



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:07 PM UTC

PDB ID : 5AA3 / pdb_00005aa3
Title : Crystal structure of MltF from *Pseudomonas aeruginosa* in the presence of tetrasaccharide and tetrapeptide
Authors : Dominguez-Gil, T.; Acebron, I.; Hermoso, J.A.
Deposited on : 2015-07-23
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

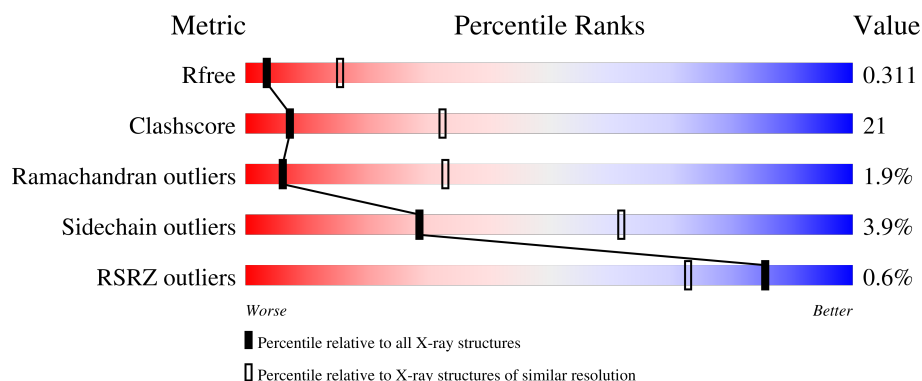
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	499	
1	B	499	
1	C	499	
1	D	499	
1	E	499	

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Mol	Chain	Length	Quality of chain
1	F	499	
1	G	499	
1	H	499	
1	I	499	
1	J	499	
1	K	499	
1	L	499	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLU	A	501	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40234 atoms, of which 8 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 MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	2	0
			3361	2121	598	633	9			
1	B	417	Total	C	N	O	S	0	1	0
			3351	2112	597	633	9			
1	C	418	Total	C	N	O	S	0	2	0
			3370	2126	599	636	9			
1	D	415	Total	C	N	O	S	0	1	0
			3333	2102	594	628	9			
1	E	418	Total	C	N	O	S	0	1	0
			3358	2117	599	633	9			
1	F	416	Total	C	N	O	S	0	2	0
			3351	2112	598	632	9			
1	G	416	Total	C	N	O	S	0	1	0
			3342	2107	596	630	9			
1	H	415	Total	C	N	O	S	0	1	0
			3333	2102	594	628	9			
1	I	418	Total	C	N	O	S	0	1	0
			3360	2118	599	634	9			
1	J	416	Total	C	N	O	S	0	1	0
			3342	2107	596	630	9			
1	K	417	Total	C	N	O	S	0	1	0
			3349	2112	597	631	9			
1	L	419	Total	C	N	O	S	0	1	0
			3366	2122	600	634	10			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP Q9HXN1
A	-7	ALA	-	expression tag	UNP Q9HXN1
A	-6	PRO	-	expression tag	UNP Q9HXN1
A	-5	SER	-	expression tag	UNP Q9HXN1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ARG	-	expression tag	UNP Q9HYN1
A	-3	LEU	-	expression tag	UNP Q9HYN1
A	-2	CYS	-	expression tag	UNP Q9HYN1
A	-1	VAL	-	expression tag	UNP Q9HYN1
A	0	TYR	-	expression tag	UNP Q9HYN1
A	1	CYS	-	expression tag	UNP Q9HYN1
A	2	ALA	-	expression tag	UNP Q9HYN1
A	3	ASP	-	expression tag	UNP Q9HYN1
A	4	VAL	-	expression tag	UNP Q9HYN1
A	5	CYS	-	expression tag	UNP Q9HYN1
A	6	PRO	-	expression tag	UNP Q9HYN1
A	7	ASP	-	expression tag	UNP Q9HYN1
A	302	LYS	LEU	conflict	UNP Q9HYN1
B	-8	MET	-	expression tag	UNP Q9HYN1
B	-7	ALA	-	expression tag	UNP Q9HYN1
B	-6	PRO	-	expression tag	UNP Q9HYN1
B	-5	SER	-	expression tag	UNP Q9HYN1
B	-4	ARG	-	expression tag	UNP Q9HYN1
B	-3	LEU	-	expression tag	UNP Q9HYN1
B	-2	CYS	-	expression tag	UNP Q9HYN1
B	-1	VAL	-	expression tag	UNP Q9HYN1
B	0	TYR	-	expression tag	UNP Q9HYN1
B	1	CYS	-	expression tag	UNP Q9HYN1
B	2	ALA	-	expression tag	UNP Q9HYN1
B	3	ASP	-	expression tag	UNP Q9HYN1
B	4	VAL	-	expression tag	UNP Q9HYN1
B	5	CYS	-	expression tag	UNP Q9HYN1
B	6	PRO	-	expression tag	UNP Q9HYN1
B	7	ASP	-	expression tag	UNP Q9HYN1
B	302	LYS	LEU	conflict	UNP Q9HYN1
C	-8	MET	-	expression tag	UNP Q9HYN1
C	-7	ALA	-	expression tag	UNP Q9HYN1
C	-6	PRO	-	expression tag	UNP Q9HYN1
C	-5	SER	-	expression tag	UNP Q9HYN1
C	-4	ARG	-	expression tag	UNP Q9HYN1
C	-3	LEU	-	expression tag	UNP Q9HYN1
C	-2	CYS	-	expression tag	UNP Q9HYN1
C	-1	VAL	-	expression tag	UNP Q9HYN1
C	0	TYR	-	expression tag	UNP Q9HYN1
C	1	CYS	-	expression tag	UNP Q9HYN1
C	2	ALA	-	expression tag	UNP Q9HYN1
C	3	ASP	-	expression tag	UNP Q9HYN1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	VAL	-	expression tag	UNP Q9HXN1
C	5	CYS	-	expression tag	UNP Q9HXN1
C	6	PRO	-	expression tag	UNP Q9HXN1
C	7	ASP	-	expression tag	UNP Q9HXN1
C	302	LYS	LEU	conflict	UNP Q9HXN1
D	-8	MET	-	expression tag	UNP Q9HXN1
D	-7	ALA	-	expression tag	UNP Q9HXN1
D	-6	PRO	-	expression tag	UNP Q9HXN1
D	-5	SER	-	expression tag	UNP Q9HXN1
D	-4	ARG	-	expression tag	UNP Q9HXN1
D	-3	LEU	-	expression tag	UNP Q9HXN1
D	-2	CYS	-	expression tag	UNP Q9HXN1
D	-1	VAL	-	expression tag	UNP Q9HXN1
D	0	TYR	-	expression tag	UNP Q9HXN1
D	1	CYS	-	expression tag	UNP Q9HXN1
D	2	ALA	-	expression tag	UNP Q9HXN1
D	3	ASP	-	expression tag	UNP Q9HXN1
D	4	VAL	-	expression tag	UNP Q9HXN1
D	5	CYS	-	expression tag	UNP Q9HXN1
D	6	PRO	-	expression tag	UNP Q9HXN1
D	7	ASP	-	expression tag	UNP Q9HXN1
D	302	LYS	LEU	conflict	UNP Q9HXN1
E	-8	MET	-	expression tag	UNP Q9HXN1
E	-7	ALA	-	expression tag	UNP Q9HXN1
E	-6	PRO	-	expression tag	UNP Q9HXN1
E	-5	SER	-	expression tag	UNP Q9HXN1
E	-4	ARG	-	expression tag	UNP Q9HXN1
E	-3	LEU	-	expression tag	UNP Q9HXN1
E	-2	CYS	-	expression tag	UNP Q9HXN1
E	-1	VAL	-	expression tag	UNP Q9HXN1
E	0	TYR	-	expression tag	UNP Q9HXN1
E	1	CYS	-	expression tag	UNP Q9HXN1
E	2	ALA	-	expression tag	UNP Q9HXN1
E	3	ASP	-	expression tag	UNP Q9HXN1
E	4	VAL	-	expression tag	UNP Q9HXN1
E	5	CYS	-	expression tag	UNP Q9HXN1
E	6	PRO	-	expression tag	UNP Q9HXN1
E	7	ASP	-	expression tag	UNP Q9HXN1
E	302	LYS	LEU	conflict	UNP Q9HXN1
F	-8	MET	-	expression tag	UNP Q9HXN1
F	-7	ALA	-	expression tag	UNP Q9HXN1
F	-6	PRO	-	expression tag	UNP Q9HXN1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	SER	-	expression tag	UNP Q9HXN1
F	-4	ARG	-	expression tag	UNP Q9HXN1
F	-3	LEU	-	expression tag	UNP Q9HXN1
F	-2	CYS	-	expression tag	UNP Q9HXN1
F	-1	VAL	-	expression tag	UNP Q9HXN1
F	0	TYR	-	expression tag	UNP Q9HXN1
F	1	CYS	-	expression tag	UNP Q9HXN1
F	2	ALA	-	expression tag	UNP Q9HXN1
F	3	ASP	-	expression tag	UNP Q9HXN1
F	4	VAL	-	expression tag	UNP Q9HXN1
F	5	CYS	-	expression tag	UNP Q9HXN1
F	6	PRO	-	expression tag	UNP Q9HXN1
F	7	ASP	-	expression tag	UNP Q9HXN1
F	302	LYS	LEU	conflict	UNP Q9HXN1
G	-8	MET	-	expression tag	UNP Q9HXN1
G	-7	ALA	-	expression tag	UNP Q9HXN1
G	-6	PRO	-	expression tag	UNP Q9HXN1
G	-5	SER	-	expression tag	UNP Q9HXN1
G	-4	ARG	-	expression tag	UNP Q9HXN1
G	-3	LEU	-	expression tag	UNP Q9HXN1
G	-2	CYS	-	expression tag	UNP Q9HXN1
G	-1	VAL	-	expression tag	UNP Q9HXN1
G	0	TYR	-	expression tag	UNP Q9HXN1
G	1	CYS	-	expression tag	UNP Q9HXN1
G	2	ALA	-	expression tag	UNP Q9HXN1
G	3	ASP	-	expression tag	UNP Q9HXN1
G	4	VAL	-	expression tag	UNP Q9HXN1
G	5	CYS	-	expression tag	UNP Q9HXN1
G	6	PRO	-	expression tag	UNP Q9HXN1
G	7	ASP	-	expression tag	UNP Q9HXN1
G	302	LYS	LEU	conflict	UNP Q9HXN1
H	-8	MET	-	expression tag	UNP Q9HXN1
H	-7	ALA	-	expression tag	UNP Q9HXN1
H	-6	PRO	-	expression tag	UNP Q9HXN1
H	-5	SER	-	expression tag	UNP Q9HXN1
H	-4	ARG	-	expression tag	UNP Q9HXN1
H	-3	LEU	-	expression tag	UNP Q9HXN1
H	-2	CYS	-	expression tag	UNP Q9HXN1
H	-1	VAL	-	expression tag	UNP Q9HXN1
H	0	TYR	-	expression tag	UNP Q9HXN1
H	1	CYS	-	expression tag	UNP Q9HXN1
H	2	ALA	-	expression tag	UNP Q9HXN1

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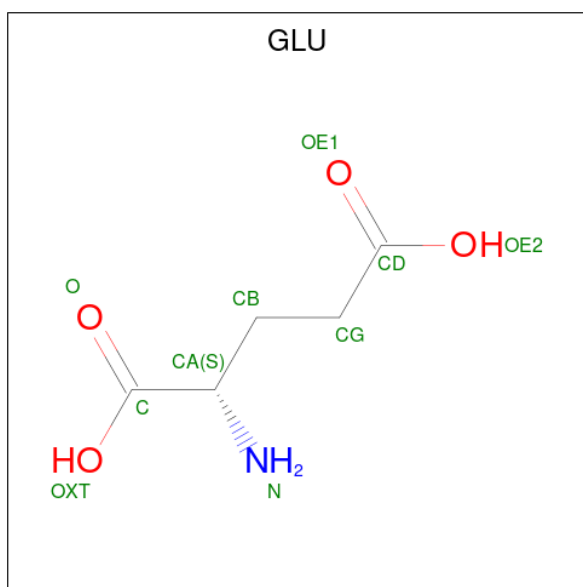
Chain	Residue	Modelled	Actual	Comment	Reference
H	3	ASP	-	expression tag	UNP Q9HYN1
H	4	VAL	-	expression tag	UNP Q9HYN1
H	5	CYS	-	expression tag	UNP Q9HYN1
H	6	PRO	-	expression tag	UNP Q9HYN1
H	7	ASP	-	expression tag	UNP Q9HYN1
H	302	LYS	LEU	conflict	UNP Q9HYN1
I	-8	MET	-	expression tag	UNP Q9HYN1
I	-7	ALA	-	expression tag	UNP Q9HYN1
I	-6	PRO	-	expression tag	UNP Q9HYN1
I	-5	SER	-	expression tag	UNP Q9HYN1
I	-4	ARG	-	expression tag	UNP Q9HYN1
I	-3	LEU	-	expression tag	UNP Q9HYN1
I	-2	CYS	-	expression tag	UNP Q9HYN1
I	-1	VAL	-	expression tag	UNP Q9HYN1
I	0	TYR	-	expression tag	UNP Q9HYN1
I	1	CYS	-	expression tag	UNP Q9HYN1
I	2	ALA	-	expression tag	UNP Q9HYN1
I	3	ASP	-	expression tag	UNP Q9HYN1
I	4	VAL	-	expression tag	UNP Q9HYN1
I	5	CYS	-	expression tag	UNP Q9HYN1
I	6	PRO	-	expression tag	UNP Q9HYN1
I	7	ASP	-	expression tag	UNP Q9HYN1
I	302	LYS	LEU	conflict	UNP Q9HYN1
J	-8	MET	-	expression tag	UNP Q9HYN1
J	-7	ALA	-	expression tag	UNP Q9HYN1
J	-6	PRO	-	expression tag	UNP Q9HYN1
J	-5	SER	-	expression tag	UNP Q9HYN1
J	-4	ARG	-	expression tag	UNP Q9HYN1
J	-3	LEU	-	expression tag	UNP Q9HYN1
J	-2	CYS	-	expression tag	UNP Q9HYN1
J	-1	VAL	-	expression tag	UNP Q9HYN1
J	0	TYR	-	expression tag	UNP Q9HYN1
J	1	CYS	-	expression tag	UNP Q9HYN1
J	2	ALA	-	expression tag	UNP Q9HYN1
J	3	ASP	-	expression tag	UNP Q9HYN1
J	4	VAL	-	expression tag	UNP Q9HYN1
J	5	CYS	-	expression tag	UNP Q9HYN1
J	6	PRO	-	expression tag	UNP Q9HYN1
J	7	ASP	-	expression tag	UNP Q9HYN1
J	302	LYS	LEU	conflict	UNP Q9HYN1
K	-8	MET	-	expression tag	UNP Q9HYN1
K	-7	ALA	-	expression tag	UNP Q9HYN1

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-6	PRO	-	expression tag	UNP Q9HYN1
K	-5	SER	-	expression tag	UNP Q9HYN1
K	-4	ARG	-	expression tag	UNP Q9HYN1
K	-3	LEU	-	expression tag	UNP Q9HYN1
K	-2	CYS	-	expression tag	UNP Q9HYN1
K	-1	VAL	-	expression tag	UNP Q9HYN1
K	0	TYR	-	expression tag	UNP Q9HYN1
K	1	CYS	-	expression tag	UNP Q9HYN1
K	2	ALA	-	expression tag	UNP Q9HYN1
K	3	ASP	-	expression tag	UNP Q9HYN1
K	4	VAL	-	expression tag	UNP Q9HYN1
K	5	CYS	-	expression tag	UNP Q9HYN1
K	6	PRO	-	expression tag	UNP Q9HYN1
K	7	ASP	-	expression tag	UNP Q9HYN1
K	302	LYS	LEU	conflict	UNP Q9HYN1
L	-8	MET	-	expression tag	UNP Q9HYN1
L	-7	ALA	-	expression tag	UNP Q9HYN1
L	-6	PRO	-	expression tag	UNP Q9HYN1
L	-5	SER	-	expression tag	UNP Q9HYN1
L	-4	ARG	-	expression tag	UNP Q9HYN1
L	-3	LEU	-	expression tag	UNP Q9HYN1
L	-2	CYS	-	expression tag	UNP Q9HYN1
L	-1	VAL	-	expression tag	UNP Q9HYN1
L	0	TYR	-	expression tag	UNP Q9HYN1
L	1	CYS	-	expression tag	UNP Q9HYN1
L	2	ALA	-	expression tag	UNP Q9HYN1
L	3	ASP	-	expression tag	UNP Q9HYN1
L	4	VAL	-	expression tag	UNP Q9HYN1
L	5	CYS	-	expression tag	UNP Q9HYN1
L	6	PRO	-	expression tag	UNP Q9HYN1
L	7	ASP	-	expression tag	UNP Q9HYN1
L	302	LYS	LEU	conflict	UNP Q9HYN1

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).

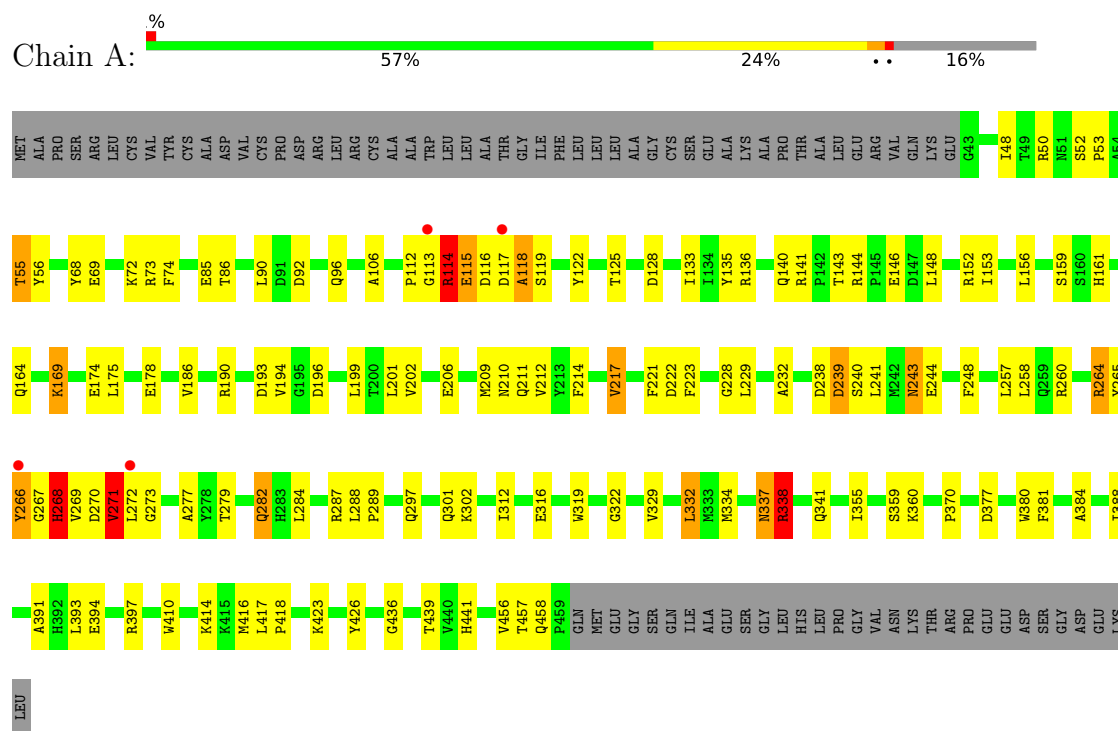


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	18	5	8	1	4	0	0

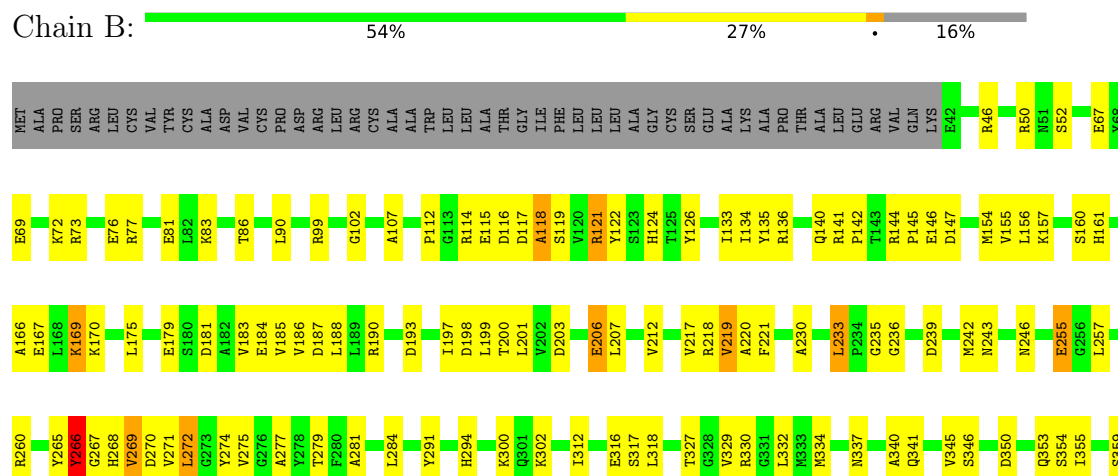
3 Residue-property plots [i](#)

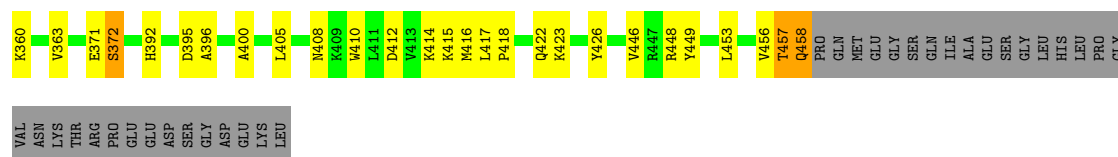
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



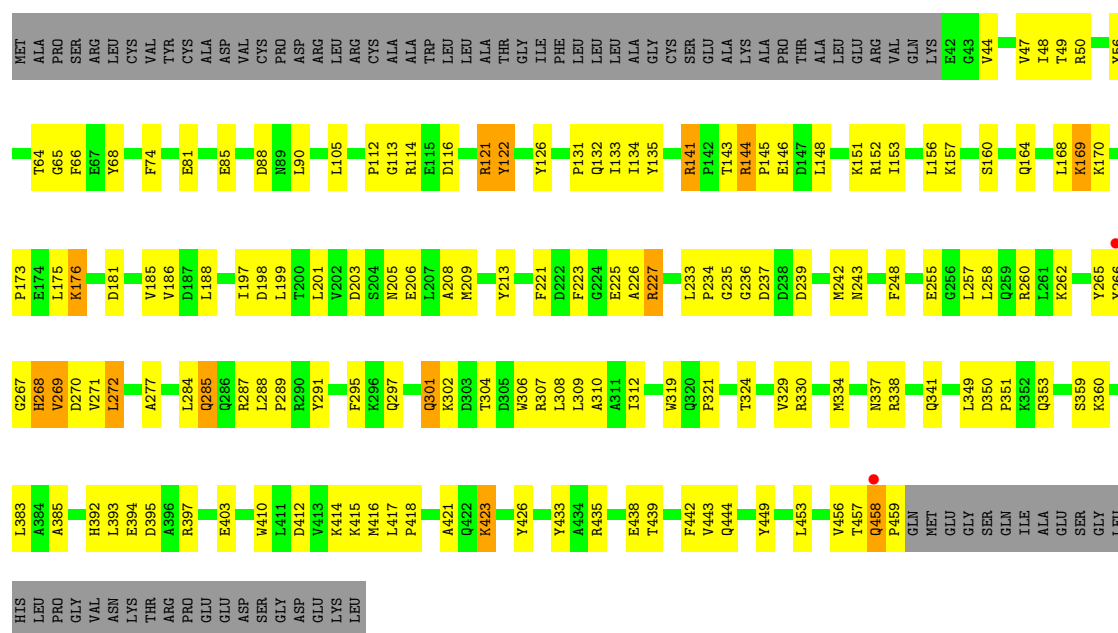
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F





