:L:280:PRO:HA	1.96	0.47
1:L:448:CYS:HA	1:L:520:SER:HB3	1.96	0.47
1:L:461:ASN:OD1	1:L:483:ASN:ND2	2.47	0.47
1:L:482:TRP:CZ2	1:L:484:CYS:HA	2.49	0.47
1:A:443:VAL:HA	1:A:516:VAL:O	2.15	0.47
1:C:361:PHE:HD1	1:C:393:PRO:HD3	1.79	0.47
1:D:110:TYR:HA	1:D:280:PRO:HA	1.97	0.47
1:D:491:GLU:HG2	1:D:491:GLU:O	2.15	0.47
1:F:243:GLY:O	1:F:246:VAL:HG12	2.14	0.47
1:H:201:LEU:O	1:H:266:ASP:HB2	2.15	0.47
1:H:593:LEU:HD13	1:H:593:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:626:ASN:O	1:H:637:ARG:NH2	2.44	0.47
1:J:160:HIS:ND1	1:J:221:TYR:CZ	2.83	0.47
1:K:601:PRO:HB3	1:K:654:LEU:HD21	1.97	0.47
1:A:28:ALA:N	1:A:288:ASP:OD1	2.48	0.47
1:A:501:ARG:NH2	1:A:696:PRO:O	2.48	0.47
1:B:9:TYR:HA	1:B:10:PRO:HA	1.69	0.47
1:B:52:ASP:O	1:B:55:VAL:N	2.42	0.47
1:C:461:ASN:HD21	1:C:483:ASN:H	1.61	0.47
1:G:112:TYR:HD1	1:G:117:PRO:HA	1.80	0.47
1:G:379:PRO:HB3	1:G:398:GLU:OE1	2.15	0.47
1:G:567:ARG:HG2	1:G:570:ARG:NH2	2.29	0.47
1:H:315:ARG:HA	1:H:356:ARG:HD2	1.97	0.47
1:H:520:SER:OG	1:H:523:ASP:OD2	2.30	0.47
1:L:22:PHE:O	1:L:57:HIS:HB2	2.15	0.47
1:A:165:THR:HB	1:A:171:LEU:HD11	1.97	0.47
1:B:37:LEU:HD12	1:B:131:THR:HG21	1.96	0.47
1:B:311:SER:OG	1:B:350:GLN:CD	2.53	0.47
1:C:403:TYR:CD1	1:C:424:ARG:HB3	2.47	0.47
1:D:67:GLN:O	1:D:134:VAL:HG23	2.15	0.47
1:E:294:ARG:HA	1:E:313:LEU:HG	1.97	0.47
1:E:446:VAL:HG13	1:E:510:LEU:HD13	1.96	0.47
1:F:90:LEU:H	1:F:125:SER:HB3	1.80	0.47
1:G:458:VAL:O	1:G:499:ARG:HG2	2.15	0.47
1:G:645:LEU:HD23	1:G:701:VAL:HG13	1.97	0.47
1:G:657:VAL:CG1	1:G:691:ARG:HD3	2.44	0.47
1:H:252:ALA:O	1:H:256:LEU:HG	2.15	0.47
1:I:88:ALA:HB3	1:I:89:LYS:HE2	1.97	0.47
1:J:418:LEU:HD23	1:J:610:ASP:O	2.14	0.47
1:K:37:LEU:HD22	1:K:41:GLY:HA2	1.97	0.47
1:K:82:GLY:O	1:K:289:ASN:HB3	2.15	0.47
1:K:269:TYR:OH	1:K:326:SER:OG	2.28	0.47
1:L:461:ASN:HD21	1:L:483:ASN:HD22	1.63	0.47
1:F:392:PHE:CE2	1:F:439:PRO:HD3	2.50	0.46
1:G:620:THR:HG22	1:G:644:LEU:HD11	1.98	0.46
1:J:289:ASN:N	1:J:290:PRO:HD2	2.30	0.46
1:J:600:THR:HG22	1:J:602:GLU:H	1.79	0.46
1:J:646:MET:HB2	1:J:700:THR:HB	1.97	0.46
1:K:171:LEU:HD22	1:K:184:HIS:CD2	2.50	0.46
1:K:178:THR:HG21	1:K:238:SER:HB3	1.97	0.46
1:L:620:THR:HA	1:L:645:LEU:O	2.16	0.46
1:A:409:ASP:OD2	1:A:416:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:THR:HA	1:B:349:ARG:HB3	1.97	0.46
1:C:648:ASN:ND2	1:C:650:SER:O	2.47	0.46
1:F:191:LEU:HB3	1:F:196:VAL:CG2	2.46	0.46
1:F:200:GLU:OE2	1:F:340:ARG:HG3	2.15	0.46
1:G:580:PHE:HD1	1:G:582:HIS:NE2	2.13	0.46
1:I:135:VAL:HG13	1:I:246:VAL:HG11	1.96	0.46
1:I:432:TYR:HB3	1:I:439:PRO:O	2.15	0.46
1:J:418:LEU:HB2	1:J:616:ALA:HB2	1.95	0.46
1:L:460:TYR:HA	1:L:487:GLU:HG3	1.97	0.46
1:B:482:TRP:CZ2	1:B:484:CYS:HA	2.50	0.46
1:C:76:PRO:HG2	1:C:83:LEU:HD13	1.98	0.46
1:E:143:ASP:O	1:E:145:ARG:N	2.47	0.46
1:E:569:ARG:O	1:E:576:ARG:HD3	2.15	0.46
1:E:601:PRO:HB3	1:E:656:PHE:CE2	2.50	0.46
1:G:146:ARG:HG2	1:G:257:HIS:CE1	2.50	0.46
1:H:313:LEU:HD23	1:H:313:LEU:HA	1.77	0.46
1:K:274:GLU:OE1	1:K:293:TYR:OH	2.14	0.46
1:L:644:LEU:HD23	1:L:702:LEU:HD12	1.96	0.46
1:B:69:TYR:CZ	1:B:132:SER:HB2	2.50	0.46
1:B:447:THR:OG1	1:B:452:PHE:O	2.33	0.46
1:B:657:VAL:O	1:B:659:PRO:HD3	2.15	0.46
1:B:661:SER:HB3	1:B:664:ARG:NE	2.28	0.46
1:C:30:HIS:CE1	1:C:76:PRO:HG3	2.50	0.46
1:C:183:ALA:HA	1:C:188:ILE:HD11	1.97	0.46
1:C:266:ASP:OD1	1:C:340:ARG:HD3	2.16	0.46
1:D:89:LYS:HA	1:D:125:SER:HB3	1.96	0.46
1:H:342:ASP:OD1	1:H:343:LEU:N	2.49	0.46
1:I:110:TYR:HD2	1:I:112:TYR:HE2	1.63	0.46
1:J:561:PHE:CD2	1:J:679:PRO:HG3	2.48	0.46
1:K:211:HIS:CD2	1:K:215:ASP:HB2	2.51	0.46
1:L:194:LEU:HA	1:L:563:ARG:HG2	1.97	0.46
1:L:618:ALA:O	1:L:619:LEU:HD23	2.15	0.46
1:A:225:ASN:HA	1:A:271:HIS:CE1	2.51	0.46
1:A:422:ALA:HB2	1:A:611:TRP:HZ3	1.80	0.46
1:C:435:ASP:HB3	1:C:437:ARG:HG3	1.97	0.46
1:D:640:ASP:OD2	1:D:641:ASP:N	2.44	0.46
1:E:607:THR:OG1	1:E:608:SER:N	2.48	0.46
1:F:194:LEU:HD12	1:F:566:VAL:HG21	1.97	0.46
1:F:397:THR:HG22	1:F:441:ALA:H	1.81	0.46
1:G:135:VAL:CG1	1:G:246:VAL:HG11	2.45	0.46
1:G:694:LEU:HD11	1:G:700:THR:OG1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:PHE:HZ	1:H:251:SER:HB3	1.79	0.46
1:K:168:HIS:O	1:K:176:ARG:NE	2.48	0.46
1:K:202:MET:O	1:K:204:VAL:HG13	2.16	0.46
1:K:321:GLN:O	1:K:325:ASP:HB2	2.16	0.46
1:L:11:LEU:HA	1:L:23:ALA:HB3	1.98	0.46
1:L:324:MET:HE3	1:L:370:VAL:HG21	1.98	0.46
1:L:447:THR:OG1	1:L:452:PHE:O	2.33	0.46
1:B:406:CYS:SG	1:B:416:ARG:NE	2.88	0.46
1:C:513:SER:O	1:C:569:ARG:NH2	2.47	0.46
1:D:28:ALA:N	1:D:288:ASP:OD1	2.48	0.46
1:D:146:ARG:HD3	1:D:337:ASP:OD1	2.16	0.46
1:E:465:ASN:OD1	1:E:532:ASN:HA	2.16	0.46
1:F:91:LEU:HD11	1:F:286:GLY:HA3	1.98	0.46
1:G:212:ARG:NH2	1:G:536:TYR:OH	2.46	0.46
1:H:344:ALA:HB3	1:H:378:GLU:H	1.79	0.46
1:H:699:LEU:HD23	1:H:700:THR:H	1.80	0.46
1:I:89:LYS:HE3	1:I:111:GLY:CA	2.45	0.46
1:I:171:LEU:HD22	1:I:184:HIS:CG	2.51	0.46
1:J:246:VAL:HG22	1:J:250:LYS:HE3	1.98	0.46
1:L:483:ASN:OD1	1:L:486:GLU:N	2.48	0.46
1:A:200:GLU:HA	1:A:264:ILE:O	2.15	0.46
1:A:336:VAL:HG12	1:A:338:GLY:H	1.80	0.46
1:C:97:ARG:HD3	1:C:329:TYR:CE1	2.51	0.46
1:C:238:SER:N	1:C:248:GLU:OE2	2.48	0.46
1:F:587:GLU:HG3	1:F:590:HIS:NE2	2.31	0.46
1:H:500:ALA:O	1:H:504:ARG:NH1	2.49	0.46
1:H:574:VAL:HG23	1:H:640:ASP:OD1	2.15	0.46
1:J:200:GLU:HA	1:J:264:ILE:O	2.16	0.46
1:J:256:LEU:HB3	1:J:261:ILE:HB	1.97	0.46
1:K:32:ILE:HB	1:K:56:ARG:HD2	1.98	0.46
1:K:167:LEU:HD22	1:K:544:TRP:HB3	1.97	0.46
1:K:392:PHE:CE2	1:K:439:PRO:HD3	2.50	0.46
1:K:646:MET:SD	1:K:656:PHE:HB3	2.56	0.46
1:L:426:THR:CG2	1:L:581:PHE:HB2	2.42	0.46
1:A:396:TRP:HE3	1:A:439:PRO:HG3	1.79	0.46
1:A:488:GLY:O	1:A:499:ARG:NH2	2.46	0.46
1:B:98:ALA:HA	1:B:231:ALA:HB1	1.98	0.46
1:B:163:GLY:HA2	1:B:544:TRP:HE3	1.80	0.46
1:B:433:GLN:HA	1:B:582:HIS:ND1	2.31	0.46
1:H:141:TRP:HB3	1:H:144:ASP:HB2	1.98	0.46
1:I:321:GLN:O	1:I:325:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:402:LYS:HB3	1:K:424:ARG:HH12	1.81	0.46
1:B:525:PHE:HE2	1:B:559:LEU:HD22	1.81	0.46
1:D:687:ALA:HB3	1:D:690:GLU:HB3	1.98	0.46
1:E:655:GLU:HA	1:E:692:VAL:O	2.15	0.46
1:F:81:ARG:HE	1:F:81:ARG:HB2	1.46	0.46
1:H:311:SER:HB2	1:H:350:GLN:HG2	1.97	0.46
1:I:110:TYR:OH	1:I:211:HIS:ND1	2.46	0.46
1:I:168:HIS:HA	1:I:547:TRP:CD1	2.51	0.46
1:J:107:GLU:HA	1:J:114:PHE:CZ	2.51	0.46
1:J:151:TYR:HE1	1:J:395:LEU:HD22	1.81	0.46
1:J:666:TRP:HA	1:J:704:ARG:HB2	1.98	0.46
1:A:146:ARG:HD2	1:A:148:ARG:HH21	1.81	0.46
