



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 01:22 AM UTC

PDB ID : 6IKM / pdb_00006ikm
Title : Crystal structure of SpuE-Spermidine in complex with ScFv5
Authors : Wu, D.; Sun, X.
Deposited on : 2018-10-16
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
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

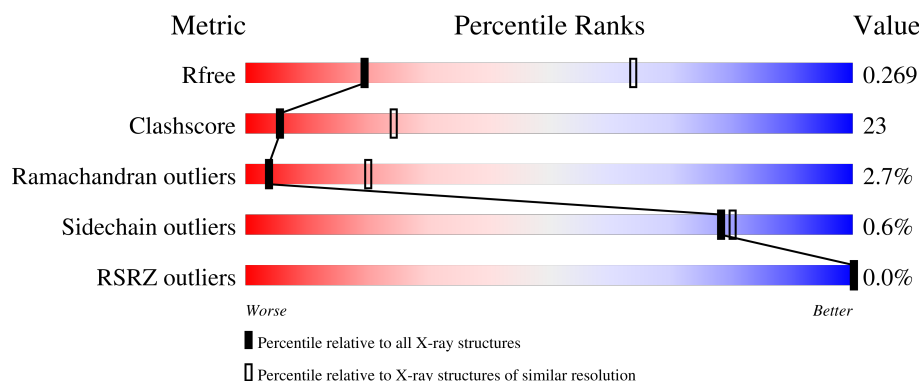
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

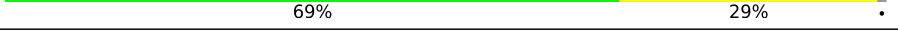
The reported resolution of this entry is 3.40 Å.

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



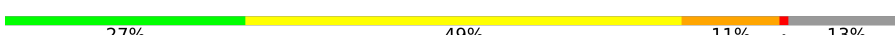
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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

Mol	Chain	Length	Quality of chain
1	A	340	 69% 29% ..
1	B	340	 68% 30% ..
1	C	340	 71% 28% .
1	D	340	 69% 29% .
1	E	340	 63% 35% .

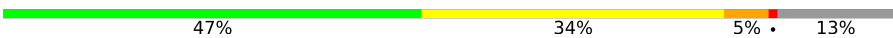
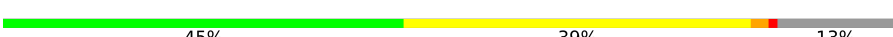
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Mol	Chain	Length	Quality of chain
1	F	340	 64% 34% ..
1	G	340	 69% 29% ..
1	H	340	 69% 28% ..
1	I	340	 60% 38% ..
1	J	340	 64% 33% ..
1	K	340	 58% 39% ..
1	L	340	 56% 39% ..
1	M	340	 62% 36% ..
1	N	340	 53% 44% ..
1	O	340	 52% 44% ..
1	P	340	 58% 38% ..
1	Q	340	 50% 47% ..
1	R	340	 49% 47% ..
2	a	258	 50% 35% • 13%
2	b	258	 49% 37% • 13%
2	c	258	 52% 34% • 13%
2	d	258	 60% 26% • 13%
2	e	258	 55% 31% • 13%
2	f	258	 55% 29% • 13%
2	g	258	 53% 32% •• 13%
2	h	258	 53% 31% • 13%
2	i	258	 48% 35% •• 13%
2	j	258	 52% 33% • 13%
2	k	258	 53% 31% • 13%
2	l	258	 27% 49% 11% • 13%

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Mol	Chain	Length	Quality of chain
2	m	258	
2	n	258	
2	o	258	
2	p	258	
2	q	258	
2	r	258	

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
3	SO4	A	403	-	-	X	-
3	SO4	G	401	-	-	X	-
3	SO4	I	402	-	-	X	-
3	SO4	M	401	-	-	X	-
3	SO4	M	402	-	-	X	-
3	SO4	N	404	-	-	X	-
3	SO4	N	406	-	-	X	-
3	SO4	O	406	-	-	X	-
3	SO4	R	401	-	-	X	-
4	SPD	N	407	-	-	X	-
4	SPD	O	407	-	-	X	-
4	SPD	Q	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 78156 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Polyamine transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	B	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	C	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	D	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	E	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	F	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	G	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	H	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	I	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	J	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	K	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	L	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	M	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	N	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	O	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	P	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			
1	R	335	Total	C	N	O	S	0	0	0
			2618	1687	424	500	7			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP A0A069QID4
A	24	PRO	-	expression tag	UNP A0A069QID4
A	25	LEU	-	expression tag	UNP A0A069QID4
A	26	GLY	-	expression tag	UNP A0A069QID4
A	27	SER	-	expression tag	UNP A0A069QID4
B	23	GLY	-	expression tag	UNP A0A069QID4
B	24	PRO	-	expression tag	UNP A0A069QID4
B	25	LEU	-	expression tag	UNP A0A069QID4
B	26	GLY	-	expression tag	UNP A0A069QID4
B	27	SER	-	expression tag	UNP A0A069QID4
C	23	GLY	-	expression tag	UNP A0A069QID4
C	24	PRO	-	expression tag	UNP A0A069QID4
C	25	LEU	-	expression tag	UNP A0A069QID4
C	26	GLY	-	expression tag	UNP A0A069QID4
C	27	SER	-	expression tag	UNP A0A069QID4
D	23	GLY	-	expression tag	UNP A0A069QID4
D	24	PRO	-	expression tag	UNP A0A069QID4
D	25	LEU	-	expression tag	UNP A0A069QID4
D	26	GLY	-	expression tag	UNP A0A069QID4
D	27	SER	-	expression tag	UNP A0A069QID4
E	23	GLY	-	expression tag	UNP A0A069QID4
E	24	PRO	-	expression tag	UNP A0A069QID4
E	25	LEU	-	expression tag	UNP A0A069QID4
E	26	GLY	-	expression tag	UNP A0A069QID4
E	27	SER	-	expression tag	UNP A0A069QID4
F	23	GLY	-	expression tag	UNP A0A069QID4
F	24	PRO	-	expression tag	UNP A0A069QID4
F	25	LEU	-	expression tag	UNP A0A069QID4
F	26	GLY	-	expression tag	UNP A0A069QID4
F	27	SER	-	expression tag	UNP A0A069QID4
G	23	GLY	-	expression tag	UNP A0A069QID4
G	24	PRO	-	expression tag	UNP A0A069QID4
G	25	LEU	-	expression tag	UNP A0A069QID4
G	26	GLY	-	expression tag	UNP A0A069QID4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	27	SER	-	expression tag	UNP A0A069QID4
H	23	GLY	-	expression tag	UNP A0A069QID4
H	24	PRO	-	expression tag	UNP A0A069QID4
H	25	LEU	-	expression tag	UNP A0A069QID4
H	26	GLY	-	expression tag	UNP A0A069QID4
H	27	SER	-	expression tag	UNP A0A069QID4
I	23	GLY	-	expression tag	UNP A0A069QID4
I	24	PRO	-	expression tag	UNP A0A069QID4
I	25	LEU	-	expression tag	UNP A0A069QID4
I	26	GLY	-	expression tag	UNP A0A069QID4
I	27	SER	-	expression tag	UNP A0A069QID4
J	23	GLY	-	expression tag	UNP A0A069QID4
J	24	PRO	-	expression tag	UNP A0A069QID4
J	25	LEU	-	expression tag	UNP A0A069QID4
J	26	GLY	-	expression tag	UNP A0A069QID4
J	27	SER	-	expression tag	UNP A0A069QID4
K	23	GLY	-	expression tag	UNP A0A069QID4
K	24	PRO	-	expression tag	UNP A0A069QID4
K	25	LEU	-	expression tag	UNP A0A069QID4
K	26	GLY	-	expression tag	UNP A0A069QID4
K	27	SER	-	expression tag	UNP A0A069QID4
L	23	GLY	-	expression tag	UNP A0A069QID4
L	24	PRO	-	expression tag	UNP A0A069QID4
L	25	LEU	-	expression tag	UNP A0A069QID4
L	26	GLY	-	expression tag	UNP A0A069QID4
L	27	SER	-	expression tag	UNP A0A069QID4
M	23	GLY	-	expression tag	UNP A0A069QID4
M	24	PRO	-	expression tag	UNP A0A069QID4
M	25	LEU	-	expression tag	UNP A0A069QID4
M	26	GLY	-	expression tag	UNP A0A069QID4
M	27	SER	-	expression tag	UNP A0A069QID4
N	23	GLY	-	expression tag	UNP A0A069QID4
N	24	PRO	-	expression tag	UNP A0A069QID4
N	25	LEU	-	expression tag	UNP A0A069QID4
N	26	GLY	-	expression tag	UNP A0A069QID4
N	27	SER	-	expression tag	UNP A0A069QID4
O	23	GLY	-	expression tag	UNP A0A069QID4
O	24	PRO	-	expression tag	UNP A0A069QID4
O	25	LEU	-	expression tag	UNP A0A069QID4
O	26	GLY	-	expression tag	UNP A0A069QID4
O	27	SER	-	expression tag	UNP A0A069QID4
P	23	GLY	-	expression tag	UNP A0A069QID4

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Chain	Residue	Modelled	Actual	Comment	Reference
P	24	PRO	-	expression tag	UNP A0A069QID4
P	25	LEU	-	expression tag	UNP A0A069QID4
P	26	GLY	-	expression tag	UNP A0A069QID4
P	27	SER	-	expression tag	UNP A0A069QID4
Q	23	GLY	-	expression tag	UNP A0A069QID4
Q	24	PRO	-	expression tag	UNP A0A069QID4
Q	25	LEU	-	expression tag	UNP A0A069QID4
Q	26	GLY	-	expression tag	UNP A0A069QID4
Q	27	SER	-	expression tag	UNP A0A069QID4
R	23	GLY	-	expression tag	UNP A0A069QID4
R	24	PRO	-	expression tag	UNP A0A069QID4
R	25	LEU	-	expression tag	UNP A0A069QID4
R	26	GLY	-	expression tag	UNP A0A069QID4
R	27	SER	-	expression tag	UNP A0A069QID4

- Molecule 2 is a protein called ScFv5.

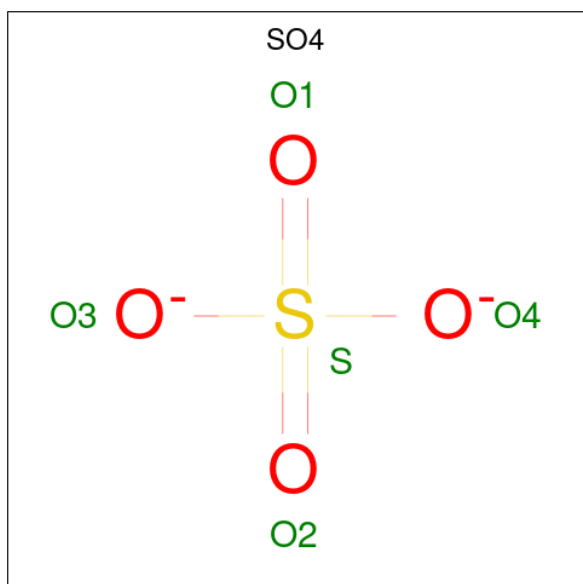
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	b	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	c	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	d	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	e	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	f	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	g	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	h	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	i	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	j	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	k	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0
2	l	225	Total 1699	C 1064	N 293	O 334	S 8	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	m	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	n	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	o	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	p	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	q	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			
2	r	225	Total	C	N	O	S	0	0	0
			1699	1064	293	334	8			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		

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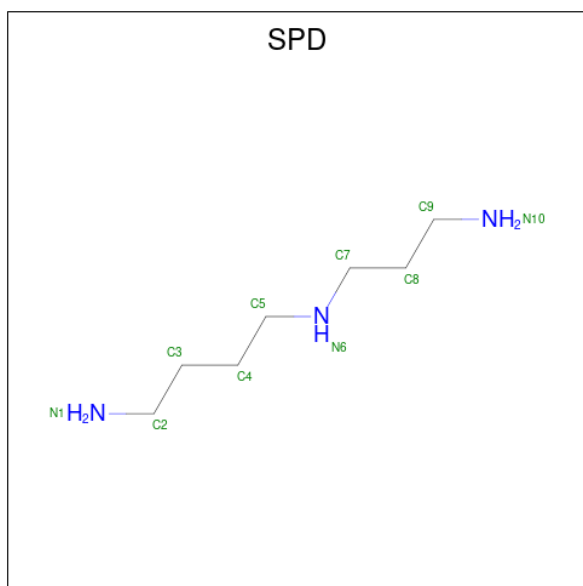
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		
3	R	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			10	7	3		
4	B	1	Total	C	N	0	0
			10	7	3		
4	C	1	Total	C	N	0	0
			10	7	3		
4	D	1	Total	C	N	0	0
			10	7	3		

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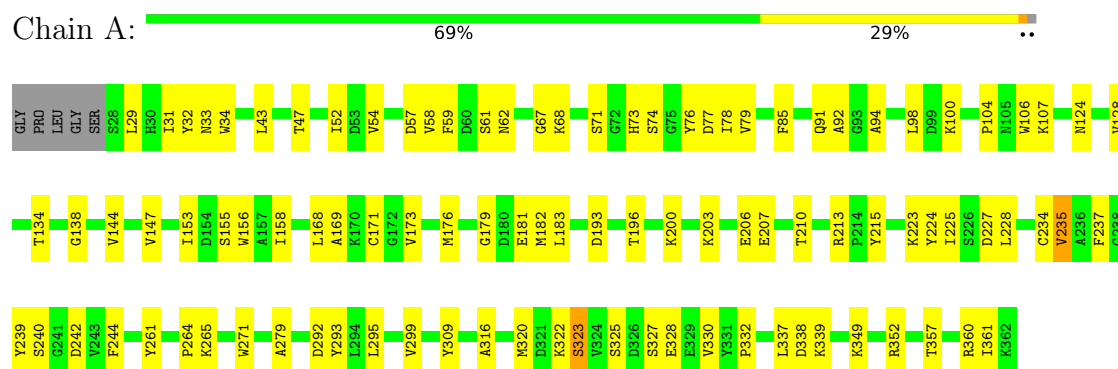
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	N	0	0
			10	7	3		
4	F	1	Total	C	N	0	0
			10	7	3		
4	G	1	Total	C	N	0	0
			10	7	3		
4	H	1	Total	C	N	0	0
			10	7	3		
4	I	1	Total	C	N	0	0
			10	7	3		
4	J	1	Total	C	N	0	0
			10	7	3		
4	K	1	Total	C	N	0	0
			10	7	3		
4	L	1	Total	C	N	0	0
			10	7	3		
4	M	1	Total	C	N	0	0
			10	7	3		
4	N	1	Total	C	N	0	0
			10	7	3		
4	O	1	Total	C	N	0	0
			10	7	3		
4	P	1	Total	C	N	0	0
			10	7	3		
4	Q	1	Total	C	N	0	0
			10	7	3		
4	R	1	Total	C	N	0	0
			10	7	3		

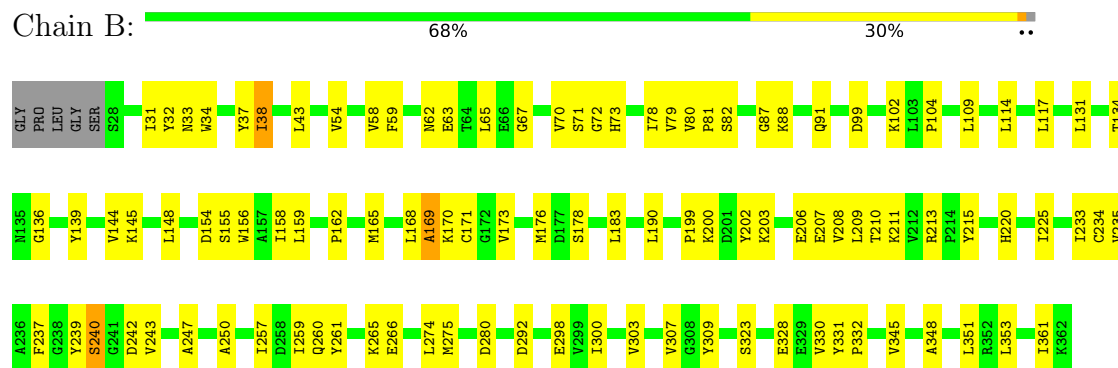
3 Residue-property plots

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

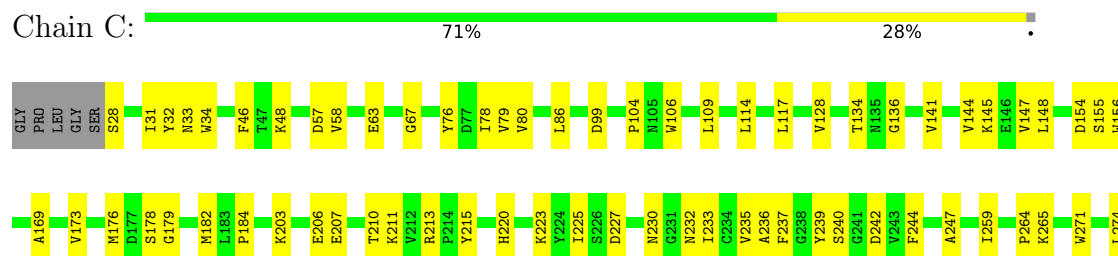
• Molecule 1: Polyamine transport protein



• Molecule 1: Polyamine transport protein



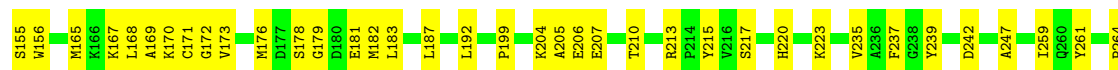
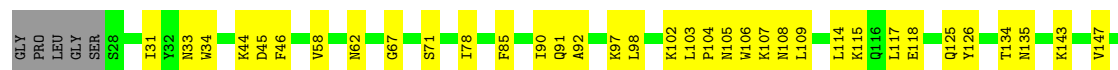
• Molecule 1: Polyamine transport protein





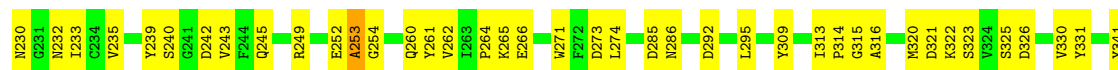
• Molecule 1: Polyamine transport protein

Chain D: 69% 29% .



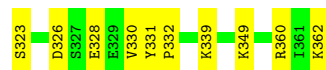
• Molecule 1: Polyamine transport protein

Chain E: 63% 35% .



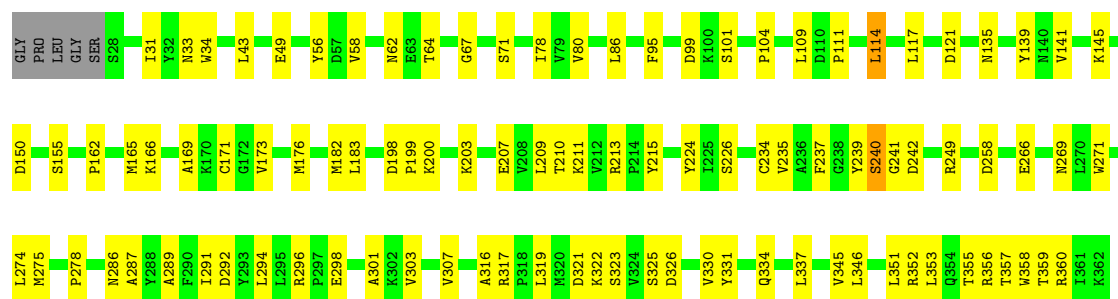
• Molecule 1: Polyamine transport protein

Chain F: 64% 34% ..



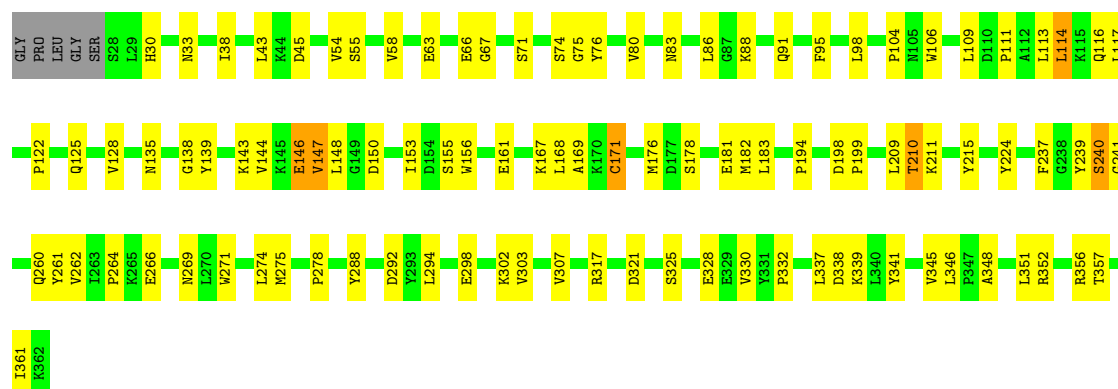
• Molecule 1: Polyamine transport protein

Chain G:  69% 29% ..



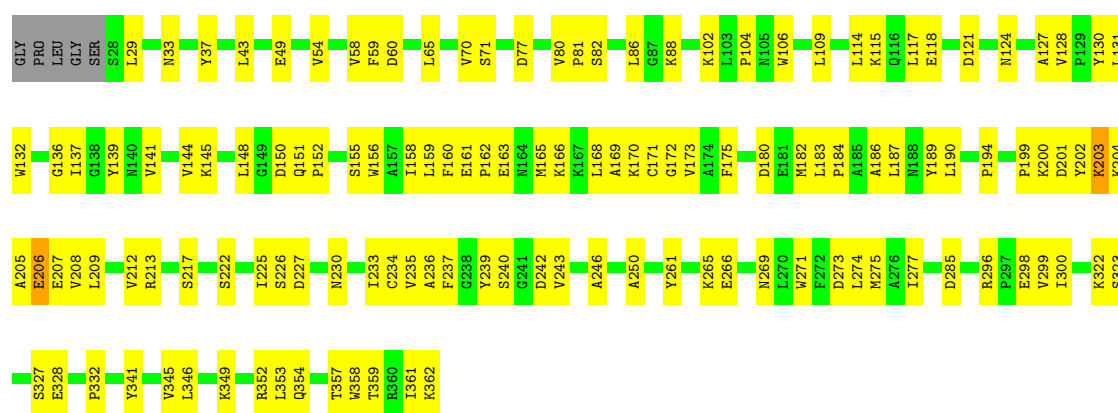
• Molecule 1: Polyamine transport protein

Chain H:  69% 28% ..



• Molecule 1: Polyamine transport protein

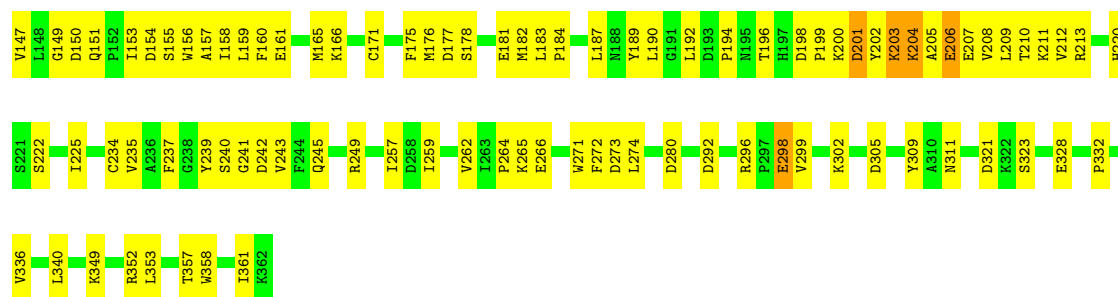
Chain I:  60% 38% ..



• Molecule 1: Polyamine transport protein

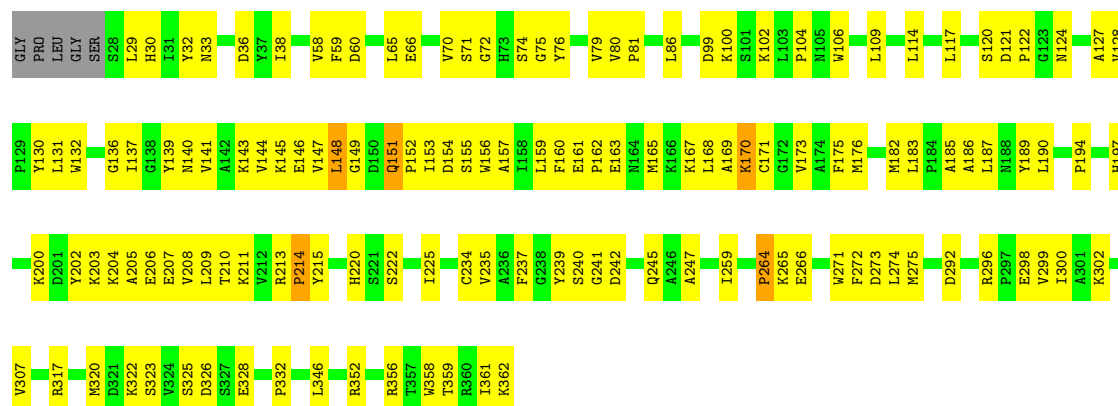
Chain J:  64% 33% ..





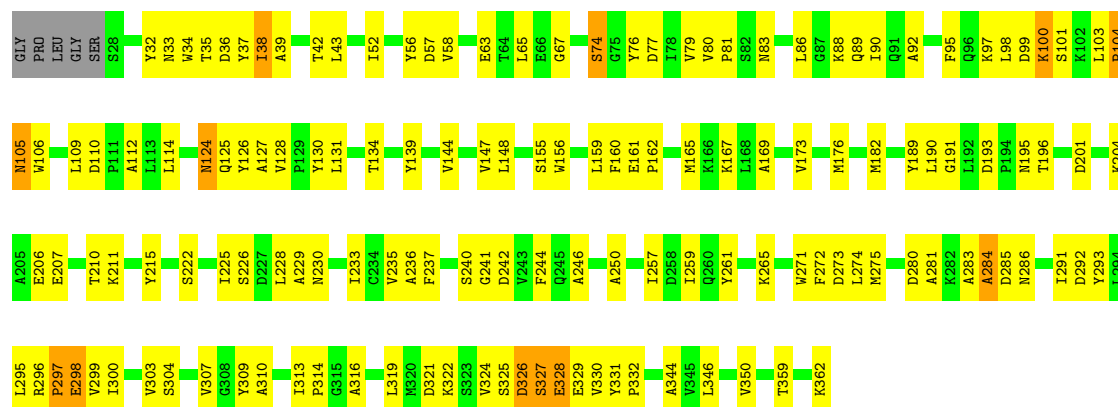
• Molecule 1: Polyamine transport protein

Chain K: 58% 39% ..



• Molecule 1: Polyamine transport protein

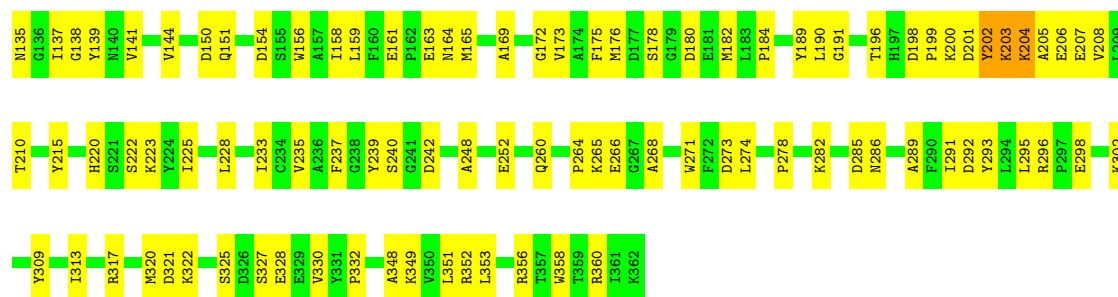
Chain L: 56% 39% ..



• Molecule 1: Polyamine transport protein

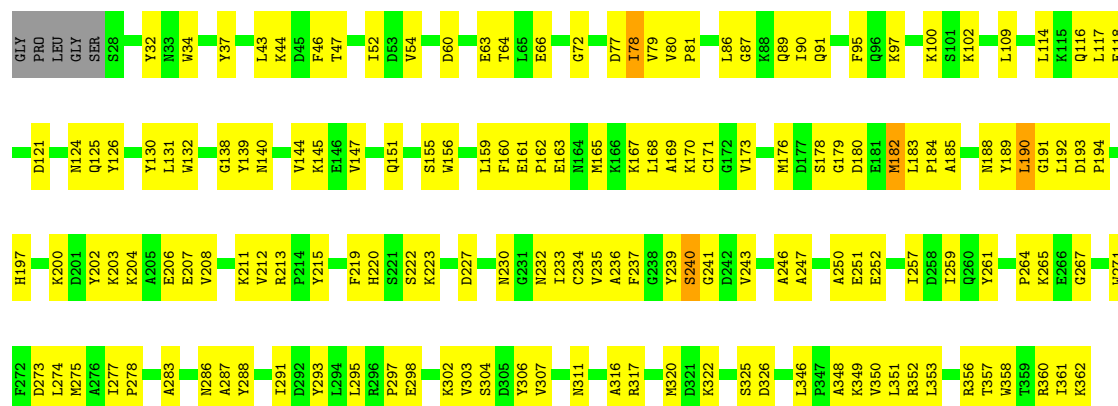
Chain M: 62% 36% ..





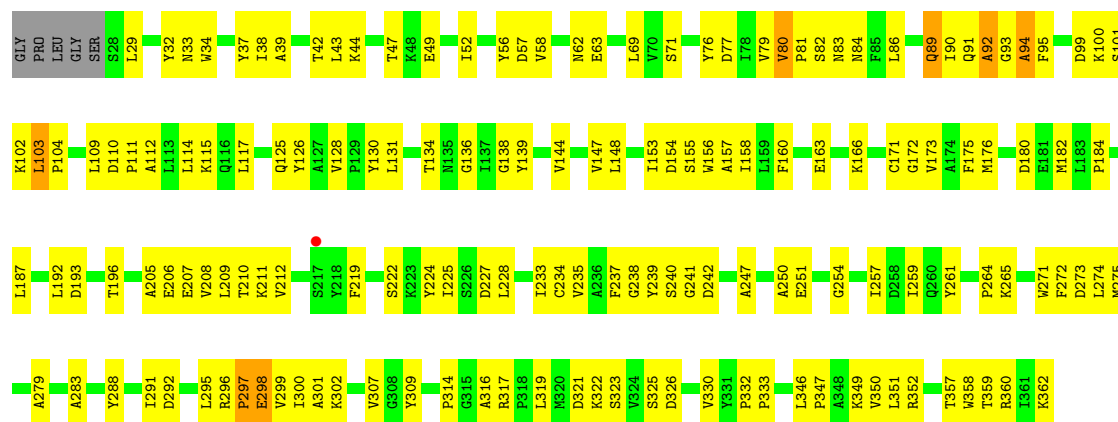
• Molecule 1: Polyamine transport protein

Chain N: 53% 44%



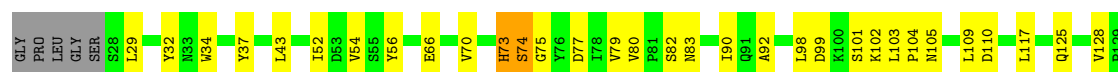
• Molecule 1: Polyamine transport protein

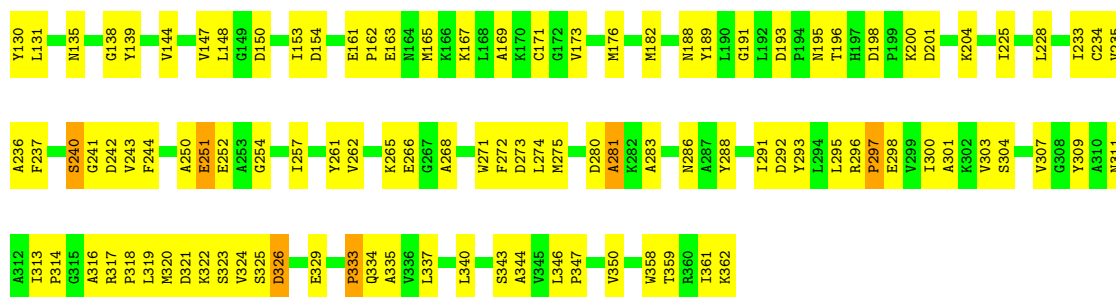
Chain O: 52% 44%



• Molecule 1: Polyamine transport protein

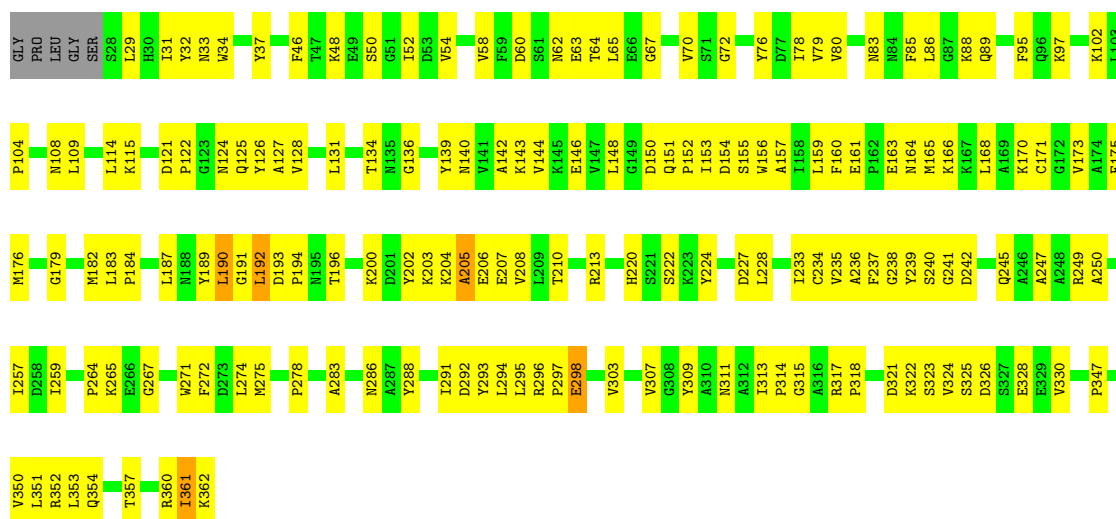
Chain P: 58% 38%





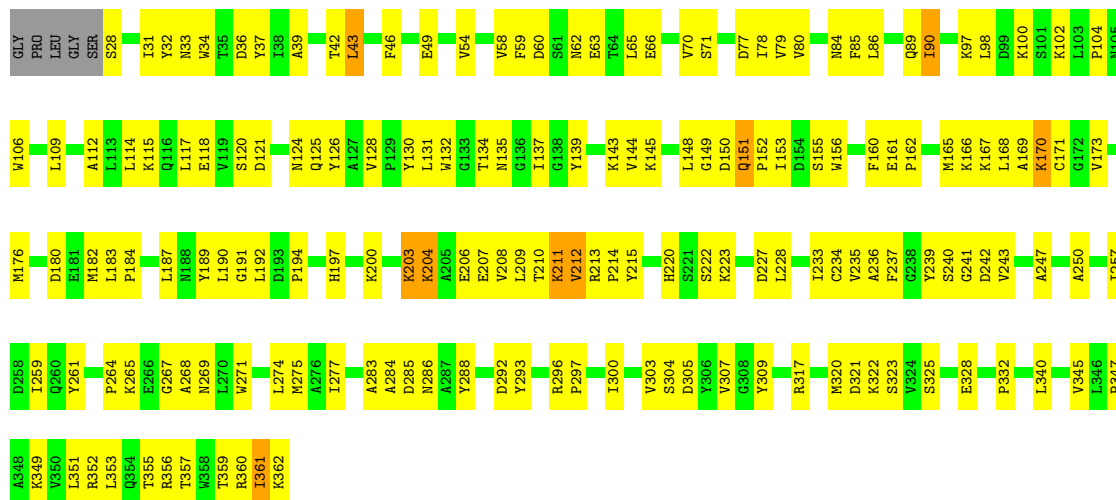
• Molecule 1: Polyamine transport protein

Chain Q: 50% 47%



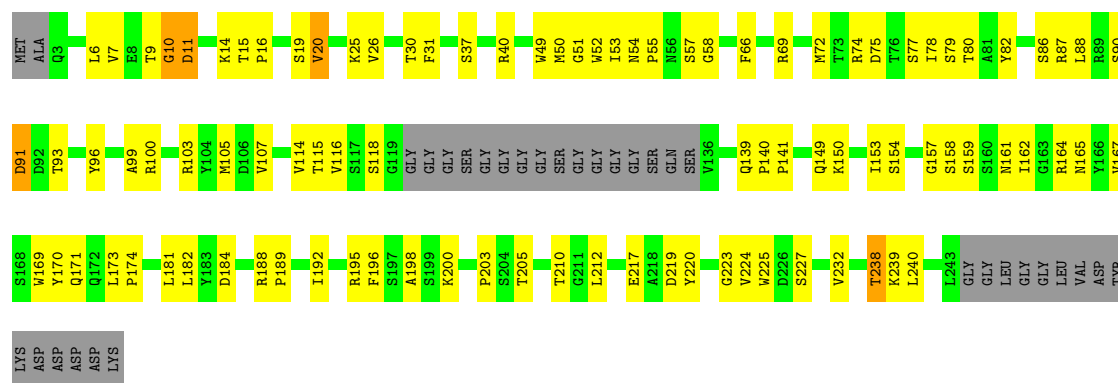
• Molecule 1: Polyamine transport protein

Chain R: 49% 47%



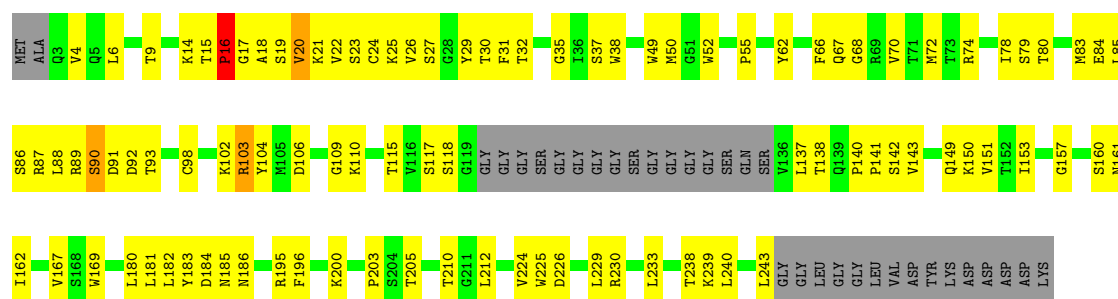
• Molecule 2: ScFv5

Chain a:  50% 35% 13%



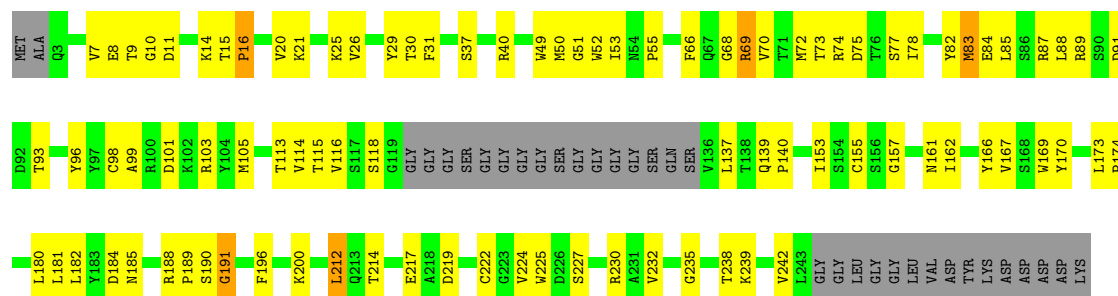
• Molecule 2: ScFv5

Chain b:  49% 37% 13%



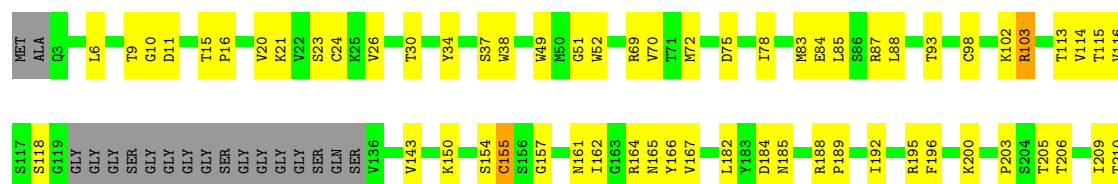
• Molecule 2: ScFv5

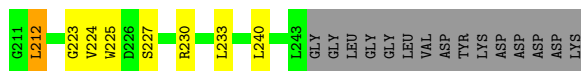
Chain c:  52% 34% 13%



• Molecule 2: ScFv5

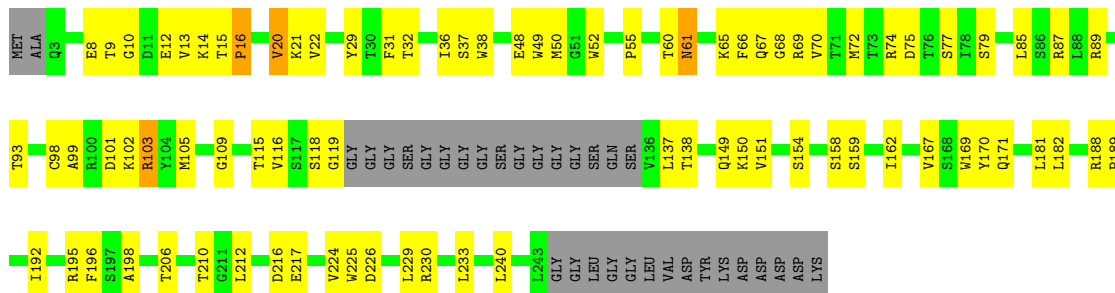
Chain d:  60% 26% 13%





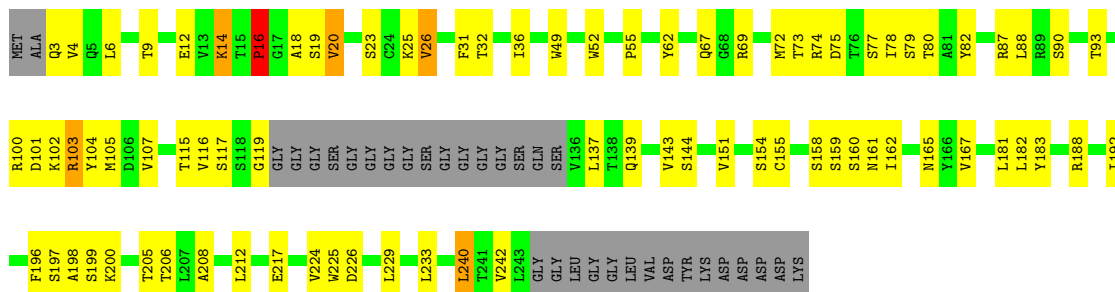
- Molecule 2: ScFv5

Chain e:



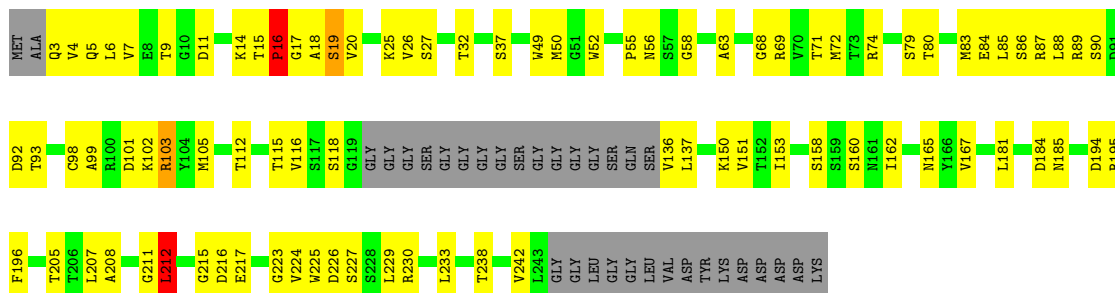
- Molecule 2: ScFv5

Chain f:



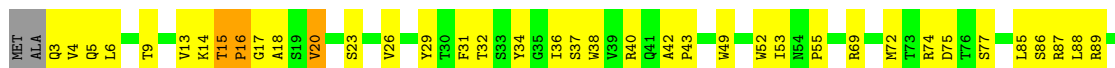
- Molecule 2: ScFv5

Chain g:

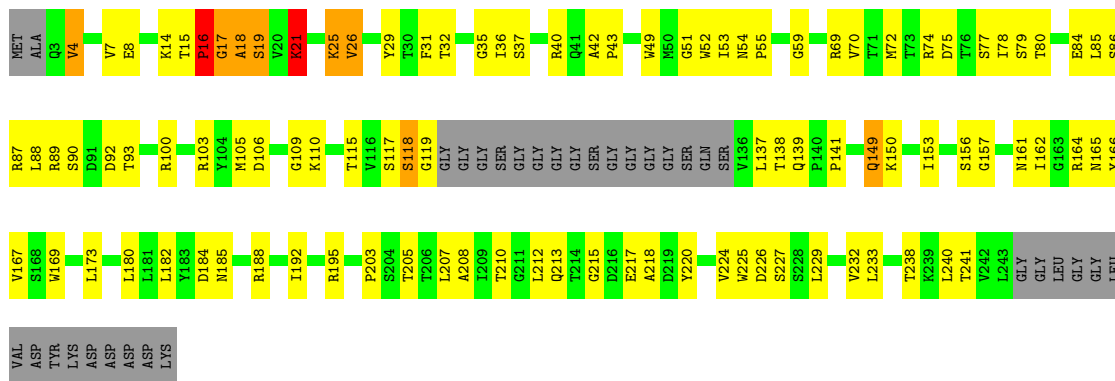


- Molecule 2: ScFv5

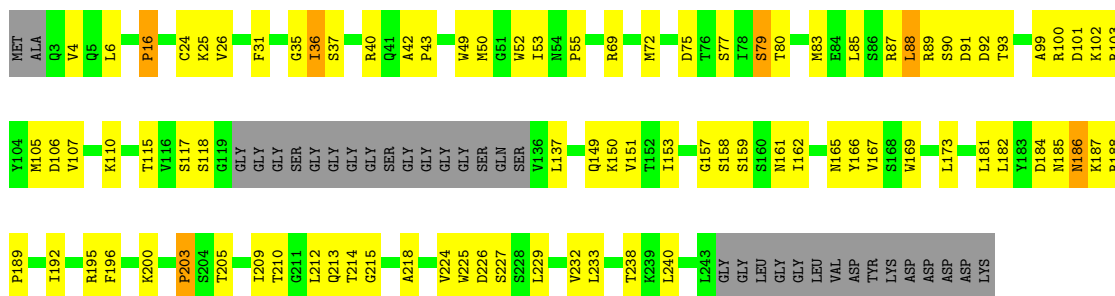
Chain h:



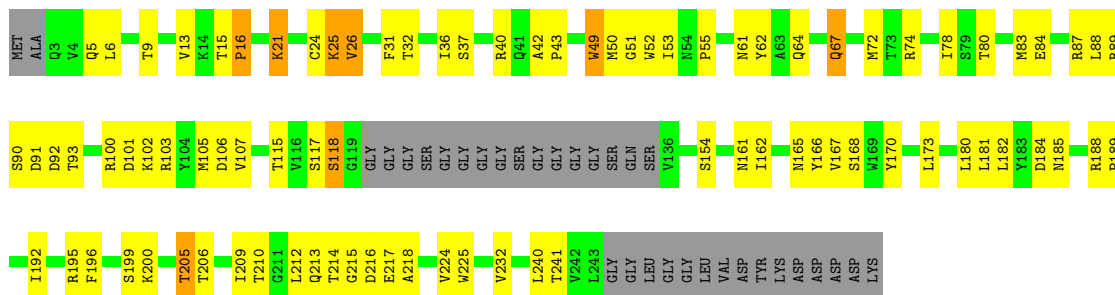
- Molecule 2: ScFv5



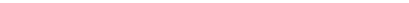
- Molecule 2: ScFv5

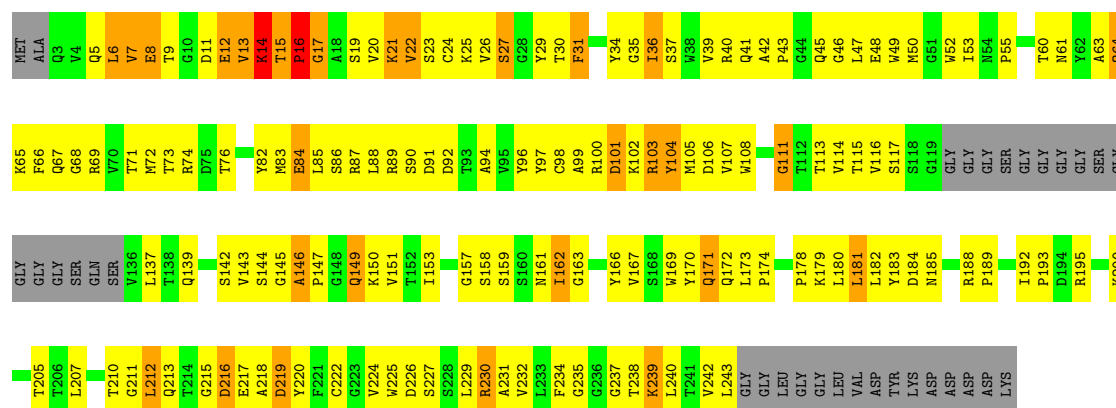


- Molecule 2: ScFv5

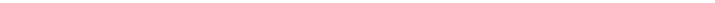


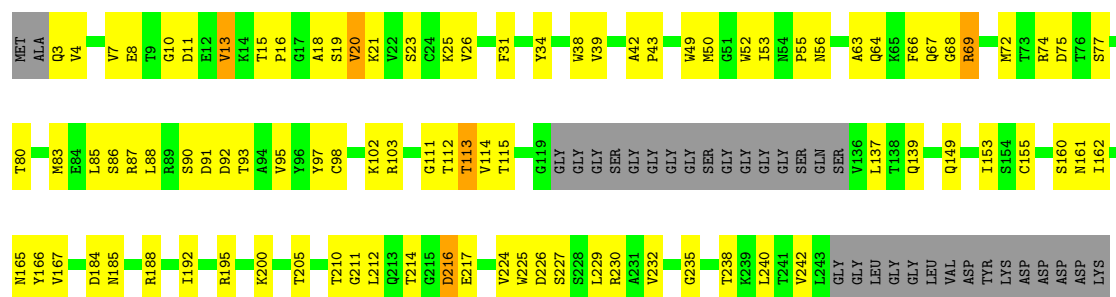
- Molecule 2: ScFv5

Chain I:  27% 49% 11% 13%



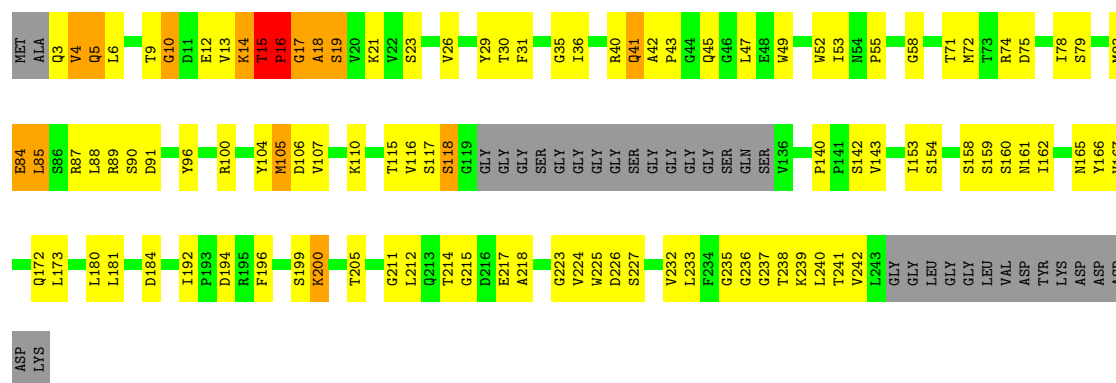
- Molecule 2: ScFv5

Chain m:  51% 34% • 13%

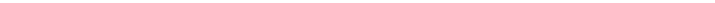


- Molecule 2: ScFv5

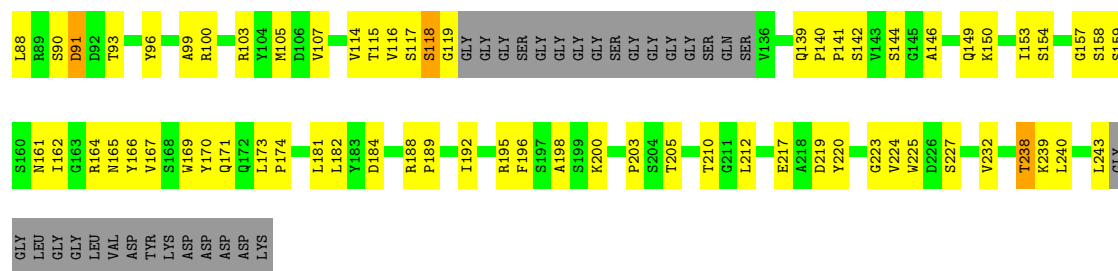
Chain n:



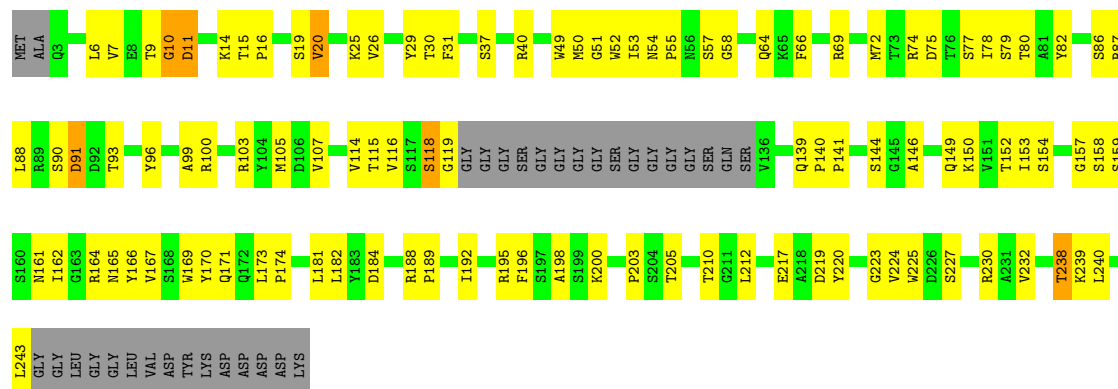
- Molecule 2: ScFv5

Chain o:  47% 38% 0 13%

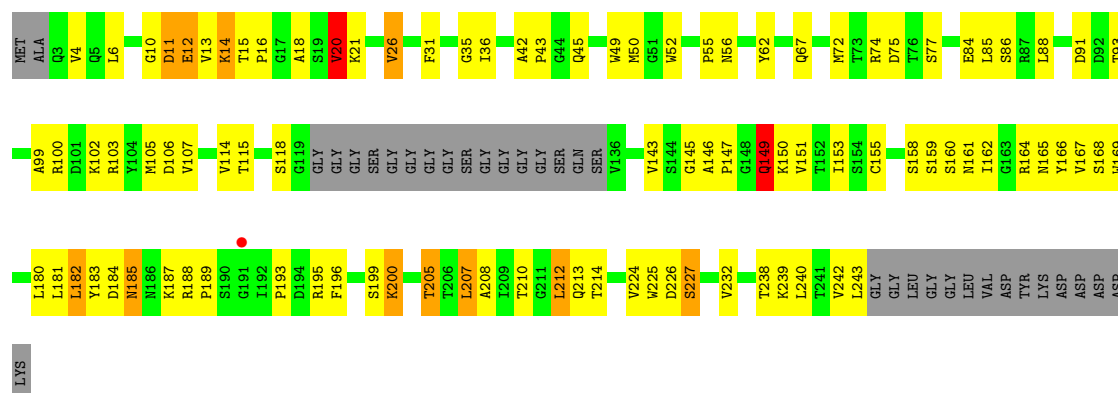




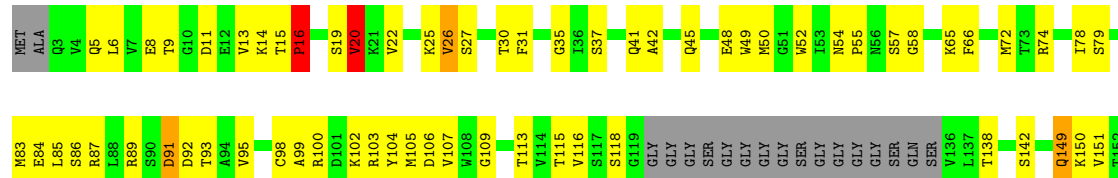
• Molecule 2: ScFv5

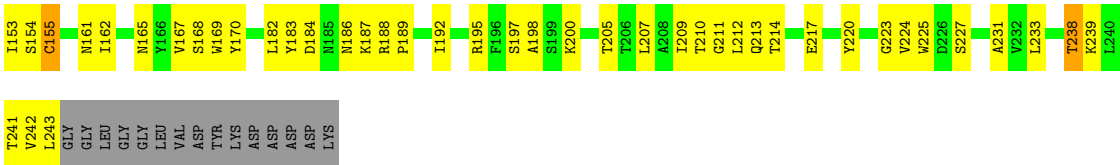


• Molecule 2: ScFv5



• Molecule 2: ScFv5





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	146.24Å 481.80Å 146.13Å 90.00° 120.08° 90.00°	Depositor
Resolution (Å)	46.47 – 3.40 46.47 – 3.40	Depositor EDS
% Data completeness (in resolution range)	89.5 (46.47-3.40) 89.4 (46.47-3.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.228 , 0.268 0.231 , 0.269	Depositor DCC
R_{free} test set	10759 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.418 for l,k,-h-l 0.418 for -h-l,k,h 0.196 for l,-k,h 0.190 for -h-l,-k,l 0.196 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	78156	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, SPD

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	0.21	0/2684	0.49	0/3653
1	B	0.23	0/2684	0.54	0/3653
1	C	0.24	0/2684	0.50	0/3653
1	D	0.23	0/2684	0.52	0/3653
1	E	0.28	0/2684	0.60	2/3653 (0.1%)
1	F	0.24	0/2684	0.55	0/3653
1	G	0.24	0/2684	0.52	0/3653
1	H	0.24	0/2684	0.65	4/3653 (0.1%)
1	I	0.35	2/2684 (0.1%)	0.67	2/3653 (0.1%)
1	J	0.29	0/2684	0.62	2/3653 (0.1%)
1	K	0.29	0/2684	0.64	2/3653 (0.1%)
1	L	0.28	0/2684	0.58	0/3653
1	M	0.25	0/2684	0.57	1/3653 (0.0%)
1	N	0.26	0/2684	0.54	0/3653
1	O	0.33	1/2684 (0.0%)	0.66	2/3653 (0.1%)
1	P	0.28	0/2684	0.62	2/3653 (0.1%)
1	Q	0.32	0/2684	0.64	2/3653 (0.1%)
1	R	0.30	0/2684	0.67	1/3653 (0.0%)
2	a	0.42	1/1736 (0.1%)	0.80	8/2358 (0.3%)
2	b	0.36	1/1736 (0.1%)	0.68	1/2358 (0.0%)
2	c	0.44	1/1736 (0.1%)	0.72	1/2358 (0.0%)
2	d	0.34	0/1736	0.66	0/2358
2	e	0.35	1/1736 (0.1%)	0.66	0/2358
2	f	0.40	2/1736 (0.1%)	0.66	1/2358 (0.0%)
2	g	0.39	1/1736 (0.1%)	0.76	2/2358 (0.1%)
2	h	0.38	0/1736	0.69	1/2358 (0.0%)
2	i	0.39	1/1736 (0.1%)	0.71	4/2358 (0.2%)
2	j	0.34	0/1736	0.70	1/2358 (0.0%)
2	k	0.46	2/1736 (0.1%)	0.79	8/2358 (0.3%)
2	l	0.47	0/1736	1.00	7/2358 (0.3%)
2	m	0.37	0/1736	0.63	0/2358
2	n	0.40	0/1736	0.88	4/2358 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	o	0.42	1/1736 (0.1%)	0.80	8/2358 (0.3%)
2	p	0.42	1/1736 (0.1%)	0.80	8/2358 (0.3%)
2	q	0.42	0/1736	0.84	3/2358 (0.1%)
2	r	0.48	1/1736 (0.1%)	0.86	4/2358 (0.2%)
All	All	0.33	16/79560 (0.0%)	0.66	81/108198 (0.1%)

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	I	0	2
1	K	0	1
1	L	0	1
1	M	0	1
1	P	0	2
1	R	0	1
2	a	0	2
2	b	0	1
2	c	0	1
2	d	0	1
2	g	0	1
2	l	0	3
2	m	0	2
2	n	0	2
2	o	0	2
2	p	0	2
2	q	0	1
All	All	0	27

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	r	238	THR	CB-CG2	10.74	1.88	1.52
2	k	26	VAL	CB-CG2	7.92	1.78	1.52
2	i	26	VAL	CB-CG2	7.36	1.76	1.52
2	c	16	PRO	C-O	-7.36	1.18	1.24
1	I	137	ILE	C-N	6.06	1.36	1.33
2	f	16	PRO	C-O	-5.92	1.16	1.24
2	b	16	PRO	C-O	-5.84	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	16	PRO	C-O	-5.52	1.16	1.24
2	g	19	SER	CA-CB	-5.47	1.47	1.53
1	O	80	VAL	CB-CG1	5.45	1.70	1.52
2	k	26	VAL	CB-CG1	5.26	1.69	1.52
1	I	345	VAL	CB-CG2	5.25	1.69	1.52
2	o	238	THR	CB-CG2	5.18	1.69	1.52
2	p	238	THR	CB-CG2	5.18	1.69	1.52
2	a	238	THR	CB-CG2	5.18	1.69	1.52
2	f	26	VAL	CB-CG2	5.10	1.69	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	147	VAL	N-CA-C	-13.36	99.60	112.96
2	g	212	LEU	CB-CG-CD2	10.82	143.15	110.70
2	n	85	LEU	CA-CB-CG	10.03	151.39	116.30
1	H	146	GLU	CA-C-N	-8.78	111.92	121.84
1	H	146	GLU	C-N-CA	-8.78	111.92	121.84
2	q	227	SER	CA-C-O	-8.72	108.03	120.51
2	n	17	GLY	N-CA-C	-8.38	102.34	115.67
1	O	80	VAL	CG1-CB-CG2	8.14	128.70	110.80
2	k	21	LYS	CA-C-N	7.63	133.16	121.71
2	k	21	LYS	C-N-CA	7.63	133.16	121.71
1	I	345	VAL	CG1-CB-CG2	7.33	126.93	110.80
2	j	16	PRO	CB-CA-C	-7.21	102.40	111.56
2	g	16	PRO	N-CA-C	7.20	127.31	112.47
2	l	84	GLU	N-CA-C	6.90	119.66	109.24
2	a	238	THR	OG1-CB-CG2	6.75	122.81	109.30
2	p	238	THR	OG1-CB-CG2	6.75	122.80	109.30
2	o	238	THR	OG1-CB-CG2	6.74	122.77	109.30
1	E	210	THR	OG1-CB-CG2	6.58	122.46	109.30
2	c	83	MET	CB-CG-SD	6.42	131.97	112.70
2	a	90	SER	CA-C-N	6.34	131.29	120.71
2	a	90	SER	C-N-CA	6.34	131.29	120.71
1	H	147	VAL	CG1-CB-CG2	6.33	124.72	110.80
2	o	90	SER	CA-C-N	6.32	131.27	120.71
2	o	90	SER	C-N-CA	6.32	131.27	120.71
2	p	90	SER	CA-C-N	6.32	131.26	120.71
2	p	90	SER	C-N-CA	6.32	131.26	120.71
2	b	16	PRO	N-CA-CB	-6.31	96.62	103.25
2	l	149	GLN	CA-C-N	6.18	133.35	121.54
2	l	149	GLN	C-N-CA	6.18	133.35	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	15	THR	CA-CB-OG1	-6.04	100.54	109.60
2	i	21	LYS	CA-C-N	5.98	130.76	121.85
2	i	21	LYS	C-N-CA	5.98	130.76	121.85
2	l	181	LEU	CB-CG-CD2	-5.97	92.78	110.70
2	l	181	LEU	CD1-CG-CD2	-5.91	97.79	110.80
2	n	15	THR	CA-C-N	5.75	127.03	119.84
2	n	15	THR	C-N-CA	5.75	127.03	119.84
1	O	103	LEU	CB-CG-CD2	-5.74	93.47	110.70
2	o	223	GLY	CA-C-N	-5.71	114.87	123.27
2	o	223	GLY	C-N-CA	-5.71	114.87	123.27
2	p	223	GLY	CA-C-N	-5.71	114.88	123.27
2	p	223	GLY	C-N-CA	-5.71	114.88	123.27
2	k	16	PRO	CB-CA-C	-5.71	104.39	111.64
1	Q	205	ALA	CA-C-N	-5.69	112.08	122.38
1	Q	205	ALA	C-N-CA	-5.69	112.08	122.38
1	J	204	LYS	N-CA-C	-5.68	106.35	113.28
2	i	25	LYS	CA-C-N	-5.67	114.45	122.34
2	i	25	LYS	C-N-CA	-5.67	114.45	122.34
2	a	223	GLY	CA-C-N	-5.66	114.95	123.27
2	a	223	GLY	C-N-CA	-5.66	114.95	123.27
2	k	25	LYS	CA-C-N	-5.64	116.24	122.27
2	k	25	LYS	C-N-CA	-5.64	116.24	122.27
2	k	205	THR	CA-C-N	5.63	132.56	123.33
2	k	205	THR	C-N-CA	5.63	132.56	123.33
2	a	11	ASP	CA-C-N	-5.57	113.06	121.86
2	a	11	ASP	C-N-CA	-5.57	113.06	121.86
2	p	11	ASP	CA-C-N	-5.55	113.10	121.86
2	p	11	ASP	C-N-CA	-5.55	113.10	121.86
1	I	206	GLU	CA-CB-CG	5.54	125.19	114.10
2	l	171	GLN	CB-CG-CD	5.52	121.99	112.60
2	o	11	ASP	CA-C-N	-5.51	113.15	121.86
2	o	11	ASP	C-N-CA	-5.51	113.15	121.86
1	M	203	LYS	N-CA-C	5.33	122.15	110.80
2	q	149	GLN	CA-CB-CG	-5.29	103.52	114.10
2	a	91	ASP	CB-CG-OD1	-5.27	106.28	118.40
1	K	148	LEU	CA-C-N	-5.27	113.80	121.44
1	K	148	LEU	C-N-CA	-5.27	113.80	121.44
2	r	238	THR	OG1-CB-CG2	5.27	119.83	109.30
2	q	182	LEU	CD1-CG-CD2	-5.26	99.22	110.80
2	o	91	ASP	CB-CG-OD1	-5.26	106.30	118.40
2	p	91	ASP	CB-CG-OD1	-5.26	106.30	118.40
1	E	210	THR	CA-CB-CG2	5.25	119.43	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	k	26	VAL	CG1-CB-CG2	5.25	122.36	110.80
1	J	203	LYS	CB-CG-CD	5.24	123.36	111.30
2	r	8	GLU	CA-C-N	5.23	130.50	120.97
2	r	8	GLU	C-N-CA	5.23	130.50	120.97
2	r	238	THR	N-CA-C	-5.18	100.96	109.40
2	l	16	PRO	N-CA-CB	-5.16	97.83	103.25
1	P	251	GLU	CA-C-N	-5.09	112.13	122.31
1	P	251	GLU	C-N-CA	-5.09	112.13	122.31
1	R	204	LYS	CB-CG-CD	-5.04	99.71	111.30
2	f	16	PRO	CB-CA-C	-5.02	103.27	111.56

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	73	HIS	Peptide
1	I	203	LYS	Peptide
1	I	361	ILE	Peptide
1	K	169	ALA	Peptide
1	L	273	ASP	Peptide
1	M	202	TYR	Peptide
1	P	333	PRO	Peptide
1	P	361	ILE	Peptide
1	R	361	ILE	Peptide
2	a	10	GLY	Peptide
2	a	11	ASP	Peptide
2	b	117	SER	Peptide
2	c	157	GLY	Peptide
2	d	157	GLY	Peptide
2	g	86	SER	Peptide
2	l	101	ASP	Peptide
2	l	219	ASP	Peptide
2	l	36	ILE	Peptide
2	m	216	ASP	Peptide
2	m	90	SER	Peptide
2	n	84	GLU	Peptide
2	n	90	SER	Peptide
2	o	10	GLY	Peptide
2	o	11	ASP	Peptide
2	p	10	GLY	Peptide
2	p	11	ASP	Peptide
2	q	212	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	2618	0	2580	80	0
1	B	2618	0	2580	79	0
1	C	2618	0	2580	67	0
1	D	2618	0	2580	76	0
1	E	2618	0	2578	102	0
1	F	2618	0	2580	87	1
1	G	2618	0	2580	77	0
1	H	2618	0	2576	75	1
1	I	2618	0	2580	109	0
1	J	2618	0	2580	129	0
1	K	2618	0	2576	127	0
1	L	2618	0	2579	124	0
1	M	2618	0	2580	110	0
1	N	2618	0	2580	148	0
1	O	2618	0	2580	151	0
1	P	2618	0	2580	127	0
1	Q	2618	0	2580	159	0
1	R	2618	0	2580	167	0
2	a	1699	0	1659	78	0
2	b	1699	0	1659	101	0
2	c	1699	0	1659	94	0
2	d	1699	0	1659	64	0
2	e	1699	0	1659	65	1
2	f	1699	0	1659	69	4
2	g	1699	0	1659	96	0
2	h	1699	0	1659	123	1
2	i	1699	0	1658	128	0
2	j	1699	0	1659	68	0
2	k	1699	0	1659	96	0
2	l	1699	0	1659	234	0
2	m	1699	0	1659	76	0
2	n	1699	0	1659	111	0
2	o	1699	0	1659	121	3
2	p	1699	0	1658	120	1
2	q	1699	0	1659	90	0
2	r	1699	0	1659	101	0
3	A	15	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	0	0	0
3	C	15	0	0	1	0
3	D	15	0	0	1	0
3	E	20	0	0	2	0
3	F	15	0	0	2	0
3	G	10	0	0	3	0
3	H	10	0	0	1	0
3	I	15	0	0	3	0
3	J	15	0	0	1	0
3	K	15	0	0	1	0
3	L	15	0	0	1	0
3	M	15	0	0	4	0
3	N	30	0	0	6	0
3	O	30	0	0	3	0
3	R	15	0	0	3	0
4	A	10	0	19	5	0
4	B	10	0	17	2	0
4	C	10	0	17	3	0
4	D	10	0	19	5	0
4	E	10	0	17	5	0
4	F	10	0	19	3	0
4	G	10	0	19	2	0
4	H	10	0	19	4	0
4	I	10	0	17	1	0
4	J	10	0	19	3	0
4	K	10	0	19	3	0
4	L	10	0	19	2	0
4	M	10	0	17	3	0
4	N	10	0	17	6	0
4	O	10	0	17	6	0
4	P	10	0	17	5	0
4	Q	10	0	19	7	0
4	R	10	0	17	3	0
All	All	78156	0	76613	3615	6

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 23.