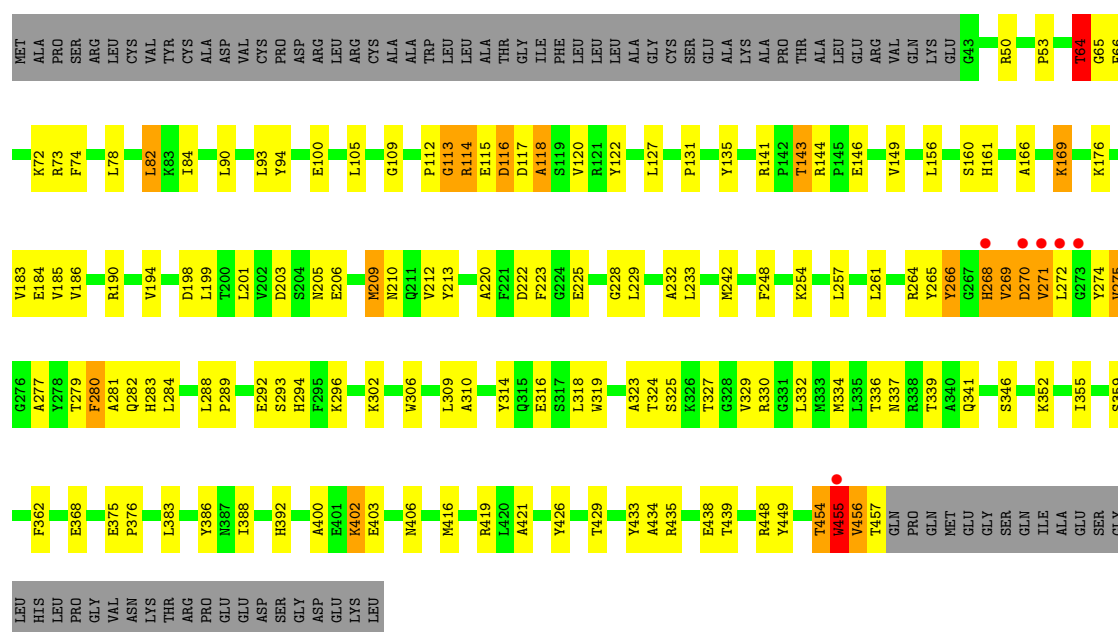
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain C: 53% 28% 16%

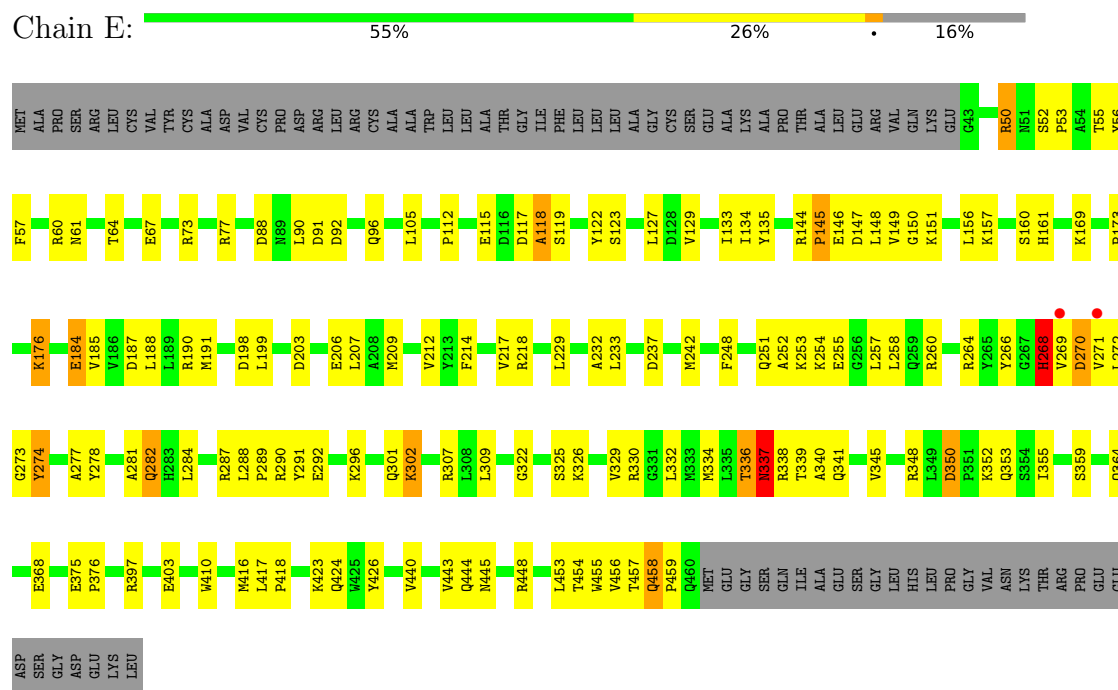


• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

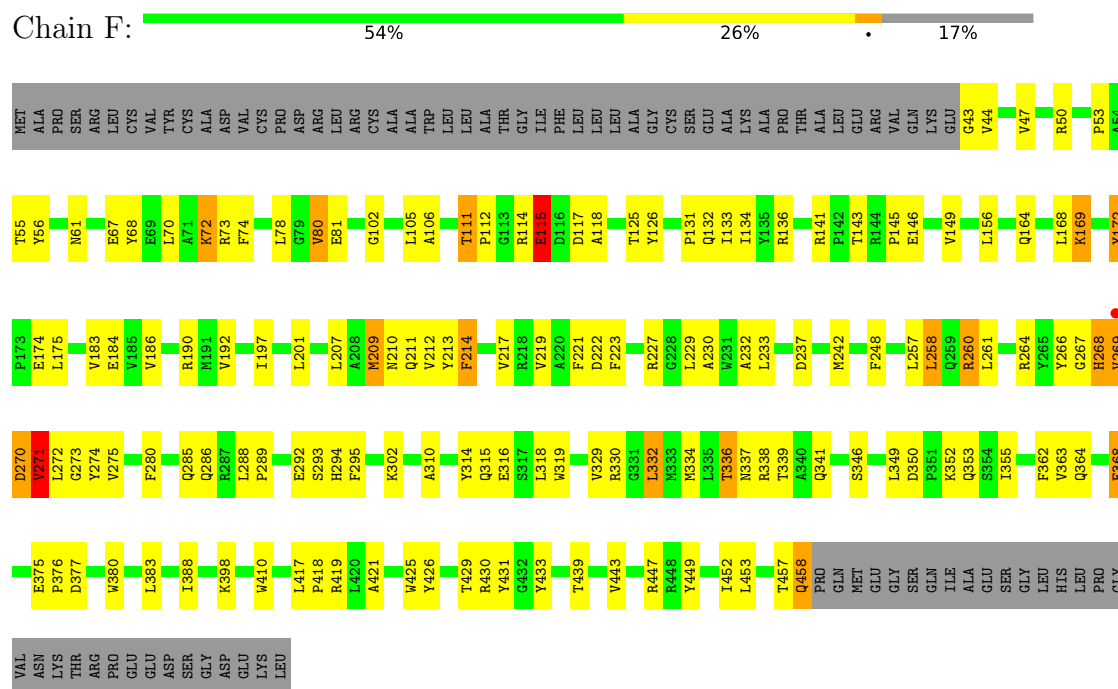
Chain D: 54% 25% 17%



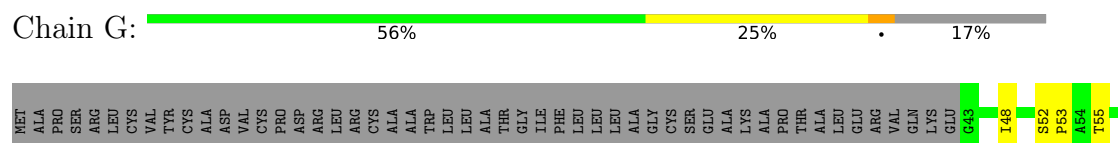
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

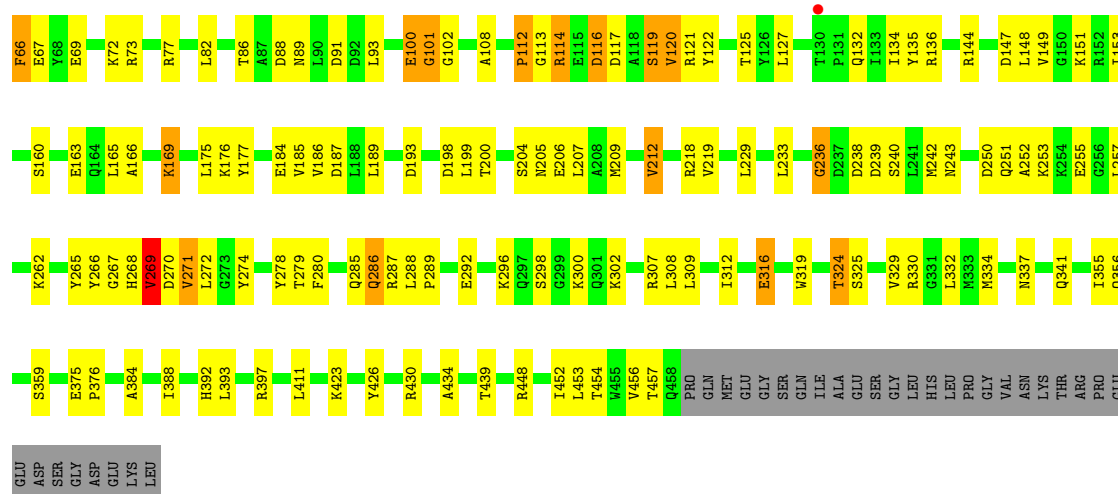


• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



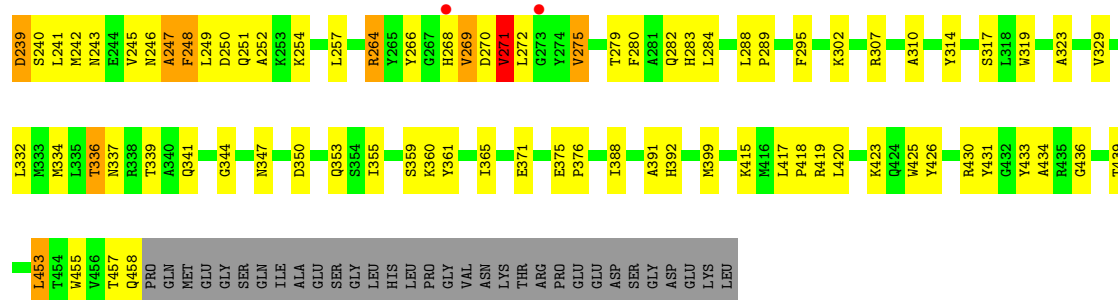


• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



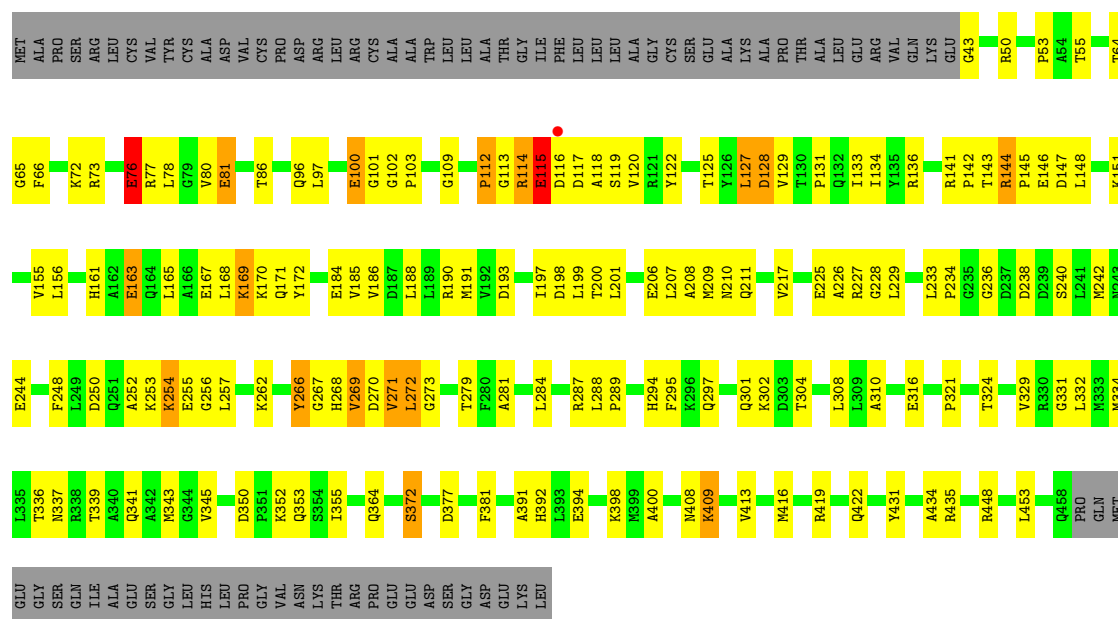
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F





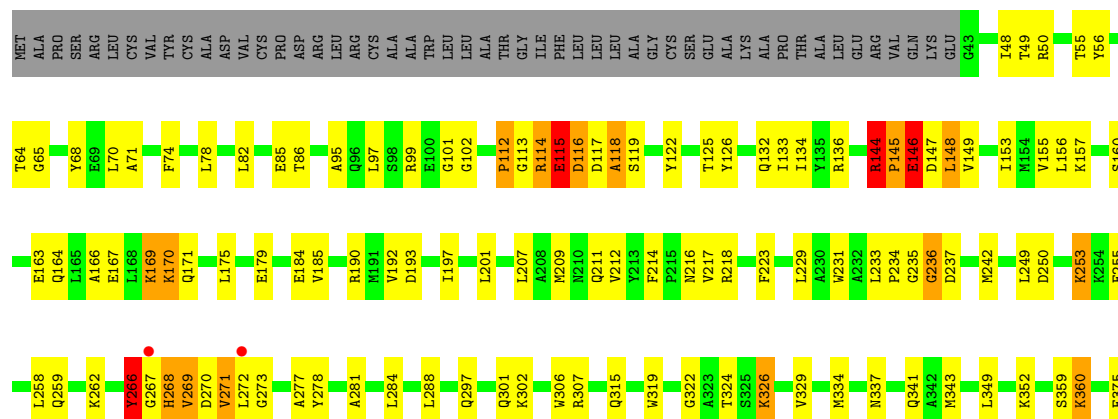
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain J: 52% 28% 17%



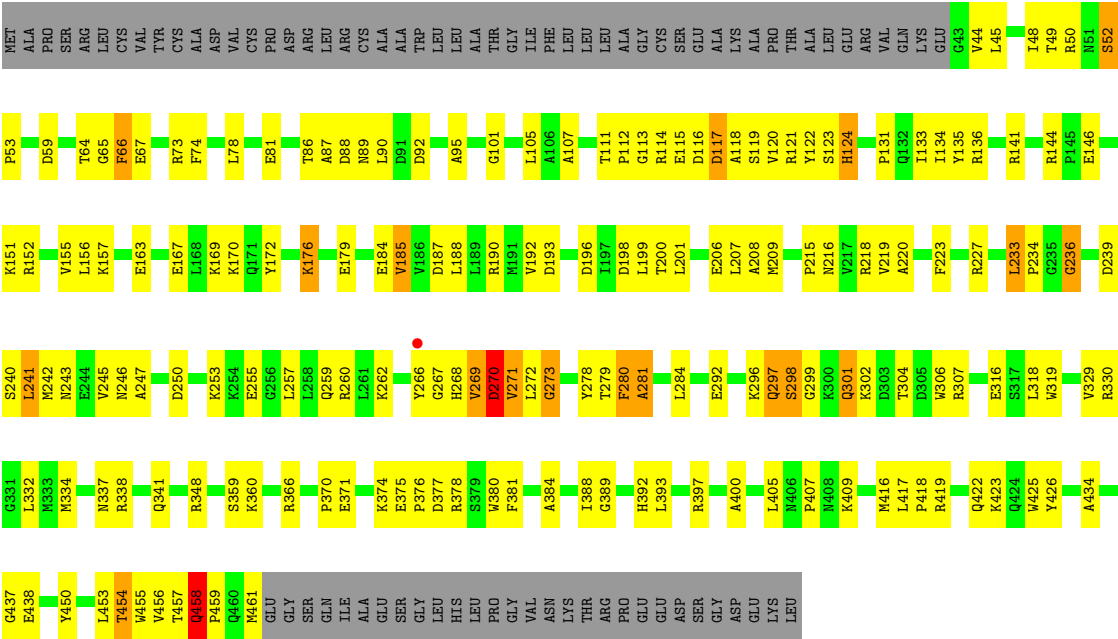
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain K: 55% 24% 16%





• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	150.60Å 136.38Å 195.39Å 90.00° 111.38° 90.00°	Depositor
Resolution (Å)	14.99 – 3.20 14.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (14.99-3.20) 98.1 (14.99-3.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.240 , 0.305 0.252 , 0.311	Depositor DCC
R_{free} test set	6091 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	40234	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 86.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2751e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.86	1/3433 (0.0%)	1.18	10/4642 (0.2%)
1	B	0.88	2/3421 (0.1%)	1.22	17/4624 (0.4%)
1	C	0.91	1/3442 (0.0%)	1.16	12/4654 (0.3%)
1	D	0.85	0/3403	1.17	10/4600 (0.2%)
1	E	0.83	0/3429	1.17	14/4636 (0.3%)
1	F	0.79	0/3421	1.13	10/4624 (0.2%)
1	G	0.79	0/3412	1.07	4/4612 (0.1%)
1	H	0.81	1/3403 (0.0%)	1.15	6/4600 (0.1%)
1	I	0.84	0/3430	1.17	12/4635 (0.3%)
1	J	0.71	1/3412 (0.0%)	1.09	6/4612 (0.1%)
1	K	0.75	0/3420	1.12	13/4624 (0.3%)
1	L	0.73	0/3437	1.11	11/4646 (0.2%)
All	All	0.81	6/41063 (0.0%)	1.15	125/55509 (0.2%)

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	A	0	1
1	D	0	1
1	I	0	2
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	116	ASP	CA-C	6.65	1.55	1.52
1	A	322	GLY	C-O	-5.78	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	443	VAL	CA-CB	-5.26	1.48	1.54
1	B	446	VAL	CA-C	-5.20	1.46	1.52
1	C	385	ALA	CA-CB	-5.18	1.45	1.53
1	B	327	THR	CA-CB	-5.09	1.44	1.53

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	148	LEU	N-CA-C	-11.31	99.51	113.20
1	H	114	ARG	N-CA-C	10.38	124.06	111.40
1	I	198	ASP	N-CA-C	10.21	132.54	110.80
1	K	277	ALA	N-CA-C	-9.04	101.33	111.82
1	A	277	ALA	N-CA-C	-8.82	101.58	111.82
1	I	199	LEU	N-CA-C	-8.78	95.64	109.50
1	E	277	ALA	N-CA-C	-8.33	102.28	111.36
1	B	277	ALA	N-CA-C	-8.20	102.31	111.82
1	J	102	GLY	CA-C-N	8.05	127.98	119.85
1	J	102	GLY	C-N-CA	8.05	127.98	119.85
1	K	255	GLU	N-CA-C	-8.00	103.10	113.17
1	H	116	ASP	N-CA-C	-7.69	103.72	113.72
1	E	118	ALA	N-CA-C	-7.58	104.53	114.31
1	B	270	ASP	N-CA-C	7.43	120.33	111.33
1	C	308	LEU	N-CA-C	-7.40	103.29	111.36
1	H	52	SER	N-CA-C	7.21	114.70	108.22
1	F	111	THR	CA-C-N	-7.19	112.91	120.03
1	F	111	THR	C-N-CA	-7.19	112.91	120.03
1	E	458	GLN	CA-C-N	-7.19	110.86	119.84
1	E	458	GLN	C-N-CA	-7.19	110.86	119.84
1	I	214	PHE	CA-C-N	7.14	127.14	119.28
1	I	214	PHE	C-N-CA	7.14	127.14	119.28
1	I	52	SER	N-CA-C	7.13	114.63	108.22
1	J	76	GLU	N-CA-C	-7.08	103.64	111.36
1	I	119	SER	N-CA-C	-6.97	104.66	113.72
1	K	115	GLU	CA-C-N	6.90	134.12	121.70
1	K	115	GLU	C-N-CA	6.90	134.12	121.70
1	C	277	ALA	N-CA-C	-6.86	103.87	111.82
1	I	283	HIS	N-CA-C	6.83	119.57	111.71
1	E	268	HIS	N-CA-C	6.69	120.43	109.72
1	H	264	ARG	N-CA-C	6.60	119.03	111.11
1	B	269	VAL	N-CA-C	6.49	117.93	108.58
1	B	266	TYR	CA-CB-CG	6.48	125.56	113.90
1	A	337	ASN	N-CA-C	6.45	118.85	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	209	MET	N-CA-C	6.43	118.37	111.36
1	G	144	ARG	CA-C-N	6.41	127.85	119.84
1	G	144	ARG	C-N-CA	6.41	127.85	119.84
1	F	273	GLY	N-CA-C	-6.34	103.42	112.81
1	L	299	GLY	N-CA-C	-6.30	105.01	112.64
1	D	392	HIS	N-CA-C	6.30	118.15	111.28
1	K	102	GLY	CA-C-N	6.25	126.16	119.85
1	K	102	GLY	C-N-CA	6.25	126.16	119.85
1	D	64	THR	CB-CA-C	-6.17	99.19	111.91
1	H	198	ASP	N-CA-C	6.10	117.73	111.14
1	B	99	ARG	N-CA-C	-6.08	102.33	110.55
1	E	337	ASN	N-CA-C	6.03	118.35	111.11
1	F	214	PHE	CA-C-N	5.99	125.87	119.28
1	F	214	PHE	C-N-CA	5.99	125.87	119.28
1	E	271	VAL	N-CA-C	-5.98	106.67	112.29
1	K	214	PHE	CA-C-N	5.88	125.75	119.28
1	K	214	PHE	C-N-CA	5.88	125.75	119.28
1	B	446	VAL	N-CA-C	-5.83	104.67	110.62
1	I	275	VAL	N-CA-C	-5.80	103.72	110.05
1	A	206	GLU	N-CA-C	-5.76	105.09	111.36
1	B	141	ARG	CA-C-N	-5.75	114.01	119.76
1	B	141	ARG	C-N-CA	-5.75	114.01	119.76
1	B	198	ASP	N-CA-C	5.68	117.15	111.07
1	C	198	ASP	N-CA-C	5.67	117.33	111.03
1	B	255	GLU	N-CA-C	-5.67	106.03	113.17
1	L	124	HIS	N-CA-C	-5.64	103.09	110.53
1	A	338	ARG	N-CA-C	-5.62	105.16	111.28
1	C	255	GLU	N-CA-C	-5.59	106.05	112.92
1	L	419	ARG	N-CA-C	-5.58	105.97	112.89
1	B	354	SER	N-CA-C	-5.57	105.11	111.07
1	D	78	LEU	N-CA-C	-5.56	105.86	113.30
1	J	144	ARG	CA-C-N	5.55	126.78	119.84
1	J	144	ARG	C-N-CA	5.55	126.78	119.84
1	A	243	ASN	N-CA-C	5.54	117.32	111.28
1	E	302	LYS	N-CA-C	5.53	119.21	111.30
1	I	136	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	A	268	HIS	N-CA-C	5.53	116.93	108.42
1	A	239	ASP	N-CA-C	-5.52	106.75	112.93
1	D	277	ALA	N-CA-C	5.50	117.35	111.36
1	D	406	ASN	CA-C-N	5.48	126.21	120.12
1	D	406	ASN	C-N-CA	5.48	126.21	120.12
1	A	52	SER	N-CA-C	5.48	113.15	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	PHE	CA-C-N	5.43	125.26	119.28
1	A	214	PHE	C-N-CA	5.43	125.26	119.28
1	L	437	GLY	N-CA-C	-5.43	107.59	114.16
1	G	204	SER	N-CA-C	5.42	117.95	111.71
1	B	233	LEU	CA-C-N	-5.40	114.36	119.76
1	B	233	LEU	C-N-CA	-5.40	114.36	119.76
1	D	280	PHE	N-CA-C	-5.39	105.31	111.14
1	L	144	ARG	CA-C-N	5.38	126.57	119.84
1	L	144	ARG	C-N-CA	5.38	126.57	119.84
1	L	185	VAL	N-CA-C	5.36	116.08	110.62
1	C	330	ARG	N-CA-C	5.35	116.65	108.52
1	C	449	TYR	N-CA-C	-5.35	105.62	111.82
1	D	82	LEU	N-CA-C	5.34	117.42	109.25
1	C	423	LYS	N-CA-C	5.34	117.10	111.28
1	I	433	TYR	N-CA-C	5.33	117.97	110.23
1	D	346	SER	N-CA-C	-5.33	106.94	113.50
1	H	452	ILE	N-CA-C	5.33	115.54	110.42
1	B	206	GLU	N-CA-C	-5.32	105.56	111.36
1	K	171	GLN	N-CA-C	5.32	117.98	111.82
1	B	102	GLY	CA-C-N	5.31	125.28	120.03
1	B	102	GLY	C-N-CA	5.31	125.28	120.03
1	C	269	VAL	N-CA-C	5.29	115.71	107.99
1	E	198	ASP	N-CA-C	5.29	116.90	111.03
1	K	266	TYR	CA-CB-CG	5.28	123.41	113.90
1	K	170	LYS	N-CA-C	-5.25	105.47	111.14
1	L	280	PHE	N-CA-C	-5.24	106.82	113.43
1	C	122	TYR	N-CA-C	5.24	118.02	109.59
1	F	237	ASP	N-CA-C	-5.22	108.17	114.75
1	K	185	VAL	N-CA-C	5.22	115.94	110.62
1	J	143	THR	N-CA-C	-5.21	107.06	113.41
1	E	184	GLU	N-CA-C	-5.19	102.51	110.14
1	I	206	GLU	N-CA-C	-5.16	105.74	111.36
1	F	355	ILE	CB-CA-C	-5.16	105.37	111.97
1	L	281	ALA	N-CA-C	-5.16	105.55	111.07
1	D	84	ILE	N-CA-C	5.15	116.22	109.21
1	E	123	SER	N-CA-C	5.15	116.57	110.19
1	I	197	ILE	N-CA-C	5.13	115.76	108.42
1	B	219	VAL	N-CA-C	-5.05	102.98	109.30
1	E	350	ASP	CA-C-N	5.05	124.65	119.05
1	E	350	ASP	C-N-CA	5.05	124.65	119.05
1	E	150	GLY	N-CA-C	5.04	121.76	115.21
1	C	144	ARG	CA-C-N	5.04	126.14	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	144	ARG	C-N-CA	5.04	126.14	119.84
1	L	52	SER	CA-C-N	5.04	124.70	119.56
1	L	52	SER	C-N-CA	5.04	124.70	119.56
1	G	316	GLU	N-CA-C	5.03	116.57	111.14
1	C	113	GLY	N-CA-C	-5.01	103.75	112.06
1	F	102	GLY	CA-C-N	5.00	124.91	119.85
1	F	102	GLY	C-N-CA	5.00	124.91	119.85

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	VAL	Peptide
1	D	114	ARG	Peptide
1	I	115	GLU	Peptide
1	I	197	ILE	Peptide
1	J	254	LYS	Peptide
1	K	146	GLU	Peptide
1	L	241	LEU	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	3361	0	3302	121	0
1	B	3351	0	3293	117	0
1	C	3370	0	3308	119	0
1	D	3333	0	3279	136	1
1	E	3358	0	3302	134	1
1	F	3351	0	3294	130	0
1	G	3342	0	3287	149	0
1	H	3333	0	3279	117	0
1	I	3360	0	3306	180	0
1	J	3342	0	3287	145	0
1	K	3349	0	3294	151	1
1	L	3366	0	3311	165	1
2	A	10	8	5	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	40226	8	39547	1640	2

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 21.