1:A:244:GLN:H	1:A:244:GLN:HG3	1.46	0.46
1:B:620:THR:HA	1:B:645:LEU:O	2.15	0.46
1:E:574:VAL:HG11	1:E:623:LEU:HB3	1.97	0.46
1:G:267:VAL:HB	1:G:269:TYR:CE1	2.51	0.46
1:G:432:TYR:HB3	1:G:439:PRO:O	2.16	0.46
1:I:159:ALA:HB1	1:I:164:LEU:HD12	1.98	0.46
1:K:655:GLU:OE1	1:K:655:GLU:N	2.49	0.46
1:B:78:ALA:N	1:B:83:LEU:O	2.48	0.45
1:B:284:MET:HA	1:B:287:LEU:HB2	1.97	0.45
1:C:27:GLU:HG2	1:C:54:PHE:CD2	2.51	0.45
1:C:43:GLU:CD	1:C:72:ARG:HH12	2.20	0.45
1:C:412:ARG:HG3	1:C:482:TRP:HB2	1.97	0.45
1:C:645:LEU:HD23	1:C:701:VAL:HG13	1.97	0.45
1:E:644:LEU:HD23	1:E:658:VAL:HG13	1.98	0.45
1:F:565:MET:HG2	1:F:679:PRO:HG3	1.97	0.45
1:F:645:LEU:HD23	1:F:701:VAL:HG13	1.98	0.45
1:I:159:ALA:HA	1:I:521:HIS:CG	2.51	0.45
1:J:91:LEU:HA	1:J:282:LEU:O	2.16	0.45
1:K:240:GLY:HA3	1:K:244:GLN:HG3	1.98	0.45
1:L:306:THR:OG1	1:L:308:THR:N	2.48	0.45
1:L:463:LYS:NZ	1:L:474:ASP:O	2.38	0.45
1:B:600:THR:HG23	1:B:601:PRO:HD2	1.98	0.45
1:C:37:LEU:HD23	1:C:43:GLU:HG3	1.98	0.45
1:C:89:LYS:HE3	1:C:111:GLY:HA2	1.98	0.45
1:D:458:VAL:HB	1:D:484:CYS:SG	2.56	0.45
1:E:354:VAL:HG23	1:E:356:ARG:HB2	1.98	0.45
1:F:404:ARG:HD3	1:F:445:PHE:CZ	2.51	0.45
1:G:221:TYR:HB2	1:G:539:ASP:HB2	1.98	0.45
1:I:394:PRO:O	1:I:395:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:387:TYR:CD2	1:K:392:PHE:HZ	2.33	0.45
1:A:500:ALA:O	1:A:504:ARG:HG3	2.16	0.45
1:B:599:PHE:N	1:B:620:THR:O	2.50	0.45
1:C:151:TYR:CE1	1:C:395:LEU:HD22	2.49	0.45
1:F:664:ARG:CG	1:F:704:ARG:HH21	2.27	0.45
1:J:504:ARG:HA	1:J:561:PHE:CE1	2.52	0.45
1:J:505:ASN:O	1:J:509:THR:OG1	2.29	0.45
1:A:289:ASN:N	1:A:290:PRO:HD2	2.30	0.45
1:A:316:SER:HB3	1:A:319:VAL:HB	1.98	0.45
1:B:409:ASP:OD2	1:B:416:ARG:HD2	2.16	0.45
1:D:380:TRP:HZ3	1:D:396:TRP:CH2	2.33	0.45
1:E:129:THR:HG22	1:E:130:MET:H	1.80	0.45
1:G:664:ARG:HD2	1:G:704:ARG:NH2	2.31	0.45
1:H:171:LEU:HD22	1:H:184:HIS:CG	2.51	0.45
1:K:460:TYR:O	1:K:481:SER:OG	2.29	0.45
1:L:34:LEU:HB2	1:L:48:LEU:HD11	1.98	0.45
1:B:225:ASN:OD1	1:B:273:ALA:HA	2.16	0.45
1:D:430:ASP:OD1	1:D:431:LEU:N	2.49	0.45
1:E:221:TYR:HB3	1:E:536:TYR:O	2.16	0.45
1:F:686:LEU:HD12	1:F:702:LEU:HD11	1.98	0.45
1:G:343:LEU:O	1:G:346:THR:N	2.50	0.45
1:G:393:PRO:C	1:G:395:LEU:H	2.18	0.45
1:G:658:VAL:HB	1:G:688:GLY:HA2	1.97	0.45
1:H:89:LYS:O	1:H:91:LEU:HD22	2.16	0.45
1:I:277:HIS:NE2	1:I:301:TYR:HD2	2.14	0.45
1:I:440:LEU:HD23	2:I:801:HOH:O	2.17	0.45
1:L:674:ASP:HA	1:L:675:PRO:HD3	1.80	0.45
1:A:585:PRO:HB2	1:A:587:GLU:OE1	2.17	0.45
1:D:335:HIS:CD2	1:D:335:HIS:N	2.85	0.45
1:F:306:THR:OG1	1:F:308:THR:OG1	2.30	0.45
1:H:89:LYS:HA	1:H:125:SER:CB	2.45	0.45
1:H:92:LEU:HD22	1:H:227:ILE:HD13	1.99	0.45
1:I:398:GLU:OE1	1:I:432:TYR:HE1	2.00	0.45
1:I:580:PHE:O	1:I:582:HIS:N	2.49	0.45
1:J:395:LEU:HA	1:J:440:LEU:HD21	1.98	0.45
1:K:245:GLN:OE1	1:K:245:GLN:N	2.34	0.45
1:K:420:GLU:O	1:K:424:ARG:HG2	2.16	0.45
1:K:658:VAL:HG12	1:K:688:GLY:HA2	1.99	0.45
1:L:34:LEU:O	1:L:45:ALA:HA	2.17	0.45
1:A:105:TRP:CH2	1:A:280:PRO:HG3	2.51	0.45
1:A:669:VAL:HG13	1:A:670:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:672:THR:HB	1:B:699:LEU:H	1.81	0.45
1:C:50:GLU:OE1	1:I:579:ARG:NH1	2.50	0.45
1:G:512:LEU:HD13	1:G:645:LEU:HD22	1.99	0.45
1:H:269:TYR:HB2	1:H:347:LEU:HD11	1.99	0.45
1:I:239:TRP:N	1:I:248:GLU:OE2	2.50	0.45
1:I:677:GLY:O	1:I:680:PRO:HD2	2.17	0.45
1:J:578:ARG:NH2	1:K:50:GLU:OE1	2.50	0.45
1:K:9:TYR:HA	1:K:10:PRO:HA	1.69	0.45
1:K:198:ALA:HB1	1:K:264:ILE:HD12	1.99	0.45
1:K:599:PHE:CE2	1:K:605:GLU:HG2	2.52	0.45
1:B:584:ARG:H	1:B:584:ARG:HE	1.64	0.45
1:C:254:ARG:C	1:C:254:ARG:HD3	2.37	0.45
1:D:25:PHE:CZ	1:D:27:GLU:HB3	2.51	0.45
1:F:466:GLU:HG3	1:F:472:ASN:HD22	1.82	0.45
1:G:529:GLN:O	1:G:542:VAL:HG13	2.16	0.45
1:J:10:PRO:HG2	1:J:14:THR:HG21	1.98	0.45
1:J:408:ARG:HB3	1:J:480:ARG:O	2.17	0.45
1:J:443:VAL:HG12	1:J:516:VAL:HB	1.99	0.45
1:K:294:ARG:NH2	1:K:303:MET:SD	2.89	0.45
1:K:580:PHE:O	1:K:582:HIS:N	2.49	0.45
1:L:30:HIS:HB2	1:L:74:HIS:O	2.17	0.45
1:L:99:VAL:HB	1:L:206:GLN:HE22	1.82	0.45
1:A:30:HIS:HB2	1:A:74:HIS:O	2.17	0.45
1:A:225:ASN:HD21	1:A:273:ALA:HA	1.81	0.45
1:A:457:LEU:HD12	1:A:481:SER:HB3	1.99	0.45
1:B:51:THR:O	1:D:579:ARG:NH2	2.45	0.45
1:B:270:ASN:ND2	1:B:343:LEU:HB2	2.32	0.45
1:B:344:ALA:HB3	1:B:378:GLU:H	1.81	0.45
1:C:580:PHE:O	1:C:582:HIS:N	2.48	0.45
1:D:461:ASN:ND2	1:D:483:ASN:HD22	2.06	0.45
1:D:667:ARG:HH11	1:D:685:GLU:HG2	1.82	0.45
1:H:495:ILE:HA	1:H:498:LEU:HB2	1.99	0.45
1:I:28:ALA:N	1:I:288:ASP:OD1	2.48	0.45
1:I:298:ASP:O	1:I:300:ARG:N	2.50	0.45
1:I:623:LEU:HD23	1:I:623:LEU:HA	1.68	0.45
1:J:482:TRP:CZ2	1:J:484:CYS:HA	2.51	0.45
1:K:595:ASP:HA	1:K:627:ALA:HB3	1.98	0.45
1:L:417:THR:HG22	1:L:419:ALA:H	1.80	0.45
1:L:687:ALA:O	1:L:689:GLY:N	2.46	0.45
1:A:340:ARG:NH2	1:A:378:GLU:OE1	2.50	0.45
1:A:580:PHE:O	1:A:582:HIS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ARG:NH2	1:C:571:GLU:OE2	2.40	0.45
1:C:423:SER:O	1:C:427:GLY:N	2.47	0.45
1:E:534:ASN:OD1	1:E:536:TYR:HD2	2.00	0.45
1:F:529:GLN:HG2	1:F:542:VAL:HG12	1.97	0.45
1:H:645:LEU:HD23	1:H:701:VAL:HG13	1.99	0.45
1:I:113:PRO:O	1:I:115:GLY:N	2.50	0.45
1:I:573:PRO:O	1:I:575:PHE:N	2.50	0.45
1:I:671:ASP:OD1	1:I:673:SER:OG	2.26	0.45
1:L:574:VAL:HG11	1:L:623:LEU:HB3	1.99	0.45
1:A:420:GLU:O	1:A:424:ARG:HG2	2.17	0.44
1:B:112:TYR:C	1:B:121:ASN:HB2	2.37	0.44
1:B:262:GLU:OE1	1:B:374:LYS:HE2	2.17	0.44
1:B:269:TYR:CE2	1:B:323:ILE:HG23	2.51	0.44
1:C:490:THR:HB	1:C:495:ILE:HD11	1.98	0.44
1:D:38:HIS:CE1	1:D:44:THR:HG1	2.34	0.44
1:D:408:ARG:HD2	1:D:446:VAL:O	2.17	0.44
1:E:19:GLY:HA2	1:E:61:PRO:HA	1.99	0.44
1:E:206:GLN:HA	1:E:233:HIS:ND1	2.32	0.44
1:E:224:TYR:HB3	1:E:268:VAL:HG21	1.99	0.44
1:E:245:GLN:O	1:E:248:GLU:HB2	2.17	0.44
1:F:129:THR:HG22	1:F:130:MET:N	2.32	0.44
1:F:322:LEU:O	1:F:326:SER:HB3	2.17	0.44
1:F:622:PHE:CE1	1:F:666:TRP:HH2	2.35	0.44
1:G:30:HIS:O	1:G:56:ARG:NH2	2.50	0.44
1:I:304:ASP:OD1	1:I:307:GLY:N	2.50	0.44
1:L:520:SER:OG	1:L:523:ASP:OD2	2.31	0.44
1:L:625:GLY:HA3	1:L:640:ASP:O	2.17	0.44
1:A:168:HIS:HB3	1:A:171:LEU:HD12	1.99	0.44
1:B:698:SER:OG	1:B:699:LEU:N	2.51	0.44
1:C:476:GLU:HB2	1:C:533:ASN:HD21	1.82	0.44
1:C:505:ASN:ND2	1:C:672:THR:HG21	2.32	0.44
1:F:504:ARG:HB2	1:F:672:THR:HG23	1.98	0.44
1:G:12:GLY:HA2	1:G:93:ASP:OD2	2.18	0.44
1:G:37:LEU:HD11	1:G:90:LEU:HD21	1.99	0.44
1:G:654:LEU:HD23	1:G:654:LEU:HA	1.76	0.44
1:H:77:TYR:CD1	1:H:120:ARG:HG3	2.52	0.44
1:H:424:ARG:NH2	1:H:430:ASP:OD2	2.50	0.44