All (3615) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:26:VAL:CB	2:k:26:VAL:CG2	1.78	1.56
2:i:26:VAL:CB	2:i:26:VAL:CG2	1.76	1.56
2:g:18:ALA:CB	2:g:88:LEU:H	1.18	1.53
2:r:238:THR:CB	2:r:238:THR:CG2	1.88	1.49
2:h:225:TRP:CZ3	2:h:227:SER:HA	1.47	1.48
2:g:18:ALA:HB3	2:g:88:LEU:N	1.12	1.45
2:g:18:ALA:HB2	2:g:88:LEU:CB	1.42	1.44
2:l:17:GLY:N	2:l:88:LEU:HB2	1.13	1.42
2:l:21:LYS:CB	2:l:83:MET:O	1.67	1.41
2:g:18:ALA:CB	2:g:88:LEU:HG	1.51	1.40
2:n:15:THR:CG2	2:n:16:PRO:HD2	1.52	1.38
2:l:21:LYS:HD2	2:l:84:GLU:CG	1.58	1.34
2:h:225:TRP:CZ3	2:h:227:SER:CA	2.12	1.33
2:n:15:THR:HG22	2:n:16:PRO:CD	1.57	1.33
2:q:13:VAL:O	2:q:14:LYS:HE2	1.19	1.31
2:k:102:LYS:NZ	2:k:106:ASP:OD2	1.62	1.31
1:J:37:TYR:CE1	1:J:131:LEU:HD12	1.68	1.26
2:l:17:GLY:HA3	2:l:88:LEU:N	1.49	1.24
2:l:21:LYS:CE	2:l:84:GLU:CD	2.12	1.23
2:g:18:ALA:CB	2:g:88:LEU:CG	2.16	1.23
2:i:118:SER:OG	2:o:119:GLY:O	1.56	1.21
2:l:17:GLY:HA2	2:l:88:LEU:CG	1.69	1.21
2:l:17:GLY:N	2:l:88:LEU:CB	2.05	1.20
2:l:17:GLY:H	2:l:88:LEU:CB	1.53	1.19
2:k:118:SER:HA	2:p:119:GLY:N	1.58	1.19
2:g:18:ALA:CB	2:g:88:LEU:CB	2.20	1.17
2:g:18:ALA:HB1	2:g:88:LEU:CG	1.73	1.17
2:i:118:SER:HA	2:o:118:SER:C	1.70	1.17
2:o:20:VAL:CG1	2:o:88:LEU:HD11	1.75	1.16
2:p:20:VAL:CG1	2:p:88:LEU:HD11	1.76	1.16
2:q:13:VAL:O	2:q:14:LYS:CE	1.92	1.16
1:I:203:LYS:NZ	1:I:357:THR:OG1	1.79	1.16
2:i:118:SER:C	2:o:118:SER:OG	1.88	1.16
2:a:20:VAL:CG1	2:a:88:LEU:HD11	1.75	1.15
2:n:5:GLN:HE22	2:n:110:LYS:NZ	1.43	1.15
2:l:15:THR:HB	2:l:16:PRO:CD	1.78	1.14
2:l:21:LYS:HB3	2:l:83:MET:O	1.47	1.13
2:l:21:LYS:HE3	2:l:84:GLU:CD	1.69	1.13
2:k:118:SER:HA	2:p:118:SER:C	1.72	1.13
2:h:225:TRP:CH2	2:h:230:ARG:HA	1.82	1.12
2:b:18:ALA:HB1	2:b:86:SER:C	1.75	1.11
2:b:18:ALA:HB2	2:b:88:LEU:H	1.09	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:68:GLY:HA2	2:i:21:LYS:CE	1.79	1.11
2:i:119:GLY:N	2:o:118:SER:OG	1.84	1.11
2:d:20:VAL:CG2	2:d:88:LEU:HD21	1.79	1.10
2:l:15:THR:CB	2:l:16:PRO:CD	2.29	1.10
2:l:219:ASP:OD2	2:l:239:LYS:NZ	1.81	1.10
2:g:18:ALA:HB2	2:g:88:LEU:HB2	1.14	1.09
2:l:21:LYS:HD2	2:l:84:GLU:HG3	1.12	1.09
2:l:21:LYS:HB2	2:l:83:MET:O	1.42	1.09
2:b:18:ALA:HB3	2:b:86:SER:O	1.53	1.09
2:l:15:THR:HB	2:l:16:PRO:HD3	1.20	1.08
2:l:17:GLY:HA2	2:l:88:LEU:HG	1.10	1.08
2:l:21:LYS:HE2	2:l:84:GLU:OE1	1.52	1.08
2:k:117:SER:C	2:p:118:SER:O	1.96	1.08
2:b:18:ALA:HB2	2:b:88:LEU:N	1.68	1.08
2:c:15:THR:CG2	2:c:16:PRO:HD2	1.84	1.08
2:l:17:GLY:CA	2:l:88:LEU:CB	2.32	1.07
2:h:225:TRP:CE3	2:h:227:SER:N	2.22	1.07
2:i:188:ARG:NH1	2:i:192:ILE:O	1.86	1.07
2:k:162:ILE:O	2:k:200:LYS:NZ	1.87	1.07
2:h:225:TRP:HZ3	2:h:227:SER:CA	1.52	1.07
1:K:170:LYS:NZ	1:K:234:CYS:SG	2.27	1.07
2:d:15:THR:HG22	2:d:16:PRO:CD	1.84	1.06
2:h:225:TRP:CZ3	2:h:227:SER:N	2.23	1.06
2:l:69:ARG:HD3	2:l:87:ARG:HG2	1.35	1.06
2:h:225:TRP:CZ3	2:h:226:ASP:C	2.35	1.04
2:b:18:ALA:CB	2:b:86:SER:O	2.06	1.04
2:h:18:ALA:HB2	2:h:88:LEU:N	1.71	1.04
2:l:17:GLY:CA	2:l:88:LEU:H	1.69	1.04
1:N:349:LYS:NZ	3:N:406:SO4:O2	1.89	1.04
2:h:3:GLN:HG2	2:h:4:VAL:H	1.21	1.04
1:N:190:LEU:HD13	2:o:243:LEU:HD22	1.38	1.04
2:h:18:ALA:HB2	2:h:87:ARG:HA	1.40	1.03
2:h:18:ALA:CB	2:h:88:LEU:H	1.70	1.03
2:l:17:GLY:CA	2:l:88:LEU:HB2	1.87	1.03
2:l:17:GLY:CA	2:l:88:LEU:N	2.20	1.03
2:l:37:SER:HB3	2:l:99:ALA:HB3	1.37	1.03
2:h:18:ALA:CB	2:h:87:ARG:HA	1.87	1.03
2:i:18:ALA:HB3	2:i:88:LEU:HD12	1.38	1.03
1:P:333:PRO:HB3	2:p:166:TYR:CE1	1.93	1.03
2:d:15:THR:CG2	2:d:16:PRO:HD2	1.88	1.03
2:b:15:THR:O	2:b:17:GLY:N	1.91	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:15:THR:HG22	2:c:16:PRO:HD2	1.05	1.02
2:h:20:VAL:HG22	2:h:88:LEU:HD11	1.39	1.02
2:g:18:ALA:HB2	2:g:88:LEU:CG	1.83	1.01
1:R:349:LYS:NZ	3:R:402:SO4:O1	1.92	1.01
2:p:20:VAL:HG12	2:p:88:LEU:CD1	1.91	1.01
2:a:20:VAL:HG12	2:a:88:LEU:CD1	1.90	1.01
2:b:18:ALA:CB	2:b:88:LEU:H	1.72	1.00
2:h:18:ALA:HB2	2:h:87:ARG:CA	1.90	1.00
2:l:17:GLY:HA3	2:l:88:LEU:H	0.84	1.00
2:l:21:LYS:HD2	2:l:84:GLU:CB	1.90	1.00
2:o:20:VAL:HG12	2:o:88:LEU:CD1	1.91	1.00
1:M:203:LYS:HD2	1:M:204:LYS:HG3	1.44	0.99
2:r:102:LYS:NZ	2:r:106:ASP:OD2	1.94	0.99
2:b:18:ALA:CB	2:b:87:ARG:HA	1.91	0.99
2:c:185:ASN:OD1	2:c:200:LYS:NZ	1.96	0.99
1:N:163:GLU:OE2	2:o:142:SER:HB2	1.63	0.99
1:N:349:LYS:NZ	3:N:406:SO4:S	2.35	0.99
1:L:193:ASP:HB3	1:L:196:THR:HG23	1.45	0.99
2:l:21:LYS:CD	2:l:84:GLU:HG3	1.94	0.98
1:O:147:VAL:HG23	1:O:148:LEU:HD13	1.41	0.98
2:l:21:LYS:CD	2:l:84:GLU:CG	2.41	0.98
2:b:49:TRP:HH2	2:b:52:TRP:HB2	1.29	0.97
2:h:18:ALA:HB1	2:h:86:SER:C	1.89	0.97
2:p:243:LEU:HD22	1:R:190:LEU:HD13	1.46	0.97
2:i:18:ALA:CB	2:i:88:LEU:HD12	1.95	0.97
1:K:100:LYS:NZ	1:K:124:ASN:O	1.97	0.97
2:p:20:VAL:HG12	2:p:88:LEU:HD11	0.97	0.97
2:d:185:ASN:OD1	2:d:200:LYS:NZ	1.95	0.97
1:N:190:LEU:HD13	2:o:243:LEU:CD2	1.95	0.97
2:a:20:VAL:HG12	2:a:88:LEU:HD11	0.97	0.96
2:q:207:LEU:HG	2:q:208:ALA:N	1.80	0.96
2:o:20:VAL:HG12	2:o:88:LEU:HD11	0.97	0.96
2:k:40:ARG:NH1	2:k:92:ASP:OD1	1.97	0.96
2:f:162:ILE:O	2:f:200:LYS:NZ	1.99	0.96
1:J:37:TYR:HE1	1:J:131:LEU:HD12	1.17	0.96
2:g:69:ARG:HH12	2:g:89:ARG:HH11	1.04	0.95
2:p:144:SER:OG	1:R:161:GLU:OE2	1.84	0.95
2:p:243:LEU:CD2	1:R:190:LEU:HD13	1.95	0.95
1:Q:161:GLU:OE2	1:Q:189:TYR:OH	1.83	0.95
1:A:176:MET:HE1	1:A:239:TYR:CE2	2.01	0.95
2:b:18:ALA:HB2	2:b:87:ARG:HA	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:68:GLY:HA2	2:i:21:LYS:HE2	1.47	0.95
2:g:68:GLY:HA2	2:i:21:LYS:HE3	1.49	0.95
2:q:153:ILE:HG21	2:q:238:THR:HG21	1.46	0.95
2:p:152:THR:OG1	1:R:265:LYS:NZ	2.00	0.94
2:h:18:ALA:CB	2:h:87:ARG:CA	2.45	0.94
2:k:37:SER:HB3	2:k:49:TRP:HZ3	1.32	0.94
2:n:15:THR:CB	2:n:16:PRO:HD2	1.95	0.94
2:f:12:GLU:OE2	2:f:14:LYS:NZ	2.01	0.94
2:b:18:ALA:CB	2:b:87:ARG:CA	2.46	0.94
1:L:131:LEU:HD13	1:L:309:TYR:HB2	1.50	0.94
2:l:149:GLN:HG3	1:Q:191:GLY:HA3	1.49	0.94
2:d:20:VAL:HG21	2:d:88:LEU:HD21	1.49	0.94
2:g:18:ALA:CB	2:g:88:LEU:N	1.92	0.93
2:d:15:THR:HG22	2:d:16:PRO:HD2	0.97	0.93
2:g:18:ALA:CB	2:g:88:LEU:CA	2.46	0.93
2:g:69:ARG:NH1	2:g:89:ARG:HH11	1.64	0.93
2:b:18:ALA:CB	2:b:86:SER:C	2.42	0.93
2:n:162:ILE:HG12	2:n:224:VAL:HG21	1.48	0.93
2:b:18:ALA:HB2	2:b:87:ARG:CA	1.98	0.93
2:l:21:LYS:O	2:l:22:VAL:O	1.87	0.93
2:l:17:GLY:HA2	2:l:88:LEU:CB	1.95	0.93
2:n:5:GLN:HE22	2:n:110:LYS:HZ3	1.14	0.92
1:P:333:PRO:CA	2:p:166:TYR:OH	2.17	0.92
1:R:353:LEU:HA	1:R:356:ARG:HE	1.35	0.92
2:h:18:ALA:CB	2:h:86:SER:O	2.18	0.92
2:k:118:SER:CA	2:p:118:SER:C	2.40	0.92
2:n:9:THR:OG1	2:n:23:SER:N	2.02	0.92
2:r:19:SER:O	2:r:85:LEU:O	1.87	0.92
1:B:71:SER:HB3	1:G:67:GLY:HA3	1.50	0.92
2:h:20:VAL:CG2	2:h:88:LEU:HD11	1.99	0.92
2:h:225:TRP:CE3	2:h:226:ASP:C	2.47	0.92
2:c:15:THR:HG22	2:c:16:PRO:CD	1.97	0.92
2:i:118:SER:HA	2:o:119:GLY:N	1.83	0.92
1:E:167:LYS:O	1:E:170:LYS:HD2	1.70	0.92
1:R:203:LYS:HG3	1:R:204:LYS:N	1.81	0.92
1:J:117:LEU:HD13	1:J:274:LEU:HD21	1.52	0.92
1:O:34:TRP:HB2	1:O:37:TYR:HD2	1.32	0.92
2:e:151:VAL:HG12	2:e:212:LEU:HD11	1.50	0.91
2:l:137:LEU:HD22	2:l:162:ILE:HD11	1.53	0.91
1:M:176:MET:HE1	1:M:239:TYR:CE2	2.05	0.91
1:K:146:GLU:HG2	1:K:147:VAL:HG13	1.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:317:ARG:NH1	2:q:103:ARG:HD3	1.86	0.91
1:N:66:GLU:HG3	1:N:89:GLN:HE21	1.36	0.91
1:M:198:ASP:HB3	1:M:201:ASP:HB2	1.53	0.91
2:i:15:THR:O	2:i:16:PRO:O	1.88	0.91
1:B:117:LEU:HD13	1:B:274:LEU:HD21	1.53	0.90
2:l:17:GLY:CA	2:l:88:LEU:CG	2.49	0.90
2:i:117:SER:HG	2:o:117:SER:HG	1.12	0.90
1:N:200:LYS:HE3	1:N:204:LYS:HG2	1.53	0.90
2:h:55:PRO:HA	2:h:74:ARG:HD3	1.53	0.90
2:g:25:LYS:HG3	2:g:80:THR:HG22	1.53	0.89
2:n:15:THR:HG22	2:n:16:PRO:HD2	0.92	0.89
2:i:15:THR:O	2:i:18:ALA:HB2	1.73	0.89
2:f:154:SER:HB3	2:f:206:THR:HG22	1.54	0.89
2:l:21:LYS:HE3	2:l:84:GLU:OE2	1.73	0.89
2:l:161:ASN:O	2:l:163:GLY:N	2.05	0.89
2:d:20:VAL:HG23	2:d:88:LEU:HD21	1.52	0.89
1:I:203:LYS:HA	1:I:206:GLU:HB3	1.53	0.88
2:k:64:GLN:HA	2:k:67:GLN:HB2	1.53	0.88
2:l:13:VAL:O	2:l:14:LYS:HB2	1.70	0.88
1:M:352:ARG:NH1	3:M:402:SO4:O3	2.05	0.88
2:c:20:VAL:HG23	2:c:88:LEU:HD21	1.55	0.88
2:l:21:LYS:HB3	2:l:84:GLU:CA	2.03	0.88
1:P:333:PRO:HB3	2:p:166:TYR:HE1	1.35	0.88
2:a:161:ASN:HB2	2:a:224:VAL:HG21	1.56	0.87
2:m:165:ASN:ND2	2:m:225:TRP:O	2.07	0.87
2:q:165:ASN:ND2	2:q:225:TRP:O	2.07	0.87
3:L:401:SO4:O3	1:R:352:ARG:NH2	2.07	0.87
1:G:321:ASP:OD2	1:G:323:SER:OG	1.93	0.87
2:g:18:ALA:HB2	2:g:88:LEU:CA	2.05	0.87
2:h:18:ALA:HB3	2:h:86:SER:O	1.73	0.87
2:l:21:LYS:HB3	2:l:83:MET:C	2.00	0.87
2:o:161:ASN:HB2	2:o:224:VAL:HG21	1.56	0.87
2:b:21:LYS:HD2	2:c:68:GLY:HA2	1.56	0.87
2:d:6:LEU:HG	2:d:26:VAL:HG12	1.56	0.86
2:g:18:ALA:HB1	2:g:88:LEU:HG	0.86	0.86
1:I:155:SER:OG	1:I:266:GLU:OE2	1.93	0.86
2:e:60:THR:O	2:e:61:ASN:ND2	2.07	0.86
2:j:40:ARG:NH1	2:j:92:ASP:OD1	2.08	0.86
2:p:161:ASN:HB2	2:p:224:VAL:HG21	1.56	0.86
2:l:17:GLY:CA	2:l:88:LEU:HG	2.02	0.86
2:h:225:TRP:HE3	2:h:227:SER:N	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:LEU:HD11	1:E:208:VAL:HG21	1.57	0.86
1:J:49:GLU:OE2	1:J:296:ARG:NH2	2.08	0.86
1:L:104:PRO:O	1:L:106:TRP:N	2.08	0.85
1:N:167:LYS:O	1:N:170:LYS:NZ	2.08	0.85
2:i:40:ARG:NH1	2:i:92:ASP:OD1	2.07	0.85
1:J:213:ARG:HG3	1:J:213:ARG:HH11	1.40	0.85
1:G:49:GLU:OE2	1:G:296:ARG:NH2	2.09	0.85
2:i:118:SER:CA	2:o:118:SER:C	2.48	0.85
1:R:176:MET:HB2	1:R:182:MET:HE3	1.58	0.85
2:l:69:ARG:HG2	2:l:86:SER:HB3	1.57	0.85
2:f:49:TRP:HH2	2:f:52:TRP:HB2	1.41	0.85
2:h:49:TRP:HH2	2:h:52:TRP:HB2	1.42	0.85
1:N:191:GLY:HA3	2:o:149:GLN:CD	2.01	0.84
2:n:167:VAL:HG11	2:n:205:THR:HG21	1.58	0.84
1:P:346:LEU:HD23	1:P:350:VAL:HG21	1.59	0.84
2:l:218:ALA:HB3	2:l:220:TYR:HE1	1.41	0.84
2:d:20:VAL:HG22	2:d:88:LEU:HD11	1.58	0.84
1:E:169:ALA:HB2	1:E:215:TYR:HB3	1.57	0.84
1:K:187:LEU:HD21	1:K:205:ALA:HB2	1.58	0.84
2:i:19:SER:HB2	2:i:86:SER:HA	1.57	0.84
2:l:15:THR:OG1	2:l:16:PRO:HD2	1.77	0.84
2:e:49:TRP:HH2	2:e:52:TRP:HB2	1.41	0.84
2:m:55:PRO:HA	2:m:74:ARG:HD3	1.59	0.83
1:N:349:LYS:NZ	3:N:406:SO4:O4	2.08	0.83
1:O:193:ASP:HB3	1:O:196:THR:HB	1.60	0.83
2:i:117:SER:C	2:o:118:SER:O	2.21	0.83
2:h:18:ALA:HB2	2:h:87:ARG:C	2.03	0.83
2:n:5:GLN:NE2	2:n:110:LYS:NZ	2.24	0.83
1:K:159:LEU:HA	1:K:165:MET:HE1	1.60	0.83
2:g:20:VAL:HG21	2:g:88:LEU:HD21	1.58	0.83
2:j:16:PRO:HD3	2:j:117:SER:O	1.78	0.83
1:N:139:TYR:HB2	1:N:144:VAL:HG21	1.60	0.83
2:k:118:SER:HB2	2:p:119:GLY:O	1.77	0.83
1:P:117:LEU:HD13	1:P:274:LEU:HD21	1.61	0.83
2:b:149:GLN:HG3	1:M:191:GLY:HA3	1.61	0.83
2:l:21:LYS:CB	2:l:83:MET:C	2.51	0.83
1:M:321:ASP:OD2	2:m:230:ARG:NH2	2.12	0.82
1:Q:203:LYS:HA	1:Q:206:GLU:OE1	1.78	0.82
1:B:73:HIS:HB3	1:B:280:ASP:OD2	1.78	0.82
1:Q:176:MET:HB2	1:Q:182:MET:HE3	1.59	0.82
1:P:34:TRP:HB2	1:P:37:TYR:HD2	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:357:THR:HA	1:N:360:ARG:HD3	1.61	0.82
1:O:176:MET:H	1:O:182:MET:HE3	1.44	0.82
1:Q:190:LEU:HD11	1:Q:208:VAL:HG21	1.62	0.82
2:q:162:ILE:HG12	2:q:224:VAL:HG11	1.59	0.82
1:O:102:LYS:HZ3	1:O:103:LEU:HD12	1.42	0.82
1:L:176:MET:H	1:L:182:MET:HE3	1.45	0.82
2:d:93:THR:HG23	2:d:115:THR:HA	1.62	0.81
2:o:165:ASN:ND2	2:o:225:TRP:O	2.13	0.81
1:F:190:LEU:HD11	1:F:208:VAL:HG21	1.62	0.81
1:B:190:LEU:HD11	1:B:208:VAL:HG21	1.62	0.81
1:P:333:PRO:N	2:p:166:TYR:OH	2.13	0.81
2:b:15:THR:C	2:b:17:GLY:H	1.88	0.81
1:K:170:LYS:CE	1:K:171:CYS:H	1.93	0.81
2:k:49:TRP:CD1	2:k:232:VAL:H	1.99	0.81
2:p:140:PRO:O	2:p:238:THR:HG23	1.81	0.81
2:r:188:ARG:HB2	2:r:192:ILE:HB	1.63	0.81
2:a:93:THR:HG23	2:a:115:THR:HA	1.62	0.81
1:N:191:GLY:CA	2:o:149:GLN:CD	2.54	0.81
2:b:243:LEU:HB3	1:M:204:LYS:HD3	1.61	0.81
1:E:168:LEU:HA	1:E:170:LYS:HZ2	1.46	0.81
1:K:190:LEU:HD11	1:K:208:VAL:HG21	1.63	0.81
1:L:327:SER:O	1:L:329:GLU:N	2.14	0.81
1:P:333:PRO:CB	2:p:166:TYR:OH	2.29	0.81
1:C:213:ARG:NH1	1:C:361:ILE:HA	1.95	0.80
1:M:41:THR:OG1	1:M:302:LYS:NZ	2.12	0.80
1:F:117:LEU:HD13	1:F:274:LEU:HD21	1.61	0.80
1:G:360:ARG:NH1	3:G:401:SO4:O3	2.15	0.80
2:a:165:ASN:ND2	2:a:225:TRP:O	2.13	0.80
1:D:213:ARG:NH1	1:D:361:ILE:O	2.13	0.80
2:l:21:LYS:HB3	2:l:84:GLU:HA	1.62	0.80
2:r:165:ASN:ND2	2:r:225:TRP:O	2.14	0.80
2:l:15:THR:CB	2:l:16:PRO:HD2	2.09	0.80
2:o:93:THR:HG23	2:o:115:THR:HA	1.62	0.80
2:p:93:THR:HG23	2:p:115:THR:HA	1.62	0.80
1:Q:317:ARG:HG2	1:Q:317:ARG:HH11	1.47	0.80
2:m:195:ARG:NH2	2:m:216:ASP:OD2	2.13	0.80
2:a:140:PRO:O	2:a:238:THR:HG23	1.81	0.79
2:k:117:SER:O	2:p:118:SER:O	1.99	0.79
2:p:165:ASN:ND2	2:p:225:TRP:O	2.13	0.79
1:R:156:TRP:NE1	1:R:267:GLY:O	2.14	0.79
2:g:195:ARG:NH2	2:g:216:ASP:OD2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:200:LYS:NZ	1:I:203:LYS:HB2	1.97	0.79
1:N:161:GLU:OE2	2:o:144:SER:OG	2.00	0.79
2:q:11:ASP:O	2:q:12:GLU:HB2	1.80	0.79
2:m:69:ARG:NH2	2:m:92:ASP:OD2	2.15	0.79
2:l:143:VAL:HG11	2:l:151:VAL:CG2	2.13	0.79
1:O:117:LEU:HD13	1:O:274:LEU:HD21	1.64	0.79
2:o:140:PRO:O	2:o:238:THR:HG23	1.81	0.79
1:R:143:LYS:HG2	1:R:170:LYS:HZ2	1.48	0.79
1:A:32:TYR:HB3	1:A:79:VAL:HG12	1.65	0.79
2:b:49:TRP:CH2	2:b:52:TRP:HB2	2.16	0.79
2:h:225:TRP:CZ2	2:h:230:ARG:HA	2.17	0.79
2:l:170:TYR:HB3	2:l:180:LEU:HA	1.62	0.79
1:N:162:PRO:HG2	1:N:211:LYS:HE2	1.64	0.79
2:c:20:VAL:CG2	2:c:88:LEU:HD21	2.13	0.79
2:h:225:TRP:CE3	2:h:227:SER:HA	2.16	0.79
2:l:69:ARG:NH1	2:l:87:ARG:HB3	1.98	0.79
1:Q:317:ARG:HH11	2:q:103:ARG:HD3	1.46	0.79
2:h:3:GLN:HG2	2:h:4:VAL:HG12	1.65	0.79
1:L:38:ILE:H	1:L:307:VAL:HG11	1.48	0.79
2:f:25:LYS:HZ2	2:f:80:THR:HB	1.45	0.78
1:H:321:ASP:OD1	2:h:230:ARG:NH2	2.15	0.78
2:l:21:LYS:CA	2:l:83:MET:O	2.32	0.78
1:N:250:ALA:HB1	1:N:257:ILE:HB	1.65	0.78
1:O:112:ALA:HA	1:O:115:LYS:HE3	1.64	0.78
2:r:225:TRP:CZ3	2:r:227:SER:HA	2.19	0.78
1:O:323:SER:OG	2:o:225:TRP:CZ3	2.36	0.78
1:P:333:PRO:HB3	2:p:166:TYR:CZ	2.18	0.78
2:o:15:THR:HG23	2:o:16:PRO:HD2	1.65	0.78
2:h:18:ALA:CB	2:h:86:SER:C	2.56	0.78
2:l:171:GLN:HG2	2:l:181:LEU:CD1	2.12	0.78
1:O:155:SER:HB2	1:O:265:LYS:HE2	1.64	0.78
1:M:161:GLU:OE2	1:M:189:TYR:OH	2.02	0.78
1:A:176:MET:HE1	1:A:239:TYR:CZ	2.19	0.78
2:b:151:VAL:HG12	2:b:212:LEU:HD11	1.66	0.78
2:k:173:LEU:HD23	2:k:218:ALA:HB2	1.66	0.78
1:N:191:GLY:HA3	2:o:149:GLN:CG	2.14	0.78
1:A:213:ARG:NH1	1:A:361:ILE:HA	1.99	0.78
2:q:13:VAL:O	2:q:14:LYS:CD	2.31	0.78
2:b:138:THR:HG21	1:M:150:ASP:OD1	1.84	0.77
2:n:18:ALA:O	2:n:19:SER:OG	2.02	0.77
2:h:18:ALA:CB	2:h:88:LEU:N	2.37	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:LYS:HE2	1:E:171:CYS:SG	2.24	0.77
2:g:7:VAL:HG23	2:g:25:LYS:HB3	1.67	0.77
1:G:321:ASP:OD1	2:g:230:ARG:NH2	2.16	0.77
2:a:15:THR:HG23	2:a:16:PRO:HD2	1.65	0.77
2:i:69:ARG:HD2	2:i:87:ARG:HG3	1.67	0.77
2:k:37:SER:HB3	2:k:49:TRP:CZ3	2.20	0.77
2:k:166:TYR:HD1	2:k:185:ASN:HD22	1.32	0.77
2:h:49:TRP:CH2	2:h:52:TRP:HB2	2.19	0.77
2:n:15:THR:HG22	2:n:16:PRO:HD3	1.61	0.77
2:p:15:THR:HG23	2:p:16:PRO:HD2	1.65	0.77
2:c:11:ASP:OD1	2:c:113:THR:N	2.18	0.77
1:I:202:TYR:OH	1:I:354:GLN:OE1	2.02	0.77
1:I:352:ARG:NH1	3:I:402:SO4:O1	2.17	0.77
1:J:37:TYR:HE1	1:J:131:LEU:CD1	1.96	0.77
2:m:7:VAL:HG23	2:m:25:LYS:HB3	1.67	0.77
1:N:360:ARG:O	1:N:362:LYS:NZ	2.18	0.77
1:C:322:LYS:HD3	2:c:225:TRP:CD1	2.19	0.77
1:J:37:TYR:CE1	1:J:131:LEU:CD1	2.61	0.77
1:K:203:LYS:O	1:K:207:GLU:N	2.15	0.77
2:k:185:ASN:OD1	2:k:200:LYS:HE2	1.85	0.77
2:m:20:VAL:HG11	2:m:114:VAL:HG21	1.67	0.77
1:P:147:VAL:HG23	1:P:148:LEU:HD13	1.66	0.77
1:R:203:LYS:HG3	1:R:204:LYS:H	1.48	0.77
1:E:230:ASN:ND2	1:E:232:ASN:OD1	2.19	0.76
2:k:49:TRP:CH2	2:k:52:TRP:HB2	2.20	0.76
2:o:55:PRO:HA	2:o:74:ARG:HD3	1.67	0.76
2:a:55:PRO:HA	2:a:74:ARG:HD3	1.67	0.76
2:b:68:GLY:O	2:b:87:ARG:NH2	2.19	0.76
2:h:18:ALA:HA	2:h:88:LEU:HG	1.68	0.76
2:n:18:ALA:O	2:n:19:SER:O	2.04	0.76
1:R:167:LYS:O	1:R:170:LYS:HG2	1.86	0.76
2:p:55:PRO:HA	2:p:74:ARG:HD3	1.67	0.76
2:b:18:ALA:HB1	2:b:87:ARG:N	1.99	0.76
1:M:176:MET:HE1	1:M:239:TYR:CD2	2.21	0.76
2:n:15:THR:HG23	2:n:117:SER:O	1.86	0.76
1:F:328:GLU:OE2	2:f:200:LYS:HE3	1.86	0.76
2:h:15:THR:O	2:h:17:GLY:N	2.19	0.76
2:p:15:THR:CG2	2:p:16:PRO:HD2	2.16	0.76
2:g:49:TRP:CH2	2:g:52:TRP:HB2	2.21	0.76
2:n:18:ALA:CB	2:n:88:LEU:H	1.99	0.76
2:a:15:THR:CG2	2:a:16:PRO:HD2	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:225:TRP:CZ3	2:g:227:SER:HA	2.21	0.75
1:C:67:GLY:HA2	1:I:70:VAL:HG13	1.69	0.75
1:D:31:ILE:HG12	1:D:78:ILE:HB	1.67	0.75
2:k:26:VAL:CG2	2:k:26:VAL:HB	2.08	0.75
2:r:149:GLN:HG2	2:r:150:LYS:H	1.51	0.75
2:f:14:LYS:HD2	2:f:19:SER:O	1.85	0.75
2:h:225:TRP:HH2	2:h:230:ARG:HG2	1.51	0.75
2:m:225:TRP:CZ3	2:m:227:SER:HA	2.22	0.75
2:o:15:THR:CG2	2:o:16:PRO:HD2	2.16	0.75
1:P:323:SER:OG	2:p:225:TRP:CZ3	2.39	0.75
1:B:71:SER:HB2	1:G:64:THR:HA	1.69	0.75
2:d:225:TRP:CZ3	2:d:227:SER:HA	2.21	0.75
2:h:225:TRP:CE3	2:h:227:SER:CA	2.66	0.75
2:i:118:SER:CA	2:o:118:SER:OG	2.34	0.75
2:k:118:SER:N	2:p:118:SER:C	2.45	0.75
2:m:93:THR:HG23	2:m:115:THR:HA	1.68	0.75
1:I:159:LEU:O	1:I:212:VAL:HG21	1.87	0.75
1:N:176:MET:HB2	1:N:182:MET:HE3	1.68	0.75
1:P:193:ASP:HB3	1:P:196:THR:HB	1.68	0.75
1:F:70:VAL:HG13	1:M:67:GLY:HA2	1.69	0.75
1:N:155:SER:HB2	1:N:265:LYS:HE2	1.69	0.75
1:R:190:LEU:HD11	1:R:208:VAL:HG21	1.68	0.75
2:r:14:LYS:HE2	2:r:20:VAL:HG23	1.68	0.75
2:b:18:ALA:CB	2:b:88:LEU:N	2.42	0.75
1:H:88:LYS:HG3	1:H:345:VAL:HG13	1.68	0.75
2:i:119:GLY:N	2:o:118:SER:HG	1.82	0.75
2:l:142:SER:OG	1:Q:163:GLU:OE2	2.05	0.75
2:c:137:LEU:HD22	2:c:162:ILE:HD11	1.67	0.75
1:K:155:SER:OG	1:K:266:GLU:OE2	2.04	0.75
2:l:40:ARG:NH2	2:l:92:ASP:OD1	2.19	0.75
2:i:26:VAL:CG2	2:i:26:VAL:HB	2.11	0.74
1:L:147:VAL:HG23	1:L:148:LEU:HD13	1.68	0.74
2:l:171:GLN:HG2	2:l:181:LEU:HD12	1.67	0.74
1:D:155:SER:HB2	1:D:265:LYS:HE2	1.68	0.74
1:L:169:ALA:HB2	1:L:215:TYR:HB3	1.70	0.74
2:k:49:TRP:HH2	2:k:52:TRP:HB2	1.51	0.74
2:p:161:ASN:HB2	2:p:224:VAL:CG2	2.18	0.74
2:r:188:ARG:NH2	2:r:197:SER:OG	2.20	0.74
1:B:155:SER:O	1:B:158:ILE:HG12	1.87	0.74
2:f:199:SER:HB2	2:f:206:THR:OG1	1.87	0.74
2:i:18:ALA:HB3	2:i:88:LEU:CD1	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:154:SER:HB3	2:k:206:THR:HG22	1.68	0.74
1:L:92:ALA:HB2	1:R:352:ARG:HG2	1.70	0.74
2:b:18:ALA:HB2	2:b:87:ARG:C	2.12	0.74
2:g:55:PRO:HA	2:g:74:ARG:HD3	1.69	0.74
2:g:69:ARG:HH12	2:g:89:ARG:NH1	1.84	0.74
1:K:117:LEU:HD13	1:K:274:LEU:HD21	1.69	0.74
1:P:182:MET:HE1	1:P:237:PHE:CG	2.22	0.74
2:i:100:ARG:NH2	2:i:106:ASP:OD2	2.19	0.74
1:J:37:TYR:OH	1:J:131:LEU:HB2	1.86	0.74
1:Q:213:ARG:HD3	1:Q:361:ILE:HG22	1.67	0.74
1:K:106:TRP:HZ3	1:K:128:VAL:HG22	1.52	0.74
2:r:15:THR:HB	2:r:16:PRO:HD2	1.69	0.74
2:d:11:ASP:OD1	2:d:113:THR:N	2.21	0.74
1:M:151:GLN:HE22	1:M:164:ASN:HD21	1.36	0.74
2:j:6:LEU:HG	2:j:26:VAL:HG12	1.70	0.73
1:L:37:TYR:OH	1:L:131:LEU:HG	1.86	0.73
1:N:182:MET:HG3	1:N:358:TRP:CH2	2.23	0.73
2:a:161:ASN:HB2	2:a:224:VAL:CG2	2.18	0.73
2:i:118:SER:N	2:o:118:SER:HA	2.03	0.73
1:J:200:LYS:HG3	1:J:203:LYS:HD3	1.70	0.73
2:k:117:SER:OG	2:p:118:SER:N	2.21	0.73
2:l:29:TYR:HB3	2:l:100:ARG:NH1	2.03	0.73
1:M:203:LYS:HD2	1:M:204:LYS:CG	2.17	0.73
2:l:21:LYS:CG	2:l:84:GLU:HB2	2.18	0.73
1:N:163:GLU:OE2	2:o:142:SER:CB	2.36	0.73
1:P:317:ARG:NH1	2:p:103:ARG:CZ	2.51	0.73
1:R:173:VAL:HG22	1:R:235:VAL:HG13	1.70	0.73
1:E:139:TYR:HB2	1:E:144:VAL:HG21	1.70	0.73
1:Q:134:THR:H	1:Q:240:SER:HB3	1.53	0.73
2:l:22:VAL:HG12	2:l:23:SER:H	1.51	0.73
2:c:153:ILE:HG21	2:c:238:THR:HG21	1.70	0.73
2:g:165:ASN:ND2	2:g:225:TRP:O	2.21	0.73
2:h:20:VAL:HG21	2:h:88:LEU:HD21	1.69	0.73
2:h:20:VAL:CG2	2:h:88:LEU:HD21	2.18	0.73
2:c:93:THR:HG23	2:c:115:THR:HA	1.69	0.73
2:g:49:TRP:HH2	2:g:52:TRP:HB2	1.51	0.73
1:B:32:TYR:CZ	1:B:59:PHE:HB3	2.24	0.73
2:o:161:ASN:HB2	2:o:224:VAL:CG2	2.18	0.73
2:c:225:TRP:CZ3	2:c:227:SER:HA	2.25	0.72
2:o:167:VAL:HG22	2:o:224:VAL:HG12	1.71	0.72
1:Q:317:ARG:NH1	2:q:103:ARG:CD	2.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:226:SER:HB3	1:G:249:ARG:HH12	1.53	0.72
1:J:210:THR:HG22	1:J:361:ILE:HG12	1.70	0.72
2:l:21:LYS:CD	2:l:84:GLU:HB2	2.19	0.72
1:Q:37:TYR:CD1	4:Q:401:SPD:H41	2.24	0.72
2:h:225:TRP:CZ3	2:h:226:ASP:O	2.42	0.72
1:O:321:ASP:OD1	1:O:322:LYS:N	2.23	0.72
2:a:167:VAL:HG22	2:a:224:VAL:HG12	1.71	0.72
2:e:49:TRP:CH2	2:e:52:TRP:HB2	2.25	0.72
2:g:32:THR:HA	2:g:55:PRO:HB2	1.70	0.72
1:N:77:ASP:OD2	1:N:283:ALA:HB3	1.89	0.72
2:a:103:ARG:NH2	2:a:184:ASP:OD1	2.23	0.72
2:g:88:LEU:HD13	2:g:116:VAL:HB	1.72	0.72
2:l:238:THR:O	2:l:240:LEU:N	2.23	0.72
1:M:200:LYS:O	1:M:203:LYS:HD3	1.89	0.72
2:d:154:SER:HA	2:d:206:THR:HG22	1.71	0.72
1:G:323:SER:HB3	2:g:225:TRP:HZ3	1.55	0.72
1:K:167:LYS:O	1:K:170:LYS:HB2	1.90	0.72
1:Q:32:TYR:HB3	1:Q:79:VAL:HG12	1.72	0.72
1:Q:182:MET:HE1	1:Q:237:PHE:CG	2.25	0.72
1:A:31:ILE:HG12	1:A:78:ILE:HB	1.70	0.72
2:c:20:VAL:HG22	2:c:88:LEU:HD11	1.72	0.72
1:K:200:LYS:NZ	1:K:203:LYS:HD2	2.05	0.72
2:l:21:LYS:CD	2:l:84:GLU:CB	2.67	0.72
1:A:67:GLY:HA2	1:K:70:VAL:HG13	1.72	0.71
2:n:55:PRO:HA	2:n:74:ARG:HD3	1.72	0.71
1:P:347:PRO:O	1:P:350:VAL:HG22	1.90	0.71
1:E:168:LEU:HD23	1:E:170:LYS:HZ2	1.56	0.71
1:J:37:TYR:CD1	1:J:131:LEU:HD12	2.24	0.71
2:j:89:ARG:O	2:j:91:ASP:N	2.23	0.71
1:N:190:LEU:O	2:o:146:ALA:CB	2.39	0.71
1:C:31:ILE:HG12	1:C:78:ILE:HB	1.72	0.71
2:c:20:VAL:CG2	2:c:88:LEU:HD11	2.20	0.71
2:h:225:TRP:HZ3	2:h:227:SER:N	1.75	0.71
1:J:190:LEU:HD11	1:J:208:VAL:HG21	1.71	0.71
1:K:213:ARG:HD3	1:K:361:ILE:HG23	1.72	0.71
1:L:100:LYS:NZ	1:L:124:ASN:O	2.21	0.71
2:l:171:GLN:HB3	2:l:220:TYR:CE1	2.25	0.71
2:o:103:ARG:NH2	2:o:184:ASP:OD1	2.23	0.71
1:P:333:PRO:HB3	2:p:166:TYR:OH	1.91	0.71
1:F:242:ASP:OD1	1:F:309:TYR:OH	2.07	0.71
2:i:7:VAL:HG22	2:i:25:LYS:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:203:LYS:HA	1:K:206:GLU:HB3	1.73	0.71
1:D:176:MET:HB2	1:D:182:MET:HE3	1.71	0.71
2:e:55:PRO:HA	2:e:74:ARG:HD3	1.72	0.71
1:L:322:LYS:HG2	2:l:225:TRP:CD1	2.26	0.71
1:L:182:MET:HE1	1:L:237:PHE:CG	2.25	0.71
1:M:203:LYS:NZ	1:M:204:LYS:HB2	2.06	0.71
2:p:167:VAL:HG22	2:p:224:VAL:HG12	1.71	0.71
2:l:171:GLN:HB3	2:l:220:TYR:CD1	2.26	0.71
1:R:148:LEU:O	1:R:151:GLN:NE2	2.24	0.71
1:R:317:ARG:NH2	1:R:325:SER:O	2.23	0.71
1:B:242:ASP:OD1	1:B:309:TYR:OH	2.07	0.71
2:c:55:PRO:HA	2:c:74:ARG:HD3	1.73	0.71
2:h:93:THR:HG23	2:h:115:THR:HA	1.72	0.71
2:n:13:VAL:C	2:n:14:LYS:CG	2.64	0.71
2:f:49:TRP:CH2	2:f:52:TRP:HB2	2.25	0.70
1:I:106:TRP:HZ3	1:I:128:VAL:HG22	1.55	0.70
1:I:187:LEU:HD12	1:I:194:PRO:HA	1.72	0.70
1:L:155:SER:HB2	1:L:265:LYS:HE2	1.73	0.70
1:M:202:TYR:N	1:M:203:LYS:HG2	2.05	0.70
1:R:162:PRO:HG3	1:R:211:LYS:HG3	1.74	0.70
2:k:21:LYS:HA	2:k:83:MET:O	1.90	0.70
1:M:348:ALA:HA	1:M:351:LEU:HD12	1.72	0.70
1:N:190:LEU:HD11	1:N:208:VAL:HG21	1.73	0.70
1:O:34:TRP:HB2	1:O:37:TYR:CD2	2.23	0.70
2:p:103:ARG:NH2	2:p:184:ASP:OD1	2.23	0.70
1:Q:184:PRO:HA	1:Q:194:PRO:HB3	1.71	0.70
2:l:15:THR:OG1	2:l:16:PRO:CD	2.38	0.70
2:d:75:ASP:OD2	2:d:78:ILE:HG13	1.91	0.70
1:G:169:ALA:HB2	1:G:215:TYR:HB3	1.74	0.70
1:L:326:ASP:HB2	2:l:166:TYR:HD2	1.57	0.70
1:O:296:ARG:HD2	1:O:298:GLU:OE2	1.90	0.70
2:i:149:GLN:O	2:i:212:LEU:HD12	1.90	0.70
1:J:203:LYS:HG2	1:J:204:LYS:H	1.56	0.70
2:j:226:ASP:OD2	2:j:229:LEU:HD13	1.91	0.70
2:h:225:TRP:HZ3	2:h:227:SER:C	1.98	0.70
1:K:328:GLU:OE2	2:k:200:LYS:HE3	1.90	0.70
1:O:102:LYS:NZ	1:O:103:LEU:HD12	2.06	0.70
1:D:167:LYS:O	1:D:170:LYS:NZ	2.25	0.70
1:D:67:GLY:HA2	1:J:70:VAL:HG13	1.74	0.70
1:E:155:SER:O	1:E:158:ILE:HG12	1.91	0.70
2:l:48:GLU:HG2	2:l:49:TRP:H	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:143:LYS:HG2	1:R:170:LYS:NZ	2.06	0.70
1:H:106:TRP:HZ3	1:H:128:VAL:HG22	1.57	0.70
2:l:21:LYS:HD2	2:l:84:GLU:HB2	1.73	0.70
2:l:29:TYR:CE1	2:l:31:PHE:HA	2.27	0.70
2:l:145:GLY:HA2	2:l:149:GLN:HE22	1.56	0.70
1:N:190:LEU:O	2:o:146:ALA:HB3	1.92	0.70
2:n:166:TYR:HD2	2:n:184:ASP:HA	1.55	0.70
1:C:155:SER:HB2	1:C:265:LYS:HE2	1.74	0.69
2:d:167:VAL:HA	2:d:224:VAL:HG12	1.74	0.69
2:h:18:ALA:HA	2:h:88:LEU:CG	2.22	0.69
2:q:20:VAL:HG21	2:q:114:VAL:HG21	1.74	0.69
1:G:352:ARG:NH1	3:G:402:SO4:O1	2.24	0.69
2:h:225:TRP:CE3	2:h:226:ASP:N	2.60	0.69
1:L:35:THR:C	1:L:37:TYR:H	1.98	0.69
1:P:98:LEU:HD23	1:P:288:TYR:HE1	1.57	0.69
2:r:195:ARG:HA	2:r:210:THR:HG22	1.73	0.69
2:r:214:THR:HA	2:r:242:VAL:HG11	1.72	0.69
1:B:165:MET:HE1	1:B:173:VAL:HG11	1.74	0.69
1:G:109:LEU:HD13	1:G:114:LEU:HD21	1.73	0.69
2:n:214:THR:HA	2:n:242:VAL:HG21	1.73	0.69
2:j:137:LEU:HD11	2:j:233:LEU:HB3	1.74	0.69
2:j:167:VAL:HA	2:j:224:VAL:HG12	1.74	0.69
2:l:25:LYS:CG	2:l:26:VAL:H	2.04	0.69
2:q:182:LEU:HD23	2:q:188:ARG:NH2	2.07	0.69
2:b:55:PRO:O	2:b:74:ARG:NE	2.26	0.69
1:J:106:TRP:HZ3	1:J:128:VAL:HG22	1.58	0.69
1:K:165:MET:HA	1:K:168:LEU:HB2	1.75	0.69
2:m:49:TRP:CD1	2:m:63:ALA:HB2	2.28	0.69
2:n:75:ASP:HB3	2:n:78:ILE:HG22	1.73	0.69
1:D:117:LEU:HD13	1:D:274:LEU:HD21	1.74	0.69
1:D:323:SER:HB3	2:d:225:TRP:CZ3	2.28	0.69
1:E:321:ASP:OD1	2:e:230:ARG:NH2	2.25	0.69
2:h:18:ALA:HB1	2:h:86:SER:O	1.89	0.69
2:l:21:LYS:C	2:l:22:VAL:O	2.36	0.69
1:P:176:MET:H	1:P:182:MET:HE3	1.58	0.69
1:C:207:GLU:HG3	1:C:211:LYS:HE3	1.73	0.69
1:E:168:LEU:HA	1:E:170:LYS:NZ	2.08	0.69
1:F:176:MET:H	1:F:182:MET:HE3	1.57	0.69
2:i:118:SER:HA	2:o:118:SER:CA	2.22	0.69
2:m:3:GLN:HG2	2:m:4:VAL:H	1.58	0.69
2:q:195:ARG:HB2	2:q:210:THR:H	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:86:LEU:HD23	1:R:120:SER:HB3	1.73	0.69
2:c:21:LYS:HE2	2:c:84:GLU:CD	2.18	0.69
1:H:45:ASP:OD2	1:H:302:LYS:NZ	2.25	0.69
2:c:137:LEU:HD12	2:c:137:LEU:O	1.93	0.68
2:f:32:THR:HA	2:f:55:PRO:HB2	1.75	0.68
1:Q:109:LEU:HD13	1:Q:114:LEU:HD21	1.75	0.68
1:F:37:TYR:CE1	4:F:404:SPD:H41	2.28	0.68
1:F:273:ASP:OD2	4:F:404:SPD:H52	1.92	0.68
2:l:99:ALA:HB1	2:l:105:MET:HB3	1.74	0.68
1:P:316:ALA:O	1:P:319:LEU:N	2.23	0.68
3:A:401:SO4:O4	1:K:352:ARG:NH2	2.27	0.68
2:e:162:ILE:HG12	2:e:224:VAL:HG11	1.75	0.68
1:J:181:GLU:OE2	1:J:239:TYR:OH	2.05	0.68
2:n:15:THR:CG2	2:n:117:SER:O	2.41	0.68
2:p:146:ALA:HB3	1:R:190:LEU:O	1.94	0.68
1:F:204:LYS:O	1:F:207:GLU:HG2	1.92	0.68
1:J:182:MET:HG3	1:J:358:TRP:CZ3	2.29	0.68
2:l:25:LYS:HG3	2:l:26:VAL:H	1.57	0.68
2:l:50:MET:O	2:l:63:ALA:N	2.27	0.68
1:Q:250:ALA:HB1	1:Q:257:ILE:HB	1.75	0.68
2:q:35:GLY:HA2	2:q:55:PRO:HD3	1.75	0.68
2:l:143:VAL:HG11	2:l:151:VAL:HG23	1.74	0.68
1:Q:48:LYS:HD3	1:Q:48:LYS:N	2.08	0.68
1:H:317:ARG:NH2	1:H:325:SER:O	2.22	0.68
2:k:16:PRO:HD2	2:k:118:SER:OG	1.94	0.68
1:R:357:THR:HG22	1:R:360:ARG:HH21	1.57	0.68
1:I:183:LEU:HD23	1:I:209:LEU:HD13	1.75	0.68
2:i:139:GLN:HE21	2:i:238:THR:H	1.39	0.68
2:m:226:ASP:OD2	2:m:229:LEU:HG	1.93	0.68
2:r:162:ILE:HG12	2:r:224:VAL:HG11	1.76	0.68
2:j:102:LYS:HD3	2:j:106:ASP:OD2	1.94	0.68
2:l:102:LYS:HB2	2:l:104:TYR:CE2	2.28	0.68
1:D:173:VAL:HG13	1:D:235:VAL:HG13	1.75	0.68
1:D:322:LYS:HD3	2:d:225:TRP:CD1	2.29	0.67
2:h:103:ARG:NH2	2:h:184:ASP:OD1	2.26	0.67
1:J:349:LYS:NZ	3:J:402:SO4:O1	2.21	0.67
1:O:103:LEU:HD21	1:O:292:ASP:HA	1.76	0.67
1:A:322:LYS:HD3	2:a:225:TRP:CD1	2.29	0.67
2:g:68:GLY:CA	2:i:21:LYS:HE2	2.22	0.67
1:I:182:MET:HG3	1:I:358:TRP:CH2	2.29	0.67
1:E:352:ARG:NH1	3:E:404:SO4:O3	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:200:LYS:HA	1:Q:203:LYS:HB3	1.77	0.67
1:A:67:GLY:HA3	1:K:71:SER:OG	1.93	0.67
2:g:217:GLU:HB2	2:g:242:VAL:HG23	1.77	0.67
1:N:182:MET:HE1	1:N:237:PHE:CG	2.30	0.67
2:p:146:ALA:CB	1:R:190:LEU:O	2.42	0.67
1:R:109:LEU:HD13	1:R:114:LEU:HD21	1.77	0.67
2:n:217:GLU:HB2	2:n:242:VAL:HG22	1.77	0.67
1:R:106:TRP:HZ3	1:R:128:VAL:HG12	1.59	0.67
2:h:167:VAL:HA	2:h:224:VAL:HG12	1.76	0.67
1:I:175:PHE:HD2	1:I:182:MET:SD	2.17	0.67
2:p:86:SER:O	2:p:87:ARG:HG3	1.94	0.67
1:E:326:ASP:OD1	2:e:103:ARG:NH1	2.26	0.67
1:R:134:THR:H	1:R:240:SER:HB3	1.59	0.67
1:C:176:MET:HB2	1:C:182:MET:HE3	1.76	0.67
1:H:147:VAL:HG23	1:H:167:LYS:HB3	1.76	0.67
1:L:35:THR:O	1:L:37:TYR:N	2.28	0.67
1:R:165:MET:HE1	1:R:173:VAL:HG11	1.75	0.67
1:A:181:GLU:OE2	4:A:404:SPD:N10	2.27	0.67
1:D:168:LEU:HD13	1:D:235:VAL:HG11	1.76	0.67
2:i:117:SER:OG	2:o:118:SER:N	2.28	0.67
1:K:74:SER:O	1:K:76:TYR:N	2.25	0.67
2:l:21:LYS:HB2	2:l:83:MET:C	2.19	0.67
2:n:49:TRP:CH2	2:n:52:TRP:HB2	2.30	0.67
1:P:317:ARG:NH1	2:p:103:ARG:NH1	2.43	0.67
2:q:182:LEU:HD23	2:q:188:ARG:CZ	2.24	0.67
2:e:93:THR:HG23	2:e:115:THR:HA	1.75	0.67
2:h:32:THR:HA	2:h:55:PRO:HB2	1.76	0.67
2:l:6:LEU:HD11	2:l:24:CYS:HB3	1.76	0.67
2:g:69:ARG:NH2	2:g:92:ASP:OD2	2.28	0.66
2:j:225:TRP:CZ3	2:j:227:SER:HA	2.30	0.66
2:o:86:SER:O	2:o:87:ARG:HG3	1.94	0.66
2:h:165:ASN:ND2	2:h:225:TRP:O	2.26	0.66
1:Q:200:LYS:HG2	1:Q:203:LYS:HB3	1.76	0.66
1:E:220:HIS:CD2	1:E:223:LYS:HB2	2.31	0.66
2:j:173:LEU:HD23	2:j:218:ALA:HB2	1.78	0.66
1:M:102:LYS:NZ	1:M:285:ASP:OD1	2.25	0.66
1:A:134:THR:O	1:A:271:TRP:NE1	2.28	0.66
2:a:86:SER:O	2:a:87:ARG:HG3	1.94	0.66
1:B:162:PRO:HD3	1:B:211:LYS:HE3	1.76	0.66
1:G:111:PRO:HA	1:G:114:LEU:HD12	1.76	0.66
1:O:109:LEU:HB3	1:O:114:LEU:HD11	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ASP:OD1	1:A:309:TYR:OH	2.13	0.66
1:C:32:TYR:HB3	1:C:79:VAL:HG12	1.77	0.66
1:F:349:LYS:NZ	3:F:403:SO4:O2	2.24	0.66
1:G:117:LEU:HD13	1:G:274:LEU:HD21	1.77	0.66
1:I:182:MET:HE2	1:I:182:MET:HA	1.77	0.66
2:l:167:VAL:HA	2:l:224:VAL:HG12	1.77	0.66
1:Q:187:LEU:HD12	1:Q:194:PRO:HA	1.76	0.66
1:Q:298:GLU:HG2	2:q:56:ASN:OD1	1.96	0.66
1:E:225:ILE:HD11	1:E:242:ASP:OD2	1.96	0.66
2:e:9:THR:HG22	2:e:10:GLY:H	1.60	0.66
1:F:226:SER:O	1:F:230:ASN:ND2	2.28	0.66
2:k:117:SER:OG	2:p:118:SER:CA	2.43	0.66
1:L:204:LYS:HD3	2:q:243:LEU:HB3	1.78	0.66
1:O:173:VAL:HG13	1:O:235:VAL:HG13	1.78	0.66
2:q:162:ILE:HG23	2:q:167:VAL:HG21	1.78	0.66
2:h:15:THR:HB	2:h:16:PRO:HD2	1.77	0.66
2:l:173:LEU:HB3	2:l:174:PRO:HD2	1.78	0.66
2:b:181:LEU:HD21	2:b:196:PHE:HD2	1.58	0.66
1:E:168:LEU:HD23	1:E:170:LYS:NZ	2.10	0.66
2:l:225:TRP:CH2	2:l:230:ARG:HA	2.31	0.66
2:n:224:VAL:HG12	2:n:225:TRP:H	1.59	0.66
2:b:162:ILE:O	2:b:200:LYS:HE3	1.96	0.66
1:C:106:TRP:HZ3	1:C:128:VAL:HG22	1.60	0.66
2:l:17:GLY:CA	2:l:88:LEU:CA	2.74	0.66
2:q:93:THR:HG23	2:q:115:THR:HA	1.78	0.66
1:A:182:MET:HE1	1:A:237:PHE:CG	2.30	0.66
1:A:349:LYS:NZ	3:A:403:SO4:O2	2.29	0.66
1:D:323:SER:HB3	2:d:225:TRP:HZ3	1.60	0.66
2:n:35:GLY:HA2	2:n:55:PRO:HD3	1.78	0.66
2:n:225:TRP:CZ3	2:n:227:SER:HA	2.30	0.66
1:P:321:ASP:OD1	1:P:322:LYS:N	2.27	0.66
1:A:171:CYS:HB3	1:A:234:CYS:SG	2.35	0.65
1:C:323:SER:HB3	2:c:225:TRP:CZ3	2.31	0.65
1:E:356:ARG:NH1	1:H:91:GLN:O	2.28	0.65
2:i:117:SER:OG	2:o:117:SER:OG	1.96	0.65
1:K:240:SER:OG	1:K:241:GLY:N	2.28	0.65
2:p:149:GLN:CD	1:R:191:GLY:HA3	2.21	0.65
2:b:137:LEU:HD11	2:b:233:LEU:HB3	1.77	0.65
2:c:217:GLU:HB2	2:c:242:VAL:HG12	1.77	0.65
1:E:228:LEU:HD23	1:E:233:ILE:HG13	1.77	0.65
2:f:161:ASN:HD22	2:f:233:LEU:HD12	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:323:SER:HB3	2:g:225:TRP:CZ3	2.31	0.65
2:l:45:GLN:CD	2:l:46:GLY:H	2.03	0.65
1:Q:283:ALA:HB1	1:Q:286:ASN:HB2	1.78	0.65
2:r:14:LYS:C	2:r:15:THR:HG23	2.21	0.65
2:c:167:VAL:HA	2:c:224:VAL:HG12	1.76	0.65
1:E:207:GLU:HA	1:E:210:THR:OG1	1.96	0.65
2:h:225:TRP:HZ3	2:h:226:ASP:C	1.91	0.65
2:l:87:ARG:HG3	2:l:87:ARG:O	1.95	0.65
2:m:214:THR:HA	2:m:242:VAL:HG11	1.77	0.65
2:i:226:ASP:OD2	2:i:229:LEU:HD12	1.96	0.65
1:K:182:MET:HG3	1:K:358:TRP:CZ3	2.32	0.65
1:K:273:ASP:OD2	4:K:404:SPD:H51	1.96	0.65
2:n:83:MET:HE1	2:n:96:TYR:CD2	2.31	0.65
1:Q:206:GLU:HG3	1:Q:360:ARG:NH1	2.12	0.65
1:Q:317:ARG:HH11	1:Q:317:ARG:CG	2.09	0.65
2:e:31:PHE:HE1	2:e:36:ILE:HD12	1.62	0.65
1:O:139:TYR:HB2	1:O:144:VAL:HG21	1.77	0.65
1:R:98:LEU:O	1:R:125:GLN:NE2	2.26	0.65
1:R:351:LEU:O	1:R:355:THR:OG1	2.12	0.65
2:g:93:THR:HG23	2:g:115:THR:HA	1.78	0.65
1:J:200:LYS:O	1:J:202:TYR:N	2.30	0.65
1:P:131:LEU:HD13	1:P:309:TYR:HB2	1.79	0.65
1:C:327:SER:HB3	1:C:330:VAL:HB	1.79	0.65
1:F:67:GLY:HA2	1:M:70:VAL:HG13	1.79	0.65
1:I:155:SER:O	1:I:158:ILE:HG12	1.96	0.65
2:k:117:SER:OG	2:p:118:SER:HA	1.95	0.65
1:R:32:TYR:HB3	1:R:79:VAL:HG12	1.79	0.65
2:r:183:TYR:HE2	2:r:187:LYS:HE3	1.61	0.65
1:E:356:ARG:NE	3:E:402:SO4:O3	2.26	0.65
2:f:25:LYS:HZ3	2:f:78:ILE:HG13	1.62	0.65
2:g:69:ARG:HE	2:g:85:LEU:HD21	1.62	0.65
1:J:200:LYS:O	1:J:203:LYS:N	2.30	0.65
2:j:162:ILE:O	2:j:200:LYS:NZ	2.23	0.65
1:L:63:GLU:OE1	1:L:63:GLU:N	2.26	0.65
2:l:13:VAL:HG22	2:l:14:LYS:H	1.62	0.65
2:f:25:LYS:NZ	2:f:80:THR:HB	2.12	0.65
1:P:163:GLU:OE2	2:r:142:SER:HB3	1.97	0.65
2:b:37:SER:HB3	2:b:49:TRP:HZ3	1.61	0.65
3:D:401:SO4:O1	1:J:352:ARG:NH2	2.30	0.65
2:l:157:GLY:HA3	2:l:162:ILE:HD12	1.79	0.65
1:N:190:LEU:CD1	2:o:243:LEU:CD2	2.74	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:156:TRP:HB2	1:R:189:TYR:HB2	1.79	0.64
2:a:162:ILE:HG12	2:a:224:VAL:HG11	1.79	0.64
2:f:154:SER:HB3	2:f:206:THR:CG2	2.27	0.64
1:M:169:ALA:HB2	1:M:215:TYR:HB3	1.79	0.64
1:P:240:SER:OG	1:P:241:GLY:N	2.30	0.64
2:p:162:ILE:HG12	2:p:224:VAL:HG11	1.79	0.64
2:q:50:MET:HE1	2:q:85:LEU:HD21	1.79	0.64
2:l:149:GLN:NE2	1:Q:190:LEU:O	2.31	0.64
2:b:18:ALA:CB	2:b:87:ARG:N	2.59	0.64
2:i:93:THR:HG23	2:i:115:THR:HG22	1.79	0.64
1:J:161:GLU:OE2	1:J:189:TYR:OH	2.16	0.64
1:N:121:ASP:OD2	1:N:124:ASN:HA	1.98	0.64
3:C:401:SO4:O1	1:I:352:ARG:NH2	2.30	0.64
2:h:219:ASP:OD1	2:h:239:LYS:HG2	1.97	0.64
2:d:162:ILE:HD13	2:d:205:THR:HG22	1.79	0.64
2:i:15:THR:HG23	2:i:16:PRO:HD2	1.80	0.64
2:k:117:SER:C	2:p:118:SER:C	2.66	0.64
1:I:180:ASP:HA	1:I:354:GLN:NE2	2.13	0.64
1:Q:29:LEU:HB3	1:Q:54:VAL:HG12	1.80	0.64
1:O:63:GLU:OE1	1:O:63:GLU:N	2.31	0.64
1:G:355:THR:O	1:G:359:THR:OG1	2.14	0.64
1:L:271:TRP:CD2	4:L:404:SPD:H91	2.33	0.64
2:l:104:TYR:HB3	2:l:180:LEU:HD11	1.80	0.64
2:q:161:ASN:HB2	2:q:224:VAL:HG21	1.80	0.64
1:M:29:LEU:HD23	1:M:54:VAL:HG12	1.79	0.64
1:N:227:ASP:HB3	1:N:233:ILE:HG23	1.80	0.64
1:P:80:VAL:HG22	1:P:275:MET:HG2	1.79	0.64
2:r:153:ILE:HD13	2:r:238:THR:HG21	1.80	0.64
2:d:212:LEU:HD11	2:d:240:LEU:HD21	1.80	0.63
1:E:359:THR:O	1:E:362:LYS:HG3	1.97	0.63
2:n:18:ALA:HB3	2:n:88:LEU:H	1.61	0.63
2:n:71:THR:O	2:n:84:GLU:N	2.30	0.63
1:K:266:GLU:CD	1:K:266:GLU:H	2.06	0.63
1:P:228:LEU:HD23	1:P:233:ILE:HG13	1.79	0.63
1:Q:31:ILE:HG12	1:Q:78:ILE:HB	1.80	0.63
2:q:158:SER:N	2:q:161:ASN:OD1	2.26	0.63
1:A:169:ALA:HB2	1:A:215:TYR:HB3	1.79	0.63
2:n:13:VAL:O	2:n:14:LYS:HG2	1.98	0.63
2:o:162:ILE:HG12	2:o:224:VAL:HG11	1.79	0.63
1:R:183:LEU:HD23	1:R:209:LEU:HD12	1.79	0.63
2:r:161:ASN:HB2	2:r:224:VAL:HG21	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LEU:HD22	1:B:54:VAL:HG21	1.81	0.63
1:E:115:LYS:HA	1:E:118:GLU:HG3	1.81	0.63
2:f:143:VAL:HG23	2:f:240:LEU:HD12	1.80	0.63
1:G:226:SER:HB3	1:G:249:ARG:NH1	2.13	0.63
2:l:40:ARG:HG3	2:l:94:ALA:CB	2.28	0.63
1:N:356:ARG:NH1	3:N:404:SO4:O4	2.32	0.63
2:n:18:ALA:CB	2:n:88:LEU:N	2.60	0.63
1:R:106:TRP:CZ3	1:R:128:VAL:HG12	2.33	0.63
1:R:169:ALA:HB2	1:R:215:TYR:HB3	1.80	0.63
2:h:69:ARG:HD2	2:h:87:ARG:HB2	1.81	0.63
2:i:217:GLU:HG3	2:i:241:THR:HA	1.79	0.63
2:l:55:PRO:HA	2:l:74:ARG:HD3	1.81	0.63
2:n:13:VAL:C	2:n:14:LYS:HG2	2.23	0.63
1:C:169:ALA:HB2	1:C:215:TYR:HB3	1.81	0.63
2:e:154:SER:CB	2:e:206:THR:HG22	2.29	0.63
1:I:200:LYS:HZ2	1:I:203:LYS:HB2	1.64	0.63
1:K:170:LYS:HE2	1:K:171:CYS:H	1.63	0.63
2:l:172:GLN:O	2:l:218:ALA:HB1	1.98	0.63
1:N:243:VAL:HG11	1:N:261:TYR:HB2	1.79	0.63
1:O:102:LYS:HZ3	1:O:103:LEU:CD1	2.10	0.63
2:q:212:LEU:HD23	2:q:242:VAL:HG22	1.80	0.63
1:A:213:ARG:HH12	1:A:361:ILE:HA	1.61	0.63
2:d:189:PRO:HD2	2:d:192:ILE:HG13	1.80	0.63
2:f:62:TYR:HB2	2:f:67:GLN:HG3	1.80	0.63
2:m:20:VAL:HG22	2:m:88:LEU:HD11	1.80	0.63
1:R:360:ARG:NH2	3:R:401:SO4:O3	2.30	0.63
2:e:226:ASP:OD2	2:e:229:LEU:HD13	1.98	0.63
1:K:175:PHE:HD2	1:K:182:MET:SD	2.22	0.63
1:N:200:LYS:HD2	1:N:203:LYS:HB3	1.81	0.63
1:O:82:SER:OG	4:O:407:SPD:H81	1.99	0.63
1:P:52:ILE:HD13	1:P:286:ASN:HB2	1.80	0.63
1:R:200:LYS:HG3	1:R:203:LYS:HD3	1.79	0.63
1:B:67:GLY:HA3	1:G:71:SER:OG	1.98	0.63
1:D:156:TRP:CE2	1:D:264:PRO:HG2	2.34	0.63
2:f:93:THR:HG23	2:f:115:THR:HA	1.79	0.63
1:I:203:LYS:HA	1:I:206:GLU:CB	2.28	0.63
1:I:349:LYS:NZ	3:I:402:SO4:O2	2.24	0.63
2:k:118:SER:HA	2:p:119:GLY:CA	2.29	0.63
1:O:43:LEU:HD11	1:O:56:TYR:CD1	2.34	0.63
1:O:99:ASP:O	1:O:102:LYS:HG3	1.99	0.63
1:A:337:LEU:O	1:A:339:LYS:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:66:PHE:O	2:c:70:VAL:HG12	1.98	0.62
1:D:271:TRP:CG	4:D:404:SPD:H92	2.33	0.62
2:i:8:GLU:H	2:i:110:LYS:HZ2	1.47	0.62
2:i:118:SER:CA	2:o:118:SER:CA	2.77	0.62
1:J:271:TRP:CE2	4:J:404:SPD:H82	2.34	0.62
2:l:21:LYS:CE	2:l:84:GLU:CG	2.74	0.62
1:D:169:ALA:HB2	1:D:215:TYR:HB3	1.81	0.62
2:d:37:SER:HB3	2:d:49:TRP:HZ3	1.65	0.62
2:j:165:ASN:ND2	2:j:225:TRP:O	2.29	0.62
1:K:99:ASP:OD2	1:K:102:LYS:HE3	1.98	0.62
2:k:165:ASN:ND2	2:k:225:TRP:O	2.26	0.62
1:L:98:LEU:HD12	1:L:126:TYR:HA	1.81	0.62
1:M:203:LYS:HZ2	1:M:205:ALA:N	1.97	0.62
1:Q:324:VAL:HG13	1:Q:330:VAL:HG11	1.81	0.62
2:h:3:GLN:HG2	2:h:4:VAL:N	2.03	0.62
1:L:128:VAL:HG21	1:L:291:ILE:HG21	1.81	0.62
1:Q:37:TYR:OH	1:Q:131:LEU:HB2	1.98	0.62
1:A:156:TRP:CE2	1:A:264:PRO:HG2	2.35	0.62
1:C:283:ALA:HB1	1:C:286:ASN:HB2	1.82	0.62
2:c:103:ARG:NH2	2:c:184:ASP:OD1	2.32	0.62
2:d:20:VAL:CG2	2:d:88:LEU:CD2	2.68	0.62
2:g:212:LEU:HD12	2:g:242:VAL:HG13	1.81	0.62
2:k:161:ASN:OD1	2:k:162:ILE:N	2.23	0.62
2:l:5:GLN:HB3	2:l:27:SER:HB3	1.82	0.62
2:l:40:ARG:HG3	2:l:94:ALA:HB2	1.81	0.62
1:M:328:GLU:OE2	2:m:200:LYS:NZ	2.32	0.62
1:D:242:ASP:OD1	1:D:309:TYR:OH	2.15	0.62
1:F:293:TYR:HD1	1:F:296:ARG:HH21	1.45	0.62
2:m:49:TRP:CH2	2:m:52:TRP:HB2	2.34	0.62
2:r:168:SER:HA	2:r:182:LEU:O	1.99	0.62
2:c:37:SER:HB3	2:c:49:TRP:HZ3	1.65	0.62
1:J:43:LEU:HD22	1:J:54:VAL:HG11	1.81	0.62
2:m:167:VAL:HA	2:m:224:VAL:HG12	1.80	0.62
1:R:211:LYS:O	1:R:214:PRO:HD3	2.00	0.62
1:I:130:TYR:O	1:I:131:LEU:HD23	2.00	0.62
1:E:147:VAL:HG11	1:E:170:LYS:HE3	1.81	0.62
2:k:213:GLN:O	2:k:215:GLY:N	2.32	0.62
1:N:348:ALA:O	1:N:352:ARG:HG3	1.98	0.62
1:P:244:PHE:CE2	1:P:329:GLU:HB2	2.35	0.62
1:F:173:VAL:HG13	1:F:235:VAL:HG13	1.82	0.62
2:f:217:GLU:HB2	2:f:242:VAL:HG23	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:117:LEU:HD13	1:H:274:LEU:HD21	1.81	0.62
1:J:206:GLU:O	1:J:210:THR:HG23	2.00	0.62
2:j:150:LYS:HG2	2:j:151:VAL:H	1.65	0.62
1:P:298:GLU:OE1	1:P:298:GLU:N	2.29	0.62
2:q:182:LEU:HB3	2:q:188:ARG:NH1	2.15	0.62
1:D:206:GLU:OE1	1:D:360:ARG:NH2	2.33	0.61
2:i:15:THR:C	2:i:16:PRO:O	2.43	0.61
1:L:293:TYR:HA	1:L:296:ARG:HD3	1.82	0.61
2:m:26:VAL:HG11	2:m:31:PHE:CD1	2.35	0.61
2:m:69:ARG:HE	2:m:85:LEU:HD21	1.63	0.61
1:P:198:ASP:OD2	1:P:200:LYS:HB3	2.00	0.61
2:k:117:SER:HB3	2:p:118:SER:O	1.99	0.61
1:L:33:ASN:OD1	1:L:34:TRP:N	2.29	0.61
1:N:86:LEU:HG	1:N:90:ILE:HD13	1.80	0.61
1:O:176:MET:N	1:O:182:MET:HE3	2.13	0.61
1:Q:143:LYS:HE3	1:Q:171:CYS:SG	2.40	0.61
1:Q:165:MET:HE1	1:Q:173:VAL:HG11	1.82	0.61
1:R:268:ALA:N	1:R:340:LEU:HD11	2.16	0.61
2:c:225:TRP:HH2	2:c:230:ARG:NH1	1.98	0.61
1:E:109:LEU:HD13	1:E:114:LEU:HD21	1.82	0.61
2:e:9:THR:HG22	2:e:10:GLY:N	2.15	0.61
2:k:166:TYR:HD1	2:k:185:ASN:ND2	1.96	0.61
2:l:104:TYR:O	2:l:105:MET:HG2	1.99	0.61
2:o:225:TRP:HD1	2:o:232:VAL:HG22	1.64	0.61
1:B:31:ILE:HG23	1:B:78:ILE:HB	1.82	0.61
2:e:37:SER:HB3	2:e:49:TRP:HZ3	1.62	0.61
1:H:43:LEU:HD22	1:H:54:VAL:HG21	1.82	0.61
2:l:149:GLN:CG	1:Q:191:GLY:HA3	2.27	0.61
1:P:37:TYR:CE1	1:P:131:LEU:HD12	2.36	0.61
2:a:225:TRP:HD1	2:a:232:VAL:HG22	1.64	0.61
1:B:239:TYR:HB2	1:B:242:ASP:HB2	1.81	0.61
2:l:69:ARG:HH11	2:l:87:ARG:H	1.49	0.61
2:p:225:TRP:HD1	2:p:232:VAL:HG22	1.64	0.61
1:K:170:LYS:HE3	1:K:171:CYS:H	1.63	0.61
1:K:182:MET:HG3	1:K:358:TRP:CH2	2.35	0.61
2:h:226:ASP:O	2:h:228:SER:N	2.33	0.61
1:J:202:TYR:O	1:J:206:GLU:HG2	2.01	0.61
2:k:189:PRO:HD2	2:k:192:ILE:HG13	1.81	0.61
1:M:201:ASP:HA	1:M:203:LYS:CD	2.31	0.61
1:O:102:LYS:HD2	1:O:103:LEU:HB2	1.82	0.61
1:R:240:SER:OG	1:R:241:GLY:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:GLU:HA	1:B:210:THR:OG1	2.01	0.61
2:b:162:ILE:HG12	2:b:224:VAL:HG11	1.83	0.61
2:f:167:VAL:HA	2:f:224:VAL:HG12	1.82	0.61
2:g:69:ARG:NH1	2:g:89:ARG:NH1	2.44	0.61
1:I:359:THR:O	1:I:362:LYS:HB2	2.01	0.61
1:O:104:PRO:HD2	1:O:292:ASP:OD2	2.00	0.61
2:i:167:VAL:HG11	2:i:205:THR:HG21	1.83	0.61
1:J:203:LYS:HG2	1:J:204:LYS:N	2.14	0.61
1:K:139:TYR:CE2	1:K:141:VAL:HG22	2.36	0.61
2:o:78:ILE:O	2:o:80:THR:HG23	2.01	0.61
1:R:135:ASN:OD1	1:R:269:ASN:N	2.31	0.61
1:B:169:ALA:HB2	1:B:215:TYR:HB3	1.83	0.61
1:I:227:ASP:HB3	1:I:233:ILE:HG23	1.83	0.61
1:L:173:VAL:HG13	1:L:235:VAL:HG13	1.82	0.61
1:P:34:TRP:HB2	1:P:37:TYR:CD2	2.31	0.61
1:A:155:SER:HB2	1:A:265:LYS:HE2	1.83	0.60
2:d:15:THR:CG2	2:d:16:PRO:CD	2.62	0.60
1:E:155:SER:HB2	1:E:265:LYS:HE3	1.83	0.60
2:h:195:ARG:NH2	2:h:216:ASP:OD2	2.33	0.60
1:L:228:LEU:HD13	1:L:259:ILE:HG21	1.83	0.60
1:M:201:ASP:HA	1:M:203:LYS:HD3	1.82	0.60
2:n:49:TRP:HH2	2:n:52:TRP:HB2	1.65	0.60
1:Q:317:ARG:NH1	1:Q:317:ARG:CG	2.64	0.60
2:f:226:ASP:OD2	2:f:229:LEU:HB2	2.00	0.60
2:g:225:TRP:HH2	2:g:230:ARG:NH1	1.99	0.60
1:H:155:SER:OG	1:H:266:GLU:OE2	2.11	0.60
1:J:120:SER:O	1:J:122:PRO:HD3	2.01	0.60
1:J:204:LYS:HA	1:J:207:GLU:HG2	1.82	0.60
1:L:110:ASP:HB3	1:L:314:PRO:HG3	1.83	0.60
2:l:11:ASP:N	2:l:11:ASP:OD1	2.33	0.60
2:p:162:ILE:HD13	2:p:205:THR:HG22	1.83	0.60
2:a:78:ILE:O	2:a:80:THR:HG23	2.01	0.60
2:b:243:LEU:HG	1:M:204:LYS:HB3	1.82	0.60
1:C:213:ARG:HH12	1:C:361:ILE:HA	1.65	0.60
1:D:182:MET:HE1	1:D:237:PHE:CG	2.35	0.60
1:J:154:ASP:O	1:J:265:LYS:N	2.32	0.60
2:a:37:SER:HB3	2:a:49:TRP:HZ3	1.66	0.60
2:p:6:LEU:HG	2:p:26:VAL:HG12	1.83	0.60
1:R:84:ASN:ND2	1:R:180:ASP:OD2	2.34	0.60
2:a:6:LEU:HG	2:a:26:VAL:HG12	1.83	0.60
1:F:169:ALA:HB2	1:F:215:TYR:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:295:LEU:HD22	1:F:313:ILE:HD11	1.82	0.60
2:g:167:VAL:HA	2:g:224:VAL:HG12	1.84	0.60
1:K:121:ASP:OD2	1:K:124:ASN:HA	2.02	0.60
1:M:196:THR:HG21	1:M:201:ASP:HB3	1.83	0.60
1:N:191:GLY:CA	2:o:149:GLN:CG	2.79	0.60
2:o:37:SER:HB3	2:o:49:TRP:HZ3	1.66	0.60
2:p:78:ILE:O	2:p:80:THR:HG23	2.01	0.60
2:p:149:GLN:CG	1:R:191:GLY:HA3	2.31	0.60
1:Q:182:MET:HE1	1:Q:237:PHE:CD1	2.36	0.60
2:a:162:ILE:HD13	2:a:205:THR:HG22	1.83	0.60
1:B:225:ILE:HD11	1:B:242:ASP:OD2	2.01	0.60
1:E:176:MET:HE1	1:E:239:TYR:OH	2.01	0.60
1:J:156:TRP:CE2	1:J:264:PRO:HG2	2.36	0.60
2:l:145:GLY:HA2	2:l:149:GLN:NE2	2.16	0.60
2:r:26:VAL:HG13	2:r:79:SER:O	2.02	0.60
2:i:8:GLU:H	2:i:110:LYS:NZ	1.99	0.60
2:q:143:VAL:HG23	2:q:240:LEU:HD13	1.83	0.60
1:J:139:TYR:CD2	1:J:144:VAL:HG21	2.36	0.60
2:j:186:ASN:OD1	2:j:187:LYS:NZ	2.33	0.60
1:K:271:TRP:CD2	4:K:404:SPD:H82	2.37	0.60
2:k:181:LEU:HD21	2:k:196:PHE:HD2	1.66	0.60
1:Q:200:LYS:HA	1:Q:203:LYS:CB	2.32	0.60
1:D:33:ASN:O	1:D:58:VAL:HA	2.02	0.60
1:F:360:ARG:NH1	3:F:402:SO4:O4	2.33	0.60
2:f:69:ARG:NH1	2:f:87:ARG:O	2.35	0.60
1:I:115:LYS:HA	1:I:118:GLU:HG3	1.84	0.60
1:J:205:ALA:O	1:J:209:LEU:HD12	2.02	0.60
2:l:41:GLN:O	2:l:94:ALA:HA	2.00	0.60
2:l:105:MET:HB2	2:l:108:TRP:CH2	2.36	0.60
2:l:218:ALA:HB3	2:l:220:TYR:CE1	2.31	0.60
1:C:147:VAL:HG23	1:C:148:LEU:HD13	1.83	0.60
2:i:165:ASN:ND2	2:i:225:TRP:O	2.34	0.60
1:J:200:LYS:HD2	1:J:203:LYS:HB3	1.84	0.60
2:k:31:PHE:HE1	2:k:36:ILE:HD12	1.66	0.60
2:l:41:GLN:H	2:l:94:ALA:HB1	1.67	0.60
1:M:220:HIS:CD2	1:M:223:LYS:HB2	2.37	0.60
2:h:220:TYR:O	2:h:237:GLY:HA2	2.02	0.59
1:J:175:PHE:HD2	1:J:182:MET:SD	2.24	0.59
1:Q:271:TRP:CE2	4:Q:401:SPD:H82	2.37	0.59
2:a:217:GLU:HG3	2:a:240:LEU:O	2.02	0.59
1:H:182:MET:HE1	1:H:237:PHE:CG	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:183:LEU:HD13	1:I:202:TYR:HE1	1.68	0.59
1:J:200:LYS:O	1:J:203:LYS:HB3	2.02	0.59
2:l:21:LYS:CE	2:l:84:GLU:OE1	2.23	0.59
2:l:153:ILE:HG12	2:l:238:THR:HG21	1.83	0.59
2:n:15:THR:HB	2:n:16:PRO:HD2	1.81	0.59
1:O:125:GLN:HG3	1:O:126:TYR:CD2	2.37	0.59
2:b:20:VAL:CG1	2:b:88:LEU:HD11	2.32	0.59
2:b:89:ARG:O	2:b:91:ASP:N	2.36	0.59
1:C:271:TRP:CH2	4:C:404:SPD:H52	2.38	0.59
1:H:109:LEU:HD13	1:H:114:LEU:HD21	1.85	0.59
1:I:139:TYR:CD2	1:I:144:VAL:HG21	2.37	0.59
1:J:202:TYR:C	1:J:205:ALA:HB3	2.28	0.59
1:K:356:ARG:NE	3:K:401:SO4:O1	2.36	0.59
2:k:21:LYS:HE2	2:m:68:GLY:HA2	1.84	0.59
2:q:49:TRP:CG	2:q:232:VAL:HB	2.38	0.59
2:r:14:LYS:CE	2:r:20:VAL:HG23	2.32	0.59
1:E:100:LYS:NZ	1:E:124:ASN:O	2.28	0.59
2:j:189:PRO:HD2	2:j:192:ILE:HG13	1.83	0.59
2:l:104:TYR:CE1	2:l:183:TYR:HB2	2.38	0.59
1:N:171:CYS:HB3	1:N:234:CYS:HB3	1.85	0.59
1:N:360:ARG:NH1	3:N:404:SO4:O1	2.36	0.59
2:n:15:THR:CG2	2:n:16:PRO:CD	2.37	0.59
1:G:182:MET:HE1	1:G:237:PHE:CG	2.37	0.59
1:J:33:ASN:O	1:J:58:VAL:HA	2.02	0.59
1:J:146:GLU:HG2	1:J:147:VAL:HG13	1.83	0.59
1:K:176:MET:HB2	1:K:182:MET:HE3	1.84	0.59
2:m:49:TRP:HD1	2:m:63:ALA:HB2	1.65	0.59
1:N:32:TYR:HB3	1:N:79:VAL:HG12	1.84	0.59
1:O:182:MET:HG3	1:O:358:TRP:CH2	2.37	0.59
2:p:37:SER:HB3	2:p:49:TRP:HZ3	1.66	0.59
1:Q:189:TYR:C	1:Q:191:GLY:H	2.09	0.59
2:q:20:VAL:O	2:q:20:VAL:HG13	2.01	0.59
2:i:16:PRO:C	2:i:18:ALA:N	2.59	0.59
1:L:128:VAL:O	1:L:275:MET:N	2.31	0.59
2:p:217:GLU:HG3	2:p:240:LEU:O	2.02	0.59
1:Q:157:ALA:O	1:Q:164:ASN:ND2	2.29	0.59
1:Q:171:CYS:HB3	1:Q:234:CYS:SG	2.42	0.59
2:r:14:LYS:O	2:r:15:THR:CG2	2.51	0.59
2:b:78:ILE:HG22	2:b:80:THR:HG23	1.85	0.59
1:C:323:SER:HB3	2:c:225:TRP:HZ3	1.68	0.59
2:h:185:ASN:HD21	2:h:200:LYS:NZ	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:149:GLN:HG3	2:i:150:LYS:N	2.16	0.59
1:J:203:LYS:CG	1:J:204:LYS:N	2.66	0.59
1:J:213:ARG:HD2	1:J:361:ILE:HG22	1.83	0.59
1:P:297:PRO:O	1:P:300:ILE:HG22	2.02	0.59
1:I:121:ASP:OD2	1:I:124:ASN:HA	2.02	0.59
1:O:242:ASP:OD1	1:O:309:TYR:OH	2.21	0.59
1:O:273:ASP:OD2	4:O:407:SPD:H52	2.02	0.59
2:e:37:SER:HB3	2:e:49:TRP:CZ3	2.37	0.59
2:h:18:ALA:CA	2:h:88:LEU:H	2.15	0.59
1:L:226:SER:O	1:L:230:ASN:HB2	2.03	0.59
2:l:192:ILE:HG13	2:l:193:PRO:HD2	1.84	0.59
2:l:220:TYR:O	2:l:237:GLY:HA2	2.03	0.59
2:m:13:VAL:O	2:m:13:VAL:HG22	2.01	0.59
1:P:323:SER:OG	2:p:225:TRP:CH2	2.55	0.59
2:q:43:PRO:O	2:q:45:GLN:NE2	2.34	0.59
1:G:165:MET:HE1	1:G:173:VAL:HG11	1.85	0.58
2:h:167:VAL:HG11	2:h:205:THR:HG21	1.84	0.58
1:I:109:LEU:HD13	1:I:114:LEU:HD21	1.83	0.58
2:k:100:ARG:HB3	2:k:107:VAL:HG22	1.85	0.58
1:P:32:TYR:HB3	1:P:79:VAL:HG12	1.85	0.58
1:C:242:ASP:OD1	1:C:309:TYR:OH	2.20	0.58
1:E:173:VAL:HG13	1:E:235:VAL:HG13	1.85	0.58
1:E:323:SER:HB3	2:e:225:TRP:HE1	1.66	0.58
2:e:20:VAL:HG13	2:e:20:VAL:O	2.01	0.58
2:i:167:VAL:HA	2:i:224:VAL:HG12	1.83	0.58
1:Q:125:GLN:HB2	1:Q:126:TYR:HD1	1.67	0.58
2:r:83:MET:HG2	2:r:84:GLU:N	2.18	0.58
2:r:89:ARG:HG3	2:r:91:ASP:HB3	1.85	0.58
2:c:181:LEU:HD11	2:c:196:PHE:CD2	2.38	0.58
1:D:213:ARG:NH1	1:D:361:ILE:HA	2.18	0.58
1:F:271:TRP:CD2	4:F:404:SPD:H82	2.38	0.58
1:M:182:MET:HE1	1:M:237:PHE:CG	2.38	0.58
1:N:192:LEU:CD2	1:N:193:ASP:H	2.16	0.58
2:p:243:LEU:CD2	1:R:190:LEU:CD1	2.77	0.58
1:E:37:TYR:CE1	4:E:405:SPD:H41	2.39	0.58
1:E:252:GLU:O	1:E:254:GLY:N	2.36	0.58
1:E:273:ASP:OD2	4:E:405:SPD:H52	2.03	0.58
2:h:75:ASP:OD1	2:h:77:SER:HB3	2.03	0.58
2:i:118:SER:HA	2:o:118:SER:OG	2.02	0.58
2:l:179:LYS:O	2:l:181:LEU:HG	2.03	0.58
1:M:158:ILE:HD13	1:M:164:ASN:HD22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:162:ILE:HD13	2:o:205:THR:HG22	1.83	0.58
2:o:217:GLU:HG3	2:o:240:LEU:O	2.02	0.58
1:B:155:SER:HB2	1:B:265:LYS:NZ	2.19	0.58
1:N:77:ASP:O	1:N:78:ILE:HG13	2.04	0.58
2:n:9:THR:HG1	2:n:23:SER:N	2.01	0.58
2:q:150:LYS:HG2	2:q:151:VAL:N	2.19	0.58
2:r:15:THR:O	2:r:16:PRO:O	2.22	0.58
1:G:271:TRP:CE2	4:G:403:SPD:H72	2.38	0.58
1:I:168:LEU:O	1:I:170:LYS:HG2	2.04	0.58
2:i:32:THR:HA	2:i:55:PRO:HB2	1.85	0.58
2:i:117:SER:HB3	2:o:118:SER:O	2.03	0.58
2:n:5:GLN:HE22	2:n:110:LYS:HZ2	1.47	0.58
1:O:94:ALA:O	1:O:279:ALA:N	2.36	0.58
1:C:156:TRP:CE2	1:C:264:PRO:HG2	2.38	0.58
1:G:326:ASP:HB3	2:g:165:ASN:HB3	1.85	0.58
2:i:15:THR:O	2:i:16:PRO:C	2.46	0.58
2:j:100:ARG:HB3	2:j:107:VAL:HG22	1.84	0.58
2:o:6:LEU:HG	2:o:26:VAL:HG12	1.83	0.58
2:o:49:TRP:CD1	2:o:232:VAL:H	2.22	0.58
2:r:14:LYS:O	2:r:15:THR:HG23	2.04	0.58
2:r:14:LYS:HG3	2:r:20:VAL:HG23	1.84	0.58
2:f:26:VAL:HG22	2:f:79:SER:HB3	1.86	0.58
2:h:18:ALA:HA	2:h:88:LEU:CB	2.34	0.58
2:l:94:ALA:HB3	2:l:96:TYR:CZ	2.38	0.58
2:i:14:LYS:HB3	2:i:18:ALA:HB1	1.86	0.58
1:J:213:ARG:HG3	1:J:213:ARG:NH1	2.14	0.58
2:n:19:SER:OG	2:n:19:SER:O	2.22	0.58
2:n:158:SER:C	2:n:160:SER:H	2.12	0.58
2:p:49:TRP:CD1	2:p:232:VAL:H	2.22	0.58
2:g:99:ALA:HB1	2:g:105:MET:HB3	1.85	0.58
2:h:18:ALA:HB1	2:h:87:ARG:N	2.18	0.58
2:k:167:VAL:HA	2:k:224:VAL:HG12	1.86	0.58
1:P:37:TYR:HE1	1:P:131:LEU:HD12	1.69	0.58
2:q:52:TRP:N	2:q:72:MET:HE1	2.19	0.58
2:r:35:GLY:HA2	2:r:55:PRO:HD3	1.86	0.58
1:D:182:MET:HE1	1:D:237:PHE:CD1	2.38	0.57
1:D:330:VAL:O	1:D:332:PRO:HD3	2.03	0.57
2:j:49:TRP:CD1	2:j:232:VAL:H	2.22	0.57
1:Q:240:SER:OG	1:Q:241:GLY:N	2.35	0.57
1:R:227:ASP:HB3	1:R:233:ILE:HG23	1.86	0.57
1:I:234:CYS:SG	1:I:235:VAL:N	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:20:VAL:HG21	2:p:114:VAL:HG21	1.87	0.57
1:Q:171:CYS:SG	1:Q:234:CYS:HB3	2.44	0.57
2:q:20:VAL:HG21	2:q:114:VAL:CG2	2.32	0.57
1:E:243:VAL:HG11	1:E:261:TYR:HB2	1.85	0.57
2:i:118:SER:N	2:o:118:SER:CA	2.66	0.57
2:j:49:TRP:HH2	2:j:52:TRP:HB2	1.68	0.57
2:l:143:VAL:HG11	2:l:151:VAL:HG21	1.86	0.57
1:N:52:ILE:HD13	1:N:286:ASN:HB2	1.85	0.57
2:o:20:VAL:HG21	2:o:114:VAL:HG21	1.87	0.57
2:o:225:TRP:CZ3	2:o:227:SER:HA	2.39	0.57
2:r:6:LEU:HD23	2:r:98:CYS:SG	2.43	0.57
1:A:33:ASN:OD1	1:A:34:TRP:N	2.36	0.57
2:b:20:VAL:HG11	2:b:88:LEU:HD11	1.87	0.57
2:d:37:SER:HB3	2:d:49:TRP:CZ3	2.38	0.57
2:f:20:VAL:O	2:f:20:VAL:HG13	2.04	0.57
2:f:31:PHE:CD2	2:f:79:SER:HA	2.38	0.57
1:K:154:ASP:O	1:K:264:PRO:HA	2.04	0.57
1:K:173:VAL:HA	1:K:235:VAL:HG12	1.86	0.57
2:l:195:ARG:NH1	2:l:216:ASP:OD2	2.37	0.57
2:n:18:ALA:HB3	2:n:88:LEU:N	2.17	0.57
1:O:90:ILE:C	1:O:92:ALA:H	2.12	0.57
1:O:128:VAL:O	1:O:275:MET:N	2.38	0.57
1:C:317:ARG:HD2	1:C:331:TYR:CE2	2.39	0.57
1:F:176:MET:H	1:F:182:MET:CE	2.17	0.57
2:g:167:VAL:H	2:g:185:ASN:HD22	1.53	0.57
2:l:29:TYR:CD1	2:l:31:PHE:HA	2.40	0.57
1:M:104:PRO:HD2	1:M:292:ASP:CG	2.30	0.57
1:N:176:MET:HE1	1:N:239:TYR:CE2	2.40	0.57
1:N:184:PRO:O	1:N:194:PRO:HB3	2.05	0.57
1:O:176:MET:H	1:O:182:MET:CE	2.17	0.57
2:a:49:TRP:CD1	2:a:232:VAL:H	2.22	0.57
1:D:62:ASN:HB3	1:D:85:PHE:CE2	2.39	0.57
1:G:166:LYS:HG2	1:G:215:TYR:CZ	2.39	0.57
1:I:165:MET:HA	1:I:168:LEU:HB2	1.87	0.57
1:N:189:TYR:C	1:N:191:GLY:H	2.13	0.57
2:q:169:TRP:HZ2	2:q:205:THR:CG2	2.18	0.57
1:R:362:LYS:NZ	1:R:362:LYS:HB3	2.19	0.57
2:r:93:THR:HG23	2:r:115:THR:HG22	1.87	0.57
1:C:271:TRP:CE2	4:C:404:SPD:H72	2.39	0.57
1:H:169:ALA:HB2	1:H:215:TYR:HB3	1.85	0.57
1:J:323:SER:HG	2:j:225:TRP:HH2	1.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:34:TYR:O	2:l:55:PRO:HG2	2.05	0.57
1:M:204:LYS:HA	1:M:207:GLU:OE1	2.04	0.57
1:O:77:ASP:OD2	1:O:283:ALA:HB3	2.04	0.57
1:A:100:LYS:NZ	1:A:124:ASN:O	2.28	0.57
2:b:18:ALA:HA	2:b:88:LEU:HG	1.87	0.57
2:d:225:TRP:HH2	2:d:230:ARG:NH1	2.03	0.57
1:R:211:LYS:O	1:R:213:ARG:N	2.38	0.57
1:D:33:ASN:OD1	1:D:34:TRP:N	2.36	0.57
1:D:179:GLY:O	1:D:183:LEU:HB2	2.04	0.57
1:H:147:VAL:CG2	1:H:167:LYS:HB3	2.35	0.57
2:i:118:SER:N	2:o:118:SER:C	2.62	0.57
2:l:35:GLY:HA3	2:l:52:TRP:CZ3	2.39	0.57
2:n:42:ALA:HB1	2:n:43:PRO:HD2	1.86	0.57
2:q:183:TYR:HD1	2:q:184:ASP:OD2	1.87	0.57
2:i:139:GLN:NE2	2:i:220:TYR:O	2.36	0.57
1:K:317:ARG:NH2	1:K:325:SER:O	2.38	0.57
2:l:29:TYR:HE1	2:l:31:PHE:HA	1.70	0.57
2:l:39:VAL:HG23	2:l:48:GLU:O	2.05	0.57
2:l:226:ASP:OD2	2:l:229:LEU:HG	2.05	0.57
1:O:33:ASN:HA	1:O:80:VAL:HG23	1.86	0.57
2:o:169:TRP:HB2	2:o:182:LEU:HB2	1.87	0.57
1:Q:317:ARG:NH1	1:Q:325:SER:O	2.37	0.57
2:r:169:TRP:HB2	2:r:182:LEU:HB2	1.86	0.57
1:C:134:THR:O	1:C:271:TRP:NE1	2.37	0.56
2:c:15:THR:CG2	2:c:16:PRO:CD	2.69	0.56
2:d:88:LEU:HD13	2:d:116:VAL:HG22	1.86	0.56
1:K:33:ASN:O	1:K:58:VAL:HA	2.05	0.56
1:L:83:ASN:OD1	1:L:272:PHE:N	2.32	0.56
1:O:102:LYS:HB2	1:O:288:TYR:HB3	1.86	0.56
1:O:110:ASP:OD2	1:O:112:ALA:HB3	2.05	0.56
1:P:250:ALA:HB1	1:P:257:ILE:HB	1.86	0.56
2:d:20:VAL:CG2	2:d:88:LEU:HD11	2.34	0.56
2:q:15:THR:HB	2:q:16:PRO:HD2	1.86	0.56
1:R:250:ALA:HB1	1:R:257:ILE:HB	1.87	0.56
2:a:225:TRP:CZ3	2:a:227:SER:HA	2.39	0.56
1:B:33:ASN:O	1:B:58:VAL:HA	2.05	0.56
1:B:225:ILE:HD11	1:B:242:ASP:CG	2.30	0.56
1:E:67:GLY:HA3	1:H:71:SER:OG	2.04	0.56
2:g:14:LYS:O	2:g:116:VAL:HA	2.05	0.56
1:H:275:MET:HE1	1:H:294:LEU:HD12	1.88	0.56
1:K:59:PHE:CE2	1:K:65:LEU:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:32:THR:HA	2:k:55:PRO:HB2	1.86	0.56
1:M:225:ILE:HD11	1:M:242:ASP:CG	2.30	0.56
2:m:20:VAL:HG11	2:m:114:VAL:CG2	2.35	0.56
1:O:62:ASN:HD21	1:O:82:SER:CB	2.18	0.56
1:O:99:ASP:O	1:O:101:SER:N	2.38	0.56
1:P:240:SER:HA	1:P:261:TYR:CZ	2.40	0.56
2:p:225:TRP:CZ3	2:p:227:SER:HA	2.39	0.56
1:Q:204:LYS:O	1:Q:207:GLU:HG2	2.04	0.56
1:R:323:SER:HB3	2:r:225:TRP:HZ3	1.69	0.56
1:E:242:ASP:OD1	1:E:309:TYR:OH	2.20	0.56
2:g:52:TRP:N	2:g:72:MET:HE1	2.21	0.56
2:h:20:VAL:HG22	2:h:88:LEU:CD1	2.25	0.56
