



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:14 AM UTC

PDB ID : 8J6V / pdb_00008j6v
Title : Structure of yeast Arginyl-tRNA-protein transferase 1
Authors : Yashiro, Y.; Tomita, K.
Deposited on : 2023-04-26
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

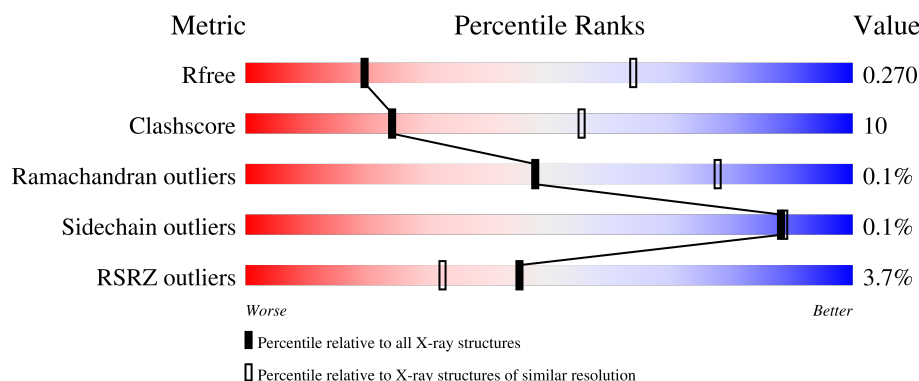
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



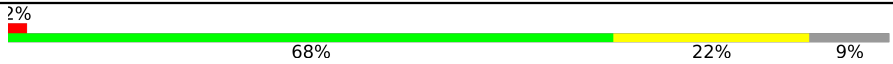
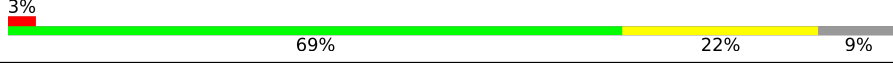
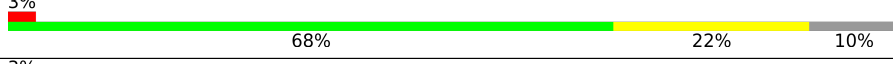
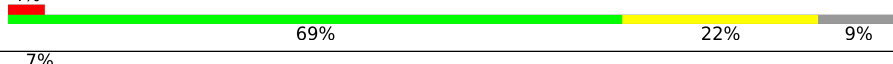
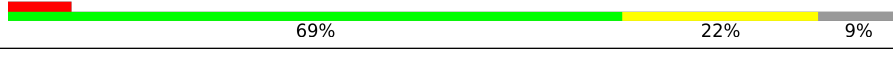
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	511	2% 70% 22% 8%
1	B	511	2% 66% 25% 9%
1	C	511	3% 69% 23% 8%
1	D	511	4% 71% 20% 10%
1	E	511	2% 65% 25% 9%

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Mol	Chain	Length	Quality of chain
1	F	511	
1	G	511	
1	H	511	
1	I	511	
1	J	511	
1	K	511	
1	L	511	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 45256 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 arginyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3817	2455	630	705	27			
1	B	465	Total	C	N	O	S	0	0	0
			3778	2431	622	698	27			
1	D	462	Total	C	N	O	S	0	0	0
			3748	2412	616	693	27			
1	F	464	Total	C	N	O	S	0	0	0
			3764	2424	618	696	26			
1	E	464	Total	C	N	O	S	0	0	0
			3768	2425	619	697	27			
1	L	465	Total	C	N	O	S	0	0	0
			3778	2431	622	698	27			
1	H	464	Total	C	N	O	S	0	0	0
			3760	2421	618	696	25			
1	G	462	Total	C	N	O	S	0	0	0
			3752	2416	616	694	26			
1	C	469	Total	C	N	O	S	0	0	0
			3812	2455	627	703	27			
1	K	465	Total	C	N	O	S	0	0	0
			3774	2429	621	698	26			
1	I	461	Total	C	N	O	S	0	0	0
			3746	2414	616	690	26			
1	J	463	Total	C	N	O	S	0	0	0
			3759	2421	618	694	26			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
A	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
A	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
A	504	LEU	-	expression tag	UNP A0A8H4C2T6
A	505	GLU	-	expression tag	UNP A0A8H4C2T6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	506	HIS	-	expression tag	UNP A0A8H4C2T6
A	507	HIS	-	expression tag	UNP A0A8H4C2T6
A	508	HIS	-	expression tag	UNP A0A8H4C2T6
A	509	HIS	-	expression tag	UNP A0A8H4C2T6
A	510	HIS	-	expression tag	UNP A0A8H4C2T6
A	511	HIS	-	expression tag	UNP A0A8H4C2T6
B	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
B	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
B	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
B	504	LEU	-	expression tag	UNP A0A8H4C2T6
B	505	GLU	-	expression tag	UNP A0A8H4C2T6
B	506	HIS	-	expression tag	UNP A0A8H4C2T6
B	507	HIS	-	expression tag	UNP A0A8H4C2T6
B	508	HIS	-	expression tag	UNP A0A8H4C2T6
B	509	HIS	-	expression tag	UNP A0A8H4C2T6
B	510	HIS	-	expression tag	UNP A0A8H4C2T6
B	511	HIS	-	expression tag	UNP A0A8H4C2T6
D	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
D	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
D	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
D	504	LEU	-	expression tag	UNP A0A8H4C2T6
D	505	GLU	-	expression tag	UNP A0A8H4C2T6
D	506	HIS	-	expression tag	UNP A0A8H4C2T6
D	507	HIS	-	expression tag	UNP A0A8H4C2T6
D	508	HIS	-	expression tag	UNP A0A8H4C2T6
D	509	HIS	-	expression tag	UNP A0A8H4C2T6
D	510	HIS	-	expression tag	UNP A0A8H4C2T6
D	511	HIS	-	expression tag	UNP A0A8H4C2T6
F	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
F	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
F	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
F	504	LEU	-	expression tag	UNP A0A8H4C2T6
F	505	GLU	-	expression tag	UNP A0A8H4C2T6
F	506	HIS	-	expression tag	UNP A0A8H4C2T6
F	507	HIS	-	expression tag	UNP A0A8H4C2T6
F	508	HIS	-	expression tag	UNP A0A8H4C2T6
F	509	HIS	-	expression tag	UNP A0A8H4C2T6
F	510	HIS	-	expression tag	UNP A0A8H4C2T6
F	511	HIS	-	expression tag	UNP A0A8H4C2T6
E	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
E	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
E	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	504	LEU	-	expression tag	UNP A0A8H4C2T6
E	505	GLU	-	expression tag	UNP A0A8H4C2T6
E	506	HIS	-	expression tag	UNP A0A8H4C2T6
E	507	HIS	-	expression tag	UNP A0A8H4C2T6
E	508	HIS	-	expression tag	UNP A0A8H4C2T6
E	509	HIS	-	expression tag	UNP A0A8H4C2T6
E	510	HIS	-	expression tag	UNP A0A8H4C2T6
E	511	HIS	-	expression tag	UNP A0A8H4C2T6
L	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
L	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
L	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
L	504	LEU	-	expression tag	UNP A0A8H4C2T6
L	505	GLU	-	expression tag	UNP A0A8H4C2T6
L	506	HIS	-	expression tag	UNP A0A8H4C2T6
L	507	HIS	-	expression tag	UNP A0A8H4C2T6
L	508	HIS	-	expression tag	UNP A0A8H4C2T6
L	509	HIS	-	expression tag	UNP A0A8H4C2T6
L	510	HIS	-	expression tag	UNP A0A8H4C2T6
L	511	HIS	-	expression tag	UNP A0A8H4C2T6
H	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
H	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
H	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
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H	505	GLU	-	expression tag	UNP A0A8H4C2T6
H	506	HIS	-	expression tag	UNP A0A8H4C2T6
H	507	HIS	-	expression tag	UNP A0A8H4C2T6
H	508	HIS	-	expression tag	UNP A0A8H4C2T6
H	509	HIS	-	expression tag	UNP A0A8H4C2T6
H	510	HIS	-	expression tag	UNP A0A8H4C2T6
H	511	HIS	-	expression tag	UNP A0A8H4C2T6
G	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
G	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
G	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
G	504	LEU	-	expression tag	UNP A0A8H4C2T6
G	505	GLU	-	expression tag	UNP A0A8H4C2T6
G	506	HIS	-	expression tag	UNP A0A8H4C2T6
G	507	HIS	-	expression tag	UNP A0A8H4C2T6
G	508	HIS	-	expression tag	UNP A0A8H4C2T6
G	509	HIS	-	expression tag	UNP A0A8H4C2T6
G	510	HIS	-	expression tag	UNP A0A8H4C2T6
G	511	HIS	-	expression tag	UNP A0A8H4C2T6
C	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
C	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
C	504	LEU	-	expression tag	UNP A0A8H4C2T6
C	505	GLU	-	expression tag	UNP A0A8H4C2T6
C	506	HIS	-	expression tag	UNP A0A8H4C2T6
C	507	HIS	-	expression tag	UNP A0A8H4C2T6
C	508	HIS	-	expression tag	UNP A0A8H4C2T6
C	509	HIS	-	expression tag	UNP A0A8H4C2T6
C	510	HIS	-	expression tag	UNP A0A8H4C2T6
C	511	HIS	-	expression tag	UNP A0A8H4C2T6
K	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
K	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
K	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
K	504	LEU	-	expression tag	UNP A0A8H4C2T6
K	505	GLU	-	expression tag	UNP A0A8H4C2T6
K	506	HIS	-	expression tag	UNP A0A8H4C2T6
K	507	HIS	-	expression tag	UNP A0A8H4C2T6
K	508	HIS	-	expression tag	UNP A0A8H4C2T6
K	509	HIS	-	expression tag	UNP A0A8H4C2T6
K	510	HIS	-	expression tag	UNP A0A8H4C2T6
K	511	HIS	-	expression tag	UNP A0A8H4C2T6
I	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
I	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
I	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
I	504	LEU	-	expression tag	UNP A0A8H4C2T6
I	505	GLU	-	expression tag	UNP A0A8H4C2T6
I	506	HIS	-	expression tag	UNP A0A8H4C2T6
I	507	HIS	-	expression tag	UNP A0A8H4C2T6
I	508	HIS	-	expression tag	UNP A0A8H4C2T6
I	509	HIS	-	expression tag	UNP A0A8H4C2T6
I	510	HIS	-	expression tag	UNP A0A8H4C2T6
I	511	HIS	-	expression tag	UNP A0A8H4C2T6
J	339	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
J	340	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
J	341	LYS	GLU	engineered mutation	UNP A0A8H4C2T6
J	504	LEU	-	expression tag	UNP A0A8H4C2T6
J	505	GLU	-	expression tag	UNP A0A8H4C2T6
J	506	HIS	-	expression tag	UNP A0A8H4C2T6
J	507	HIS	-	expression tag	UNP A0A8H4C2T6
J	508	HIS	-	expression tag	UNP A0A8H4C2T6
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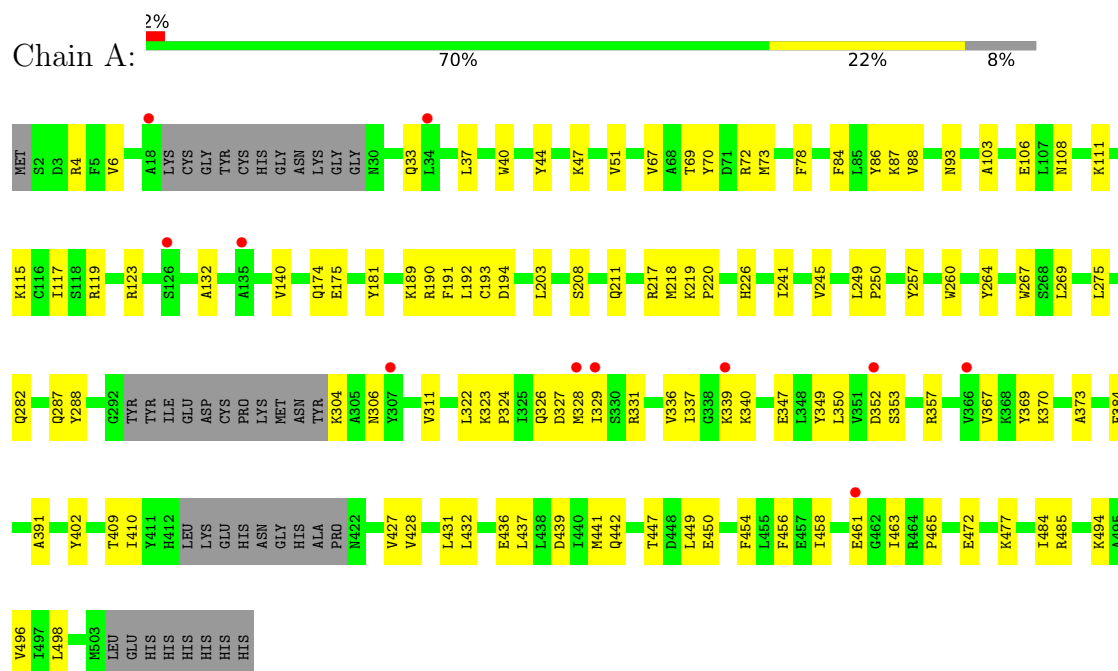
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Chain	Residue	Modelled	Actual	Comment	Reference
J	511	HIS	-	expression tag	UNP A0A8H4C2T6

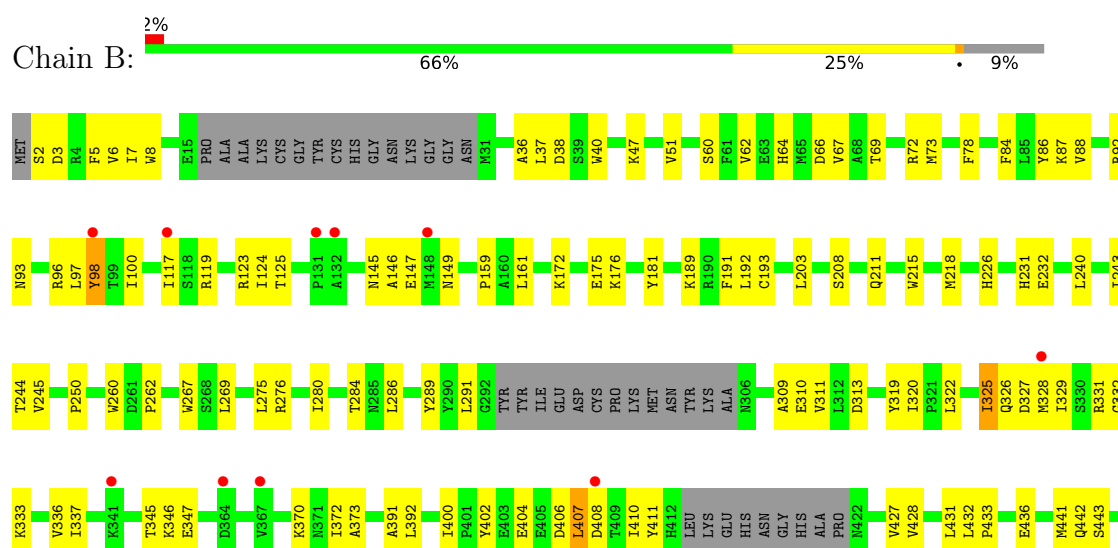
3 Residue-property plots [i](#)