1:J:284:MET:HB3	1:J:292:TYR:CD1	2.53	0.44
1:J:403:TYR:CE2	1:J:444:ASN:HB3	2.52	0.44
1:J:446:VAL:HG22	1:J:510:LEU:HD13	1.99	0.44
1:J:461:ASN:ND2	1:J:482:TRP:HA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:156:ILE:HA	1:K:198:ALA:HB3	1.98	0.44
1:L:381:ASP:HA	1:L:386:GLY:HA2	1.99	0.44
1:L:507:LEU:HA	1:L:507:LEU:HD23	1.68	0.44
1:A:642:SER:N	1:A:704:ARG:O	2.43	0.44
1:A:677:GLY:O	1:A:681:GLN:HG2	2.18	0.44
1:D:296:ALA:C	1:D:298:ASP:H	2.21	0.44
1:F:37:LEU:HD21	1:F:43:GLU:HG3	1.99	0.44
1:G:179:TYR:N	1:G:236:TYR:O	2.46	0.44
1:H:139:PHE:HE1	1:H:247:LEU:HG	1.83	0.44
1:H:233:HIS:CE1	1:H:235:ALA:HB3	2.53	0.44
1:H:262:GLU:OE2	1:H:374:LYS:NZ	2.49	0.44
1:I:97:ARG:HD3	1:I:329:TYR:CE1	2.53	0.44
1:K:584:ARG:HG2	1:K:584:ARG:HH11	1.83	0.44
1:L:483:ASN:H	1:L:483:ASN:ND2	2.15	0.44
1:L:568:LEU:HG	1:L:572:HIS:HD2	1.83	0.44
1:A:584:ARG:HD2	1:A:595:ASP:OD2	2.16	0.44
1:B:271:HIS:CG	1:B:308:THR:HG21	2.53	0.44
1:C:4:TRP:N	1:C:4:TRP:CD1	2.84	0.44
1:C:53:ALA:HA	1:I:435:ASP:HA	2.00	0.44
1:C:405:ASP:OD2	1:C:480:ARG:NE	2.50	0.44
1:C:432:TYR:HB3	1:C:439:PRO:O	2.18	0.44
1:E:151:TYR:CE1	1:E:395:LEU:HD22	2.53	0.44
1:G:48:LEU:HD22	1:G:58:ALA:HB3	1.98	0.44
1:G:68:ARG:HB3	1:G:131:THR:HG21	1.99	0.44
1:G:425:LEU:HD23	1:G:513:SER:HA	1.98	0.44
1:H:183:ALA:HA	1:H:188:ILE:HD11	1.99	0.44
1:H:211:HIS:NE2	1:H:215:ASP:OD2	2.51	0.44
1:J:570:ARG:O	1:J:576:ARG:NH2	2.47	0.44
1:J:579:ARG:NH1	1:K:52:ASP:OD1	2.48	0.44
1:K:179:TYR:HB2	1:K:248:GLU:OE1	2.17	0.44
1:L:27:GLU:HA	1:L:54:PHE:CD1	2.52	0.44
1:L:162:LYS:HA	1:L:177:GLY:HA2	1.99	0.44
1:L:190:HIS:CD2	1:L:547:TRP:HZ3	2.36	0.44
1:L:528:THR:CG2	1:L:530:GLY:H	2.27	0.44
1:A:660:ASP:HB3	1:A:666:TRP:NE1	2.27	0.44
1:B:452:PHE:HB3	1:B:456:ASP:HB2	2.00	0.44
1:C:68:ARG:HD3	1:C:242:ARG:HE	1.81	0.44
1:C:652:LYS:CA	1:C:696:PRO:HB3	2.48	0.44
1:D:274:GLU:O	1:D:285:ARG:NH2	2.51	0.44
1:E:72:ARG:HD3	1:E:87:ALA:O	2.18	0.44
1:F:241:ASP:O	1:F:245:GLN:NE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:664:ARG:CB	1:G:704:ARG:HE	2.29	0.44
1:H:194:LEU:HD12	1:H:563:ARG:HG3	2.00	0.44
1:I:141:TRP:HB3	1:I:144:ASP:HB2	1.99	0.44
1:I:658:VAL:O	1:I:660:ASP:N	2.51	0.44
1:J:239:TRP:HB2	1:J:248:GLU:HG3	1.98	0.44
1:K:246:VAL:O	1:K:250:LYS:HG3	2.18	0.44
1:L:396:TRP:HD1	1:L:439:PRO:HG3	1.82	0.44
1:B:125:SER:OG	1:B:129:THR:OG1	2.35	0.44
1:B:205:HIS:CE1	1:B:267:VAL:HG12	2.53	0.44
1:B:403:TYR:CE2	1:B:444:ASN:HB3	2.52	0.44
1:B:433:GLN:HG2	1:B:438:ARG:HB2	1.99	0.44
1:C:406:CYS:SG	1:C:420:GLU:HG2	2.58	0.44
1:D:322:LEU:O	1:D:326:SER:N	2.37	0.44
1:E:403:TYR:CE2	1:E:444:ASN:HB3	2.52	0.44
1:I:470:GLU:HB3	1:I:474:ASP:OD1	2.17	0.44
1:I:512:LEU:HD22	1:I:575:PHE:CE1	2.53	0.44
1:K:344:ALA:HB3	1:K:378:GLU:H	1.82	0.44
1:L:417:THR:HB	1:L:420:GLU:HB3	2.00	0.44
1:B:426:THR:CG2	1:B:581:PHE:HB2	2.48	0.44
1:C:22:PHE:CE1	1:C:60:LEU:HD12	2.53	0.44
1:C:168:HIS:CE1	1:C:170:ASP:HB2	2.53	0.44
1:C:289:ASN:N	1:C:290:PRO:HD2	2.32	0.44
1:D:668:MET:HE1	1:D:684:PRO:HD2	2.00	0.44
1:G:483:ASN:H	1:G:483:ASN:HD22	1.66	0.44
1:H:465:ASN:ND2	1:H:533:ASN:OD1	2.41	0.44
1:I:272:THR:OG1	1:I:312:LEU:HD11	2.17	0.44
1:I:393:PRO:O	1:I:395:LEU:N	2.47	0.44
1:L:68:ARG:HD3	1:L:242:ARG:CZ	2.48	0.44
1:B:105:TRP:CB	1:B:211:HIS:HD2	2.31	0.44
1:C:135:VAL:CG1	1:C:246:VAL:HG11	2.45	0.44
1:C:329:TYR:HD2	1:C:330:TRP:CD1	2.36	0.44
1:D:195:GLY:O	1:D:566:VAL:HG11	2.17	0.44
1:D:225:ASN:HA	1:D:271:HIS:HE1	1.82	0.44
1:E:49:ARG:HA	1:E:49:ARG:HD2	1.72	0.44
1:G:175:LEU:HD22	1:G:180:ALA:HB3	1.98	0.44
1:G:525:PHE:HE2	1:G:559:LEU:HD22	1.82	0.44
1:H:72:ARG:NH2	1:H:126:ALA:HB2	2.33	0.44
1:H:508:ALA:O	1:H:512:LEU:HG	2.18	0.44
1:I:89:LYS:NZ	1:I:123:LEU:O	2.48	0.44
1:I:705:PRO:HG2	1:K:567:ARG:CZ	2.48	0.44
1:J:11:LEU:HD12	1:J:95:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:112:TYR:CE2	1:J:278:LEU:HA	2.53	0.44
1:K:16:ASP:O	1:K:18:ALA:N	2.47	0.44
1:K:417:THR:HG22	1:K:420:GLU:H	1.83	0.44
1:L:210:ASP:OD1	1:L:210:ASP:N	2.49	0.44
1:A:620:THR:HA	1:A:645:LEU:O	2.18	0.44
1:B:191:LEU:HD22	1:B:196:VAL:HG21	2.00	0.44
1:C:461:ASN:ND2	1:C:483:ASN:HD22	2.14	0.44
1:F:201:LEU:HD23	1:F:204:VAL:HG11	2.00	0.44
1:H:154:THR:HA	1:H:197:THR:OG1	2.17	0.44
1:H:182:LEU:HD22	1:H:256:LEU:HD11	2.00	0.44
1:H:270:ASN:ND2	1:H:343:LEU:HB2	2.33	0.44
1:L:408:ARG:NH2	1:L:479:ASN:HB3	2.31	0.44
1:A:678:MET:HA	1:A:681:GLN:HB2	2.00	0.43
1:C:112:TYR:CD1	1:C:117:PRO:HA	2.52	0.43
1:C:224:TYR:HA	1:C:268:VAL:HG21	1.99	0.43
1:C:456:ASP:OD2	1:C:528:THR:HG23	2.18	0.43
1:G:154:THR:HA	1:G:197:THR:OG1	2.18	0.43
1:G:670:VAL:O	1:G:700:THR:HA	2.17	0.43
1:I:645:LEU:HD23	1:I:701:VAL:HG13	1.99	0.43
1:J:361:PHE:CZ	1:J:380:TRP:HH2	2.35	0.43
1:L:78:ALA:HB3	1:L:81:ARG:HH21	1.82	0.43
1:L:125:SER:OG	1:L:129:THR:OG1	2.36	0.43
1:L:205:HIS:HB2	1:L:226:THR:HG21	2.00	0.43
1:A:270:ASN:ND2	1:A:343:LEU:HB2	2.33	0.43
1:B:264:ILE:HA	1:B:338:GLY:O	2.18	0.43
1:C:24:VAL:HG22	1:C:25:PHE:H	1.83	0.43
1:C:470:GLU:C	1:C:473:ARG:HH21	2.21	0.43
1:D:161:VAL:HG11	1:D:179:TYR:CE2	2.53	0.43
1:D:447:THR:OG1	1:D:452:PHE:O	2.37	0.43
1:D:514:GLN:NE2	1:D:574:VAL:O	2.51	0.43
1:E:398:GLU:OE2	1:E:439:PRO:HG2	2.17	0.43
1:F:175:LEU:O	1:F:178:THR:OG1	2.33	0.43
1:H:277:HIS:ND1	1:H:278:LEU:HG	2.33	0.43
1:I:221:TYR:CD2	1:I:222:TRP:HD1	2.36	0.43
1:I:233:HIS:HB3	1:I:236:TYR:CD2	2.53	0.43
1:I:296:ALA:C	1:I:298:ASP:H	2.22	0.43
1:I:549:LYS:HA	1:I:549:LYS:HD2	1.65	0.43
1:J:92:LEU:O	1:J:94:PRO:HD3	2.18	0.43
1:J:399:TRP:HD1	1:J:443:VAL:HG21	1.83	0.43
1:L:618:ALA:HA	1:L:647:PHE:O	2.18	0.43
1:A:512:LEU:HD22	1:A:575:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:TRP:N	1:B:248:GLU:OE2	2.52	0.43
1:B:454:LEU:HD12	1:B:457:LEU:HD23	2.00	0.43
1:D:146:ARG:HH22	1:D:331:VAL:HG12	1.83	0.43
1:D:159:ALA:HA	1:D:521:HIS:ND1	2.33	0.43
1:D:595:ASP:HA	1:D:627:ALA:HB3	2.00	0.43
1:E:377:ALA:HB3	1:E:396:TRP:CH2	2.53	0.43
1:F:607:THR:O	1:F:611:TRP:N	2.51	0.43
1:G:53:ALA:HA	1:L:435:ASP:O	2.18	0.43
1:G:313:LEU:CD2	1:G:315:ARG:HG2	2.49	0.43
1:H:225:ASN:O	1:H:225:ASN:ND2	2.51	0.43
1:I:578:ARG:NH1	1:I:578:ARG:HB3	2.32	0.43
1:J:110:TYR:HA	1:J:280:PRO:HA	2.00	0.43
1:J:154:THR:HA	1:J:197:THR:OG1	2.17	0.43
1:K:37:LEU:HD12	1:K:131:THR:HG21	2.00	0.43
1:L:31:ARG:HH21	1:L:74:HIS:CD2	2.36	0.43
1:L:50:GLU:O	1:L:56:ARG:HA	2.18	0.43
1:A:433:GLN:HA	1:A:582:HIS:CD2	2.53	0.43
1:B:442:SER:OG	1:B:444:ASN:OD1	2.34	0.43
1:E:622:PHE:HB2	1:E:644:LEU:HD13	2.00	0.43