2:h:212:LEU:HD23	2:h:242:VAL:HG22	1.87	0.56
2:i:225:TRP:CZ3	2:i:227:SER:HA	2.41	0.56
1:J:207:GLU:HA	1:J:210:THR:OG1	2.05	0.56
1:M:203:LYS:HZ3	1:M:204:LYS:HB2	1.69	0.56
1:O:240:SER:OG	1:O:241:GLY:N	2.38	0.56
1:Q:142:ALA:O	1:Q:146:GLU:HB2	2.06	0.56
2:a:167:VAL:HG22	2:a:224:VAL:CG1	2.34	0.56
2:b:62:TYR:HB2	2:b:67:GLN:HG3	1.88	0.56
1:I:170:LYS:HD3	1:I:234:CYS:SG	2.45	0.56
1:N:163:GLU:O	1:N:167:LYS:HG2	2.05	0.56
2:b:185:ASN:OD1	2:b:200:LYS:NZ	2.38	0.56
1:G:198:ASP:OD1	1:G:200:LYS:N	2.30	0.56
1:J:177:ASP:HA	1:J:358:TRP:HZ2	1.71	0.56
1:L:97:LYS:HD3	1:L:126:TYR:CE1	2.40	0.56
2:l:73:THR:HG22	2:l:82:TYR:HB2	1.88	0.56
1:P:333:PRO:HA	2:p:166:TYR:OH	2.05	0.56
2:a:169:TRP:HB2	2:a:182:LEU:HB2	1.87	0.56
2:c:37:SER:HB3	2:c:49:TRP:CZ3	2.40	0.56
1:O:205:ALA:O	1:O:209:LEU:HD12	2.06	0.56
2:o:167:VAL:HG22	2:o:224:VAL:CG1	2.35	0.56
2:a:25:LYS:HA	2:a:80:THR:HG22	1.88	0.56
2:c:26:VAL:HB	2:c:29:TYR:CE1	2.40	0.56
2:f:182:LEU:CD2	2:f:188:ARG:HG2	2.35	0.56
2:h:85:LEU:HD12	2:h:86:SER:H	1.69	0.56
2:j:166:TYR:HD2	2:j:184:ASP:HA	1.70	0.56
1:L:207:GLU:O	1:L:211:LYS:HG3	2.06	0.56
2:l:84:GLU:HG2	2:l:85:LEU:N	2.21	0.56
1:M:248:ALA:O	1:M:252:GLU:HG2	2.06	0.56
2:m:225:TRP:CZ2	2:m:230:ARG:HA	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:125:GLN:HB2	1:Q:126:TYR:CD1	2.41	0.56
1:R:170:LYS:NZ	1:R:234:CYS:HB3	2.21	0.56
1:A:104:PRO:HD2	1:A:292:ASP:CG	2.30	0.56
1:I:183:LEU:HD23	1:I:209:LEU:CD1	2.35	0.56
1:L:130:TYR:CE2	1:L:275:MET:HE3	2.40	0.56
2:l:42:ALA:HB1	2:l:43:PRO:HD2	1.88	0.56
2:n:26:VAL:HG12	2:n:79:SER:HB3	1.86	0.56
1:Q:122:PRO:O	1:Q:125:GLN:HG3	2.05	0.56
1:R:353:LEU:HA	1:R:356:ARG:NE	2.14	0.56
1:B:109:LEU:HD13	1:B:114:LEU:HD21	1.87	0.56
1:I:207:GLU:OE1	1:I:207:GLU:N	2.39	0.56
2:i:37:SER:HB3	2:i:49:TRP:HZ3	1.71	0.56
2:k:93:THR:HG23	2:k:115:THR:HA	1.87	0.56
1:L:196:THR:HG21	1:L:201:ASP:OD2	2.06	0.56
1:N:271:TRP:CG	4:N:407:SPD:H91	2.41	0.56
2:n:53:ILE:HD11	2:n:74:ARG:HG2	1.88	0.56
1:A:29:LEU:HD12	1:A:77:ASP:OD2	2.05	0.55
2:a:20:VAL:HG21	2:a:114:VAL:HG21	1.86	0.55
2:d:70:VAL:HA	2:d:84:GLU:O	2.06	0.55
2:f:197:SER:HB2	2:f:208:ALA:HB3	1.88	0.55
1:I:203:LYS:CA	1:I:206:GLU:HB3	2.30	0.55
2:p:167:VAL:HG22	2:p:224:VAL:CG1	2.34	0.55
1:Q:155:SER:HB2	1:Q:265:LYS:NZ	2.21	0.55
1:J:159:LEU:HA	1:J:165:MET:HE1	1.88	0.55
1:K:60:ASP:HB2	1:K:222:SER:HB3	1.89	0.55
2:k:118:SER:CB	2:p:119:GLY:O	2.52	0.55
1:L:159:LEU:O	1:L:165:MET:HG3	2.06	0.55
1:M:298:GLU:HG2	2:m:56:ASN:ND2	2.20	0.55
1:N:125:GLN:HG3	1:N:126:TYR:HD1	1.70	0.55
2:n:18:ALA:C	2:n:19:SER:HG	2.10	0.55
2:n:83:MET:HE1	2:n:96:TYR:CE2	2.41	0.55
2:r:26:VAL:HG11	2:r:31:PHE:CD1	2.41	0.55
2:a:20:VAL:CG1	2:a:88:LEU:HD21	2.37	0.55
1:I:165:MET:HE1	1:I:173:VAL:HG11	1.89	0.55
1:I:170:LYS:HE2	1:I:171:CYS:SG	2.46	0.55
1:L:56:TYR:HE1	1:L:58:VAL:HG12	1.71	0.55
2:l:21:LYS:HB3	2:l:84:GLU:N	2.21	0.55
2:m:75:ASP:OD1	2:m:77:SER:HB3	2.06	0.55
2:p:169:TRP:HB2	2:p:182:LEU:HB2	1.87	0.55
2:r:89:ARG:O	2:r:116:VAL:HG21	2.07	0.55
1:A:330:VAL:O	1:A:332:PRO:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:MET:HE1	1:G:239:TYR:CD2	2.41	0.55
1:K:156:TRP:O	1:K:159:LEU:N	2.30	0.55
2:l:173:LEU:HA	2:l:218:ALA:HB2	1.89	0.55
2:l:182:LEU:HD23	2:l:188:ARG:HA	1.87	0.55
1:M:201:ASP:C	1:M:203:LYS:HG2	2.32	0.55
2:n:106:ASP:HA	2:n:180:LEU:HB2	1.87	0.55
2:o:20:VAL:CG1	2:o:88:LEU:HD21	2.37	0.55
1:P:139:TYR:HB2	1:P:144:VAL:HG21	1.88	0.55
2:c:21:LYS:HG2	2:c:84:GLU:HB2	1.89	0.55
2:c:162:ILE:O	2:c:200:LYS:HE3	2.07	0.55
1:G:240:SER:OG	1:G:241:GLY:N	2.34	0.55
2:j:181:LEU:HD21	2:j:196:PHE:HD2	1.71	0.55
2:k:21:LYS:HG3	2:k:21:LYS:O	2.06	0.55
2:p:25:LYS:HA	2:p:80:THR:HG22	1.88	0.55
1:Q:242:ASP:OD1	1:Q:309:TYR:OH	2.24	0.55
1:Q:322:LYS:HD3	2:q:225:TRP:NE1	2.22	0.55
1:R:97:LYS:HG2	1:R:126:TYR:CE1	2.42	0.55
1:F:182:MET:HE1	1:F:237:PHE:CG	2.41	0.55
1:I:88:LYS:HE2	1:I:346:LEU:O	2.07	0.55
1:I:233:ILE:HD11	1:I:236:ALA:HB2	1.87	0.55
1:M:165:MET:HE1	1:M:173:VAL:HG11	1.88	0.55
2:o:25:LYS:HA	2:o:80:THR:HG22	1.88	0.55
1:Q:163:GLU:HA	1:Q:166:LYS:HG3	1.87	0.55
1:Q:317:ARG:HH12	1:Q:325:SER:C	2.14	0.55
1:Q:328:GLU:HG2	2:q:166:TYR:CE1	2.41	0.55
2:q:199:SER:OG	2:q:200:LYS:N	2.34	0.55
1:R:115:LYS:HA	1:R:118:GLU:HG3	1.89	0.55
1:R:187:LEU:HD12	1:R:194:PRO:HA	1.89	0.55
1:A:322:LYS:HD3	2:a:225:TRP:NE1	2.21	0.55
2:f:90:SER:HA	2:f:116:VAL:HG13	1.88	0.55
1:H:111:PRO:HA	1:H:114:LEU:HD12	1.89	0.55
1:I:168:LEU:C	1:I:170:LYS:HG2	2.32	0.55
2:i:19:SER:O	2:i:19:SER:OG	2.24	0.55
1:M:111:PRO:HA	1:M:114:LEU:HD12	1.88	0.55
1:O:176:MET:HE1	1:O:239:TYR:CD2	2.42	0.55
2:p:20:VAL:CG1	2:p:88:LEU:HD21	2.37	0.55
2:b:18:ALA:CA	2:b:88:LEU:H	2.19	0.55
2:c:69:ARG:HE	2:c:85:LEU:HD21	1.72	0.55
1:K:120:SER:O	1:K:122:PRO:HD3	2.07	0.55
2:l:225:TRP:HD1	2:l:232:VAL:HG22	1.72	0.55
1:N:191:GLY:HA2	2:o:149:GLN:CD	2.29	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:82:SER:OG	4:P:401:SPD:H81	2.07	0.55
1:Q:350:VAL:C	1:Q:352:ARG:H	2.15	0.55
1:R:197:HIS:CD2	1:R:347:PRO:HG2	2.42	0.55
1:R:268:ALA:H	1:R:340:LEU:HD11	1.70	0.55
1:A:337:LEU:C	1:A:339:LYS:H	2.15	0.55
2:c:26:VAL:HB	2:c:29:TYR:HE1	1.71	0.55
2:h:167:VAL:HG22	2:h:224:VAL:HG11	1.89	0.55
2:i:153:ILE:HG21	2:i:238:THR:HG21	1.88	0.55
2:k:78:ILE:HD11	2:m:64:GLN:NE2	2.22	0.55
1:L:110:ASP:OD2	1:L:112:ALA:HB3	2.06	0.55
2:l:225:TRP:CZ3	2:l:227:SER:HA	2.42	0.55
2:i:117:SER:O	2:o:118:SER:O	2.25	0.55
2:i:139:GLN:NE2	2:i:238:THR:HG22	2.22	0.55
1:K:359:THR:O	1:K:362:LYS:NZ	2.35	0.55
2:l:21:LYS:HD3	2:l:21:LYS:N	2.22	0.55
2:l:85:LEU:HD22	2:l:88:LEU:HD23	1.89	0.55
1:P:317:ARG:HH12	2:p:103:ARG:CZ	2.18	0.55
2:r:187:LYS:NZ	2:r:189:PRO:HA	2.22	0.55
1:B:173:VAL:HG22	1:B:235:VAL:HG12	1.88	0.54
1:E:147:VAL:HG21	1:E:170:LYS:HE3	1.88	0.54
1:N:176:MET:HA	1:N:220:HIS:O	2.06	0.54
2:q:183:TYR:CD1	2:q:184:ASP:OD2	2.59	0.54
2:r:52:TRP:N	2:r:72:MET:HE1	2.22	0.54
1:F:139:TYR:CD2	1:F:144:VAL:HG21	2.43	0.54
2:f:75:ASP:OD1	2:f:77:SER:HB3	2.06	0.54
1:H:104:PRO:HD2	1:H:292:ASP:CG	2.32	0.54
2:i:26:VAL:HG11	2:i:31:PHE:CD1	2.42	0.54
1:Q:204:LYS:O	1:Q:208:VAL:HG23	2.06	0.54
1:R:43:LEU:HD22	1:R:54:VAL:HG21	1.88	0.54
2:r:153:ILE:HG21	2:r:238:THR:HG21	1.89	0.54
1:A:176:MET:HB2	1:A:182:MET:HE3	1.88	0.54
1:B:99:ASP:OD2	1:B:102:LYS:HG3	2.06	0.54
1:C:330:VAL:O	1:C:332:PRO:HD3	2.06	0.54
1:G:155:SER:OG	1:G:266:GLU:OE2	2.24	0.54
1:I:187:LEU:CD2	1:I:205:ALA:HB2	2.36	0.54
1:I:200:LYS:NZ	1:I:203:LYS:CB	2.67	0.54
2:j:182:LEU:HD21	2:j:188:ARG:HG2	1.89	0.54
2:l:11:ASP:O	2:l:12:GLU:HB2	2.07	0.54
1:O:346:LEU:HB2	1:O:351:LEU:HD21	1.89	0.54
1:R:322:LYS:HD3	2:r:225:TRP:CD1	2.42	0.54
2:h:31:PHE:HE1	2:h:36:ILE:HD12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:225:TRP:HZ3	2:h:226:ASP:O	1.86	0.54
2:i:16:PRO:O	2:i:18:ALA:N	2.41	0.54
2:i:26:VAL:CG2	2:i:26:VAL:CA	2.77	0.54
2:k:195:ARG:NH2	2:k:216:ASP:OD2	2.41	0.54
1:M:156:TRP:CE2	1:M:264:PRO:HG2	2.42	0.54
1:M:173:VAL:HG13	1:M:235:VAL:HG13	1.88	0.54
2:m:49:TRP:HH2	2:m:52:TRP:HB2	1.72	0.54
1:N:66:GLU:HG3	1:N:89:GLN:NE2	2.16	0.54
2:n:71:THR:N	2:n:84:GLU:O	2.40	0.54
1:O:83:ASN:OD1	1:O:272:PHE:N	2.38	0.54
1:P:244:PHE:CZ	1:P:329:GLU:HB2	2.42	0.54
2:p:139:GLN:HG3	2:p:154:SER:O	2.08	0.54
1:B:213:ARG:NH1	1:B:361:ILE:HA	2.22	0.54
1:H:122:PRO:O	1:H:125:GLN:HG3	2.07	0.54
1:I:106:TRP:CZ3	1:I:128:VAL:HG22	2.40	0.54
2:i:31:PHE:HE1	2:i:36:ILE:HD12	1.73	0.54
2:i:139:GLN:HE21	2:i:238:THR:N	2.04	0.54
1:J:176:MET:HG3	1:J:237:PHE:CD1	2.42	0.54
1:M:203:LYS:HG3	1:M:204:LYS:N	2.23	0.54
1:Q:37:TYR:CZ	1:Q:131:LEU:HB2	2.43	0.54
1:Q:350:VAL:O	1:Q:352:ARG:N	2.41	0.54
2:q:102:LYS:HD3	2:q:106:ASP:OD2	2.08	0.54
1:E:165:MET:SD	1:E:173:VAL:HG11	2.48	0.54
1:H:143:LYS:HA	1:H:146:GLU:HB3	1.89	0.54
1:H:328:GLU:OE2	2:h:200:LYS:NZ	2.41	0.54
1:L:131:LEU:CD1	1:L:309:TYR:HB2	2.30	0.54
1:A:106:TRP:HZ3	1:A:128:VAL:HG22	1.72	0.54
2:a:139:GLN:HG3	2:a:154:SER:O	2.08	0.54
2:b:153:ILE:HG21	2:b:238:THR:HG21	1.89	0.54
1:E:172:GLY:HA3	1:E:233:ILE:HG22	1.88	0.54
1:I:80:VAL:HG22	1:I:275:MET:HG2	1.89	0.54
1:M:201:ASP:HA	1:M:203:LYS:CE	2.38	0.54
1:N:326:ASP:HB3	2:n:165:ASN:HB3	1.89	0.54
2:o:139:GLN:HG3	2:o:154:SER:O	2.08	0.54
1:P:297:PRO:HA	1:P:313:ILE:HG21	1.89	0.54
1:Q:322:LYS:HA	1:Q:325:SER:OG	2.06	0.54
1:R:139:TYR:HB2	1:R:144:VAL:HG21	1.88	0.54
1:R:320:MET:HB2	1:R:325:SER:HB3	1.90	0.54
1:A:323:SER:HB3	2:a:225:TRP:HZ3	1.73	0.54
2:b:184:ASP:O	2:b:186:ASN:N	2.38	0.54
1:E:213:ARG:HH11	1:E:361:ILE:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:104:TYR:CD2	2:f:183:TYR:HB2	2.42	0.54
1:H:88:LYS:HE2	1:H:346:LEU:O	2.08	0.54
1:N:191:GLY:CA	2:o:149:GLN:HG3	2.38	0.54
2:r:238:THR:CG2	2:r:238:THR:CA	2.77	0.54
2:b:21:LYS:HG3	2:b:84:GLU:HB2	1.90	0.54
2:b:37:SER:HB3	2:b:49:TRP:CZ3	2.41	0.54
1:C:86:LEU:HD22	1:C:274:LEU:HD13	1.89	0.54
1:C:282:LYS:HG3	1:C:283:ALA:N	2.23	0.54
2:d:161:ASN:HB2	2:d:224:VAL:CG2	2.38	0.54
2:k:49:TRP:CG	2:k:232:VAL:HB	2.43	0.54
1:L:240:SER:HA	1:L:261:TYR:CZ	2.43	0.54
2:m:49:TRP:CE3	2:m:232:VAL:HB	2.42	0.54
2:n:199:SER:OG	2:n:200:LYS:N	2.40	0.54
2:b:14:LYS:HD2	2:b:19:SER:O	2.07	0.54
2:b:93:THR:HG23	2:b:115:THR:HA	1.90	0.54
2:c:214:THR:HA	2:c:242:VAL:HG11	1.88	0.54
2:h:18:ALA:CB	2:h:87:ARG:N	2.71	0.54
2:l:21:LYS:HG3	2:l:84:GLU:HB2	1.90	0.54
1:M:360:ARG:NH1	3:M:401:SO4:O3	2.41	0.54
1:N:357:THR:O	1:N:361:ILE:HG13	2.08	0.54
2:n:13:VAL:HG22	2:n:115:THR:HB	1.90	0.54
2:n:167:VAL:HG13	2:n:224:VAL:HG22	1.89	0.54
2:o:20:VAL:CG1	2:o:88:LEU:CD1	2.68	0.54
1:R:66:GLU:HG3	1:R:89:GLN:HE21	1.72	0.54
1:E:320:MET:HB2	1:E:325:SER:HB3	1.89	0.53
1:F:33:ASN:ND2	1:F:56:TYR:OH	2.28	0.53
2:k:55:PRO:O	2:k:74:ARG:NE	2.41	0.53
1:M:203:LYS:HZ2	1:M:204:LYS:HB2	1.73	0.53
1:O:99:ASP:C	1:O:101:SER:H	2.16	0.53
2:q:182:LEU:HB3	2:q:188:ARG:CZ	2.38	0.53
2:c:166:TYR:HD1	2:c:185:ASN:ND2	2.06	0.53
1:D:204:LYS:N	1:D:204:LYS:HD2	2.24	0.53
1:I:182:MET:HE1	1:I:237:PHE:CD2	2.42	0.53
2:j:31:PHE:HE1	2:j:36:ILE:HD12	1.73	0.53
1:L:43:LEU:HD11	1:L:56:TYR:HD2	1.72	0.53
2:l:35:GLY:HA3	2:l:52:TRP:HZ3	1.74	0.53
2:l:96:TYR:HE2	2:l:114:VAL:HB	1.73	0.53
1:M:291:ILE:O	1:M:295:LEU:HG	2.08	0.53
1:O:298:GLU:HG3	1:O:299:VAL:H	1.71	0.53
1:R:34:TRP:HZ2	1:R:62:ASN:OD1	1.90	0.53
1:R:200:LYS:HE3	1:R:203:LYS:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:207:GLU:HA	1:R:210:THR:OG1	2.09	0.53
1:R:284:ALA:O	1:R:288:TYR:HD1	1.91	0.53
1:A:323:SER:HB3	2:a:225:TRP:CZ3	2.44	0.53
2:e:12:GLU:OE2	2:e:14:LYS:HE2	2.08	0.53
2:f:20:VAL:CG1	2:f:88:LEU:HD11	2.38	0.53
2:j:157:GLY:O	2:j:203:PRO:HB2	2.09	0.53
1:L:297:PRO:O	1:L:299:VAL:N	2.41	0.53
2:n:214:THR:HA	2:n:242:VAL:CG2	2.38	0.53
1:Q:357:THR:O	1:Q:360:ARG:HB2	2.09	0.53
1:R:355:THR:O	1:R:359:THR:OG1	2.24	0.53
2:r:200:LYS:HD2	2:r:205:THR:CB	2.38	0.53
1:C:233:ILE:HD12	1:C:236:ALA:HB2	1.89	0.53
1:I:266:GLU:CD	1:I:266:GLU:H	2.16	0.53
1:K:66:GLU:O	1:K:70:VAL:HG12	2.09	0.53
1:L:33:ASN:O	1:L:58:VAL:HA	2.08	0.53
2:n:235:GLY:O	2:n:237:GLY:N	2.41	0.53
1:O:250:ALA:HB1	1:O:257:ILE:HB	1.91	0.53
2:o:164:ARG:HG2	2:o:165:ASN:OD1	2.09	0.53
1:A:34:TRP:CE3	4:A:404:SPD:H42	2.43	0.53
1:B:34:TRP:HA	1:B:59:PHE:O	2.09	0.53
1:B:207:GLU:O	1:B:211:LYS:HB2	2.08	0.53
2:k:43:PRO:HD3	2:k:93:THR:O	2.08	0.53
2:k:118:SER:N	2:p:118:SER:HA	2.23	0.53
2:k:196:PHE:HA	2:k:209:ILE:HG22	1.89	0.53
2:m:42:ALA:HB1	2:m:43:PRO:HD2	1.91	0.53
2:m:217:GLU:HA	2:m:240:LEU:O	2.08	0.53
2:n:6:LEU:HG	2:n:26:VAL:HG23	1.90	0.53
1:O:71:SER:O	1:O:71:SER:OG	2.25	0.53
1:P:304:SER:O	1:P:324:VAL:HG11	2.08	0.53
2:a:164:ARG:HG2	2:a:165:ASN:OD1	2.08	0.53
1:B:323:SER:HB3	2:b:225:TRP:HE1	1.73	0.53
2:c:20:VAL:HG11	2:c:114:VAL:HG21	1.91	0.53
1:E:156:TRP:CE2	1:E:264:PRO:HG2	2.43	0.53
2:e:167:VAL:HA	2:e:224:VAL:HG12	1.90	0.53
2:f:158:SER:OG	2:f:159:SER:N	2.42	0.53
2:h:3:GLN:CG	2:h:4:VAL:H	2.06	0.53
2:h:69:ARG:CD	2:h:87:ARG:HB2	2.37	0.53
1:Q:176:MET:HE1	1:Q:239:TYR:CE2	2.43	0.53
1:B:200:LYS:HA	1:B:203:LYS:HB2	1.90	0.53
1:B:243:VAL:HG11	1:B:261:TYR:HB2	1.91	0.53
2:g:162:ILE:HD13	2:g:205:THR:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:6:LEU:HD23	2:j:24:CYS:SG	2.48	0.53
1:L:90:ILE:C	1:L:92:ALA:H	2.17	0.53
1:M:63:GLU:OE1	1:M:63:GLU:N	2.42	0.53
2:n:41:GLN:HE22	2:n:172:GLN:HE22	1.56	0.53
1:Q:80:VAL:HG22	1:Q:275:MET:HG2	1.91	0.53
2:a:167:VAL:HG11	2:a:205:THR:HG21	1.90	0.53
2:b:19:SER:HA	2:b:85:LEU:O	2.08	0.53
1:C:182:MET:HE1	1:C:237:PHE:CG	2.43	0.53
2:g:207:LEU:HD12	2:g:208:ALA:H	1.73	0.53
2:g:225:TRP:CZ2	2:g:230:ARG:HA	2.43	0.53
1:I:37:TYR:OH	1:I:273:ASP:HB2	2.08	0.53
1:M:106:TRP:HA	1:M:109:LEU:HD12	1.90	0.53
1:R:200:LYS:HE3	1:R:203:LYS:CB	2.39	0.53
1:F:49:GLU:CD	1:F:296:ARG:HH22	2.17	0.53
1:F:74:SER:O	1:F:76:TYR:N	2.40	0.53
1:F:323:SER:HB3	2:f:225:TRP:HE1	1.74	0.53
2:g:17:GLY:HA2	2:g:87:ARG:CZ	2.39	0.53
2:j:26:VAL:CG2	2:j:79:SER:HB3	2.39	0.53
1:K:211:LYS:O	1:K:214:PRO:HD2	2.08	0.53
2:l:97:TYR:CG	2:l:108:TRP:HD1	2.27	0.53
1:N:77:ASP:CG	1:N:283:ALA:HB3	2.34	0.53
1:O:38:ILE:N	1:O:307:VAL:HG11	2.24	0.53
1:O:102:LYS:HG2	1:O:288:TYR:CG	2.44	0.53
2:p:149:GLN:HG2	2:p:150:LYS:H	1.74	0.53
2:p:167:VAL:HG11	2:p:205:THR:HG21	1.90	0.53
1:D:210:THR:HG23	1:D:361:ILE:HG12	1.90	0.53
1:J:106:TRP:CZ3	1:J:128:VAL:HG22	2.42	0.53
1:K:32:TYR:HB3	1:K:79:VAL:HG12	1.91	0.53
2:k:154:SER:CB	2:k:206:THR:HG22	2.38	0.53
2:l:158:SER:OG	2:l:159:SER:N	2.42	0.53
1:M:154:ASP:O	1:M:265:LYS:N	2.40	0.53
1:M:298:GLU:HG2	2:m:56:ASN:HD21	1.73	0.53
1:N:34:TRP:HB3	4:N:407:SPD:H22	1.91	0.53
2:n:3:GLN:HG2	2:n:4:VAL:HG12	1.90	0.53
2:o:195:ARG:O	2:o:210:THR:HG23	2.09	0.53
1:P:98:LEU:HD23	1:P:288:TYR:CE1	2.40	0.53
1:Q:203:LYS:HG3	1:Q:206:GLU:OE2	2.09	0.53
2:q:184:ASP:O	2:q:185:ASN:HB2	2.08	0.53
2:q:193:PRO:HG2	2:q:196:PHE:CD2	2.44	0.53
1:R:283:ALA:HB1	1:R:286:ASN:HB2	1.91	0.53
1:B:176:MET:HA	1:B:220:HIS:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:140:PRO:O	2:b:238:THR:HB	2.09	0.52
1:E:144:VAL:O	1:E:148:LEU:HB2	2.09	0.52
1:I:296:ARG:HB2	1:I:299:VAL:HG23	1.92	0.52
2:l:139:GLN:OE1	2:l:235:GLY:HA3	2.09	0.52
2:n:17:GLY:O	2:n:18:ALA:C	2.52	0.52
1:O:33:ASN:O	1:O:58:VAL:HA	2.09	0.52
1:O:62:ASN:HD21	1:O:82:SER:HB2	1.73	0.52
1:O:352:ARG:NH2	3:O:406:SO4:O3	2.38	0.52
1:Q:60:ASP:HB2	1:Q:222:SER:HB3	1.90	0.52
1:Q:139:TYR:HB2	1:Q:144:VAL:HG21	1.92	0.52
1:Q:159:LEU:HA	1:Q:165:MET:SD	2.48	0.52
2:q:195:ARG:NH1	2:q:213:GLN:OE1	2.42	0.52
1:R:200:LYS:HA	1:R:203:LYS:HB3	1.91	0.52
2:b:161:ASN:OD1	2:b:162:ILE:N	2.37	0.52
1:E:154:ASP:O	1:E:265:LYS:N	2.43	0.52
1:E:239:TYR:CE1	4:E:405:SPD:H81	2.45	0.52
1:K:183:LEU:O	1:K:187:LEU:HG	2.09	0.52
1:L:37:TYR:CZ	1:L:131:LEU:HG	2.43	0.52
1:L:43:LEU:HD11	1:L:56:TYR:CD2	2.44	0.52
1:N:220:HIS:CG	1:N:223:LYS:HG2	2.44	0.52
1:R:80:VAL:HA	1:R:274:LEU:O	2.09	0.52
2:b:226:ASP:HB3	2:b:229:LEU:HB2	1.91	0.52
2:d:195:ARG:O	2:d:210:THR:HG23	2.09	0.52
1:G:207:GLU:O	1:G:211:LYS:HB2	2.09	0.52
1:N:251:GLU:HG3	1:N:252:GLU:N	2.24	0.52
1:Q:189:TYR:O	1:Q:191:GLY:N	2.43	0.52
1:R:204:LYS:O	1:R:208:VAL:HG23	2.08	0.52
2:r:58:GLY:HA3	2:r:74:ARG:NH1	2.24	0.52
1:F:99:ASP:OD2	1:F:102:LYS:HG3	2.10	0.52
1:H:356:ARG:NE	3:H:401:SO4:O1	2.42	0.52
2:l:39:VAL:HG13	2:l:97:TYR:HB2	1.91	0.52
2:l:162:ILE:CG1	2:l:224:VAL:HG21	2.39	0.52
2:l:170:TYR:HH	2:l:234:PHE:HE1	1.57	0.52
1:M:203:LYS:CG	1:M:204:LYS:N	2.69	0.52
2:i:78:ILE:HG13	2:i:80:THR:HG23	1.90	0.52
2:j:43:PRO:HD3	2:j:93:THR:O	2.10	0.52
2:l:100:ARG:NE	2:l:106:ASP:OD2	2.39	0.52
1:Q:207:GLU:HA	1:Q:210:THR:OG1	2.09	0.52
2:a:14:LYS:O	2:a:116:VAL:HA	2.10	0.52
1:E:102:LYS:NZ	1:E:285:ASP:OD1	2.42	0.52
1:E:143:LYS:O	1:E:147:VAL:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:32:THR:HA	2:e:55:PRO:HB2	1.92	0.52
1:F:45:ASP:OD2	1:F:302:LYS:NZ	2.42	0.52
2:i:19:SER:HA	2:i:85:LEU:O	2.08	0.52
1:M:349:LYS:NZ	3:M:402:SO4:O1	2.37	0.52
1:N:34:TRP:CD2	4:N:407:SPD:H42	2.44	0.52
1:O:155:SER:O	1:O:158:ILE:HG12	2.09	0.52
2:o:167:VAL:HG11	2:o:205:THR:HG21	1.90	0.52
1:Q:233:ILE:HD12	1:Q:236:ALA:HB2	1.92	0.52
2:r:198:ALA:HB2	2:r:207:LEU:HA	1.90	0.52
2:d:150:LYS:HB2	2:d:210:THR:HA	1.92	0.52
1:F:66:GLU:O	1:F:70:VAL:HG12	2.10	0.52
2:h:18:ALA:HB3	2:h:87:ARG:HA	1.83	0.52
1:J:187:LEU:HD21	1:J:205:ALA:HB2	1.90	0.52
1:J:199:PRO:HA	1:J:353:LEU:HD21	1.92	0.52
2:k:118:SER:N	2:p:118:SER:CA	2.73	0.52
2:l:139:GLN:NE2	2:l:238:THR:OG1	2.42	0.52
2:m:95:VAL:HG12	2:m:111:GLY:HA3	1.91	0.52
1:R:170:LYS:HZ1	1:R:234:CYS:HB3	1.74	0.52
2:r:150:LYS:HG2	2:r:151:VAL:N	2.25	0.52
2:c:88:LEU:HB3	2:c:116:VAL:HG11	1.92	0.52
1:E:266:GLU:H	1:E:266:GLU:CD	2.15	0.52
1:I:161:GLU:OE2	1:I:189:TYR:OH	2.28	0.52
1:J:198:ASP:HB3	1:J:201:ASP:HB2	1.92	0.52
2:q:100:ARG:HB3	2:q:107:VAL:HG13	1.92	0.52
2:r:104:TYR:CE1	2:r:183:TYR:CD1	2.98	0.52
1:C:33:ASN:OD1	1:C:34:TRP:N	2.35	0.52
2:c:153:ILE:CG2	2:c:238:THR:HG21	2.38	0.52
2:f:137:LEU:HD11	2:f:233:LEU:HB3	1.91	0.52
1:G:78:ILE:HG13	1:G:287:ALA:HB1	1.91	0.52
1:J:182:MET:HG3	1:J:358:TRP:CH2	2.45	0.52
1:K:182:MET:HE1	1:K:237:PHE:CG	2.45	0.52
2:k:199:SER:HB2	2:k:206:THR:OG1	2.09	0.52
2:l:73:THR:CG2	2:l:82:TYR:HB2	2.40	0.52
2:o:14:LYS:O	2:o:116:VAL:HA	2.10	0.52
2:o:149:GLN:HG2	2:o:150:LYS:H	1.74	0.52
2:p:140:PRO:C	2:p:238:THR:HG23	2.35	0.52
2:p:164:ARG:HG2	2:p:165:ASN:OD1	2.09	0.52
1:R:132:TRP:HA	1:R:271:TRP:CZ3	2.45	0.52
2:r:188:ARG:HD3	2:r:192:ILE:O	2.09	0.52
2:a:195:ARG:O	2:a:210:THR:HG23	2.09	0.52
1:G:173:VAL:HG13	1:G:235:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:212:LEU:HD12	2:g:242:VAL:CG1	2.40	0.52
1:I:33:ASN:O	1:I:58:VAL:HA	2.09	0.52
1:K:152:PRO:O	1:K:154:ASP:N	2.42	0.52
1:P:344:ALA:O	1:P:346:LEU:HD12	2.09	0.52
2:a:140:PRO:C	2:a:238:THR:HG23	2.35	0.51
1:B:91:GLN:O	1:G:356:ARG:NH1	2.43	0.51
2:c:21:LYS:HA	2:c:83:MET:O	2.10	0.51
1:G:86:LEU:HD21	1:G:121:ASP:HB2	1.91	0.51
2:h:195:ARG:HD2	2:h:211:GLY:HA3	1.92	0.51
2:i:4:VAL:HG21	2:i:100:ARG:NH1	2.25	0.51
1:J:213:ARG:NH1	1:J:213:ARG:CG	2.72	0.51
2:j:185:ASN:OD1	2:j:200:LYS:HD2	2.10	0.51
1:N:151:GLN:OE1	2:o:140:PRO:HA	2.10	0.51
1:O:207:GLU:HA	1:O:210:THR:OG1	2.10	0.51
1:O:349:LYS:HA	1:O:352:ARG:NH1	2.26	0.51
1:O:359:THR:O	1:O:362:LYS:HG3	2.10	0.51
2:p:195:ARG:O	2:p:210:THR:HG23	2.09	0.51
1:C:182:MET:HE1	1:C:237:PHE:CD1	2.45	0.51
2:c:189:PRO:O	2:c:191:GLY:N	2.43	0.51
1:E:136:GLY:HA2	1:E:156:TRP:CH2	2.46	0.51
1:E:170:LYS:HD3	1:E:170:LYS:N	2.25	0.51
1:G:43:LEU:HD11	1:G:56:TYR:CD1	2.46	0.51
2:g:167:VAL:HG22	2:g:224:VAL:HG11	1.92	0.51
1:H:88:LYS:HG3	1:H:345:VAL:CG1	2.39	0.51
1:H:147:VAL:HG22	1:H:148:LEU:HD13	1.93	0.51
1:J:139:TYR:CE2	1:J:141:VAL:HG22	2.45	0.51
1:J:187:LEU:CD2	1:J:205:ALA:HB2	2.41	0.51
2:k:6:LEU:HD23	2:k:24:CYS:SG	2.50	0.51
1:O:102:LYS:HZ3	1:O:103:LEU:CG	2.23	0.51
2:p:14:LYS:O	2:p:116:VAL:HA	2.10	0.51
2:q:106:ASP:HA	2:q:180:LEU:HD22	1.93	0.51
1:R:97:LYS:HG2	1:R:126:TYR:HE1	1.75	0.51
1:B:70:VAL:CG1	1:G:67:GLY:HA2	2.41	0.51
1:C:239:TYR:CE1	4:C:404:SPD:H71	2.44	0.51
1:D:213:ARG:HH12	1:D:361:ILE:HA	1.74	0.51
2:d:83:MET:HE3	2:d:85:LEU:N	2.25	0.51
2:h:225:TRP:CH2	2:h:230:ARG:CA	2.75	0.51
1:I:200:LYS:C	1:I:202:TYR:N	2.67	0.51
2:i:15:THR:O	2:i:18:ALA:CB	2.53	0.51
2:q:169:TRP:CZ2	2:q:205:THR:CG2	2.93	0.51
2:q:193:PRO:HG2	2:q:196:PHE:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:14:LYS:C	2:r:15:THR:CG2	2.83	0.51
2:r:19:SER:HA	2:r:86:SER:HA	1.92	0.51
1:B:154:ASP:O	1:B:265:LYS:HG3	2.11	0.51
2:e:14:LYS:O	2:e:116:VAL:HA	2.11	0.51
2:h:15:THR:C	2:h:17:GLY:H	2.12	0.51
1:L:35:THR:C	1:L:37:TYR:N	2.60	0.51
1:N:291:ILE:O	1:N:295:LEU:HG	2.09	0.51
2:o:140:PRO:C	2:o:238:THR:HG23	2.35	0.51
2:q:99:ALA:HB1	2:q:105:MET:HB3	1.91	0.51
1:R:170:LYS:CE	1:R:171:CYS:H	2.23	0.51
1:R:323:SER:HB3	2:r:225:TRP:CZ3	2.44	0.51
2:r:161:ASN:HB2	2:r:224:VAL:CG2	2.40	0.51
2:d:9:THR:HG1	2:d:23:SER:H	1.56	0.51
1:H:156:TRP:CE2	1:H:264:PRO:HG2	2.46	0.51
1:I:136:GLY:HA2	1:I:156:TRP:CH2	2.45	0.51
1:I:328:GLU:HG2	2:i:166:TYR:CE1	2.45	0.51
2:i:49:TRP:CD1	2:i:232:VAL:H	2.28	0.51
1:J:159:LEU:HA	1:J:165:MET:CE	2.40	0.51
2:j:75:ASP:OD1	2:j:77:SER:HB3	2.10	0.51
2:m:38:TRP:CZ3	2:m:98:CYS:HB2	2.45	0.51
1:N:168:LEU:HD13	1:N:235:VAL:HG11	1.93	0.51
1:B:34:TRP:CD2	4:B:405:SPD:H42	2.45	0.51
1:C:33:ASN:O	1:C:58:VAL:HA	2.09	0.51
1:D:206:GLU:CD	1:D:360:ARG:HH21	2.19	0.51
2:h:69:ARG:NH1	2:h:87:ARG:O	2.43	0.51
2:m:166:TYR:HD1	2:m:185:ASN:HD22	1.58	0.51
1:O:271:TRP:CG	4:O:407:SPD:H91	2.46	0.51
1:Q:63:GLU:O	1:Q:65:LEU:N	2.44	0.51
1:Q:121:ASP:OD2	1:Q:124:ASN:HA	2.11	0.51
2:q:21:LYS:HG3	2:q:84:GLU:HB2	1.92	0.51
2:r:168:SER:HB2	2:r:170:TYR:CE2	2.46	0.51
1:A:224:TYR:O	1:A:228:LEU:N	2.41	0.51
2:a:149:GLN:HG2	2:a:150:LYS:H	1.74	0.51
2:c:161:ASN:HB2	2:c:224:VAL:CG2	2.40	0.51
2:e:154:SER:HB2	2:e:206:THR:HG22	1.92	0.51
2:g:223:GLY:HA2	2:g:233:LEU:O	2.11	0.51
1:I:183:LEU:HD12	1:I:354:GLN:HG3	1.92	0.51
2:l:169:TRP:CH2	2:l:222:CYS:HB3	2.45	0.51
2:l:171:GLN:H	2:l:181:LEU:CD1	2.24	0.51
1:M:199:PRO:C	1:M:201:ASP:H	2.19	0.51
1:P:77:ASP:OD2	1:P:283:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:322:LYS:HD3	2:r:225:TRP:NE1	2.25	0.51
2:r:217:GLU:HG3	2:r:241:THR:HA	1.92	0.51
1:A:357:THR:O	1:A:361:ILE:HG13	2.10	0.51
2:h:184:ASP:O	2:h:185:ASN:HB2	2.10	0.51
2:i:16:PRO:C	2:i:18:ALA:H	2.18	0.51
2:i:225:TRP:HD1	2:i:232:VAL:HG22	1.76	0.51
2:l:225:TRP:HZ3	2:l:227:SER:HA	1.76	0.51
1:Q:62:ASN:HB3	1:Q:85:PHE:CE1	2.46	0.51
1:R:173:VAL:HG22	1:R:235:VAL:CG1	2.39	0.51
1:C:206:GLU:CD	1:C:360:ARG:HH21	2.18	0.51
2:c:51:GLY:C	2:c:72:MET:HE1	2.36	0.51
1:G:275:MET:HE1	1:G:294:LEU:HD12	1.93	0.51
2:h:100:ARG:HB3	2:h:107:VAL:HG13	1.92	0.51
2:i:212:LEU:HD21	2:i:240:LEU:HD21	1.92	0.51
1:K:147:VAL:HG21	1:K:170:LYS:HG3	1.92	0.51
1:L:106:TRP:HA	1:L:295:LEU:HD13	1.92	0.51
1:L:228:LEU:HD22	1:L:259:ILE:HD12	1.92	0.51
2:l:29:TYR:HB3	2:l:100:ARG:HH11	1.75	0.51
2:l:68:GLY:O	2:l:69:ARG:HG3	2.11	0.51
1:N:182:MET:HE1	1:N:237:PHE:CD2	2.45	0.51
1:N:230:ASN:O	1:N:230:ASN:ND2	2.33	0.51
1:N:356:ARG:HD2	3:N:404:SO4:O3	2.11	0.51
2:n:85:LEU:HD12	2:n:88:LEU:CD2	2.41	0.51
1:O:346:LEU:HD13	1:O:350:VAL:HG11	1.93	0.51
2:o:162:ILE:O	2:o:200:LYS:HE3	2.11	0.51
1:R:150:ASP:OD1	1:R:150:ASP:N	2.37	0.51
2:c:16:PRO:O	2:c:16:PRO:HG2	2.11	0.51
2:e:38:TRP:CZ3	2:e:98:CYS:HB2	2.46	0.51
1:H:348:ALA:O	1:H:352:ARG:HG3	2.11	0.51
2:h:18:ALA:HA	2:h:88:LEU:HB2	1.93	0.51
1:I:184:PRO:HA	1:I:187:LEU:HG	1.93	0.51
1:L:134:THR:H	1:L:240:SER:HB3	1.76	0.51
2:n:18:ALA:N	2:n:88:LEU:H	2.09	0.51
2:n:161:ASN:HA	2:n:226:ASP:HA	1.93	0.51
1:O:33:ASN:HA	1:O:80:VAL:CG2	2.40	0.51
1:O:225:ILE:HD11	1:O:242:ASP:CG	2.36	0.51
1:Q:350:VAL:O	1:Q:353:LEU:HG	2.11	0.51
1:R:359:THR:O	1:R:362:LYS:HB2	2.11	0.51
1:A:203:LYS:NZ	1:A:207:GLU:OE1	2.41	0.50
1:D:207:GLU:HA	1:D:210:THR:OG1	2.11	0.50
1:D:317:ARG:HD2	1:D:331:TYR:CE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:ILE:HG21	1:F:313:ILE:HB	1.94	0.50
2:i:117:SER:CB	2:o:117:SER:HG	2.20	0.50
2:i:137:LEU:HD11	2:i:233:LEU:HB3	1.92	0.50
2:i:166:TYR:HD2	2:i:184:ASP:HA	1.75	0.50
1:K:328:GLU:O	1:K:332:PRO:HA	2.11	0.50
2:l:17:GLY:H	2:l:88:LEU:HB2	0.69	0.50
2:l:173:LEU:HA	2:l:218:ALA:CB	2.41	0.50
1:N:159:LEU:HA	1:N:165:MET:SD	2.51	0.50
1:N:317:ARG:NH2	1:N:325:SER:O	2.32	0.50
1:O:131:LEU:HD13	1:O:309:TYR:HB2	1.93	0.50
1:F:137:ILE:HB	1:F:262:VAL:HG13	1.92	0.50
2:g:71:THR:HB	2:g:84:GLU:HB3	1.91	0.50
1:L:225:ILE:HD11	1:L:242:ASP:CG	2.36	0.50
2:l:69:ARG:CG	2:l:86:SER:HB3	2.37	0.50
2:m:50:MET:HE1	2:m:85:LEU:HD12	1.93	0.50
1:P:291:ILE:O	1:P:295:LEU:HG	2.11	0.50
2:p:162:ILE:O	2:p:200:LYS:HE3	2.11	0.50
1:R:197:HIS:HD2	1:R:347:PRO:HG2	1.77	0.50
2:c:21:LYS:HE3	2:c:84:GLU:OE2	2.11	0.50
1:E:70:VAL:HG13	1:H:67:GLY:HA2	1.94	0.50
1:I:200:LYS:C	1:I:202:TYR:H	2.18	0.50
1:J:37:TYR:OH	1:J:273:ASP:HB2	2.11	0.50
1:K:296:ARG:HB2	1:K:299:VAL:HG23	1.92	0.50
2:n:12:GLU:O	2:n:13:VAL:HG23	2.10	0.50
1:R:271:TRP:CG	4:R:404:SPD:H91	2.47	0.50
1:A:240:SER:HA	1:A:261:TYR:CZ	2.46	0.50
2:a:69:ARG:HG2	2:a:87:ARG:NH1	2.27	0.50
2:a:162:ILE:O	2:a:200:LYS:HE3	2.11	0.50
1:B:134:THR:O	1:B:240:SER:N	2.40	0.50
2:b:195:ARG:O	2:b:210:THR:HG23	2.12	0.50
2:e:101:ASP:C	2:e:103:ARG:H	2.19	0.50
1:G:141:VAL:HG12	1:G:258:ASP:HB3	1.93	0.50
2:g:55:PRO:HA	2:g:74:ARG:CD	2.39	0.50
2:g:158:SER:C	2:g:160:SER:H	2.20	0.50
2:g:226:ASP:OD2	2:g:229:LEU:HB2	2.11	0.50
2:h:93:THR:OG1	2:h:116:VAL:HG22	2.11	0.50
2:i:26:VAL:CG2	2:i:26:VAL:C	2.85	0.50
2:j:161:ASN:OD1	2:j:162:ILE:N	2.44	0.50
2:l:85:LEU:HD23	2:l:86:SER:N	2.26	0.50
2:l:85:LEU:HD23	2:l:86:SER:H	1.75	0.50
1:O:171:CYS:HB3	1:O:234:CYS:SG	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:317:ARG:HB2	1:P:318:PRO:HD3	1.93	0.50
1:Q:227:ASP:HB3	1:Q:233:ILE:HG23	1.93	0.50
1:R:34:TRP:CE3	4:R:404:SPD:H42	2.47	0.50
1:R:98:LEU:N	1:R:125:GLN:OE1	2.45	0.50
2:c:219:ASP:OD2	2:c:239:LYS:HG2	2.12	0.50
1:F:67:GLY:HA2	1:M:70:VAL:CG1	2.41	0.50
2:f:9:THR:HG23	2:f:23:SER:HB2	1.92	0.50
2:g:11:ASP:HA	2:g:112:THR:HG23	1.94	0.50
1:H:337:LEU:C	1:H:339:LYS:H	2.20	0.50
1:K:161:GLU:OE2	1:K:189:TYR:OH	2.29	0.50
1:K:200:LYS:HZ2	1:K:203:LYS:HD2	1.77	0.50
2:k:162:ILE:HG12	2:k:224:VAL:HG11	1.93	0.50
2:k:217:GLU:HG3	2:k:241:THR:HA	1.94	0.50
1:L:33:ASN:ND2	1:L:80:VAL:HG21	2.27	0.50
1:L:250:ALA:HB1	1:L:257:ILE:HB	1.92	0.50
1:L:328:GLU:O	1:L:332:PRO:HA	2.12	0.50
1:M:207:GLU:HA	1:M:210:THR:HG22	1.94	0.50
1:N:220:HIS:CD2	1:N:223:LYS:NZ	2.80	0.50
1:P:333:PRO:CD	2:p:166:TYR:OH	2.59	0.50
2:p:20:VAL:CG1	2:p:88:LEU:CD1	2.68	0.50
1:Q:154:ASP:O	1:Q:265:LYS:N	2.41	0.50
1:A:225:ILE:HD11	1:A:242:ASP:CG	2.37	0.50
1:E:170:LYS:HD3	1:E:171:CYS:H	1.77	0.50
1:I:226:SER:O	1:I:230:ASN:ND2	2.41	0.50
2:i:75:ASP:OD1	2:i:77:SER:HB3	2.12	0.50
1:P:337:LEU:HD23	1:P:340:LEU:HD12	1.94	0.50
2:p:69:ARG:HG2	2:p:87:ARG:NH1	2.27	0.50
2:r:162:ILE:HD13	2:r:205:THR:HG22	1.92	0.50
1:A:33:ASN:O	1:A:58:VAL:HA	2.11	0.50
1:A:193:ASP:HB3	1:A:196:THR:HB	1.92	0.50
1:C:230:ASN:OD1	1:C:232:ASN:N	2.43	0.50
2:e:99:ALA:HB1	2:e:105:MET:HB3	1.94	0.50
2:f:16:PRO:CD	2:f:117:SER:O	2.59	0.50
1:G:78:ILE:HD11	1:G:291:ILE:HG13	1.94	0.50
1:I:117:LEU:HD13	1:I:274:LEU:HD21	1.92	0.50
2:j:93:THR:HG23	2:j:115:THR:HA	1.93	0.50
1:L:244:PHE:HZ	1:L:329:GLU:OE1	1.95	0.50
1:N:197:HIS:HA	1:N:350:VAL:HG11	1.94	0.50
1:O:330:VAL:O	1:O:332:PRO:HD3	2.12	0.50
2:o:69:ARG:HG2	2:o:87:ARG:NH1	2.27	0.50
1:P:83:ASN:HB3	1:P:272:PHE:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:317:ARG:NH2	1:Q:325:SER:O	2.41	0.50
1:B:32:TYR:OH	1:B:59:PHE:HB3	2.11	0.50
2:b:18:ALA:HB3	2:b:87:ARG:HA	1.88	0.50
1:C:109:LEU:HD13	1:C:114:LEU:HD21	1.93	0.50
1:H:33:ASN:O	1:H:58:VAL:HA	2.11	0.50
2:i:182:LEU:HD21	2:i:188:ARG:HG2	1.94	0.50
2:l:89:ARG:HG3	2:l:91:ASP:H	1.75	0.50
2:n:224:VAL:O	2:n:232:VAL:HA	2.11	0.50
1:O:176:MET:HE3	1:O:238:GLY:HA2	1.93	0.50
2:o:54:ASN:ND2	2:o:57:SER:OG	2.45	0.50
1:P:323:SER:HG	2:p:225:TRP:HZ3	1.42	0.50
1:Q:83:ASN:OD1	1:Q:83:ASN:N	2.45	0.50
1:R:121:ASP:OD2	1:R:124:ASN:HA	2.12	0.50
1:R:322:LYS:HB2	2:r:225:TRP:CE2	2.47	0.50
1:A:179:GLY:O	1:A:183:LEU:HB2	2.12	0.50
1:B:32:TYR:HD2	1:B:65:LEU:HD13	1.77	0.50
2:b:153:ILE:CG2	2:b:238:THR:HG21	2.42	0.50
2:g:68:GLY:CA	2:i:21:LYS:CE	2.71	0.50
2:g:102:LYS:O	2:g:103:ARG:HB2	2.12	0.50
2:h:147:PRO:HD3	2:h:243:LEU:C	2.37	0.50
2:j:37:SER:HB3	2:j:49:TRP:HZ3	1.75	0.50
1:K:170:LYS:HG2	1:K:171:CYS:SG	2.51	0.50
2:k:195:ARG:HB3	2:k:210:THR:H	1.76	0.50
1:L:326:ASP:O	1:L:328:GLU:N	2.45	0.50
2:l:8:GLU:OE2	2:l:24:CYS:N	2.45	0.50
1:N:125:GLN:HG3	1:N:126:TYR:CD1	2.46	0.50
2:p:54:ASN:ND2	2:p:57:SER:OG	2.45	0.50
2:c:167:VAL:H	2:c:185:ASN:ND2	2.09	0.49
1:G:135:ASN:CG	1:G:269:ASN:HB3	2.37	0.49
1:K:162:PRO:HD2	1:K:163:GLU:OE2	2.12	0.49
2:k:117:SER:CB	2:p:118:SER:O	2.60	0.49
1:L:300:ILE:HG21	1:L:313:ILE:HG13	1.94	0.49
2:l:89:ARG:HE	2:l:91:ASP:HB2	1.76	0.49
1:M:203:LYS:NZ	1:M:205:ALA:N	2.59	0.49
2:o:173:LEU:HB3	2:o:174:PRO:HD2	1.94	0.49
1:Q:80:VAL:HA	1:Q:274:LEU:O	2.11	0.49
2:b:70:VAL:HB	2:b:85:LEU:HD22	1.94	0.49
2:c:184:ASP:O	2:c:185:ASN:HB2	2.12	0.49
1:E:330:VAL:HG12	1:E:331:TYR:CD1	2.47	0.49
2:f:160:SER:HB2	2:f:226:ASP:OD1	2.12	0.49
1:I:127:ALA:HB1	1:I:274:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:102:LYS:O	1:J:104:PRO:HD3	2.11	0.49
1:K:225:ILE:HD11	1:K:242:ASP:CG	2.37	0.49
2:l:6:LEU:O	2:l:7:VAL:HG13	2.12	0.49
1:O:44:LYS:HE2	1:O:47:THR:HG21	1.95	0.49
2:q:214:THR:HG22	2:q:242:VAL:HG11	1.94	0.49
1:E:169:ALA:HB2	1:E:215:TYR:CB	2.38	0.49
1:G:109:LEU:HB3	1:G:114:LEU:HD11	1.94	0.49
2:g:20:VAL:CG2	2:g:88:LEU:HD21	2.34	0.49
1:H:176:MET:HB2	1:H:182:MET:HE3	1.93	0.49
1:J:155:SER:O	1:J:158:ILE:HG12	2.13	0.49
1:K:206:GLU:HG3	1:K:210:THR:HG23	1.94	0.49
1:L:32:TYR:HB3	1:L:79:VAL:HG12	1.92	0.49
2:l:98:CYS:O	2:l:108:TRP:HA	2.12	0.49
2:l:215:GLY:O	2:l:217:GLU:N	2.45	0.49
1:M:286:ASN:O	1:M:289:ALA:N	2.42	0.49
2:n:162:ILE:HA	2:n:224:VAL:HG11	1.94	0.49
1:O:93:GLY:O	1:O:95:PHE:N	2.45	0.49
1:A:168:LEU:HD13	1:A:235:VAL:HG11	1.93	0.49
1:B:176:MET:HG3	1:B:237:PHE:CD1	2.47	0.49
1:C:213:ARG:HH11	1:C:361:ILE:HA	1.73	0.49
2:c:49:TRP:CD1	2:c:232:VAL:H	2.31	0.49
2:c:66:PHE:C	2:c:70:VAL:HG12	2.36	0.49
2:h:89:ARG:C	2:h:116:VAL:HG21	2.38	0.49
2:h:185:ASN:HD21	2:h:200:LYS:HZ3	1.59	0.49
1:M:137:ILE:HG12	1:M:159:LEU:HD11	1.94	0.49
2:m:34:TYR:CE1	2:m:102:LYS:HE3	2.47	0.49
1:O:103:LEU:HD23	1:O:292:ASP:OD2	2.12	0.49
1:P:196:THR:HG21	1:P:201:ASP:OD2	2.13	0.49
1:R:155:SER:HB2	1:R:265:LYS:HD3	1.94	0.49
1:B:159:LEU:HA	1:B:165:MET:SD	2.52	0.49
2:b:142:SER:OG	1:M:163:GLU:CD	2.56	0.49
2:d:103:ARG:NH2	2:d:184:ASP:OD1	2.44	0.49
1:E:112:ALA:HA	1:E:115:LYS:HE3	1.93	0.49
1:E:271:TRP:CD2	4:E:405:SPD:H82	2.47	0.49
1:M:239:TYR:CZ	4:M:404:SPD:H82	2.47	0.49
1:O:111:PRO:O	1:O:115:LYS:HG3	2.12	0.49
1:O:352:ARG:NH2	3:O:406:SO4:O4	2.44	0.49
1:Q:202:TYR:C	1:Q:204:LYS:H	2.20	0.49
1:R:160:PHE:HA	1:R:212:VAL:HG11	1.94	0.49
2:r:167:VAL:HG22	2:r:224:VAL:HG12	1.95	0.49
1:B:155:SER:HB2	1:B:265:LYS:HZ3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:PRO:HA	1:B:353:LEU:HD21	1.95	0.49
2:f:20:VAL:O	2:f:20:VAL:HG22	2.13	0.49
1:H:176:MET:HE1	1:H:239:TYR:CD2	2.48	0.49
1:H:194:PRO:HG3	1:H:341:TYR:CG	2.48	0.49
1:J:296:ARG:HB2	1:J:299:VAL:HG23	1.94	0.49
2:j:26:VAL:HG22	2:j:79:SER:HB3	1.94	0.49
2:j:213:GLN:O	2:j:215:GLY:N	2.45	0.49
1:L:327:SER:O	1:L:330:VAL:N	2.40	0.49
2:m:16:PRO:O	2:m:16:PRO:HG2	2.13	0.49
2:m:188:ARG:HD2	2:m:192:ILE:HG22	1.93	0.49
2:n:117:SER:O	2:n:118:SER:HB2	2.11	0.49
2:o:189:PRO:HD2	2:o:192:ILE:HG13	1.95	0.49
1:P:266:GLU:CD	1:P:266:GLU:H	2.17	0.49
1:Q:144:VAL:O	1:Q:148:LEU:HB2	2.13	0.49
1:R:128:VAL:HG23	1:R:275:MET:HB2	1.94	0.49
1:A:200:LYS:O	1:A:203:LYS:HB3	2.12	0.49
2:a:86:SER:OG	2:f:12:GLU:OE2	2.27	0.49
1:F:171:CYS:HB3	1:F:234:CYS:HB3	1.94	0.49
2:h:20:VAL:HG21	2:h:88:LEU:HD11	1.88	0.49
2:i:138:THR:OG1	2:i:156:SER:HB2	2.13	0.49
2:i:212:LEU:CD2	2:i:240:LEU:HD21	2.43	0.49
1:J:60:ASP:HB2	1:J:222:SER:HB3	1.95	0.49
1:J:240:SER:OG	1:J:241:GLY:N	2.46	0.49
1:K:163:GLU:H	1:K:163:GLU:HG3	1.27	0.49
1:K:190:LEU:HD11	1:K:208:VAL:CG2	2.37	0.49
1:L:67:GLY:HA2	1:R:70:VAL:HG13	1.94	0.49
1:L:281:ALA:CB	1:L:284:ALA:HB2	2.42	0.49
1:M:190:LEU:HD21	1:M:208:VAL:HG21	1.94	0.49
2:n:140:PRO:HD2	2:n:154:SER:O	2.13	0.49
1:P:225:ILE:HD11	1:P:242:ASP:CG	2.37	0.49
1:P:233:ILE:HD12	1:P:236:ALA:HB2	1.95	0.49
1:R:63:GLU:O	1:R:66:GLU:N	2.46	0.49
1:R:234:CYS:SG	1:R:235:VAL:HG12	2.53	0.49
1:F:165:MET:HE1	1:F:173:VAL:HG11	1.94	0.49
2:j:101:ASP:OD1	2:j:103:ARG:N	2.45	0.49
1:M:172:GLY:HA3	1:M:233:ILE:HA	1.95	0.49
1:M:199:PRO:HA	1:M:353:LEU:HD21	1.93	0.49
1:R:39:ALA:HB3	1:R:42:THR:OG1	2.13	0.49
1:R:317:ARG:HD3	2:r:103:ARG:NH1	2.28	0.49
1:A:34:TRP:CD2	4:A:404:SPD:H42	2.48	0.49
2:b:35:GLY:HA2	2:b:55:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:243:LEU:HB3	1:M:204:LYS:CD	2.36	0.49
2:e:75:ASP:OD1	2:e:77:SER:HB3	2.13	0.49
1:G:325:SER:HB2	2:g:103:ARG:HD3	1.94	0.49
2:g:7:VAL:CG2	2:g:25:LYS:HB3	2.41	0.49
2:g:15:THR:HB	2:g:16:PRO:HD2	1.95	0.49
2:h:34:TYR:CE2	2:h:102:LYS:HD3	2.48	0.49
2:i:153:ILE:CG2	2:i:238:THR:HG21	2.42	0.49
1:K:206:GLU:O	1:K:210:THR:OG1	2.28	0.49
1:L:99:ASP:O	1:L:101:SER:N	2.46	0.49
2:m:225:TRP:HH2	2:m:230:ARG:NH1	2.11	0.49
1:P:326:ASP:HB3	2:p:165:ASN:HB3	1.94	0.49
2:p:37:SER:HB3	2:p:49:TRP:CZ3	2.47	0.49
2:r:89:ARG:NH1	2:r:91:ASP:HB2	2.28	0.49
2:a:54:ASN:ND2	2:a:57:SER:OG	2.45	0.49
2:b:29:TYR:CE1	2:b:31:PHE:HA	2.47	0.49
1:D:97:LYS:HE3	1:D:125:GLN:OE1	2.13	0.49
2:i:164:ARG:HG2	2:i:165:ASN:OD1	2.13	0.49
1:J:353:LEU:HD12	1:J:353:LEU:O	2.13	0.49
1:N:357:THR:HA	1:N:360:ARG:CD	2.40	0.49
1:O:37:TYR:CE2	4:O:407:SPD:H41	2.48	0.49
1:P:176:MET:HG3	1:P:237:PHE:CD1	2.47	0.49
1:Q:187:LEU:HD23	1:Q:205:ALA:HB2	1.94	0.49
1:Q:203:LYS:HA	1:Q:206:GLU:CD	2.38	0.49
2:q:224:VAL:HG23	2:q:225:TRP:N	2.28	0.49
1:R:182:MET:HE1	1:R:237:PHE:CG	2.47	0.49
1:R:233:ILE:HD12	1:R:236:ALA:HB2	1.94	0.49
1:B:207:GLU:HA	1:B:210:THR:HG1	1.77	0.48
2:d:143:VAL:HG23	2:d:240:LEU:HD12	1.94	0.48
1:F:67:GLY:HA3	1:M:71:SER:OG	2.13	0.48
1:F:225:ILE:HD11	1:F:242:ASP:OD2	2.13	0.48
2:g:3:GLN:OE1	2:g:4:VAL:HG12	2.13	0.48
1:H:239:TYR:CE1	4:H:403:SPD:H82	2.48	0.48
2:h:20:VAL:CG2	2:h:88:LEU:CD1	2.83	0.48
1:J:328:GLU:HG2	2:j:166:TYR:CE1	2.48	0.48
2:j:167:VAL:HG11	2:j:205:THR:HG21	1.94	0.48
1:N:190:LEU:O	2:o:146:ALA:HB2	2.11	0.48
1:Q:213:ARG:HD3	1:Q:361:ILE:CG2	2.39	0.48
1:R:125:GLN:OE1	1:R:125:GLN:O	2.31	0.48
1:R:242:ASP:OD1	1:R:309:TYR:OH	2.29	0.48
2:r:20:VAL:O	2:r:20:VAL:HG12	2.13	0.48
2:a:189:PRO:HD2	2:a:192:ILE:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:105:MET:O	2:e:170:TYR:HE2	1.96	0.48
1:G:357:THR:HG23	1:G:360:ARG:NH2	2.27	0.48
1:K:187:LEU:CD2	1:K:205:ALA:HB2	2.36	0.48
2:l:99:ALA:CB	2:l:105:MET:HB3	2.42	0.48
2:n:52:TRP:N	2:n:72:MET:HE1	2.27	0.48
2:b:9:THR:HB	2:b:23:SER:H	1.77	0.48
1:C:176:MET:HE1	1:C:239:TYR:CE2	2.48	0.48
1:F:259:ILE:O	1:F:260:GLN:HG2	2.12	0.48
1:G:203:LYS:O	1:G:207:GLU:HG3	2.13	0.48
2:k:182:LEU:HD23	2:k:188:ARG:HB3	1.95	0.48
2:l:13:VAL:HG13	2:l:14:LYS:N	2.28	0.48
1:M:220:HIS:CD2	1:M:223:LYS:HD3	2.48	0.48
1:N:156:TRP:NE1	1:N:267:GLY:O	2.43	0.48
2:n:18:ALA:H	2:n:88:LEU:H	1.60	0.48
2:n:31:PHE:HE1	2:n:36:ILE:HD11	1.77	0.48
1:P:43:LEU:HD11	1:P:56:TYR:CD1	2.47	0.48
2:a:20:VAL:CG1	2:a:88:LEU:CD1	2.67	0.48
2:b:137:LEU:HD12	2:b:137:LEU:H	1.77	0.48
2:c:26:VAL:HG21	2:c:31:PHE:CD1	2.47	0.48
1:D:90:ILE:C	1:D:92:ALA:H	2.21	0.48
1:E:207:GLU:O	1:E:211:LYS:N	2.46	0.48
1:H:80:VAL:HA	1:H:274:LEU:O	2.14	0.48
1:H:168:LEU:O	1:H:171:CYS:HB3	2.12	0.48
1:I:102:LYS:NZ	1:I:285:ASP:OD1	2.46	0.48
1:I:182:MET:HE1	1:I:237:PHE:CG	2.49	0.48
1:K:203:LYS:NZ	1:K:206:GLU:OE1	2.45	0.48
2:l:30:THR:O	2:l:30:THR:OG1	2.22	0.48
1:O:176:MET:HE1	1:O:239:TYR:HD2	1.78	0.48
1:O:227:ASP:HB3	1:O:233:ILE:HG12	1.96	0.48
1:P:182:MET:HE1	1:P:237:PHE:CD2	2.48	0.48
2:p:49:TRP:CZ2	2:p:52:TRP:HB2	2.49	0.48
2:p:153:ILE:HD13	2:p:238:THR:OG1	2.13	0.48
1:Q:176:MET:CB	1:Q:182:MET:HE3	2.38	0.48
1:R:90:ILE:HD12	1:R:120:SER:O	2.12	0.48
1:A:320:MET:HB2	1:A:325:SER:HB3	1.95	0.48
1:B:183:LEU:HD23	1:B:209:LEU:HD12	1.94	0.48
1:B:266:GLU:H	1:B:266:GLU:CD	2.21	0.48
1:D:67:GLY:HA2	1:J:70:VAL:CG1	2.41	0.48
1:G:356:ARG:NE	3:G:401:SO4:O1	2.46	0.48
2:g:83:MET:HG2	2:g:84:GLU:N	2.27	0.48
1:I:170:LYS:HG3	1:I:171:CYS:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:200:LYS:HZ2	1:I:203:LYS:CB	2.27	0.48
2:j:49:TRP:HH2	2:j:52:TRP:CB	2.26	0.48
1:K:80:VAL:HG22	1:K:275:MET:HG2	1.96	0.48
1:N:165:MET:HE1	1:N:173:VAL:HG11	1.96	0.48
1:O:110:ASP:HB3	1:O:314:PRO:HG2	1.96	0.48
1:O:156:TRP:HB3	1:O:160:PHE:CD2	2.48	0.48
1:Q:143:LYS:HG2	1:Q:171:CYS:SG	2.53	0.48
1:R:203:LYS:HE3	1:R:204:LYS:HD2	1.96	0.48
2:r:183:TYR:CE2	2:r:187:LYS:HE3	2.43	0.48
1:A:182:MET:HE1	1:A:237:PHE:CD1	2.48	0.48
2:a:7:VAL:HG23	2:a:25:LYS:HB3	1.96	0.48
2:e:31:PHE:CE1	2:e:36:ILE:HD12	2.46	0.48
2:f:14:LYS:CD	2:f:19:SER:O	2.58	0.48
2:g:215:GLY:C	2:g:217:GLU:H	2.21	0.48
1:N:44:LYS:HA	1:N:47:THR:HG22	1.96	0.48
2:n:31:PHE:CD2	2:n:79:SER:HA	2.49	0.48
2:n:142:SER:OG	2:n:143:VAL:N	2.46	0.48
2:n:162:ILE:HG23	2:n:167:VAL:HG21	1.96	0.48
1:P:323:SER:OG	2:p:230:ARG:NH1	2.46	0.48
2:p:189:PRO:HD2	2:p:192:ILE:HG13	1.95	0.48
2:q:167:VAL:HG13	2:q:224:VAL:HG12	1.95	0.48
2:r:54:ASN:ND2	2:r:57:SER:HB3	2.28	0.48
2:r:98:CYS:O	2:r:109:GLY:N	2.41	0.48
2:f:20:VAL:HG11	2:f:88:LEU:HD11	1.96	0.48
2:h:53:ILE:HB	2:h:72:MET:HE2	1.96	0.48
2:l:53:ILE:HG13	2:l:60:THR:HB	1.94	0.48
2:n:5:GLN:NE2	2:n:110:LYS:HZ2	2.05	0.48
1:O:138:GLY:O	1:O:235:VAL:HA	2.14	0.48
1:P:182:MET:HG3	1:P:358:TRP:CH2	2.49	0.48
2:r:210:THR:O	2:r:210:THR:HG23	2.14	0.48
2:a:173:LEU:HB3	2:a:174:PRO:HD2	1.94	0.48
2:d:49:TRP:CZ2	2:d:52:TRP:HB2	2.49	0.48
1:E:104:PRO:HD2	1:E:292:ASP:CG	2.39	0.48
2:g:211:GLY:O	2:g:212:LEU:C	2.56	0.48
2:i:18:ALA:HB1	2:i:88:LEU:HD12	1.92	0.48
2:i:52:TRP:HE3	2:i:53:ILE:C	2.21	0.48
1:J:134:THR:O	1:J:240:SER:HB3	2.14	0.48
1:L:98:LEU:CD1	1:L:126:TYR:C	2.86	0.48
1:L:229:ALA:HB2	1:L:246:ALA:O	2.14	0.48
1:L:240:SER:OG	1:L:241:GLY:N	2.44	0.48
1:L:321:ASP:OD1	1:L:322:LYS:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:17:GLY:H	2:l:88:LEU:CG	2.23	0.48
2:l:36:ILE:HA	2:l:99:ALA:O	2.14	0.48
1:N:156:TRP:HB3	1:N:160:PHE:CE2	2.48	0.48
1:N:251:GLU:HG3	1:N:252:GLU:H	1.79	0.48
1:O:90:ILE:O	1:O:92:ALA:N	2.46	0.48
1:O:102:LYS:NZ	1:O:103:LEU:HB2	2.27	0.48
2:o:49:TRP:CZ2	2:o:52:TRP:HB2	2.49	0.48
1:P:103:LEU:HD23	1:P:292:ASP:HB2	1.95	0.48
2:p:173:LEU:HB3	2:p:174:PRO:HD2	1.94	0.48
1:A:34:TRP:HB3	4:A:404:SPD:H22	1.95	0.48
2:a:9:THR:HG22	2:a:10:GLY:N	2.29	0.48
2:c:50:MET:HG2	2:c:66:PHE:CE2	2.48	0.48
2:c:89:ARG:O	2:c:116:VAL:HG21	2.14	0.48
2:c:140:PRO:O	2:c:238:THR:HB	2.13	0.48
2:d:49:TRP:HZ2	2:d:52:TRP:HB2	1.77	0.48
2:d:166:TYR:HA	2:d:185:ASN:HD21	1.78	0.48
1:F:330:VAL:O	1:F:332:PRO:HD3	2.14	0.48
1:I:160:PHE:HB2	1:I:189:TYR:CE2	2.49	0.48
2:i:161:ASN:OD1	2:i:162:ILE:N	2.38	0.48
1:J:200:LYS:HD2	1:J:203:LYS:CB	2.44	0.48
1:K:102:LYS:O	1:K:104:PRO:HD3	2.13	0.48
2:o:37:SER:HB3	2:o:49:TRP:CZ3	2.47	0.48
2:o:153:ILE:HD13	2:o:238:THR:OG1	2.14	0.48
2:b:143:VAL:O	2:b:240:LEU:HA	2.14	0.48
2:b:167:VAL:HG11	2:b:205:THR:HG21	1.96	0.48
1:G:286:ASN:O	1:G:289:ALA:N	2.46	0.48
2:g:153:ILE:HG12	2:g:238:THR:HG21	1.96	0.48
2:h:209:ILE:HD11	2:h:212:LEU:HG	1.96	0.48
1:I:86:LEU:HD11	1:I:127:ALA:HB2	1.95	0.48
1:J:187:LEU:HB2	1:J:194:PRO:HA	1.96	0.48
1:K:104:PRO:HD2	1:K:292:ASP:CG	2.38	0.48
1:M:117:LEU:HD13	1:M:274:LEU:HD21	1.95	0.48
2:n:172:GLN:O	2:n:218:ALA:HB1	2.14	0.48
1:O:357:THR:HA	1:O:360:ARG:NH1	2.28	0.48
2:o:69:ARG:HG2	2:o:87:ARG:HH11	1.79	0.48
1:P:303:VAL:O	1:P:307:VAL:HG22	2.13	0.48
2:p:161:ASN:OD1	2:p:162:ILE:N	2.47	0.48
1:R:37:TYR:HD1	1:R:130:TYR:HE2	1.60	0.48
2:b:160:SER:HB2	2:b:226:ASP:OD1	2.14	0.47
1:C:337:LEU:O	1:C:340:LEU:N	2.44	0.47
2:c:69:ARG:HH12	2:c:89:ARG:CD	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LYS:C	1:D:104:PRO:HD3	2.39	0.47
2:d:164:ARG:HG2	2:d:165:ASN:OD1	2.14	0.47
2:f:188:ARG:NH1	2:f:192:ILE:O	2.46	0.47
1:G:80:VAL:HA	1:G:274:LEU:O	2.14	0.47
1:H:210:THR:HG22	1:H:361:ILE:HG23	1.97	0.47
1:I:144:VAL:HG12	1:I:145:LYS:N	2.29	0.47
2:i:7:VAL:CG2	2:i:25:LYS:HB3	2.41	0.47
1:J:213:ARG:NE	1:J:361:ILE:O	2.47	0.47
2:j:31:PHE:CE2	2:j:55:PRO:HB3	2.49	0.47
1:L:316:ALA:O	1:L:319:LEU:N	2.44	0.47
2:l:52:TRP:CE3	2:l:101:ASP:OD2	2.66	0.47
2:m:210:THR:OG1	2:m:211:GLY:N	2.46	0.47
1:N:247:ALA:HB2	1:N:259:ILE:HB	1.95	0.47
1:Q:37:TYR:CE1	4:Q:401:SPD:H52	2.49	0.47
1:B:144:VAL:O	1:B:148:LEU:HB2	2.14	0.47
1:B:348:ALA:HA	1:B:351:LEU:HD12	1.95	0.47
2:b:20:VAL:O	2:b:20:VAL:HG22	2.14	0.47
2:c:225:TRP:CH2	2:c:230:ARG:HA	2.49	0.47
1:H:348:ALA:HA	1:H:351:LEU:HD12	1.96	0.47
2:i:162:ILE:HG12	2:i:224:VAL:HG11	1.96	0.47
2:j:35:GLY:O	2:j:36:ILE:HG12	2.15	0.47
2:k:9:THR:HG21	2:m:87:ARG:NH2	2.28	0.47
1:M:81:PRO:HG2	1:M:86:LEU:HB2	1.96	0.47
1:N:102:LYS:HB2	1:N:288:TYR:CD2	2.48	0.47
1:O:37:TYR:HE1	1:O:131:LEU:HD12	1.78	0.47
2:o:7:VAL:HG23	2:o:25:LYS:HB3	1.96	0.47
1:P:37:TYR:CE2	4:P:401:SPD:H41	2.49	0.47
1:P:150:ASP:OD1	2:r:138:THR:HG21	2.15	0.47
1:Q:143:LYS:HG3	1:Q:146:GLU:OE1	2.14	0.47
1:R:37:TYR:CE2	4:R:404:SPD:H41	2.48	0.47
1:R:340:LEU:HD12	1:R:340:LEU:HA	1.48	0.47
2:r:149:GLN:HB3	2:r:212:LEU:HD13	1.94	0.47
1:A:59:PHE:HD2	1:A:61:SER:O	1.97	0.47
2:c:161:ASN:HB2	2:c:224:VAL:HG21	1.95	0.47
2:d:21:LYS:HG2	2:d:84:GLU:HB2	1.96	0.47
1:E:314:PRO:O	1:E:316:ALA:N	2.47	0.47
1:F:33:ASN:O	1:F:58:VAL:HA	2.14	0.47
1:F:97:LYS:NZ	1:F:125:GLN:OE1	2.34	0.47
1:F:165:MET:HE3	1:F:165:MET:HB3	1.66	0.47
2:f:4:VAL:HG22	2:f:107:VAL:HG11	1.96	0.47
2:i:55:PRO:O	2:i:74:ARG:NE	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:203:LYS:HG3	1:K:206:GLU:HB3	1.96	0.47
2:k:42:ALA:HB1	2:k:43:PRO:HD2	1.97	0.47
1:N:34:TRP:CE3	4:N:407:SPD:H42	2.49	0.47
1:Q:108:ASN:O	1:Q:314:PRO:HD2	2.15	0.47
1:Q:303:VAL:O	1:Q:307:VAL:HG22	2.13	0.47
1:Q:317:ARG:NH1	1:Q:325:SER:HB2	2.30	0.47
1:R:102:LYS:NZ	1:R:285:ASP:OD1	2.27	0.47
2:a:49:TRP:CZ2	2:a:52:TRP:HB2	2.49	0.47
1:G:150:ASP:OD1	1:G:150:ASP:N	2.47	0.47
1:G:162:PRO:HG2	1:G:211:LYS:HE3	1.96	0.47
1:H:74:SER:O	1:H:76:TYR:N	2.39	0.47
2:k:100:ARG:O	2:k:105:MET:HA	2.14	0.47
1:N:37:TYR:CE2	4:N:407:SPD:H41	2.50	0.47
1:P:138:GLY:HA3	1:P:243:VAL:HG21	1.95	0.47
2:p:7:VAL:HG23	2:p:25:LYS:HB3	1.96	0.47
2:p:9:THR:HG22	2:p:10:GLY:N	2.29	0.47
1:Q:139:TYR:CD2	1:Q:144:VAL:HG21	2.50	0.47
1:Q:350:VAL:C	1:Q:352:ARG:N	2.72	0.47
2:b:98:CYS:O	2:b:109:GLY:N	2.47	0.47
2:c:9:THR:HG22	2:c:10:GLY:H	1.79	0.47
1:H:357:THR:O	1:H:361:ILE:HG13	2.14	0.47
1:I:204:LYS:HA	1:I:207:GLU:OE2	2.14	0.47
1:J:239:TYR:O	1:J:243:VAL:HG23	2.14	0.47
2:k:106:ASP:HA	2:k:180:LEU:HD22	1.95	0.47
1:N:32:TYR:CB	1:N:79:VAL:HG12	2.44	0.47
1:N:77:ASP:O	1:N:277:ILE:HG23	2.13	0.47
1:P:90:ILE:C	1:P:92:ALA:H	2.23	0.47
1:P:188:ASN:ND2	1:P:266:GLU:O	2.42	0.47
2:p:69:ARG:HG2	2:p:87:ARG:HH11	1.79	0.47
1:Q:34:TRP:HE3	4:Q:401:SPD:H22	1.79	0.47
2:r:5:GLN:HG2	2:r:27:SER:HB3	1.95	0.47
1:A:67:GLY:HA2	1:K:70:VAL:CG1	2.40	0.47
1:A:239:TYR:CZ	4:A:404:SPD:H82	2.50	0.47
1:D:143:LYS:O	1:D:147:VAL:HG23	2.14	0.47
1:E:194:PRO:HG3	1:E:341:TYR:CG	2.49	0.47
1:F:106:TRP:HZ3	1:F:128:VAL:HG22	1.79	0.47
2:h:185:ASN:ND2	2:h:200:LYS:NZ	2.62	0.47
1:J:46:PHE:HE2	1:J:52:ILE:HB	1.79	0.47
1:J:127:ALA:HB1	1:J:274:LEU:HB3	1.95	0.47
1:L:39:ALA:HB3	1:L:42:THR:OG1	2.14	0.47
2:m:95:VAL:CG1	2:m:111:GLY:HA3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:86:LEU:HA	1:O:89:GLN:OE1	2.15	0.47
2:o:9:THR:HG22	2:o:10:GLY:N	2.29	0.47
1:P:154:ASP:O	1:P:265:LYS:N	2.47	0.47
1:Q:193:ASP:HB3	1:Q:196:THR:HG23	1.96	0.47
1:R:121:ASP:CG	1:R:125:GLN:H	2.23	0.47
2:a:158:SER:N	2:a:161:ASN:OD1	2.48	0.47
1:D:134:THR:O	1:D:261:TYR:OH	2.26	0.47
2:e:69:ARG:NH1	2:e:87:ARG:O	2.46	0.47
1:F:267:GLY:HA3	1:F:339:LYS:O	2.15	0.47
2:f:55:PRO:O	2:f:74:ARG:NE	2.48	0.47
2:g:20:VAL:CG2	2:g:88:LEU:HD11	2.45	0.47
1:J:37:TYR:CZ	1:J:131:LEU:HB2	2.50	0.47
1:J:99:ASP:OD1	1:J:101:SER:OG	2.23	0.47
1:J:204:LYS:O	1:J:208:VAL:HB	2.14	0.47
1:K:38:ILE:N	1:K:307:VAL:HG11	2.29	0.47
1:K:328:GLU:HG2	2:k:166:TYR:CE1	2.49	0.47
2:l:5:GLN:CG	2:l:27:SER:HB3	2.45	0.47
2:l:159:SER:O	2:l:159:SER:OG	2.25	0.47
2:m:39:VAL:O	2:m:97:TYR:HB2	2.15	0.47
2:m:103:ARG:NH2	2:m:184:ASP:OD1	2.47	0.47
1:N:160:PHE:HD2	1:N:189:TYR:CD2	2.32	0.47
1:N:233:ILE:CD1	1:N:236:ALA:HB2	2.45	0.47
2:n:194:ASP:OD1	2:n:194:ASP:N	2.39	0.47
2:o:161:ASN:OD1	2:o:162:ILE:N	2.47	0.47
1:Q:140:ASN:ND2	1:Q:143:LYS:HE2	2.29	0.47
1:R:128:VAL:CG2	1:R:275:MET:HB2	2.45	0.47
2:a:153:ILE:HD13	2:a:238:THR:OG1	2.14	0.47
2:h:14:LYS:HG3	2:h:20:VAL:HG13	1.97	0.47
2:i:25:LYS:HB2	2:i:80:THR:HG22	1.96	0.47
1:J:37:TYR:CE1	1:J:131:LEU:HB2	2.50	0.47
2:l:13:VAL:O	2:l:14:LYS:CB	2.53	0.47
2:l:149:GLN:NE2	1:Q:190:LEU:C	2.73	0.47
1:N:116:GLN:C	1:N:118:GLU:H	2.23	0.47
1:N:220:HIS:CE1	1:N:223:LYS:H	2.32	0.47
2:n:173:LEU:H	2:n:173:LEU:HD12	1.80	0.47
2:o:26:VAL:HG21	2:o:31:PHE:CD1	2.50	0.47
1:P:195:ASN:OD1	1:P:343:SER:HA	2.14	0.47
2:p:26:VAL:HG21	2:p:31:PHE:CD1	2.50	0.47
2:b:25:LYS:HB2	2:b:80:THR:HG22	1.96	0.47
1:E:80:VAL:HA	1:E:274:LEU:O	2.14	0.47
1:E:158:ILE:HA	1:E:164:ASN:HD22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:LEU:HD13	1:F:235:VAL:HG11	1.97	0.47
2:f:25:LYS:NZ	2:f:78:ILE:HG13	2.29	0.47
1:H:95:PHE:HA	1:H:278:PRO:HA	1.97	0.47
2:h:9:THR:HB	2:h:23:SER:HB2	1.96	0.47
1:I:29:LEU:HD12	1:I:77:ASP:HB2	1.97	0.47
1:L:86:LEU:HD21	1:L:127:ALA:HB2	1.97	0.47
2:l:21:LYS:HB3	2:l:84:GLU:CB	2.45	0.47
1:N:349:LYS:HA	1:N:349:LYS:HD2	1.62	0.47
1:O:155:SER:HA	1:O:264:PRO:HB3	1.96	0.47
1:P:77:ASP:HA	1:P:281:ALA:HB1	1.96	0.47
2:q:225:TRP:CZ3	2:q:227:SER:HA	2.50	0.47
2:r:13:VAL:C	2:r:14:LYS:HG2	2.39	0.47
1:B:155:SER:OG	1:B:266:GLU:OE2	2.23	0.47
1:B:328:GLU:OE2	2:b:200:LYS:NZ	2.48	0.47
2:e:29:TYR:CE1	2:e:31:PHE:HA	2.50	0.47
1:F:207:GLU:HA	1:F:210:THR:OG1	2.15	0.47
2:f:199:SER:HB2	2:f:206:THR:HG1	1.77	0.47
1:G:239:TYR:HB2	1:G:242:ASP:HB2	1.97	0.47
1:G:271:TRP:CZ2	4:G:403:SPD:H72	2.50	0.47
1:H:337:LEU:O	1:H:339:LYS:N	2.48	0.47
2:h:42:ALA:HB1	2:h:43:PRO:HD2	1.97	0.47
1:M:203:LYS:HZ2	1:M:204:LYS:C	2.22	0.47
1:Q:293:TYR:HD1	1:Q:296:ARG:NH2	2.12	0.47
2:q:182:LEU:CB	2:q:188:ARG:HG2	2.45	0.47
2:r:223:GLY:HA2	2:r:233:LEU:O	2.14	0.47
2:a:69:ARG:HG2	2:a:87:ARG:HH11	1.79	0.46
2:b:18:ALA:HA	2:b:88:LEU:HB2	1.96	0.46
2:b:106:ASP:HA	2:b:180:LEU:HD22	1.97	0.46
1:D:336:VAL:O	1:D:340:LEU:HG	2.15	0.46
2:e:217:GLU:HG3	2:e:240:LEU:O	2.15	0.46
1:F:176:MET:HG3	1:F:237:PHE:CD1	2.50	0.46
1:G:182:MET:HE1	1:G:237:PHE:CD1	2.50	0.46
1:G:357:THR:HG23	1:G:360:ARG:HH21	1.79	0.46
2:i:52:TRP:C	2:i:72:MET:HE1	2.40	0.46
1:J:242:ASP:OD1	4:J:404:SPD:H21	2.15	0.46
2:m:64:GLN:O	2:m:67:GLN:HG2	2.15	0.46
2:n:26:VAL:HG22	2:n:29:TYR:CE1	2.50	0.46
2:n:40:ARG:HG2	2:n:41:GLN:H	1.79	0.46
1:P:252:GLU:O	1:P:252:GLU:HG2	2.15	0.46
1:B:136:GLY:HA2	1:B:156:TRP:CH2	2.51	0.46
1:E:145:LYS:C	1:E:147:VAL:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:322:LYS:HD3	2:e:225:TRP:CE3	2.51	0.46
2:h:154:SER:HA	2:h:206:THR:HA	1.97	0.46
1:I:362:LYS:HE2	1:I:362:LYS:O	2.15	0.46
1:J:149:GLY:O	1:J:151:GLN:N	2.44	0.46
1:J:204:LYS:HG2	1:J:207:GLU:CG	2.46	0.46
2:j:31:PHE:CE1	2:j:36:ILE:HD12	2.49	0.46
2:k:26:VAL:CG2	2:k:26:VAL:CA	2.85	0.46
1:L:89:GLN:HB3	1:L:95:PHE:HE2	1.79	0.46
1:L:99:ASP:C	1:L:101:SER:H	2.22	0.46
1:L:283:ALA:O	1:L:285:ASP:N	2.48	0.46
1:L:303:VAL:O	1:L:307:VAL:HG22	2.15	0.46
2:l:96:TYR:CE2	2:l:114:VAL:HB	2.49	0.46
1:M:60:ASP:HB2	1:M:222:SER:HB3	1.96	0.46
1:N:208:VAL:O	1:N:212:VAL:HG13	2.15	0.46
1:P:130:TYR:O	1:P:131:LEU:HD23	2.16	0.46
2:q:42:ALA:HB3	2:q:45:GLN:HG2	1.97	0.46
2:q:168:SER:HA	2:q:182:LEU:CD1	2.46	0.46
1:R:300:ILE:HD12	1:R:303:VAL:HG21	1.96	0.46
2:r:50:MET:HA	2:r:66:PHE:CE2	2.51	0.46
2:a:26:VAL:HG21	2:a:31:PHE:CD1	2.50	0.46
2:d:166:TYR:HA	2:d:185:ASN:ND2	2.30	0.46
1:G:95:PHE:HA	1:G:278:PRO:HA	1.97	0.46
2:g:6:LEU:HD23	2:g:98:CYS:SG	2.55	0.46
2:g:150:LYS:HG2	2:g:151:VAL:N	2.31	0.46
2:g:181:LEU:HD21	2:g:196:PHE:CD2	2.50	0.46
1:H:139:TYR:HB2	1:H:144:VAL:HG21	1.96	0.46
1:K:213:ARG:O	1:K:215:TYR:N	2.47	0.46
1:L:104:PRO:C	1:L:106:TRP:N	2.72	0.46
2:l:14:LYS:HD3	2:l:14:LYS:HA	1.38	0.46
2:l:86:SER:O	2:l:87:ARG:C	2.58	0.46
2:l:102:LYS:HB2	2:l:104:TYR:CD2	2.51	0.46
2:l:195:ARG:O	2:l:210:THR:HG22	2.15	0.46
1:M:199:PRO:C	1:M:201:ASP:N	2.74	0.46
1:O:153:ILE:HG23	1:O:158:ILE:HG13	1.97	0.46
2:p:182:LEU:HD13	2:p:198:ALA:HB2	1.97	0.46
2:a:37:SER:HB3	2:a:49:TRP:CZ3	2.47	0.46
2:b:102:LYS:O	2:b:103:ARG:HB2	2.14	0.46
1:C:104:PRO:HD2	1:C:292:ASP:CG	2.40	0.46
1:E:271:TRP:CE2	4:E:405:SPD:H82	2.51	0.46
2:e:102:LYS:O	2:e:103:ARG:HB2	2.15	0.46
1:H:176:MET:HE2	1:H:224:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:199:PRO:O	1:I:203:LYS:HG2	2.15	0.46
1:K:182:MET:O	1:K:185:ALA:N	2.48	0.46
2:k:181:LEU:HD11	2:k:196:PHE:CD2	2.51	0.46
2:l:40:ARG:NH2	2:l:85:LEU:CD1	2.79	0.46
1:N:191:GLY:HA3	2:o:149:GLN:CB	2.45	0.46
2:n:4:VAL:HG22	2:n:107:VAL:HG21	1.97	0.46
2:n:143:VAL:HG13	2:n:240:LEU:HD13	1.97	0.46
1:P:163:GLU:CD	1:P:163:GLU:H	2.21	0.46
2:q:225:TRP:HD1	2:q:232:VAL:HG22	1.80	0.46
2:r:220:TYR:HB2	2:r:238:THR:HG23	1.96	0.46
1:B:63:GLU:OE2	1:B:178:SER:OG	2.26	0.46
2:b:137:LEU:HD11	2:b:233:LEU:CB	2.46	0.46
2:b:150:LYS:HG3	2:b:210:THR:HA	1.98	0.46
2:d:34:TYR:HD1	2:d:102:LYS:HB3	1.81	0.46
1:E:145:LYS:C	1:E:147:VAL:N	2.73	0.46
2:e:182:LEU:CD2	2:e:188:ARG:HG2	2.44	0.46
1:G:183:LEU:HD23	1:G:209:LEU:HD12	1.95	0.46
1:I:362:LYS:O	1:I:362:LYS:HG2	2.16	0.46
2:k:103:ARG:NH2	2:k:184:ASP:OD1	2.48	0.46
1:L:156:TRP:HB3	1:L:160:PHE:CD2	2.50	0.46
1:M:322:LYS:NZ	2:m:103:ARG:HA	2.30	0.46
1:N:109:LEU:HD13	1:N:114:LEU:HD21	1.97	0.46
1:N:298:GLU:O	1:N:302:LYS:HG3	2.15	0.46
1:P:109:LEU:HD21	1:P:295:LEU:HD22	1.97	0.46
2:p:49:TRP:CH2	2:p:52:TRP:HB2	2.51	0.46
1:A:293:TYR:CE1	1:A:299:VAL:HG21	2.50	0.46
2:a:49:TRP:CH2	2:a:52:TRP:HB2	2.51	0.46
2:d:16:PRO:HG2	2:d:16:PRO:O	2.15	0.46
2:d:225:TRP:HZ3	2:d:227:SER:HA	1.76	0.46
1:F:286:ASN:O	1:F:289:ALA:N	2.49	0.46
2:f:73:THR:OG1	2:f:82:TYR:HB2	2.16	0.46
2:f:198:ALA:HA	2:f:206:THR:O	2.15	0.46
2:h:226:ASP:C	2:h:228:SER:H	2.24	0.46
1:I:77:ASP:O	1:I:277:ILE:HG23	2.16	0.46
1:J:200:LYS:O	1:J:201:ASP:C	2.59	0.46
2:j:42:ALA:HB1	2:j:43:PRO:HD2	1.97	0.46
2:k:37:SER:CB	2:k:49:TRP:HZ3	2.15	0.46
1:L:105:ASN:O	1:L:295:LEU:HB3	2.16	0.46
1:L:207:GLU:HA	1:L:210:THR:OG1	2.16	0.46
2:l:162:ILE:HG13	2:l:224:VAL:HG21	1.96	0.46
2:n:71:THR:HB	2:n:84:GLU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:217:GLU:HG3	2:n:241:THR:HA	1.97	0.46
1:O:155:SER:CB	1:O:265:LYS:HE2	2.42	0.46
2:o:182:LEU:HD13	2:o:198:ALA:HB2	1.97	0.46
2:q:214:THR:HA	2:q:242:VAL:HG11	1.97	0.46
2:r:37:SER:HB3	2:r:49:TRP:HE1	1.81	0.46
1:C:80:VAL:HG22	1:C:275:MET:HG2	1.98	0.46
2:c:75:ASP:OD1	2:c:77:SER:HB3	2.16	0.46
1:E:115:LYS:HG3	1:E:116:GLN:N	2.31	0.46
1:E:153:ILE:HG22	1:E:262:VAL:HG11	1.97	0.46
2:f:25:LYS:HZ3	2:f:78:ILE:CG1	2.28	0.46
1:H:182:MET:HE1	1:H:237:PHE:CD1	2.51	0.46
1:H:298:GLU:H	1:H:298:GLU:HG3	1.45	0.46
2:i:105:MET:O	2:i:180:LEU:HB2	2.15	0.46
2:j:169:TRP:HB2	2:j:182:LEU:HB2	1.98	0.46
1:K:247:ALA:HB2	1:K:259:ILE:HB	1.98	0.46
1:L:242:ASP:OD1	1:L:309:TYR:OH	2.32	0.46
1:L:326:ASP:HB2	2:l:166:TYR:CD2	2.44	0.46
1:M:158:ILE:HD13	1:M:164:ASN:ND2	2.30	0.46
1:N:202:TYR:O	1:N:206:GLU:N	2.44	0.46
1:O:102:LYS:HD2	1:O:103:LEU:N	2.30	0.46
1:O:182:MET:HE1	1:O:237:PHE:CG	2.50	0.46
1:P:189:TYR:C	1:P:191:GLY:H	2.24	0.46
1:P:359:THR:O	1:P:362:LYS:HB2	2.16	0.46
1:R:211:LYS:HD2	1:R:211:LYS:C	2.41	0.46
1:R:220:HIS:CG	1:R:223:LYS:HG2	2.51	0.46
1:C:352:ARG:NH1	3:I:403:SO4:O1	2.44	0.46
2:i:25:LYS:CB	2:i:80:THR:HG22	2.46	0.46
1:J:176:MET:HA	1:J:220:HIS:O	2.15	0.46
1:K:159:LEU:CA	1:K:165:MET:HE1	2.39	0.46
1:K:170:LYS:HG2	1:K:171:CYS:N	2.31	0.46
2:k:21:LYS:CA	2:k:83:MET:O	2.61	0.46
2:l:210:THR:HG23	2:l:210:THR:O	2.15	0.46
2:m:139:GLN:HB2	2:m:155:CYS:HB2	1.98	0.46
2:m:149:GLN:O	2:m:212:LEU:HB2	2.16	0.46
1:N:43:LEU:HD22	1:N:54:VAL:HG21	1.98	0.46
1:N:191:GLY:HA2	2:o:149:GLN:NE2	2.30	0.46
2:o:100:ARG:HB3	2:o:107:VAL:HG13	1.98	0.46
1:R:165:MET:HA	1:R:168:LEU:HB3	1.97	0.46
1:R:187:LEU:O	1:R:192:LEU:HB2	2.16	0.46
1:A:206:GLU:CD	1:A:360:ARG:HH21	2.23	0.46
2:b:157:GLY:O	2:b:203:PRO:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:GLY:HA3	1:I:71:SER:OG	2.16	0.46
1:F:220:HIS:CD2	1:F:223:LYS:HD3	2.50	0.46
1:G:33:ASN:O	1:G:58:VAL:HA	2.15	0.46
1:H:30:HIS:ND1	1:H:55:SER:HB2	2.31	0.46
2:h:37:SER:HB3	2:h:49:TRP:HZ3	1.80	0.46
2:h:38:TRP:CD1	2:h:72:MET:HE3	2.51	0.46
1:I:225:ILE:HD11	1:I:242:ASP:CG	2.41	0.46
1:I:328:GLU:O	1:I:332:PRO:HA	2.16	0.46
1:P:98:LEU:HD11	1:P:128:VAL:HG23	1.98	0.46
1:Q:170:LYS:H	1:Q:170:LYS:HG2	1.54	0.46
1:R:36:ASP:O	1:R:307:VAL:HG23	2.15	0.46
1:R:303:VAL:O	1:R:307:VAL:HG12	2.16	0.46
1:E:33:ASN:O	1:E:58:VAL:HA	2.16	0.46
2:f:3:GLN:HG2	2:f:4:VAL:H	1.81	0.46
2:f:143:VAL:CG2	2:f:240:LEU:HD12	2.46	0.46
1:K:176:MET:HA	1:K:220:HIS:O	2.16	0.46
1:K:326:ASP:HB3	2:k:165:ASN:HB3	1.98	0.46
1:L:32:TYR:HD2	1:L:65:LEU:HD13	1.81	0.46
2:l:219:ASP:C	2:l:220:TYR:HD1	2.24	0.46
1:M:180:ASP:O	1:M:184:PRO:HG2	2.15	0.46
1:O:160:PHE:C	1:O:212:VAL:HG11	2.41	0.46
2:o:49:TRP:CH2	2:o:52:TRP:HB2	2.51	0.46
2:p:16:PRO:O	2:p:88:LEU:O	2.35	0.46
2:p:88:LEU:HD23	2:p:88:LEU:HA	1.78	0.46
2:q:182:LEU:HB2	2:q:187:LYS:O	2.15	0.46
2:a:182:LEU:HD13	2:a:198:ALA:HB2	1.97	0.45
1:C:176:MET:HE1	1:C:239:TYR:CD2	2.51	0.45
1:C:227:ASP:HB3	1:C:233:ILE:HG12	1.98	0.45
2:c:8:GLU:OE2	2:c:98:CYS:HB3	2.16	0.45