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: arginyltransferase

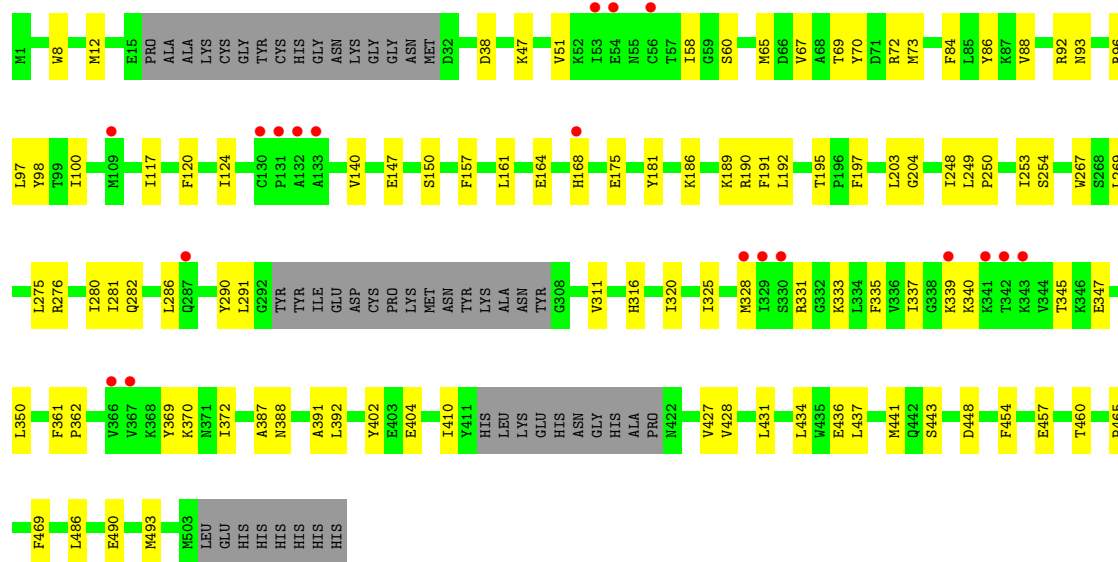


• Molecule 1: arginyltransferase

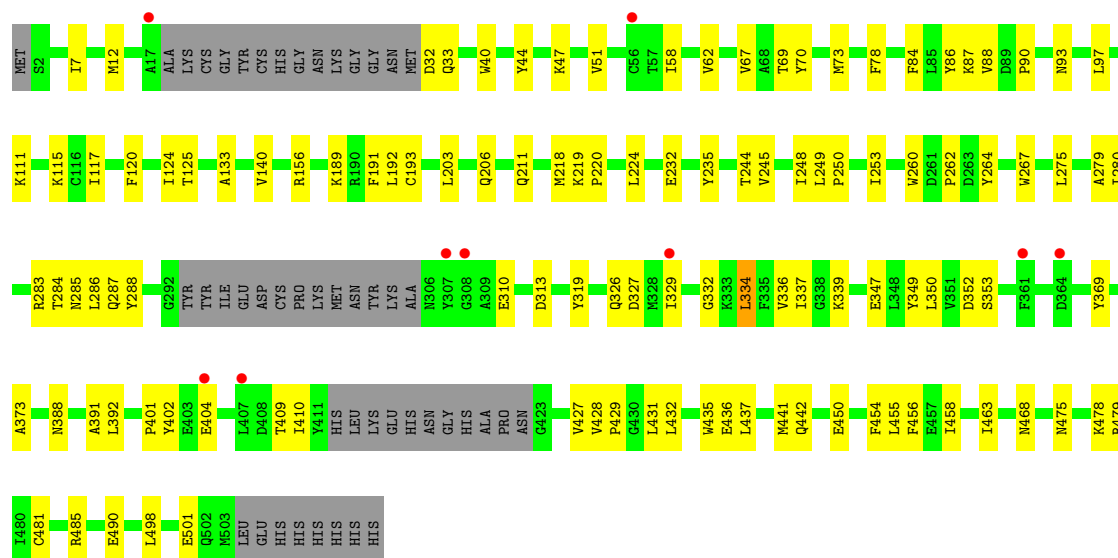




• Molecule 1: arginyltransferase

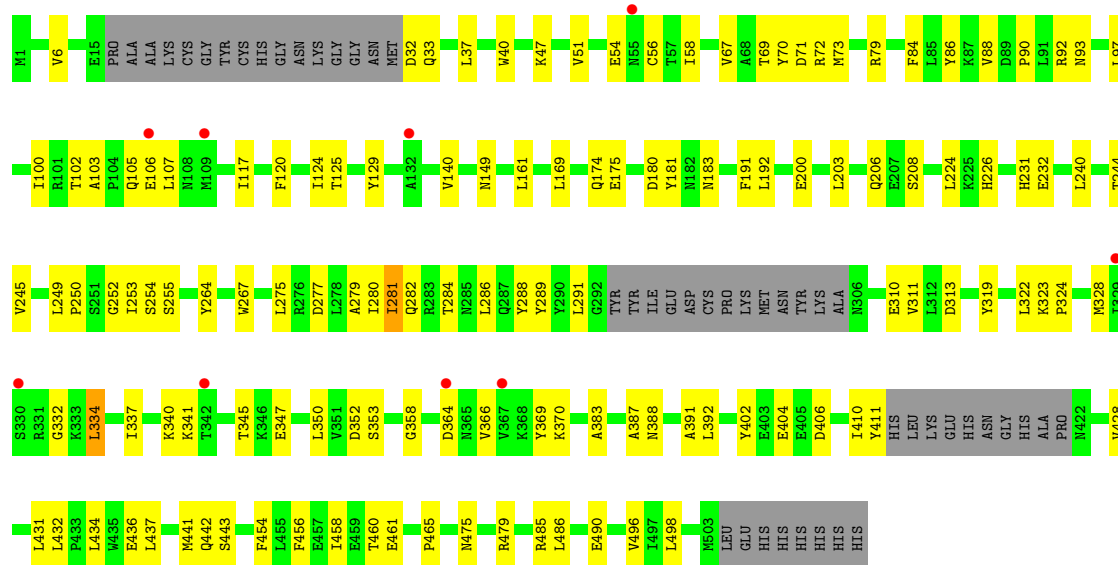


• Molecule 1: arginyltransferase

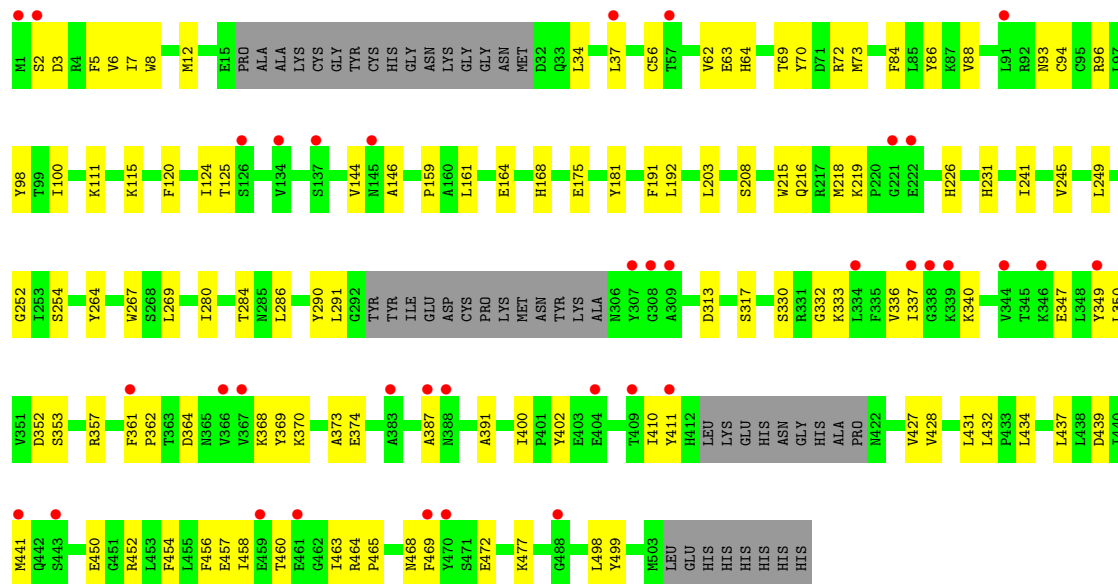


• Molecule 1: arginyltransferase

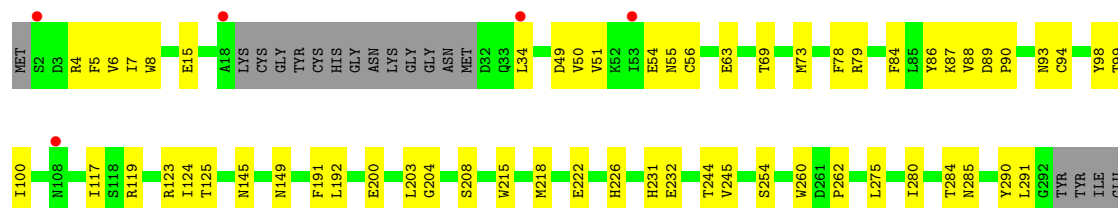


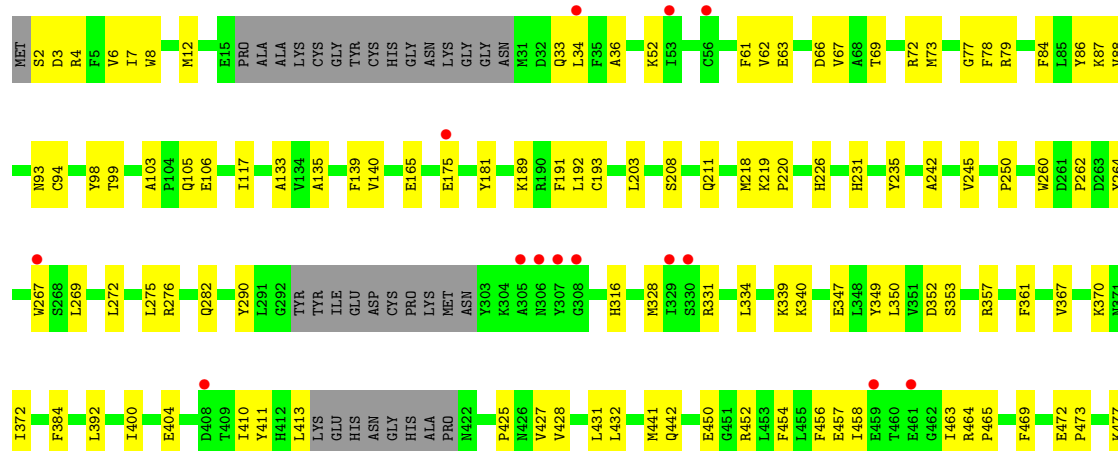


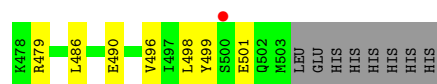
• Molecule 1: arginyltransferase



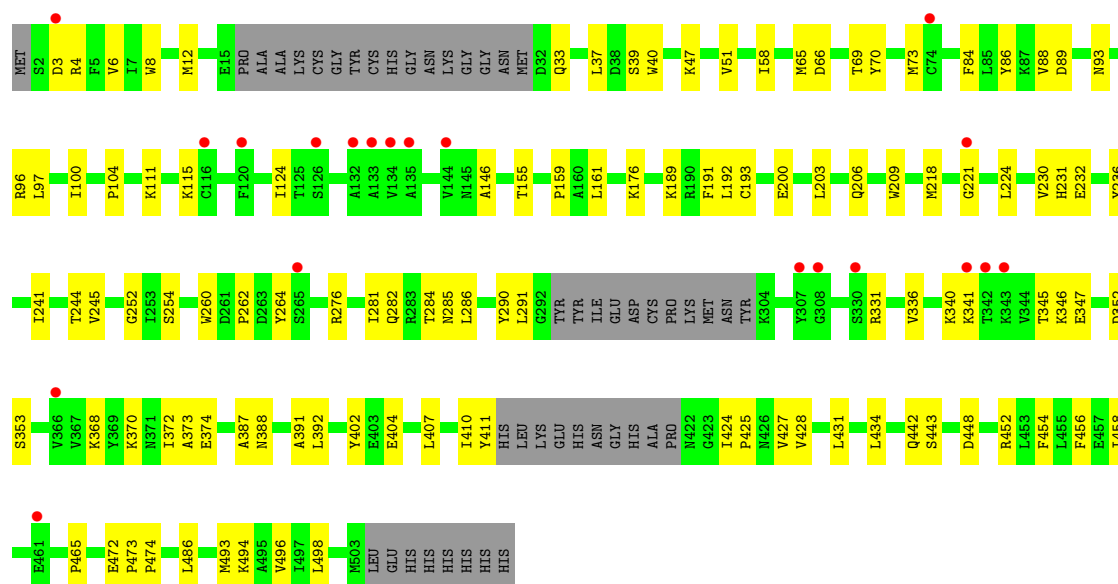
• Molecule 1: arginyltransferase



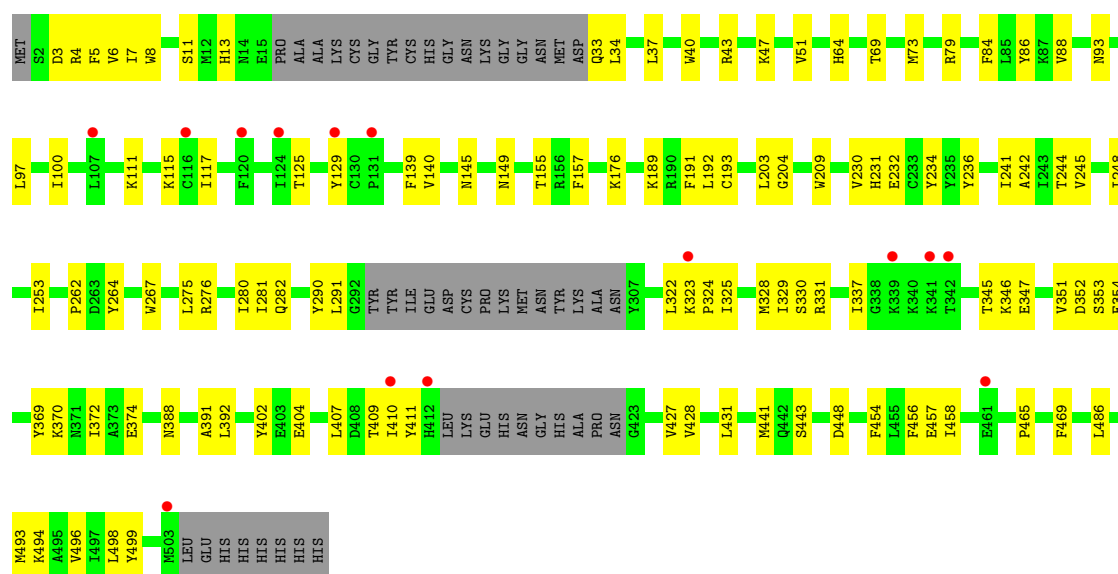




- Molecule 1: arginyltransferase

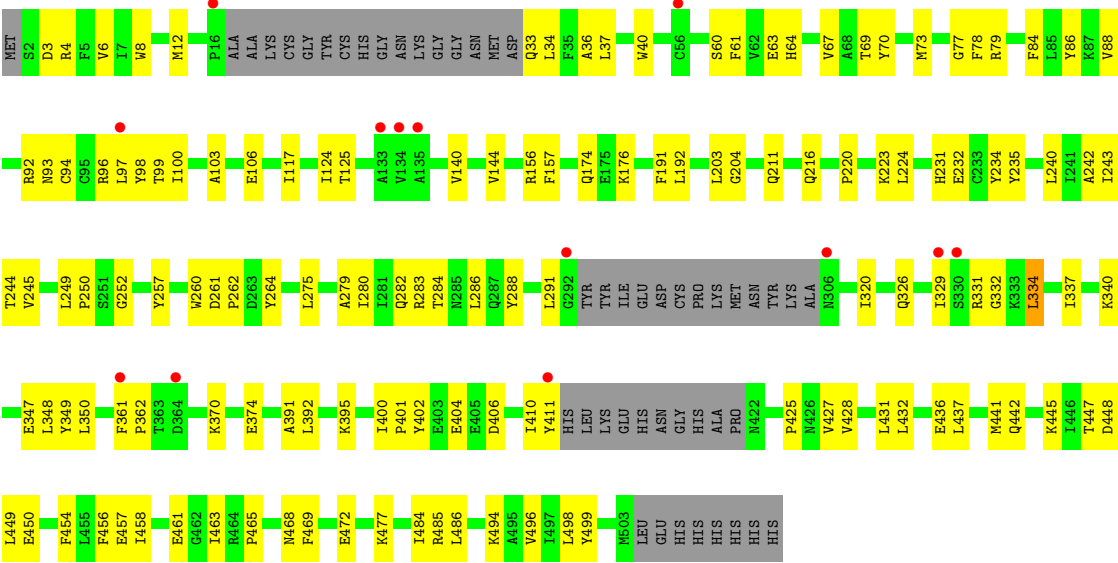


- Molecule 1: arginyltransferase



- Molecule 1: arginyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	235.66Å 235.66Å 171.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 3.40 48.56 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.56-3.40) 99.9 (48.56-3.40)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.238 , 0.270 0.240 , 0.270	Depositor DCC
R_{free} test set	6441 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	82.1	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	45256	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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	0.15	0/3909	0.42	0/5279
1	B	0.14	0/3869	0.43	1/5224 (0.0%)
1	C	0.14	0/3904	0.40	0/5271
1	D	0.14	0/3837	0.40	0/5180
1	E	0.14	0/3858	0.42	0/5209
1	F	0.14	0/3855	0.41	0/5207
1	G	0.13	0/3842	0.40	0/5188
1	H	0.16	0/3851	0.45	0/5203
1	I	0.15	0/3837	0.41	0/5181
1	J	0.15	0/3850	0.41	0/5200
1	K	0.14	0/3864	0.40	0/5217
1	L	0.13	0/3869	0.40	0/5224
All	All	0.14	0/46345	0.41	1/62583 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	TYR	N-CA-C	6.42	119.19	108.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3817	0	3775	74	0
1	B	3778	0	3734	97	0
1	C	3812	0	3772	80	0
1	D	3748	0	3715	66	0
1	E	3768	0	3730	89	0
1	F	3764	0	3724	76	0
1	G	3752	0	3712	78	0
1	H	3760	0	3718	84	0
1	I	3746	0	3709	75	0
1	J	3759	0	3721	96	0
1	K	3774	0	3736	81	0
1	L	3778	0	3737	79	0
All	All	45256	0	44783	900	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 10.