1:F:300:ARG:HD2	1:F:301:TYR:CZ	2.54	0.43
1:G:242:ARG:C	1:G:244:GLN:H	2.21	0.43
1:G:330:TRP:O	1:G:334:MET:HB2	2.18	0.43
1:H:65:PRO:HG2	1:H:136:ASN:HB2	2.00	0.43
1:H:296:ALA:HA	1:H:303:MET:HG3	2.00	0.43
1:I:644:LEU:HD12	1:I:644:LEU:HA	1.77	0.43
1:J:410:LEU:HD23	1:J:411:TRP:CE2	2.54	0.43
1:J:417:THR:HB	1:J:420:GLU:CB	2.48	0.43
1:J:494:GLY:O	1:J:498:LEU:HB2	2.19	0.43
1:K:14:THR:O	1:K:20:THR:HA	2.17	0.43
1:K:147:PRO:O	1:K:149:THR:N	2.49	0.43
1:K:622:PHE:CE2	1:K:624:ASN:HB2	2.54	0.43
1:L:379:PRO:HD3	1:L:398:GLU:HB3	2.01	0.43
1:L:589:THR:O	1:L:594:THR:HG21	2.17	0.43
1:L:618:ALA:HB1	1:L:656:PHE:CZ	2.53	0.43
1:L:699:LEU:HD23	1:L:700:THR:H	1.84	0.43
1:A:650:SER:OG	1:A:651:ALA:N	2.50	0.43
1:B:86:ASN:ND2	1:B:89:LYS:HE2	2.34	0.43
1:B:100:SER:HB2	1:B:241:ASP:OD1	2.19	0.43
1:B:644:LEU:HB2	1:B:666:TRP:CZ3	2.54	0.43
1:E:86:ASN:ND2	1:E:121:ASN:O	2.51	0.43
1:E:495:ILE:HG13	1:E:496:THR:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:580:PHE:O	1:F:582:HIS:N	2.44	0.43
1:G:271:HIS:CG	1:G:308:THR:HG1	2.36	0.43
1:G:642:SER:N	1:G:704:ARG:O	2.51	0.43
1:H:108:ALA:HA	1:H:123:LEU:HD13	2.00	0.43
1:H:192:ARG:CD	1:H:259:ALA:HB1	2.49	0.43
1:H:458:VAL:HG11	1:H:502:GLN:HB3	2.00	0.43
1:J:50:GLU:O	1:J:56:ARG:HA	2.18	0.43
1:J:554:ALA:O	1:J:558:LEU:HB2	2.17	0.43
1:K:113:PRO:HG2	1:K:119:ALA:HB3	2.00	0.43
1:K:204:VAL:HG21	1:K:265:LEU:HD22	2.00	0.43
1:K:289:ASN:N	1:K:290:PRO:HD2	2.33	0.43
1:K:646:MET:HB2	1:K:700:THR:HB	2.00	0.43
1:L:343:LEU:HD23	1:L:343:LEU:HA	1.80	0.43
1:A:233:HIS:CE1	1:A:235:ALA:HB3	2.53	0.43
1:B:345:ALA:HA	1:B:380:TRP:HB3	2.00	0.43
1:B:424:ARG:HD3	1:B:424:ARG:HA	1.55	0.43
1:C:24:VAL:HB	1:C:71:PHE:CE1	2.54	0.43
1:C:225:ASN:HA	1:C:271:HIS:HE1	1.84	0.43
1:C:361:PHE:CD1	1:C:393:PRO:HD3	2.54	0.43
1:C:418:LEU:HD22	1:C:611:TRP:CE3	2.52	0.43
1:C:422:ALA:HA	1:C:598:TRP:CH2	2.53	0.43
1:C:452:PHE:HB3	1:C:456:ASP:CB	2.48	0.43
1:C:652:LYS:HA	1:C:696:PRO:HB3	2.00	0.43
1:D:364:VAL:HG13	1:D:370:VAL:HG12	2.00	0.43
1:G:19:GLY:HA3	1:G:61:PRO:HA	2.00	0.43
1:G:157:TYR:HB2	1:G:196:VAL:HG11	2.00	0.43
1:H:502:GLN:HA	1:H:505:ASN:HD22	1.83	0.43
1:I:143:ASP:H	1:I:254:ARG:NH2	2.16	0.43
1:I:561:PHE:HA	1:I:679:PRO:HG2	2.00	0.43
1:J:699:LEU:HD23	1:J:700:THR:H	1.84	0.43
1:K:404:ARG:HG2	1:K:408:ARG:HD3	2.00	0.43
1:L:159:ALA:HA	1:L:521:HIS:HB3	1.99	0.43
1:L:363:LEU:O	1:L:366:GLN:HG3	2.18	0.43
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.88	0.43
1:B:619:LEU:HD23	1:B:619:LEU:HA	1.87	0.43
1:C:89:LYS:O	1:C:91:LEU:HD22	2.18	0.43
1:C:377:ALA:O	1:C:398:GLU:HA	2.19	0.43
1:G:239:TRP:CD2	1:G:248:GLU:HG3	2.54	0.43
1:H:13:ALA:HB1	1:H:134:VAL:HG22	2.00	0.43
1:J:89:LYS:NZ	1:J:108:ALA:O	2.44	0.43
1:J:125:SER:OG	1:J:129:THR:OG1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:294:ARG:NH1	1:J:353:GLU:HG3	2.30	0.43
1:K:244:GLN:O	1:K:247:LEU:HB2	2.19	0.43
1:A:490:THR:HG22	1:A:492:ASP:H	1.84	0.43
1:B:121:ASN:HD21	1:B:123:LEU:HD12	1.84	0.43
1:B:418:LEU:HD23	1:B:610:ASP:O	2.18	0.43
1:C:296:ALA:C	1:C:298:ASP:H	2.23	0.43
1:C:511:MET:CE	1:C:519:LEU:HD21	2.48	0.43
1:C:561:PHE:CE1	1:C:565:MET:HG3	2.54	0.43
1:C:586:VAL:O	1:C:598:TRP:NE1	2.50	0.43
1:D:157:TYR:HB2	1:D:196:VAL:HG11	2.01	0.43
1:D:184:HIS:HB3	1:D:187:VAL:HG23	2.01	0.43
1:D:679:PRO:HG2	1:D:680:PRO:HD3	2.01	0.43
1:E:580:PHE:O	1:E:582:HIS:N	2.46	0.43
1:G:116:ARG:HA	1:G:117:PRO:HD3	1.93	0.43
1:H:522:GLY:HA3	1:H:527:ARG:HB2	2.00	0.43
1:I:699:LEU:HD23	1:I:700:THR:N	2.34	0.43
1:J:11:LEU:HA	1:J:23:ALA:HB3	2.00	0.43
1:J:285:ARG:HD2	1:J:302:TYR:HH	1.84	0.43
1:J:668:MET:HA	1:J:702:LEU:HA	2.01	0.43
1:K:319:VAL:O	1:K:323:ILE:HG13	2.19	0.43
1:L:590:HIS:HB3	1:L:605:GLU:OE2	2.18	0.43
1:L:678:MET:HG2	1:L:681:GLN:O	2.19	0.43
1:B:86:ASN:OD1	1:B:87:ALA:N	2.52	0.43
1:B:154:THR:HA	1:B:197:THR:OG1	2.18	0.43
1:C:387:TYR:CD2	1:C:392:PHE:HZ	2.37	0.43
1:D:343:LEU:HB3	1:D:346:THR:HB	2.01	0.43
1:D:678:MET:HG2	1:D:681:GLN:O	2.19	0.43
1:H:644:LEU:HB3	1:H:702:LEU:HB2	2.00	0.43
1:I:577:ARG:HH12	1:I:595:ASP:HB2	1.83	0.43
1:J:141:TRP:HB3	1:J:144:ASP:HB2	2.01	0.43
1:J:328:ARG:NH1	1:J:367:ASP:OD1	2.52	0.43
1:J:668:MET:HG3	1:J:701:VAL:O	2.19	0.43
1:K:30:HIS:C	1:K:31:ARG:HD2	2.39	0.43
1:L:488:GLY:O	1:L:499:ARG:NH2	2.50	0.43
1:L:584:ARG:HB2	1:L:585:PRO:CD	2.49	0.43
1:D:108:ALA:HA	1:D:123:LEU:HD12	2.00	0.43
1:D:448:CYS:HA	1:D:520:SER:HB3	2.01	0.43
1:F:80:GLU:CD	1:F:80:GLU:H	2.22	0.43
1:G:175:LEU:HD22	1:G:180:ALA:CB	2.49	0.43
1:H:63:VAL:HG13	1:H:67:GLN:HG2	2.00	0.43
1:H:455:ARG:HG3	1:H:526:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:76:PRO:O	1:I:83:LEU:HB3	2.19	0.43
1:I:221:TYR:HE1	1:I:544:TRP:HZ3	1.66	0.43
1:I:352:HIS:C	1:I:354:VAL:H	2.22	0.43
1:J:37:LEU:HB2	1:J:68:ARG:HB2	2.00	0.43
1:K:4:TRP:HB3	1:K:5:PRO:HD2	2.00	0.43
1:K:336:VAL:HG12	1:K:338:GLY:H	1.84	0.43
1:L:93:ASP:HB3	1:L:96:ALA:HB2	2.00	0.43
1:L:404:ARG:HE	1:L:408:ARG:NH1	2.17	0.43
1:L:432:TYR:O	1:L:582:HIS:CD2	2.71	0.43
1:L:678:MET:N	1:L:679:PRO:HD2	2.33	0.43
1:C:151:TYR:CE2	1:C:397:THR:HG21	2.54	0.42
1:C:574:VAL:HG11	1:C:623:LEU:HB3	2.01	0.42
1:F:159:ALA:HB1	1:F:164:LEU:HG	2.01	0.42
1:F:580:PHE:C	1:F:582:HIS:H	2.22	0.42
1:G:105:TRP:CZ3	1:G:211:HIS:HB2	2.53	0.42
1:G:620:THR:HA	1:G:645:LEU:O	2.18	0.42
1:G:695:ALA:HB1	1:G:696:PRO:HD2	1.99	0.42
1:H:564:SER:O	1:H:567:ARG:HB2	2.19	0.42
1:J:324:MET:HG3	1:J:363:LEU:HD21	2.01	0.42
1:J:425:LEU:HD12	1:J:598:TRP:HH2	1.84	0.42
1:K:381:ASP:HA	1:K:386:GLY:O	2.19	0.42
1:L:227:ILE:HD12	1:L:228:GLY:H	1.84	0.42
1:L:444:ASN:N	1:L:516:VAL:O	2.51	0.42
1:A:484:CYS:O	1:A:495:ILE:HG23	2.19	0.42
1:B:78:ALA:HB3	1:B:83:LEU:HB2	2.01	0.42
1:B:241:ASP:HA	1:B:245:GLN:OE1	2.18	0.42
1:B:584:ARG:H	1:B:584:ARG:NE	2.16	0.42
1:C:461:ASN:OD1	1:C:483:ASN:ND2	2.52	0.42
1:D:80:GLU:H	1:D:80:GLU:CD	2.23	0.42
1:E:525:PHE:HE2	1:E:559:LEU:HD22	1.84	0.42
1:E:667:ARG:NH1	1:E:685:GLU:OE2	2.52	0.42
1:H:699:LEU:HD23	1:H:700:THR:N	2.34	0.42
1:I:314:MET:HB2	1:I:354:VAL:HG21	2.01	0.42
1:J:165:THR:HB	1:J:171:LEU:CD1	2.49	0.42
1:J:336:VAL:HG12	1:J:338:GLY:H	1.85	0.42
1:K:4:TRP:CZ2	1:K:61:PRO:HG3	2.54	0.42
1:K:154:THR:HA	1:K:197:THR:OG1	2.19	0.42
1:K:564:SER:HA	1:K:567:ARG:HB2	2.01	0.42
1:B:71:PHE:HE1	1:B:93:ASP:HB2	1.83	0.42
1:D:210:ASP:N	1:D:210:ASP:OD1	2.51	0.42
1:D:564:SER:HB3	1:D:567:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:619:LEU:HD23	1:D:619:LEU:HA	1.78	0.42