1:D:45:ASP:OD2	1:D:302:LYS:NZ	2.49	0.45
1:E:170:LYS:HD3	1:E:171:CYS:N	2.32	0.45
2:e:12:GLU:HG2	2:e:13:VAL:H	1.80	0.45
1:F:225:ILE:HD11	1:F:242:ASP:CG	2.41	0.45
2:g:15:THR:HB	2:g:16:PRO:CD	2.46	0.45
2:h:34:TYR:HE2	2:h:102:LYS:HD3	1.80	0.45
2:h:185:ASN:ND2	2:h:200:LYS:HZ3	2.14	0.45
2:h:225:TRP:CH2	2:h:230:ARG:HG2	2.40	0.45
1:I:269:ASN:HB2	1:I:341:TYR:CE1	2.51	0.45
1:J:155:SER:OG	1:J:266:GLU:OE2	2.17	0.45
1:J:208:VAL:O	1:J:212:VAL:HG13	2.16	0.45
1:K:29:LEU:HD12	1:K:30:HIS:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:106:ASP:CG	2:l:107:VAL:HG23	2.41	0.45
2:l:172:GLN:HB2	2:l:178:PRO:HG3	1.98	0.45
1:N:243:VAL:O	1:N:246:ALA:N	2.45	0.45
1:P:293:TYR:HD1	1:P:296:ARG:NH1	2.13	0.45
2:p:158:SER:N	2:p:161:ASN:OD1	2.48	0.45
1:A:47:THR:HG22	1:A:52:ILE:O	2.16	0.45
1:A:104:PRO:HD2	1:A:292:ASP:OD2	2.16	0.45
2:a:16:PRO:O	2:a:88:LEU:O	2.35	0.45
2:b:50:MET:HE2	2:b:50:MET:HB3	1.49	0.45
2:d:9:THR:HG22	2:d:10:GLY:H	1.81	0.45
1:f:326:ASP:HB3	2:f:165:ASN:HB3	1.98	0.45
1:H:303:VAL:O	1:H:307:VAL:HG22	2.16	0.45
2:h:18:ALA:HA	2:h:88:LEU:H	1.80	0.45
1:I:200:LYS:HA	1:I:200:LYS:HD2	1.36	0.45
2:i:19:SER:H	2:i:88:LEU:HG	1.82	0.45
2:k:100:ARG:NH2	2:k:102:LYS:HZ1	2.14	0.45
1:M:204:LYS:HA	1:M:207:GLU:HB2	1.99	0.45
2:m:38:TRP:HD1	2:m:72:MET:HE3	1.81	0.45
2:m:167:VAL:HG11	2:m:205:THR:HG21	1.97	0.45
1:N:81:PRO:HD2	1:N:274:LEU:O	2.17	0.45
2:o:19:SER:O	2:o:19:SER:OG	2.28	0.45
2:o:158:SER:N	2:o:161:ASN:OD1	2.48	0.45
1:Q:271:TRP:C	1:Q:272:PHE:CD1	2.95	0.45
1:R:77:ASP:O	1:R:277:ILE:HG23	2.16	0.45
1:R:211:LYS:C	1:R:213:ARG:H	2.24	0.45
1:B:134:THR:H	1:B:240:SER:HB2	1.81	0.45
2:c:170:TYR:CE1	2:c:180:LEU:HD13	2.51	0.45
2:c:185:ASN:CG	2:c:200:LYS:HZ2	2.08	0.45
1:D:206:GLU:OE1	1:D:357:THR:HG23	2.16	0.45
2:d:182:LEU:HD21	2:d:188:ARG:HG2	1.98	0.45
1:E:62:ASN:HD21	1:E:82:SER:CB	2.29	0.45
2:e:89:ARG:O	2:e:116:VAL:HG11	2.17	0.45
1:H:86:LEU:HD22	1:H:274:LEU:HD13	1.97	0.45
1:H:176:MET:HE1	1:H:239:TYR:CE2	2.51	0.45
1:I:148:LEU:HG	1:I:148:LEU:O	2.16	0.45
2:i:35:GLY:HA2	2:i:55:PRO:HD3	1.97	0.45
2:i:53:ILE:HG13	2:i:59:GLY:O	2.17	0.45
1:J:206:GLU:C	1:J:210:THR:HG23	2.41	0.45
2:j:83:MET:HE3	2:j:85:LEU:H	1.81	0.45
1:K:132:TRP:HA	1:K:271:TRP:CZ3	2.51	0.45
1:K:200:LYS:CE	1:K:203:LYS:HD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:50:MET:HG2	2:l:66:PHE:CE2	2.52	0.45
2:l:84:GLU:CG	2:l:85:LEU:N	2.79	0.45
2:r:161:ASN:OD1	2:r:162:ILE:N	2.39	0.45
1:B:38:ILE:N	1:B:307:VAL:HG11	2.31	0.45
2:c:40:ARG:HD2	2:c:96:TYR:OH	2.15	0.45
2:d:223:GLY:HA2	2:d:233:LEU:O	2.17	0.45
1:E:239:TYR:HB2	1:E:242:ASP:HB2	1.97	0.45
2:g:37:SER:HB3	2:g:49:TRP:HZ3	1.81	0.45
2:g:167:VAL:H	2:g:185:ASN:ND2	2.15	0.45
1:J:273:ASP:OD2	4:J:404:SPD:H71	2.16	0.45
1:K:145:LYS:HA	1:K:149:GLY:O	2.17	0.45
1:K:176:MET:HE1	1:K:239:TYR:CD2	2.50	0.45
2:l:90:SER:CB	2:l:117:SER:HA	2.47	0.45
2:l:169:TRP:HB2	2:l:182:LEU:HB2	1.98	0.45
1:M:176:MET:HE1	1:M:239:TYR:CZ	2.50	0.45
2:m:160:SER:HB2	2:m:226:ASP:OD1	2.16	0.45
1:O:224:TYR:O	1:O:228:LEU:HB2	2.16	0.45
1:O:323:SER:OG	2:o:225:TRP:CH2	2.66	0.45
2:o:16:PRO:O	2:o:88:LEU:O	2.35	0.45
1:P:101:SER:OG	1:P:102:LYS:HE3	2.17	0.45
1:R:161:GLU:OE2	1:R:189:TYR:OH	2.34	0.45
1:R:176:MET:HE1	1:R:239:TYR:CE2	2.52	0.45
2:r:239:LYS:HE2	2:r:239:LYS:HB3	1.53	0.45
1:A:43:LEU:HB3	1:A:54:VAL:HG21	1.99	0.45
1:A:156:TRP:CD2	1:A:264:PRO:HG2	2.52	0.45
1:C:220:HIS:CD2	1:C:223:LYS:HB2	2.50	0.45
2:c:21:LYS:HE2	2:c:84:GLU:OE1	2.16	0.45
2:e:137:LEU:HD11	2:e:233:LEU:HB3	1.99	0.45
1:F:37:TYR:OH	1:F:131:LEU:HB2	2.17	0.45
2:h:6:LEU:HD22	2:h:98:CYS:SG	2.57	0.45
1:J:131:LEU:HD13	1:J:309:TYR:HB2	1.98	0.45
1:J:183:LEU:O	1:J:187:LEU:HG	2.16	0.45
1:K:317:ARG:HA	1:K:320:MET:SD	2.57	0.45
1:L:327:SER:C	1:L:329:GLU:H	2.23	0.45
1:M:175:PHE:HB3	1:M:182:MET:HE3	1.98	0.45
1:Q:37:TYR:HH	1:Q:131:LEU:HB2	1.82	0.45
1:Q:353:LEU:HD12	1:Q:354:GLN:N	2.32	0.45
2:r:149:GLN:HG2	2:r:150:LYS:N	2.24	0.45
1:D:271:TRP:CD2	4:D:404:SPD:H92	2.52	0.45
1:E:43:LEU:HD22	1:E:54:VAL:HG21	1.98	0.45
1:E:159:LEU:O	1:E:165:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:THR:HG22	1:G:213:ARG:NH1	2.31	0.45
1:I:266:GLU:OE1	1:I:266:GLU:N	2.42	0.45
2:i:117:SER:C	2:o:118:SER:C	2.85	0.45
1:J:182:MET:HE2	1:J:182:MET:HA	1.98	0.45
1:J:298:GLU:H	1:J:298:GLU:HG3	1.57	0.45
2:j:53:ILE:HB	2:j:72:MET:HE2	1.99	0.45
1:L:114:LEU:HB3	1:L:124:ASN:ND2	2.31	0.45
2:m:184:ASP:O	2:m:185:ASN:HB2	2.16	0.45
1:N:87:GLY:O	1:N:91:GLN:HG3	2.17	0.45
1:N:161:GLU:OE2	1:N:189:TYR:OH	2.30	0.45
1:O:44:LYS:HD3	1:O:44:LYS:HA	1.39	0.45
2:p:100:ARG:HB3	2:p:107:VAL:HG13	1.98	0.45
1:Q:168:LEU:HD13	1:Q:235:VAL:HG11	1.98	0.45
1:R:46:PHE:HB2	1:R:293:TYR:CD2	2.51	0.45
1:R:233:ILE:CD1	1:R:236:ALA:HB2	2.46	0.45
2:a:75:ASP:OD1	2:a:78:ILE:HG13	2.17	0.45
1:B:80:VAL:HG22	1:B:275:MET:HG2	1.98	0.45
1:C:28:SER:O	1:C:286:ASN:ND2	2.43	0.45
1:E:165:MET:HE1	1:E:173:VAL:HG11	1.99	0.45
2:e:31:PHE:CD2	2:e:79:SER:HA	2.52	0.45
2:e:195:ARG:NH2	2:e:216:ASP:OD2	2.42	0.45
1:G:269:ASN:OD1	1:G:271:TRP:HD1	1.98	0.45
2:g:5:GLN:O	2:g:6:LEU:HD12	2.17	0.45
1:H:153:ILE:O	1:H:262:VAL:HG11	2.17	0.45
1:M:132:TRP:HA	1:M:271:TRP:CZ3	2.51	0.45
1:M:327:SER:HB3	1:M:330:VAL:HB	1.99	0.45
1:N:240:SER:OG	1:N:241:GLY:N	2.49	0.45
1:O:171:CYS:SG	1:O:234:CYS:HB3	2.57	0.45
1:Q:34:TRP:CE3	4:Q:401:SPD:H22	2.50	0.45
1:Q:321:ASP:OD2	1:Q:323:SER:HB2	2.17	0.45
1:R:240:SER:HA	1:R:261:TYR:CZ	2.51	0.45
1:R:349:LYS:O	1:R:349:LYS:HG3	2.17	0.45
2:b:90:SER:OG	2:l:67:GLN:HG3	2.16	0.45
1:C:99:ASP:N	1:C:288:TYR:OH	2.39	0.45
1:C:328:GLU:O	1:C:332:PRO:HA	2.17	0.45
2:c:91:ASP:C	2:c:93:THR:H	2.25	0.45
1:D:199:PRO:HA	1:D:353:LEU:HD21	1.99	0.45
1:F:32:TYR:HB3	1:F:79:VAL:HG12	1.98	0.45
2:f:6:LEU:HG	2:f:26:VAL:HG12	1.98	0.45
2:j:149:GLN:O	2:j:212:LEU:HD12	2.17	0.45
1:K:130:TYR:O	1:K:131:LEU:HD23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:300:ILE:HD12	1:K:300:ILE:HA	1.86	0.45
2:k:62:TYR:HB2	2:k:67:GLN:HG2	1.99	0.45
1:L:37:TYR:HE2	1:L:131:LEU:HB2	1.82	0.45
1:L:127:ALA:HB1	1:L:274:LEU:HB3	1.97	0.45
1:M:135:ASN:OD1	1:M:268:ALA:HB1	2.16	0.45
1:N:60:ASP:HB2	1:N:222:SER:HB3	1.97	0.45
1:N:182:MET:O	1:N:185:ALA:N	2.46	0.45
2:n:100:ARG:O	2:n:105:MET:HA	2.17	0.45
1:O:130:TYR:O	1:O:131:LEU:HD23	2.16	0.45
1:Q:50:SER:C	1:Q:52:ILE:H	2.25	0.45
2:q:102:LYS:O	2:q:103:ARG:HB2	2.17	0.45
1:A:223:LYS:O	1:A:227:ASP:HB2	2.17	0.45
1:B:168:LEU:O	1:B:170:LYS:N	2.50	0.45
1:D:67:GLY:CA	1:J:70:VAL:HG13	2.44	0.45
1:E:213:ARG:HD3	1:E:361:ILE:HG23	1.98	0.45
1:E:314:PRO:C	1:E:316:ALA:H	2.25	0.45
2:e:74:ARG:HG3	2:e:74:ARG:O	2.15	0.45
1:F:168:LEU:O	1:F:170:LYS:N	2.50	0.45
1:F:330:VAL:HG12	1:F:331:TYR:CD1	2.51	0.45
2:j:195:ARG:O	2:j:210:THR:HG23	2.17	0.45
1:K:204:LYS:H	1:K:204:LYS:HG2	1.47	0.45
1:M:109:LEU:HB3	1:M:114:LEU:HD11	1.98	0.45
1:O:333:PRO:HB3	2:o:166:TYR:OH	2.17	0.45
1:Q:192:LEU:HB3	1:Q:193:ASP:H	1.61	0.45
1:Q:322:LYS:HB2	2:q:225:TRP:CE2	2.52	0.45
2:r:209:ILE:HG13	2:r:209:ILE:O	2.16	0.45
2:a:157:GLY:HA3	2:a:161:ASN:OD1	2.17	0.45
2:c:166:TYR:HA	2:c:185:ASN:HD21	1.81	0.45
1:F:115:LYS:HB2	1:F:115:LYS:HE3	1.63	0.45
1:G:99:ASP:OD1	1:G:101:SER:OG	2.31	0.45
1:G:176:MET:HE2	1:G:224:TYR:CE2	2.52	0.45
1:H:138:GLY:HA2	1:H:260:GLN:O	2.16	0.45
1:H:337:LEU:C	1:H:339:LYS:N	2.75	0.45
2:i:157:GLY:O	2:i:203:PRO:HB2	2.17	0.45
2:l:71:THR:C	2:l:72:MET:HG3	2.42	0.45
2:l:170:TYR:OH	2:l:234:PHE:HE1	2.00	0.45
1:M:37:TYR:OH	1:M:131:LEU:HB2	2.17	0.45
1:M:220:HIS:CG	1:M:223:LYS:HB2	2.52	0.45
1:N:80:VAL:HA	1:N:274:LEU:O	2.17	0.45
1:N:100:LYS:HZ1	1:N:125:GLN:HA	1.82	0.45
1:N:132:TRP:HA	1:N:271:TRP:CZ3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:156:TRP:CE2	1:N:264:PRO:HG2	2.52	0.45
1:N:304:SER:C	1:N:306:TYR:H	2.24	0.45
1:O:182:MET:HE1	1:O:237:PHE:CB	2.47	0.45
1:P:150:ASP:OD1	1:P:150:ASP:N	2.47	0.45
1:P:271:TRP:CD1	4:P:401:SPD:H91	2.52	0.45
2:p:75:ASP:OD1	2:p:78:ILE:HG13	2.17	0.45
2:b:93:THR:HG23	2:b:115:THR:HG22	1.99	0.44
1:C:329:GLU:H	1:C:329:GLU:HG2	1.37	0.44
1:D:239:TYR:CE1	4:D:404:SPD:H91	2.52	0.44
2:d:93:THR:HA	2:d:114:VAL:O	2.16	0.44
2:e:225:TRP:CZ2	2:e:230:ARG:HA	2.52	0.44
2:g:49:TRP:CD1	2:g:63:ALA:HB2	2.52	0.44
1:J:234:CYS:SG	1:J:235:VAL:HG23	2.57	0.44
2:k:213:GLN:C	2:k:215:GLY:N	2.75	0.44
2:l:145:GLY:O	2:l:242:VAL:HG13	2.17	0.44
2:l:184:ASP:O	2:l:185:ASN:HB2	2.17	0.44
2:l:195:ARG:NH1	2:l:216:ASP:OD1	2.51	0.44
1:O:42:THR:HA	1:O:302:LYS:NZ	2.32	0.44
1:Q:86:LEU:HD11	1:Q:127:ALA:HB2	1.99	0.44
1:Q:317:ARG:NH1	1:Q:317:ARG:HG2	2.22	0.44
2:q:13:VAL:O	2:q:14:LYS:HD3	2.15	0.44
1:R:117:LEU:HD13	1:R:274:LEU:HD21	1.98	0.44
1:R:210:THR:HG22	1:R:361:ILE:HG23	1.99	0.44
2:r:14:LYS:HG3	2:r:20:VAL:CG2	2.47	0.44
1:A:176:MET:H	1:A:182:MET:HE3	1.81	0.44
2:d:6:LEU:HD23	2:d:24:CYS:SG	2.57	0.44
2:e:21:LYS:HB2	2:e:21:LYS:HE3	1.78	0.44
1:I:43:LEU:HD22	1:I:54:VAL:HG11	1.99	0.44
1:J:203:LYS:O	1:J:206:GLU:HB2	2.17	0.44
1:L:37:TYR:CE2	1:L:131:LEU:HG	2.52	0.44
1:L:321:ASP:O	1:L:325:SER:OG	2.31	0.44
1:M:273:ASP:OD2	4:M:404:SPD:H52	2.17	0.44
2:m:8:GLU:OE2	2:m:98:CYS:HB3	2.18	0.44
1:N:189:TYR:O	1:N:191:GLY:N	2.47	0.44
1:O:128:VAL:HG21	1:O:291:ILE:HG21	1.97	0.44
1:O:166:LYS:HB3	1:O:166:LYS:HE3	1.74	0.44
1:O:240:SER:HA	1:O:261:TYR:CZ	2.53	0.44
2:o:75:ASP:OD1	2:o:78:ILE:HG13	2.17	0.44
1:P:110:ASP:HB3	1:P:314:PRO:CG	2.47	0.44
1:Q:247:ALA:HA	1:Q:259:ILE:HB	1.98	0.44
2:q:167:VAL:HG22	2:q:224:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:28:SER:O	1:R:286:ASN:ND2	2.50	0.44
2:a:100:ARG:HB3	2:a:107:VAL:HG13	1.98	0.44
2:c:21:LYS:CE	2:c:84:GLU:OE2	2.65	0.44
2:e:181:LEU:HD21	2:e:196:PHE:HD2	1.82	0.44
2:f:18:ALA:O	2:f:88:LEU:HG	2.17	0.44
1:I:81:PRO:HD2	1:I:274:LEU:O	2.17	0.44
1:I:159:LEU:HD21	1:I:235:VAL:HG11	1.99	0.44
1:I:322:LYS:HD2	2:i:52:TRP:HE1	1.82	0.44
2:i:14:LYS:HB3	2:i:18:ALA:CB	2.48	0.44
2:j:212:LEU:HD23	2:j:240:LEU:HD21	1.99	0.44
1:K:170:LYS:HE2	1:K:170:LYS:HB3	1.38	0.44
1:L:33:ASN:CG	1:L:34:TRP:H	2.21	0.44
1:L:37:TYR:CE1	1:L:130:TYR:CE2	3.06	0.44
1:M:356:ARG:NE	3:M:401:SO4:O1	2.50	0.44
1:N:78:ILE:CD1	1:N:287:ALA:HB1	2.48	0.44
1:O:160:PHE:HB3	1:O:208:VAL:CG1	2.48	0.44
1:O:297:PRO:O	1:O:300:ILE:HG22	2.17	0.44
1:P:165:MET:HE3	1:P:165:MET:HB3	1.88	0.44
1:Q:102:LYS:HG3	1:Q:288:TYR:CD1	2.52	0.44
2:a:181:LEU:HD11	2:a:196:PHE:CD2	2.53	0.44
1:C:244:PHE:HZ	1:C:329:GLU:CD	2.26	0.44
2:c:173:LEU:HB3	2:c:174:PRO:HD2	1.98	0.44
2:d:38:TRP:CE2	2:d:83:MET:HB2	2.51	0.44
1:F:68:LYS:O	1:F:71:SER:HB3	2.18	0.44
2:f:217:GLU:HG3	2:f:240:LEU:O	2.17	0.44
2:g:26:VAL:HG22	2:g:79:SER:O	2.17	0.44
1:J:46:PHE:CE2	1:J:52:ILE:HB	2.52	0.44
1:J:176:MET:HB2	1:J:182:MET:HE3	1.99	0.44
1:J:176:MET:HE1	1:J:239:TYR:CD2	2.51	0.44
2:j:153:ILE:HG12	2:j:238:THR:HG21	1.99	0.44
2:k:25:LYS:HA	2:k:80:THR:HA	1.99	0.44
1:L:104:PRO:HD2	1:L:292:ASP:OD1	2.18	0.44
1:L:182:MET:HE1	1:L:237:PHE:CD1	2.53	0.44
2:l:137:LEU:HD12	2:l:137:LEU:O	2.17	0.44
2:l:180:LEU:HD21	2:l:183:TYR:HB3	1.99	0.44
2:l:181:LEU:HA	2:l:181:LEU:HD23	1.42	0.44
2:l:217:GLU:HA	2:l:240:LEU:HD23	1.99	0.44
1:O:103:LEU:HD13	1:O:295:LEU:HD12	1.99	0.44
1:Q:206:GLU:HB2	1:Q:357:THR:CG2	2.48	0.44
2:q:15:THR:HB	2:q:16:PRO:CD	2.47	0.44
2:q:55:PRO:HA	2:q:74:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:228:LEU:HD22	1:R:259:ILE:HD12	2.00	0.44
1:R:305:ASP:OD1	1:R:321:ASP:N	2.47	0.44
2:r:220:TYR:O	2:r:238:THR:HG22	2.16	0.44
2:a:161:ASN:OD1	2:a:162:ILE:N	2.47	0.44
1:B:88:LYS:HG2	1:B:345:VAL:HG13	1.99	0.44
2:b:143:VAL:HG13	2:b:240:LEU:HD13	2.00	0.44
2:c:53:ILE:O	2:c:55:PRO:HD3	2.18	0.44
2:c:225:TRP:CE3	2:c:227:SER:HA	2.52	0.44
1:F:100:LYS:HE2	1:F:106:TRP:CH2	2.53	0.44
1:F:266:GLU:CD	1:F:266:GLU:H	2.25	0.44
1:G:317:ARG:C	1:G:319:LEU:H	2.25	0.44
1:H:181:GLU:OE2	4:H:403:SPD:N10	2.50	0.44
2:i:25:LYS:HA	2:i:80:THR:HG22	1.98	0.44
2:i:29:TYR:CE1	2:i:31:PHE:HA	2.52	0.44
1:J:213:ARG:CD	1:J:361:ILE:HG22	2.48	0.44
2:k:168:SER:HB2	2:k:170:TYR:CE1	2.53	0.44
1:L:88:LYS:HA	1:L:88:LYS:HD2	1.67	0.44
2:l:106:ASP:OD2	2:l:107:VAL:HG23	2.17	0.44
2:m:18:ALA:O	2:m:86:SER:O	2.36	0.44
1:N:204:LYS:HA	1:N:207:GLU:OE2	2.17	0.44
1:P:167:LYS:C	1:P:169:ALA:H	2.26	0.44
2:p:99:ALA:HB1	2:p:105:MET:HB3	1.99	0.44
1:Q:32:TYR:HB2	1:Q:76:TYR:CD1	2.52	0.44
1:Q:136:GLY:HA2	1:Q:156:TRP:CH2	2.52	0.44
2:q:147:PRO:HG3	2:q:214:THR:HG22	1.98	0.44
1:R:356:ARG:HD2	3:R:401:SO4:O1	2.18	0.44
1:A:328:GLU:O	1:A:332:PRO:HA	2.17	0.44
2:a:99:ALA:HB1	2:a:105:MET:HB3	1.99	0.44
1:B:62:ASN:HD21	1:B:82:SER:CB	2.30	0.44
1:D:176:MET:HE1	1:D:239:TYR:CD2	2.53	0.44
2:d:164:ARG:HE	2:d:164:ARG:HB2	1.48	0.44
1:E:34:TRP:HA	1:E:59:PHE:O	2.17	0.44
1:E:113:LEU:O	1:E:116:GLN:N	2.50	0.44
1:E:163:GLU:O	1:E:167:LYS:HD3	2.18	0.44
1:H:98:LEU:HD23	1:H:288:TYR:HE1	1.81	0.44
2:h:161:ASN:HB2	2:h:224:VAL:HG23	1.99	0.44
1:J:336:VAL:O	1:J:340:LEU:HG	2.18	0.44
1:K:36:ASP:HB3	1:K:245:GLN:HE22	1.82	0.44
1:K:202:TYR:C	1:K:205:ALA:HB3	2.43	0.44
1:K:302:LYS:HB2	1:K:302:LYS:HE3	1.69	0.44
1:L:310:ALA:HB1	1:L:331:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:104:TYR:O	2:n:106:ASP:N	2.51	0.44
1:O:49:GLU:HG2	1:O:49:GLU:O	2.18	0.44
2:o:51:GLY:C	2:o:72:MET:HE1	2.43	0.44
2:o:99:ALA:HB1	2:o:105:MET:HB3	1.99	0.44
2:o:158:SER:OG	2:o:159:SER:N	2.51	0.44
1:P:52:ILE:HG21	1:P:286:ASN:HD22	1.82	0.44
2:p:181:LEU:HD11	2:p:196:PHE:CD2	2.53	0.44
1:Q:179:GLY:O	1:Q:183:LEU:HB2	2.17	0.44
2:c:50:MET:HA	2:c:66:PHE:CD2	2.52	0.44
2:c:73:THR:OG1	2:c:82:TYR:HB2	2.17	0.44
1:E:137:ILE:HB	1:E:262:VAL:HG13	2.00	0.44
1:E:138:GLY:HA2	1:E:260:GLN:O	2.17	0.44
1:E:160:PHE:HD2	1:E:189:TYR:CD2	2.36	0.44
2:e:151:VAL:CG1	2:e:212:LEU:HD11	2.36	0.44
2:g:58:GLY:HA2	2:g:74:ARG:HE	1.81	0.44
1:H:239:TYR:CZ	4:H:403:SPD:H82	2.51	0.44
2:h:26:VAL:HG21	2:h:31:PHE:CD1	2.53	0.44
1:I:159:LEU:HD23	1:I:165:MET:SD	2.57	0.44
1:K:86:LEU:HD11	1:K:127:ALA:HB2	1.99	0.44
1:K:170:LYS:CG	1:K:171:CYS:N	2.81	0.44
2:m:20:VAL:CG2	2:m:88:LEU:HD11	2.47	0.44
1:N:192:LEU:HD23	1:N:193:ASP:H	1.83	0.44
2:n:13:VAL:C	2:n:14:LYS:HG3	2.41	0.44
1:O:297:PRO:O	1:O:299:VAL:N	2.50	0.44
2:o:181:LEU:HD11	2:o:196:PHE:CD2	2.53	0.44
1:P:200:LYS:HE2	1:P:204:LYS:HZ1	1.83	0.44
2:p:51:GLY:C	2:p:72:MET:HE1	2.43	0.44
1:Q:362:LYS:H	1:Q:362:LYS:HG2	1.47	0.44
2:q:42:ALA:HB1	2:q:43:PRO:HD2	1.99	0.44
1:R:357:THR:O	1:R:361:ILE:HG13	2.18	0.44
2:r:41:GLN:HB3	2:r:95:VAL:HG13	2.00	0.44
1:A:67:GLY:CA	1:K:70:VAL:HG13	2.43	0.44
2:a:91:ASP:OD1	2:a:91:ASP:C	2.59	0.44
1:B:213:ARG:HH11	1:B:361:ILE:C	2.25	0.44
2:b:32:THR:HA	2:b:55:PRO:HB2	1.99	0.44
1:C:225:ILE:HD11	1:C:242:ASP:CG	2.43	0.44
2:d:196:PHE:CD2	2:d:209:ILE:HG22	2.52	0.44
2:e:85:LEU:HD23	2:e:85:LEU:HA	1.86	0.44
1:F:193:ASP:HB3	1:F:196:THR:HB	1.97	0.44
2:f:151:VAL:HG11	2:f:240:LEU:HD11	1.99	0.44
1:I:102:LYS:C	1:I:104:PRO:HD3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:200:LYS:HZ1	1:I:203:LYS:HB2	1.77	0.44
1:L:125:GLN:HG3	1:L:126:TYR:CE2	2.52	0.44
1:N:316:ALA:O	1:N:320:MET:HG3	2.18	0.44
1:O:99:ASP:C	1:O:101:SER:N	2.76	0.44
1:O:317:ARG:NH2	1:O:325:SER:O	2.49	0.44
1:Q:156:TRP:CE2	1:Q:264:PRO:HG2	2.53	0.44
1:R:43:LEU:O	1:R:46:PHE:HB3	2.18	0.44
2:r:49:TRP:HZ2	2:r:52:TRP:HB2	1.83	0.44
2:r:100:ARG:HB3	2:r:107:VAL:HG13	2.00	0.44
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.78	0.44
1:A:244:PHE:CE2	1:A:330:VAL:HG23	2.53	0.44
1:B:250:ALA:HB1	1:B:257:ILE:HB	2.00	0.44
2:b:38:TRP:CE2	2:b:83:MET:HB2	2.53	0.44
1:C:117:LEU:HD13	1:C:274:LEU:HD21	2.00	0.44
1:G:322:LYS:HA	1:G:325:SER:OG	2.17	0.44
2:h:105:MET:HG3	2:h:170:TYR:OH	2.18	0.44
2:i:8:GLU:OE2	2:i:109:GLY:HA3	2.17	0.44
1:J:156:TRP:HB2	1:J:189:TYR:HB2	1.99	0.44
1:J:225:ILE:HD11	1:J:242:ASP:CG	2.43	0.44
2:j:158:SER:OG	2:j:159:SER:N	2.50	0.44
1:K:165:MET:HG2	1:K:215:TYR:HB2	2.00	0.44
1:L:37:TYR:C	1:L:37:TYR:CD1	2.96	0.44
1:L:77:ASP:OD2	1:L:283:ALA:HB3	2.17	0.44
1:L:104:PRO:HB2	1:L:105:ASN:H	1.55	0.44
2:l:195:ARG:NH1	2:l:216:ASP:CG	2.75	0.44
1:M:80:VAL:HA	1:M:274:LEU:O	2.17	0.44
1:N:247:ALA:HA	1:N:259:ILE:HB	2.00	0.44
2:n:29:TYR:O	2:n:31:PHE:N	2.51	0.44
2:p:158:SER:OG	2:p:159:SER:N	2.51	0.44
1:Q:245:GLN:HG3	1:Q:307:VAL:O	2.18	0.44
1:R:162:PRO:HB3	1:R:211:LYS:HE3	2.00	0.44
1:R:247:ALA:HB2	1:R:259:ILE:HB	2.00	0.44
1:A:94:ALA:O	1:A:279:ALA:N	2.46	0.43
2:a:75:ASP:OD1	2:a:77:SER:HB3	2.18	0.43
2:c:75:ASP:CG	2:c:78:ILE:HG13	2.43	0.43
1:E:63:GLU:OE2	1:E:178:SER:OG	2.32	0.43
1:F:62:ASN:HD21	1:F:82:SER:CB	2.31	0.43
2:f:100:ARG:O	2:f:105:MET:HA	2.18	0.43
1:I:159:LEU:HD21	1:I:235:VAL:CG1	2.48	0.43
1:I:165:MET:O	1:I:169:ALA:N	2.51	0.43
2:j:6:LEU:CG	2:j:26:VAL:HG12	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:69:ARG:HG3	2:j:87:ARG:NH1	2.33	0.43
1:K:165:MET:HE3	1:K:165:MET:HB2	1.53	0.43
1:L:206:GLU:O	1:L:210:THR:HG23	2.16	0.43
2:m:52:TRP:N	2:m:72:MET:HE1	2.32	0.43
1:N:188:ASN:HB2	1:N:194:PRO:HD3	1.98	0.43
2:n:9:THR:HG22	2:n:10:GLY:N	2.33	0.43
2:n:41:GLN:HE21	2:n:47:LEU:HD23	1.83	0.43
1:O:90:ILE:HD13	1:O:126:TYR:CD2	2.53	0.43
1:Q:328:GLU:HG2	2:q:166:TYR:HE1	1.83	0.43
1:R:349:LYS:HA	1:R:352:ARG:NH2	2.32	0.43
1:A:62:ASN:HB3	1:A:85:PHE:CE2	2.53	0.43
2:c:53:ILE:HB	2:c:72:MET:HE2	2.00	0.43
2:c:89:ARG:C	2:c:91:ASP:N	2.73	0.43
1:D:247:ALA:HA	1:D:259:ILE:HB	2.00	0.43
1:F:250:ALA:HA	1:F:253:ALA:HB2	1.99	0.43
2:f:31:PHE:HE1	2:f:36:ILE:CD1	2.32	0.43
2:f:49:TRP:HH2	2:f:52:TRP:CB	2.23	0.43
2:g:101:ASP:OD1	2:g:103:ARG:N	2.46	0.43
1:H:271:TRP:CE2	4:H:403:SPD:H71	2.52	0.43
2:j:213:GLN:C	2:j:215:GLY:N	2.77	0.43
1:K:160:PHE:HB3	1:K:208:VAL:CG1	2.48	0.43
2:m:137:LEU:HD22	2:m:162:ILE:HD11	2.00	0.43
1:O:38:ILE:H	1:O:307:VAL:HG11	1.83	0.43
1:O:175:PHE:O	1:O:219:PHE:HA	2.18	0.43
1:P:173:VAL:HA	1:P:235:VAL:O	2.18	0.43
2:p:157:GLY:HA3	2:p:161:ASN:OD1	2.17	0.43
1:Q:175:PHE:HD2	1:Q:182:MET:SD	2.41	0.43
2:r:11:ASP:OD1	2:r:11:ASP:N	2.50	0.43
2:a:50:MET:HG2	2:a:66:PHE:HE2	1.84	0.43
2:a:51:GLY:C	2:a:72:MET:HE1	2.43	0.43
1:B:34:TRP:CE3	4:B:405:SPD:H42	2.54	0.43
2:b:89:ARG:C	2:b:91:ASP:N	2.75	0.43
1:G:31:ILE:HG12	1:G:78:ILE:HB	1.99	0.43
2:g:50:MET:HE2	2:g:50:MET:HB3	1.94	0.43
2:g:90:SER:HA	2:g:116:VAL:HG13	2.00	0.43
2:h:52:TRP:N	2:h:72:MET:HE1	2.33	0.43
2:h:225:TRP:CE3	2:h:225:TRP:C	2.96	0.43
2:k:101:ASP:OD1	2:k:103:ARG:N	2.51	0.43
2:l:39:VAL:CG1	2:l:97:TYR:HB2	2.48	0.43
1:N:138:GLY:HA3	1:N:243:VAL:HG21	2.00	0.43
1:O:251:GLU:O	1:O:254:GLY:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:271:TRP:CD1	4:O:407:SPD:H91	2.53	0.43
2:q:151:VAL:HG12	2:q:212:LEU:HD11	1.99	0.43
2:r:11:ASP:HB3	2:r:113:THR:HB	2.00	0.43
1:C:104:PRO:HD2	1:C:292:ASP:OD1	2.18	0.43
2:c:139:GLN:OE1	2:c:235:GLY:HA3	2.18	0.43
1:D:357:THR:O	1:D:361:ILE:HG13	2.19	0.43
1:E:81:PRO:HD2	1:E:274:LEU:O	2.17	0.43
1:E:173:VAL:HG13	1:E:235:VAL:CG1	2.48	0.43
2:f:52:TRP:N	2:f:72:MET:HE1	2.32	0.43
1:H:211:LYS:HA	1:H:211:LYS:HD2	1.78	0.43
2:h:40:ARG:NH1	2:h:92:ASP:OD1	2.50	0.43
1:J:196:THR:HG21	1:J:201:ASP:HB3	1.99	0.43
1:L:67:GLY:HA3	1:R:71:SER:OG	2.19	0.43
1:L:99:ASP:C	1:L:101:SER:N	2.77	0.43
2:l:63:ALA:HB3	2:l:66:PHE:HD2	1.82	0.43
2:l:146:ALA:HB1	2:l:147:PRO:CD	2.48	0.43
1:M:202:TYR:C	1:M:203:LYS:CG	2.91	0.43
2:m:153:ILE:HG12	2:m:238:THR:HG21	1.99	0.43
1:N:46:PHE:HB2	1:N:293:TYR:CD2	2.53	0.43
1:N:95:PHE:HA	1:N:278:PRO:HA	2.00	0.43
1:O:38:ILE:HG12	1:O:39:ALA:O	2.18	0.43
2:o:157:GLY:HA3	2:o:161:ASN:OD1	2.17	0.43
1:P:301:ALA:O	1:P:304:SER:N	2.52	0.43
2:p:72:MET:HA	2:p:82:TYR:O	2.19	0.43
2:p:75:ASP:OD1	2:p:77:SER:HB3	2.18	0.43
1:Q:347:PRO:HB2	1:Q:350:VAL:HG23	2.01	0.43
1:R:165:MET:HE3	1:R:165:MET:HB3	1.89	0.43
1:A:144:VAL:O	1:A:147:VAL:N	2.52	0.43
1:B:79:VAL:HG23	1:B:81:PRO:HD3	2.01	0.43
2:c:7:VAL:HG22	2:c:25:LYS:HB3	1.99	0.43
1:G:303:VAL:O	1:G:307:VAL:HG22	2.19	0.43
2:g:69:ARG:HH12	2:g:89:ARG:CD	2.32	0.43
2:g:83:MET:CE	2:g:85:LEU:HB2	2.48	0.43
1:J:184:PRO:O	1:J:194:PRO:HB3	2.18	0.43
1:K:137:ILE:HD11	1:K:264:PRO:HG3	1.99	0.43
1:K:151:GLN:HA	1:K:152:PRO:HD3	1.94	0.43
2:k:118:SER:CA	2:p:118:SER:CA	2.96	0.43
2:l:104:TYR:C	2:l:105:MET:HG2	2.40	0.43
2:l:243:LEU:HD12	2:l:243:LEU:HA	1.88	0.43
2:m:25:LYS:HG3	2:m:80:THR:HG22	1.99	0.43
2:m:50:MET:HG2	2:m:66:PHE:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:303:VAL:O	1:N:307:VAL:HG22	2.17	0.43
2:n:49:TRP:CZ2	2:n:52:TRP:HB2	2.53	0.43
2:o:72:MET:HA	2:o:82:TYR:O	2.19	0.43
2:o:75:ASP:OD1	2:o:77:SER:HB3	2.18	0.43
1:P:73:HIS:O	1:P:74:SER:C	2.60	0.43
2:p:149:GLN:CD	1:R:191:GLY:CA	2.90	0.43
1:Q:151:GLN:NE2	1:Q:164:ASN:OD1	2.46	0.43
1:Q:234:CYS:SG	1:Q:235:VAL:HG12	2.59	0.43
1:R:322:LYS:HB2	2:r:225:TRP:CD2	2.53	0.43
2:r:104:TYR:CZ	2:r:183:TYR:CD1	3.06	0.43
1:B:145:LYS:HA	1:B:145:LYS:HD3	1.83	0.43
1:D:109:LEU:HD13	1:D:114:LEU:HD21	2.00	0.43
1:E:204:LYS:HA	1:E:204:LYS:HD3	1.52	0.43
1:E:348:ALA:HA	1:E:351:LEU:HD12	1.99	0.43
1:F:29:LEU:N	1:F:53:ASP:O	2.51	0.43
1:H:240:SER:HA	1:H:261:TYR:CZ	2.53	0.43
2:j:25:LYS:HB2	2:j:80:THR:HG22	2.00	0.43
2:k:53:ILE:HB	2:k:72:MET:HE2	2.01	0.43
2:l:69:ARG:HG2	2:l:86:SER:CB	2.39	0.43
2:l:88:LEU:HD13	2:l:116:VAL:HG21	2.01	0.43
1:P:73:HIS:O	1:P:75:GLY:N	2.51	0.43
1:Q:115:LYS:HA	1:Q:115:LYS:HD3	1.73	0.43
1:Q:150:ASP:N	1:Q:150:ASP:OD1	2.52	0.43
1:Q:160:PHE:HD2	1:Q:189:TYR:CD2	2.36	0.43
2:q:181:LEU:C	2:q:188:ARG:HH11	2.26	0.43
2:r:15:THR:C	2:r:16:PRO:O	2.62	0.43
1:A:138:GLY:O	1:A:235:VAL:HA	2.19	0.43
1:D:115:LYS:HE3	1:D:118:GLU:OE1	2.18	0.43
2:d:20:VAL:HG23	2:d:88:LEU:CD2	2.37	0.43
1:E:153:ILE:HD12	1:E:158:ILE:HG21	1.99	0.43
1:F:100:LYS:HE2	1:F:106:TRP:CZ2	2.54	0.43
1:F:322:LYS:HD3	2:f:225:TRP:CE3	2.53	0.43
1:H:109:LEU:HB3	1:H:114:LEU:HD11	2.00	0.43
1:H:198:ASP:HA	1:H:199:PRO:HD3	1.84	0.43
1:I:132:TRP:HB2	1:I:271:TRP:O	2.19	0.43
2:i:42:ALA:HB1	2:i:43:PRO:HD2	2.00	0.43
2:i:195:ARG:HG2	2:i:210:THR:HG22	2.01	0.43
1:J:160:PHE:HE1	1:J:175:PHE:HE2	1.67	0.43
1:J:182:MET:HE1	1:J:237:PHE:CD2	2.54	0.43
1:J:245:GLN:O	1:J:249:ARG:HG3	2.18	0.43
2:j:225:TRP:HD1	2:j:232:VAL:HG22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:64:GLN:O	2:l:66:PHE:N	2.46	0.43
1:M:33:ASN:O	1:M:58:VAL:HA	2.18	0.43
1:O:347:PRO:HA	3:O:403:SO4:O4	2.18	0.43
1:Q:228:LEU:HD23	1:Q:228:LEU:HA	1.78	0.43
1:B:34:TRP:HH2	1:B:62:ASN:ND2	2.16	0.43
2:d:161:ASN:HB2	2:d:224:VAL:HG21	1.99	0.43
1:E:117:LEU:HD13	1:E:274:LEU:HD11	2.01	0.43
1:G:334:GLN:HG2	1:G:337:LEU:HD12	2.01	0.43
1:J:153:ILE:O	1:J:262:VAL:HG11	2.19	0.43
2:j:110:LYS:HE2	2:j:110:LYS:HB3	1.74	0.43
1:K:271:TRP:CD1	4:K:404:SPD:H101	2.36	0.43
1:K:322:LYS:HD3	2:k:225:TRP:CE3	2.54	0.43
2:k:50:MET:HE2	2:k:50:MET:HB3	1.83	0.43
1:M:202:TYR:O	1:M:206:GLU:N	2.41	0.43
1:M:293:TYR:O	1:M:296:ARG:HG2	2.18	0.43
1:O:154:ASP:N	1:O:154:ASP:OD1	2.48	0.43
1:P:200:LYS:HE2	1:P:204:LYS:NZ	2.34	0.43
1:Q:224:TYR:CZ	1:Q:238:GLY:HA2	2.53	0.43
2:q:31:PHE:HE1	2:q:36:ILE:HD11	1.84	0.43
1:R:169:ALA:O	1:R:170:LYS:C	2.62	0.43
1:A:92:ALA:HB2	1:K:352:ARG:HG2	2.01	0.43
2:a:158:SER:OG	2:a:159:SER:N	2.51	0.43
1:B:330:VAL:HG12	1:B:331:TYR:CD1	2.54	0.43
2:c:49:TRP:CZ2	2:c:52:TRP:HB2	2.54	0.43
2:c:99:ALA:HB1	2:c:105:MET:HB3	2.01	0.43
2:d:38:TRP:CD1	2:d:72:MET:HE3	2.54	0.43
1:E:265:LYS:HE3	1:E:265:LYS:HB2	1.85	0.43
1:F:304:SER:HB3	1:F:320:MET:HE3	1.99	0.43
2:g:49:TRP:CZ2	2:g:52:TRP:HB2	2.54	0.43
2:g:136:VAL:HG22	2:g:137:LEU:H	1.84	0.43
2:h:104:TYR:CD2	2:h:183:TYR:HB2	2.53	0.43
2:i:153:ILE:HD13	2:i:238:THR:CG2	2.49	0.43
1:J:171:CYS:HB3	1:J:234:CYS:HB3	2.00	0.43
1:J:204:LYS:HG2	1:J:207:GLU:CD	2.43	0.43
1:J:305:ASP:CG	1:J:321:ASP:H	2.27	0.43
1:L:97:LYS:H	1:L:97:LYS:HG2	1.50	0.43
1:L:98:LEU:HD23	1:L:103:LEU:HD12	2.01	0.43
2:l:17:GLY:HA2	2:l:88:LEU:N	2.24	0.43
1:M:176:MET:H	1:M:182:MET:CE	2.32	0.43
1:M:201:ASP:HA	1:M:203:LYS:HE3	2.01	0.43
1:M:320:MET:HB2	1:M:325:SER:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:53:ILE:HB	2:m:72:MET:HE2	2.01	0.43
2:n:88:LEU:HD13	2:n:116:VAL:CG1	2.48	0.43
2:q:164:ARG:HG2	2:q:165:ASN:OD1	2.19	0.43
1:R:59:PHE:CE2	1:R:65:LEU:HB2	2.53	0.43
1:A:207:GLU:HA	1:A:210:THR:OG1	2.18	0.43
2:c:137:LEU:HD12	2:c:235:GLY:HA2	2.00	0.43
2:d:51:GLY:C	2:d:72:MET:HE1	2.44	0.43
1:E:210:THR:HG22	1:E:213:ARG:NH1	2.34	0.43
2:e:48:GLU:CD	2:e:65:LYS:HZ3	2.27	0.43
1:F:31:ILE:HG23	1:F:78:ILE:HB	2.00	0.43
1:F:298:GLU:H	1:F:298:GLU:HG3	1.30	0.43
2:g:5:GLN:C	2:g:6:LEU:HD12	2.44	0.43
2:g:20:VAL:HG21	2:g:88:LEU:HD11	2.01	0.43
2:h:161:ASN:HB2	2:h:224:VAL:CG2	2.49	0.43
1:I:170:LYS:HE3	1:I:170:LYS:HB2	1.70	0.43
2:j:53:ILE:O	2:j:55:PRO:HD3	2.18	0.43
2:j:99:ALA:HB1	2:j:105:MET:HB3	2.00	0.43
1:K:165:MET:HG2	1:K:215:TYR:CB	2.49	0.43
1:K:323:SER:HB3	2:k:225:TRP:HE1	1.83	0.43
2:k:25:LYS:HB2	2:k:25:LYS:HE3	1.82	0.43
1:L:362:LYS:HB2	1:L:362:LYS:HE3	1.72	0.43
2:l:26:VAL:HG21	2:l:31:PHE:HB2	2.00	0.43
2:l:162:ILE:HG12	2:l:224:VAL:HG21	2.01	0.43
2:m:10:GLY:O	2:m:112:THR:HG23	2.18	0.43
2:m:161:ASN:HB2	2:m:224:VAL:CG2	2.49	0.43
2:n:212:LEU:HD23	2:n:242:VAL:HG12	2.01	0.43
1:O:125:GLN:HG3	1:O:126:TYR:CE2	2.54	0.43
1:O:206:GLU:OE2	1:O:360:ARG:HD2	2.19	0.43
1:Q:37:TYR:CE1	4:Q:401:SPD:C5	3.01	0.43
1:Q:139:TYR:HD2	1:Q:144:VAL:HG21	1.83	0.43
1:Q:189:TYR:C	1:Q:191:GLY:N	2.75	0.43
2:q:164:ARG:HE	2:q:164:ARG:HB2	1.70	0.43
2:q:200:LYS:HA	2:q:205:THR:HA	2.01	0.43
2:a:53:ILE:HB	2:a:72:MET:HE2	2.01	0.42
2:a:225:TRP:CD1	2:a:232:VAL:HG22	2.50	0.42
1:B:173:VAL:HG13	1:B:235:VAL:HG13	2.01	0.42
1:C:296:ARG:HB2	1:C:299:VAL:HG23	2.01	0.42
2:c:50:MET:HA	2:c:66:PHE:CE2	2.54	0.42
2:c:169:TRP:CH2	2:c:222:CYS:HB3	2.54	0.42
1:E:183:LEU:HD11	1:E:357:THR:HB	2.01	0.42
1:F:173:VAL:HG13	1:F:235:VAL:CG1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:MET:N	1:F:182:MET:HE3	2.28	0.42
2:f:139:GLN:HB3	2:f:155:CYS:HB2	2.01	0.42
2:f:162:ILE:HG12	2:f:224:VAL:HG11	2.01	0.42
1:G:34:TRP:HH2	1:G:62:ASN:ND2	2.17	0.42
1:H:38:ILE:N	1:H:307:VAL:HG11	2.33	0.42
1:I:49:GLU:OE2	1:I:296:ARG:NH2	2.43	0.42
1:I:151:GLN:HG3	1:I:152:PRO:HD2	2.01	0.42
1:I:172:GLY:HA2	1:I:217:SER:OG	2.19	0.42
1:I:323:SER:O	1:I:327:SER:HB2	2.19	0.42
2:k:167:VAL:HG11	2:k:205:THR:HG21	2.00	0.42
1:L:139:TYR:HB2	1:L:144:VAL:HG21	2.00	0.42
2:l:29:TYR:HB3	2:l:100:ARG:HH12	1.80	0.42
1:N:169:ALA:HB2	1:N:215:TYR:HB3	2.01	0.42
1:N:220:HIS:HE1	1:N:222:SER:OG	2.02	0.42
1:N:346:LEU:HB3	1:N:351:LEU:HG	2.01	0.42
2:n:181:LEU:HD11	2:n:196:PHE:CD2	2.54	0.42
1:O:103:LEU:HD23	1:O:103:LEU:HA	1.59	0.42
1:O:187:LEU:HD23	1:O:205:ALA:HB2	2.01	0.42
2:o:50:MET:HG2	2:o:66:PHE:HE2	1.84	0.42
2:p:53:ILE:HB	2:p:72:MET:HE2	2.01	0.42
1:Q:97:LYS:HB2	1:Q:97:LYS:HE3	1.86	0.42
1:Q:140:ASN:ND2	1:Q:143:LYS:HB2	2.34	0.42
2:q:85:LEU:HD12	2:q:88:LEU:HD23	2.00	0.42
1:R:104:PRO:HD2	1:R:292:ASP:CG	2.44	0.42
1:A:107:LYS:HA	1:A:107:LYS:HD2	1.59	0.42
1:A:352:ARG:NH2	3:A:403:SO4:O3	2.43	0.42
1:D:187:LEU:HD23	1:D:205:ALA:HB2	2.02	0.42
1:E:245:GLN:OE1	1:E:249:ARG:NH2	2.52	0.42
2:e:50:MET:HE2	2:e:50:MET:HB3	1.71	0.42
1:F:109:LEU:HD13	1:F:114:LEU:HD21	2.00	0.42
1:G:298:GLU:HG2	2:g:56:ASN:ND2	2.34	0.42
1:H:63:GLU:O	1:H:66:GLU:N	2.53	0.42
1:I:205:ALA:O	1:I:208:VAL:HG12	2.19	0.42
2:k:78:ILE:HD11	2:m:64:GLN:HE22	1.84	0.42
1:L:280:ASP:OD1	1:L:280:ASP:N	2.52	0.42
1:M:139:TYR:HB2	1:M:144:VAL:HG21	2.00	0.42
2:m:102:LYS:O	2:m:103:ARG:HB2	2.18	0.42
2:m:192:ILE:HD13	2:m:192:ILE:HA	1.85	0.42
1:N:213:ARG:HD2	1:N:361:ILE:O	2.19	0.42
2:n:158:SER:C	2:n:160:SER:N	2.77	0.42
2:o:31:PHE:CD2	2:o:79:SER:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:103:LEU:HD21	1:P:291:ILE:HG22	2.00	0.42
2:p:50:MET:HG2	2:p:66:PHE:HE2	1.84	0.42
1:Q:176:MET:HA	1:Q:220:HIS:O	2.19	0.42
2:q:62:TYR:HD2	2:q:67:GLN:OE1	2.02	0.42
2:q:147:PRO:O	2:q:149:GLN:NE2	2.52	0.42
1:R:33:ASN:O	1:R:58:VAL:HA	2.19	0.42
1:R:37:TYR:CD1	1:R:130:TYR:HE2	2.37	0.42
1:R:166:LYS:HA	1:R:166:LYS:HD2	1.77	0.42
1:R:190:LEU:HD11	1:R:208:VAL:CG2	2.45	0.42
2:r:85:LEU:HD13	2:r:92:ASP:OD2	2.19	0.42
2:r:99:ALA:CB	2:r:105:MET:HB3	2.48	0.42
2:a:72:MET:HA	2:a:82:TYR:O	2.19	0.42
2:a:188:ARG:HD2	2:a:196:PHE:O	2.19	0.42
1:B:260:GLN:HG3	1:B:261:TYR:H	1.84	0.42
1:B:328:GLU:O	1:B:332:PRO:HA	2.20	0.42
1:C:203:LYS:HD2	1:C:203:LYS:HA	1.75	0.42
1:D:283:ALA:HB1	1:D:286:ASN:HB2	2.01	0.42
1:H:135:ASN:OD1	1:H:269:ASN:HB3	2.19	0.42
1:I:60:ASP:HB2	1:I:222:SER:HB2	2.00	0.42
1:J:137:ILE:HD11	1:J:264:PRO:HG3	2.00	0.42
1:K:187:LEU:HB2	1:K:194:PRO:HA	2.00	0.42
1:L:233:ILE:HD12	1:L:236:ALA:HB2	2.01	0.42
1:O:84:ASN:ND2	1:O:180:ASP:OD2	2.51	0.42
2:q:18:ALA:O	2:q:86:SER:O	2.38	0.42
1:R:137:ILE:HD11	1:R:264:PRO:HG3	2.00	0.42
1:R:182:MET:HE1	1:R:237:PHE:CD2	2.54	0.42
1:A:91:GLN:O	1:K:356:ARG:NH1	2.52	0.42
2:a:31:PHE:CD2	2:a:79:SER:HA	2.55	0.42
2:c:188:ARG:HD2	2:c:196:PHE:O	2.20	0.42
1:D:46:PHE:HB2	1:D:293:TYR:CE2	2.53	0.42
1:D:143:LYS:HG2	1:D:171:CYS:SG	2.59	0.42
1:D:156:TRP:CD2	1:D:264:PRO:HG2	2.53	0.42
1:D:207:GLU:HG2	1:D:210:THR:OG1	2.20	0.42
1:I:213:ARG:HE	1:I:213:ARG:HB3	1.54	0.42
1:I:265:LYS:HE2	1:I:265:LYS:HB3	1.67	0.42
2:j:4:VAL:HG21	2:j:100:ARG:NH1	2.33	0.42
2:j:37:SER:CB	2:j:49:TRP:HZ3	2.32	0.42
1:K:143:LYS:O	1:K:147:VAL:HG22	2.19	0.42
1:K:265:LYS:HA	1:K:265:LYS:HD2	1.90	0.42
1:L:97:LYS:HD3	1:L:126:TYR:HE1	1.82	0.42
2:l:25:LYS:HG3	2:l:26:VAL:N	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:113:THR:HG22	2:l:115:THR:HG23	2.01	0.42
1:M:266:GLU:H	1:M:266:GLU:CD	2.28	0.42
1:N:145:LYS:C	1:N:147:VAL:H	2.27	0.42
1:N:178:SER:C	1:N:180:ASP:H	2.27	0.42
1:N:178:SER:O	1:N:180:ASP:N	2.53	0.42
1:N:243:VAL:CG1	1:N:261:TYR:HB2	2.48	0.42
2:n:89:ARG:O	2:n:116:VAL:HG21	2.19	0.42
1:O:176:MET:SD	1:O:239:TYR:HE2	2.42	0.42
1:O:207:GLU:O	1:O:211:LYS:HB2	2.19	0.42
1:P:34:TRP:CE3	4:P:401:SPD:H42	2.54	0.42
1:P:244:PHE:HE2	1:P:329:GLU:HB2	1.82	0.42
1:Q:315:GLY:O	1:Q:318:PRO:HD2	2.19	0.42
1:R:102:LYS:HG3	1:R:288:TYR:CE2	2.54	0.42
1:A:337:LEU:C	1:A:339:LYS:N	2.78	0.42
2:c:14:LYS:O	2:c:116:VAL:HA	2.19	0.42
2:c:169:TRP:HB2	2:c:182:LEU:HB2	2.02	0.42
1:D:44:LYS:HE3	1:D:44:LYS:HB2	1.73	0.42
2:e:68:GLY:O	2:e:87:ARG:NH2	2.52	0.42
2:e:226:ASP:HB3	2:e:229:LEU:HB2	2.00	0.42
1:G:346:LEU:HB2	1:G:351:LEU:HD21	2.00	0.42
1:I:82:SER:OG	4:I:404:SPD:H81	2.19	0.42
2:i:103:ARG:NH2	2:i:184:ASP:OD1	2.47	0.42
1:K:117:LEU:HD21	1:K:272:PHE:HB2	2.02	0.42
2:l:171:GLN:HE22	2:l:207:LEU:CD2	2.33	0.42
1:M:138:GLY:HA2	1:M:260:GLN:O	2.19	0.42
2:m:212:LEU:HA	2:m:212:LEU:HD12	1.58	0.42
2:o:91:ASP:OD1	2:o:91:ASP:C	2.59	0.42
2:p:105:MET:HG3	2:p:170:TYR:OH	2.20	0.42
1:R:307:VAL:HG22	1:R:309:TYR:HD2	1.84	0.42
2:r:153:ILE:HD13	2:r:238:THR:CG2	2.48	0.42
1:D:181:GLU:OE2	4:D:404:SPD:N10	2.53	0.42
1:D:220:HIS:CD2	1:D:223:LYS:HB2	2.55	0.42
1:E:165:MET:HE3	1:E:165:MET:HB3	1.70	0.42
2:e:138:THR:HG21	1:G:150:ASP:OD1	2.20	0.42
2:e:150:LYS:HG3	2:e:210:THR:HG22	2.01	0.42
1:F:137:ILE:O	1:F:261:TYR:HA	2.20	0.42
2:f:102:LYS:O	2:f:103:ARG:HB2	2.19	0.42
2:f:151:VAL:HG12	2:f:212:LEU:HD11	2.01	0.42
2:f:181:LEU:HD21	2:f:196:PHE:HD2	1.82	0.42
1:G:139:TYR:HE2	1:G:141:VAL:HG23	1.84	0.42
2:g:184:ASP:O	2:g:185:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:330:VAL:O	1:H:332:PRO:HD3	2.19	0.42
2:i:137:LEU:HB3	2:i:156:SER:O	2.20	0.42
2:i:169:TRP:HZ2	2:i:205:THR:HG23	1.85	0.42
1:J:257:ILE:HG22	1:J:259:ILE:HG12	2.02	0.42
1:K:170:LYS:CG	1:K:171:CYS:H	2.32	0.42
1:M:62:ASN:ND2	1:M:85:PHE:CG	2.88	0.42
1:M:182:MET:HG3	1:M:358:TRP:CH2	2.55	0.42
1:N:170:LYS:HE2	1:N:170:LYS:HB2	1.72	0.42
1:N:173:VAL:HA	1:N:235:VAL:O	2.19	0.42
1:N:178:SER:C	1:N:180:ASP:N	2.77	0.42
1:O:33:ASN:CG	1:O:34:TRP:H	2.26	0.42
1:O:326:ASP:HB3	2:o:165:ASN:HB3	2.01	0.42
2:o:40:ARG:HD2	2:o:96:TYR:OH	2.20	0.42
1:P:128:VAL:HG21	1:P:291:ILE:HG21	2.01	0.42
1:P:242:ASP:OD1	1:P:309:TYR:OH	2.32	0.42
1:P:275:MET:HB3	1:P:291:ILE:HD11	2.01	0.42
1:P:346:LEU:HB3	1:P:350:VAL:HG21	2.02	0.42
1:Q:104:PRO:HD2	1:Q:292:ASP:CG	2.45	0.42
2:q:100:ARG:HB3	2:q:107:VAL:CG1	2.49	0.42
1:R:182:MET:HE1	1:R:237:PHE:CD1	2.55	0.42
1:R:208:VAL:O	1:R:212:VAL:HG13	2.20	0.42
2:r:49:TRP:CZ3	2:r:231:ALA:HA	2.55	0.42
2:r:99:ALA:HB1	2:r:105:MET:HB3	2.02	0.42
2:a:40:ARG:HD2	2:a:96:TYR:OH	2.20	0.42
2:b:66:PHE:HB3	2:b:70:VAL:HG12	2.02	0.42
1:D:67:GLY:HA3	1:J:71:SER:OG	2.20	0.42
1:D:135:ASN:CG	1:D:269:ASN:HB3	2.45	0.42
1:D:210:THR:CG2	1:D:361:ILE:HG12	2.50	0.42
2:h:29:TYR:CG	2:h:100:ARG:NH1	2.88	0.42
1:J:104:PRO:HD2	1:J:292:ASP:CG	2.45	0.42
1:J:159:LEU:HD21	1:J:235:VAL:HG11	2.02	0.42
2:j:213:GLN:C	2:j:215:GLY:H	2.28	0.42
2:k:100:ARG:CB	2:k:107:VAL:HG22	2.49	0.42
1:L:32:TYR:HA	1:L:57:ASP:O	2.20	0.42
1:L:98:LEU:HD21	1:L:128:VAL:CG2	2.50	0.42
2:l:52:TRP:CD1	2:l:61:ASN:OD1	2.73	0.42
2:m:8:GLU:HA	2:m:23:SER:O	2.20	0.42
2:m:38:TRP:CD2	2:m:83:MET:HB2	2.54	0.42
1:N:160:PHE:HA	1:N:212:VAL:HG11	2.01	0.42
2:n:223:GLY:HA2	2:n:233:LEU:O	2.20	0.42
1:O:47:THR:HG22	1:O:52:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:247:ALA:HA	1:O:259:ILE:HB	2.01	0.42
1:P:29:LEU:CD1	1:P:77:ASP:HB2	2.50	0.42
1:P:128:VAL:O	1:P:275:MET:N	2.52	0.42
1:P:135:ASN:O	1:P:268:ALA:HB1	2.20	0.42
2:p:225:TRP:CD1	2:p:232:VAL:HG22	2.50	0.42
2:q:10:GLY:O	2:q:11:ASP:O	2.37	0.42
1:A:316:ALA:O	1:A:320:MET:HG3	2.19	0.42
2:a:58:GLY:HA2	2:a:74:ARG:HE	1.85	0.42
2:b:9:THR:HG21	2:b:22:VAL:HA	2.01	0.42
1:F:97:LYS:HG2	1:F:126:TYR:CE1	2.55	0.42
2:f:16:PRO:HD3	2:f:117:SER:O	2.19	0.42
2:g:90:SER:O	2:g:93:THR:OG1	2.25	0.42
1:H:113:LEU:O	1:H:116:GLN:N	2.52	0.42
1:H:147:VAL:HG22	1:H:148:LEU:CD1	2.50	0.42
1:I:243:VAL:HG11	1:I:261:TYR:HB2	2.02	0.42
2:i:70:VAL:HA	2:i:84:GLU:O	2.20	0.42
2:i:207:LEU:HD12	2:i:208:ALA:N	2.35	0.42
1:J:207:GLU:O	1:J:211:LYS:N	2.50	0.42
1:O:155:SER:C	1:O:157:ALA:N	2.77	0.42
1:P:171:CYS:HB3	1:P:234:CYS:SG	2.60	0.42
1:P:191:GLY:HA3	2:r:149:GLN:HG3	2.02	0.42
2:a:105:MET:HG3	2:a:170:TYR:OH	2.20	0.42
1:B:183:LEU:HD13	1:B:202:TYR:CD2	2.55	0.42
2:b:25:LYS:CB	2:b:80:THR:HG22	2.50	0.42
2:b:167:VAL:HA	2:b:224:VAL:HG12	2.02	0.42
1:C:46:PHE:CE1	1:C:290:PHE:HA	2.53	0.42
1:C:63:GLU:OE1	1:C:63:GLU:N	2.49	0.42
2:d:20:VAL:HG21	2:d:88:LEU:CD2	2.34	0.42
2:d:154:SER:O	2:d:155:CYS:HB2	2.19	0.42
1:E:249:ARG:O	1:E:253:ALA:HB2	2.20	0.42
1:F:72:GLY:O	1:F:73:HIS:C	2.62	0.42
1:G:145:LYS:HD2	1:G:150:ASP:HA	2.02	0.42
1:H:88:LYS:HE3	1:H:348:ALA:HB2	2.01	0.42
2:i:49:TRP:CZ2	2:i:51:GLY:HA2	2.55	0.42
2:i:118:SER:HA	2:o:118:SER:CB	2.50	0.42
1:K:136:GLY:HA2	1:K:156:TRP:CH2	2.54	0.42
1:L:74:SER:O	1:L:76:TYR:N	2.46	0.42
2:l:162:ILE:O	2:l:200:LYS:HE2	2.20	0.42
2:l:212:LEU:HD23	2:l:213:GLN:O	2.20	0.42
1:N:189:TYR:C	1:N:191:GLY:N	2.77	0.42
2:n:142:SER:HB3	1:O:163:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:53:ILE:HB	2:o:72:MET:HE2	2.01	0.42
2:p:31:PHE:CD2	2:p:79:SER:HA	2.55	0.42
2:p:188:ARG:HD2	2:p:196:PHE:O	2.19	0.42
2:q:145:GLY:O	2:q:242:VAL:HA	2.20	0.42
2:r:42:ALA:HB3	2:r:45:GLN:HB2	2.02	0.42
2:r:213:GLN:HG3	2:r:214:THR:N	2.35	0.42
1:B:247:ALA:HA	1:B:259:ILE:HB	2.01	0.42
2:d:167:VAL:HG22	2:d:224:VAL:HG11	2.02	0.42
2:e:154:SER:HA	2:e:206:THR:HA	2.01	0.42
1:F:32:TYR:HB2	1:F:76:TYR:CG	2.55	0.42
1:F:155:SER:HB2	1:F:265:LYS:HD3	2.01	0.42
1:F:322:LYS:O	1:F:326:ASP:HB2	2.19	0.42
2:f:165:ASN:ND2	2:f:225:TRP:O	2.45	0.42
1:G:301:ALA:HB2	1:G:316:ALA:HB1	2.02	0.42
1:H:83:ASN:OD1	1:H:83:ASN:N	2.52	0.42
2:i:117:SER:O	2:i:118:SER:HB2	2.18	0.42
2:i:139:GLN:NE2	2:i:238:THR:H	2.12	0.42
1:K:81:PRO:HD2	1:K:274:LEU:O	2.20	0.42
1:L:109:LEU:HD12	1:L:109:LEU:C	2.45	0.42
1:L:148:LEU:HD12	1:L:167:LYS:HE2	2.02	0.42
1:L:283:ALA:C	1:L:285:ASP:N	2.77	0.42
1:L:346:LEU:HD13	1:L:350:VAL:HG11	2.01	0.42
2:n:18:ALA:HA	2:n:88:LEU:HD12	1.76	0.42
2:n:88:LEU:HB3	2:n:116:VAL:HG11	2.02	0.42
1:O:38:ILE:CD1	1:O:43:LEU:HG	2.49	0.42
1:O:180:ASP:O	1:O:184:PRO:HG2	2.20	0.42
1:O:316:ALA:O	1:O:319:LEU:N	2.53	0.42
2:o:105:MET:HG3	2:o:170:TYR:OH	2.20	0.42
2:o:188:ARG:HD2	2:o:196:PHE:O	2.19	0.42
1:Q:67:GLY:HA2	1:Q:70:VAL:HG12	2.01	0.42
1:Q:245:GLN:O	1:Q:249:ARG:HG3	2.20	0.42
1:Q:294:LEU:HD23	1:Q:294:LEU:HA	1.87	0.42
2:q:207:LEU:CG	2:q:208:ALA:N	2.67	0.42
1:B:37:TYR:OH	1:B:131:LEU:HB2	2.20	0.41
1:B:171:CYS:O	1:B:233:ILE:HA	2.20	0.41
1:C:48:LYS:HE3	1:C:48:LYS:HB2	1.71	0.41
1:C:141:VAL:O	1:C:145:LYS:HG2	2.20	0.41
1:C:210:THR:CG2	1:C:361:ILE:HG12	2.50	0.41
2:e:31:PHE:HE1	2:e:36:ILE:CD1	2.31	0.41
2:h:167:VAL:HG23	2:h:185:ASN:OD1	2.19	0.41
2:h:226:ASP:C	2:h:228:SER:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:109:LEU:HD13	1:K:114:LEU:HD21	2.02	0.41
1:K:204:LYS:HA	1:K:207:GLU:HB2	2.01	0.41
2:l:97:TYR:CZ	2:l:178:PRO:HD2	2.54	0.41
2:l:167:VAL:HG11	2:l:205:THR:HG21	2.02	0.41
1:M:95:PHE:HA	1:M:278:PRO:HA	2.02	0.41
2:m:85:LEU:HD23	2:m:86:SER:N	2.35	0.41
2:m:162:ILE:HD13	2:m:205:THR:HG22	2.02	0.41
1:N:37:TYR:CE1	1:N:131:LEU:HD12	2.55	0.41
2:n:224:VAL:HG12	2:n:225:TRP:N	2.30	0.41
1:P:243:VAL:HG11	1:P:261:TYR:HB2	2.02	0.41
1:P:280:ASP:OD1	1:P:281:ALA:N	2.52	0.41
1:Q:33:ASN:O	1:Q:58:VAL:HA	2.20	0.41
2:b:31:PHE:CD2	2:b:79:SER:HA	2.55	0.41
2:c:182:LEU:CD2	2:c:188:ARG:HG3	2.49	0.41
1:D:298:GLU:H	1:D:298:GLU:HG2	1.27	0.41
2:d:6:LEU:HD23	2:d:98:CYS:SG	2.60	0.41
1:E:113:LEU:O	1:E:116:GLN:HB3	2.20	0.41
1:E:295:LEU:HD22	1:E:313:ILE:HD11	2.02	0.41
2:e:158:SER:OG	2:e:159:SER:N	2.52	0.41
1:G:104:PRO:HD2	1:G:292:ASP:CG	2.45	0.41
1:G:141:VAL:HG11	1:G:258:ASP:OD2	2.20	0.41
1:I:186:ALA:O	1:I:190:LEU:HG	2.20	0.41
2:i:89:ARG:O	2:i:92:ASP:N	2.35	0.41
1:J:323:SER:HA	2:j:225:TRP:CZ3	2.55	0.41
2:m:11:ASP:OD1	2:m:113:THR:N	2.53	0.41
1:N:37:TYR:HD1	1:N:130:TYR:CE2	2.37	0.41
1:N:183:LEU:HB2	1:N:184:PRO:HD3	2.02	0.41
1:N:247:ALA:CA	1:N:259:ILE:HB	2.50	0.41
1:N:357:THR:O	1:N:360:ARG:HG2	2.19	0.41
2:n:161:ASN:OD1	2:n:162:ILE:N	2.38	0.41
1:P:110:ASP:HB3	1:P:314:PRO:HG2	2.01	0.41
1:P:251:GLU:O	1:P:254:GLY:N	2.52	0.41
2:p:40:ARG:HD2	2:p:96:TYR:OH	2.20	0.41
1:Q:34:TRP:HB3	4:Q:401:SPD:H42	2.01	0.41
1:Q:128:VAL:HG21	1:Q:291:ILE:HG21	2.02	0.41
2:q:158:SER:C	2:q:160:SER:H	2.27	0.41
1:A:68:LYS:O	1:A:71:SER:HB3	2.20	0.41
1:A:327:SER:HB3	1:A:330:VAL:HB	2.02	0.41
2:c:21:LYS:CE	2:c:84:GLU:CD	2.90	0.41
1:D:107:LYS:H	1:D:107:LYS:HG3	1.62	0.41
2:e:13:VAL:HA	2:e:115:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:GLY:HA2	1:F:260:GLN:O	2.19	0.41
2:i:149:GLN:HG3	2:i:150:LYS:O	2.19	0.41
1:J:156:TRP:CD2	1:J:264:PRO:HG2	2.56	0.41
1:K:139:TYR:HB3	1:K:235:VAL:HG23	2.02	0.41
1:K:241:GLY:O	1:K:245:GLN:HB2	2.20	0.41
1:L:195:ASN:ND2	1:L:344:ALA:H	2.17	0.41
1:L:297:PRO:HB2	1:L:298:GLU:H	1.60	0.41
2:l:102:LYS:O	2:l:103:ARG:HG3	2.20	0.41
2:l:143:VAL:CG1	2:l:144:SER:N	2.82	0.41
1:N:97:LYS:HB3	1:N:97:LYS:HE2	1.75	0.41
2:n:158:SER:N	2:n:161:ASN:OD1	2.51	0.41
1:O:37:TYR:CE1	1:O:131:LEU:HD12	2.55	0.41
1:O:93:GLY:O	1:O:94:ALA:C	2.63	0.41
1:R:49:GLU:OE2	1:R:296:ARG:NH2	2.44	0.41
1:R:100:LYS:HE3	1:R:106:TRP:CZ2	2.55	0.41
2:r:9:THR:HB	2:r:22:VAL:HG13	2.02	0.41
2:r:154:SER:OG	2:r:155:CYS:N	2.52	0.41
1:B:104:PRO:HD2	1:B:292:ASP:CG	2.46	0.41
2:b:110:LYS:HB3	2:b:110:LYS:HE2	1.78	0.41
2:b:225:TRP:CZ2	2:b:230:ARG:HA	2.55	0.41
1:D:46:PHE:CD2	1:D:290:PHE:HD1	2.38	0.41
1:D:282:LYS:HA	1:D:282:LYS:HD3	1.85	0.41
2:e:189:PRO:HD2	2:e:192:ILE:HG13	2.01	0.41
1:F:176:MET:HE1	1:F:239:TYR:CD2	2.56	0.41
1:H:176:MET:H	1:H:182:MET:HE3	1.85	0.41
2:h:161:ASN:OD1	2:h:162:ILE:N	2.50	0.41
2:j:87:ARG:O	2:j:88:LEU:C	2.63	0.41
1:K:132:TRP:HB2	1:K:271:TRP:O	2.20	0.41
2:k:16:PRO:HD2	2:k:118:SER:HG	1.84	0.41
2:l:103:ARG:NH2	2:l:184:ASP:OD1	2.52	0.41
1:M:34:TRP:CD2	4:M:404:SPD:H42	2.55	0.41
1:N:46:PHE:HB2	1:N:293:TYR:CE2	2.56	0.41
1:O:34:TRP:CE3	4:O:407:SPD:H42	2.55	0.41
2:o:225:TRP:CD1	2:o:232:VAL:HG22	2.50	0.41
1:P:176:MET:N	1:P:182:MET:HE3	2.32	0.41
1:R:304:SER:HA	1:R:307:VAL:CG1	2.50	0.41
2:r:184:ASP:O	2:r:186:ASN:N	2.50	0.41
1:A:106:TRP:HA	1:A:295:LEU:HD13	2.03	0.41
1:B:154:ASP:O	1:B:265:LYS:N	2.52	0.41
2:b:18:ALA:HA	2:b:88:LEU:CB	2.49	0.41
2:c:101:ASP:OD1	2:c:103:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:TYR:OH	4:D:404:SPD:H32	2.20	0.41
1:F:243:VAL:HG11	1:F:261:TYR:HB2	2.02	0.41
2:f:167:VAL:HG11	2:f:205:THR:HG21	2.03	0.41
1:G:171:CYS:HB3	1:G:234:CYS:SG	2.61	0.41
2:h:89:ARG:O	2:h:116:VAL:HG21	2.21	0.41
1:I:102:LYS:O	1:I:104:PRO:HD3	2.21	0.41
2:i:78:ILE:O	2:i:79:SER:HB2	2.20	0.41
1:J:187:LEU:N	1:J:187:LEU:HD23	2.36	0.41
1:K:140:ASN:O	1:K:144:VAL:HG23	2.20	0.41
1:K:182:MET:HE1	1:K:237:PHE:CD2	2.55	0.41
2:k:5:GLN:C	2:k:6:LEU:HD12	2.45	0.41
2:l:14:LYS:O	2:l:116:VAL:HG12	2.21	0.41
2:l:17:GLY:H	2:l:88:LEU:CD1	2.34	0.41
2:l:243:LEU:HG	1:Q:204:LYS:CE	2.50	0.41
1:N:273:ASP:OD2	4:N:407:SPD:N6	2.53	0.41
1:O:79:VAL:HG22	1:O:95:PHE:HE1	1.85	0.41
1:O:323:SER:OG	2:o:225:TRP:HZ3	1.92	0.41
2:o:219:ASP:OD1	2:o:239:LYS:HG3	2.21	0.41
1:P:83:ASN:N	1:P:272:PHE:O	2.52	0.41
1:Q:70:VAL:C	1:Q:72:GLY:N	2.78	0.41
1:Q:97:LYS:HB3	1:Q:126:TYR:CE1	2.55	0.41
1:A:153:ILE:HG23	1:A:158:ILE:HG13	2.03	0.41
1:B:300:ILE:HD12	1:B:303:VAL:HB	2.03	0.41
2:b:88:LEU:HA	2:b:92:ASP:OD2	2.19	0.41
1:D:102:LYS:NZ	1:D:285:ASP:OD1	2.54	0.41
1:D:108:ASN:O	1:D:314:PRO:HD2	2.21	0.41
1:D:165:MET:HE3	1:D:165:MET:HB3	1.79	0.41
1:E:43:LEU:HB3	1:E:54:VAL:HG21	2.03	0.41
2:e:149:GLN:HG3	2:e:150:LYS:N	2.34	0.41
2:e:182:LEU:HD13	2:e:198:ALA:HB2	2.03	0.41
1:F:73:HIS:HA	1:F:280:ASP:OD2	2.19	0.41
1:F:156:TRP:CD2	1:F:264:PRO:HG2	2.56	0.41
1:I:163:GLU:H	1:I:163:GLU:HG3	1.48	0.41
2:i:19:SER:CB	2:i:86:SER:HA	2.39	0.41
2:i:52:TRP:HZ3	2:i:54:ASN:HB2	1.86	0.41
2:j:25:LYS:HA	2:j:80:THR:HG22	2.03	0.41
1:K:160:PHE:HB3	1:K:208:VAL:HG12	2.03	0.41
1:L:304:SER:O	1:L:324:VAL:HG11	2.20	0.41
2:l:144:SER:HB2	1:Q:190:LEU:CD2	2.50	0.41
1:M:108:ASN:HB3	1:M:313:ILE:HG23	2.02	0.41
2:m:20:VAL:HG21	2:m:114:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:353:LEU:O	1:N:357:THR:HG23	2.20	0.41
2:n:18:ALA:C	2:n:19:SER:O	2.61	0.41
2:o:58:GLY:HA2	2:o:74:ARG:HE	1.85	0.41
1:P:153:ILE:O	1:P:262:VAL:HG21	2.21	0.41
2:p:219:ASP:OD1	2:p:239:LYS:HG3	2.21	0.41
1:R:180:ASP:O	1:R:184:PRO:HG2	2.21	0.41
2:r:189:PRO:HD2	2:r:192:ILE:HG13	2.01	0.41
1:B:37:TYR:CE1	1:B:131:LEU:HD12	2.56	0.41
1:B:206:GLU:O	1:B:210:THR:HG23	2.20	0.41
1:C:136:GLY:HA2	1:C:156:TRP:CH2	2.56	0.41
1:D:104:PRO:HD2	1:D:292:ASP:CG	2.46	0.41
1:E:52:ILE:HG21	1:E:286:ASN:HB3	2.01	0.41
1:F:72:GLY:O	1:F:74:SER:N	2.54	0.41
2:f:101:ASP:OD1	2:f:103:ARG:N	2.48	0.41
2:g:167:VAL:HG23	2:g:185:ASN:ND2	2.35	0.41
1:H:135:ASN:CG	1:H:269:ASN:HB3	2.44	0.41
2:h:188:ARG:HD2	2:h:192:ILE:HG22	2.02	0.41
1:I:246:ALA:O	1:I:250:ALA:N	2.49	0.41
1:K:183:LEU:HD23	1:K:209:LEU:HD13	2.03	0.41
1:K:197:HIS:HE1	1:K:346:LEU:HD22	1.85	0.41
1:L:281:ALA:HB3	1:L:284:ALA:HB2	2.01	0.41
2:l:50:MET:HG2	2:l:66:PHE:HE2	1.85	0.41
1:N:220:HIS:ND1	1:N:223:LYS:HG2	2.35	0.41
2:n:85:LEU:CD1	2:n:88:LEU:HD23	2.50	0.41
1:P:66:GLU:O	1:P:70:VAL:HG12	2.21	0.41
2:p:171:GLN:HG3	2:p:220:TYR:CE1	2.56	0.41
1:Q:88:LYS:HG3	1:Q:89:GLN:N	2.35	0.41
2:q:168:SER:HA	2:q:182:LEU:HD12	2.02	0.41
2:r:200:LYS:HD2	2:r:205:THR:HB	2.01	0.41
2:b:104:TYR:CD2	2:b:183:TYR:HB2	2.56	0.41
1:C:203:LYS:NZ	1:C:207:GLU:OE1	2.44	0.41
2:c:225:TRP:HZ3	2:c:227:SER:HA	1.78	0.41
1:D:117:LEU:HD22	1:D:274:LEU:HD11	2.02	0.41
1:D:172:GLY:HA2	1:D:217:SER:OG	2.20	0.41
2:d:16:PRO:O	2:d:16:PRO:CG	2.69	0.41
2:e:8:GLU:OE2	2:e:109:GLY:HA3	2.21	0.41
2:h:106:ASP:HA	2:h:180:LEU:HD22	2.01	0.41
2:h:225:TRP:CZ3	2:h:227:SER:C	2.83	0.41
1:J:139:TYR:HE1	1:J:262:VAL:CG2	2.34	0.41
2:k:26:VAL:CG2	2:k:26:VAL:C	2.94	0.41
2:k:212:LEU:HD23	2:k:240:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:189:TYR:C	1:L:191:GLY:H	2.29	0.41
2:l:41:GLN:HB2	2:l:47:LEU:HD23	2.02	0.41
1:M:39:ALA:HB3	1:M:42:THR:OG1	2.21	0.41
1:M:317:ARG:HG2	1:M:325:SER:HB2	2.01	0.41
1:N:176:MET:O	1:N:219:PHE:HB3	2.20	0.41
2:n:58:GLY:HA2	2:n:74:ARG:HE	1.86	0.41
2:n:192:ILE:HD13	2:n:192:ILE:HA	1.87	0.41
2:n:239:LYS:HE2	2:n:239:LYS:HB3	1.50	0.41
1:O:29:LEU:HD12	1:O:77:ASP:HB2	2.02	0.41
1:P:37:TYR:CE1	1:P:131:LEU:HB2	2.55	0.41
1:P:304:SER:OG	1:P:311:ASN:ND2	2.47	0.41
1:P:317:ARG:NH2	1:P:325:SER:O	2.47	0.41
1:Q:184:PRO:CA	1:Q:194:PRO:HB3	2.45	0.41
1:Q:200:LYS:HG2	1:Q:203:LYS:CB	2.49	0.41
1:Q:317:ARG:HB3	1:Q:318:PRO:HD3	2.01	0.41
1:R:112:ALA:HA	1:R:115:LYS:NZ	2.36	0.41
1:R:145:LYS:HA	1:R:149:GLY:O	2.21	0.41
1:A:173:VAL:HG13	1:A:235:VAL:HG13	2.03	0.41
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.86	0.41
2:a:171:GLN:HG3	2:a:220:TYR:CE1	2.56	0.41
2:a:219:ASP:OD1	2:a:239:LYS:HG3	2.21	0.41
2:b:4:VAL:HA	2:b:27:SER:O	2.21	0.41
2:b:89:ARG:O	2:b:90:SER:C	2.64	0.41
2:b:169:TRP:HB2	2:b:182:LEU:HB2	2.03	0.41
2:b:239:LYS:HE3	2:b:239:LYS:HB2	1.70	0.41
1:C:57:ASP:OD2	1:C:76:TYR:HE1	2.04	0.41
1:C:179:GLY:O	1:C:184:PRO:HD3	2.20	0.41
1:C:247:ALA:HA	1:C:259:ILE:HB	2.01	0.41
2:d:85:LEU:HD23	2:d:85:LEU:HA	1.72	0.41
1:F:67:GLY:CA	1:M:70:VAL:HG13	2.50	0.41
1:G:199:PRO:HA	1:G:353:LEU:HD21	2.02	0.41
1:H:139:TYR:CE1	1:H:260:GLN:HB2	2.56	0.41
1:H:150:ASP:OD1	1:H:150:ASP:N	2.42	0.41
2:h:31:PHE:HE1	2:h:36:ILE:CD1	2.34	0.41
2:h:197:SER:O	2:h:207:LEU:HD12	2.21	0.41
2:i:37:SER:CB	2:i:49:TRP:HZ3	2.33	0.41
1:J:117:LEU:HD21	1:J:272:PHE:HB2	2.02	0.41
1:J:132:TRP:NE1	1:J:311:ASN:O	2.48	0.41
1:J:134:THR:O	1:J:240:SER:N	2.51	0.41
1:J:177:ASP:HA	1:J:358:TRP:CZ2	2.54	0.41
1:K:298:GLU:H	1:K:298:GLU:HG2	1.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:21:LYS:HB3	2:k:84:GLU:HB2	2.03	0.41
2:k:51:GLY:C	2:k:72:MET:HE1	2.46	0.41
2:k:51:GLY:HA2	2:k:61:ASN:O	2.20	0.41
2:k:89:ARG:C	2:k:91:ASP:N	2.79	0.41
1:L:283:ALA:C	1:L:285:ASP:H	2.28	0.41
2:l:36:ILE:O	2:l:52:TRP:HB2	2.21	0.41
2:l:149:GLN:HE21	1:Q:190:LEU:C	2.28	0.41
1:N:247:ALA:CB	1:N:259:ILE:HB	2.50	0.41
1:O:134:THR:O	1:O:240:SER:N	2.48	0.41
2:o:171:GLN:HG3	2:o:220:TYR:CE1	2.56	0.41
1:P:104:PRO:HD2	1:P:292:ASP:OD2	2.21	0.41
1:Q:156:TRP:NE1	1:Q:267:GLY:O	2.47	0.41
1:Q:204:LYS:HA	1:Q:204:LYS:HD3	1.41	0.41
1:Q:291:ILE:O	1:Q:295:LEU:HG	2.21	0.41
1:R:37:TYR:CE1	1:R:131:LEU:HB2	2.55	0.41
1:R:135:ASN:OD1	1:R:268:ALA:HB1	2.21	0.41
1:R:239:TYR:O	1:R:243:VAL:HG23	2.21	0.41
1:A:224:TYR:HA	1:A:227:ASP:HB2	2.02	0.41
1:B:176:MET:HG3	1:B:237:PHE:HD1	1.84	0.41
2:c:20:VAL:CG2	2:c:88:LEU:CD2	2.95	0.41
1:D:98:LEU:HD22	1:D:103:LEU:HD11	2.03	0.41
1:E:122:PRO:O	1:E:125:GLN:HG3	2.20	0.41
1:E:176:MET:HE3	1:E:221:SER:OG	2.21	0.41
2:e:66:PHE:O	2:e:70:VAL:HG12	2.21	0.41
1:F:328:GLU:O	1:F:332:PRO:HA	2.20	0.41
1:H:240:SER:OG	1:H:241:GLY:N	2.53	0.41
2:h:116:VAL:O	2:h:116:VAL:HG23	2.21	0.41
1:I:59:PHE:CE2	1:I:65:LEU:HB2	2.55	0.41
1:J:157:ALA:O	1:J:161:GLU:HB2	2.21	0.41
1:J:328:GLU:O	1:J:332:PRO:HA	2.21	0.41
2:j:150:LYS:HG2	2:j:151:VAL:N	2.32	0.41
2:j:195:ARG:O	2:j:209:ILE:HA	2.20	0.41
1:K:167:LYS:HE2	1:K:167:LYS:HB3	1.82	0.41
1:K:186:ALA:O	1:K:190:LEU:HG	2.21	0.41
1:L:52:ILE:HD13	1:L:286:ASN:HB2	2.03	0.41
1:L:81:PRO:HD2	1:L:274:LEU:O	2.21	0.41
1:L:161:GLU:HA	1:L:162:PRO:HD3	1.90	0.41
1:M:228:LEU:HD23	1:M:233:ILE:HG13	2.03	0.41
2:m:139:GLN:OE1	2:m:235:GLY:HA3	2.21	0.41
1:N:140:ASN:HB2	1:N:259:ILE:HD13	2.02	0.41
1:N:322:LYS:HA	1:N:325:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:357:THR:HA	1:O:360:ARG:HH12	1.85	0.41
1:P:98:LEU:HB2	1:P:125:GLN:O	2.21	0.41
1:Q:46:PHE:HB2	1:Q:293:TYR:CE2	2.55	0.41
2:q:6:LEU:HD23	2:q:26:VAL:HG12	2.03	0.41
2:q:180:LEU:HD23	2:q:189:PRO:HG3	2.02	0.41
1:A:213:ARG:NH1	1:A:361:ILE:O	2.53	0.40
1:B:87:GLY:HA3	1:B:345:VAL:HG21	2.03	0.40
1:B:165:MET:HE3	1:B:165:MET:HB3	1.85	0.40
1:C:173:VAL:HG13	1:C:235:VAL:HG13	2.02	0.40
2:c:137:LEU:HD13	2:c:155:CYS:SG	2.61	0.40
2:e:169:TRP:HB2	2:e:182:LEU:HB2	2.02	0.40
1:F:34:TRP:HA	1:F:59:PHE:O	2.21	0.40
1:F:60:ASP:HB2	1:F:222:SER:HB3	2.02	0.40
1:F:360:ARG:C	1:F:362:LYS:N	2.79	0.40
1:G:139:TYR:CE2	1:G:141:VAL:HG23	2.55	0.40
2:g:167:VAL:HG11	2:g:205:THR:HG21	2.03	0.40
1:H:183:LEU:HD23	1:H:209:LEU:HD12	2.03	0.40
2:h:106:ASP:OD1	2:h:107:VAL:HG12	2.21	0.40
1:I:239:TYR:O	1:I:243:VAL:HG23	2.20	0.40
2:i:213:GLN:C	2:i:215:GLY:N	2.76	0.40
1:J:302:LYS:HB2	1:J:302:LYS:HE3	1.88	0.40
2:j:50:MET:HE2	2:j:50:MET:HB3	1.95	0.40
2:l:25:LYS:HE2	2:l:25:LYS:HB2	1.92	0.40
2:l:97:TYR:HB3	2:l:108:TRP:CD1	2.56	0.40
2:m:224:VAL:O	2:m:232:VAL:HA	2.21	0.40
2:n:153:ILE:HD13	2:n:238:THR:HB	2.03	0.40
1:O:32:TYR:HA	1:O:57:ASP:O	2.21	0.40
1:O:89:GLN:O	1:O:90:ILE:C	2.63	0.40
1:O:110:ASP:HB3	1:O:314:PRO:CG	2.51	0.40
1:P:161:GLU:HA	1:P:162:PRO:HD3	1.95	0.40
1:P:304:SER:HB3	1:P:320:MET:HE3	2.03	0.40
1:P:334:GLN:O	1:P:337:LEU:N	2.54	0.40
2:p:26:VAL:HB	2:p:29:TYR:CE1	2.56	0.40
1:Q:95:PHE:HA	1:Q:278:PRO:HA	2.02	0.40
2:r:48:GLU:OE2	2:r:65:LYS:HE2	2.21	0.40
2:b:6:LEU:HG	2:b:26:VAL:HG12	2.03	0.40
1:D:97:LYS:HG3	1:D:126:TYR:CE1	2.55	0.40
1:D:192:LEU:H	1:D:192:LEU:HG	1.74	0.40
2:d:88:LEU:HD23	2:d:88:LEU:HA	1.85	0.40
1:E:243:VAL:CG1	1:E:261:TYR:HB2	2.52	0.40
2:e:171:GLN:HB2	2:e:181:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:69:ARG:HH21	2:g:85:LEU:HD21	1.86	0.40
2:h:151:VAL:HG12	2:h:212:LEU:HD11	2.03	0.40
2:i:166:TYR:CD2	2:i:185:ASN:ND2	2.89	0.40
2:i:173:LEU:HD23	2:i:218:ALA:HB2	2.03	0.40
1:J:182:MET:HE1	1:J:237:PHE:CG	2.57	0.40
1:J:187:LEU:HD12	1:J:194:PRO:HA	2.02	0.40
1:K:200:LYS:HD2	1:K:200:LYS:HA	1.46	0.40
1:K:322:LYS:O	1:K:326:ASP:HB2	2.21	0.40
2:k:13:VAL:HA	2:k:115:THR:O	2.21	0.40
2:n:58:GLY:CA	2:n:74:ARG:HE	2.33	0.40
2:n:104:TYR:HD2	2:n:180:LEU:HD22	1.87	0.40
2:n:224:VAL:O	2:n:233:LEU:N	2.49	0.40
1:O:32:TYR:HB2	1:O:76:TYR:CG	2.56	0.40
1:O:297:PRO:HB2	1:O:298:GLU:H	1.67	0.40
1:O:298:GLU:O	1:O:301:ALA:HB3	2.21	0.40
1:O:362:LYS:HE3	1:O:362:LYS:HB2	1.82	0.40
1:P:99:ASP:O	1:P:102:LYS:HG2	2.21	0.40
1:Q:311:ASN:OD1	1:Q:313:ILE:N	2.46	0.40
1:Q:326:ASP:HB3	2:q:165:ASN:HB3	2.02	0.40
1:R:135:ASN:HD22	1:R:237:PHE:HE1	1.68	0.40
1:R:187:LEU:HA	1:R:187:LEU:HD23	1.84	0.40
1:R:305:ASP:CG	1:R:321:ASP:H	2.28	0.40
2:r:25:LYS:HE2	2:r:78:ILE:HG22	2.03	0.40
2:b:9:THR:HG22	2:b:22:VAL:HG13	2.03	0.40
1:C:144:VAL:O	1:C:147:VAL:N	2.52	0.40
2:c:89:ARG:H	2:c:89:ARG:HG2	1.63	0.40
2:e:149:GLN:O	2:e:210:THR:O	2.40	0.40
1:F:105:ASN:ND2	1:F:292:ASP:OD1	2.40	0.40
1:G:145:LYS:HA	1:G:145:LYS:HD3	1.82	0.40
1:G:330:VAL:HG12	1:G:331:TYR:CD1	2.56	0.40
1:I:162:PRO:O	1:I:166:LYS:HG2	2.21	0.40
1:I:298:GLU:H	1:I:298:GLU:HG2	1.69	0.40
1:I:300:ILE:HD12	1:I:300:ILE:HA	1.88	0.40
2:i:16:PRO:O	2:i:17:GLY:C	2.64	0.40
2:i:213:GLN:C	2:i:215:GLY:H	2.30	0.40
2:j:83:MET:HE3	2:j:85:LEU:N	2.37	0.40
2:l:83:MET:SD	2:l:84:GLU:N	2.95	0.40
1:M:242:ASP:OD1	1:M:309:TYR:OH	2.39	0.40
1:O:81:PRO:HD2	1:O:274:LEU:O	2.21	0.40
1:O:99:ASP:O	1:O:99:ASP:CG	2.65	0.40
1:O:136:GLY:HA2	1:O:156:TRP:CH2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:172:GLY:HA3	1:O:233:ILE:HG22	2.04	0.40
2:o:26:VAL:HB	2:o:29:TYR:CE1	2.56	0.40
1:P:29:LEU:HB3	1:P:54:VAL:HG12	2.02	0.40
2:q:75:ASP:OD1	2:q:77:SER:HB3	2.20	0.40
1:R:60:ASP:HB2	1:R:222:SER:HB3	2.04	0.40
1:A:57:ASP:OD2	1:A:76:TYR:HE1	2.04	0.40
1:B:139:TYR:HA	1:B:234:CYS:O	2.21	0.40
2:b:102:LYS:HE3	2:b:102:LYS:HB2	1.88	0.40
2:b:185:ASN:CG	2:b:200:LYS:HZ2	2.29	0.40
2:c:212:LEU:HD12	2:c:212:LEU:HA	1.85	0.40
2:c:225:TRP:CZ2	2:c:230:ARG:HA	2.57	0.40
2:e:52:TRP:C	2:e:72:MET:HE1	2.47	0.40
1:G:182:MET:HG3	1:G:358:TRP:CH2	2.57	0.40
1:J:183:LEU:HD11	1:J:357:THR:HB	2.04	0.40
1:L:81:PRO:HG2	1:L:86:LEU:HB2	2.04	0.40
1:L:127:ALA:HA	1:L:275:MET:O	2.21	0.40
1:L:359:THR:O	1:L:362:LYS:HG3	2.22	0.40
2:l:108:TRP:HH2	2:l:170:TYR:CZ	2.39	0.40
1:M:282:LYS:HD2	1:M:282:LYS:C	2.46	0.40
1:M:330:VAL:O	1:M:332:PRO:HD3	2.22	0.40
2:n:215:GLY:C	2:n:217:GLU:H	2.29	0.40
1:O:90:ILE:C	1:O:92:ALA:N	2.78	0.40
2:p:58:GLY:HA2	2:p:74:ARG:HE	1.85	0.40
2:p:91:ASP:OD1	2:p:91:ASP:C	2.59	0.40
2:q:239:LYS:HB3	2:q:239:LYS:NZ	2.36	0.40
1:R:62:ASN:ND2	1:R:85:PHE:CD2	2.90	0.40
1:R:328:GLU:O	1:R:332:PRO:HA	2.21	0.40
2:r:106:ASP:OD1	2:r:107:VAL:N	2.53	0.40
2:b:24:CYS:HB2	2:b:38:TRP:CH2	2.56	0.40
2:b:62:TYR:HH	2:b:72:MET:H	1.70	0.40
1:C:295:LEU:HD22	1:C:313:ILE:HD11	2.03	0.40
1:D:105:ASN:C	1:D:107:LYS:N	2.80	0.40
1:J:187:LEU:O	1:J:192:LEU:HB2	2.21	0.40
4:L:404:SPD:HN6	4:L:404:SPD:H31	1.46	0.40
2:l:40:ARG:HB2	2:l:96:TYR:CE1	2.56	0.40
2:l:96:TYR:O	2:l:111:GLY:HA2	2.21	0.40
2:l:97:TYR:CG	2:l:108:TRP:CD1	3.07	0.40
1:M:203:LYS:HZ2	1:M:204:LYS:CB	2.35	0.40
1:N:63:GLU:OE2	1:N:178:SER:OG	2.30	0.40
1:N:80:VAL:HG22	1:N:275:MET:HG2	2.03	0.40
1:N:207:GLU:H	1:N:207:GLU:HG2	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:42:ALA:HB3	2:n:45:GLN:HB2	2.03	0.40
1:O:69:LEU:HD12	1:O:89:GLN:HE21	1.87	0.40
1:P:204:LYS:HD2	2:r:243:LEU:HB3	2.02	0.40
1:P:273:ASP:OD2	4:P:401:SPD:H72	2.22	0.40
1:R:31:ILE:HG23	1:R:78:ILE:HB	2.04	0.40
1:R:37:TYR:CE1	1:R:131:LEU:HD12	2.56	0.40