All (900) 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:B:98:TYR:CZ	1:B:328:MET:HG2	1.83	1.13
1:K:340:LYS:HG2	1:K:370:LYS:HD3	1.52	0.91
1:F:220:PRO:HB3	1:C:219:LYS:HD3	1.54	0.90
1:B:98:TYR:CE1	1:B:328:MET:HG2	2.08	0.87
1:D:340:LYS:HG2	1:D:370:LYS:HD3	1.57	0.84
1:B:98:TYR:OH	1:B:332:GLY:HA2	1.79	0.83
1:H:336:VAL:H	1:H:373:ALA:HB2	1.44	0.83
1:L:349:TYR:HB3	1:G:443:SER:HB3	1.61	0.82
1:H:15:GLU:N	1:H:55:ASN:HD21	1.76	0.82
1:L:219:LYS:HD3	1:J:220:PRO:HB3	1.61	0.81
1:B:98:TYR:CE1	1:B:328:MET:CG	2.64	0.80
1:E:311:VAL:HG13	1:E:322:LEU:HD11	1.62	0.80
1:E:79:ARG:HH12	1:E:254:SER:HB2	1.47	0.79
1:B:320:ILE:HD12	1:B:337:ILE:HD12	1.65	0.78
1:G:340:LYS:HG2	1:G:370:LYS:HD3	1.66	0.78
1:I:43:ARG:HH22	1:I:409:THR:HG22	1.49	0.77
1:C:52:LYS:HE3	1:C:413:LEU:HD12	1.65	0.76
1:H:100:ILE:HD11	1:H:291:LEU:HD12	1.68	0.76
1:K:284:THR:HG22	1:K:285:ASN:H	1.52	0.75
1:G:96:ARG:HH21	1:G:332:GLY:H	1.35	0.74
1:G:350:LEU:N	1:G:436:GLU:OE2	2.20	0.74
1:K:12:MET:HG2	1:K:58:ILE:HG12	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:ILE:HD12	1:D:328:MET:HE1	1.70	0.74
1:E:284:THR:HG23	1:E:286:LEU:HD23	1.69	0.74
1:A:220:PRO:HB3	1:F:219:LYS:HD3	1.70	0.73
1:C:340:LYS:HG2	1:C:370:LYS:HD3	1.70	0.72
1:B:98:TYR:CE2	1:B:328:MET:HG2	2.22	0.72
1:K:96:ARG:NH2	1:K:331:ARG:O	2.21	0.72
1:J:33:GLN:HB3	1:J:331:ARG:HG2	1.72	0.71
1:E:100:ILE:HG23	1:E:291:LEU:HB2	1.72	0.71
1:K:33:GLN:HB3	1:K:331:ARG:HG3	1.73	0.71
1:K:391:ALA:HB1	1:K:402:TYR:HB3	1.72	0.71
1:A:442:GLN:HB3	1:B:345:THR:HB	1.73	0.71
1:F:284:THR:HG23	1:F:286:LEU:HD23	1.72	0.71
1:H:15:GLU:H	1:H:55:ASN:HD21	1.38	0.70
1:F:349:TYR:HB3	1:E:443:SER:HB3	1.72	0.70
1:K:442:GLN:HE22	1:J:348:LEU:HA	1.56	0.70
1:K:224:LEU:HG	1:K:284:THR:HG21	1.72	0.70
1:I:33:GLN:HG3	1:I:34:LEU:H	1.56	0.69
1:J:350:LEU:N	1:J:436:GLU:OE2	2.26	0.69
1:H:322:LEU:HD21	1:H:329:ILE:HD12	1.74	0.69
1:J:392:LEU:HD11	1:J:404:GLU:OE2	1.92	0.69
1:D:100:ILE:HG23	1:D:291:LEU:HB2	1.75	0.69
1:A:349:TYR:HB3	1:B:443:SER:HB3	1.75	0.69
1:E:310:GLU:HG2	1:E:319:TYR:HB3	1.74	0.68
1:A:456:PHE:HD2	1:A:498:LEU:HG	1.59	0.68
1:E:350:LEU:N	1:E:436:GLU:OE2	2.26	0.68
1:E:174:GLN:HG2	1:E:183:ASN:HD21	1.59	0.67
1:E:277:ASP:O	1:E:281:ILE:HD12	1.93	0.67
1:H:442:GLN:HB3	1:I:345:THR:HB	1.76	0.67
1:E:174:GLN:HG3	1:E:180:ASP:HB3	1.76	0.67
1:K:443:SER:HB3	1:J:349:TYR:HB3	1.76	0.67
1:F:336:VAL:H	1:F:373:ALA:HB2	1.60	0.67
1:C:33:GLN:HG3	1:C:331:ARG:HB3	1.76	0.66
1:L:468:ASN:HD21	1:G:341:LYS:HD2	1.60	0.66
1:J:456:PHE:HD2	1:J:498:LEU:HG	1.61	0.66
1:F:280:ILE:O	1:F:284:THR:HG22	1.96	0.65
1:E:431:LEU:HD22	1:E:486:LEU:HA	1.77	0.65
1:H:4:ARG:HD2	1:H:496:VAL:HG23	1.78	0.65
1:A:340:LYS:HG2	1:A:370:LYS:HD2	1.77	0.65
1:K:8:TRP:HH2	1:K:458:ILE:HD11	1.61	0.65
1:K:345:THR:HB	1:J:442:GLN:HB3	1.78	0.65
1:D:431:LEU:HD22	1:D:486:LEU:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:12:MET:HE1	1:J:425:PRO:HD3	1.79	0.65
1:C:189:LYS:HA	1:C:193:CYS:HB2	1.78	0.65
1:B:98:TYR:OH	1:B:332:GLY:CA	2.45	0.65
1:B:313:ASP:OD2	1:B:337:ILE:HG22	1.97	0.65
1:F:442:GLN:HB3	1:E:345:THR:HB	1.78	0.65
1:C:8:TRP:CH2	1:C:458:ILE:HD11	2.32	0.65
1:J:326:GLN:O	1:J:329:ILE:HG12	1.97	0.65
1:D:350:LEU:N	1:D:436:GLU:OE2	2.30	0.64
1:G:387:ALA:HB1	1:G:434:LEU:HD12	1.79	0.64
1:J:320:ILE:HD12	1:J:337:ILE:HD12	1.79	0.64
1:L:340:LYS:HG2	1:L:370:LYS:HD3	1.79	0.64
1:L:452:ARG:NH1	1:K:206:GLN:OE1	2.30	0.64
1:J:284:THR:HG23	1:J:286:LEU:HD23	1.78	0.64
1:H:454:PHE:HD2	1:G:203:LEU:HD13	1.63	0.64
1:K:8:TRP:CH2	1:K:458:ILE:HD11	2.33	0.64
1:K:336:VAL:H	1:K:373:ALA:HB2	1.63	0.64
1:J:88:VAL:HG11	1:J:97:LEU:HD13	1.79	0.64
1:C:392:LEU:HD11	1:C:404:GLU:OE2	1.98	0.63
1:A:175:GLU:HB2	1:A:181:TYR:CE1	2.33	0.63
1:A:391:ALA:HB1	1:A:402:TYR:HB3	1.79	0.63
1:F:224:LEU:HG	1:F:284:THR:OG1	1.98	0.63
1:F:334:LEU:HD11	1:F:429:PRO:HG2	1.80	0.63
1:G:327:ASP:HB2	1:G:333:LYS:HD2	1.80	0.63
1:A:103:ALA:HB3	1:A:106:GLU:HG2	1.80	0.63
1:B:432:LEU:HG	1:B:436:GLU:OE2	1.99	0.62
1:E:224:LEU:HG	1:E:284:THR:OG1	1.99	0.62
1:D:391:ALA:HB1	1:D:402:TYR:HB3	1.81	0.62
1:L:456:PHE:HD2	1:L:498:LEU:HG	1.63	0.62
1:H:340:LYS:HG2	1:H:370:LYS:HD3	1.80	0.62
1:B:400:ILE:HD11	1:B:441:MET:HE2	1.81	0.62
1:C:4:ARG:NH1	1:C:452:ARG:O	2.32	0.62
1:C:456:PHE:HD2	1:C:498:LEU:HG	1.65	0.62
1:K:111:LYS:HE2	1:K:115:LYS:HE3	1.81	0.62
1:I:330:SER:O	1:I:331:ARG:HG2	2.00	0.62
1:E:280:ILE:O	1:E:284:THR:HG22	2.00	0.62
1:H:449:LEU:HD11	1:H:484:ILE:HD11	1.82	0.62
1:D:392:LEU:HD11	1:D:404:GLU:OE2	2.00	0.61
1:B:336:VAL:H	1:B:373:ALA:HB2	1.65	0.61
1:F:12:MET:HG2	1:F:58:ILE:HG12	1.81	0.61
1:L:96:ARG:HH21	1:L:332:GLY:HA3	1.64	0.61
1:C:88:VAL:HB	1:C:93:ASN:HD22	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:222:GLU:O	1:H:285:ASN:ND2	2.30	0.61
1:H:313:ASP:OD2	1:H:337:ILE:HG22	2.00	0.61
1:K:189:LYS:HA	1:K:193:CYS:HB2	1.82	0.61
1:J:103:ALA:HB3	1:J:106:GLU:HG2	1.82	0.61
1:B:392:LEU:HD11	1:B:404:GLU:OE2	2.00	0.61
1:E:90:PRO:HB2	1:E:334:LEU:HD13	1.82	0.61
1:I:4:ARG:HD2	1:I:496:VAL:HG23	1.83	0.61
1:A:203:LEU:HD13	1:D:454:PHE:HD2	1.65	0.61
1:K:221:GLY:C	1:K:285:ASN:HD21	2.09	0.61
1:J:449:LEU:HD11	1:J:484:ILE:HD11	1.83	0.61
1:A:339:LYS:HE2	1:A:367:VAL:HG11	1.83	0.60
1:G:96:ARG:HE	1:G:332:GLY:HA3	1.64	0.60
1:K:3:ASP:HB2	1:K:66:ASP:HB3	1.83	0.60
1:G:208:SER:HB2	1:G:226:HIS:HB2	1.83	0.60
1:H:208:SER:HB2	1:H:226:HIS:HB2	1.83	0.60
1:C:103:ALA:HB3	1:C:106:GLU:HG2	1.84	0.60
1:K:252:GLY:HA2	1:K:286:LEU:HB3	1.83	0.60
1:I:325:ILE:HG23	1:I:328:MET:HB3	1.83	0.60
1:B:2:SER:N	1:B:66:ASP:OD2	2.34	0.60
1:K:370:LYS:HE3	1:K:372:ILE:HG22	1.84	0.60
1:A:350:LEU:N	1:A:436:GLU:OE2	2.35	0.60
1:F:350:LEU:N	1:F:436:GLU:OE2	2.33	0.60
1:C:117:ILE:HD11	1:C:275:LEU:HD13	1.84	0.60
1:A:322:LEU:HD21	1:A:329:ILE:HD13	1.85	0.59
1:B:88:VAL:HB	1:B:93:ASN:HD22	1.67	0.59
1:E:454:PHE:HD2	1:C:203:LEU:HD13	1.68	0.59
1:A:117:ILE:HD11	1:A:275:LEU:HD13	1.83	0.59
1:I:410:ILE:HG23	1:I:411:TYR:CD2	2.37	0.59
1:B:452:ARG:NE	1:F:206:GLN:OE1	2.36	0.59
1:H:328:MET:SD	1:H:335:PHE:HB3	2.42	0.59
1:J:3:ASP:OD2	1:J:64:HIS:NE2	2.25	0.59
1:F:310:GLU:HG2	1:F:319:TYR:HB3	1.84	0.59
1:K:392:LEU:HD11	1:K:404:GLU:OE2	2.03	0.59
1:L:8:TRP:HH2	1:L:458:ILE:HD11	1.66	0.59
1:D:72:ARG:NH2	1:D:490:GLU:OE2	2.36	0.59
1:J:88:VAL:HG21	1:J:97:LEU:H	1.68	0.59
1:G:88:VAL:HB	1:G:93:ASN:HD22	1.66	0.58
1:J:117:ILE:HD11	1:J:275:LEU:HD13	1.84	0.58
1:A:347:GLU:OE2	1:A:427:VAL:HG13	2.03	0.58
1:B:447:THR:O	1:B:450:GLU:HG2	2.02	0.58
1:K:124:ILE:HD11	1:K:146:ALA:HB1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:117:ILE:HD11	1:I:275:LEU:HD13	1.85	0.58
1:D:96:ARG:NH1	1:D:331:ARG:O	2.36	0.58
1:E:92:ARG:NH2	1:E:406:ASP:OD2	2.37	0.58
1:E:117:ILE:HD11	1:E:275:LEU:HD13	1.84	0.58
1:L:347:GLU:OE2	1:L:427:VAL:HG13	2.03	0.58
1:C:8:TRP:HH2	1:C:458:ILE:HD11	1.68	0.58
1:J:447:THR:O	1:J:450:GLU:HG2	2.02	0.58
1:B:8:TRP:O	1:B:60:SER:OG	2.21	0.58
1:D:328:MET:SD	1:D:328:MET:N	2.76	0.58
1:F:117:ILE:HD11	1:F:275:LEU:HD13	1.86	0.58
1:C:3:ASP:OD2	1:C:66:ASP:HB3	2.04	0.58
1:J:96:ARG:NH2	1:J:331:ARG:O	2.37	0.58
1:G:103:ALA:HB3	1:G:106:GLU:HG2	1.84	0.58
1:J:280:ILE:O	1:J:284:THR:HG22	2.03	0.58
1:A:6:VAL:HG22	1:A:496:VAL:HB	1.85	0.58
1:H:347:GLU:OE2	1:H:427:VAL:HG13	2.04	0.58
1:F:44:TYR:OH	1:F:409:THR:OG1	2.22	0.57
1:K:346:LYS:NZ	1:J:442:GLN:OE1	2.36	0.57
1:B:98:TYR:CZ	1:B:328:MET:CG	2.73	0.57
1:L:441:MET:HE1	1:L:469:PHE:HE2	1.68	0.57
1:G:240:LEU:HD21	1:G:243:ILE:HD11	1.86	0.57
1:A:447:THR:O	1:A:450:GLU:HG2	2.04	0.57
1:L:457:GLU:HB3	1:L:499:TYR:CE2	2.39	0.57
1:H:54:GLU:HG2	1:H:55:ASN:N	2.19	0.57
1:K:387:ALA:HB1	1:K:434:LEU:HD12	1.86	0.57
1:D:88:VAL:HG21	1:D:97:LEU:H	1.69	0.57
1:K:340:LYS:HG3	1:K:368:LYS:HE3	1.85	0.57
1:I:8:TRP:CH2	1:I:458:ILE:HD11	2.40	0.57
1:B:461:GLU:HA	1:F:189:LYS:HZ1	1.69	0.57
1:H:8:TRP:HH2	1:H:458:ILE:HD11	1.70	0.57
1:A:463:ILE:HG23	1:D:161:LEU:HD22	1.87	0.57
1:D:88:VAL:HG11	1:D:97:LEU:HD13	1.86	0.56
1:H:231:HIS:CD2	1:H:245:VAL:HG22	2.40	0.56
1:B:232:GLU:HG2	1:B:244:THR:HB	1.86	0.56
1:B:310:GLU:HG2	1:B:319:TYR:HB3	1.87	0.56
1:B:100:ILE:HG23	1:B:291:LEU:HB2	1.86	0.56
1:G:313:ASP:OD2	1:G:337:ILE:HG22	2.05	0.56
1:G:428:VAL:HB	1:G:431:LEU:HD12	1.86	0.56
1:L:284:THR:O	1:L:286:LEU:N	2.31	0.56
1:I:454:PHE:CE2	1:J:203:LEU:HD22	2.41	0.56
1:J:78:PHE:O	1:J:79:ARG:NH1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:ILE:HD11	1:D:361:PHE:CE1	2.40	0.56
1:B:145:ASN:OD1	1:B:149:ASN:ND2	2.38	0.56
1:D:311:VAL:HG21	1:D:328:MET:HE2	1.88	0.56
1:G:472:GLU:CD	1:G:473:PRO:HD2	2.30	0.56
1:D:69:THR:O	1:D:73:MET:HG2	2.05	0.56
1:F:44:TYR:HH	1:F:409:THR:HG1	1.54	0.56
1:F:192:LEU:HD22	1:F:245:VAL:HG21	1.86	0.56
1:L:2:SER:HB3	1:L:64:HIS:NE2	2.21	0.56
1:E:392:LEU:HD11	1:E:404:GLU:OE2	2.06	0.56
1:B:98:TYR:HH	1:B:332:GLY:C	2.13	0.56
1:B:203:LEU:HD13	1:F:454:PHE:HD2	1.71	0.56
1:K:431:LEU:HD22	1:K:486:LEU:HA	1.86	0.55
1:B:124:ILE:HD11	1:B:146:ALA:HB1	1.89	0.55
1:B:311:VAL:HG13	1:B:322:LEU:HD13	1.88	0.55
1:E:391:ALA:HB1	1:E:402:TYR:HB3	1.87	0.55
1:L:203:LEU:HD22	1:K:454:PHE:CE2	2.41	0.55
1:B:88:VAL:HG21	1:B:97:LEU:H	1.71	0.55
1:H:392:LEU:HD11	1:H:404:GLU:OE2	2.06	0.55
1:K:6:VAL:HG22	1:K:496:VAL:HB	1.88	0.55
1:J:260:TRP:CZ3	1:J:262:PRO:HA	2.42	0.55
1:A:4:ARG:NH2	1:D:204:GLY:O	2.40	0.55
1:A:174:GLN:OE1	1:A:257:TYR:OH	2.22	0.55
1:K:192:LEU:HD22	1:K:245:VAL:HG21	1.87	0.55
1:I:351:VAL:HG13	1:I:354:GLU:HB2	1.88	0.55
1:A:88:VAL:HB	1:A:93:ASN:HD22	1.71	0.55
1:B:98:TYR:OH	1:B:332:GLY:C	2.49	0.55
1:B:325:ILE:HG23	1:B:327:ASP:OD1	2.07	0.55
1:G:472:GLU:OE2	1:G:476:VAL:HG11	2.07	0.55
1:C:339:LYS:HE2	1:C:367:VAL:HG11	1.89	0.55
1:C:472:GLU:HG3	1:C:473:PRO:HD2	1.89	0.55
1:D:12:MET:HG2	1:D:58:ILE:HG12	1.89	0.55
1:C:352:ASP:OD2	1:C:490:GLU:HG3	2.07	0.55
1:C:410:ILE:HG22	1:C:411:TYR:H	1.72	0.54
1:H:339:LYS:HG2	1:H:367:VAL:HG11	1.89	0.54
1:H:463:ILE:HG23	1:G:161:LEU:HD22	1.89	0.54
1:I:204:GLY:O	1:J:4:ARG:NH1	2.39	0.54
1:E:340:LYS:HG2	1:E:370:LYS:HD2	1.88	0.54
1:E:313:ASP:OD2	1:E:337:ILE:HG22	2.06	0.54
1:C:72:ARG:NH1	1:C:357:ARG:HE	2.06	0.54
1:J:224:LEU:HG	1:J:284:THR:OG1	2.07	0.54
1:D:195:THR:HB	1:D:197:PHE:HD2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:THR:HB	1:C:442:GLN:HB3	1.89	0.54