All (1640) 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:A:117:ASP:O	1:A:119:SER:N	1.63	1.31
1:K:144:ARG:HG3	1:K:145:PRO:HD2	1.27	1.14
1:B:457:THR:HA	1:B:458:GLN:HB2	1.28	1.14
1:A:212:VAL:HG21	1:A:269:VAL:HG22	1.17	1.12
1:D:114:ARG:HB2	1:D:115:GLU:HG3	1.21	1.10
1:E:144:ARG:HG3	1:E:145:PRO:HD2	1.20	1.09
1:C:457:THR:HA	1:C:458:GLN:HB3	1.35	1.07
1:D:114:ARG:CB	1:D:115:GLU:HG3	1.87	1.04
1:L:242:MET:HG3	1:L:243:ASN:H	1.16	1.02
1:K:212:VAL:HG21	1:K:269:VAL:HG23	1.42	1.02
1:I:116:ASP:O	1:I:118:ALA:N	1.92	1.01
1:I:197:ILE:HB	1:I:198:ASP:HB3	1.43	1.01
1:K:375:GLU:HG3	1:K:376:PRO:HA	1.42	1.01
1:A:244:GLU:OE1	1:A:244:GLU:N	1.92	1.00
1:E:307:ARG:HH11	1:E:454:THR:HG22	1.27	1.00
1:I:271:VAL:HB	1:I:272:LEU:HA	1.41	0.99
1:K:70:LEU:HD13	1:K:231:TRP:HZ2	1.24	0.97
1:K:117:ASP:O	1:K:119:SER:N	1.98	0.96
1:L:242:MET:CG	1:L:243:ASN:H	1.77	0.96
1:K:144:ARG:HG3	1:K:145:PRO:CD	1.95	0.96
1:K:115:GLU:N	1:K:116:ASP:HB2	1.81	0.95
1:H:50:ARG:NH1	1:H:184:GLU:OE2	2.00	0.94
1:L:243:ASN:O	1:L:247:ALA:N	2.01	0.93
1:I:167:GLU:HG3	1:I:170:LYS:HE2	1.47	0.93
1:E:270:ASP:HA	1:E:272:LEU:HD12	1.46	0.93
1:F:269:VAL:HG13	1:F:270:ASP:H	1.33	0.93
1:L:269:VAL:HG13	1:L:270:ASP:H	1.33	0.93
1:I:212:VAL:CG1	1:I:270:ASP:HB3	1.99	0.93
1:J:78:LEU:HD21	1:J:244:GLU:HG2	1.48	0.93
1:C:272:LEU:HD12	1:C:272:LEU:H	1.34	0.92
1:E:253:LYS:HD2	1:E:258:LEU:CD1	2.00	0.92
1:J:250:ASP:HA	1:J:253:LYS:HG2	1.52	0.91
1:B:272:LEU:HD22	1:B:272:LEU:H	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:LYS:HD2	1:E:258:LEU:HD12	1.50	0.91
1:J:294:HIS:HD2	1:J:352:LYS:HD2	1.31	0.91
1:D:114:ARG:HB3	1:D:115:GLU:HA	1.49	0.91
1:E:282:GLN:N	1:E:282:GLN:OE1	2.03	0.91
1:A:156:LEU:HD12	2:A:501:GLU:HA	1.52	0.90
1:F:156:LEU:CD2	1:F:183:VAL:HG23	2.01	0.90
1:J:268:HIS:HB3	1:J:269:VAL:HG12	1.53	0.90
1:A:241:LEU:HA	1:A:244:GLU:OE2	1.70	0.90
1:A:212:VAL:HG21	1:A:269:VAL:CG2	2.00	0.89
1:B:117:ASP:O	1:B:119:SER:N	2.04	0.89
1:G:252:ALA:HA	1:G:255:GLU:HG2	1.54	0.88
1:L:271:VAL:HG12	1:L:272:LEU:HA	1.54	0.88
1:L:239:ASP:O	1:L:242:MET:HB2	1.73	0.88
1:I:264:ARG:HG3	1:I:264:ARG:HH11	1.37	0.88
1:E:270:ASP:HA	1:E:272:LEU:CD1	2.03	0.88
1:L:262:LYS:O	1:L:266:TYR:HB3	1.72	0.88
1:G:212:VAL:HG11	1:G:269:VAL:HG21	1.55	0.88
1:H:205:ASN:HB2	1:H:266:TYR:CE2	2.09	0.88
1:I:136:ARG:HH12	1:I:198:ASP:N	1.70	0.88
1:A:112:PRO:HA	1:A:122:TYR:CE2	2.09	0.88
1:I:136:ARG:HD3	1:I:136:ARG:H	1.36	0.88
1:I:271:VAL:CB	1:I:272:LEU:HA	2.03	0.87
1:G:268:HIS:HA	1:G:269:VAL:HB	1.54	0.87
1:J:114:ARG:HH12	1:J:163:GLU:HG3	1.39	0.87
1:K:268:HIS:HB2	1:K:269:VAL:HB	1.57	0.86
1:K:144:ARG:CG	1:K:145:PRO:HD2	2.06	0.85
1:D:115:GLU:HB3	1:D:117:ASP:H	1.41	0.85
1:G:148:LEU:HD23	1:G:151:LYS:HZ1	1.41	0.85
1:L:457:THR:O	1:L:459:PRO:HD3	1.75	0.84
1:J:112:PRO:HA	1:J:122:TYR:CD2	2.13	0.84
1:B:167:GLU:HG2	1:B:170:LYS:HE2	1.60	0.84
1:G:112:PRO:HA	1:G:122:TYR:CE2	2.13	0.84
1:K:233:LEU:HD22	1:K:242:MET:HE2	1.60	0.84
1:E:307:ARG:NH1	1:E:454:THR:HG22	1.93	0.83
1:B:457:THR:CA	1:B:458:GLN:HB2	2.09	0.83
1:D:302:LYS:HB2	1:D:302:LYS:HZ2	1.44	0.83
1:E:307:ARG:HD3	1:E:457:THR:HG21	1.58	0.83
1:L:112:PRO:HA	1:L:122:TYR:CE2	2.14	0.83
1:L:271:VAL:CG1	1:L:272:LEU:HA	2.07	0.83
1:E:144:ARG:CG	1:E:145:PRO:HD2	2.05	0.83
1:I:117:ASP:O	1:I:119:SER:N	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:114:ARG:NH1	1:K:117:ASP:HB2	1.93	0.83
1:C:457:THR:HA	1:C:458:GLN:CB	2.07	0.83
1:G:169:LYS:NZ	1:G:177:TYR:OH	2.12	0.82
1:D:114:ARG:HB2	1:D:115:GLU:CG	2.09	0.82
1:L:272:LEU:HG	1:L:273:GLY:H	1.45	0.82
1:D:319:TRP:HA	1:D:332:LEU:HD11	1.62	0.81
1:K:149:VAL:HG22	1:K:175:LEU:CA	2.10	0.81
1:E:212:VAL:HG23	1:E:269:VAL:HG23	1.61	0.81
1:L:112:PRO:HA	1:L:122:TYR:CD2	2.15	0.81
1:D:294:HIS:CD2	1:D:352:LYS:HE2	2.15	0.81
1:I:197:ILE:CB	1:I:198:ASP:HB3	2.10	0.81
1:F:336:THR:HG23	1:F:339:THR:HB	1.63	0.81
1:K:268:HIS:HB2	1:K:269:VAL:CG1	2.11	0.80
1:F:209:MET:HE3	1:F:266:TYR:CE1	2.15	0.80
1:J:262:LYS:HE3	1:J:266:TYR:CE2	2.16	0.80
1:A:55:THR:HG22	1:A:56:TYR:N	1.96	0.80
1:G:148:LEU:HA	1:G:151:LYS:HE2	1.62	0.80
1:D:115:GLU:HA	1:D:116:ASP:HB3	1.64	0.80
1:G:268:HIS:HA	1:G:269:VAL:CB	2.10	0.80
1:I:250:ASP:OD1	1:I:251:GLN:N	2.15	0.80
1:L:250:ASP:O	1:L:253:LYS:HB3	1.81	0.80
1:H:112:PRO:HA	1:H:122:TYR:CE2	2.17	0.80
1:D:143:THR:HG22	1:D:144:ARG:HG2	1.62	0.80
1:L:208:ALA:HB1	1:L:266:TYR:CD1	2.17	0.80
1:K:207:LEU:HD21	1:K:211:GLN:OE1	1.81	0.79
1:D:115:GLU:HB3	1:D:117:ASP:N	1.96	0.79
1:D:456:VAL:HG23	1:D:457:THR:H	1.47	0.79
1:H:207:LEU:CD2	1:H:219:VAL:HG22	2.13	0.79
1:H:269:VAL:HB	1:H:270:ASP:C	2.07	0.79
1:I:329:VAL:HG23	1:I:334:MET:HE3	1.65	0.79
1:K:147:ASP:HB2	1:K:149:VAL:HG23	1.66	0.78
1:C:302:LYS:HZ2	1:C:302:LYS:HB2	1.45	0.78
1:I:121:ARG:NH1	1:I:234:PRO:O	2.16	0.78
1:L:242:MET:HG3	1:L:243:ASN:N	1.97	0.78
1:J:117:ASP:O	1:J:119:SER:N	2.16	0.78
1:F:156:LEU:HD21	1:F:183:VAL:HG23	1.64	0.78
1:F:50:ARG:NH1	1:F:184:GLU:OE1	2.17	0.78
1:F:164:GLN:NE2	1:F:223:PHE:O	2.17	0.77
1:H:209:MET:HE3	1:H:266:TYR:CD1	2.19	0.77
1:D:156:LEU:CD2	1:D:183:VAL:HG23	2.14	0.77
1:K:147:ASP:OD2	1:K:149:VAL:HB	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:HG2	1:A:264:ARG:HH11	1.50	0.77
1:I:48:ILE:HG23	1:I:93:LEU:HD11	1.64	0.77
1:K:149:VAL:HG22	1:K:175:LEU:HA	1.66	0.77
1:C:302:LYS:HB2	1:C:302:LYS:NZ	1.99	0.77
1:H:302:LYS:HB2	1:H:302:LYS:NZ	1.99	0.77
1:I:264:ARG:HH11	1:I:264:ARG:CG	1.97	0.77
1:G:250:ASP:OD1	1:G:251:GLN:N	2.17	0.77
1:D:114:ARG:HB3	1:D:115:GLU:CA	2.16	0.76
1:E:117:ASP:OD1	1:E:119:SER:OG	2.01	0.76
1:K:147:ASP:HB2	1:K:149:VAL:CG2	2.16	0.76
1:C:185:VAL:HG21	1:C:206:GLU:OE2	1.85	0.76
1:H:99:ARG:HG2	1:H:100:GLU:CG	2.15	0.76
1:H:127:LEU:HD21	1:H:266:TYR:HE2	1.50	0.76
1:E:212:VAL:CG2	1:E:269:VAL:HG23	2.15	0.76
1:I:270:ASP:CG	1:I:271:VAL:HA	2.10	0.76
1:B:112:PRO:HA	1:B:122:TYR:CE2	2.21	0.76
1:C:44:VAL:HG22	1:C:81:GLU:CG	2.14	0.76
1:F:294:HIS:CD2	1:F:352:LYS:HE2	2.21	0.76
1:K:148:LEU:HB3	1:K:153:ILE:HD11	1.68	0.76
1:H:394:GLU:OE2	1:H:397:ARG:NH1	2.18	0.76
1:I:302:LYS:HB2	1:I:302:LYS:HZ2	1.50	0.75
1:K:268:HIS:CB	1:K:269:VAL:HB	2.16	0.75
1:C:50:ARG:HD2	1:C:90:LEU:HD21	1.67	0.75
1:C:185:VAL:HG11	1:C:206:GLU:CD	2.11	0.75
1:G:302:LYS:HB2	1:G:302:LYS:HZ2	1.51	0.75
1:I:212:VAL:HG12	1:I:270:ASP:HB3	1.68	0.75
1:K:307:ARG:HD3	1:K:457:THR:HG21	1.67	0.75
1:K:268:HIS:HB2	1:K:269:VAL:CB	2.16	0.75
1:B:135:TYR:CD1	1:B:220:ALA:HB2	2.21	0.75
1:G:148:LEU:HA	1:G:151:LYS:CE	2.17	0.75
1:J:127:LEU:HD22	1:J:129:VAL:HG13	1.67	0.75
1:B:302:LYS:HB2	1:B:302:LYS:HZ2	1.51	0.75
1:C:458:GLN:H	1:C:459:PRO:HD3	1.52	0.75
1:K:115:GLU:HG3	1:K:116:ASP:N	1.99	0.75
1:J:337:ASN:O	1:J:341:GLN:HG3	1.86	0.75
1:F:50:ARG:HD2	1:F:184:GLU:OE2	1.86	0.74
1:F:302:LYS:HB2	1:F:302:LYS:HZ2	1.52	0.74
1:K:302:LYS:HB2	1:K:302:LYS:HZ2	1.53	0.74
1:I:144:ARG:NH1	1:I:146:GLU:OE1	2.17	0.74
1:I:270:ASP:OD1	1:I:271:VAL:HA	1.87	0.74
1:L:271:VAL:CB	1:L:272:LEU:HA	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:ARG:HG3	1:E:145:PRO:CD	2.10	0.74
1:G:169:LYS:HE3	1:G:177:TYR:CE2	2.22	0.74
1:E:292:GLU:OE2	1:E:296:LYS:NZ	2.17	0.74
1:J:171:GLN:HG3	1:J:172:TYR:CD1	2.24	0.73
1:F:302:LYS:HB2	1:F:302:LYS:NZ	2.03	0.73
1:L:50:ARG:HD2	1:L:184:GLU:OE2	1.89	0.73
1:D:135:TYR:HD1	1:D:220:ALA:HB2	1.50	0.73
1:G:66:PHE:CD2	1:G:266:TYR:HE1	2.07	0.73
1:J:64:THR:HG22	1:J:65:GLY:N	2.04	0.73
1:D:233:LEU:HD22	1:D:242:MET:HE2	1.71	0.73
1:E:269:VAL:O	1:E:270:ASP:HB2	1.89	0.73
1:I:270:ASP:OD2	1:I:271:VAL:HG13	1.89	0.73
1:H:207:LEU:HD21	1:H:219:VAL:HG22	1.71	0.73
1:I:275:VAL:HG21	1:I:314:TYR:OH	1.89	0.73
1:K:70:LEU:HD13	1:K:231:TRP:CZ2	2.16	0.73
1:E:322:GLY:HA3	1:K:117:ASP:HA	1.69	0.73
1:C:151:LYS:HD2	1:C:199:LEU:HD11	1.71	0.72
1:F:209:MET:HE3	1:F:266:TYR:CD1	2.24	0.72
1:I:144:ARG:HH12	1:I:146:GLU:CD	1.96	0.72
1:C:112:PRO:HA	1:C:122:TYR:CE2	2.23	0.72
1:G:88:ASP:O	1:G:423:LYS:NZ	2.15	0.72
1:G:332:LEU:HD23	1:G:355:ILE:CG1	2.20	0.72
1:H:269:VAL:HB	1:H:270:ASP:O	1.88	0.72
1:L:74:PHE:CE1	1:L:245:VAL:HA	2.23	0.72
1:I:197:ILE:HG13	1:I:198:ASP:CG	2.15	0.72
1:I:430:ARG:HG2	1:I:430:ARG:HH11	1.55	0.72
1:C:272:LEU:H	1:C:272:LEU:CD1	2.03	0.72
1:D:302:LYS:HB2	1:D:302:LYS:NZ	2.02	0.72
1:H:214:PHE:O	1:H:217:VAL:HG12	1.89	0.72
1:H:184:GLU:HG3	1:H:185:VAL:H	1.54	0.72
1:J:125:THR:HG21	1:J:228:GLY:HA3	1.72	0.71
1:D:332:LEU:HD23	1:D:355:ILE:HD11	1.71	0.71
1:K:115:GLU:HB3	1:K:116:ASP:OD2	1.90	0.71
1:E:270:ASP:CA	1:E:272:LEU:HD12	2.21	0.71
1:I:142:PRO:HG3	1:I:199:LEU:HD13	1.72	0.71
1:J:329:VAL:CG2	1:J:334:MET:HE3	2.19	0.71
1:C:457:THR:CA	1:C:458:GLN:HB3	2.18	0.71
1:C:44:VAL:HG22	1:C:81:GLU:HG3	1.70	0.71
1:D:292:GLU:OE2	1:D:296:LYS:NZ	2.18	0.71
1:E:290:ARG:HG3	1:E:291:TYR:CE2	2.26	0.71
1:L:208:ALA:HB1	1:L:266:TYR:CE1	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:268:HIS:HA	1:J:269:VAL:HB	1.71	0.71
1:K:115:GLU:H	1:K:116:ASP:HB2	1.55	0.71
1:A:50:ARG:NH1	2:A:501:GLU:OXT	2.24	0.71
1:G:239:ASP:O	1:G:243:ASN:ND2	2.23	0.70
1:K:146:GLU:CD	1:K:147:ASP:H	1.98	0.70
1:L:123:SER:OG	1:L:124:HIS:N	2.18	0.70
1:I:271:VAL:HB	1:I:272:LEU:CA	2.20	0.70
1:F:233:LEU:HD22	1:F:242:MET:HE2	1.71	0.70
1:G:148:LEU:HA	1:G:151:LYS:NZ	2.06	0.70
1:I:43:GLY:HA2	1:I:80:VAL:HG12	1.74	0.70
1:L:146:GLU:HG3	1:L:172:TYR:CZ	2.26	0.70
1:L:242:MET:HE3	1:L:243:ASN:ND2	2.06	0.70
1:F:168:LEU:HD23	1:F:175:LEU:HD22	1.73	0.70
1:D:73:ARG:HH11	1:D:257:LEU:CD1	2.04	0.70
1:G:302:LYS:HB2	1:G:302:LYS:NZ	2.06	0.70
1:I:192:VAL:HG22	1:I:198:ASP:OD1	1.92	0.70
1:A:112:PRO:O	1:A:114:ARG:N	2.24	0.69
1:G:212:VAL:HG11	1:G:269:VAL:HG11	1.73	0.69
1:K:337:ASN:O	1:K:341:GLN:HG3	1.92	0.69
1:C:121:ARG:NH1	1:C:236:GLY:HA2	2.08	0.69
1:K:166:ALA:HB1	1:K:169:LYS:NZ	2.08	0.69
1:D:332:LEU:CD2	1:D:355:ILE:HD11	2.22	0.69
1:H:209:MET:HE3	1:H:266:TYR:CE1	2.27	0.69
1:B:72:LYS:O	1:B:76:GLU:HG3	1.92	0.69
1:J:114:ARG:HG2	1:J:114:ARG:HH11	1.56	0.69
1:L:316:GLU:OE1	1:L:334:MET:HB2	1.92	0.69
1:L:281:ALA:O	1:L:284:LEU:HB2	1.92	0.69
1:D:135:TYR:CD1	1:D:220:ALA:HB2	2.27	0.69
1:H:337:ASN:O	1:H:341:GLN:HG3	1.93	0.69
1:H:269:VAL:HG12	1:H:271:VAL:HG23	1.73	0.68
1:G:271:VAL:HG22	1:G:272:LEU:HA	1.75	0.68
1:L:121:ARG:CZ	1:L:236:GLY:HA2	2.23	0.68
1:L:307:ARG:NH1	1:L:454:THR:HG22	2.08	0.68
1:A:337:ASN:O	1:A:341:GLN:HG3	1.93	0.68
1:G:116:ASP:O	1:J:324:THR:HG22	1.93	0.68
1:L:281:ALA:HA	1:L:284:LEU:HD12	1.76	0.68
1:F:421:ALA:HA	1:F:433:TYR:CE1	2.28	0.68
1:I:95:ALA:O	1:I:99:ARG:HG3	1.93	0.68
1:K:149:VAL:HG22	1:K:175:LEU:CB	2.24	0.68
1:E:454:THR:HA	1:E:457:THR:HG22	1.74	0.68
1:D:205:ASN:HB2	1:D:266:TYR:CE2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:TYR:HD1	1:C:68:TYR:HB2	1.56	0.68
1:G:332:LEU:HD23	1:G:355:ILE:HD11	1.75	0.68
1:L:242:MET:CG	1:L:243:ASN:N	2.56	0.68
1:L:337:ASN:O	1:L:341:GLN:HG3	1.93	0.68
1:I:116:ASP:C	1:I:118:ALA:H	1.98	0.68
1:G:288:LEU:N	1:G:289:PRO:HD2	2.08	0.68
1:J:144:ARG:HG3	1:J:145:PRO:HD2	1.75	0.67
1:D:233:LEU:HD13	1:D:242:MET:HE1	1.77	0.67
1:G:136:ARG:NH1	1:G:193:ASP:O	2.27	0.67
1:A:384:ALA:O	1:A:388:ILE:HG22	1.94	0.67
1:H:403:GLU:OE2	1:L:136:ARG:NH2	2.27	0.67
1:C:403:GLU:HG2	1:C:416:MET:HE1	1.75	0.67
1:I:112:PRO:HA	1:I:122:TYR:CE2	2.30	0.67
1:I:419:ARG:HD3	1:I:425:TRP:CD2	2.29	0.67
1:B:167:GLU:HG2	1:B:170:LYS:CE	2.25	0.67
1:B:456:VAL:O	1:B:457:THR:OG1	2.12	0.67
1:C:265:TYR:O	1:C:267:GLY:HA2	1.95	0.67
1:F:43:GLY:C	1:F:80:VAL:HG12	2.19	0.67
1:A:297:GLN:O	1:A:301:GLN:HG3	1.95	0.67
1:A:456:VAL:HG23	1:A:457:THR:HG23	1.77	0.67
1:B:212:VAL:HG21	1:B:269:VAL:HB	1.76	0.67
1:J:268:HIS:HB3	1:J:269:VAL:CG1	2.24	0.67
1:C:225:GLU:OE1	1:C:226:ALA:N	2.28	0.67
1:E:187:ASP:O	1:E:191:MET:HG3	1.94	0.67
1:L:243:ASN:HA	1:L:246:ASN:HB2	1.77	0.67
1:I:136:ARG:HD3	1:I:136:ARG:N	2.10	0.67
1:E:269:VAL:HG22	1:E:272:LEU:HD11	1.77	0.66
1:I:142:PRO:HG3	1:I:199:LEU:CD1	2.24	0.66
1:J:250:ASP:CA	1:J:253:LYS:HG2	2.25	0.66
1:J:400:ALA:HB2	1:J:416:MET:HG3	1.77	0.66
1:A:174:GLU:N	1:A:174:GLU:OE1	2.29	0.66
1:A:338:ARG:HH11	1:A:338:ARG:HG2	1.61	0.66
1:C:185:VAL:HG11	1:C:206:GLU:OE2	1.96	0.66
1:C:272:LEU:HD12	1:C:272:LEU:N	2.10	0.66
1:G:120:VAL:HG12	1:G:122:TYR:CE1	2.30	0.66
1:G:233:LEU:HD22	1:G:242:MET:HE2	1.78	0.66
1:I:121:ARG:HG2	1:I:121:ARG:HH11	1.60	0.66
1:K:64:THR:HG22	1:K:65:GLY:N	2.10	0.66
1:G:48:ILE:HG23	1:G:93:LEU:HD11	1.76	0.66
1:L:105:LEU:HB3	1:L:233:LEU:CD1	2.25	0.66
1:E:55:THR:HA	1:E:67:GLU:HG2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:250:ASP:HA	1:J:253:LYS:CG	2.25	0.66
1:D:190:ARG:O	1:D:194:VAL:HG23	1.96	0.66
1:E:302:LYS:HZ3	1:E:359:SER:HB3	1.61	0.66
1:D:265:TYR:C	1:D:266:TYR:HD1	2.04	0.66
1:D:332:LEU:HD23	1:D:355:ILE:CG1	2.26	0.66
1:K:430:ARG:HG2	1:K:430:ARG:HH11	1.61	0.66
1:B:121:ARG:HH21	1:B:236:GLY:CA	2.08	0.65
1:E:129:VAL:HG21	1:E:229:LEU:HD21	1.77	0.65
1:B:136:ARG:NH1	1:B:193:ASP:O	2.29	0.65
1:I:167:GLU:O	1:I:170:LYS:HG2	1.96	0.65
1:K:166:ALA:HB1	1:K:169:LYS:HZ3	1.61	0.65
1:E:302:LYS:HZ3	1:E:359:SER:CB	2.09	0.65
1:J:394:GLU:HG3	1:J:398:LYS:HE2	1.78	0.65
1:H:99:ARG:HG2	1:H:100:GLU:HG2	1.78	0.65
1:K:268:HIS:HB2	1:K:269:VAL:HG12	1.79	0.65
1:L:302:LYS:HD3	1:L:360:LYS:HG2	1.79	0.65
1:C:337:ASN:O	1:C:341:GLN:HG3	1.96	0.65
1:I:329:VAL:CG2	1:I:334:MET:HE3	2.26	0.65
1:E:281:ALA:O	1:E:284:LEU:HB2	1.96	0.65
1:J:281:ALA:O	1:J:284:LEU:HB2	1.96	0.65
1:G:268:HIS:CA	1:G:269:VAL:HB	2.25	0.65
1:J:208:ALA:HB1	1:J:266:TYR:CD1	2.32	0.65
1:H:267:GLY:O	1:H:268:HIS:ND1	2.29	0.65
1:K:149:VAL:HG22	1:K:175:LEU:HB2	1.78	0.65
1:A:50:ARG:HH12	2:A:501:GLU:C	2.04	0.65
1:E:273:GLY:HA3	1:E:445:ASN:ND2	2.12	0.65
1:F:134:ILE:CG2	1:F:217:VAL:HG13	2.26	0.65
1:G:280:PHE:CE2	1:G:452:ILE:HG21	2.31	0.65
1:H:99:ARG:HG2	1:H:100:GLU:HG3	1.78	0.65
1:I:121:ARG:NH1	1:I:235:GLY:HA2	2.12	0.64
1:J:332:LEU:HD23	1:J:355:ILE:HG13	1.78	0.64
1:A:338:ARG:HH11	1:A:338:ARG:CG	2.10	0.64
1:E:253:LYS:HD2	1:E:258:LEU:HD13	1.79	0.64
1:B:272:LEU:HD22	1:B:272:LEU:N	2.09	0.64
1:C:360:LYS:HD2	1:I:371:GLU:OE2	1.98	0.64
1:K:302:LYS:HB2	1:K:302:LYS:NZ	2.12	0.64
1:A:143:THR:OG1	1:A:144:ARG:HG3	1.97	0.64
1:D:66:PHE:CE1	1:D:261:LEU:HB3	2.31	0.64
1:D:454:THR:O	1:D:456:VAL:HG22	1.96	0.64
1:I:350:ASP:HB3	1:I:353:GLN:HG2	1.78	0.64
1:B:458:GLN:HA	1:B:458:GLN:OE1	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:GLN:OE1	1:H:282:GLN:HA	1.97	0.64
1:G:212:VAL:CG1	1:G:269:VAL:HG21	2.27	0.64
1:A:288:LEU:HD22	1:A:319:TRP:CH2	2.32	0.64
1:K:125:THR:HA	1:K:229:LEU:O	1.98	0.64
1:D:100:GLU:OE2	1:I:344:GLY:HA3	1.98	0.64
1:K:457:THR:O	1:K:458:GLN:HB2	1.97	0.64
1:J:302:LYS:HB2	1:J:302:LYS:NZ	2.13	0.64
1:K:147:ASP:CG	1:K:149:VAL:HB	2.22	0.64
1:B:302:LYS:HE2	1:B:360:LYS:N	2.13	0.63
1:B:184:GLU:HG3	1:B:185:VAL:H	1.63	0.63
1:A:265:TYR:O	1:A:267:GLY:HA2	1.97	0.63
1:F:421:ALA:HA	1:F:433:TYR:CD1	2.33	0.63
1:I:271:VAL:CG1	1:I:272:LEU:HA	2.28	0.63
1:G:307:ARG:CZ	1:G:454:THR:HG22	2.28	0.63
1:L:417:LEU:HB2	1:L:418:PRO:HD3	1.79	0.63
1:B:169:LYS:HD2	1:B:175:LEU:O	1.98	0.63
1:J:372:SER:HB2	1:J:408:ASN:OD1	1.99	0.63
1:L:269:VAL:HG22	1:L:272:LEU:HB2	1.81	0.63
1:B:115:GLU:HG3	1:B:116:ASP:N	2.11	0.63
1:B:157:LYS:HE2	1:B:179:GLU:OE2	1.99	0.63
1:K:117:ASP:C	1:K:119:SER:H	2.01	0.63
1:G:280:PHE:HE2	1:G:452:ILE:HG21	1.63	0.63
1:C:114:ARG:HD3	1:C:116:ASP:HB3	1.79	0.63
1:E:52:SER:HB2	1:E:53:PRO:HD2	1.80	0.63
1:L:157:LYS:HE2	1:L:179:GLU:OE2	2.00	0.62
1:E:156:LEU:CD1	1:E:188:LEU:HD11	2.30	0.62
1:F:125:THR:HA	1:F:229:LEU:O	1.98	0.62
1:H:184:GLU:HG3	1:H:185:VAL:N	2.14	0.62
1:H:336:THR:HG23	1:H:339:THR:HB	1.80	0.62
1:I:136:ARG:NH1	1:I:198:ASP:N	2.46	0.62
1:I:252:ALA:HB1	1:I:257:LEU:HB3	1.81	0.62
1:J:112:PRO:C	1:J:114:ARG:H	2.07	0.62
1:J:294:HIS:HD2	1:J:352:LYS:CD	2.08	0.62
1:K:297:GLN:OE1	1:K:352:LYS:NZ	2.33	0.62
1:L:271:VAL:HB	1:L:272:LEU:HA	1.80	0.62
1:A:302:LYS:HB2	1:A:302:LYS:NZ	2.14	0.62
1:I:198:ASP:OD1	1:I:198:ASP:C	2.41	0.62
1:A:156:LEU:HB2	2:A:501:GLU:HG2	1.80	0.62
1:D:271:VAL:HG12	1:D:272:LEU:N	2.15	0.62
1:E:337:ASN:OD1	1:E:348:ARG:NH2	2.33	0.62
1:F:292:GLU:HG3	1:F:293:SER:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:423:LYS:HA	1:G:426:TYR:CE2	2.34	0.62
1:E:290:ARG:HG3	1:E:291:TYR:CZ	2.35	0.62
1:K:56:TYR:HD1	1:K:68:TYR:HB2	1.63	0.62
1:A:209:MET:HE3	1:A:266[B]:TYR:CE2	2.35	0.62
1:H:148:LEU:HB3	1:H:153:ILE:HD11	1.81	0.62
1:G:287:ARG:C	1:G:289:PRO:HD2	2.25	0.62
1:I:74:PHE:HB2	1:I:248:PHE:CE2	2.35	0.62
1:E:332:LEU:HD23	1:E:355:ILE:HG12	1.81	0.62
1:I:457:THR:N	1:I:458:GLN:HA	2.15	0.62
1:D:73:ARG:HH11	1:D:257:LEU:HD11	1.65	0.61
1:E:156:LEU:HD12	1:E:188:LEU:HD11	1.81	0.61
1:K:133:ILE:HD13	1:K:201:LEU:HD13	1.83	0.61
1:E:336:THR:HG23	1:E:339:THR:HB	1.80	0.61
1:J:332:LEU:HD23	1:J:355:ILE:CG1	2.30	0.61
1:L:423:LYS:HA	1:L:426:TYR:CE2	2.35	0.61
1:E:332:LEU:CD2	1:E:355:ILE:HD11	2.31	0.61
1:F:269:VAL:HG13	1:F:270:ASP:N	2.11	0.61
1:H:149:VAL:HG13	1:H:175:LEU:HA	1.83	0.61
1:H:209:MET:CE	1:H:266:TYR:CE1	2.84	0.61
1:I:136:ARG:NH1	1:I:198:ASP:O	2.33	0.61
1:K:166:ALA:HA	1:K:169:LYS:HD3	1.82	0.61
1:C:74:PHE:HB2	1:C:248:PHE:CE2	2.35	0.61
1:I:48:ILE:HG23	1:I:93:LEU:CD1	2.30	0.61
1:I:212:VAL:HG11	1:I:270:ASP:HB3	1.83	0.61
1:J:268:HIS:CA	1:J:269:VAL:HB	2.31	0.61
1:L:458:GLN:HA	1:L:458:GLN:OE1	1.99	0.61
1:B:274:TYR:CZ	1:B:448:ARG:HD2	2.36	0.61
1:E:302:LYS:NZ	1:E:359:SER:HB3	2.14	0.61
1:F:426:TYR:HA	1:F:429:THR:HG23	1.82	0.61
1:G:151:LYS:NZ	1:G:199:LEU:HD11	2.15	0.61
1:J:109:GLY:CA	1:J:229:LEU:HD13	2.31	0.61
1:C:112:PRO:HA	1:C:122:TYR:CD2	2.36	0.61
1:K:115:GLU:HB3	1:K:116:ASP:CG	2.25	0.61
1:K:115:GLU:CA	1:K:116:ASP:HB2	2.30	0.61
1:L:270:ASP:O	1:L:271:VAL:HG23	2.01	0.61
1:L:329:VAL:CG2	1:L:334:MET:HE3	2.31	0.61
1:G:332:LEU:CD2	1:G:355:ILE:HD11	2.30	0.61
1:J:269:VAL:O	1:J:272:LEU:HD12	2.01	0.61
1:L:185:VAL:HG21	1:L:206:GLU:OE1	2.01	0.61
1:H:329:VAL:HG23	1:H:334:MET:HE3	1.83	0.61
1:B:115:GLU:HG3	1:B:116:ASP:CB	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:337:ASN:O	1:G:341:GLN:HG3	2.00	0.60
1:H:73:ARG:HD2	1:H:257:LEU:HD21	1.83	0.60
1:J:372:SER:HB2	1:J:408:ASN:CG	2.26	0.60
1:L:134:ILE:HB	1:L:200:THR:HG22	1.83	0.60
1:F:43:GLY:O	1:F:80:VAL:HG12	2.00	0.60
1:F:117:ASP:O	1:F:118:ALA:HB3	2.02	0.60
1:G:384:ALA:O	1:G:388:ILE:HG22	2.01	0.60
1:J:64:THR:CG2	1:J:65:GLY:N	2.64	0.60
1:L:329:VAL:HG23	1:L:334:MET:HE3	1.83	0.60
1:K:97:LEU:O	1:K:234:PRO:HB3	2.02	0.60
1:A:264:ARG:HH11	1:A:264:ARG:CG	2.12	0.60
1:D:332:LEU:HD23	1:D:355:ILE:CD1	2.32	0.60
1:B:117:ASP:C	1:B:119:SER:H	2.07	0.60
1:D:203:ASP:O	1:D:206:GLU:HB2	2.01	0.60
1:E:91:ASP:OD2	1:E:157:LYS:NZ	2.34	0.60
1:I:159:SER:O	1:I:163:GLU:HG3	2.00	0.60
1:J:190:ARG:CZ	1:J:422:GLN:HG2	2.31	0.60
1:K:136:ARG:HD2	1:K:192:VAL:O	2.02	0.60
1:D:456:VAL:HG23	1:D:457:THR:N	2.16	0.60
1:J:125:THR:CG2	1:J:228:GLY:HA3	2.31	0.60
1:G:147:ASP:O	1:G:151:LYS:NZ	2.33	0.60
1:K:329:VAL:HG23	1:K:334:MET:HE3	1.83	0.60
1:D:118:ALA:O	1:D:120:VAL:N	2.28	0.60
1:D:156:LEU:HD21	1:D:183:VAL:HG23	1.83	0.60
1:J:270:ASP:OD1	1:J:271:VAL:N	2.34	0.60
1:G:265:TYR:O	1:G:267:GLY:HA3	2.02	0.59
1:H:149:VAL:HG22	1:H:175:LEU:HB2	1.83	0.59
1:H:233:LEU:HD22	1:H:242:MET:HE2	1.84	0.59
1:C:410:TRP:CZ2	1:C:443:VAL:HG11	2.38	0.59
1:G:100:GLU:O	1:G:102:GLY:N	2.34	0.59
1:G:332:LEU:HD23	1:G:355:ILE:CD1	2.32	0.59
1:I:145:PRO:HB3	1:I:168:LEU:HD11	1.83	0.59
1:I:197:ILE:HG13	1:I:198:ASP:OD2	2.02	0.59
1:I:332:LEU:HD23	1:I:355:ILE:HD11	1.84	0.59
1:L:242:MET:HG3	1:L:243:ASN:CG	2.27	0.59
1:C:456:VAL:HG23	1:C:457:THR:HG23	1.84	0.59
1:H:273:GLY:HA2	1:H:274:TYR:O	2.01	0.59
1:L:208:ALA:HB1	1:L:266:TYR:HD1	1.68	0.59
1:F:156:LEU:HD23	1:F:183:VAL:HG23	1.81	0.59
1:G:66:PHE:HD2	1:G:266:TYR:HE1	1.48	0.59
1:I:116:ASP:C	1:I:118:ALA:N	2.58	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:233:LEU:HG	1:L:234:PRO:HD2	1.84	0.59
1:G:430:ARG:HG2	1:G:430:ARG:HH11	1.68	0.59
1:E:184:GLU:HG3	1:E:185:VAL:H	1.67	0.59
1:I:149:VAL:HG11	1:I:174:GLU:HG3	1.84	0.59
1:D:209:MET:O	1:D:268:HIS:NE2	2.29	0.59
1:H:329:VAL:CG2	1:H:334:MET:HE3	2.32	0.59
1:I:264:ARG:CG	1:I:264:ARG:NH1	2.63	0.59
1:L:269:VAL:HG13	1:L:270:ASP:N	2.10	0.59
1:A:114:ARG:O	1:A:115:GLU:HG2	2.03	0.59
1:G:114:ARG:NH2	1:G:116:ASP:OD2	2.36	0.59
1:I:191:MET:SD	1:I:197:ILE:HD13	2.43	0.59
1:J:72:LYS:O	1:J:76:GLU:HG2	2.03	0.59
1:J:345:VAL:HG13	1:J:353:GLN:HB3	1.84	0.59
1:H:66:PHE:CD1	1:H:66:PHE:C	2.81	0.58
1:J:329:VAL:HG21	1:J:334:MET:HE3	1.84	0.58
1:K:155:VAL:HG22	1:K:156:LEU:N	2.18	0.58
1:K:157:LYS:HE2	1:K:179:GLU:OE2	2.03	0.58
1:A:74:PHE:HB2	1:A:248:PHE:CE2	2.38	0.58
1:A:169:LYS:HD2	1:A:175:LEU:O	2.03	0.58
1:B:260:ARG:HG3	1:B:260:ARG:HH11	1.68	0.58
1:D:184:GLU:HG3	1:D:185:VAL:H	1.68	0.58
1:H:212:VAL:HG23	1:H:271:VAL:HG22	1.85	0.58
1:L:405:LEU:O	1:L:407:PRO:HD3	2.03	0.58
1:A:302:LYS:HZ3	1:A:359:SER:HB3	1.69	0.58
1:G:268:HIS:CG	1:G:269:VAL:HB	2.38	0.58
1:K:147:ASP:C	1:K:149:VAL:N	2.60	0.58
1:G:53:PRO:HG3	1:G:186:VAL:HG21	1.85	0.58
1:A:288:LEU:HB2	1:A:319:TRP:CZ3	2.38	0.58
1:D:74:PHE:HB2	1:D:248:PHE:CE2	2.39	0.58
1:H:66:PHE:C	1:H:66:PHE:HD1	2.11	0.58
1:H:271:VAL:O	1:H:272:LEU:HB2	2.04	0.58
1:F:73:ARG:HH11	1:F:257:LEU:CD1	2.16	0.58
1:J:112:PRO:O	1:J:114:ARG:N	2.36	0.58
1:L:135:TYR:CZ	1:L:141:ARG:HD3	2.37	0.58
1:A:68:TYR:OH	1:A:72:LYS:HE2	2.03	0.58
1:A:209:MET:HE3	1:A:266[B]:TYR:CD2	2.39	0.58
1:E:457:THR:HG23	1:E:457:THR:O	2.03	0.58
1:I:47:VAL:HG22	1:I:105:LEU:HG	1.84	0.58
1:L:233:LEU:HD11	1:L:241:LEU:HD23	1.85	0.58
1:D:362:PHE:CE1	1:D:383:LEU:HD23	2.39	0.58
1:E:350:ASP:HB3	1:E:353:GLN:CD	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:LEU:HA	1:G:151:LYS:HZ1	1.68	0.58
1:I:41:LYS:HB3	1:I:42:GLU:C	2.29	0.58
1:K:419:ARG:HG2	1:K:419:ARG:HH11	1.69	0.58
1:L:271:VAL:HG12	1:L:272:LEU:CA	2.31	0.58
1:E:332:LEU:HD22	1:E:355:ILE:HD11	1.86	0.58
1:F:114:ARG:O	1:F:115:GLU:HB2	2.03	0.58
1:A:279:THR:O	1:A:282:GLN:HB2	2.04	0.58
1:C:144:ARG:NH2	1:C:146:GLU:OE1	2.37	0.58
1:F:50:ARG:HH11	1:F:184:GLU:CD	2.12	0.58
1:G:121:ARG:CZ	1:G:236:GLY:HA2	2.34	0.58
1:G:325:SER:HB3	1:G:329:VAL:HG22	1.86	0.58
1:I:112:PRO:HA	1:I:122:TYR:CD2	2.38	0.58
1:K:144:ARG:HG3	1:K:145:PRO:N	2.18	0.58
1:K:458:GLN:OE1	1:K:459:PRO:HD3	2.02	0.58
1:G:116:ASP:C	1:J:324:THR:HG22	2.29	0.57
1:I:247:ALA:O	1:I:250:ASP:N	2.28	0.57
1:B:239:ASP:O	1:B:243:ASN:ND2	2.36	0.57
1:E:269:VAL:HG22	1:E:270:ASP:N	2.19	0.57
1:H:273:GLY:HA2	1:H:274:TYR:C	2.28	0.57
1:A:238:ASP:CG	1:A:240:SER:HB2	2.29	0.57
1:C:349:LEU:HD21	1:D:118:ALA:HB3	1.86	0.57
1:I:113:GLY:HA3	1:I:114:ARG:O	2.04	0.57
1:I:419:ARG:HD3	1:I:425:TRP:CE2	2.39	0.57
1:J:114:ARG:HH22	1:J:163:GLU:CD	2.12	0.57
1:J:294:HIS:CD2	1:J:352:LYS:HD2	2.23	0.57
1:D:266:TYR:N	1:D:266:TYR:CD1	2.72	0.57
1:F:380:TRP:CZ3	1:F:447:ARG:HD3	2.39	0.57
1:I:157:LYS:HA	1:I:179:GLU:HG2	1.86	0.57
1:K:193:ASP:OD1	1:K:216:ASN:HB2	2.04	0.57
1:I:319:TRP:HA	1:I:332:LEU:HD11	1.86	0.57
1:J:329:VAL:HG23	1:J:334:MET:HE3	1.86	0.57
1:B:50:ARG:HD2	1:B:184:GLU:OE2	2.04	0.57
1:C:295:PHE:CE1	1:C:310:ALA:HA	2.39	0.57
1:A:241:LEU:CA	1:A:244:GLU:OE2	2.51	0.57
1:F:285[B]:GLN:HG2	1:F:286:GLN:N	2.19	0.57
1:L:242:MET:HG3	1:L:243:ASN:OD1	2.04	0.57
1:B:134:ILE:HB	1:B:200:THR:HG22	1.85	0.57
1:F:426:TYR:CE2	1:F:433:TYR:HB2	2.40	0.57
1:G:119:SER:O	1:G:120:VAL:HB	2.04	0.57
1:A:73:ARG:HD2	1:A:257:LEU:HD22	1.86	0.57
1:D:426:TYR:CE2	1:D:433:TYR:HB2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:ARG:CD	1:E:457:THR:HG21	2.32	0.57
1:J:267:GLY:O	1:J:268:HIS:HB2	2.04	0.57
1:K:147:ASP:HB2	1:K:149:VAL:CB	2.34	0.57
1:C:121:ARG:HH11	1:C:236:GLY:CA	2.18	0.56
1:F:380:TRP:CH2	1:F:447:ARG:HD2	2.40	0.56
1:H:127:LEU:HD23	1:H:229:LEU:HD12	1.87	0.56
1:H:336:THR:HG23	1:H:339:THR:CB	2.35	0.56
1:I:198:ASP:OD1	1:I:199:LEU:N	2.37	0.56
1:J:343:MET:HE1	1:J:364:GLN:OE1	2.05	0.56
1:L:269:VAL:O	1:L:270:ASP:HB2	2.04	0.56
1:B:330:ARG:HD3	1:E:118:ALA:HB1	1.87	0.56
1:D:184:GLU:HG3	1:D:185:VAL:N	2.19	0.56
1:J:134:ILE:HB	1:J:200:THR:HG22	1.87	0.56
1:K:147:ASP:HB2	1:K:149:VAL:HB	1.87	0.56
1:D:156:LEU:HD23	1:D:183:VAL:HG23	1.85	0.56
1:E:57:PHE:CE1	1:E:64:THR:HG23	2.40	0.56
1:G:147:ASP:C	1:G:151:LYS:HZ3	2.13	0.56
1:H:209:MET:CE	1:H:266:TYR:CD1	2.88	0.56
1:H:212:VAL:CG2	1:H:271:VAL:HG22	2.36	0.56
1:I:92:ASP:O	1:I:96:GLN:HG2	2.05	0.56
1:J:64:THR:HG22	1:J:65:GLY:H	1.70	0.56
1:J:64:THR:CG2	1:J:65:GLY:H	2.19	0.56
1:L:307:ARG:CZ	1:L:454:THR:HG22	2.35	0.56
1:B:124:HIS:HD1	1:B:246:ASN:CG	2.13	0.56
1:B:136:ARG:NH2	1:D:403:GLU:OE2	2.39	0.56