All (6) 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)
2:f:119:GLY:O	2:o:64:GLN:OE1[2_657]	1.51	0.69
2:f:119:GLY:O	2:o:64:GLN:CG[2_657]	1.59	0.61
2:f:119:GLY:O	2:o:64:GLN:CD[2_657]	1.66	0.54
1:F:163:GLU:OE1	2:h:142:SER:OG[2_757]	2.09	0.11
2:e:119:GLY:O	2:p:64:GLN:CG[1_554]	2.16	0.04
2:f:144:SER:OG	1:H:161:GLU:OE2[2_757]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/340 (98%)	301 (90%)	28 (8%)	4 (1%)	10	35
1	B	333/340 (98%)	300 (90%)	28 (8%)	5 (2%)	8	30
1	C	333/340 (98%)	301 (90%)	28 (8%)	4 (1%)	10	35
1	D	333/340 (98%)	305 (92%)	24 (7%)	4 (1%)	10	35
1	E	333/340 (98%)	298 (90%)	30 (9%)	5 (2%)	8	30
1	F	333/340 (98%)	297 (89%)	28 (8%)	8 (2%)	4	22
1	G	333/340 (98%)	304 (91%)	26 (8%)	3 (1%)	14	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	333/340 (98%)	305 (92%)	21 (6%)	7 (2%)	5	24
1	I	333/340 (98%)	291 (87%)	39 (12%)	3 (1%)	14	42
1	J	333/340 (98%)	281 (84%)	44 (13%)	8 (2%)	4	22
1	K	333/340 (98%)	293 (88%)	31 (9%)	9 (3%)	4	20
1	L	333/340 (98%)	284 (85%)	34 (10%)	15 (4%)	2	12
1	M	333/340 (98%)	293 (88%)	35 (10%)	5 (2%)	8	30
1	N	333/340 (98%)	282 (85%)	40 (12%)	11 (3%)	3	17
1	O	333/340 (98%)	285 (86%)	39 (12%)	9 (3%)	4	20
1	P	333/340 (98%)	281 (84%)	46 (14%)	6 (2%)	6	26
1	Q	333/340 (98%)	275 (83%)	49 (15%)	9 (3%)	4	20
1	R	333/340 (98%)	274 (82%)	49 (15%)	10 (3%)	3	18
2	a	221/258 (86%)	187 (85%)	28 (13%)	6 (3%)	4	20
2	b	221/258 (86%)	197 (89%)	18 (8%)	6 (3%)	4	20
2	c	221/258 (86%)	193 (87%)	21 (10%)	7 (3%)	3	17
2	d	221/258 (86%)	187 (85%)	26 (12%)	8 (4%)	2	16
2	e	221/258 (86%)	202 (91%)	16 (7%)	3 (1%)	9	31
2	f	221/258 (86%)	196 (89%)	24 (11%)	1 (0%)	24	54
2	g	221/258 (86%)	187 (85%)	29 (13%)	5 (2%)	5	23
2	h	221/258 (86%)	190 (86%)	25 (11%)	6 (3%)	4	20
2	i	221/258 (86%)	189 (86%)	24 (11%)	8 (4%)	2	16
2	j	221/258 (86%)	185 (84%)	29 (13%)	7 (3%)	3	17
2	k	221/258 (86%)	189 (86%)	25 (11%)	7 (3%)	3	17
2	l	221/258 (86%)	146 (66%)	46 (21%)	29 (13%)	0	1
2	m	221/258 (86%)	181 (82%)	37 (17%)	3 (1%)	9	31
2	n	221/258 (86%)	173 (78%)	32 (14%)	16 (7%)	1	5
2	o	221/258 (86%)	186 (84%)	29 (13%)	6 (3%)	4	20
2	p	221/258 (86%)	186 (84%)	29 (13%)	6 (3%)	4	20
2	q	221/258 (86%)	171 (77%)	36 (16%)	14 (6%)	1	7
2	r	221/258 (86%)	179 (81%)	32 (14%)	10 (4%)	2	12
All	All	9972/10764 (93%)	8574 (86%)	1125 (11%)	273 (3%)	4	20