1:F:327:ASP:O	1:F:332:GLY:N	2.31	0.54
1:B:322:LEU:HD11	1:B:328:MET:HE2	1.89	0.54
1:E:58:ILE:HG22	1:E:486:LEU:HD11	1.90	0.54
1:F:347:GLU:OE2	1:F:427:VAL:HG13	2.08	0.54
1:F:391:ALA:HB1	1:F:402:TYR:HB3	1.89	0.54
1:L:428:VAL:HB	1:L:431:LEU:HD12	1.89	0.54
1:H:4:ARG:NH2	1:G:204:GLY:O	2.40	0.54
1:I:325:ILE:HG22	1:I:329:ILE:HG23	1.90	0.54
1:G:145:ASN:OD1	1:G:149:ASN:ND2	2.41	0.54
1:I:3:ASP:OD2	1:I:64:HIS:NE2	2.41	0.54
1:A:449:LEU:HD11	1:A:484:ILE:HD11	1.89	0.54
1:A:456:PHE:CD2	1:A:498:LEU:HG	2.41	0.54
1:B:147:GLU:OE2	1:B:276:ARG:NE	2.36	0.54
1:D:362:PRO:HB3	1:E:206:GLN:HE21	1.73	0.54
1:A:111:LYS:HE2	1:A:115:LYS:HE3	1.90	0.53
1:G:73:MET:HB3	1:G:78:PHE:HD2	1.74	0.53
1:J:432:LEU:HB3	1:J:485:ARG:HA	1.89	0.53
1:J:437:LEU:O	1:J:441:MET:HG2	2.08	0.53
1:E:69:THR:O	1:E:73:MET:HG2	2.08	0.53
1:E:208:SER:HB2	1:E:226:HIS:HB2	1.90	0.53
1:A:454:PHE:HD2	1:D:203:LEU:HD13	1.72	0.53
1:H:325:ILE:CG2	1:H:328:MET:HG2	2.38	0.53
1:I:391:ALA:HB1	1:I:402:TYR:HB3	1.89	0.53
1:E:328:MET:HA	1:E:332:GLY:HA2	1.90	0.53
1:B:88:VAL:HG11	1:B:97:LEU:HD13	1.89	0.53
1:B:117:ILE:HD11	1:B:275:LEU:HD13	1.90	0.53
1:I:454:PHE:HE2	1:J:203:LEU:HD22	1.73	0.53
1:A:4:ARG:HD3	1:A:494:LYS:O	2.08	0.53
1:A:72:ARG:HH12	1:A:357:ARG:NE	2.06	0.53
1:C:242:ALA:HB2	1:C:269:LEU:HD13	1.89	0.53
1:L:454:PHE:HD2	1:K:203:LEU:HD13	1.74	0.53
1:B:211:GLN:HE21	1:B:218:MET:HE3	1.74	0.53
1:F:189:LYS:HA	1:F:193:CYS:HB2	1.89	0.53
1:I:125:THR:HG21	1:I:129:TYR:CD1	2.44	0.53
1:B:336:VAL:N	1:B:373:ALA:HB2	2.24	0.53
1:F:388:ASN:HB3	1:F:404:GLU:HG2	1.91	0.53
1:A:69:THR:O	1:A:73:MET:HG2	2.09	0.53
1:B:370:LYS:HE3	1:B:372:ILE:HG22	1.91	0.53
1:J:395:LYS:HD3	1:J:401:PRO:HA	1.90	0.53
1:B:69:THR:O	1:B:73:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:GLN:HA	1:G:331:ARG:HE	1.73	0.52
1:K:191:PHE:HD2	1:K:192:LEU:HG	1.74	0.52
1:B:441:MET:HE1	1:B:469:PHE:CE2	2.44	0.52
1:D:88:VAL:HB	1:D:93:ASN:HD22	1.73	0.52
1:A:119:ARG:HB3	1:A:123:ARG:NH1	2.25	0.52
1:B:78:PHE:CE1	1:B:87:LYS:HD2	2.44	0.52
1:L:364:ASP:OD1	1:L:369:TYR:OH	2.24	0.52
1:L:457:GLU:HA	1:L:499:TYR:O	2.09	0.52
1:C:34:LEU:HD22	1:C:94:CYS:HB2	1.90	0.52
1:B:84:PHE:CE2	1:B:86:TYR:HB3	2.44	0.52
1:F:133:ALA:HB1	1:C:133:ALA:HB3	1.91	0.52
1:G:100:ILE:HG23	1:G:291:LEU:HB2	1.90	0.52
1:G:264:TYR:HB3	1:G:267:TRP:CD1	2.45	0.52
1:B:172:LYS:HE3	1:B:176:LYS:HZ2	1.75	0.52
1:F:88:VAL:HB	1:F:93:ASN:HD22	1.75	0.52
1:H:325:ILE:HG21	1:H:328:MET:HG2	1.90	0.52
1:C:78:PHE:CE1	1:C:87:LYS:HD2	2.44	0.52
1:K:104:PRO:HB2	1:K:282:GLN:HB2	1.92	0.52
1:A:428:VAL:HB	1:A:431:LEU:HD12	1.91	0.52
1:B:454:PHE:CE2	1:F:203:LEU:HD22	2.45	0.52
1:L:69:THR:O	1:L:73:MET:HG2	2.10	0.52
1:C:347:GLU:OE2	1:C:427:VAL:HG13	2.09	0.52
1:K:454:PHE:CD1	1:K:465:PRO:HA	2.45	0.52
1:F:285:ASN:OD1	1:C:219:LYS:NZ	2.40	0.52
1:E:125:THR:HG21	1:E:129:TYR:CD1	2.45	0.52
1:I:203:LEU:HD13	1:J:454:PHE:HD2	1.73	0.52
1:F:326:GLN:HA	1:F:329:ILE:HD13	1.91	0.52
1:H:56:CYS:SG	1:H:89:ASP:HB3	2.50	0.52
1:K:100:ILE:HG23	1:K:291:LEU:HB2	1.91	0.52
1:I:191:PHE:CD2	1:I:192:LEU:HG	2.45	0.52
1:J:191:PHE:CD2	1:J:192:LEU:HG	2.45	0.52
1:L:218:MET:SD	1:L:284:THR:HG22	2.50	0.51
1:G:232:GLU:HG2	1:G:244:THR:HB	1.91	0.51
1:C:6:VAL:HG22	1:C:496:VAL:HB	1.90	0.51
1:C:410:ILE:HG22	1:C:411:TYR:N	2.25	0.51
1:A:219:LYS:HD2	1:C:220:PRO:HB3	1.91	0.51
1:B:456:PHE:HD2	1:B:498:LEU:HG	1.75	0.51
1:L:100:ILE:HG23	1:L:291:LEU:HB2	1.92	0.51
1:H:191:PHE:HD2	1:H:192:LEU:HG	1.75	0.51
1:H:192:LEU:HD22	1:H:245:VAL:HG21	1.92	0.51
1:C:69:THR:O	1:C:73:MET:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:HE3	1:B:176:LYS:NZ	2.26	0.51
1:H:69:THR:O	1:H:73:MET:HG2	2.11	0.51
1:H:90:PRO:HG2	1:H:429:PRO:HB2	1.92	0.51
1:A:70:TYR:HD2	1:A:249:LEU:HD21	1.76	0.51
1:E:88:VAL:HB	1:E:93:ASN:HD22	1.75	0.51
1:C:192:LEU:HD22	1:C:245:VAL:HG21	1.92	0.51
1:I:111:LYS:HG2	1:I:115:LYS:HE3	1.92	0.51
1:I:392:LEU:HD11	1:I:404:GLU:OE2	2.11	0.51
1:J:79:ARG:HH22	1:J:99:THR:HG23	1.75	0.51
1:B:96:ARG:NH2	1:B:331:ARG:O	2.43	0.51
1:B:309:ALA:HB3	1:B:322:LEU:HD22	1.93	0.51
1:E:231:HIS:CD2	1:E:245:VAL:HG22	2.45	0.51
1:H:447:THR:O	1:H:450:GLU:HG2	2.11	0.51
1:I:337:ILE:HG23	1:I:369:TYR:HB3	1.91	0.51
1:D:70:TYR:HD2	1:D:249:LEU:HD21	1.75	0.51
1:L:387:ALA:HB1	1:L:434:LEU:HD12	1.93	0.51
1:J:458:ILE:H	1:J:458:ILE:HD12	1.75	0.51
1:D:267:TRP:HE3	1:D:269:LEU:HD21	1.76	0.51
1:F:392:LEU:HD11	1:F:404:GLU:OE2	2.11	0.51
1:E:232:GLU:CG	1:E:244:THR:HB	2.41	0.51
1:B:98:TYR:CD1	1:B:328:MET:HG3	2.46	0.50
1:B:327:ASP:OD1	1:B:327:ASP:N	2.42	0.50
1:J:231:HIS:CD2	1:J:245:VAL:HG22	2.46	0.50
1:E:387:ALA:HB1	1:E:434:LEU:HD12	1.93	0.50
1:L:252:GLY:HA2	1:L:286:LEU:HB3	1.93	0.50
1:C:472:GLU:O	1:C:477:LYS:HE3	2.11	0.50
1:I:157:PHE:HZ	1:I:280:ILE:HD13	1.76	0.50
1:I:370:LYS:NZ	1:I:372:ILE:HG22	2.27	0.50
1:B:37:LEU:HB2	1:B:40:TRP:HD1	1.75	0.50
1:E:337:ILE:HG13	1:E:369:TYR:HB3	1.93	0.50
1:L:441:MET:HE1	1:L:469:PHE:CE2	2.46	0.50
1:G:350:LEU:HD12	1:G:432:LEU:HA	1.93	0.50
1:I:4:ARG:HD3	1:I:494:LYS:O	2.10	0.50
1:I:69:THR:O	1:I:73:MET:HG2	2.12	0.50
1:I:88:VAL:HB	1:I:93:ASN:HD22	1.75	0.50
1:A:67:VAL:HG12	1:A:250:PRO:HD3	1.93	0.50
1:E:388:ASN:HB3	1:E:404:GLU:HG2	1.94	0.50
1:H:454:PHE:CD1	1:H:465:PRO:HA	2.47	0.50
1:G:192:LEU:HD22	1:G:245:VAL:HG21	1.93	0.50
1:E:264:TYR:HB3	1:E:267:TRP:CD1	2.47	0.50
1:L:37:LEU:HD13	1:L:374:GLU:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:254:SER:HA	1:L:290:TYR:HB2	1.94	0.50
1:C:431:LEU:HD22	1:C:486:LEU:HA	1.94	0.50
1:C:231:HIS:CD2	1:C:245:VAL:HG22	2.47	0.50
1:A:132:ALA:HB2	1:C:135:ALA:HB2	1.94	0.50
1:L:464:ARG:NH2	1:L:472:GLU:OE1	2.44	0.50
1:G:370:LYS:HE3	1:G:372:ILE:HG22	1.93	0.50
1:A:4:ARG:HD2	1:A:496:VAL:HG23	1.92	0.50
1:A:33:GLN:OE1	1:A:331:ARG:NH2	2.44	0.50
1:A:327:ASP:OD1	1:A:328:MET:N	2.45	0.50
1:E:125:THR:HG23	1:E:149:ASN:O	2.12	0.50
1:L:144:VAL:HG13	1:L:216:GLN:HB3	1.94	0.50
1:K:232:GLU:CG	1:K:244:THR:HB	2.41	0.50
1:J:69:THR:O	1:J:73:MET:HG2	2.11	0.50
1:E:454:PHE:CD1	1:E:465:PRO:HA	2.47	0.50
1:H:232:GLU:CG	1:H:244:THR:HB	2.42	0.50
1:G:195:THR:HB	1:G:197:PHE:HD2	1.77	0.50
1:I:428:VAL:HB	1:I:431:LEU:HD12	1.93	0.50
1:G:78:PHE:CE1	1:G:87:LYS:HD2	2.47	0.49
1:C:316:HIS:CG	1:C:361:PHE:HZ	2.30	0.49
1:K:336:VAL:N	1:K:373:ALA:HB2	2.27	0.49
1:J:391:ALA:HB1	1:J:402:TYR:HB3	1.93	0.49
1:D:191:PHE:CD2	1:D:192:LEU:HG	2.47	0.49
1:F:70:TYR:HD2	1:F:249:LEU:HD21	1.76	0.49
1:F:352:ASP:O	1:F:353:SER:OG	2.25	0.49
1:F:69:THR:O	1:F:73:MET:HG2	2.11	0.49
1:L:175:GLU:HB2	1:L:181:TYR:CE1	2.48	0.49
1:K:89:ASP:H	1:K:93:ASN:ND2	2.10	0.49
1:B:175:GLU:HB2	1:B:181:TYR:CE1	2.47	0.49
1:F:388:ASN:HD22	1:F:404:GLU:HA	1.78	0.49
1:E:432:LEU:HB3	1:E:485:ARG:HA	1.93	0.49
1:C:12:MET:SD	1:C:425:PRO:HD3	2.52	0.49
1:J:261:ASP:HB3	1:J:264:TYR:HD2	1.78	0.49
1:J:441:MET:HE1	1:J:469:PHE:CE2	2.47	0.49
1:D:67:VAL:HG12	1:D:250:PRO:HD3	1.94	0.49
1:H:4:ARG:HD3	1:H:494:LYS:O	2.13	0.49
1:K:4:ARG:NH1	1:K:452:ARG:O	2.43	0.49
1:J:347:GLU:OE2	1:J:427:VAL:HG13	2.12	0.49
1:A:461:GLU:O	1:D:189:LYS:HD2	2.13	0.49
1:G:224:LEU:HD12	1:G:286:LEU:HD21	1.94	0.49
1:D:370:LYS:HE3	1:D:372:ILE:HG22	1.95	0.49
1:F:352:ASP:OD2	1:F:490:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:GLN:OE1	1:E:282:GLN:NE2	2.46	0.49
1:K:88:VAL:HG21	1:K:97:LEU:H	1.78	0.49
1:K:159:PRO:HB2	1:K:161:LEU:HG	1.95	0.49
1:I:431:LEU:HD22	1:I:486:LEU:HA	1.94	0.49
1:H:215:TRP:CD2	1:H:280:ILE:HG12	2.48	0.49
1:C:352:ASP:O	1:C:353:SER:OG	2.28	0.49
1:C:464:ARG:NH2	1:C:472:GLU:OE2	2.40	0.49
1:J:92:ARG:NH2	1:J:406:ASP:OD2	2.39	0.49
1:B:232:GLU:CG	1:B:244:THR:HB	2.43	0.49
1:B:322:LEU:HD11	1:B:328:MET:CE	2.43	0.49
1:C:479:ARG:HH22	1:C:501:GLU:HA	1.77	0.49
1:K:448:ASP:HB3	1:K:493:MET:HE2	1.94	0.49
1:B:119:ARG:HB3	1:B:123:ARG:NH1	2.28	0.48
1:L:454:PHE:CE2	1:K:203:LEU:HD22	2.47	0.48
1:G:74:CYS:SG	1:G:79:ARG:NH1	2.87	0.48
1:B:98:TYR:CE1	1:B:328:MET:HG3	2.46	0.48
1:F:90:PRO:HB2	1:F:334:LEU:HD12	1.94	0.48
1:K:88:VAL:HG11	1:K:97:LEU:HD13	1.95	0.48
1:B:231:HIS:CD2	1:B:245:VAL:HG22	2.49	0.48
1:E:37:LEU:HB2	1:E:40:TRP:HD1	1.78	0.48
1:K:84:PHE:CE2	1:K:86:TYR:HB3	2.48	0.48
1:I:441:MET:HE1	1:I:469:PHE:CE2	2.49	0.48
1:E:203:LEU:HD22	1:C:454:PHE:CE2	2.49	0.48
1:G:232:GLU:CG	1:G:244:THR:HB	2.44	0.48
1:B:36:ALA:O	1:B:333:LYS:HB2	2.13	0.48
1:H:428:VAL:HB	1:H:431:LEU:HD12	1.96	0.48
1:C:165:GLU:OE2	1:C:235:TYR:OH	2.29	0.48
1:C:370:LYS:HE3	1:C:372:ILE:HG22	1.95	0.48
1:J:454:PHE:CD1	1:J:465:PRO:HA	2.49	0.48
1:B:410:ILE:HD11	1:B:411:TYR:CE2	2.48	0.48
1:L:164:GLU:HG3	1:L:168:HIS:NE2	2.29	0.48
1:H:6:VAL:HG12	1:H:63:GLU:HB3	1.96	0.48
1:C:33:GLN:CD	1:C:331:ARG:HD2	2.39	0.48
1:C:72:ARG:HH12	1:C:357:ARG:HE	1.60	0.48
1:I:47:LYS:O	1:I:51:VAL:HG23	2.13	0.48
1:I:88:VAL:HG21	1:I:97:LEU:H	1.79	0.48
1:F:428:VAL:HB	1:F:431:LEU:HD12	1.95	0.48
1:E:437:LEU:O	1:E:441:MET:HG2	2.14	0.48
1:L:340:LYS:HA	1:L:370:LYS:HE2	1.96	0.48
1:A:191:PHE:CD2	1:A:192:LEU:HG	2.49	0.48
1:A:203:LEU:HD22	1:D:454:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ILE:HD12	1:A:458:ILE:H	1.79	0.48
1:F:456:PHE:HD2	1:F:498:LEU:HG	1.79	0.48
1:L:5:PHE:CE2	1:L:7:ILE:HD13	2.49	0.48
1:H:328:MET:SD	1:H:333:LYS:HB2	2.53	0.48
1:J:340:LYS:HA	1:J:370:LYS:HE2	1.95	0.48
1:B:47:LYS:O	1:B:51:VAL:HG23	2.14	0.48
1:E:456:PHE:HD2	1:E:498:LEU:HG	1.78	0.48
1:H:401:PRO:HG2	1:H:478:LYS:HD2	1.96	0.48
1:G:254:SER:HA	1:G:290:TYR:HB2	1.95	0.48
1:G:260:TRP:CZ3	1:G:262:PRO:HA	2.49	0.48
1:G:320:ILE:HD11	1:G:335:PHE:CE2	2.48	0.48
1:K:4:ARG:HG3	1:K:494:LYS:O	2.14	0.48
1:I:176:LYS:HB2	1:I:262:PRO:HG2	1.94	0.48
1:J:410:ILE:HG13	1:J:411:TYR:CD2	2.49	0.48
1:A:337:ILE:HG23	1:A:369:TYR:HB3	1.95	0.47
1:J:8:TRP:CD1	1:J:61:PHE:HD2	2.32	0.47
1:A:439:ASP:OD1	1:B:346:LYS:NZ	2.39	0.47
1:B:407:LEU:HD12	1:B:408:ASP:H	1.78	0.47
1:D:47:LYS:O	1:D:51:VAL:HG23	2.14	0.47
1:H:370:LYS:HE3	1:H:372:ILE:HG22	1.95	0.47
1:C:400:ILE:HD11	1:C:441:MET:HE2	1.96	0.47
1:I:236:TYR:HB3	1:I:241:ILE:HG21	1.96	0.47
1:J:156:ARG:NH2	1:J:235:TYR:OH	2.47	0.47
1:A:352:ASP:O	1:A:353:SER:OG	2.30	0.47
1:D:186:LYS:HE3	1:D:190:ARG:HH21	1.78	0.47
1:D:437:LEU:O	1:D:441:MET:HG2	2.15	0.47