1:F:78:LEU:HB2	1:F:80:VAL:HG23	1.87	0.56
1:I:113:GLY:HA3	1:I:114:ARG:C	2.29	0.56
1:K:268:HIS:CA	1:K:269:VAL:HB	2.36	0.56
1:B:275:VAL:HG22	1:B:449:TYR:OH	2.06	0.56
1:I:66:PHE:CD1	1:I:66:PHE:C	2.83	0.56
1:K:95:ALA:O	1:K:99:ARG:HG3	2.05	0.56
1:A:329:VAL:HG23	1:A:334:MET:HE3	1.86	0.56
1:D:269:VAL:O	1:D:270:ASP:HB2	2.05	0.56
1:H:118:ALA:HB2	1:K:324:THR:HB	1.88	0.56
1:L:187:ASP:HA	1:L:190:ARG:HH12	1.69	0.56
1:F:329:VAL:CG2	1:F:334:MET:HE3	2.36	0.56
1:H:295:PHE:CE1	1:H:310:ALA:HA	2.41	0.56
1:C:208:ALA:HB3	1:C:266[A]:TYR:CD2	2.40	0.56
1:H:393:LEU:O	1:H:397:ARG:HG3	2.06	0.56
1:L:392:HIS:CE1	1:L:434:ALA:HB2	2.41	0.56
1:A:381:PHE:HD2	1:A:393:LEU:HD21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:OH	1:A:141:ARG:HD2	2.06	0.55
1:A:267:GLY:O	1:A:268:HIS:ND1	2.36	0.55
1:H:302:LYS:HB2	1:H:302:LYS:HZ2	1.68	0.55
1:L:135:TYR:OH	1:L:141:ARG:HD3	2.06	0.55
1:A:260:ARG:HG3	1:A:260:ARG:HH11	1.71	0.55
1:G:148:LEU:HD22	1:G:199:LEU:HD13	1.89	0.55
1:H:170:LYS:NZ	1:H:170:LYS:HB3	2.20	0.55
1:I:332:LEU:HD23	1:I:355:ILE:HG13	1.88	0.55
1:F:141:ARG:HH12	1:F:143:THR:HG22	1.71	0.55
1:F:268:HIS:CE1	1:F:270:ASP:HB2	2.41	0.55
1:K:269:VAL:O	1:K:269:VAL:HG22	2.07	0.55
1:L:377:ASP:HA	1:L:380:TRP:CD1	2.42	0.55
1:D:294:HIS:NE2	1:D:352:LYS:HE2	2.21	0.55
1:E:332:LEU:HD23	1:E:355:ILE:CG1	2.36	0.55
1:I:332:LEU:HD23	1:I:355:ILE:CG1	2.37	0.55
1:K:268:HIS:HE1	1:K:326:LYS:HE2	1.72	0.55
1:A:117:ASP:C	1:A:119:SER:N	2.60	0.55
1:E:410:TRP:CZ2	1:E:443:VAL:HG11	2.42	0.55
1:C:148:LEU:HD12	1:C:168:LEU:CD2	2.37	0.55
1:H:205:ASN:HB2	1:H:266:TYR:CD2	2.42	0.55
1:A:152:ARG:NH1	1:A:196:ASP:O	2.40	0.55
1:B:350:ASP:OD2	1:B:353:GLN:HG3	2.07	0.55
1:C:205:ASN:HA	1:C:266[A]:TYR:CE2	2.42	0.55
1:H:120:VAL:HG12	1:H:122:TYR:CE1	2.42	0.55
1:K:253:LYS:HD3	1:K:258:LEU:HD12	1.89	0.55
1:C:133:ILE:C	1:C:134:ILE:HD13	2.31	0.55
1:F:207:LEU:CD2	1:F:219:VAL:HG22	2.37	0.55
1:A:69:GLU:OE2	1:A:265:TYR:OH	2.21	0.55
1:E:273:GLY:O	1:E:274:TYR:HB3	2.07	0.55
1:F:350:ASP:OD2	1:F:353:GLN:HG2	2.07	0.55
1:G:73:ARG:HD3	1:G:257:LEU:HD21	1.88	0.55
1:B:284:LEU:HD21	1:B:453:LEU:HD21	1.89	0.54
1:D:232:ALA:C	1:D:233:LEU:HD12	2.32	0.54
1:G:66:PHE:CD1	1:G:66:PHE:C	2.84	0.54
1:J:233:LEU:HD22	1:J:242:MET:HE2	1.88	0.54
1:J:127:LEU:HD23	1:J:128:ASP:N	2.22	0.54
1:L:49:THR:OG1	1:L:107:ALA:O	2.24	0.54
1:B:337:ASN:O	1:B:341:GLN:HG3	2.08	0.54
1:E:212:VAL:HG21	1:E:269:VAL:HA	1.88	0.54
1:H:148:LEU:HD22	1:H:199:LEU:HD13	1.88	0.54
1:H:166:ALA:O	1:H:169:LYS:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ARG:HG3	1:B:146:GLU:HG2	1.89	0.54
1:J:53:PRO:HG3	1:J:186:VAL:HG21	1.88	0.54
1:F:380:TRP:CZ2	1:F:447:ARG:HD2	2.42	0.54
1:L:450:TYR:O	1:L:454:THR:OG1	2.26	0.54
1:J:419:ARG:HG2	1:J:419:ARG:HH11	1.73	0.54
1:K:126:TYR:HA	1:K:253:LYS:NZ	2.22	0.54
1:C:209:MET:HE1	1:C:266[B]:TYR:CE1	2.42	0.54
1:D:279:THR:HG22	1:D:283:HIS:CE1	2.42	0.54
1:G:148:LEU:HD22	1:G:199:LEU:CD1	2.37	0.54
1:G:423:LYS:HA	1:G:426:TYR:CD2	2.43	0.54
1:I:284:LEU:HD21	1:I:453:LEU:HD11	1.90	0.54
1:K:64:THR:CG2	1:K:65:GLY:N	2.70	0.54
1:D:114:ARG:CB	1:D:115:GLU:CG	2.74	0.54
1:E:129:VAL:CG2	1:E:229:LEU:HD21	2.37	0.54
1:E:281:ALA:HB3	1:E:282:GLN:OE1	2.08	0.54
1:H:52:SER:HB2	1:H:53:PRO:HD2	1.89	0.54
1:H:257:LEU:HA	1:H:260:ARG:NH1	2.22	0.54
1:J:288:LEU:N	1:J:289:PRO:CD	2.71	0.54
1:C:458:GLN:H	1:C:459:PRO:CD	2.21	0.54
1:D:118:ALA:C	1:D:120:VAL:H	2.16	0.54
1:K:164:GLN:NE2	1:K:223:PHE:O	2.41	0.54
1:C:121:ARG:HH11	1:C:236:GLY:HA2	1.73	0.54
1:G:55:THR:HG22	1:G:67:GLU:HG3	1.89	0.54
1:J:238:ASP:OD1	1:J:240:SER:N	2.34	0.54
1:K:284:LEU:CD2	1:K:288:LEU:HD23	2.37	0.54
1:A:112:PRO:HA	1:A:122:TYR:CD2	2.41	0.53
1:C:306:TRP:CE2	1:C:307:ARG:HG3	2.43	0.53
1:E:364:GLN:O	1:E:368:GLU:HG3	2.08	0.53
1:K:125:THR:O	1:K:253:LYS:NZ	2.38	0.53
1:B:115:GLU:HG3	1:B:116:ASP:HB2	1.90	0.53
1:C:121:ARG:NH1	1:C:236:GLY:CA	2.71	0.53
1:D:288:LEU:HB3	1:D:289:PRO:HD3	1.89	0.53
1:E:232:ALA:C	1:E:233:LEU:HD12	2.33	0.53
1:F:419:ARG:HD3	1:F:425:TRP:CD2	2.44	0.53
1:I:66:PHE:C	1:I:66:PHE:HD1	2.16	0.53
1:F:73:ARG:HH11	1:F:257:LEU:HD13	1.74	0.53
1:H:134:ILE:CG2	1:H:217:VAL:CG2	2.86	0.53
1:J:269:VAL:HG22	1:J:272:LEU:CD1	2.38	0.53
1:K:268:HIS:CE1	1:K:326:LYS:HE2	2.42	0.53
1:L:44:VAL:HG22	1:L:81:GLU:OE1	2.08	0.53
1:L:48:ILE:HD11	1:L:87:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:VAL:HG13	1:E:270:ASP:OD1	2.08	0.53
1:F:336:THR:HG23	1:F:339:THR:CB	2.36	0.53
1:H:283:HIS:ND1	1:H:314:TYR:OH	2.20	0.53
1:I:350:ASP:HB3	1:I:353:GLN:CG	2.39	0.53
1:L:370:PRO:HG2	1:L:397:ARG:NH1	2.23	0.53
1:I:125:THR:HA	1:I:229:LEU:O	2.08	0.53
1:I:134:ILE:O	1:I:199:LEU:HA	2.08	0.53
1:K:281:ALA:O	1:K:284:LEU:HB2	2.07	0.53
1:L:381:PHE:HD2	1:L:393:LEU:HD21	1.74	0.53
1:C:105:LEU:HD12	1:C:105:LEU:C	2.34	0.53
1:D:135:TYR:HB3	1:D:199:LEU:CD2	2.39	0.53
1:J:168:LEU:HD12	1:J:171:GLN:HE21	1.73	0.53
1:A:266[A]:TYR:HD1	1:A:266[A]:TYR:C	2.17	0.53
1:G:324:THR:CG2	1:G:330:ARG:HE	2.21	0.53
1:I:239:ASP:O	1:I:243:ASN:ND2	2.42	0.53
1:B:156:LEU:HD21	1:B:183:VAL:O	2.08	0.53
1:B:410:TRP:O	1:B:414:LYS:HB3	2.08	0.53
1:E:251:GLN:HG3	1:E:255:GLU:OE2	2.09	0.53
1:E:253:LYS:CD	1:E:258:LEU:CD1	2.83	0.53
1:I:239:ASP:HB3	1:I:243:ASN:HD21	1.73	0.53
1:D:337:ASN:O	1:D:341:GLN:HG3	2.08	0.53
1:E:454:THR:CA	1:E:457:THR:HG22	2.39	0.53
1:F:47:VAL:HG13	1:F:105:LEU:HD12	1.89	0.53
1:I:144:ARG:NH1	1:I:146:GLU:HB3	2.24	0.53
1:I:239:ASP:HB3	1:I:243:ASN:ND2	2.24	0.53
1:I:317:SER:HB2	1:I:323:ALA:CB	2.38	0.53
1:A:144:ARG:NH2	1:A:146:GLU:OE2	2.36	0.53
1:A:238:ASP:OD2	1:A:240:SER:HB2	2.07	0.53
1:B:312:ILE:O	1:B:316:GLU:HG2	2.09	0.53
1:G:127:LEU:HD11	1:G:262:LYS:HE3	1.90	0.53
1:H:126:TYR:CE2	1:H:230:ALA:HA	2.44	0.53
1:I:64:THR:OG1	1:I:65:GLY:N	2.42	0.53
1:I:184:GLU:HG2	1:I:423:LYS:HD2	1.90	0.53
1:J:262:LYS:HE3	1:J:266:TYR:CZ	2.43	0.53
1:K:343:MET:SD	1:K:360:LYS:CG	2.97	0.53
1:L:280:PHE:HE1	1:L:319:TRP:CH2	2.27	0.53
1:D:53:PRO:HG3	1:D:186:VAL:HG21	1.92	0.52
1:E:253:LYS:CD	1:E:258:LEU:HD12	2.30	0.52
1:F:330:ARG:HD3	1:F:349:LEU:HD21	1.91	0.52
1:L:78:LEU:HD12	1:L:78:LEU:O	2.09	0.52
1:L:269:VAL:CG1	1:L:270:ASP:H	2.15	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ARG:HG2	1:A:338:ARG:NH1	2.20	0.52
1:C:135:TYR:CZ	1:C:141:ARG:HB2	2.44	0.52
1:E:325:SER:HB3	1:E:329:VAL:HG22	1.91	0.52
1:E:336:THR:HG23	1:E:339:THR:CB	2.39	0.52
1:H:140:GLN:O	1:H:142:PRO:HD3	2.09	0.52
1:H:232:ALA:C	1:H:233:LEU:HD12	2.34	0.52
1:H:421:ALA:HA	1:H:433:TYR:CD1	2.43	0.52
1:D:64:THR:HG22	1:D:65:GLY:H	1.73	0.52
1:I:391:ALA:HB1	1:I:431:TYR:CD2	2.45	0.52
1:L:115:GLU:HG3	1:L:116:ASP:CG	2.34	0.52
1:E:284:LEU:O	1:E:289:PRO:HD3	2.08	0.52
1:I:41:LYS:HG3	1:I:43:GLY:N	2.25	0.52
1:K:118:ALA:O	1:K:235:GLY:HA3	2.09	0.52
1:K:144:ARG:O	1:K:145:PRO:C	2.50	0.52
1:E:322:GLY:HA3	1:K:117:ASP:CA	2.39	0.52
1:E:453:LEU:O	1:E:457:THR:HG22	2.09	0.52
1:K:167:GLU:HA	1:K:170:LYS:HE3	1.90	0.52
1:L:240:SER:C	1:L:242:MET:HB2	2.34	0.52
1:A:423:LYS:HA	1:A:426:TYR:CE2	2.44	0.52
1:B:121:ARG:HH21	1:B:236:GLY:HA3	1.74	0.52
1:C:267:GLY:O	1:C:268:HIS:ND1	2.32	0.52
1:D:73:ARG:HH11	1:D:257:LEU:HD13	1.74	0.52
1:F:316:GLU:HA	1:F:316:GLU:OE1	2.09	0.52
1:G:298:SER:HB3	1:G:356:GLN:OE1	2.08	0.52
1:L:146:GLU:HG3	1:L:172:TYR:CE1	2.45	0.52
1:L:375:GLU:OE2	1:L:378:ARG:HB3	2.09	0.52
1:B:154:MET:HB3	1:B:197:ILE:HD12	1.91	0.52
1:C:271:VAL:HG22	1:C:438:GLU:OE1	2.10	0.52
1:D:161:HIS:HB3	1:D:201:LEU:HG	1.92	0.52
1:E:190:ARG:HA	1:E:214:PHE:CE1	2.44	0.52
1:J:329:VAL:HG23	1:J:334:MET:CE	2.39	0.52
1:B:146:GLU:HG3	1:B:147:ASP:OD1	2.10	0.52
1:B:329:VAL:HG23	1:B:334:MET:HE3	1.92	0.52
1:F:294:HIS:NE2	1:F:352:LYS:HE2	2.24	0.52
1:I:238:ASP:OD1	1:I:240:SER:HB2	2.10	0.52
1:I:269:VAL:HG12	1:I:269:VAL:O	2.08	0.52
1:I:347:ASN:HB3	1:I:353:GLN:HE21	1.75	0.52
1:J:114:ARG:HG2	1:J:114:ARG:NH1	2.25	0.52
1:A:287:ARG:C	1:A:289:PRO:HD2	2.34	0.52
1:B:417:LEU:N	1:B:418:PRO:CD	2.73	0.52
1:C:126:TYR:O	1:C:258:LEU:HD13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:VAL:CG2	1:C:206:GLU:OE2	2.56	0.52
1:D:114:ARG:CB	1:D:115:GLU:CA	2.88	0.52
1:E:456:VAL:C	1:E:458:GLN:H	2.18	0.52
1:G:100:GLU:O	1:G:101:GLY:C	2.52	0.52
1:E:161:HIS:NE2	1:E:203:ASP:OD1	2.43	0.52
1:H:93:LEU:HD21	1:H:110:LEU:HD11	1.92	0.52
1:L:215:PRO:O	1:L:218:ARG:NH1	2.37	0.52
1:L:272:LEU:HD13	1:L:438:GLU:OE1	2.10	0.52
1:A:266[A]:TYR:C	1:A:266[A]:TYR:CD1	2.88	0.51
1:G:66:PHE:C	1:G:66:PHE:HD1	2.17	0.51
1:G:238:ASP:OD1	1:G:240:SER:HB2	2.10	0.51
1:G:257:LEU:HD12	1:G:257:LEU:O	2.10	0.51
1:J:141:ARG:O	1:J:141:ARG:HG3	2.09	0.51
1:L:105:LEU:HB3	1:L:233:LEU:HD11	1.92	0.51
1:A:388:ILE:HB	1:A:439:THR:OG1	2.10	0.51
1:D:115:GLU:CA	1:D:116:ASP:HB3	2.38	0.51
1:E:169:LYS:O	1:E:173:PRO:HA	2.10	0.51
1:E:284:LEU:HD21	1:E:453:LEU:HD21	1.92	0.51
1:I:47:VAL:HG13	1:I:105:LEU:HD12	1.93	0.51
1:I:332:LEU:HD23	1:I:355:ILE:CD1	2.39	0.51
1:B:184:GLU:HG3	1:B:185:VAL:N	2.26	0.51
1:D:288:LEU:N	1:D:289:PRO:CD	2.73	0.51
1:I:152:ARG:NE	1:I:178:GLU:OE2	2.39	0.51
1:J:302:LYS:HB2	1:J:302:LYS:HZ2	1.73	0.51
1:A:202:VAL:HG12	2:A:501:GLU:OE1	2.10	0.51
1:C:169:LYS:HD2	1:C:175:LEU:O	2.10	0.51
1:F:212:VAL:HG21	1:F:270:ASP:O	2.09	0.51
1:G:151:LYS:HE3	1:G:199:LEU:CD1	2.40	0.51
1:J:295:PHE:CE1	1:J:310:ALA:HA	2.46	0.51
1:D:105:LEU:C	1:D:105:LEU:HD12	2.34	0.51
1:G:388:ILE:HB	1:G:439:THR:OG1	2.10	0.51
1:H:156:LEU:CD2	1:H:183:VAL:HG23	2.40	0.51
1:I:149:VAL:HG13	1:I:175:LEU:HA	1.93	0.51
1:K:457:THR:O	1:K:457:THR:HG22	2.10	0.51
1:A:50:ARG:O	1:A:55:THR:HG21	2.11	0.51
1:B:316:GLU:HA	1:B:316:GLU:OE1	2.10	0.51
1:C:309:LEU:HD13	1:C:359:SER:OG	2.11	0.51
1:G:272:LEU:HD23	1:G:274:TYR:O	2.10	0.51
1:C:152:ARG:HD3	1:C:197:ILE:HG22	1.92	0.51
1:D:93:LEU:C	1:D:93:LEU:HD23	2.36	0.51
1:E:440:VAL:O	1:E:444[A]:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:LEU:HD23	1:F:175:LEU:CD2	2.38	0.51
1:H:361:TYR:CZ	1:H:365:ILE:HD11	2.46	0.51
1:I:108:ALA:HB3	1:I:110:LEU:HD21	1.93	0.51
1:I:307:ARG:HD3	1:I:457:THR:HG21	1.92	0.51
1:J:50:ARG:HD2	1:J:184:GLU:OE2	2.10	0.51
1:K:50:ARG:HD2	1:K:184:GLU:OE2	2.10	0.51
1:A:410:TRP:O	1:A:414:LYS:HB3	2.11	0.51
1:B:239:ASP:HB3	1:B:243:ASN:ND2	2.26	0.51
1:F:329:VAL:HG21	1:F:334:MET:HE3	1.93	0.51
1:G:288:LEU:N	1:G:289:PRO:CD	2.73	0.51
1:I:302:LYS:HB2	1:I:302:LYS:NZ	2.24	0.51
1:J:131:PRO:CG	1:J:227:ARG:HH21	2.23	0.51
1:K:288:LEU:HB2	1:K:319:TRP:CZ3	2.46	0.51
1:C:121:ARG:HD3	1:C:234:PRO:O	2.11	0.51
1:G:280:PHE:HE2	1:G:452:ILE:CG2	2.24	0.51
1:J:142:PRO:HB3	1:J:147:ASP:HB2	1.93	0.51
1:J:262:LYS:HE3	1:J:266:TYR:HE2	1.73	0.51
1:K:147:ASP:C	1:K:149:VAL:H	2.11	0.51
1:L:52:SER:HB2	1:L:53:PRO:HD2	1.92	0.51
1:J:78:LEU:HD21	1:J:244:GLU:CG	2.33	0.51
1:J:297:GLN:O	1:J:301:GLN:HG3	2.11	0.51
1:K:306:TRP:CE2	1:K:307:ARG:HG3	2.46	0.51
1:L:296:LYS:HA	1:L:306:TRP:HB2	1.93	0.51
1:B:332:LEU:HD13	1:B:355:ILE:HD11	1.93	0.50
1:D:210:ASN:OD1	1:D:435:ARG:NH2	2.33	0.50
1:E:454:THR:HA	1:E:457:THR:CG2	2.40	0.50
1:H:97:LEU:O	1:H:234:PRO:HG3	2.11	0.50
1:I:152:ARG:O	1:I:198:ASP:HB2	2.11	0.50
1:I:423:LYS:HA	1:I:426:TYR:CE2	2.46	0.50
1:K:302:LYS:HZ1	1:K:359:SER:HB3	1.76	0.50
1:A:117:ASP:O	1:A:118:ALA:C	2.38	0.50
1:B:396:ALA:HB2	1:B:417:LEU:HD23	1.93	0.50
1:E:148:LEU:HD22	1:E:199:LEU:HD13	1.93	0.50
1:G:278:TYR:O	1:G:278:TYR:HD1	1.94	0.50
1:J:131:PRO:HG2	1:J:227:ARG:HH21	1.76	0.50
1:J:238:ASP:OD1	1:J:240:SER:HB2	2.11	0.50
1:K:132:GLN:O	1:K:201:LEU:HD12	2.11	0.50
1:A:56:TYR:HD1	1:A:68:TYR:HB2	1.75	0.50
1:A:238:ASP:OD1	1:A:240:SER:HB2	2.11	0.50
1:A:423:LYS:HA	1:A:426:TYR:CD2	2.46	0.50
1:B:115:GLU:CG	1:B:116:ASP:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LYS:NZ	1:C:302:LYS:CB	2.73	0.50
1:D:274:TYR:O	1:D:275:VAL:HG22	2.11	0.50
1:G:198:ASP:O	1:G:199:LEU:HD23	2.10	0.50
1:G:239:ASP:HB3	1:G:243:ASN:ND2	2.26	0.50
1:G:278:TYR:CD1	1:G:278:TYR:C	2.89	0.50
1:K:375:GLU:OE1	1:K:378:ARG:HB3	2.11	0.50
1:F:275:VAL:HG21	1:F:314:TYR:OH	2.10	0.50
1:G:53:PRO:O	1:G:209:MET:HE1	2.11	0.50
1:G:185:VAL:HG21	1:G:206:GLU:OE1	2.11	0.50
1:H:302:LYS:HB2	1:H:302:LYS:HZ3	1.75	0.50
1:I:264:ARG:HG3	1:I:264:ARG:NH1	2.16	0.50
1:K:249:LEU:O	1:K:253:LYS:HG2	2.12	0.50
1:D:455:TRP:O	1:D:457:THR:N	2.45	0.50
1:E:73:ARG:HH11	1:E:257:LEU:HD11	1.77	0.50
1:G:132:GLN:HB3	1:G:219:VAL:HG13	1.94	0.50
1:K:400:ALA:HB2	1:K:416:MET:HG3	1.93	0.50
1:E:233:LEU:HD12	1:E:233:LEU:N	2.27	0.50
1:F:314:TYR:CZ	1:F:318:LEU:HD22	2.47	0.50
1:G:205:ASN:HB2	1:G:266:TYR:CE2	2.46	0.50
1:I:51:ASN:HB2	1:I:86:THR:HG21	1.93	0.50
1:B:400:ALA:HB2	1:B:416:MET:HG3	1.93	0.50
1:D:306:TRP:O	1:D:310:ALA:N	2.35	0.50
1:F:272:LEU:HD22	1:F:315:GLN:HE22	1.77	0.50
1:G:253:LYS:O	1:G:253:LYS:HG3	2.12	0.50
1:H:127:LEU:HD21	1:H:266:TYR:CE2	2.40	0.50
1:H:403:GLU:CD	1:L:136:ARG:HH22	2.20	0.50
1:J:190:ARG:NH2	1:J:422:GLN:HG2	2.27	0.50
1:E:73:ARG:HH11	1:E:257:LEU:CD1	2.25	0.50
1:A:122:TYR:N	1:A:122:TYR:CD1	2.80	0.49
1:B:135:TYR:HB3	1:B:199:LEU:CD2	2.42	0.49
1:C:226:ALA:C	1:C:227:ARG:HG3	2.36	0.49
1:F:141:ARG:NH1	1:F:143:THR:HG22	2.27	0.49
1:G:52:SER:HB2	1:G:53:PRO:HD2	1.93	0.49
1:I:74:PHE:CZ	1:I:78:LEU:HD11	2.47	0.49
1:L:233:LEU:HG	1:L:234:PRO:CD	2.42	0.49
1:B:207:LEU:HD22	1:B:219:VAL:HG22	1.94	0.49
1:C:47:VAL:HG13	1:C:105:LEU:HD12	1.93	0.49
1:K:297:GLN:CD	1:K:352:LYS:HZ1	2.19	0.49
1:B:190:ARG:CZ	1:B:422:GLN:HG2	2.42	0.49
1:J:100:GLU:CD	1:J:100:GLU:H	2.19	0.49
1:K:133:ILE:O	1:K:134:ILE:HD13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:207:LEU:HD23	1:K:211:GLN:HB2	1.93	0.49
1:L:198:ASP:O	1:L:199:LEU:HD23	2.13	0.49
1:A:266[A]:TYR:HD1	1:A:266[A]:TYR:O	1.94	0.49
1:E:147:ASP:O	1:E:151:LYS:HE2	2.12	0.49
1:E:184:GLU:HG3	1:E:185:VAL:N	2.26	0.49
1:F:337:ASN:O	1:F:341:GLN:HG3	2.12	0.49
1:G:239:ASP:HB3	1:G:243:ASN:HD21	1.78	0.49
1:H:207:LEU:HD21	1:H:219:VAL:CG2	2.40	0.49
1:I:56:TYR:HD1	1:I:68:TYR:HB2	1.78	0.49
1:I:124:HIS:CE1	1:I:246:ASN:HD22	2.29	0.49
1:I:192:VAL:HG22	1:I:198:ASP:CG	2.37	0.49
1:J:155:VAL:HG21	1:J:161:HIS:HB2	1.94	0.49
1:L:187:ASP:OD1	1:L:422:GLN:HA	2.12	0.49
1:A:270:ASP:O	1:A:271:VAL:HG23	2.12	0.49
1:A:302:LYS:NZ	1:A:302:LYS:CB	2.75	0.49
1:B:154:MET:HB3	1:B:197:ILE:CD1	2.42	0.49
1:F:421:ALA:HA	1:F:433:TYR:HE1	1.78	0.49
1:J:148:LEU:HD12	1:J:168:LEU:CD2	2.41	0.49
1:L:417:LEU:N	1:L:418:PRO:CD	2.75	0.49
1:D:309:LEU:HD13	1:D:359:SER:OG	2.13	0.49
1:D:324:THR:CG2	1:D:325:SER:N	2.75	0.49
1:F:126:TYR:HB2	1:F:258:LEU:CD1	2.43	0.49
1:D:146:GLU:O	1:D:149:VAL:HG23	2.13	0.49
1:E:273:GLY:O	1:E:274:TYR:CB	2.60	0.49
1:F:280:PHE:CE2	1:F:452:ILE:HG21	2.47	0.49
1:J:43:GLY:C	1:J:80:VAL:HG13	2.37	0.49
1:L:240:SER:O	1:L:242:MET:CB	2.61	0.49
1:B:371:GLU:O	1:B:371:GLU:HG2	2.13	0.49
1:C:205:ASN:HB2	1:C:266[B]:TYR:CE2	2.48	0.49
1:F:209:MET:HG2	1:F:210:ASN:ND2	2.27	0.49
1:I:329:VAL:HG23	1:I:334:MET:CE	2.41	0.49
1:J:136:ARG:NH1	1:J:193:ASP:O	2.40	0.49
1:D:112:PRO:HA	1:D:122:TYR:CE2	2.48	0.49
1:E:278:TYR:CZ	1:E:282:GLN:NE2	2.81	0.49
1:K:284:LEU:HD23	1:K:288:LEU:HD23	1.94	0.49
1:L:375:GLU:HB3	1:L:376:PRO:HA	1.95	0.49
1:A:257:LEU:HD12	1:A:257:LEU:O	2.13	0.49
1:G:302:LYS:NZ	1:G:302:LYS:CB	2.76	0.49
1:J:185:VAL:HG21	1:J:206:GLU:OE1	2.13	0.49
1:L:239:ASP:O	1:L:242:MET:CB	2.55	0.49
1:G:119:SER:O	1:G:120:VAL:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:187:ASP:HA	1:L:190:ARG:NH1	2.26	0.48
1:A:55:THR:HG22	1:A:56:TYR:HB3	1.95	0.48
1:B:154:MET:CB	1:B:197:ILE:HD12	2.43	0.48
1:B:329:VAL:CG2	1:B:334:MET:HE3	2.43	0.48
1:C:392:HIS:O	1:C:395:ASP:HB2	2.13	0.48
1:D:212:VAL:HG21	1:D:270:ASP:HB3	1.95	0.48
1:H:193:ASP:OD1	1:H:216:ASN:HB2	2.12	0.48
1:L:151:LYS:HD2	1:L:199:LEU:HD11	1.95	0.48
1:L:271:VAL:HB	1:L:272:LEU:HD13	1.94	0.48
1:G:309:LEU:HD22	1:G:359:SER:OG	2.13	0.48
1:K:144:ARG:O	1:K:146:GLU:HG3	2.13	0.48
1:K:147:ASP:CB	1:K:149:VAL:HB	2.43	0.48
1:K:259:GLN:OE1	1:K:262:LYS:NZ	2.28	0.48
1:L:74:PHE:HE1	1:L:245:VAL:HA	1.75	0.48
1:A:106:ALA:HB3	1:A:232:ALA:HB3	1.94	0.48
1:A:302:LYS:HE2	1:A:360:LYS:N	2.29	0.48
1:A:391:ALA:O	1:A:394:GLU:HB3	2.13	0.48
1:D:109:GLY:HA2	1:D:229:LEU:HD13	1.95	0.48
1:D:213:TYR:HE2	1:D:438:GLU:HG3	1.78	0.48
1:F:457:THR:HG22	1:F:457:THR:O	2.13	0.48
1:I:198:ASP:OD1	1:I:199:LEU:C	2.56	0.48
1:L:388:ILE:HG23	1:L:389:GLY:O	2.13	0.48
1:G:122:TYR:N	1:G:122:TYR:CD1	2.81	0.48
1:G:212:VAL:HG11	1:G:269:VAL:CG2	2.33	0.48
1:H:270:ASP:HB2	1:H:271:VAL:HA	1.95	0.48
1:I:279:THR:O	1:I:282:GLN:HB3	2.13	0.48
1:J:156:LEU:N	1:J:156:LEU:HD12	2.29	0.48
1:L:114:ARG:HG3	1:L:115:GLU:H	1.79	0.48
1:D:302:LYS:NZ	1:D:302:LYS:CB	2.74	0.48
1:F:44:VAL:HG22	1:F:81:GLU:HB3	1.94	0.48
1:F:56:TYR:HD1	1:F:68:TYR:HB2	1.78	0.48
1:G:212:VAL:CG1	1:G:269:VAL:HG11	2.43	0.48
1:I:121:ARG:NH1	1:I:236:GLY:HA2	2.29	0.48
1:I:209:MET:HE3	1:I:266:TYR:CD1	2.49	0.48
1:J:391:ALA:HB1	1:J:431:TYR:CD1	2.48	0.48
1:A:264:ARG:CG	1:A:264:ARG:NH1	2.74	0.48
1:B:235:GLY:HA2	1:B:236:GLY:HA3	1.54	0.48
1:C:350:ASP:HB3	1:C:353:GLN:HG3	1.96	0.48
1:C:412:ASP:HA	1:C:415:LYS:HE3	1.96	0.48
1:I:164:GLN:HG2	1:I:223:PHE:CE2	2.48	0.48
1:J:269:VAL:CG2	1:J:272:LEU:HD11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:55:THR:OG1	1:K:56:TYR:N	2.47	0.48
1:L:296:LYS:HA	1:L:306:TRP:CB	2.43	0.48
1:A:153:ILE:HG12	1:A:199:LEU:HB2	1.96	0.48
1:C:114:ARG:C	1:C:116:ASP:H	2.22	0.48
1:D:135:TYR:HE1	1:D:220:ALA:HA	1.79	0.48
1:F:131:PRO:HG2	1:F:227:ARG:NH2	2.29	0.48
1:J:77:ARG:HD2	1:J:248:PHE:HD1	1.79	0.48
1:K:49:THR:O	1:K:86:THR:HA	2.13	0.48
1:K:190:ARG:NH1	1:K:422:GLN:HG2	2.28	0.48
1:L:233:LEU:HD21	1:L:241:LEU:HB3	1.94	0.48
1:L:240:SER:O	1:L:242:MET:HB3	2.13	0.48
1:L:255:GLU:HG2	1:L:260:ARG:NH2	2.28	0.48
1:A:116:ASP:C	1:A:118:ALA:H	2.22	0.48
1:B:423:LYS:HA	1:B:426:TYR:CD2	2.48	0.48
1:H:421:ALA:HA	1:H:433:TYR:CE1	2.49	0.48
1:I:197:ILE:CG1	1:I:198:ASP:HB3	2.44	0.48
1:J:225:GLU:HG2	1:J:226:ALA:O	2.14	0.48
1:B:142:PRO:HG3	1:B:199:LEU:HD11	1.96	0.48
1:C:156:LEU:N	1:C:156:LEU:HD12	2.29	0.48
1:D:50:ARG:NH2	1:D:184:GLU:OE2	2.41	0.48
1:E:375:GLU:HB3	1:E:376:PRO:HA	1.95	0.48
1:H:153:ILE:HG12	1:H:199:LEU:HB2	1.94	0.48
1:I:388:ILE:HB	1:I:439:THR:OG1	2.13	0.48
1:K:112:PRO:HA	1:K:122:TYR:CE2	2.48	0.48
1:A:190:ARG:O	1:A:194:VAL:HG22	2.14	0.47
1:B:115:GLU:HG3	1:B:116:ASP:CG	2.39	0.47
1:F:149:VAL:HG11	1:F:174:GLU:HG3	1.96	0.47
1:F:319:TRP:HA	1:F:332:LEU:HD11	1.96	0.47
1:L:88:ASP:O	1:L:423:LYS:NZ	2.38	0.47
1:L:400:ALA:HB2	1:L:416:MET:HG3	1.96	0.47
1:D:324:THR:HG22	1:D:325:SER:N	2.29	0.47
1:E:269:VAL:O	1:E:270:ASP:CB	2.61	0.47
1:E:284:LEU:HD21	1:E:453:LEU:CD2	2.44	0.47
1:G:116:ASP:OD1	1:G:117:ASP:N	2.47	0.47
1:H:73:ARG:HD2	1:H:257:LEU:CD2	2.43	0.47
1:I:271:VAL:HG12	1:I:272:LEU:HA	1.94	0.47
1:J:448:ARG:HG3	1:J:448:ARG:HH11	1.79	0.47
1:B:423:LYS:HA	1:B:426:TYR:CE2	2.49	0.47
1:C:393:LEU:O	1:C:397:ARG:HG3	2.15	0.47
1:E:148:LEU:HD22	1:E:199:LEU:CD1	2.45	0.47
1:E:268:HIS:CE1	1:E:326:LYS:NZ	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:126:TYR:CE2	1:H:231:TRP:CD1	3.02	0.47
1:H:375:GLU:HB3	1:H:376:PRO:HA	1.95	0.47
1:L:338:ARG:HG2	1:L:338:ARG:HH11	1.78	0.47
1:G:73:ARG:O	1:G:77:ARG:HG2	2.14	0.47
1:G:166:ALA:HA	1:G:169:LYS:NZ	2.30	0.47
1:G:184:GLU:O	1:G:187:ASP:HB2	2.15	0.47
1:K:117:ASP:C	1:K:119:SER:N	2.68	0.47
1:K:343:MET:SD	1:K:360:LYS:HG3	2.55	0.47
1:A:388:ILE:HG12	1:A:388:ILE:O	2.15	0.47
1:C:141:ARG:NH1	1:C:141:ARG:HG2	2.28	0.47
1:D:135:TYR:CZ	1:D:141:ARG:HB2	2.49	0.47
1:H:176:LYS:NZ	1:H:177:TYR:O	2.48	0.47
1:I:238:ASP:C	1:I:240:SER:H	2.22	0.47
1:I:336:THR:HG23	1:I:339:THR:HB	1.96	0.47
1:C:48:ILE:HA	1:C:85:GLU:O	2.14	0.47
1:C:288:LEU:N	1:C:289:PRO:CD	2.77	0.47
1:C:426:TYR:CE2	1:C:433:TYR:HB2	2.49	0.47
1:F:111:THR:HG22	1:F:112:PRO:O	2.15	0.47
1:G:151:LYS:CE	1:G:199:LEU:HD11	2.44	0.47
1:A:244:GLU:H	1:A:244:GLU:CD	2.04	0.47
1:D:144:ARG:NH1	1:D:146:GLU:OE1	2.36	0.47
1:D:316:GLU:OE2	1:D:386:TYR:HE1	1.98	0.47
1:G:308:LEU:O	1:G:312:ILE:HG13	2.15	0.47
1:I:42:GLU:O	1:I:44:VAL:HG23	2.14	0.47
1:I:183:VAL:HG11	1:I:191:MET:HE1	1.96	0.47
1:I:415:LYS:HB3	1:I:415:LYS:HE3	1.78	0.47
1:J:55:THR:O	1:J:65:GLY:HA3	2.14	0.47
1:K:167:GLU:HG2	1:K:170:LYS:HE3	1.95	0.47
1:K:272:LEU:HD13	1:K:441:HIS:ND1	2.30	0.47
1:L:292:GLU:O	1:L:296:LYS:HB2	2.15	0.47
1:A:288:LEU:HD12	1:A:288:LEU:O	2.15	0.47
1:A:417:LEU:O	1:A:436:GLY:HA3	2.13	0.47
1:H:329:VAL:HG23	1:H:334:MET:CE	2.45	0.47
1:I:419:ARG:HH11	1:I:419:ARG:HG2	1.79	0.47
1:K:455:TRP:CE3	1:K:456:VAL:HG13	2.50	0.47
1:L:49:THR:O	1:L:86:THR:HA	2.15	0.47
1:L:269:VAL:O	1:L:270:ASP:CB	2.62	0.47
1:C:170:LYS:O	1:C:173:PRO:HD3	2.15	0.47
1:D:375:GLU:HB3	1:D:376:PRO:HA	1.96	0.47
1:F:55:THR:OG1	1:F:56:TYR:N	2.48	0.47
1:G:69:GLU:OE2	1:G:265:TYR:OH	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:156:LEU:HD23	1:L:156:LEU:HA	1.66	0.47
1:L:302:LYS:CD	1:L:360:LYS:HG2	2.44	0.47
1:L:423:LYS:HA	1:L:426:TYR:CD2	2.50	0.47
1:A:115:GLU:HG3	1:A:116:ASP:H	1.79	0.47
1:A:148:LEU:CD2	1:A:199:LEU:HD13	2.45	0.47
1:C:66:PHE:CD1	1:C:66:PHE:C	2.92	0.47
1:C:233:LEU:HD22	1:C:242:MET:HE2	1.96	0.47
1:D:112:PRO:HA	1:D:122:TYR:CD2	2.50	0.47
1:D:400:ALA:HB2	1:D:416:MET:HG3	1.97	0.47
1:F:131:PRO:HB2	1:F:223:PHE:O	2.15	0.47
1:K:146:GLU:OE2	1:K:147:ASP:O	2.31	0.47
1:K:207:LEU:HD23	1:K:207:LEU:O	2.15	0.47
1:D:332:LEU:HD23	1:D:355:ILE:HG13	1.97	0.46
1:E:52:SER:CB	1:E:53:PRO:HD2	2.45	0.46
1:J:269:VAL:O	1:J:269:VAL:HG22	2.15	0.46
1:K:297:GLN:O	1:K:301:GLN:HG3	2.15	0.46
1:L:105:LEU:CB	1:L:233:LEU:HD12	2.45	0.46
1:D:421:ALA:HA	1:D:433:TYR:CD1	2.50	0.46
1:E:112:PRO:HA	1:E:122:TYR:CE2	2.51	0.46
1:E:287:ARG:O	1:E:290:ARG:HG2	2.15	0.46
1:E:448:ARG:HG3	1:E:448:ARG:HH11	1.80	0.46
1:G:329:VAL:CG2	1:G:334:MET:HE3	2.44	0.46
1:H:316:GLU:OE1	1:H:316:GLU:HA	2.16	0.46
1:J:171:GLN:HG3	1:J:172:TYR:CE1	2.50	0.46
1:L:302:LYS:HE2	1:L:360:LYS:HG2	1.97	0.46
1:C:157:LYS:HB3	1:C:181:ASP:OD1	2.14	0.46
1:D:388:ILE:HD11	1:D:434:ALA:HB1	1.96	0.46
1:E:77:ARG:HD2	1:E:248:PHE:HD1	1.80	0.46
1:E:135:TYR:CE1	1:E:218:ARG:HB2	2.51	0.46
1:F:257:LEU:HD12	1:F:257:LEU:O	2.16	0.46
1:G:151:LYS:HE3	1:G:199:LEU:HD11	1.95	0.46
1:G:285:GLN:HG3	1:G:286:GLN:N	2.30	0.46
1:H:198:ASP:O	1:H:199:LEU:HD23	2.15	0.46
1:H:385:ALA:HB2	1:H:393:LEU:HD22	1.97	0.46
1:I:77:ARG:O	1:I:77:ARG:HG2	2.15	0.46
1:I:232:ALA:C	1:I:233:LEU:HD12	2.40	0.46
1:L:271:VAL:CB	1:L:272:LEU:CA	2.91	0.46
1:A:258:LEU:HD23	1:A:258:LEU:HA	1.38	0.46
1:D:66:PHE:CE1	1:D:261:LEU:CB	2.98	0.46
1:D:416:MET:O	1:D:419:ARG:HB2	2.16	0.46
1:E:233:LEU:HD22	1:E:242:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:ALA:HB1	1:E:257:LEU:HB3	1.97	0.46
1:E:348:ARG:NH2	1:K:237:ASP:OD1	2.49	0.46
1:F:169:LYS:HD2	1:F:175:LEU:O	2.16	0.46
1:I:198:ASP:CG	1:I:199:LEU:N	2.70	0.46
1:A:135:TYR:CE2	1:A:141:ARG:HB2	2.51	0.46
1:F:72:LYS:HD2	1:F:72:LYS:O	2.16	0.46
1:L:298:SER:HA	1:L:301:GLN:HB2	1.96	0.46
1:A:416:MET:HE2	1:A:416:MET:HA	1.97	0.46
1:E:260:ARG:HG3	1:E:260:ARG:HH11	1.80	0.46
1:H:114:ARG:HB2	1:H:116:ASP:H	1.80	0.46
1:I:337:ASN:O	1:I:341:GLN:HG3	2.15	0.46
1:J:78:LEU:CD2	1:J:244:GLU:HG2	2.35	0.46
1:K:268:HIS:HE1	1:K:326:LYS:CE	2.28	0.46
1:L:74:PHE:CZ	1:L:245:VAL:HG22	2.51	0.46
1:A:302:LYS:CB	1:A:302:LYS:HZ2	2.28	0.46
1:C:145:PRO:HD3	1:C:221:PHE:CE2	2.51	0.46
1:C:164:GLN:NE2	1:C:223:PHE:O	2.46	0.46
1:D:115:GLU:CB	1:D:117:ASP:H	2.20	0.46
1:D:279:THR:CG2	1:D:283:HIS:CE1	2.99	0.46
1:E:60:ARG:HG3	1:E:61:ASN:OD1	2.15	0.46
1:F:136:ARG:HD2	1:F:192:VAL:O	2.16	0.46
1:F:380:TRP:CH2	1:F:447:ARG:CD	2.98	0.46
1:F:419:ARG:HG2	1:F:419:ARG:HH11	1.80	0.46
1:G:319:TRP:HA	1:G:332:LEU:HD11	1.98	0.46
1:J:96:GLN:O	1:J:103:PRO:HD2	2.16	0.46
1:J:156:LEU:HD12	1:J:188:LEU:HD11	1.98	0.46
1:J:208:ALA:CB	1:J:266:TYR:CD1	2.99	0.46
1:K:64:THR:CG2	1:K:65:GLY:H	2.28	0.46
1:A:148:LEU:HB2	1:A:175:LEU:HD13	1.98	0.46
1:A:312:ILE:O	1:A:316:GLU:HG2	2.15	0.46
1:C:141:ARG:HG2	1:C:141:ARG:HH11	1.81	0.46
1:F:426:TYR:HA	1:F:429:THR:CG2	2.45	0.46
1:I:241:LEU:CD1	1:I:245:VAL:HG23	2.46	0.46
1:J:66:PHE:CD1	1:J:66:PHE:C	2.93	0.46
1:J:80:VAL:HG12	1:J:81:GLU:N	2.30	0.46
1:K:114:ARG:NH1	1:K:116:ASP:O	2.40	0.46
1:C:47:VAL:HG13	1:C:105:LEU:CD1	2.46	0.46
1:D:90:LEU:HA	1:D:90:LEU:HD23	1.70	0.46
1:I:152:ARG:O	1:I:198:ASP:CA	2.64	0.46
1:I:302:LYS:HZ1	1:I:359:SER:HB3	1.80	0.46
1:K:329:VAL:CG2	1:K:334:MET:HE3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLN:NE2	1:A:223:PHE:CD2	2.84	0.46
1:B:135:TYR:HD1	1:B:220:ALA:HB2	1.75	0.46
1:C:239:ASP:HB3	1:C:243:ASN:OD1	2.16	0.46
1:D:265:TYR:C	1:D:266:TYR:CD1	2.89	0.46