1:E:225:ASN:OD1	1:E:273:ALA:HA	2.19	0.42
1:E:254:ARG:NH1	1:E:258:GLN:OE1	2.52	0.42
1:E:277:HIS:H	1:E:302:TYR:HD2	1.66	0.42
1:F:9:TYR:HA	1:F:10:PRO:HA	1.79	0.42
1:F:157:TYR:CE2	1:F:159:ALA:HB2	2.55	0.42
1:H:166:MET:HA	1:H:176:ARG:HB3	2.02	0.42
1:H:447:THR:HG23	1:H:520:SER:OG	2.19	0.42
1:I:492:ASP:HB3	1:I:495:ILE:HG12	2.01	0.42
1:I:574:VAL:HG12	1:I:623:LEU:HD13	2.00	0.42
1:K:470:GLU:OE2	1:K:474:ASP:HB3	2.20	0.42
1:A:644:LEU:HD12	1:A:644:LEU:HA	1.88	0.42
1:B:52:ASP:OD1	1:D:579:ARG:NH2	2.48	0.42
1:D:589:THR:O	1:D:594:THR:HB	2.19	0.42
1:F:135:VAL:CG1	1:F:246:VAL:HG11	2.50	0.42
1:J:237:ALA:HA	1:J:248:GLU:OE1	2.18	0.42
1:K:68:ARG:HB3	1:K:131:THR:HG21	2.00	0.42
1:A:143:ASP:H	1:A:254:ARG:NH2	2.17	0.42
1:A:296:ALA:HB3	1:A:303:MET:CG	2.49	0.42
1:B:69:TYR:HE2	1:B:133:VAL:C	2.22	0.42
1:B:184:HIS:CG	1:B:185:PRO:HD2	2.55	0.42
1:B:679:PRO:HG2	1:B:680:PRO:HD3	2.01	0.42
1:D:175:LEU:HD22	1:D:180:ALA:HB3	2.02	0.42
1:D:677:GLY:O	1:D:680:PRO:HD2	2.20	0.42
1:E:267:VAL:HB	1:E:269:TYR:CE1	2.55	0.42
1:E:274:GLU:OE2	1:E:283:SER:N	2.45	0.42
1:F:171:LEU:HD22	1:F:184:HIS:CG	2.54	0.42
1:F:426:THR:CG2	1:F:581:PHE:HB2	2.46	0.42
1:H:648:ASN:HB2	1:H:656:PHE:CE1	2.53	0.42
1:K:35:CYS:SG	1:K:72:ARG:NH1	2.92	0.42
1:K:51:THR:HA	1:K:55:VAL:O	2.20	0.42
1:K:98:ALA:HB1	1:K:245:GLN:NE2	2.34	0.42
1:K:112:TYR:C	1:K:121:ASN:HB2	2.39	0.42
1:K:671:ASP:H	1:K:678:MET:HG2	1.84	0.42
1:L:102:ARG:HD3	1:L:102:ARG:N	2.26	0.42
1:A:1:MET:HB3	1:A:2:GLN:H	1.60	0.42
1:A:393:PRO:C	1:A:395:LEU:H	2.23	0.42
1:A:471:GLY:HA3	1:A:473:ARG:HH21	1.84	0.42
1:B:35:CYS:SG	1:B:72:ARG:HG3	2.60	0.42
1:B:162:LYS:HD3	1:B:544:TRP:HH2	1.84	0.42
1:C:72:ARG:NH2	1:C:124:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:VAL:H	1:D:197:THR:HG1	1.59	0.42
1:D:249:PHE:HZ	1:D:265:LEU:HD23	1.84	0.42
1:D:423:SER:HA	1:D:426:THR:OG1	2.18	0.42
1:E:377:ALA:O	1:E:398:GLU:HA	2.20	0.42
1:E:380:TRP:CZ3	1:E:396:TRP:HH2	2.36	0.42
1:F:344:ALA:HB3	1:F:378:GLU:H	1.85	0.42
1:F:393:PRO:O	1:F:395:LEU:N	2.52	0.42
1:F:565:MET:HE2	1:F:565:MET:HA	2.00	0.42
1:G:631:PRO:HA	1:G:636:GLU:O	2.20	0.42
1:H:97:ARG:HD3	1:H:329:TYR:CE1	2.54	0.42
1:I:30:HIS:HB3	1:I:31:ARG:HD2	2.02	0.42
1:I:77:TYR:CD1	1:I:120:ARG:HG3	2.55	0.42
1:I:200:GLU:HG3	1:I:264:ILE:O	2.18	0.42
1:I:397:THR:HB	1:I:443:VAL:HG23	2.01	0.42
1:J:579:ARG:NH2	1:K:50:GLU:OE1	2.52	0.42
1:K:168:HIS:CE1	1:K:170:ASP:HB2	2.55	0.42
1:K:335:HIS:N	1:K:335:HIS:CD2	2.88	0.42
1:K:479:ASN:HD21	1:K:533:ASN:HD22	1.66	0.42
1:L:512:LEU:HD13	1:L:645:LEU:HD21	2.01	0.42
1:B:1:MET:HB3	1:B:2:GLN:H	1.60	0.42
1:B:121:ASN:OD1	1:B:123:LEU:HG	2.20	0.42
1:B:233:HIS:CD2	1:B:235:ALA:HB3	2.54	0.42
1:B:301:TYR:CE1	1:C:467:ALA:HA	2.54	0.42
1:B:411:TRP:HB3	1:B:502:GLN:HE22	1.85	0.42
1:B:620:THR:HG23	1:B:646:MET:HG2	2.02	0.42
1:B:687:ALA:HB3	1:B:690:GLU:HG2	2.02	0.42
1:C:19:GLY:CA	1:C:62:GLY:H	2.33	0.42
1:C:25:PHE:CZ	1:C:27:GLU:HG3	2.55	0.42
1:C:410:LEU:HD22	1:C:421:PHE:CE2	2.54	0.42
1:C:579:ARG:NH2	1:I:52:ASP:OD1	2.50	0.42
1:D:667:ARG:HA	1:D:685:GLU:HA	2.00	0.42
1:F:88:ALA:HB3	1:F:89:LYS:HE2	2.02	0.42
1:F:313:LEU:HD23	1:F:313:LEU:HA	1.82	0.42
1:H:408:ARG:HG2	1:H:457:LEU:HD11	2.01	0.42
1:I:565:MET:HE2	1:I:679:PRO:HB3	2.02	0.42
1:I:622:PHE:HE1	1:I:642:SER:HB3	1.84	0.42
1:J:168:HIS:CE1	1:J:170:ASP:HB2	2.55	0.42
1:L:80:GLU:OE1	1:L:80:GLU:N	2.43	0.42
1:A:225:ASN:ND2	1:A:273:ALA:HA	2.35	0.42
1:A:434:ASP:HB2	1:A:440:LEU:HD12	2.01	0.42
1:C:214:VAL:HA	1:C:218:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:ALA:HA	1:C:380:TRP:HB3	2.01	0.42
1:D:356:ARG:HA	1:D:359:SER:OG	2.20	0.42
1:F:89:LYS:HA	1:F:125:SER:CB	2.50	0.42
1:F:301:TYR:CZ	1:J:467:ALA:HA	2.55	0.42
1:F:328:ARG:HG2	1:F:369:VAL:HB	2.00	0.42
1:F:538:GLN:HG3	1:F:540:ASN:OD1	2.19	0.42
1:G:213:LEU:HD23	1:G:219:SER:C	2.40	0.42
1:G:599:PHE:CD1	1:G:659:PRO:HG2	2.54	0.42
1:G:644:LEU:O	1:G:701:VAL:HA	2.20	0.42
1:H:461:ASN:OD1	1:H:483:ASN:HB3	2.20	0.42
1:H:574:VAL:HG12	1:H:623:LEU:HD13	2.01	0.42
1:H:698:SER:OG	1:H:699:LEU:N	2.53	0.42
1:J:379:PRO:HD3	1:J:398:GLU:HB3	2.01	0.42
1:L:92:LEU:HD21	1:L:130:MET:HB2	2.02	0.42
1:A:379:PRO:HD3	1:A:398:GLU:HB3	2.02	0.42
1:B:89:LYS:O	1:B:91:LEU:HD22	2.20	0.42
1:B:205:HIS:HE1	1:B:267:VAL:HG12	1.84	0.42
1:C:15:TYR:CE2	1:C:17:GLY:HA2	2.55	0.42
1:E:153:HIS:O	1:E:197:THR:HG21	2.19	0.42
1:E:200:GLU:HA	1:E:264:ILE:O	2.20	0.42
1:E:227:ILE:HD12	1:E:228:GLY:H	1.85	0.42
1:G:210:ASP:N	1:G:210:ASP:OD1	2.53	0.42
1:H:476:GLU:H	1:H:533:ASN:HD21	1.67	0.42
1:H:549:LYS:HA	1:H:549:LYS:HD2	1.57	0.42
1:J:602:GLU:H	1:J:602:GLU:HG3	1.72	0.42
1:J:670:VAL:HB	1:J:701:VAL:HB	2.01	0.42
1:K:609:ARG:O	1:K:609:ARG:HD3	2.19	0.42
1:L:440:LEU:HD23	1:L:440:LEU:H	1.85	0.42
1:L:560:ARG:O	1:L:680:PRO:HG3	2.20	0.42
1:L:668:MET:HE3	1:L:684:PRO:HD2	2.01	0.42
1:B:86:ASN:HD21	1:B:89:LYS:HE2	1.85	0.42
1:B:670:VAL:HA	1:B:678:MET:O	2.19	0.42
1:B:677:GLY:O	1:B:680:PRO:HD2	2.20	0.42
1:C:226:THR:HG1	1:C:229:PHE:HE1	1.68	0.42
1:C:488:GLY:O	1:C:499:ARG:NH1	2.52	0.42
1:C:490:THR:CB	1:C:495:ILE:HD11	2.50	0.42
1:C:699:LEU:HD23	1:C:700:THR:N	2.35	0.42
1:E:476:GLU:N	1:E:533:ASN:HD21	2.18	0.42
1:G:25:PHE:CE1	1:G:27:GLU:HB3	2.55	0.42
1:G:690:GLU:OE2	1:G:692:VAL:HG22	2.20	0.42
1:H:100:SER:HA	1:H:241:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:164:LEU:HD23	1:H:547:TRP:HZ2	1.84	0.42
1:I:538:GLN:HG3	1:I:540:ASN:HD21	1.85	0.42
1:J:527:ARG:HE	1:J:527:ARG:HB3	1.77	0.42
1:J:585:PRO:HG2	1:J:588:GLY:N	2.28	0.42
1:K:343:LEU:HD23	1:K:343:LEU:HA	1.72	0.42
1:K:408:ARG:HD2	1:K:446:VAL:O	2.20	0.42
1:L:112:TYR:CD1	1:L:117:PRO:HA	2.54	0.42
1:L:160:HIS:ND1	1:L:221:TYR:CZ	2.84	0.42
1:L:671:ASP:OD1	1:L:672:THR:N	2.53	0.42
1:A:61:PRO:HB2	1:F:61:PRO:O	2.20	0.41
1:A:71:PHE:CE1	1:A:93:ASP:HB2	2.55	0.41
1:A:393:PRO:HG2	1:A:396:TRP:HD1	1.85	0.41
1:C:426:THR:HG23	1:C:581:PHE:HB2	2.00	0.41
1:D:80:GLU:HG3	1:D:300:ARG:HE	1.85	0.41
1:D:418:LEU:HD12	1:D:418:LEU:HA	1.73	0.41
1:D:426:THR:CG2	1:D:581:PHE:HB2	2.45	0.41
1:D:645:LEU:HD23	1:D:701:VAL:HG13	2.02	0.41
1:E:478:TYR:HE1	1:E:480:ARG:HH21	1.68	0.41
1:E:646:MET:O	1:E:699:LEU:HD23	2.20	0.41
1:F:296:ALA:C	1:F:298:ASP:H	2.24	0.41
1:F:313:LEU:HD22	1:F:315:ARG:HG2	2.02	0.41
1:H:32:ILE:HD12	1:H:56:ARG:HG3	2.02	0.41
1:H:102:ARG:NH1	1:H:209:ASN:H	2.18	0.41
1:I:92:LEU:O	1:I:94:PRO:HD3	2.19	0.41
1:J:77:TYR:CD1	1:J:120:ARG:HG3	2.55	0.41
1:K:4:TRP:CE2	1:K:61:PRO:HG3	2.55	0.41