1:L:72:ARG:HH12	1:L:357:ARG:HE	1.62	0.47
1:H:232:GLU:HG2	1:H:244:THR:HB	1.95	0.47
1:G:447:THR:O	1:G:450:GLU:HG2	2.14	0.47
1:D:441:MET:HE1	1:D:469:PHE:CE2	2.49	0.47
1:H:8:TRP:CH2	1:H:458:ILE:HD11	2.49	0.47
1:D:316:HIS:CG	1:D:361:PHE:HZ	2.33	0.47
1:H:331:ARG:HG2	1:H:333:LYS:NZ	2.29	0.47
1:H:456:PHE:HD2	1:H:498:LEU:HG	1.79	0.47
1:G:392:LEU:HD11	1:G:404:GLU:OE2	2.14	0.47
1:K:284:THR:HG22	1:K:285:ASN:N	2.24	0.47
1:I:84:PHE:CE2	1:I:86:TYR:HB3	2.49	0.47
1:J:77:GLY:HA2	1:J:99:THR:OG1	2.14	0.47
1:J:428:VAL:HB	1:J:431:LEU:HD12	1.97	0.47
1:A:33:GLN:HE22	1:A:331:ARG:HG2	1.80	0.47
1:B:6:VAL:HG22	1:B:496:VAL:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:TRP:CZ3	1:B:262:PRO:HA	2.50	0.47
1:F:218:MET:O	1:F:283:ARG:NH1	2.46	0.47
1:E:456:PHE:CD2	1:E:498:LEU:HG	2.50	0.47
1:H:191:PHE:CD2	1:H:192:LEU:HG	2.49	0.47
1:C:175:GLU:HB2	1:C:181:TYR:CE1	2.50	0.47
1:K:254:SER:HA	1:K:290:TYR:HB2	1.97	0.47
1:I:4:ARG:NH2	1:J:204:GLY:O	2.47	0.47
1:E:47:LYS:O	1:E:51:VAL:HG23	2.15	0.47
1:H:15:GLU:H	1:H:55:ASN:ND2	2.09	0.47
1:H:88:VAL:HB	1:H:93:ASN:HD22	1.79	0.47
1:H:335:PHE:CG	1:H:335:PHE:O	2.66	0.47
1:K:388:ASN:HB3	1:K:404:GLU:HG2	1.97	0.47
1:K:428:VAL:HB	1:K:431:LEU:HD12	1.96	0.47
1:J:211:GLN:NE2	1:J:223:LYS:O	2.33	0.47
1:E:252:GLY:HA3	1:E:288:TYR:O	2.15	0.47
1:L:203:LEU:HD22	1:K:454:PHE:HE2	1.80	0.47
1:G:216:GLN:O	1:G:283:ARG:NH2	2.48	0.47
1:J:4:ARG:HD2	1:J:496:VAL:HG23	1.97	0.47
1:D:454:PHE:CD1	1:D:465:PRO:HA	2.50	0.47
1:L:391:ALA:HB1	1:L:402:TYR:HB3	1.97	0.47
1:G:70:TYR:HD2	1:G:249:LEU:HD21	1.80	0.47
1:I:264:TYR:HB3	1:I:267:TRP:CD1	2.50	0.47
1:J:67:VAL:HG12	1:J:250:PRO:HD3	1.97	0.47
1:J:406:ASP:CG	1:J:410:ILE:HG22	2.40	0.47
1:B:189:LYS:HA	1:B:193:CYS:HB2	1.97	0.47
1:F:78:PHE:HD1	1:F:87:LYS:HB3	1.80	0.47
1:F:339:LYS:HE2	1:F:369:TYR:HE1	1.79	0.47
1:E:253:ILE:HB	1:E:281:ILE:HD11	1.96	0.47
1:H:49:ASP:OD1	1:H:49:ASP:N	2.48	0.47
1:G:253:ILE:HB	1:G:281:ILE:HD11	1.97	0.47
1:C:67:VAL:HG12	1:C:250:PRO:HD3	1.97	0.47
1:J:70:TYR:HD2	1:J:249:LEU:HD21	1.80	0.47
1:J:100:ILE:HG23	1:J:291:LEU:HB2	1.97	0.47
1:B:191:PHE:CD2	1:B:192:LEU:HG	2.50	0.46
1:E:103:ALA:HB3	1:E:106:GLU:HG2	1.97	0.46
1:L:203:LEU:HD12	1:K:4:ARG:HD2	1.96	0.46
1:H:119:ARG:HB3	1:H:123:ARG:NH1	2.30	0.46
1:C:428:VAL:HB	1:C:431:LEU:HD12	1.97	0.46
1:K:39:SER:OG	1:K:374:GLU:OE2	2.28	0.46
1:A:349:TYR:H	1:B:442:GLN:HE22	1.62	0.46
1:A:454:PHE:CD1	1:A:465:PRO:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:ASP:OD1	1:F:33:GLN:N	2.48	0.46
1:F:47:LYS:O	1:F:51:VAL:HG23	2.15	0.46
1:F:435:TRP:CZ2	1:E:442:GLN:NE2	2.83	0.46
1:L:6:VAL:HG12	1:L:63:GLU:HB3	1.96	0.46
1:L:8:TRP:CH2	1:L:458:ILE:HD11	2.49	0.46
1:C:140:VAL:HG21	1:C:282:GLN:OE1	2.15	0.46
1:C:211:GLN:HE21	1:C:218:MET:HE3	1.80	0.46
1:K:472:GLU:HG3	1:K:473:PRO:HD2	1.97	0.46
1:B:391:ALA:HB1	1:B:402:TYR:HB3	1.97	0.46
1:B:428:VAL:HB	1:B:431:LEU:HD12	1.98	0.46
1:D:84:PHE:CE2	1:D:86:TYR:HB3	2.50	0.46
1:H:124:ILE:HG13	1:H:125:THR:HG23	1.98	0.46
1:H:352:ASP:O	1:H:353:SER:OG	2.31	0.46
1:G:191:PHE:CD2	1:G:192:LEU:HG	2.50	0.46
1:G:437:LEU:O	1:G:441:MET:HG2	2.15	0.46
1:C:73:MET:HB3	1:C:78:PHE:HD2	1.80	0.46
1:K:12:MET:SD	1:K:425:PRO:HD3	2.56	0.46
1:K:176:LYS:HB2	1:K:262:PRO:HG2	1.98	0.46
1:B:92:ARG:NH2	1:B:406:ASP:OD2	2.48	0.46
1:L:7:ILE:HG22	1:L:62:VAL:HG22	1.97	0.46
1:I:352:ASP:O	1:I:353:SER:OG	2.29	0.46
1:J:284:THR:CG2	1:J:286:LEU:HD23	2.46	0.46
1:B:431:LEU:HD22	1:B:486:LEU:HA	1.96	0.46
1:D:254:SER:HA	1:D:290:TYR:HB2	1.97	0.46
1:F:111:LYS:HE2	1:F:115:LYS:HE3	1.97	0.46
1:H:34:LEU:HD22	1:H:94:CYS:HB2	1.96	0.46
1:K:352:ASP:O	1:K:353:SER:OG	2.28	0.46
1:J:457:GLU:HA	1:J:499:TYR:O	2.15	0.46
1:F:84:PHE:CE2	1:F:86:TYR:HB3	2.51	0.46
1:E:88:VAL:HG21	1:E:97:LEU:H	1.80	0.46
1:H:78:PHE:CE1	1:H:87:LYS:HD2	2.51	0.46
1:H:400:ILE:HD11	1:H:441:MET:HE2	1.97	0.46
1:H:439:ASP:OD1	1:I:346:LYS:NZ	2.40	0.46
1:G:65:MET:HE3	1:G:70:TYR:HB2	1.98	0.46
1:G:241:ILE:HB	1:G:264:TYR:HD2	1.81	0.46
1:I:11:SER:OG	1:I:13:HIS:NE2	2.49	0.46
1:I:234:TYR:HB2	1:I:242:ALA:HB3	1.97	0.46
1:B:458:ILE:HD12	1:B:458:ILE:H	1.81	0.46
1:E:460:THR:O	1:E:461:GLU:HG3	2.15	0.46
1:L:400:ILE:HD11	1:L:441:MET:HE2	1.98	0.46
1:L:472:GLU:O	1:L:477:LYS:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144:VAL:HG13	1:J:216:GLN:HB3	1.98	0.46
1:A:260:TRP:HB2	1:A:269:LEU:HD12	1.98	0.46
1:F:7:ILE:HG22	1:F:62:VAL:HA	1.96	0.46
1:F:260:TRP:CZ3	1:F:262:PRO:HA	2.50	0.46
1:L:98:TYR:OH	1:L:333:LYS:O	2.32	0.46
1:H:472:GLU:O	1:H:477:LYS:HE3	2.15	0.46
1:I:40:TRP:CZ3	1:I:410:ILE:HG22	2.50	0.46
1:B:5:PHE:CE2	1:B:7:ILE:HD13	2.51	0.46
1:D:175:GLU:HB2	1:D:181:TYR:CE1	2.51	0.46
1:E:140:VAL:HG22	1:E:279:ALA:HA	1.98	0.46
1:E:458:ILE:HD12	1:E:458:ILE:H	1.81	0.46
1:C:77:GLY:HA2	1:C:99:THR:OG1	2.16	0.46
1:K:33:GLN:OE1	1:K:331:ARG:NE	2.48	0.46
1:K:410:ILE:HG13	1:K:411:TYR:CD2	2.50	0.46
1:J:252:GLY:HA3	1:J:288:TYR:O	2.15	0.46
1:A:264:TYR:HB3	1:A:267:TRP:CD1	2.51	0.45
1:F:475:ASN:O	1:F:479:ARG:HG3	2.17	0.45
1:L:88:VAL:HB	1:L:93:ASN:HD22	1.80	0.45
1:L:313:ASP:O	1:L:317:SER:N	2.49	0.45
1:L:410:ILE:HG13	1:L:411:TYR:CD2	2.52	0.45
1:H:461:GLU:O	1:G:189:LYS:HD2	2.16	0.45
1:G:175:GLU:HG3	1:G:181:TYR:CZ	2.51	0.45
1:K:37:LEU:HB2	1:K:40:TRP:HD1	1.81	0.45
1:J:8:TRP:O	1:J:60:SER:OG	2.34	0.45
1:L:231:HIS:CD2	1:L:245:VAL:HG22	2.51	0.45
1:L:267:TRP:HE3	1:L:269:LEU:HD21	1.80	0.45
1:G:432:LEU:HB3	1:G:485:ARG:HA	1.99	0.45
1:K:260:TRP:CZ3	1:K:262:PRO:HA	2.51	0.45
1:J:84:PHE:CE2	1:J:86:TYR:HB3	2.51	0.45
1:L:203:LEU:HD13	1:K:454:PHE:HD2	1.79	0.45
1:L:361:PHE:CG	1:L:362:PRO:HD2	2.51	0.45
1:G:147:GLU:OE2	1:G:276:ARG:NH2	2.49	0.45
1:C:264:TYR:HB3	1:C:267:TRP:CD1	2.51	0.45
1:I:232:GLU:HG2	1:I:244:THR:HB	1.98	0.45
1:A:44:TYR:OH	1:A:409:THR:HG23	2.16	0.45
1:A:287:GLN:HG3	1:A:288:TYR:CD2	2.52	0.45
1:D:157:PHE:HZ	1:D:280:ILE:HD13	1.82	0.45
1:E:350:LEU:HD12	1:E:432:LEU:HA	1.99	0.45
1:L:215:TRP:CD2	1:L:280:ILE:HG12	2.51	0.45
1:L:313:ASP:OD2	1:L:337:ILE:HG22	2.16	0.45
1:L:454:PHE:CD1	1:L:465:PRO:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:437:LEU:O	1:H:441:MET:HG2	2.17	0.45
1:J:79:ARG:NH2	1:J:99:THR:HG23	2.30	0.45
1:F:432:LEU:HB3	1:F:485:ARG:HA	1.98	0.45
1:L:111:LYS:HE2	1:L:115:LYS:HE3	1.98	0.45
1:A:304:LYS:O	1:A:329:ILE:HD11	2.16	0.45
1:F:437:LEU:O	1:F:441:MET:HG2	2.16	0.45
1:H:454:PHE:CE2	1:G:203:LEU:HD22	2.51	0.45
1:C:84:PHE:CE2	1:C:86:TYR:HB3	2.51	0.45
1:C:441:MET:HE1	1:C:469:PHE:CE2	2.52	0.45
1:J:6:VAL:HG22	1:J:496:VAL:HB	1.99	0.45
1:E:461:GLU:O	1:C:189:LYS:HD2	2.16	0.45
1:L:191:PHE:CD2	1:L:192:LEU:HG	2.50	0.45
1:L:208:SER:HB2	1:L:226:HIS:HB2	1.99	0.45
1:G:5:PHE:CE2	1:G:7:ILE:HD13	2.51	0.45
1:C:79:ARG:HH22	1:C:290:TYR:HB3	1.82	0.45
1:K:368:LYS:HE2	1:K:368:LYS:HB3	1.63	0.45
1:I:454:PHE:CD2	1:J:203:LEU:HD13	2.52	0.45
1:K:69:THR:O	1:K:73:MET:HG2	2.17	0.45
1:B:72:ARG:NH2	1:B:490:GLU:OE2	2.50	0.45
1:L:34:LEU:HD22	1:L:94:CYS:HB2	1.97	0.45
1:L:437:LEU:O	1:L:441:MET:HG2	2.17	0.45
1:L:456:PHE:CD1	1:L:463:ILE:HG22	2.52	0.45
1:G:312:LEU:HB2	1:G:319:TYR:CE1	2.52	0.45
1:C:454:PHE:CD1	1:C:465:PRO:HA	2.52	0.45
1:J:456:PHE:HB2	1:J:463:ILE:HG12	1.98	0.45
1:A:437:LEU:O	1:A:441:MET:HG2	2.17	0.45
1:B:100:ILE:HD11	1:B:322:LEU:HD22	1.99	0.45
1:F:437:LEU:HD21	1:F:481:CYS:HB3	1.99	0.45
1:I:388:ASN:HB3	1:I:404:GLU:HG2	1.97	0.45
1:F:211:GLN:HE21	1:F:218:MET:HE3	1.81	0.44
1:E:475:ASN:O	1:E:479:ARG:HG3	2.17	0.44
1:C:6:VAL:HG12	1:C:63:GLU:HB3	1.98	0.44
1:B:3:ASP:OD2	1:B:64:HIS:NE2	2.49	0.44
1:B:347:GLU:OE2	1:B:427:VAL:HG13	2.17	0.44
1:H:254:SER:HA	1:H:290:TYR:HB2	2.00	0.44
1:G:215:TRP:CD2	1:G:280:ILE:HG12	2.53	0.44
1:I:454:PHE:CD1	1:I:465:PRO:HA	2.52	0.44
1:B:326:GLN:O	1:B:329:ILE:HG12	2.17	0.44
1:B:452:ARG:HB3	1:B:493:MET:O	2.17	0.44
1:E:102:THR:HG21	1:E:107:LEU:HD12	1.99	0.44
1:E:428:VAL:HB	1:E:431:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:THR:HG21	1:G:229:PRO:HG3	1.99	0.44
1:K:224:LEU:HG	1:K:284:THR:CG2	2.44	0.44
1:J:140:VAL:HG21	1:J:282:GLN:OE1	2.17	0.44
1:A:84:PHE:CE2	1:A:86:TYR:HB3	2.53	0.44
1:B:215:TRP:CD2	1:B:280:ILE:HG12	2.53	0.44
1:E:161:LEU:HD22	1:C:463:ILE:HG23	2.00	0.44
1:E:255:SER:HG	1:E:289:TYR:HH	1.64	0.44
1:H:331:ARG:HG2	1:H:333:LYS:HZ3	1.83	0.44
1:H:441:MET:HE1	1:H:469:PHE:CE2	2.52	0.44
1:G:340:LYS:HA	1:G:370:LYS:HE2	1.98	0.44
1:K:340:LYS:HA	1:K:370:LYS:HE2	1.98	0.44
1:D:387:ALA:HB1	1:D:434:LEU:HD12	1.99	0.44
1:G:253:ILE:HD12	1:G:281:ILE:HG13	1.99	0.44
1:K:47:LYS:O	1:K:51:VAL:HG23	2.16	0.44
1:I:117:ILE:HD13	1:I:139:PHE:HB2	1.99	0.44
1:B:267:TRP:HE3	1:B:269:LEU:HD21	1.82	0.44
1:B:280:ILE:O	1:B:284:THR:HG22	2.17	0.44
1:D:140:VAL:HG21	1:D:282:GLN:OE1	2.18	0.44
1:F:156:ARG:NH2	1:F:235:TYR:OH	2.51	0.44
1:E:203:LEU:HD13	1:C:454:PHE:HD2	1.82	0.44
1:E:232:GLU:HG2	1:E:244:THR:HB	1.98	0.44
1:I:232:GLU:CG	1:I:244:THR:HB	2.47	0.44
1:J:4:ARG:HD3	1:J:494:LYS:O	2.18	0.44
1:D:320:ILE:HD12	1:D:335:PHE:HE2	1.82	0.44
1:D:320:ILE:HD13	1:D:337:ILE:HG21	1.98	0.44
1:D:347:GLU:OE2	1:D:427:VAL:HG13	2.18	0.44
1:J:340:LYS:HG2	1:J:370:LYS:HD3	2.00	0.44
1:D:8:TRP:O	1:D:60:SER:OG	2.35	0.44
1:E:328:MET:SD	1:E:328:MET:N	2.86	0.44
1:L:120:PHE:O	1:L:124:ILE:HG12	2.17	0.44
1:L:330:SER:HB3	1:L:333:LYS:HB2	1.99	0.44
1:B:98:TYR:OH	1:B:328:MET:HA	2.17	0.44
1:L:159:PRO:HB2	1:L:161:LEU:HG	2.00	0.44
1:H:340:LYS:HA	1:H:370:LYS:HE2	2.00	0.44
1:G:35:PHE:O	1:G:331:ARG:NH1	2.51	0.44
1:G:124:ILE:HG13	1:G:125:THR:HG23	2.00	0.44
1:C:384:PHE:CE1	1:C:410:ILE:HD11	2.53	0.44
1:E:70:TYR:HD2	1:E:249:LEU:HD21	1.83	0.43
1:E:79:ARG:NH1	1:E:254:SER:HB2	2.25	0.43
1:E:347:GLU:OE2	1:E:383:ALA:HB1	2.18	0.43
1:E:364:ASP:OD1	1:E:366:VAL:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:350:LEU:HD12	1:L:432:LEU:HA	2.00	0.43
1:L:450:GLU:OE1	1:G:339:LYS:HE3	2.18	0.43
1:H:322:LEU:HD11	1:H:329:ILE:HB	1.98	0.43
1:I:8:TRP:HH2	1:I:458:ILE:HD11	1.82	0.43
1:I:140:VAL:HG21	1:I:282:GLN:OE1	2.18	0.43
1:L:12:MET:HE2	1:L:56:CYS:SG	2.58	0.43
1:H:98:TYR:OH	1:H:332:GLY:O	2.34	0.43
1:I:6:VAL:HG22	1:I:496:VAL:HB	1.98	0.43
1:F:264:TYR:HB3	1:F:267:TRP:CD1	2.54	0.43
1:E:175:GLU:HB2	1:E:181:TYR:CE1	2.52	0.43
1:L:457:GLU:HG2	1:L:460:THR:OG1	2.17	0.43