1:E:144:ARG:CG	1:E:145:PRO:CD	2.84	0.46
1:H:275:VAL:HA	1:H:276:GLY:HA3	1.73	0.46
1:J:377:ASP:OD2	1:J:409:LYS:HA	2.16	0.46
1:C:156:LEU:HD12	1:C:188:LEU:HD11	1.98	0.45
1:E:403:GLU:HG3	1:E:416:MET:SD	2.56	0.45
1:H:50:ARG:HD2	1:H:184:GLU:OE2	2.16	0.45
1:I:154:MET:O	1:I:200:THR:OG1	2.32	0.45
1:J:97:LEU:O	1:J:234:PRO:HG3	2.15	0.45
1:L:131:PRO:HB2	1:L:223:PHE:O	2.16	0.45
1:A:115:GLU:C	1:A:116:ASP:CG	2.84	0.45
1:B:281:ALA:O	1:B:284:LEU:HB2	2.16	0.45
1:D:205:ASN:HB2	1:D:266:TYR:HE2	1.78	0.45
1:J:381:PHE:CZ	1:J:413:VAL:HG21	2.51	0.45
1:L:88:ASP:HB2	1:L:89:ASN:ND2	2.31	0.45
1:B:145:PRO:HD3	1:B:221:PHE:CE2	2.50	0.45
1:C:148:LEU:HB3	1:C:153:ILE:HD11	1.98	0.45
1:E:105:LEU:HD12	1:E:105:LEU:C	2.41	0.45
1:F:261:LEU:HD23	1:F:264:ARG:NH1	2.32	0.45
1:A:92:ASP:O	1:A:96:GLN:HG2	2.16	0.45
1:G:265:TYR:O	1:G:267:GLY:CA	2.64	0.45
1:G:278:TYR:HD1	1:G:278:TYR:C	2.25	0.45
1:G:456:VAL:HG23	1:G:457:THR:HG23	1.98	0.45
1:H:149:VAL:HG11	1:H:174:GLU:HG3	1.99	0.45
1:J:254:LYS:C	1:J:256:GLY:H	2.24	0.45
1:L:329:VAL:HG23	1:L:334:MET:CE	2.45	0.45
1:B:284:LEU:HD23	1:B:284:LEU:HA	1.83	0.45
1:B:340:ALA:HB1	1:B:345:VAL:HB	1.97	0.45
1:C:329:VAL:CG2	1:C:334:MET:HE3	2.47	0.45
1:F:222:ASP:OD1	1:F:222:ASP:N	2.48	0.45
1:F:458:GLN:OE1	1:F:458:GLN:HA	2.17	0.45
1:I:198:ASP:OD1	1:I:199:LEU:CA	2.64	0.45
1:I:250:ASP:OD1	1:I:251:GLN:HG3	2.17	0.45
1:J:321:PRO:O	1:J:331:GLY:HA2	2.17	0.45
1:K:209:MET:HB2	1:K:209:MET:HE3	1.67	0.45
1:L:257:LEU:O	1:L:257:LEU:HD12	2.16	0.45
1:L:271:VAL:HB	1:L:272:LEU:CA	2.45	0.45
1:A:272:LEU:HD11	1:A:441:HIS:ND1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:252:ALA:HA	1:G:255:GLU:CG	2.37	0.45
1:G:411:LEU:HD23	1:G:411:LEU:O	2.17	0.45
1:I:243:ASN:HA	1:I:246:ASN:OD1	2.17	0.45
1:I:247:ALA:O	1:I:248:PHE:C	2.59	0.45
1:J:145:PRO:O	1:J:148:LEU:HG	2.17	0.45
1:B:161:HIS:NE2	1:B:203:ASP:OD1	2.47	0.45
1:C:64:THR:OG1	1:C:65:GLY:N	2.50	0.45
1:D:281:ALA:O	1:D:284:LEU:HB2	2.16	0.45
1:F:47:VAL:HG13	1:F:105:LEU:CD1	2.47	0.45
1:F:55:THR:HA	1:F:67:GLU:HG2	1.98	0.45
1:F:172:TYR:O	1:F:174:GLU:N	2.50	0.45
1:G:125:THR:HA	1:G:229:LEU:O	2.17	0.45
1:G:274:TYR:CE1	1:G:448:ARG:HG2	2.51	0.45
1:I:51:ASN:HB2	1:I:86:THR:CG2	2.47	0.45
1:J:114:ARG:O	1:J:115:GLU:HB2	2.17	0.45
1:L:134:ILE:O	1:L:199:LEU:HA	2.17	0.45
1:B:126:TYR:CE2	1:B:230:ALA:HA	2.52	0.45
1:C:175:LEU:HD12	1:C:176:LYS:N	2.32	0.45
1:F:73:ARG:NH1	1:F:257:LEU:HD13	2.32	0.45
1:F:453:LEU:HA	1:F:453:LEU:HD23	1.64	0.45
1:H:92:ASP:O	1:H:96:GLN:HG2	2.17	0.45
1:H:209:MET:HE1	1:H:266:TYR:HE1	1.82	0.45
1:I:191:MET:HB3	1:I:197:ILE:HG12	1.99	0.45
1:K:148:LEU:CB	1:K:153:ILE:HD11	2.41	0.45
1:K:284:LEU:HD23	1:K:288:LEU:CD2	2.46	0.45
1:A:209:MET:HE3	1:A:209:MET:HB2	1.65	0.45
1:C:141:ARG:HH11	1:C:141:ARG:CG	2.30	0.45
1:C:185:VAL:CG1	1:C:206:GLU:OE2	2.64	0.45
1:C:329:VAL:HG23	1:C:334:MET:HE3	1.98	0.45
1:D:254:LYS:HA	1:D:254:LYS:HD3	1.77	0.45
1:H:127:LEU:CD1	1:H:262:LYS:HG3	2.45	0.45
1:I:302:LYS:HE2	1:I:360:LYS:N	2.31	0.45
1:L:133:ILE:HD13	1:L:201:LEU:HD13	1.99	0.45
1:H:122:TYR:N	1:H:122:TYR:CD1	2.85	0.45
1:I:121:ARG:NH1	1:I:121:ARG:HG2	2.28	0.45
1:I:176:LYS:HD2	1:I:176:LYS:HA	1.77	0.45
1:I:239:ASP:CB	1:I:243:ASN:HD21	2.30	0.45
1:J:165:LEU:O	1:J:169:LYS:N	2.50	0.45
1:L:370:PRO:HG2	1:L:397:ARG:HH12	1.81	0.45
1:A:284:LEU:HD23	1:A:288:LEU:HD23	2.00	0.44
1:B:46:ARG:HG2	1:B:83:LYS:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:SER:HB2	1:B:408:ASN:OD1	2.16	0.44
1:E:350:ASP:HB3	1:E:353:GLN:OE1	2.17	0.44
1:F:74:PHE:HB2	1:F:248:PHE:CE2	2.52	0.44
1:K:70:LEU:HD12	1:K:71:ALA:N	2.32	0.44
1:K:114:ARG:HH11	1:K:114:ARG:HB3	1.83	0.44
1:L:371:GLU:O	1:L:374:LYS:NZ	2.39	0.44
1:L:381:PHE:CD2	1:L:393:LEU:HD21	2.52	0.44
1:A:73:ARG:HD2	1:A:257:LEU:CD2	2.47	0.44
1:A:159:SER:HB2	2:A:501:GLU:N	2.32	0.44
1:A:302:LYS:NZ	1:A:359:SER:HB3	2.32	0.44
1:B:457:THR:CA	1:B:458:GLN:CB	2.87	0.44
1:E:229:LEU:N	1:E:229:LEU:HD23	2.32	0.44
1:E:352:LYS:HG2	1:E:353:GLN:N	2.31	0.44
1:G:185:VAL:HG11	1:G:206:GLU:HB3	1.98	0.44
1:H:152:ARG:NH1	1:H:196:ASP:O	2.50	0.44
1:H:235:GLY:HA2	1:H:236:GLY:HA3	1.72	0.44
1:J:147:ASP:O	1:J:151:LYS:HE2	2.16	0.44
1:A:53:PRO:HG3	1:A:186:VAL:HG21	1.99	0.44
1:A:241:LEU:O	1:A:244:GLU:CD	2.60	0.44
1:C:49:THR:OG1	1:C:50:ARG:N	2.51	0.44
1:D:233:LEU:HD12	1:D:233:LEU:N	2.32	0.44
1:E:185:VAL:HG21	1:E:206:GLU:OE1	2.16	0.44
1:G:72:LYS:HA	1:G:82:LEU:HD22	1.99	0.44
1:G:134:ILE:HB	1:G:200:THR:HG22	1.99	0.44
1:J:207:LEU:HD21	1:J:211:GLN:OE1	2.17	0.44
1:L:133:ILE:O	1:L:134:ILE:HD13	2.18	0.44
1:D:336:THR:HG23	1:D:339:THR:HB	2.00	0.44
1:H:412:ASP:O	1:H:415:LYS:HB2	2.16	0.44
1:I:136:ARG:N	1:I:136:ARG:CD	2.79	0.44
1:J:50:ARG:NH1	1:J:184:GLU:OE2	2.50	0.44
1:J:77:ARG:O	1:J:77:ARG:HG2	2.17	0.44
1:J:254:LYS:C	1:J:256:GLY:N	2.73	0.44
1:J:392:HIS:CD2	1:J:434:ALA:HB2	2.52	0.44
1:K:302:LYS:HE2	1:K:360:LYS:N	2.33	0.44
1:L:92:ASP:HA	1:L:95:ALA:HB3	2.00	0.44
1:L:384:ALA:O	1:L:388:ILE:HG22	2.17	0.44
1:A:48:ILE:HA	1:A:85:GLU:O	2.17	0.44
1:B:118:ALA:O	1:H:349:LEU:HD13	2.17	0.44
1:B:203:ASP:O	1:B:206:GLU:HB2	2.18	0.44
1:B:260:ARG:HG3	1:B:260:ARG:NH1	2.32	0.44
1:C:291:TYR:OH	1:C:321:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:ALA:HA	1:C:433:TYR:CD1	2.52	0.44
1:D:336:THR:HG23	1:D:339:THR:CB	2.47	0.44
1:E:161:HIS:HE2	1:E:203:ASP:CG	2.25	0.44
1:F:126:TYR:O	1:F:258:LEU:HD13	2.17	0.44
1:F:156:LEU:HD23	1:F:156:LEU:HA	1.71	0.44
1:F:426:TYR:CD1	1:F:426:TYR:C	2.95	0.44
1:G:148:LEU:HD23	1:G:151:LYS:NZ	2.23	0.44
1:I:171:GLN:O	1:I:172:TYR:CD1	2.70	0.44
1:I:269:VAL:O	1:I:270:ASP:HB2	2.17	0.44
1:I:288:LEU:N	1:I:289:PRO:CD	2.80	0.44
1:K:284:LEU:HD21	1:K:453:LEU:CD2	2.48	0.44
1:L:241:LEU:HD12	1:L:241:LEU:O	2.17	0.44
1:A:210:ASN:O	1:A:211:GLN:C	2.59	0.44
1:F:419:ARG:HD3	1:F:425:TRP:CE2	2.53	0.44
1:G:113:GLY:O	1:G:114:ARG:C	2.60	0.44
1:H:297:GLN:O	1:H:301:GLN:HG3	2.17	0.44
1:I:209:MET:HE3	1:I:209:MET:HB2	1.70	0.44
1:J:142:PRO:CB	1:J:147:ASP:HB2	2.47	0.44
1:K:288:LEU:HD12	1:K:288:LEU:O	2.18	0.44
1:A:125:THR:HA	1:A:229:LEU:O	2.17	0.44
1:B:456:VAL:C	1:B:457:THR:HG1	2.20	0.44
1:D:329:VAL:HG23	1:D:334:MET:HE3	2.00	0.44
1:E:88:ASP:O	1:E:423:LYS:NZ	2.47	0.44
1:E:337:ASN:O	1:E:341:GLN:HG3	2.18	0.44
1:G:207:LEU:O	1:G:207:LEU:HG	2.17	0.44
1:H:168:LEU:HD23	1:H:175:LEU:HD13	2.00	0.44
1:J:127:LEU:CD2	1:J:129:VAL:HG13	2.41	0.44
1:K:112:PRO:HB2	1:K:113:GLY:H	1.55	0.44
1:L:50:ARG:NH1	1:L:184:GLU:OE1	2.51	0.44
1:A:302:LYS:HE2	1:A:359:SER:C	2.43	0.44
1:B:114:ARG:HG2	1:B:115:GLU:N	2.33	0.44
1:B:302:LYS:HD2	1:B:363:VAL:HG21	2.00	0.44
1:C:260:ARG:HH11	1:C:260:ARG:HG3	1.83	0.44
1:D:271:VAL:HG12	1:D:272:LEU:H	1.80	0.44
1:D:388:ILE:HG12	1:D:388:ILE:O	2.18	0.44
1:E:50:ARG:HD3	1:E:90:LEU:HD21	1.99	0.44
1:E:55:THR:OG1	1:E:56:TYR:N	2.51	0.44
1:F:288:LEU:N	1:F:289:PRO:CD	2.81	0.44
1:G:268:HIS:HA	1:G:269:VAL:CG2	2.46	0.44
1:I:332:LEU:CD2	1:I:355:ILE:HD11	2.46	0.44
1:I:336:THR:HG23	1:I:339:THR:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:392:HIS:CD2	1:I:434:ALA:HB2	2.53	0.44
1:K:322:GLY:HA2	1:K:349:LEU:HD22	2.00	0.44
1:A:133:ILE:HD13	1:A:201:LEU:HD13	1.99	0.44
1:A:338:ARG:CG	1:A:338:ARG:NH1	2.76	0.44
1:D:280:PHE:O	1:D:284:LEU:N	2.44	0.44
1:F:272:LEU:HD22	1:F:315:GLN:NE2	2.32	0.44
1:L:64:THR:OG1	1:L:65:GLY:N	2.51	0.44
1:L:67:GLU:OE1	1:L:107:ALA:HB1	2.18	0.44
1:B:122:TYR:CD1	1:B:122:TYR:N	2.86	0.43
1:I:233:LEU:HD22	1:I:242:MET:HE2	1.99	0.43
1:I:295:PHE:CZ	1:I:310:ALA:HA	2.53	0.43
1:I:417:LEU:N	1:I:418:PRO:CD	2.80	0.43
1:K:115:GLU:CB	1:K:116:ASP:CG	2.90	0.43
1:L:302:LYS:HZ3	1:L:359:SER:CB	2.30	0.43
1:L:423:LYS:C	1:L:425:TRP:N	2.75	0.43
1:B:233:LEU:HD13	1:B:242:MET:CE	2.49	0.43
1:C:133:ILE:O	1:C:134:ILE:HD13	2.18	0.43
1:D:213:TYR:CE2	1:D:438:GLU:HG3	2.54	0.43
1:F:126:TYR:CE1	1:F:230:ALA:HA	2.52	0.43
1:H:105:LEU:C	1:H:105:LEU:HD12	2.43	0.43
1:H:134:ILE:HG21	1:H:217:VAL:CG2	2.48	0.43
1:H:176:LYS:HE3	1:L:157:LYS:HE3	2.00	0.43
1:K:148:LEU:HB2	1:K:175:LEU:HD11	2.00	0.43
1:A:161:HIS:CE1	2:A:501:GLU:HB2	2.53	0.43
1:B:156:LEU:HA	1:B:156:LEU:HD23	1.80	0.43
1:F:209:MET:CE	1:F:266:TYR:CE1	2.96	0.43
1:H:350:ASP:HB3	1:H:353:GLN:HB2	2.00	0.43
1:L:307:ARG:CZ	1:L:454:THR:CG2	2.96	0.43
1:B:161:HIS:HB3	1:B:201:LEU:HD23	2.00	0.43
1:B:291:TYR:O	1:B:294:HIS:HB2	2.19	0.43
1:F:105:LEU:HD12	1:F:105:LEU:C	2.44	0.43
1:F:106:ALA:N	1:F:232:ALA:O	2.37	0.43
1:F:364:GLN:O	1:F:368:GLU:HG2	2.19	0.43
1:H:270:ASP:CB	1:H:271:VAL:HA	2.49	0.43
1:H:388:ILE:HB	1:H:439:THR:OG1	2.19	0.43
1:J:73:ARG:HA	1:J:76:GLU:HG3	2.00	0.43
1:J:252:ALA:HA	1:J:255:GLU:HB3	2.00	0.43
1:J:400:ALA:CB	1:J:416:MET:HG3	2.47	0.43
1:L:297:GLN:NE2	1:L:297:GLN:HA	2.33	0.43
1:C:439:THR:O	1:C:442:PHE:HB3	2.18	0.43
1:D:72:LYS:HA	1:D:82:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144:ARG:HG2	1:J:146:GLU:H	1.83	0.43
1:K:133:ILE:C	1:K:134:ILE:HD13	2.44	0.43
1:A:50:ARG:HD3	1:A:90:LEU:HD21	2.01	0.43
1:A:55:THR:HG22	1:A:56:TYR:CB	2.49	0.43
1:C:209:MET:HB2	1:C:209:MET:HE3	1.65	0.43
1:C:414:LYS:NZ	1:C:444[A]:GLN:HG3	2.33	0.43
1:G:148:LEU:CD2	1:G:151:LYS:HZ1	2.22	0.43
1:G:316:GLU:HA	1:G:316:GLU:OE1	2.19	0.43
1:H:70:LEU:HD12	1:H:70:LEU:HA	1.75	0.43
1:I:197:ILE:HG13	1:I:198:ASP:CB	2.48	0.43
1:A:122:TYR:N	1:A:122:TYR:HD1	2.16	0.43
1:A:288:LEU:N	1:A:289:PRO:CD	2.81	0.43
1:B:77:ARG:O	1:B:77:ARG:HG2	2.18	0.43
1:B:412:ASP:O	1:B:415:LYS:HB2	2.18	0.43
1:C:213:TYR:CE2	1:C:435:ARG:CZ	3.02	0.43
1:G:163:GLU:O	1:G:166:ALA:HB3	2.19	0.43
1:K:155:VAL:CG2	1:K:156:LEU:N	2.81	0.43
1:K:405:LEU:HB3	1:K:412:ASP:OD2	2.19	0.43
1:B:392:HIS:O	1:B:395:ASP:HB2	2.19	0.43
1:C:203:ASP:HB3	1:C:205:ASN:OD1	2.19	0.43
1:F:146:GLU:HG3	1:F:172:TYR:HE2	1.83	0.43
1:G:288:LEU:HA	1:G:288:LEU:HD12	1.68	0.43
1:I:152:ARG:O	1:I:198:ASP:CB	2.67	0.43
1:J:120:VAL:HG12	1:J:122:TYR:CE1	2.53	0.43
1:J:170:LYS:CG	1:J:171:GLN:N	2.81	0.43
1:K:115:GLU:CG	1:K:116:ASP:CG	2.92	0.43
1:L:135:TYR:CD1	1:L:220:ALA:HB2	2.53	0.43
1:L:318:LEU:HA	1:L:318:LEU:HD23	1.81	0.43
1:L:453:LEU:O	1:L:457:THR:HG23	2.19	0.43
1:A:221:PHE:HD2	1:A:222:ASP:O	2.00	0.43
1:B:302:LYS:NZ	1:B:359:SER:HB3	2.33	0.43
1:E:290:ARG:HE	1:E:290:ARG:HB3	1.69	0.43
1:F:132:GLN:O	1:F:201:LEU:HD12	2.18	0.43
1:F:133:ILE:HD12	1:F:133:ILE:HG23	1.73	0.43
1:G:66:PHE:HD2	1:G:266:TYR:CE1	2.33	0.43
1:G:114:ARG:NE	1:G:117:ASP:OD2	2.37	0.43
1:H:118:ALA:O	1:H:120:VAL:N	2.51	0.43
1:H:233:LEU:HD12	1:H:233:LEU:N	2.33	0.43
1:I:136:ARG:CZ	1:I:198:ASP:O	2.67	0.43
1:I:347:ASN:HB3	1:I:353:GLN:NE2	2.34	0.43
1:I:423:LYS:HA	1:I:426:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:268:HIS:CB	1:J:269:VAL:HB	2.49	0.43
1:K:74:PHE:CZ	1:K:78:LEU:HD11	2.54	0.43
1:L:117:ASP:HA	1:L:118:ALA:HA	1.61	0.43
1:L:176:LYS:HB3	1:L:176:LYS:HE2	1.75	0.43
1:A:50:ARG:O	1:A:55:THR:CG2	2.67	0.43
1:B:269:VAL:HG22	1:B:271:VAL:H	1.83	0.43
1:C:50:ARG:HD2	1:C:90:LEU:CD2	2.43	0.43
1:C:312:ILE:HD11	1:C:383:LEU:HD21	2.01	0.43
1:E:61:ASN:HB3	1:E:338:ARG:HH21	1.84	0.43
1:F:72:LYS:HD2	1:F:72:LYS:C	2.43	0.43
1:F:375:GLU:HB3	1:F:376:PRO:HA	2.00	0.43
1:G:66:PHE:CD2	1:G:266:TYR:CE1	2.98	0.43
1:G:89:ASN:OD1	1:G:91:ASP:HB2	2.19	0.43
1:H:369:LEU:O	1:H:370:PRO:C	2.61	0.43
1:J:281:ALA:HA	1:J:284:LEU:HD12	2.01	0.43
1:A:426:TYR:CD1	1:A:426:TYR:C	2.97	0.42
1:B:134:ILE:HB	1:B:200:THR:CG2	2.48	0.42
1:C:88:ASP:O	1:C:423:LYS:NZ	2.36	0.42
1:H:175:LEU:C	1:H:175:LEU:HD23	2.44	0.42
1:I:455:TRP:O	1:I:455:TRP:CG	2.72	0.42
1:K:48:ILE:HG13	1:K:85:GLU:O	2.19	0.42
1:L:188:LEU:HA	1:L:188:LEU:HD23	1.64	0.42
1:A:148:LEU:HD22	1:A:199:LEU:HD13	2.01	0.42
1:C:122:TYR:CD1	1:C:122:TYR:N	2.87	0.42
1:C:205:ASN:HA	1:C:266[A]:TYR:HE2	1.83	0.42
1:E:61:ASN:HB3	1:E:338:ARG:NH2	2.34	0.42
1:F:190:ARG:HA	1:F:214:PHE:CE1	2.55	0.42
1:G:239:ASP:CB	1:G:243:ASN:HD21	2.31	0.42
1:G:271:VAL:HG13	1:G:272:LEU:N	2.34	0.42
1:H:209:MET:CE	1:H:266:TYR:HE1	2.31	0.42
1:I:55:THR:HG22	1:I:67:GLU:HG3	2.00	0.42
1:J:112:PRO:C	1:J:114:ARG:N	2.75	0.42
1:J:167:GLU:O	1:J:170:LYS:HG2	2.20	0.42
1:J:266:TYR:HA	1:J:267:GLY:HA2	1.69	0.42
1:L:259:GLN:OE1	1:L:262:LYS:HD3	2.19	0.42
1:L:270:ASP:O	1:L:271:VAL:CB	2.67	0.42
1:A:417:LEU:N	1:A:418:PRO:CD	2.81	0.42
1:B:69:GLU:OE2	1:B:265:TYR:OH	2.31	0.42
1:B:90:LEU:HD23	1:B:90:LEU:HA	1.83	0.42
1:B:187:ASP:CG	1:B:190:ARG:HH22	2.27	0.42
1:C:324:THR:HG22	1:D:116:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:ILE:C	1:E:134:ILE:HD13	2.45	0.42
1:F:211:GLN:C	1:F:213:TYR:N	2.77	0.42
1:F:362:PHE:CE1	1:F:383:LEU:HD23	2.54	0.42
1:K:392:HIS:CE1	1:K:434:ALA:HB2	2.54	0.42
1:L:105:LEU:HB3	1:L:233:LEU:HD12	1.99	0.42
1:L:271:VAL:HB	1:L:272:LEU:CD1	2.49	0.42
1:L:304:THR:OG1	1:L:366:ARG:NH2	2.44	0.42
1:L:388:ILE:HG12	1:L:392:HIS:HB2	2.01	0.42
1:B:81:GLU:CD	1:F:398:LYS:HZ1	2.26	0.42
1:B:302:LYS:HB2	1:B:302:LYS:NZ	2.26	0.42
1:C:453:LEU:HD23	1:C:453:LEU:HA	1.82	0.42
1:D:127:LEU:O	1:D:228:GLY:HA2	2.20	0.42
1:D:314:TYR:O	1:D:318:LEU:HD12	2.20	0.42
1:E:92:ASP:O	1:E:96:GLN:HG2	2.20	0.42
1:F:211:GLN:O	1:F:214:PHE:N	2.36	0.42
1:F:302:LYS:HD2	1:F:363:VAL:HG21	2.00	0.42
1:F:314:TYR:CD1	1:F:318:LEU:HA	2.53	0.42
1:H:176:LYS:HA	1:H:176:LYS:HD2	1.63	0.42
1:I:142:PRO:HG3	1:I:199:LEU:HD11	2.00	0.42
1:J:127:LEU:O	1:J:228:GLY:HA2	2.19	0.42
1:K:134:ILE:HG23	1:K:218:ARG:O	2.19	0.42
1:K:144:ARG:CG	1:K:145:PRO:CD	2.81	0.42
1:K:268:HIS:CE1	1:K:326:LYS:CE	3.02	0.42
1:L:269:VAL:HG22	1:L:272:LEU:CB	2.47	0.42
1:F:197:ILE:HD13	1:F:197:ILE:HG21	1.69	0.42
1:F:329:VAL:HG23	1:F:334:MET:HE3	2.02	0.42
1:G:250:ASP:OD1	1:G:250:ASP:C	2.60	0.42
1:I:135:TYR:HB3	1:I:199:LEU:HD22	1.99	0.42
1:J:287:ARG:O	1:J:288:LEU:C	2.61	0.42
1:J:350:ASP:OD2	1:J:352:LYS:HB3	2.20	0.42
1:L:167:GLU:HG2	1:L:170:LYS:NZ	2.33	0.42
1:C:208:ALA:HB3	1:C:266[A]:TYR:CE2	2.55	0.42
1:G:135:TYR:CE1	1:G:218:ARG:HB2	2.55	0.42
1:G:212:VAL:HG11	1:G:269:VAL:CG1	2.45	0.42
1:I:430:ARG:NH1	1:I:431:TYR:CE1	2.88	0.42
1:I:453:LEU:HD12	1:I:453:LEU:HA	1.78	0.42
1:K:250:ASP:HA	1:K:253:LYS:HG2	2.01	0.42
1:K:430:ARG:HG2	1:K:430:ARG:NH1	2.33	0.42
1:L:136:ARG:HD2	1:L:192:VAL:O	2.20	0.42
1:A:272:LEU:CD1	1:A:441:HIS:ND1	2.82	0.42
1:B:266:TYR:HA	1:B:267:GLY:HA2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ARG:CA	1:D:115:GLU:HG3	2.47	0.42
1:D:233:LEU:HD13	1:D:242:MET:CE	2.48	0.42
1:F:417:LEU:N	1:F:418:PRO:CD	2.82	0.42
1:G:53:PRO:CG	1:G:186:VAL:HG21	2.49	0.42
1:G:393:LEU:O	1:G:397:ARG:HG3	2.19	0.42
1:G:430:ARG:HH11	1:G:430:ARG:CG	2.30	0.42
1:I:41:LYS:HG3	1:I:43:GLY:H	1.84	0.42
1:I:188:LEU:O	1:I:192:VAL:HG23	2.19	0.42
1:L:118:ALA:C	1:L:120:VAL:H	2.26	0.42
1:D:115:GLU:HB3	1:D:117:ASP:CA	2.49	0.42
1:D:269:VAL:HG13	1:D:270:ASP:N	2.35	0.42
1:E:176:LYS:HE2	1:E:176:LYS:HB3	1.75	0.42
1:F:330:ARG:NH1	1:J:236:GLY:O	2.53	0.42
1:G:148:LEU:HB3	1:G:153:ILE:HD11	2.02	0.42
1:G:271:VAL:HG13	1:G:272:LEU:HA	2.01	0.42
1:G:292:GLU:OE2	1:G:296:LYS:NZ	2.48	0.42
1:G:375:GLU:HB3	1:G:376:PRO:HA	2.02	0.42
1:J:284:LEU:HD21	1:J:453:LEU:CD2	2.50	0.42
1:J:316:GLU:OE1	1:J:316:GLU:HA	2.20	0.42
1:L:207:LEU:HD22	1:L:219:VAL:HG22	2.00	0.42
1:B:236:GLY:O	1:H:330:ARG:NH1	2.53	0.42
1:B:400:ALA:O	1:B:405:LEU:HB2	2.20	0.42
1:C:225:GLU:OE1	1:C:225:GLU:CA	2.67	0.42
1:C:257:LEU:O	1:C:257:LEU:HD12	2.20	0.42
1:D:362:PHE:HE1	1:D:383:LEU:HD23	1.85	0.42
1:E:127:LEU:HD22	1:E:266:TYR:HE2	1.85	0.42
1:E:301:GLN:O	1:E:301:GLN:HG2	2.18	0.42
1:F:221:PHE:N	1:F:221:PHE:CD1	2.88	0.42
1:I:250:ASP:O	1:I:254:LYS:HD3	2.20	0.42
1:I:280:PHE:HZ	1:I:453:LEU:HD13	1.85	0.42
1:J:250:ASP:C	1:J:253:LYS:HG2	2.44	0.42
1:J:269:VAL:CG2	1:J:272:LEU:CD1	2.98	0.42
1:B:73:ARG:HD3	1:B:257:LEU:HD21	2.02	0.42
1:B:154:MET:HB3	1:B:188:LEU:HD22	2.02	0.42
1:C:131:PRO:HD3	1:C:227:ARG:HE	1.85	0.42
1:D:166:ALA:O	1:D:169:LYS:HB3	2.19	0.42
1:D:323:ALA:O	1:D:330:ARG:HG3	2.19	0.42
1:E:455:TRP:CE3	1:E:456:VAL:CG2	3.02	0.42
1:F:70:LEU:HA	1:F:70:LEU:HD12	1.46	0.42
1:F:274:TYR:CD1	1:F:449:TYR:CE1	3.07	0.42
1:F:417:LEU:HA	1:F:417:LEU:HD23	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:271:VAL:O	1:K:315:GLN:NE2	2.53	0.42
1:L:193:ASP:OD1	1:L:216:ASN:HB2	2.19	0.42
1:A:136:ARG:NH1	1:A:193:ASP:O	2.52	0.41
1:B:67:GLU:OE1	1:B:107:ALA:HB1	2.19	0.41
1:D:222:ASP:N	1:D:222:ASP:OD1	2.53	0.41
1:E:423:LYS:O	1:E:424:GLN:C	2.62	0.41
1:F:210:ASN:O	1:F:213:TYR:HB2	2.20	0.41
1:G:392:HIS:CE1	1:G:434:ALA:HB2	2.55	0.41
1:K:329:VAL:HB	1:K:334:MET:O	2.20	0.41
1:K:417:LEU:HB2	1:K:418:PRO:HD3	2.00	0.41
1:L:113:GLY:HA2	1:L:114:ARG:HA	1.64	0.41
1:A:125:THR:HG21	1:A:228:GLY:HA3	2.02	0.41
1:B:255:GLU:O	1:B:260:ARG:NH2	2.45	0.41
1:C:185:VAL:HG21	1:C:206:GLU:CD	2.43	0.41
1:D:314:TYR:CD1	1:D:318:LEU:HA	2.55	0.41
1:E:455:TRP:CE3	1:E:456:VAL:HG22	2.56	0.41
1:F:274:TYR:CE1	1:F:449:TYR:CE1	3.09	0.41
1:F:274:TYR:CE1	1:F:449:TYR:HE1	2.38	0.41
1:H:350:ASP:OD2	1:H:353:GLN:HG3	2.20	0.41
1:I:136:ARG:NH1	1:I:198:ASP:CA	2.83	0.41
1:I:430:ARG:HG2	1:I:430:ARG:NH1	2.29	0.41
1:L:66:PHE:HD1	1:L:66:PHE:C	2.28	0.41
1:B:140:GLN:O	1:B:142:PRO:HD3	2.21	0.41
1:B:300:LYS:HA	1:B:300:LYS:HD2	1.86	0.41
1:C:288:LEU:HB2	1:C:319:TRP:CZ3	2.55	0.41
1:E:309:LEU:HD13	1:E:359:SER:OG	2.21	0.41
1:E:340:ALA:HB1	1:E:345:VAL:HB	2.02	0.41
1:F:53:PRO:HG3	1:F:186:VAL:HG21	2.02	0.41
1:H:306:TRP:CE2	1:H:307:ARG:HG3	2.56	0.41
1:J:381:PHE:HZ	1:J:413:VAL:HG21	1.85	0.41
1:A:370:PRO:HG2	1:A:397:ARG:NH1	2.34	0.41
1:D:275:VAL:HB	1:D:448:ARG:NH1	2.35	0.41
1:E:330:ARG:NH1	1:K:236:GLY:O	2.53	0.41
1:E:426:TYR:CD1	1:E:426:TYR:C	2.98	0.41
1:F:430:ARG:HB3	1:F:431:TYR:CD2	2.55	0.41
1:G:169:LYS:H	1:G:169:LYS:HG3	1.66	0.41
1:H:415:LYS:HB3	1:H:415:LYS:HE2	1.86	0.41
1:J:133:ILE:HD13	1:J:201:LEU:HD13	2.02	0.41
1:J:191:MET:HB3	1:J:197:ILE:HD13	2.02	0.41
1:K:149:VAL:CG2	1:K:175:LEU:HB2	2.47	0.41
1:L:270:ASP:O	1:L:271:VAL:CG2	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLU:OE2	1:F:398:LYS:NZ	2.47	0.41
1:D:327:THR:OG1	1:D:329:VAL:HG22	2.20	0.41
1:E:290:ARG:HG3	1:E:291:TYR:CD2	2.54	0.41
1:F:388:ILE:HB	1:F:439:THR:OG1	2.20	0.41
1:G:112:PRO:HB2	1:G:113:GLY:H	1.78	0.41
1:G:149:VAL:HG13	1:G:175:LEU:HA	2.02	0.41
1:H:133:ILE:C	1:H:134:ILE:HD13	2.46	0.41
1:I:164:GLN:NE2	1:I:223:PHE:O	2.53	0.41
1:I:247:ALA:O	1:I:249:LEU:N	2.53	0.41
1:J:207:LEU:HD12	1:J:207:LEU:HA	1.94	0.41
1:J:210:ASN:OD1	1:J:435:ARG:NH2	2.53	0.41
1:J:329:VAL:HB	1:J:334:MET:O	2.21	0.41
1:K:266:TYR:CD1	1:K:266:TYR:O	2.74	0.41
1:B:52:SER:HB2	1:B:184:GLU:HG2	2.03	0.41
1:B:133:ILE:HD13	1:B:133:ILE:HA	1.72	0.41
1:B:181:ASP:OD2	1:D:176:LYS:HD3	2.21	0.41
1:D:131:PRO:HB2	1:D:223:PHE:O	2.20	0.41
1:D:426:TYR:HA	1:D:429:THR:HG23	2.03	0.41
1:E:417:LEU:N	1:E:418:PRO:CD	2.84	0.41
1:F:270:ASP:O	1:F:271:VAL:HG23	2.21	0.41
1:F:302:LYS:NZ	1:F:302:LYS:CB	2.78	0.41
1:G:324:THR:HG23	1:G:330:ARG:HG3	2.03	0.41
1:G:332:LEU:HA	1:G:332:LEU:HD12	1.80	0.41
1:J:109:GLY:HA3	1:J:229:LEU:HD13	2.02	0.41
1:L:66:PHE:C	1:L:66:PHE:CD1	2.97	0.41
1:L:111:THR:CG2	1:L:227:ARG:HD3	2.50	0.41
1:L:209:MET:HE3	1:L:209:MET:HB2	1.54	0.41
1:A:332:LEU:HD22	1:A:355:ILE:CG1	2.51	0.41
1:B:233:LEU:HD13	1:B:242:MET:HE1	2.03	0.41
1:C:297:GLN:O	1:C:301:GLN:HB2	2.20	0.41
1:D:402:LYS:HB2	1:D:402:LYS:HE3	1.49	0.41
1:E:233:LEU:N	1:E:233:LEU:CD1	2.84	0.41
1:E:288:LEU:HD12	1:E:288:LEU:O	2.20	0.41
1:G:176:LYS:HA	1:G:176:LYS:HD2	1.41	0.41
1:J:209:MET:HB2	1:J:209:MET:HE3	1.66	0.41
1:K:258:LEU:HD23	1:K:258:LEU:HA	1.78	0.41
1:A:211:GLN:NE2	1:A:217:VAL:O	2.51	0.41
1:B:217:VAL:C	1:B:218:ARG:HG2	2.45	0.41
1:D:93:LEU:HD23	1:D:94:TYR:N	2.36	0.41
1:D:314:TYR:HD2	1:D:449:TYR:CE2	2.38	0.41
1:E:146:GLU:O	1:E:149:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:LEU:HD12	1:E:272:LEU:H	1.86	0.41
1:F:73:ARG:HH11	1:F:257:LEU:HD11	1.84	0.41
1:F:377:ASP:HA	1:F:380:TRP:CD1	2.56	0.41
1:G:332:LEU:HD23	1:G:355:ILE:HG13	1.97	0.41
1:G:430:ARG:CG	1:G:430:ARG:NH1	2.83	0.41
1:H:448:ARG:HG3	1:H:448:ARG:HH11	1.84	0.41
1:I:74:PHE:CZ	1:I:245:VAL:HG22	2.55	0.41
1:I:420:LEU:HD23	1:I:420:LEU:HA	1.89	0.41
1:K:212:VAL:CG2	1:K:269:VAL:HG23	2.31	0.41
1:K:267:GLY:O	1:K:268:HIS:CG	2.74	0.41
1:L:152:ARG:NH1	1:L:196:ASP:O	2.53	0.41
1:L:269:VAL:CG2	1:L:272:LEU:CB	2.99	0.41
1:B:114:ARG:HG2	1:B:115:GLU:HG2	2.02	0.41
1:B:166:ALA:O	1:B:169:LYS:HB3	2.21	0.41
1:C:44:VAL:HG13	1:C:81:GLU:HG3	2.03	0.41
1:C:426:TYR:CD1	1:C:426:TYR:C	2.99	0.41
1:D:66:PHE:CD1	1:D:261:LEU:HB3	2.56	0.41
1:D:115:GLU:HG2	1:D:117:ASP:HB3	2.03	0.41
1:D:198:ASP:O	1:D:199:LEU:HD23	2.21	0.41
1:E:258:LEU:HD23	1:E:258:LEU:HA	1.94	0.41
1:G:165:LEU:HB3	1:G:177:TYR:CE2	2.56	0.41
1:H:111:THR:CG2	1:H:227:ARG:HD3	2.51	0.41
1:I:375:GLU:HB3	1:I:376:PRO:HA	2.03	0.41
1:J:198:ASP:O	1:J:199:LEU:HD23	2.20	0.41
1:K:410:TRP:O	1:K:414:LYS:HB3	2.21	0.41
1:L:302:LYS:NZ	1:L:359:SER:C	2.79	0.41
1:L:455:TRP:CE3	1:L:456:VAL:CG1	3.03	0.41
1:C:132:GLN:O	1:C:201:LEU:HD12	2.20	0.41
1:C:350:ASP:O	1:C:351:PRO:C	2.61	0.41
1:C:394:GLU:OE1	1:C:394:GLU:HA	2.21	0.41
1:C:417:LEU:HB2	1:C:418:PRO:HD3	2.02	0.41
1:G:112:PRO:HB3	1:G:122:TYR:CG	2.56	0.41
1:I:250:ASP:CG	1:I:251:GLN:N	2.79	0.41
1:I:254:LYS:HD3	1:I:254:LYS:N	2.36	0.41
1:B:302:LYS:HE2	1:B:360:LYS:CA	2.50	0.40
1:C:235:GLY:HA2	1:C:236:GLY:HA3	1.65	0.40
1:C:262:LYS:HG2	1:C:266[A]:TYR:HD1	1.86	0.40
1:E:273:GLY:HA3	1:E:445:ASN:HD21	1.81	0.40
1:E:329:VAL:CG2	1:E:334:MET:HE3	2.51	0.40
1:F:106:ALA:HB3	1:F:232:ALA:HB3	2.02	0.40
1:G:147:ASP:O	1:G:151:LYS:HD3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:157:LYS:HB3	1:I:181:ASP:OD1	2.20	0.40
1:J:287:ARG:C	1:J:289:PRO:HD2	2.46	0.40
1:J:308:LEU:HA	1:J:308:LEU:HD12	1.77	0.40
1:L:118:ALA:O	1:L:120:VAL:N	2.49	0.40
1:B:317:SER:O	1:B:318:LEU:HB2	2.21	0.40
1:C:287:ARG:C	1:C:289:PRO:HD2	2.46	0.40
1:D:112:PRO:O	1:D:113:GLY:O	2.40	0.40
1:D:264:ARG:HE	1:D:264:ARG:HB2	1.51	0.40
1:D:270:ASP:HA	1:D:272:LEU:N	2.36	0.40
1:F:61:ASN:O	1:F:338:ARG:NH2	2.54	0.40
1:F:295:PHE:CZ	1:F:310:ALA:HA	2.56	0.40
1:F:410:TRP:CZ2	1:F:443:VAL:HG11	2.56	0.40
1:G:453:LEU:O	1:G:456:VAL:HG22	2.20	0.40
1:I:361:TYR:CZ	1:I:365:ILE:HD11	2.55	0.40
1:L:59:ASP:OD1	1:L:59:ASP:C	2.64	0.40
1:L:90:LEU:HD23	1:L:90:LEU:HA	1.89	0.40
1:L:330:ARG:HB3	1:L:348:ARG:CZ	2.52	0.40
1:A:239:ASP:HB3	1:A:243:ASN:OD1	2.22	0.40
1:B:133:ILE:HD12	1:B:133:ILE:HG23	1.62	0.40
1:D:388:ILE:HB	1:D:439:THR:OG1	2.22	0.40
1:D:456:VAL:CG2	1:D:457:THR:H	2.26	0.40
1:H:53:PRO:HG3	1:H:186:VAL:HG21	2.03	0.40
1:H:156:LEU:HD23	1:H:183:VAL:HG23	2.03	0.40
1:J:73:ARG:HG2	1:J:257:LEU:HD11	2.03	0.40
1:J:134:ILE:CG2	1:J:217:VAL:HB	2.51	0.40
1:K:48:ILE:HA	1:K:85:GLU:O	2.21	0.40
1:K:71:ALA:C	1:K:82:LEU:HD22	2.46	0.40
1:K:268:HIS:HA	1:K:269:VAL:HB	2.03	0.40
1:L:155:VAL:HG22	1:L:156:LEU:N	2.35	0.40
1:A:377:ASP:HA	1:A:380:TRP:CD1	2.57	0.40
1:B:330:ARG:HD3	1:E:118:ALA:CB	2.51	0.40
1:C:145:PRO:O	1:C:148:LEU:HG	2.21	0.40
1:E:251:GLN:O	1:E:255:GLU:HG2	2.21	0.40
1:F:260:ARG:HG3	1:F:260:ARG:HH11	1.86	0.40
1:G:189:LEU:HA	1:G:189:LEU:HD23	1.81	0.40
1:G:423:LYS:CA	1:G:426:TYR:CE2	3.04	0.40
1:H:253:LYS:O	1:H:253:LYS:HG3	2.22	0.40
1:H:309:LEU:HD23	1:H:309:LEU:HA	1.90	0.40
1:I:270:ASP:CG	1:I:271:VAL:HG13	2.46	0.40
1:I:399:MET:SD	1:I:419:ARG:HD2	2.62	0.40
1:I:434:ALA:O	1:I:436:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:336:THR:OG1	1:J:339:THR:HB	2.21	0.40
1:K:201:LEU:HD12	1:K:201:LEU:HA	1.62	0.40
1:L:45:LEU:HD21	1:L:74:PHE:CD2	2.57	0.40
1:C:414:LYS:NZ	1:C:444[B]:GLN:OE1	2.54	0.40
1:D:421:ALA:HA	1:D:433:TYR:CE1	2.57	0.40
1:G:112:PRO:HA	1:G:122:TYR:CZ	2.55	0.40
1:I:112:PRO:HB3	1:I:122:TYR:CG	2.57	0.40
1:K:114:ARG:NH1	1:K:114:ARG:HB3	2.37	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:GLU:OE1	1:L:278:TYR:OH[1_545]	2.10	0.10
1:D:292:GLU:OE1	1:K:278:TYR:OH[1_655]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	417/499 (84%)	389 (93%)	21 (5%)	7 (2%)	7	35
1	B	416/499 (83%)	398 (96%)	16 (4%)	2 (0%)	24	59
1	C	418/499 (84%)	396 (95%)	19 (4%)	3 (1%)	18	52
1	D	414/499 (83%)	392 (95%)	14 (3%)	8 (2%)	6	33
1	E	417/499 (84%)	395 (95%)	17 (4%)	5 (1%)	10	42
1	F	416/499 (83%)	391 (94%)	19 (5%)	6 (1%)	9	39
1	G	415/499 (83%)	393 (95%)	12 (3%)	10 (2%)	4	28
1	H	414/499 (83%)	393 (95%)	16 (4%)	5 (1%)	10	42
1	I	417/499 (84%)	387 (93%)	19 (5%)	11 (3%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	415/499 (83%)	387 (93%)	19 (5%)	9 (2%)	5	29
1	K	416/499 (83%)	383 (92%)	17 (4%)	16 (4%)	2	18
1	L	418/499 (84%)	385 (92%)	21 (5%)	12 (3%)	3	24
All	All	4993/5988 (83%)	4689 (94%)	210 (4%)	94 (2%)	6	33