All (273) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	ASP
2	a	118	SER
2	b	16	PRO
2	b	90	SER
2	b	118	SER
2	c	118	SER
2	d	118	SER
2	d	155	CYS
2	e	61	ASN
2	e	118	SER
1	F	73	HIS
1	F	163	GLU
2	g	9	THR
2	g	118	SER
1	H	114	LEU
2	h	103	ARG
2	h	212	LEU
2	i	16	PRO
1	J	201	ASP
1	J	206	GLU
2	j	88	LEU
2	j	90	SER
2	j	118	SER
1	L	36	ASP
1	L	38	ILE
1	L	105	ASN
1	L	297	PRO
1	L	298	GLU
1	L	328	GLU
2	l	6	LEU
2	l	9	THR
2	l	12	GLU
2	l	14	LYS
2	l	15	THR
2	l	22	VAL
2	l	27	SER
2	l	104	TYR
2	l	146	ALA
2	l	150	LYS
2	l	162	ILE
2	l	216	ASP
2	l	239	LYS
2	m	91	ASP

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Mol	Chain	Res	Type
1	N	232	ASN
1	N	240	SER
2	n	30	THR
2	n	41	GLN
2	n	87	ARG
2	n	91	ASP
2	n	105	MET
2	n	118	SER
1	O	91	GLN
1	O	94	ALA
1	O	297	PRO
1	O	298	GLU
2	o	118	SER
1	P	74	SER
1	P	335	ALA
2	p	118	SER
2	q	4	VAL
2	q	11	ASP
2	q	12	GLU
2	q	118	SER
2	q	149	GLN
2	q	155	CYS
2	q	200	LYS
1	R	170	LYS
2	r	16	PRO
2	r	87	ARG
2	r	149	GLN
2	r	155	CYS
2	a	212	LEU
1	B	72	GLY
1	B	169	ALA
1	B	240	SER
2	b	30	THR
2	b	103	ARG
2	c	30	THR
2	c	190	SER
2	d	103	ARG
1	E	253	ALA
2	e	103	ARG
1	F	75	GLY
1	F	252	GLU
2	f	103	ARG