1:H:260:TRP:CZ3	1:H:262:PRO:HA	2.54	0.43
1:D:117:ILE:HD11	1:D:275:LEU:HD13	1.99	0.43
1:F:73:MET:HB3	1:F:78:PHE:HD2	1.82	0.43
1:F:336:VAL:N	1:F:373:ALA:HB2	2.31	0.43
1:H:203:LEU:HD22	1:G:454:PHE:CZ	2.53	0.43
1:G:472:GLU:HG3	1:G:476:VAL:HB	2.01	0.43
1:J:6:VAL:HG12	1:J:63:GLU:HB3	1.99	0.43
1:J:232:GLU:CG	1:J:244:THR:HB	2.48	0.43
1:A:241:ILE:HG22	1:A:264:TYR:HE2	1.84	0.43
1:E:323:LYS:HG3	1:E:324:PRO:HD3	2.01	0.43
1:H:145:ASN:OD1	1:H:149:ASN:ND2	2.51	0.43
1:G:479:ARG:NH1	1:G:499:TYR:HB2	2.34	0.43
1:C:208:SER:HB2	1:C:226:HIS:HB2	2.01	0.43
1:I:370:LYS:HZ2	1:I:372:ILE:HG22	1.84	0.43
1:B:98:TYR:CD1	1:B:328:MET:CG	2.99	0.43
1:E:6:VAL:HG22	1:E:496:VAL:HB	2.01	0.43
1:L:340:LYS:HE3	1:L:368:LYS:O	2.19	0.43
1:G:231:HIS:CD2	1:G:245:VAL:HG22	2.53	0.43
1:E:454:PHE:CE2	1:C:203:LEU:HD22	2.54	0.43
1:G:98:TYR:OH	1:G:332:GLY:O	2.32	0.43
1:C:98:TYR:CE1	1:C:328:MET:HE2	2.53	0.43
1:K:209:TRP:CH2	1:K:230:VAL:HG12	2.53	0.43
1:I:145:ASN:OD1	1:I:149:ASN:ND2	2.51	0.43
1:I:209:TRP:CH2	1:I:230:VAL:HG12	2.53	0.43
1:J:176:LYS:HD2	1:J:262:PRO:HG2	2.01	0.43
1:B:67:VAL:HG12	1:B:250:PRO:HD3	2.01	0.43
1:F:67:VAL:HG12	1:F:250:PRO:HD3	2.01	0.43
1:I:189:LYS:HA	1:I:193:CYS:HB2	2.01	0.43
1:I:322:LEU:HD11	1:I:329:ILE:HD13	2.00	0.43
1:J:234:TYR:CD2	1:J:242:ALA:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:SER:HB2	1:A:226:HIS:HB2	1.99	0.43
1:L:457:GLU:O	1:L:460:THR:OG1	2.30	0.43
1:L:468:ASN:ND2	1:G:341:LYS:HD2	2.30	0.43
1:H:56:CYS:SG	1:H:93:ASN:HB2	2.59	0.43
1:H:218:MET:SD	1:H:284:THR:HG22	2.59	0.43
1:G:456:PHE:HD1	1:G:463:ILE:HB	1.84	0.43
1:C:7:ILE:HG22	1:C:62:VAL:HG22	2.01	0.43
1:K:65:MET:HE3	1:K:70:TYR:HB2	2.01	0.43
1:I:347:GLU:OE2	1:I:427:VAL:HG13	2.19	0.43
1:A:189:LYS:HA	1:A:193:CYS:HB2	2.00	0.43
1:A:349:TYR:CD1	1:A:436:GLU:OE2	2.72	0.43
1:D:124:ILE:O	1:D:150:SER:OG	2.27	0.43
1:F:401:PRO:HG2	1:F:478:LYS:HD2	2.00	0.43
1:E:191:PHE:CD2	1:E:192:LEU:HG	2.54	0.43
1:E:284:THR:CG2	1:E:286:LEU:HD23	2.45	0.43
1:L:336:VAL:H	1:L:373:ALA:HB2	1.83	0.43
1:K:155:THR:HG21	1:K:276:ARG:CZ	2.48	0.43
1:I:203:LEU:HD22	1:J:454:PHE:CE2	2.54	0.43
1:A:217:ARG:HD3	1:C:105:GLN:OE1	2.19	0.42
1:D:120:PHE:O	1:D:124:ILE:HG12	2.18	0.42
1:L:439:ASP:OD1	1:G:346:LYS:NZ	2.37	0.42
1:H:5:PHE:CE2	1:H:7:ILE:HD13	2.54	0.42
1:H:79:ARG:HH22	1:H:99:THR:HG23	1.84	0.42
1:K:236:TYR:HB3	1:K:241:ILE:HG21	2.01	0.42
1:J:232:GLU:HG2	1:J:244:THR:HB	2.00	0.42
1:J:361:PHE:CG	1:J:362:PRO:HD2	2.53	0.42
1:A:326:GLN:O	1:A:329:ILE:HG22	2.19	0.42
1:D:281:ILE:HG23	1:D:286:LEU:HB2	2.01	0.42
1:D:388:ASN:HB3	1:D:404:GLU:HG2	2.01	0.42
1:E:323:LYS:CG	1:E:324:PRO:HD3	2.49	0.42
1:C:8:TRP:HD1	1:C:61:PHE:O	2.03	0.42
1:C:350:LEU:HD12	1:C:432:LEU:HA	2.01	0.42
1:J:192:LEU:HD22	1:J:245:VAL:HG21	2.01	0.42
1:B:289:TYR:HE2	1:B:291:LEU:HD23	1.84	0.42
1:D:362:PRO:HG2	1:D:369:TYR:OH	2.20	0.42
1:F:232:GLU:CG	1:F:244:THR:HB	2.49	0.42
1:F:475:ASN:ND2	1:F:501:GLU:OE2	2.52	0.42
1:E:54:GLU:HG3	1:E:56:CYS:SG	2.59	0.42
1:E:337:ILE:HD11	1:E:369:TYR:CG	2.55	0.42
1:L:124:ILE:HG13	1:L:125:THR:HG23	2.02	0.42
1:G:337:ILE:HG13	1:G:369:TYR:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:456:PHE:CD2	1:K:498:LEU:HG	2.54	0.42
1:J:279:ALA:O	1:J:283:ARG:HG2	2.19	0.42
1:J:431:LEU:HD22	1:J:486:LEU:HA	2.01	0.42
1:B:203:LEU:HD22	1:F:454:PHE:CE2	2.55	0.42
1:D:443:SER:HB3	1:C:349:TYR:HB3	2.01	0.42
1:E:140:VAL:HG21	1:E:282:GLN:OE1	2.19	0.42
1:L:84:PHE:CE2	1:L:86:TYR:HB3	2.53	0.42
1:L:241:ILE:HG22	1:L:264:TYR:HE2	1.83	0.42
1:G:69:THR:O	1:G:73:MET:HG2	2.19	0.42
1:I:248:ILE:HD13	1:I:253:ILE:HG12	2.01	0.42
1:J:98:TYR:OH	1:J:332:GLY:O	2.24	0.42
1:A:78:PHE:CE1	1:A:87:LYS:HD2	2.55	0.42
1:E:169:LEU:HD22	1:E:240:LEU:HG	2.00	0.42
1:H:84:PHE:CE2	1:H:86:TYR:HB3	2.54	0.42
1:I:231:HIS:CD2	1:I:245:VAL:HG22	2.54	0.42
1:I:456:PHE:CD2	1:I:498:LEU:HG	2.53	0.42
1:J:34:LEU:HD22	1:J:94:CYS:HB2	2.02	0.42
1:A:73:MET:HB3	1:A:78:PHE:HD2	1.85	0.42
1:B:433:PRO:HD2	1:B:436:GLU:OE2	2.19	0.42
1:B:454:PHE:HD2	1:F:203:LEU:HD13	1.84	0.42
1:D:65:MET:HE3	1:D:70:TYR:HB2	2.01	0.42
1:H:331:ARG:HE	1:H:333:LYS:HE2	1.83	0.42
1:K:12:MET:SD	1:K:424:ILE:HA	2.59	0.42
1:I:5:PHE:CE2	1:I:7:ILE:HD13	2.55	0.42
1:J:36:ALA:HB1	1:J:334:LEU:HD22	2.01	0.42
1:F:40:TRP:CZ2	1:F:410:ILE:HD13	2.53	0.42
1:E:352:ASP:O	1:E:353:SER:OG	2.31	0.42
1:K:241:ILE:HG22	1:K:264:TYR:HE2	1.85	0.42
1:K:341:LYS:HD3	1:J:468:ASN:ND2	2.34	0.42
1:K:456:PHE:HD2	1:K:498:LEU:HG	1.85	0.42
1:A:311:VAL:HG13	1:A:322:LEU:HD12	2.01	0.42
1:A:336:VAL:H	1:A:373:ALA:HB2	1.84	0.42
1:A:432:LEU:HB3	1:A:485:ARG:HA	2.01	0.42
1:C:191:PHE:CD2	1:C:192:LEU:HG	2.54	0.42
1:C:272:LEU:O	1:C:276:ARG:HG3	2.20	0.42
1:I:100:ILE:HG23	1:I:291:LEU:HB3	2.02	0.42
1:I:457:GLU:HG2	1:I:499:TYR:CE2	2.55	0.42
1:J:156:ARG:O	1:J:232:GLU:HA	2.19	0.42
1:J:240:LEU:HD21	1:J:243:ILE:HD11	2.02	0.42
1:A:384:PHE:CE1	1:A:410:ILE:HD12	2.55	0.42
1:B:124:ILE:HG13	1:B:125:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:GLU:OE2	1:D:276:ARG:NH2	2.53	0.42
1:G:431:LEU:HD22	1:G:486:LEU:HA	2.01	0.42
1:J:400:ILE:HG12	1:J:477:LYS:HB3	2.01	0.42
1:B:7:ILE:HG22	1:B:62:VAL:HG22	2.01	0.42
1:F:124:ILE:HG13	1:F:125:THR:HG23	2.02	0.42
1:F:313:ASP:OD2	1:F:337:ILE:HG22	2.20	0.42
1:L:96:ARG:NH2	1:L:332:GLY:HA3	2.33	0.42
1:H:349:TYR:HB3	1:I:443:SER:HB3	2.02	0.42
1:F:450:GLU:OE2	1:F:468:ASN:HA	2.20	0.41
1:F:458:ILE:HD12	1:F:458:ILE:H	1.85	0.41
1:H:73:MET:HB3	1:H:78:PHE:HD2	1.84	0.41
1:K:218:MET:HE1	1:K:284:THR:HG23	2.02	0.41
1:K:347:GLU:OE2	1:K:427:VAL:HG13	2.20	0.41
1:A:140:VAL:HG21	1:A:282:GLN:OE1	2.20	0.41
1:D:92:ARG:HG2	1:D:410:ILE:HD13	2.01	0.41
1:D:248:ILE:HD13	1:D:253:ILE:HG12	2.03	0.41
1:L:70:TYR:HD2	1:L:249:LEU:HD21	1.85	0.41
1:L:124:ILE:HD11	1:L:146:ALA:HB1	2.01	0.41
1:H:200:GLU:O	1:H:204:GLY:N	2.50	0.41
1:G:159:PRO:HB2	1:G:161:LEU:HG	2.02	0.41
1:K:231:HIS:CD2	1:K:245:VAL:HG22	2.54	0.41
1:J:445:LYS:HD2	1:J:448:ASP:OD2	2.19	0.41
1:A:37:LEU:HB2	1:A:40:TRP:HD1	1.86	0.41
1:B:159:PRO:HB2	1:B:161:LEU:HG	2.01	0.41
1:D:448:ASP:HB3	1:D:493:MET:HE2	2.02	0.41
1:L:3:ASP:HB2	1:K:200:GLU:OE1	2.20	0.41
1:J:224:LEU:HD12	1:J:286:LEU:HD21	2.02	0.41
1:A:211:GLN:HE21	1:A:218:MET:HE3	1.86	0.41
1:E:67:VAL:HG12	1:E:250:PRO:HD3	2.02	0.41
1:E:72:ARG:NH2	1:E:490:GLU:OE2	2.54	0.41
1:E:410:ILE:HG22	1:E:411:TYR:N	2.36	0.41
1:G:312:LEU:HD13	1:G:319:TYR:CZ	2.55	0.41
1:I:79:ARG:HH22	1:I:290:TYR:HB3	1.85	0.41
1:B:38:ASP:OD2	1:B:333:LYS:NZ	2.53	0.41
1:F:287:GLN:HG3	1:F:288:TYR:CD2	2.56	0.41
1:H:78:PHE:HD1	1:H:87:LYS:HB3	1.85	0.41
1:H:98:TYR:CE1	1:H:335:PHE:HE1	2.38	0.41
1:C:260:TRP:CZ3	1:C:262:PRO:HA	2.56	0.41
1:E:319:TYR:HE2	1:E:358:GLY:HA2	1.85	0.41
1:K:281:ILE:HG23	1:K:286:LEU:HB2	2.03	0.41
1:I:8:TRP:CZ3	1:I:458:ILE:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:472:GLU:O	1:J:477:LYS:HE3	2.19	0.41
1:C:457:GLU:HA	1:C:499:TYR:O	2.21	0.41
1:F:120:PHE:O	1:F:124:ILE:HG12	2.20	0.41
1:I:37:LEU:HD22	1:I:374:GLU:OE2	2.20	0.41
1:I:448:ASP:HB3	1:I:493:MET:HE2	2.03	0.41
1:A:47:LYS:O	1:A:51:VAL:HG23	2.21	0.41
1:A:192:LEU:HD22	1:A:245:VAL:HG21	2.02	0.41
1:A:323:LYS:HB3	1:A:324:PRO:HD3	2.03	0.41
1:B:240:LEU:HD21	1:B:243:ILE:HD11	2.03	0.41
1:B:284:THR:HG23	1:B:286:LEU:HG	2.03	0.41
1:D:164:GLU:O	1:D:168:HIS:ND1	2.47	0.41
1:D:339:LYS:NZ	1:C:450:GLU:OE1	2.43	0.41
1:D:428:VAL:HB	1:D:431:LEU:HD12	2.03	0.41
1:F:455:LEU:O	1:F:463:ILE:HG13	2.20	0.41
1:E:32:ASP:OD1	1:E:33:GLN:N	2.53	0.41
1:E:84:PHE:CE2	1:E:86:TYR:HB3	2.56	0.41
1:L:352:ASP:O	1:L:353:SER:OG	2.29	0.41
1:G:79:ARG:HH22	1:G:99:THR:HG23	1.86	0.41
1:I:253:ILE:HD12	1:I:281:ILE:HG13	2.02	0.41
1:I:324:PRO:HG2	1:I:325:ILE:HG12	2.03	0.41
1:J:157:PHE:HZ	1:J:280:ILE:HD13	1.85	0.41
1:A:472:GLU:O	1:A:477:LYS:HE3	2.21	0.41
1:H:117:ILE:HD11	1:H:275:LEU:HD13	2.03	0.41
1:G:175:GLU:HG3	1:G:181:TYR:CE1	2.56	0.41
1:G:349:TYR:HA	1:G:436:GLU:OE2	2.20	0.41
1:J:174:GLN:OE1	1:J:257:TYR:OH	2.31	0.41
1:D:457:GLU:O	1:D:460:THR:OG1	2.27	0.40
1:F:140:VAL:HG22	1:F:279:ALA:HA	2.02	0.40
1:F:191:PHE:CD2	1:F:192:LEU:HG	2.56	0.40
1:E:71:ASP:HA	1:E:249:LEU:HD13	2.02	0.40
1:H:333:LYS:HA	1:H:333:LYS:HD3	1.83	0.40
1:H:410:ILE:HG22	1:H:411:TYR:N	2.35	0.40
1:I:191:PHE:HD2	1:I:192:LEU:HG	1.86	0.40
1:J:37:LEU:HD22	1:J:374:GLU:OE2	2.21	0.40
1:J:124:ILE:HG13	1:J:125:THR:HG23	2.03	0.40
1:A:190:ARG:HA	1:A:194:ASP:OD2	2.21	0.40
1:D:98:TYR:CE2	1:D:328:MET:HG3	2.56	0.40
1:I:189:LYS:NZ	1:J:461:GLU:O	2.40	0.40
1:I:323:LYS:HG3	1:I:324:PRO:HD3	2.03	0.40
1:J:88:VAL:HB	1:J:93:ASN:HD22	1.86	0.40
1:F:88:VAL:HG11	1:F:97:LEU:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:GLU:CD	1:C:2:SER:HB3	2.45	0.40
1:H:203:LEU:HD13	1:G:454:PHE:CD2	2.56	0.40
1:H:450:GLU:OE1	1:H:468:ASN:HA	2.22	0.40
1:G:338:GLY:HA3	1:G:372:ILE:HD13	2.03	0.40
1:C:36:ALA:O	1:C:334:LEU:N	2.47	0.40
1:C:117:ILE:HD13	1:C:139:PHE:HB2	2.03	0.40
1:K:473:PRO:HA	1:K:474:PRO:HD3	1.97	0.40
1:A:108:ASN:OD1	1:A:306:ASN:ND2	2.55	0.40
1:F:248:ILE:HD13	1:F:253:ILE:HG12	2.03	0.40
1:E:120:PHE:CZ	1:E:124:ILE:HD13	2.55	0.40
1:I:155:THR:HG21	1:I:276:ARG:CZ	2.50	0.40
1:B:208:SER:HB2	1:B:226:HIS:HB2	2.04	0.40
1:D:38:ASP:H	1:D:333:LYS:NZ	2.19	0.40
1:D:337:ILE:HD11	1:D:361:PHE:CZ	2.57	0.40
1:F:468:ASN:ND2	1:E:341:LYS:HD2	2.37	0.40
1:G:47:LYS:O	1:G:51:VAL:HG23	2.22	0.40
1:J:37:LEU:HB2	1:J:40:TRP:HD1	1.86	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	463/511 (91%)	437 (94%)	26 (6%)	0	100	100
1	B	457/511 (89%)	437 (96%)	20 (4%)	0	100	100
1	C	461/511 (90%)	439 (95%)	22 (5%)	0	100	100
1	D	454/511 (89%)	432 (95%)	22 (5%)	0	100	100
1	E	456/511 (89%)	438 (96%)	17 (4%)	1 (0%)	43	71
1	F	456/511 (89%)	438 (96%)	17 (4%)	1 (0%)	43	71
1	G	454/511 (89%)	440 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	456/511 (89%)	431 (94%)	25 (6%)	0	100	100
1	I	453/511 (89%)	442 (98%)	10 (2%)	1 (0%)	43	71
1	J	455/511 (89%)	435 (96%)	19 (4%)	1 (0%)	43	71
1	K	457/511 (89%)	433 (95%)	23 (5%)	1 (0%)	43	71
1	L	457/511 (89%)	435 (95%)	22 (5%)	0	100	100
All	All	5479/6132 (89%)	5237 (96%)	237 (4%)	5 (0%)	48	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	334	LEU
1	E	334	LEU
1	K	407	LEU
1	J	334	LEU
1	I	407	LEU