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	GLY
1	A	115	GLU
1	A	118	ALA
1	A	271	VAL
1	B	118	ALA
1	B	457	THR
1	C	270	ASP
1	C	458	GLN
1	D	113	GLY
1	D	456	VAL
1	E	115	GLU
1	E	270	ASP
1	E	274	TYR
1	F	115	GLU
1	F	269	VAL
1	G	100	GLU
1	G	101	GLY
1	G	112	PRO
1	G	116	ASP
1	I	116	ASP
1	I	117	ASP
1	I	118	ALA
1	I	237	ASP
1	I	248	PHE
1	I	269	VAL
1	J	113	GLY
1	J	115	GLU
1	J	118	ALA
1	J	269	VAL
1	K	112	PRO
1	K	118	ALA
1	K	253	LYS
1	K	266	TYR

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Mol	Chain	Res	Type
1	K	268	HIS
1	K	269	VAL
1	L	119	SER
1	L	267	GLY
1	L	268	HIS
1	L	269	VAL
1	L	271	VAL
1	L	273	GLY
1	A	114	ARG
1	A	458	GLN
1	D	116	ASP
1	D	270	ASP
1	D	455	TRP
1	E	237	ASP
1	F	268	HIS
1	G	114	ARG
1	G	120	VAL
1	G	236	GLY
1	G	269	VAL
1	H	101	GLY
1	H	236	GLY
1	H	272	LEU
1	I	113	GLY
1	I	271	VAL
1	J	114	ARG
1	J	273	GLY
1	K	101	GLY
1	K	116	ASP
1	K	146	GLU
1	K	236	GLY
1	K	273	GLY
1	L	101	GLY
1	L	298	SER
1	D	118	ALA
1	D	271	VAL
1	D	275	VAL
1	G	119	SER
1	I	247	ALA
1	J	271	VAL
1	K	114	ARG
1	K	144	ARG
1	K	270	ASP