1:K:479:ASN:OD1	1:K:479:ASN:N	2.53	0.41
1:L:618:ALA:HB1	1:L:656:PHE:HZ	1.84	0.41
1:L:694:LEU:HD11	1:L:700:THR:OG1	2.19	0.41
1:A:100:SER:HB2	1:A:241:ASP:CG	2.39	0.41
1:A:294:ARG:HH11	1:A:296:ALA:HB2	1.84	0.41
1:A:453:THR:O	1:A:457:LEU:N	2.45	0.41
1:B:426:THR:HG23	1:B:581:PHE:CD2	2.55	0.41
1:C:274:GLU:O	1:C:280:PRO:HD2	2.20	0.41
1:C:418:LEU:HA	1:C:616:ALA:HB2	2.02	0.41
1:D:83:LEU:HD23	1:D:83:LEU:HA	1.73	0.41
1:D:578:ARG:HB3	1:D:578:ARG:NH1	2.35	0.41
1:E:426:THR:HG22	1:E:581:PHE:HB2	2.02	0.41
1:F:461:ASN:ND2	1:F:482:TRP:HA	2.35	0.41
1:F:644:LEU:O	1:F:701:VAL:HA	2.20	0.41
1:I:112:TYR:CZ	1:I:278:LEU:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:399:TRP:CD1	1:J:443:VAL:HG21	2.54	0.41
1:L:431:LEU:HB2	1:L:432:TYR:CD2	2.54	0.41
1:A:380:TRP:CD1	1:A:382:VAL:HG23	2.55	0.41
1:A:501:ARG:NE	1:A:673:SER:HA	2.36	0.41
1:A:585:PRO:HG2	1:A:588:GLY:N	2.29	0.41
1:B:403:TYR:O	1:B:407:VAL:HG23	2.20	0.41
1:B:578:ARG:HH22	1:B:631:PRO:HD2	1.85	0.41
1:B:602:GLU:O	1:B:657:VAL:HG21	2.20	0.41
1:C:204:VAL:O	1:C:233:HIS:N	2.54	0.41
1:D:2:GLN:CD	1:D:4:TRP:HE1	2.23	0.41
1:D:504:ARG:HB3	1:D:561:PHE:CZ	2.56	0.41
1:E:313:LEU:HD22	1:E:315:ARG:HG2	2.01	0.41
1:F:194:LEU:O	1:F:566:VAL:HG11	2.20	0.41
1:F:360:PHE:O	1:F:364:VAL:N	2.48	0.41
1:F:368:PRO:HD3	1:H:328:ARG:CZ	2.50	0.41
1:F:478:TYR:HD2	1:F:479:ASN:H	1.67	0.41
1:F:522:GLY:HA3	1:F:527:ARG:HB2	2.02	0.41
1:G:427:GLY:CA	1:G:514:GLN:HB2	2.49	0.41
1:H:607:THR:HG23	1:H:610:ASP:H	1.85	0.41
1:I:486:GLU:O	1:I:499:ARG:NH2	2.53	0.41
1:I:584:ARG:HB2	1:I:585:PRO:HD2	2.02	0.41
1:J:91:LEU:HD11	1:J:286:GLY:HA3	2.02	0.41
1:J:178:THR:HG21	1:J:238:SER:HB3	2.03	0.41
1:K:313:LEU:HD23	1:K:313:LEU:HA	1.87	0.41
1:K:460:TYR:HA	1:K:487:GLU:CG	2.50	0.41
1:L:102:ARG:NH1	1:L:102:ARG:O	2.53	0.41
1:L:105:TRP:CD2	1:L:211:HIS:HB2	2.55	0.41
1:L:458:VAL:HG11	1:L:502:GLN:HB3	2.01	0.41
1:D:330:TRP:CE3	1:D:334:MET:HG3	2.55	0.41
1:F:68:ARG:HB3	1:F:131:THR:CG2	2.50	0.41
1:F:224:TYR:O	1:F:271:HIS:NE2	2.53	0.41
1:H:265:LEU:HG	1:H:336:VAL:HG11	2.01	0.41
1:I:578:ARG:HH12	1:I:579:ARG:NH1	2.18	0.41
1:J:405:ASP:O	1:J:416:ARG:NH2	2.53	0.41
1:J:432:TYR:HB3	1:J:439:PRO:O	2.21	0.41
1:K:585:PRO:HG2	1:K:588:GLY:HA2	2.01	0.41
1:L:143:ASP:H	1:L:254:ARG:NH2	2.19	0.41
1:L:212:ARG:NH2	1:L:536:TYR:OH	2.53	0.41
1:A:34:LEU:HD12	1:A:35:CYS:H	1.85	0.41
1:A:312:LEU:O	1:A:319:VAL:HG11	2.20	0.41
1:B:456:ASP:OD2	1:B:528:THR:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:TRP:CE3	1:C:248:GLU:HG2	2.54	0.41
1:C:368:PRO:HD3	1:I:328:ARG:NH2	2.35	0.41
1:D:68:ARG:HB3	1:D:131:THR:CG2	2.50	0.41
1:E:11:LEU:H	1:E:11:LEU:HG	1.68	0.41
1:E:78:ALA:N	1:E:83:LEU:O	2.48	0.41
1:E:92:LEU:H	1:E:283:SER:HA	1.86	0.41
1:E:288:ASP:OD2	1:E:291:SER:OG	2.26	0.41
1:F:37:LEU:CD2	1:F:43:GLU:HG3	2.50	0.41
1:F:153:HIS:O	1:F:197:THR:HG21	2.20	0.41
1:F:686:LEU:HD23	1:F:686:LEU:HA	1.87	0.41
1:G:253:VAL:HG22	1:G:263:VAL:HG21	2.01	0.41
1:G:408:ARG:HG2	1:G:457:LEU:HD11	2.02	0.41
1:H:577:ARG:HB2	1:H:580:PHE:HA	2.02	0.41
1:I:67:GLN:O	1:I:134:VAL:HG23	2.20	0.41
1:I:393:PRO:C	1:I:395:LEU:H	2.23	0.41
1:I:640:ASP:OD2	1:I:641:ASP:N	2.53	0.41
1:J:395:LEU:HA	1:J:395:LEU:HD23	1.84	0.41
1:J:648:ASN:OD1	1:J:654:LEU:HD12	2.20	0.41
1:J:665:TYR:O	1:J:704:ARG:HG3	2.20	0.41
1:K:205:HIS:NE2	1:K:267:VAL:HG12	2.35	0.41
1:K:274:GLU:OE2	1:K:282:LEU:N	2.44	0.41
1:L:37:LEU:HD11	1:L:90:LEU:CD2	2.47	0.41
1:A:66:GLY:O	1:A:242:ARG:NH2	2.51	0.41
1:B:242:ARG:O	1:G:40:ASP:HB3	2.19	0.41
1:B:313:LEU:HB3	1:B:316:SER:OG	2.20	0.41
1:B:579:ARG:NH2	1:D:52:ASP:OD1	2.53	0.41
1:B:670:VAL:HB	1:B:701:VAL:HB	2.03	0.41
1:C:347:LEU:HD23	1:C:347:LEU:O	2.20	0.41
1:E:454:LEU:HD12	1:E:454:LEU:HA	1.85	0.41
1:F:52:ASP:OD1	1:H:579:ARG:NH2	2.54	0.41
1:G:461:ASN:ND2	1:G:482:TRP:HA	2.35	0.41
1:J:86:ASN:ND2	1:J:121:ASN:O	2.36	0.41
1:J:653:GLU:HG2	2:J:836:HOH:O	2.20	0.41
1:K:151:TYR:HE1	1:K:397:THR:CG2	2.34	0.41
1:K:412:ARG:CZ	1:K:414:GLU:HG3	2.51	0.41
1:K:417:THR:HB	1:K:420:GLU:HB3	2.02	0.41
1:L:105:TRP:CE3	1:L:211:HIS:HB2	2.56	0.41
1:L:149:THR:HG22	1:L:150:GLU:O	2.20	0.41
1:A:97:ARG:HD3	1:A:329:TYR:CE1	2.56	0.41
1:B:404:ARG:HE	1:B:408:ARG:NH1	2.18	0.41
1:B:433:GLN:HG3	1:B:435:ASP:CB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:ALA:O	1:C:537:CYS:N	2.53	0.41
1:D:14:THR:O	1:D:20:THR:HA	2.20	0.41
1:D:47:GLU:O	1:D:49:ARG:HG3	2.21	0.41
1:D:586:VAL:O	1:D:598:TRP:NE1	2.54	0.41
1:E:200:GLU:HA	1:E:264:ILE:HB	2.02	0.41
1:F:172:PRO:O	1:F:176:ARG:HG3	2.21	0.41
1:F:667:ARG:HA	1:F:685:GLU:HA	2.03	0.41
1:F:674:ASP:HA	1:F:675:PRO:HD3	1.86	0.41
1:I:142:GLY:H	1:I:254:ARG:NH1	2.19	0.41
1:I:483:ASN:H	1:I:483:ASN:HD22	1.68	0.41
1:I:641:ASP:HB3	1:I:704:ARG:O	2.20	0.41
1:J:156:ILE:O	1:J:518:MET:HA	2.21	0.41
1:J:165:THR:HB	1:J:171:LEU:HD11	2.02	0.41
1:K:205:HIS:HB2	1:K:226:THR:HG21	2.02	0.41
1:L:36:LEU:HB2	1:L:44:THR:HB	2.01	0.41
1:A:443:VAL:HG22	1:A:516:VAL:HB	2.02	0.41
1:C:239:TRP:CD2	1:C:248:GLU:HG2	2.56	0.41
1:E:255:ALA:O	1:E:258:GLN:HB2	2.20	0.41
1:F:51:THR:OG1	1:F:56:ARG:HG2	2.21	0.41
1:G:202:MET:HB3	1:G:203:PRO:HD2	2.03	0.41
1:H:255:ALA:O	1:H:258:GLN:HB2	2.20	0.41
1:H:398:GLU:HB2	2:H:802:HOH:O	2.21	0.41
1:H:670:VAL:HA	1:H:678:MET:O	2.20	0.41
1:I:345:ALA:HB2	1:I:379:PRO:O	2.20	0.41
1:I:404:ARG:NH1	1:I:405:ASP:OD1	2.54	0.41
1:I:432:TYR:CD2	1:I:442:SER:HB3	2.56	0.41
1:J:37:LEU:HD12	1:J:131:THR:HG21	2.02	0.41
1:J:129:THR:HG22	1:J:130:MET:N	2.35	0.41
1:J:222:TRP:HB3	1:J:224:TYR:CD1	2.56	0.41
1:J:426:THR:HG22	1:J:581:PHE:HB2	2.03	0.41
1:J:634:GLN:HA	1:K:4:TRP:CD2	2.56	0.41
1:J:652:LYS:C	1:J:696:PRO:HB3	2.41	0.41
1:K:632:GLY:N	1:K:636:GLU:O	2.54	0.41
1:L:168:HIS:HB3	1:L:171:LEU:HG	2.03	0.41
1:L:601:PRO:HA	1:L:656:PHE:HD2	1.86	0.41
1:A:379:PRO:HB3	1:A:398:GLU:OE1	2.20	0.41
1:A:433:GLN:HA	1:A:582:HIS:HD2	1.86	0.41
1:A:564:SER:HA	1:A:567:ARG:HB2	2.02	0.41
1:B:141:TRP:HB3	1:B:144:ASP:HB2	2.03	0.41
1:C:304:ASP:CG	1:C:309:GLY:H	2.24	0.41
1:C:585:PRO:HG2	1:C:588:GLY:N	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:ILE:HG22	1:F:48:LEU:HD12	2.02	0.41
1:F:213:LEU:HD21	1:F:536:TYR:HE1	1.85	0.41
1:F:424:ARG:NH2	1:F:431:LEU:HD11	2.35	0.41
1:F:564:SER:OG	1:F:679:PRO:HB2	2.21	0.41
1:G:4:TRP:CE2	1:G:61:PRO:HG3	2.56	0.41
1:G:16:ASP:O	1:G:18:ALA:N	2.50	0.41
1:G:16:ASP:C	1:G:18:ALA:H	2.24	0.41
1:G:92:LEU:O	1:G:94:PRO:HD3	2.20	0.41