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	419/453 (92%)	419 (100%)	0	100	100
1	B	416/453 (92%)	414 (100%)	2 (0%)	81	81
1	C	419/453 (92%)	419 (100%)	0	100	100
1	D	413/453 (91%)	413 (100%)	0	100	100
1	E	415/453 (92%)	414 (100%)	1 (0%)	87	85
1	F	414/453 (91%)	414 (100%)	0	100	100
1	G	413/453 (91%)	413 (100%)	0	100	100
1	H	413/453 (91%)	411 (100%)	2 (0%)	81	81
1	I	412/453 (91%)	412 (100%)	0	100	100
1	J	414/453 (91%)	414 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	415/453 (92%)	415 (100%)	0	100	100
1	L	416/453 (92%)	416 (100%)	0	100	100
All	All	4979/5436 (92%)	4974 (100%)	5 (0%)	88	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	325	ILE
1	B	407	LEU
1	E	281	ILE
1	H	50	VAL
1	H	51	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	B	182	ASN
1	B	211	GLN
1	D	442	GLN
1	F	174	GLN
1	F	316	HIS
1	E	183	ASN
1	E	282	GLN
1	L	75	ASN
1	L	149	ASN
1	L	226	HIS
1	H	55	ASN
1	H	149	ASN
1	H	206	GLN
1	H	306	ASN
1	H	316	HIS
1	G	55	ASN
1	G	105	GLN
1	G	149	ASN
1	G	206	GLN
1	C	149	ASN
1	C	183	ASN
1	I	149	ASN
1	I	183	ASN