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Mol	Chain	Res	Type
1	C	237	ASP
1	F	271	VAL
1	H	275	VAL
1	I	114	ARG
1	K	115	GLU
1	L	117	ASP
1	L	236	GLY
1	L	270	ASP
1	G	108	ALA
1	A	273	GLY
1	F	270	ASP
1	I	239	ASP
1	K	271	VAL
1	F	267	GLY
1	J	101	GLY
1	J	112	PRO
1	L	458	GLN
1	E	459	PRO
1	H	267	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/413 (84%)	334 (96%)	15 (4%)	26	59
1	B	348/413 (84%)	335 (96%)	13 (4%)	30	63
1	C	350/413 (85%)	334 (95%)	16 (5%)	24	58
1	D	346/413 (84%)	331 (96%)	15 (4%)	26	59
1	E	349/413 (84%)	335 (96%)	14 (4%)	28	61
1	F	348/413 (84%)	334 (96%)	14 (4%)	28	61
1	G	347/413 (84%)	335 (96%)	12 (4%)	32	64
1	H	346/413 (84%)	335 (97%)	11 (3%)	34	65
1	I	349/413 (84%)	338 (97%)	11 (3%)	34	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	347/413 (84%)	332 (96%)	15 (4%)	26	59
1	K	348/413 (84%)	337 (97%)	11 (3%)	34	65
1	L	350/413 (85%)	335 (96%)	15 (4%)	26	59
All	All	4177/4956 (84%)	4015 (96%)	162 (4%)	28	62