1:G:107:GLU:OE2	1:G:114:PHE:HB2	2.21	0.41
1:G:124:ASP:OD1	1:G:125:SER:N	2.54	0.41
1:H:201:LEU:HD23	1:H:204:VAL:HG11	2.03	0.41
1:H:266:ASP:OD1	1:H:340:ARG:HD3	2.21	0.41
1:H:276:ASN:C	1:H:285:ARG:HH12	2.24	0.41
1:H:330:TRP:CE3	1:H:334:MET:HG3	2.56	0.41
1:H:471:GLY:HA3	1:H:473:ARG:HE	1.85	0.41
1:H:617:GLN:OE1	1:H:650:SER:HA	2.21	0.41
1:H:619:LEU:HD23	1:H:619:LEU:HA	1.88	0.41
1:I:342:ASP:OD2	1:I:343:LEU:HG	2.21	0.41
1:J:361:PHE:HZ	1:J:380:TRP:HH2	1.69	0.41
1:J:398:GLU:OE1	1:J:432:TYR:HE1	2.04	0.41
1:J:512:LEU:HD22	1:J:575:PHE:CE2	2.56	0.41
1:J:560:ARG:NH1	1:J:676:GLU:O	2.45	0.41
1:J:600:THR:O	1:J:603:GLY:N	2.54	0.41
1:J:624:ASN:HB3	1:J:627:ALA:HB3	2.03	0.41
1:K:100:SER:HB2	1:K:241:ASP:OD1	2.20	0.41
1:K:426:THR:HG23	1:K:581:PHE:CD2	2.56	0.41
1:L:573:PRO:O	1:L:576:ARG:N	2.42	0.41
1:L:652:LYS:C	1:L:696:PRO:HB3	2.40	0.41
1:A:224:TYR:HA	1:A:268:VAL:HG21	2.03	0.41
1:B:68:ARG:HD3	1:B:242:ARG:NH1	2.36	0.41
1:D:598:TRP:CE3	1:D:619:LEU:HD13	2.56	0.41
1:E:116:ARG:HA	1:E:117:PRO:HD3	1.98	0.41
1:E:222:TRP:CD2	1:E:536:TYR:HA	2.55	0.41
1:H:70:GLY:HA3	1:H:90:LEU:HD11	2.03	0.41
1:H:275:GLY:O	1:H:310:ASN:ND2	2.54	0.41
1:H:565:MET:HE1	1:H:568:LEU:HD22	2.03	0.41
1:J:380:TRP:NE1	1:J:387:TYR:HA	2.35	0.41
1:J:541:GLU:HA	1:J:544:TRP:CD1	2.56	0.41
1:J:644:LEU:HB3	1:J:702:LEU:HB2	2.03	0.41
1:L:97:ARG:HB2	1:L:135:VAL:HG21	2.03	0.41
1:A:112:TYR:C	1:A:121:ASN:HB2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:SER:HA	1:A:426:THR:HB	2.04	0.40
1:B:135:VAL:HG13	1:B:246:VAL:HG11	2.03	0.40
1:B:577:ARG:HB2	1:B:580:PHE:HA	2.02	0.40
1:C:159:ALA:HB1	1:C:164:LEU:HG	2.04	0.40
1:C:461:ASN:ND2	1:C:483:ASN:H	2.18	0.40
1:D:568:LEU:HG	1:D:572:HIS:CD2	2.55	0.40
1:F:321:GLN:O	1:F:325:ASP:HB2	2.21	0.40
1:F:398:GLU:OE1	1:F:432:TYR:HE1	2.04	0.40
1:G:281:THR:HG23	1:G:285:ARG:HG2	2.03	0.40
1:J:239:TRP:CE3	1:J:248:GLU:HG2	2.56	0.40
1:K:457:LEU:HD12	1:K:481:SER:HB2	2.02	0.40
1:L:527:ARG:NH1	1:L:545:VAL:HG22	2.37	0.40
1:L:645:LEU:HA	1:L:645:LEU:HD23	1.74	0.40
1:A:227:ILE:CG2	1:A:273:ALA:HB3	2.46	0.40
1:B:409:ASP:OD1	1:B:412:ARG:HD3	2.21	0.40
1:D:482:TRP:CZ3	1:D:484:CYS:HA	2.56	0.40
1:D:549:LYS:O	1:D:551:ASN:N	2.55	0.40
1:E:314:MET:SD	1:E:351:PHE:CE2	3.14	0.40
1:E:418:LEU:HB3	1:E:611:TRP:O	2.22	0.40
1:F:19:GLY:HA3	1:F:60:LEU:O	2.21	0.40
1:F:622:PHE:HE1	1:F:666:TRP:HH2	1.69	0.40
1:G:68:ARG:HB3	1:G:131:THR:CG2	2.52	0.40
1:H:262:GLU:HB3	1:H:337:ASP:HB2	2.03	0.40
1:H:447:THR:OG1	1:H:452:PHE:O	2.35	0.40
1:I:27:GLU:HG3	1:I:54:PHE:CD2	2.56	0.40
1:I:461:ASN:ND2	1:I:482:TRP:HA	2.36	0.40
1:K:424:ARG:HA	1:K:424:ARG:HD3	1.73	0.40
1:L:81:ARG:HE	1:L:81:ARG:HB2	1.47	0.40
1:L:622:PHE:CE2	1:L:660:ASP:OD2	2.74	0.40
1:B:53:ALA:HA	1:D:435:ASP:O	2.22	0.40
1:B:632:GLY:HA3	1:B:636:GLU:OE2	2.20	0.40
1:C:403:TYR:CZ	1:C:407:VAL:HG21	2.56	0.40
1:C:587:GLU:HG2	1:C:611:TRP:CZ2	2.55	0.40
1:D:593:LEU:O	1:D:627:ALA:HB2	2.20	0.40
1:E:32:ILE:HD12	1:E:56:ARG:HG3	2.03	0.40
1:E:159:ALA:HB1	1:E:164:LEU:HD12	2.04	0.40
1:E:453:THR:O	1:E:457:LEU:N	2.54	0.40
1:G:70:GLY:HA3	1:G:90:LEU:HD11	2.02	0.40
1:G:502:GLN:NE2	1:G:697:LEU:HB3	2.37	0.40
1:H:179:TYR:HB2	1:H:248:GLU:HB3	2.03	0.40
1:J:213:LEU:HD21	1:J:536:TYR:HE1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:412:ARG:HH11	1:J:480:ARG:HA	1.85	0.40
1:J:674:ASP:OD2	1:J:678:MET:HB2	2.21	0.40
1:L:180:ALA:N	1:L:248:GLU:OE1	2.48	0.40
1:L:406:CYS:SG	1:L:416:ARG:NH2	2.95	0.40
1:L:648:ASN:ND2	1:L:654:LEU:HB2	2.36	0.40
1:L:652:LYS:CA	1:L:696:PRO:HB3	2.51	0.40
1:A:32:ILE:HG12	1:A:73:VAL:HG22	2.03	0.40
1:A:565:MET:HE1	1:A:568:LEU:HD22	2.04	0.40
1:B:625:GLY:HA3	1:B:640:ASP:O	2.21	0.40
1:D:3:VAL:HG21	1:D:46:VAL:HG13	2.03	0.40
1:D:107:GLU:HG3	1:D:114:PHE:CG	2.56	0.40
1:D:262:GLU:HB3	1:D:337:ASP:HB2	2.04	0.40
1:E:159:ALA:HA	1:E:521:HIS:CG	2.57	0.40
1:E:268:VAL:HG22	1:E:342:ASP:HB3	2.04	0.40
1:E:321:GLN:HG2	1:E:325:ASP:OD1	2.21	0.40
1:E:598:TRP:CD1	1:E:598:TRP:N	2.89	0.40
1:F:65:PRO:HG2	1:F:136:ASN:HB2	2.04	0.40
1:F:184:HIS:O	1:F:188:ILE:HG13	2.22	0.40
1:G:100:SER:HB2	1:G:241:ASP:OD1	2.21	0.40
1:G:171:LEU:HD22	1:G:184:HIS:CG	2.57	0.40
1:I:319:VAL:O	1:I:322:LEU:HB3	2.22	0.40
1:I:600:THR:CG2	1:I:601:PRO:HD2	2.51	0.40
1:J:348:ALA:HA	1:J:351:PHE:HB2	2.03	0.40
1:K:414:GLU:HA	1:K:415:PRO:HD3	1.86	0.40
1:L:427:GLY:N	1:L:514:GLN:HB2	2.36	0.40
1:L:501:ARG:HG3	1:L:672:THR:HG22	2.04	0.40
1:L:586:VAL:O	1:L:598:TRP:NE1	2.55	0.40
1:A:65:PRO:HD2	1:F:38:HIS:ND1	2.37	0.40
1:A:351:PHE:CZ	1:A:360:PHE:HB2	2.56	0.40
1:A:418:LEU:HD23	1:A:611:TRP:CZ3	2.57	0.40
1:A:601:PRO:HG3	1:A:618:ALA:HB3	2.03	0.40
1:B:574:VAL:HG23	1:B:640:ASP:OD1	2.21	0.40
1:D:574:VAL:HG12	1:D:623:LEU:HD13	2.02	0.40
1:E:166:MET:C	1:E:167:LEU:HD12	2.42	0.40
1:E:501:ARG:HA	1:E:504:ARG:HB2	2.03	0.40
1:G:94:PRO:HG3	1:G:283:SER:OG	2.21	0.40
1:G:157:TYR:N	1:G:198:ALA:O	2.52	0.40
1:G:173:GLU:HA	1:G:176:ARG:HD2	2.04	0.40
1:G:242:ARG:HG2	1:G:242:ARG:HH11	1.86	0.40
1:G:500:ALA:O	1:G:504:ARG:HG3	2.21	0.40
1:H:184:HIS:O	1:H:187:VAL:N	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:263:VAL:O	1:H:336:VAL:HG13	2.21	0.40
1:H:270:ASN:HD22	1:H:343:LEU:HB2	1.87	0.40
1:H:345:ALA:HA	1:H:380:TRP:HB3	2.04	0.40
1:H:528:THR:HG22	1:H:530:GLY:H	1.86	0.40
1:J:30:HIS:O	1:J:31:ARG:HD2	2.21	0.40
1:J:105:TRP:CH2	1:J:280:PRO:HG3	2.57	0.40
1:J:294:ARG:HH22	1:J:353:GLU:HG3	1.87	0.40
1:J:668:MET:CE	1:J:684:PRO:HD2	2.52	0.40
1:L:91:LEU:HD11	1:L:281:THR:HG22	2.03	0.40
1:L:98:ALA:HB1	1:L:245:GLN:NE2	2.36	0.40
1:L:315:ARG:HA	1:L:356:ARG:HG3	2.03	0.40
1:L:404:ARG:HB2	1:L:445:PHE:O	2.22	0.40
1:L:645:LEU:HD22	1:L:699:LEU:HD21	2.04	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	699/709 (99%)	620 (89%)	79 (11%)	0	100	100
1	B	703/709 (99%)	636 (90%)	67 (10%)	0	100	100
1	C	693/709 (98%)	614 (89%)	79 (11%)	0	100	100
1	D	696/709 (98%)	604 (87%)	92 (13%)	0	100	100
1	E	694/709 (98%)	628 (90%)	66 (10%)	0	100	100
1	F	692/709 (98%)	617 (89%)	75 (11%)	0	100	100
1	G	692/709 (98%)	612 (88%)	80 (12%)	0	100	100
1	H	695/709 (98%)	623 (90%)	72 (10%)	0	100	100
1	I	697/709 (98%)	622 (89%)	75 (11%)	0	100	100
1	J	694/709 (98%)	622 (90%)	72 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	697/709 (98%)	619 (89%)	78 (11%)	0	100	100
1	L	695/709 (98%)	617 (89%)	78 (11%)	0	100	100
All	All	8347/8508 (98%)	7434 (89%)	913 (11%)	0	100	100

There are no Ramachandran outliers to report.