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Mol	Chain	Res	Type
1	I	316	HIS
1	J	13	HIS
1	J	55	ASN
1	J	206	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	471/511 (92%)	0.23	11 (2%)	61	46	39, 69, 132, 165	0
1	B	465/511 (90%)	0.29	11 (2%)	59	45	42, 77, 142, 179	0
1	C	469/511 (91%)	0.34	15 (3%)	50	37	43, 77, 140, 171	0
1	D	462/511 (90%)	0.29	19 (4%)	41	29	39, 71, 134, 170	0
1	E	464/511 (90%)	0.37	9 (1%)	66	51	48, 80, 142, 167	0
1	F	464/511 (90%)	0.29	9 (1%)	66	51	43, 77, 136, 161	0
1	G	462/511 (90%)	0.72	34 (7%)	20	17	55, 103, 157, 175	0
1	H	464/511 (90%)	0.41	14 (3%)	52	39	42, 79, 140, 174	0
1	I	461/511 (90%)	0.23	14 (3%)	52	39	38, 70, 131, 175	0
1	J	463/511 (90%)	0.25	13 (2%)	55	41	37, 69, 133, 165	0
1	K	465/511 (90%)	0.52	20 (4%)	40	29	52, 87, 154, 191	0
1	L	465/511 (90%)	0.74	37 (7%)	18	16	54, 101, 149, 172	0
All	All	5575/6132 (90%)	0.39	206 (3%)	45	32	37, 79, 143, 191	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	342	THR	4.6
1	D	329	ILE	4.2
1	H	53	ILE	4.2
1	G	439	ASP	4.0
1	A	18	ALA	4.0
1	D	330	SER	3.9
1	G	109	MET	3.7
1	C	408	ASP	3.6
1	A	366	VAL	3.5
1	E	330	SER	3.5
1	D	328	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	335	PHE	3.4
1	A	135	ALA	3.4
1	K	120	PHE	3.3
1	I	342	THR	3.3
1	J	133	ALA	3.3
1	L	308	GLY	3.3
1	L	411	TYR	3.2
1	C	330	SER	3.2
1	F	329	ILE	3.2
1	B	328	MET	3.2
1	K	308	GLY	3.2
1	J	292	GLY	3.2
1	L	1	MET	3.2
1	H	18	ALA	3.2
1	C	308	GLY	3.2
1	H	306	ASN	3.2
1	L	470	TYR	3.2
1	H	366	VAL	3.1
1	K	343	LYS	3.1
1	A	329	ILE	3.1
1	L	443	SER	3.1
1	G	403	GLU	3.1
1	C	53	ILE	3.0
1	B	98	TYR	3.0
1	K	342	THR	3.0
1	L	366	VAL	3.0
1	G	394	LEU	2.9
1	K	132	ALA	2.9
1	L	145	ASN	2.9
1	F	404	GLU	2.9
1	J	134	VAL	2.9
1	E	364	ASP	2.8
1	J	135	ALA	2.8
1	A	34	LEU	2.8
1	L	334	LEU	2.8
1	C	34	LEU	2.8
1	H	328	MET	2.8
1	H	329	ILE	2.8
1	K	116	CYS	2.8
1	H	2	SER	2.8
1	K	265	SER	2.8
1	L	388	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	56	CYS	2.7
1	F	361	PHE	2.7
1	L	338	GLY	2.7
1	B	117	ILE	2.7
1	H	335	PHE	2.7
1	G	328	MET	2.7
1	C	329	ILE	2.6
1	G	307	TYR	2.6
1	E	55	ASN	2.6
1	L	459	GLU	2.6
1	J	56	CYS	2.6
1	E	367	VAL	2.6
1	L	367	VAL	2.6
1	B	131	PRO	2.6
1	I	410	ILE	2.6
1	L	91	LEU	2.6
1	G	91	LEU	2.6
1	G	337	ILE	2.5
1	H	307	TYR	2.5
1	J	97	LEU	2.5
1	C	56	CYS	2.5
1	I	129	TYR	2.5
1	K	341	LYS	2.5
1	K	330	SER	2.5
1	I	124	ILE	2.5
1	L	488	GLY	2.5
1	G	336	VAL	2.5
1	C	305	ALA	2.5
1	K	133	ALA	2.5
1	L	222	GLU	2.5
1	D	341	LYS	2.5
1	I	341	LYS	2.4
1	J	364	ASP	2.4
1	L	37	LEU	2.4
1	J	411	TYR	2.4
1	D	367	VAL	2.4
1	L	2	SER	2.4
1	K	126	SER	2.4
1	B	341	LYS	2.4
1	C	461	GLU	2.4
1	G	459	GLU	2.4
1	G	56	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	412	HIS	2.4
1	L	469	PHE	2.4
1	K	144	VAL	2.4
1	F	308	GLY	2.3
1	I	461	GLU	2.3
1	G	367	VAL	2.3
1	J	330	SER	2.3
1	E	132	ALA	2.3
1	L	221	GLY	2.3
1	B	132	ALA	2.3
1	K	135	ALA	2.3
1	E	109	MET	2.3
1	H	334	LEU	2.3
1	D	287	GLN	2.3
1	L	339	LYS	2.3
1	G	271	LYS	2.3
1	G	329	ILE	2.3
1	D	133	ALA	2.3
1	G	383	ALA	2.3
1	L	126	SER	2.3
1	B	364	ASP	2.3
1	G	442	GLN	2.3
1	I	339	LYS	2.3
1	A	461	GLU	2.3
1	B	367	VAL	2.3
1	B	461	GLU	2.3
1	H	367	VAL	2.3
1	E	329	ILE	2.3
1	J	329	ILE	2.3
1	L	383	ALA	2.3
1	A	339	LYS	2.3
1	D	339	LYS	2.3
1	F	364	ASP	2.3
1	K	461	GLU	2.2
1	D	131	PRO	2.2
1	D	132	ALA	2.2
1	C	306	ASN	2.2
1	G	342	THR	2.2
1	G	137	SER	2.2
1	G	390	SER	2.2
1	L	404	GLU	2.2
1	G	352	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	437	LEU	2.2
1	L	346	LYS	2.2
1	G	393	GLU	2.2
1	J	306	ASN	2.2
1	F	407	LEU	2.2
1	G	132	ALA	2.2
1	J	16	PRO	2.2
1	I	323	LYS	2.2
1	D	168	HIS	2.2
1	D	366	VAL	2.2
1	L	349	TYR	2.2
1	L	137	SER	2.2
1	G	386	SER	2.2
1	H	34	LEU	2.2
1	A	328	MET	2.2
1	D	109	MET	2.2
1	I	503	MET	2.2
1	D	343	LYS	2.2
1	D	56	CYS	2.2
1	C	267	TRP	2.2
1	G	344	VAL	2.1
1	F	307	TYR	2.1
1	G	402	TYR	2.1
1	G	411	TYR	2.1
1	L	441	MET	2.1
1	D	54	GLU	2.1
1	L	409	THR	2.1
1	C	307	TYR	2.1
1	F	17	ALA	2.1
1	I	120	PHE	2.1
1	A	352	ASP	2.1
1	E	342	THR	2.1
1	L	57	THR	2.1
1	G	57	THR	2.1
1	I	131	PRO	2.1
1	G	311	VAL	2.1
1	G	339	LYS	2.1
1	L	337	ILE	2.1
1	A	307	TYR	2.1
1	L	307	TYR	2.1
1	L	387	ALA	2.1
1	E	106	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	361	PHE	2.1
1	C	500	SER	2.1
1	G	410	ILE	2.1
1	G	438	LEU	2.1
1	K	307	TYR	2.1
1	L	361	PHE	2.1
1	L	461	GLU	2.1
1	K	366	VAL	2.0
1	D	53	ILE	2.0
1	H	337	ILE	2.0
1	I	107	LEU	2.0
1	B	148	MET	2.0
1	L	309	ALA	2.0
1	K	74	CYS	2.0
1	I	116	CYS	2.0
1	K	221	GLY	2.0
1	C	459	GLU	2.0
1	L	344	VAL	2.0
1	K	134	VAL	2.0
1	A	126	SER	2.0
1	H	108	ASN	2.0
1	B	408	ASP	2.0
1	K	3	ASP	2.0
1	D	130	CYS	2.0
1	L	134	VAL	2.0
1	G	366	VAL	2.0
1	C	175	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.