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	THR
1	A	86	THR
1	A	114	ARG
1	A	128	ASP
1	A	140	GLN
1	A	169	LYS
1	A	178	GLU
1	A	217	VAL
1	A	264	ARG
1	A	266[A]	TYR
1	A	266[B]	TYR
1	A	268	HIS
1	A	282	GLN
1	A	332	LEU
1	A	338	ARG
1	B	86	THR
1	B	121	ARG
1	B	155	VAL
1	B	160	SER
1	B	169	LYS
1	B	186	VAL
1	B	266	TYR
1	B	268	HIS
1	B	272	LEU
1	B	279	THR
1	B	346	SER
1	B	372	SER
1	B	458	GLN
1	C	121	ARG
1	C	141	ARG
1	C	143	THR
1	C	160	SER
1	C	169	LYS

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Mol	Chain	Res	Type
1	C	176	LYS
1	C	186	VAL
1	C	227	ARG
1	C	268	HIS
1	C	269	VAL
1	C	272	LEU
1	C	284	LEU
1	C	285	GLN
1	C	301	GLN
1	C	304	THR
1	C	338	ARG
1	D	64	THR
1	D	143	THR
1	D	160	SER
1	D	169	LYS
1	D	209	MET
1	D	225	GLU
1	D	266	TYR
1	D	268	HIS
1	D	269	VAL
1	D	282	GLN
1	D	293	SER
1	D	368	GLU
1	D	402	LYS
1	D	454	THR
1	D	455	TRP
1	E	50	ARG
1	E	145	PRO
1	E	160	SER
1	E	176	LYS
1	E	207	LEU
1	E	209	MET
1	E	217	VAL
1	E	254	LYS
1	E	264	ARG
1	E	268	HIS
1	E	282	GLN
1	E	336	THR
1	E	337	ASN
1	E	397	ARG
1	F	72	LYS
1	F	80	VAL

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Mol	Chain	Res	Type
1	F	115	GLU
1	F	145	PRO
1	F	169	LYS
1	F	172	TYR
1	F	258	LEU
1	F	260	ARG
1	F	271	VAL
1	F	332	LEU
1	F	336	THR
1	F	346	SER
1	F	368	GLU
1	F	458	GLN
1	G	66	PHE
1	G	86	THR
1	G	160	SER
1	G	169	LYS
1	G	212	VAL
1	G	269	VAL
1	G	270	ASP
1	G	271	VAL
1	G	279	THR
1	G	286	GLN
1	G	300	LYS
1	G	324	THR
1	H	66	PHE
1	H	100	GLU
1	H	169	LYS
1	H	170	LYS
1	H	178	GLU
1	H	266	TYR
1	H	268	HIS
1	H	272	LEU
1	H	332	LEU
1	H	336	THR
1	H	415	LYS
1	I	66	PHE
1	I	136	ARG
1	I	169	LYS
1	I	198	ASP
1	I	209	MET
1	I	217	VAL
1	I	264	ARG

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Mol	Chain	Res	Type
1	I	268	HIS
1	I	271	VAL
1	I	336	THR
1	I	453	LEU
1	J	76	GLU
1	J	81	GLU
1	J	86	THR
1	J	100	GLU
1	J	115	GLU
1	J	127	LEU
1	J	128	ASP
1	J	163	GLU
1	J	169	LYS
1	J	266	TYR
1	J	272	LEU
1	J	279	THR
1	J	304	THR
1	J	372	SER
1	J	409	LYS
1	K	115	GLU
1	K	144	ARG
1	K	145	PRO
1	K	160	SER
1	K	163	GLU
1	K	169	LYS
1	K	197	ILE
1	K	217	VAL
1	K	266	TYR
1	K	326	LYS
1	K	360	LYS
1	L	66	PHE
1	L	73	ARG
1	L	163	GLU
1	L	169	LYS
1	L	176	LYS
1	L	233	LEU
1	L	270	ASP
1	L	279	THR
1	L	297	GLN
1	L	301	GLN
1	L	332	LEU
1	L	409	LYS

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Mol	Chain	Res	Type
1	L	454	THR
1	L	458	GLN
1	L	461	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	137	ASN
1	A	140	GLN
1	A	164	GLN
1	A	301	GLN
1	A	320	GLN
1	A	356	GLN
1	A	458	GLN
1	B	61	ASN
1	B	137	ASN
1	B	205	ASN
1	C	315	GLN
1	D	61	ASN
1	D	282	GLN
1	D	286	GLN
1	D	408	ASN
1	E	387	ASN
1	E	408	ASN
1	F	58	GLN
1	F	132	GLN
1	F	286	GLN
1	F	315	GLN
1	F	353	GLN
1	G	132	GLN
1	G	171	GLN
1	G	243	ASN
1	G	315	GLN
1	G	445	ASN
1	H	132	GLN
1	H	164	GLN
1	H	301	GLN
1	H	315	GLN
1	H	337	ASN
1	I	58	GLN
1	I	132	GLN

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Mol	Chain	Res	Type
1	I	243	ASN
1	I	246	ASN
1	I	356	GLN
1	I	424	GLN
1	J	61	ASN
1	J	137	ASN
1	J	285	GLN
1	J	294	HIS
1	J	301	GLN
1	J	315	GLN
1	K	89	ASN
1	K	161	HIS
1	K	268	HIS
1	K	315	GLN
1	K	387	ASN
1	L	89	ASN
1	L	137	ASN

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLU	A	501	-	8,9,9	1.37	1 (12%)	8,11,11	1.04	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	A	501	-	-	4/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	GLU	CG-CD	2.07	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GLU	O-C-CA-N
2	A	501	GLU	OXT-C-CA-N
2	A	501	GLU	O-C-CA-CB
2	A	501	GLU	OXT-C-CA-CB

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GLU	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	417/499 (83%)	-0.45	4 (0%) 79 63	23, 60, 97, 136	2 (0%)
1	B	417/499 (83%)	-0.50	0 100 100	22, 58, 92, 159	1 (0%)
1	C	418/499 (83%)	-0.43	2 (0%) 87 76	23, 60, 92, 134	2 (0%)
1	D	415/499 (83%)	-0.43	6 (1%) 73 54	28, 64, 99, 141	1 (0%)
1	E	418/499 (83%)	-0.45	2 (0%) 87 76	28, 65, 97, 150	1 (0%)
1	F	416/499 (83%)	-0.51	1 (0%) 91 85	31, 65, 96, 135	2 (0%)
1	G	416/499 (83%)	-0.40	1 (0%) 91 85	32, 72, 107, 148	1 (0%)
1	H	415/499 (83%)	-0.39	4 (0%) 79 63	28, 68, 104, 160	1 (0%)
1	I	418/499 (83%)	-0.35	4 (0%) 79 63	28, 69, 105, 144	1 (0%)
1	J	416/499 (83%)	-0.25	1 (0%) 91 85	34, 85, 118, 135	1 (0%)
1	K	417/499 (83%)	-0.26	2 (0%) 87 76	31, 81, 118, 154	1 (0%)
1	L	419/499 (83%)	-0.24	1 (0%) 91 85	31, 80, 120, 179	1 (0%)
All	All	5002/5988 (83%)	-0.39	28 (0%) 85 73	22, 70, 108, 179	15 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	266	TYR	3.8
1	A	117	ASP	3.4
1	A	272	LEU	3.4
1	E	271	VAL	3.3
1	C	266[A]	TYR	3.2
1	F	269	VAL	3.2
1	I	198	ASP	3.1
1	D	272	LEU	3.0
1	A	266[A]	TYR	2.9
1	D	273	GLY	2.9
1	I	268	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	116	ASP	2.8
1	H	269	VAL	2.7
1	C	458	GLN	2.6
1	I	273	GLY	2.6
1	K	272	LEU	2.5
1	H	268	HIS	2.4
1	H	272	LEU	2.4
1	D	270	ASP	2.4
1	H	100	GLU	2.4
1	D	455	TRP	2.3
1	D	268	HIS	2.3
1	G	130	THR	2.3
1	A	113	GLY	2.1
1	E	269	VAL	2.1
1	I	136	ARG	2.1
1	K	267	GLY	2.1
1	D	271	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLU	A	501	10/10	0.70	0.21	19,81,82,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.