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	576/590 (98%)	551 (96%)	25 (4%)	29	62
1	B	580/590 (98%)	549 (95%)	31 (5%)	22	56
1	C	575/590 (98%)	546 (95%)	29 (5%)	24	58
1	D	578/590 (98%)	548 (95%)	30 (5%)	23	57
1	E	579/590 (98%)	548 (95%)	31 (5%)	22	56
1	F	576/590 (98%)	544 (94%)	32 (6%)	21	55
1	G	577/590 (98%)	544 (94%)	33 (6%)	20	54
1	H	577/590 (98%)	544 (94%)	33 (6%)	20	54
1	I	580/590 (98%)	557 (96%)	23 (4%)	31	64
1	J	577/590 (98%)	548 (95%)	29 (5%)	24	58
1	K	580/590 (98%)	554 (96%)	26 (4%)	27	62
1	L	577/590 (98%)	549 (95%)	28 (5%)	25	59
All	All	6932/7080 (98%)	6582 (95%)	350 (5%)	24	58

All (350) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	40	ASP
1	A	116	ARG
1	A	125	SER

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Mol	Chain	Res	Type
1	A	170	ASP
1	A	254	ARG
1	A	283	SER
1	A	297	ASP
1	A	300	ARG
1	A	340	ARG
1	A	351	PHE
1	A	359	SER
1	A	367	ASP
1	A	393	PRO
1	A	404	ARG
1	A	416	ARG
1	A	434	ASP
1	A	478	TYR
1	A	527	ARG
1	A	546	ARG
1	A	560	ARG
1	A	579	ARG
1	A	619	LEU
1	A	623	LEU
1	A	678	MET
1	B	40	ASP
1	B	100	SER
1	B	107	GLU
1	B	116	ARG
1	B	125	SER
1	B	151	TYR
1	B	190	HIS
1	B	212	ARG
1	B	297	ASP
1	B	313	LEU
1	B	322	LEU
1	B	349	ARG
1	B	391	ASN
1	B	396	TRP
1	B	399	TRP
1	B	400	ASN
1	B	423	SER
1	B	442	SER
1	B	455	ARG
1	B	501	ARG
1	B	537	CYS

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Mol	Chain	Res	Type
1	B	546	ARG
1	B	569	ARG
1	B	579	ARG
1	B	584	ARG
1	B	610	ASP
1	B	612	GLN
1	B	674	ASP
1	B	678	MET
1	B	682	GLN
1	B	698	SER
1	C	30	HIS
1	C	52	ASP
1	C	56	ARG
1	C	116	ARG
1	C	151	TYR
1	C	164	LEU
1	C	199	LEU
1	C	210	ASP
1	C	220	ASN
1	C	245	GLN
1	C	254	ARG
1	C	297	ASP
1	C	311	SER
1	C	400	ASN
1	C	434	ASP
1	C	455	ARG
1	C	470	GLU
1	C	478	TYR
1	C	487	GLU
1	C	498	LEU
1	C	537	CYS
1	C	546	ARG
1	C	565	MET
1	C	569	ARG
1	C	648	ASN
1	C	650	SER
1	C	674	ASP
1	C	678	MET
1	C	681	GLN
1	D	114	PHE
1	D	116	ARG
1	D	125	SER

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Mol	Chain	Res	Type
1	D	130	MET
1	D	139	PHE
1	D	151	TYR
1	D	170	ASP
1	D	210	ASP
1	D	277	HIS
1	D	351	PHE
1	D	358	SER
1	D	371	SER
1	D	400	ASN
1	D	405	ASP
1	D	420	GLU
1	D	423	SER
1	D	448	CYS
1	D	455	ARG
1	D	478	TYR
1	D	483	ASN
1	D	544	TRP
1	D	546	ARG
1	D	549	LYS
1	D	577	ARG
1	D	584	ARG
1	D	612	GLN
1	D	665	TYR
1	D	667	ARG
1	D	674	ASP
1	D	703	ARG
1	E	40	ASP
1	E	116	ARG
1	E	125	SER
1	E	143	ASP
1	E	173	GLU
1	E	190	HIS
1	E	241	ASP
1	E	294	ARG
1	E	313	LEU
1	E	340	ARG
1	E	349	ARG
1	E	350	GLN
1	E	400	ASN
1	E	404	ARG
1	E	455	ARG

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Mol	Chain	Res	Type
1	E	463	LYS
1	E	473	ARG
1	E	476	GLU
1	E	502	GLN
1	E	538	GLN
1	E	544	TRP
1	E	546	ARG
1	E	576	ARG
1	E	579	ARG
1	E	584	ARG
1	E	612	GLN
1	E	648	ASN
1	E	665	TYR
1	E	673	SER
1	E	699	LEU
1	E	704	ARG
1	F	9	TYR
1	F	16	ASP
1	F	31	ARG
1	F	40	ASP
1	F	107	GLU
1	F	116	ARG
1	F	151	TYR
1	F	168	HIS
1	F	229	PHE
1	F	242	ARG
1	F	245	GLN
1	F	283	SER
1	F	311	SER
1	F	313	LEU
1	F	326	SER
1	F	351	PHE
1	F	359	SER
1	F	400	ASN
1	F	405	ASP
1	F	433	GLN
1	F	437	ARG
1	F	445	PHE
1	F	455	ARG
1	F	478	TYR
1	F	544	TRP
1	F	579	ARG

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Mol	Chain	Res	Type
1	F	590	HIS
1	F	611	TRP
1	F	665	TYR
1	F	674	ASP
1	F	699	LEU
1	F	704	ARG
1	G	7	GLN
1	G	21	ASN
1	G	30	HIS
1	G	69	TYR
1	G	100	SER
1	G	104	ARG
1	G	107	GLU
1	G	114	PHE
1	G	116	ARG
1	G	125	SER
1	G	151	TYR
1	G	170	ASP
1	G	271	HIS
1	G	294	ARG
1	G	322	LEU
1	G	343	LEU
1	G	425	LEU
1	G	433	GLN
1	G	438	ARG
1	G	442	SER
1	G	455	ARG
1	G	476	GLU
1	G	478	TYR
1	G	538	GLN
1	G	544	TRP
1	G	546	ARG
1	G	580	PHE
1	G	591	ASP
1	G	609	ARG
1	G	610	ASP
1	G	664	ARG
1	G	665	TYR
1	G	694	LEU
1	H	40	ASP
1	H	49	ARG
1	H	52	ASP

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Mol	Chain	Res	Type
1	H	104	ARG
1	H	107	GLU
1	H	116	ARG
1	H	123	LEU
1	H	151	TYR
1	H	254	ARG
1	H	271	HIS
1	H	298	ASP
1	H	311	SER
1	H	313	LEU
1	H	316	SER
1	H	333	GLU
1	H	340	ARG
1	H	371	SER
1	H	381	ASP
1	H	414	GLU
1	H	431	LEU
1	H	455	ARG
1	H	478	TYR
1	H	527	ARG
1	H	537	CYS
1	H	544	TRP
1	H	546	ARG
1	H	569	ARG
1	H	584	ARG
1	H	619	LEU
1	H	662	HIS
1	H	665	TYR
1	H	674	ASP
1	H	682	GLN
1	I	21	ASN
1	I	40	ASP
1	I	74	HIS
1	I	104	ARG
1	I	116	ARG
1	I	150	GLU
1	I	168	HIS
1	I	242	ARG
1	I	266	ASP
1	I	313	LEU
1	I	340	ARG
1	I	351	PHE

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Mol	Chain	Res	Type
1	I	367	ASP
1	I	406	CYS
1	I	416	ARG
1	I	420	GLU
1	I	455	ARG
1	I	478	TYR
1	I	521	HIS
1	I	546	ARG
1	I	580	PHE
1	I	584	ARG
1	I	609	ARG
1	J	9	TYR
1	J	43	GLU
1	J	67	GLN
1	J	102	ARG
1	J	116	ARG
1	J	146	ARG
1	J	151	TYR
1	J	212	ARG
1	J	254	ARG
1	J	297	ASP
1	J	340	ARG
1	J	351	PHE
1	J	359	SER
1	J	409	ASP
1	J	434	ASP
1	J	438	ARG
1	J	472	ASN
1	J	476	GLU
1	J	478	TYR
1	J	527	ARG
1	J	536	TYR
1	J	537	CYS
1	J	544	TRP
1	J	546	ARG
1	J	560	ARG
1	J	612	GLN
1	J	650	SER
1	J	660	ASP
1	J	704	ARG
1	K	16	ASP
1	K	49	ARG

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Mol	Chain	Res	Type
1	K	52	ASP
1	K	56	ARG
1	K	116	ARG
1	K	185	PRO
1	K	215	ASP
1	K	219	SER
1	K	249	PHE
1	K	270	ASN
1	K	294	ARG
1	K	313	LEU
1	K	340	ARG
1	K	365	GLN
1	K	371	SER
1	K	455	ARG
1	K	478	TYR
1	K	479	ASN
1	K	480	ARG
1	K	576	ARG
1	K	580	PHE
1	K	582	HIS
1	K	584	ARG
1	K	609	ARG
1	K	664	ARG
1	K	699	LEU
1	L	30	HIS
1	L	102	ARG
1	L	116	ARG
1	L	118	ASP
1	L	125	SER
1	L	143	ASP
1	L	151	TYR
1	L	164	LEU
1	L	170	ASP
1	L	210	ASP
1	L	266	ASP
1	L	297	ASP
1	L	311	SER
1	L	404	ARG
1	L	409	ASP
1	L	440	LEU
1	L	455	ARG
1	L	478	TYR

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Mol	Chain	Res	Type
1	L	483	ASN
1	L	546	ARG
1	L	576	ARG
1	L	580	PHE
1	L	590	HIS
1	L	610	ASP
1	L	626	ASN
1	L	664	ARG
1	L	674	ASP
1	L	704	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	225	ASN
1	A	233	HIS
1	A	271	HIS
1	A	433	GLN
1	A	461	ASN
1	A	483	ASN
1	A	505	ASN
1	B	205	HIS
1	B	211	HIS
1	B	234	ASN
1	B	271	HIS
1	B	277	HIS
1	B	289	ASN
1	B	350	GLN
1	B	391	ASN
1	B	502	GLN
1	B	505	ASN
1	C	153	HIS
1	C	190	HIS
1	C	225	ASN
1	C	258	GLN
1	C	270	ASN
1	C	365	GLN
1	C	391	ASN
1	C	461	ASN
1	C	483	ASN
1	C	505	ASN

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Mol	Chain	Res	Type
1	C	681	GLN
1	D	271	HIS
1	D	352	HIS
1	D	483	ASN
1	D	502	GLN
1	D	572	HIS
1	D	648	ASN
1	E	350	GLN
1	E	372	GLN
1	E	391	ASN
1	E	461	ASN
1	E	483	ASN
1	F	205	HIS
1	F	400	ASN
1	F	461	ASN
1	F	483	ASN
1	G	505	ASN
1	G	533	ASN
1	H	233	HIS
1	H	648	ASN
1	I	505	ASN
1	I	617	GLN
1	I	681	GLN
1	J	152	HIS
1	J	289	ASN
1	J	391	ASN
1	K	67	GLN
1	K	206	GLN
1	K	461	ASN
1	K	483	ASN
1	L	350	GLN
1	L	365	GLN
1	L	391	ASN
1	L	461	ASN
1	L	483	ASN
1	L	521	HIS
1	L	529	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	703/709 (99%)	-0.31	0 100 100	26, 44, 73, 95	0
1	B	705/709 (99%)	-0.34	4 (0%) 89 81	27, 41, 69, 102	0
1	C	699/709 (98%)	-0.45	0 100 100	25, 41, 70, 93	0
1	D	700/709 (98%)	-0.44	1 (0%) 95 93	28, 45, 73, 112	0
1	E	700/709 (98%)	-0.34	3 (0%) 92 87	27, 46, 72, 106	0
1	F	698/709 (98%)	-0.35	4 (0%) 89 81	26, 43, 72, 98	0
1	G	698/709 (98%)	-0.08	11 (1%) 72 59	30, 56, 87, 113	0
1	H	701/709 (98%)	-0.35	3 (0%) 92 87	30, 43, 73, 96	0
1	I	701/709 (98%)	-0.39	1 (0%) 95 93	29, 45, 75, 96	0
1	J	700/709 (98%)	-0.34	5 (0%) 87 79	27, 44, 74, 103	0
1	K	701/709 (98%)	-0.30	4 (0%) 89 81	31, 49, 79, 122	0
1	L	701/709 (98%)	-0.32	1 (0%) 95 93	34, 50, 78, 102	0
All	All	8407/8508 (98%)	-0.33	37 (0%) 92 87	25, 45, 76, 122	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	615	HIS	4.4
1	F	615	HIS	3.9
1	G	306	THR	3.6
1	K	615	HIS	3.6
1	D	615	HIS	3.5
1	K	117	PRO	3.5
1	G	583	GLY	3.1
1	J	684	PRO	3.1
1	F	614	ALA	3.0
1	B	616	ALA	2.8
1	B	687	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	689	GLY	2.6
1	G	615	HIS	2.6
1	K	297	ASP	2.5
1	J	614	ALA	2.4
1	G	617	GLN	2.4
1	G	307	GLY	2.4
1	G	520	SER	2.4
1	L	118	ASP	2.3
1	B	597	ALA	2.3
1	G	667	ARG	2.3
1	B	615	HIS	2.3
1	H	614	ALA	2.3
1	G	509	THR	2.3
1	J	619	LEU	2.3
1	H	693	THR	2.2
1	J	589	THR	2.1
1	J	553	GLU	2.1
1	I	615	HIS	2.1
1	G	679	PRO	2.1
1	F	567	ARG	2.1
1	E	620	THR	2.1
1	K	614	ALA	2.1
1	G	656	PHE	2.1
1	F	616	ALA	2.0
1	E	619	LEU	2.0
1	H	687	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.