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Mol	Chain	Res	Type
1	G	114	LEU
2	g	16	PRO
2	g	27	SER
1	H	171	CYS
1	H	240	SER
2	h	227	SER
1	I	201	ASP
2	i	90	SER
2	i	149	GLN
2	j	214	THR
1	K	72	GLY
1	K	75	GLY
1	K	153	ILE
2	k	87	ARG
2	k	88	LEU
2	k	90	SER
2	k	214	THR
1	L	74	SER
1	L	104	PRO
1	L	124	ASN
1	L	190	LEU
1	L	284	ALA
1	L	327	SER
2	l	8	GLU
2	l	17	GLY
2	l	65	LYS
2	l	76	THR
2	l	103	ARG
2	l	111	GLY
2	l	231	ALA
1	M	114	LEU
1	M	204	LYS
1	N	117	LEU
2	n	10	GLY
2	n	19	SER
2	n	236	GLY
2	o	212	LEU
1	P	281	ALA
2	p	212	LEU
1	Q	64	THR
1	Q	190	LEU
1	Q	351	LEU

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Mol	Chain	Res	Type
2	q	91	ASP
2	q	185	ASN
1	R	153	ILE
1	R	203	LYS
1	A	323	SER
2	a	19	SER
2	a	30	THR
1	C	338	ASP
2	c	87	ARG
1	D	71	SER
1	D	91	GLN
2	d	69	ARG
1	E	315	GLY
1	F	169	ALA
1	G	240	SER
2	g	103	ARG
1	H	338	ASP
2	h	5	GLN
2	h	16	PRO
1	I	240	SER
2	i	17	GLY
1	J	150	ASP
1	J	166	LYS
1	J	298	GLU
1	K	151	GLN
1	K	170	LYS
2	k	49	TRP
2	k	67	GLN
2	k	118	SER
1	L	100	LYS
1	L	326	ASP
2	l	31	PHE
2	l	211	GLY
2	l	212	LEU
2	l	230	ARG
1	M	141	VAL
1	M	240	SER
2	m	69	ARG
1	N	64	THR
1	N	190	LEU
2	n	5	GLN
2	n	16	PRO

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Mol	Chain	Res	Type
2	n	18	ALA
2	n	159	SER
1	O	100	LYS
1	O	192	LEU
2	o	19	SER
2	o	30	THR
1	P	297	PRO
2	p	19	SER
2	p	30	THR
1	R	43	LEU
1	R	212	VAL
2	r	30	THR
2	r	91	ASP
1	A	74	SER
2	a	203	PRO
1	C	178	SER
1	D	106	TRP
2	d	30	THR
1	E	210	THR
1	F	240	SER
2	h	200	LYS
2	i	18	ALA
2	i	19	SER
1	J	117	LEU
2	j	79	SER
2	j	186	ASN
1	L	222	SER
2	l	7	VAL
2	l	64	GLN
1	N	78	ILE
1	O	89	GLN
1	O	92	ALA
1	O	222	SER
2	o	203	PRO
2	p	203	PRO
2	q	226	ASP
1	B	298	GLU
2	c	69	ARG
2	c	212	LEU
2	d	87	ARG
2	d	212	LEU
1	E	240	SER

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Mol	Chain	Res	Type
1	I	150	ASP
1	J	178	SER
1	J	280	ASP
1	K	148	LEU
1	K	157	ALA
2	l	16	PRO
2	l	189	PRO
1	M	178	SER
2	m	113	THR
1	N	182	MET
1	N	311	ASN
2	n	200	LYS
1	P	105	ASN
1	P	240	SER
1	Q	192	LEU
2	q	159	SER
1	R	152	PRO
1	R	206	GLU
1	R	211	LYS
2	r	20	VAL
2	r	118	SER
1	C	154	ASP
1	C	240	SER
1	D	178	SER
1	G	345	VAL
1	H	75	GLY
1	H	178	SER
1	H	210	THR
2	i	118	SER
1	N	179	GLY
1	N	297	PRO
2	n	211	GLY
1	Q	297	PRO
1	Q	298	GLU
2	r	211	GLY
2	c	191	GLY
1	F	256	GLY
1	Q	153	ILE
2	q	146	ALA
1	R	297	PRO
1	B	38	ILE
2	l	13	VAL

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Mol	Chain	Res	Type
1	N	72	GLY
1	Q	361	ILE
2	b	141	PRO
2	d	203	PRO
1	K	214	PRO
2	n	4	VAL
2	q	26	VAL
2	r	26	VAL
1	A	235	VAL
2	a	141	PRO
1	F	162	PRO
2	j	203	PRO
1	K	264	PRO
2	o	141	PRO
2	p	141	PRO
1	Q	152	PRO
1	E	40	PRO
2	i	141	PRO
2	q	20	VAL
1	R	345	VAL

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	279/282 (99%)	279 (100%)	0	100	100
1	B	279/282 (99%)	279 (100%)	0	100	100
1	C	279/282 (99%)	279 (100%)	0	100	100
1	D	279/282 (99%)	279 (100%)	0	100	100
1	E	279/282 (99%)	279 (100%)	0	100	100
1	F	279/282 (99%)	279 (100%)	0	100	100
1	G	279/282 (99%)	279 (100%)	0	100	100
1	H	279/282 (99%)	279 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	279/282 (99%)	277 (99%)	2 (1%)	76	78
1	J	279/282 (99%)	279 (100%)	0	100	100
1	K	279/282 (99%)	279 (100%)	0	100	100
1	L	279/282 (99%)	279 (100%)	0	100	100
1	M	279/282 (99%)	278 (100%)	1 (0%)	84	83
1	N	279/282 (99%)	279 (100%)	0	100	100
1	O	279/282 (99%)	279 (100%)	0	100	100
1	P	279/282 (99%)	277 (99%)	2 (1%)	76	78
1	Q	279/282 (99%)	279 (100%)	0	100	100
1	R	279/282 (99%)	277 (99%)	2 (1%)	76	78
2	a	186/203 (92%)	185 (100%)	1 (0%)	81	81
2	b	186/203 (92%)	184 (99%)	2 (1%)	65	74
2	c	186/203 (92%)	186 (100%)	0	100	100
2	d	186/203 (92%)	186 (100%)	0	100	100
2	e	186/203 (92%)	181 (97%)	5 (3%)	39	60
2	f	186/203 (92%)	182 (98%)	4 (2%)	45	63
2	g	186/203 (92%)	182 (98%)	4 (2%)	45	63
2	h	186/203 (92%)	184 (99%)	2 (1%)	65	74
2	i	186/203 (92%)	183 (98%)	3 (2%)	55	68
2	j	186/203 (92%)	185 (100%)	1 (0%)	81	81
2	k	186/203 (92%)	185 (100%)	1 (0%)	81	81
2	l	186/203 (92%)	182 (98%)	4 (2%)	45	63
2	m	186/203 (92%)	181 (97%)	5 (3%)	39	60
2	n	186/203 (92%)	182 (98%)	4 (2%)	45	63
2	o	186/203 (92%)	185 (100%)	1 (0%)	81	81
2	p	186/203 (92%)	185 (100%)	1 (0%)	81	81
2	q	186/203 (92%)	182 (98%)	4 (2%)	45	63
2	r	186/203 (92%)	184 (99%)	2 (1%)	65	74
All	All	8370/8730 (96%)	8319 (99%)	51 (1%)	78	80

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	a	20	VAL
2	b	16	PRO
2	b	20	VAL
2	e	15	THR
2	e	16	PRO
2	e	20	VAL
2	e	22	VAL
2	e	67	GLN
2	f	14	LYS
2	f	16	PRO
2	f	20	VAL
2	f	240	LEU
2	g	16	PRO
2	g	19	SER
2	g	194	ASP
2	g	212	LEU
2	h	13	VAL
2	h	20	VAL
1	I	141	VAL
1	I	353	LEU
2	i	4	VAL
2	i	16	PRO
2	i	21	LYS
2	j	36	ILE
2	k	15	THR
2	l	14	LYS
2	l	19	SER
2	l	20	VAL
2	l	21	LYS
1	M	88	LYS
2	m	13	VAL
2	m	15	THR
2	m	19	SER
2	m	20	VAL
2	m	21	LYS
2	n	14	LYS
2	n	15	THR
2	n	16	PRO
2	n	21	LYS
2	o	20	VAL
1	P	73	HIS
1	P	326	ASP
2	p	20	VAL

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Mol	Chain	Res	Type
2	q	14	LYS
2	q	20	VAL
2	q	205	THR
2	q	207	LEU
1	R	90	ILE
1	R	151	GLN
2	r	16	PRO
2	r	20	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	220	HIS
1	A	232	ASN
1	A	311	ASN
2	a	54	ASN
1	B	96	GLN
1	B	125	GLN
1	B	188	ASN
1	B	230	ASN
2	b	56	ASN
1	C	96	GLN
1	D	30	HIS
1	D	220	HIS
1	D	232	ASN
2	d	149	GLN
1	E	89	GLN
1	E	96	GLN
1	E	124	ASN
1	E	230	ASN
1	E	354	GLN
2	e	54	ASN
2	e	165	ASN
1	F	151	GLN
1	F	197	HIS
1	F	354	GLN
2	f	165	ASN
1	G	96	GLN
2	g	56	ASN
2	g	185	ASN
1	I	96	GLN

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Mol	Chain	Res	Type
2	i	139	GLN
1	J	62	ASN
1	J	96	GLN
1	J	197	HIS
2	j	3	GLN
2	j	171	GLN
1	K	73	HIS
1	K	151	GLN
1	K	164	ASN
1	K	245	GLN
1	K	260	GLN
2	k	213	GLN
1	L	220	HIS
1	L	311	ASN
1	L	334	GLN
2	l	149	GLN
1	M	89	GLN
1	M	151	GLN
1	M	232	ASN
1	M	334	GLN
2	m	41	GLN
2	m	56	ASN
2	m	64	GLN
2	m	172	GLN
1	N	89	GLN
1	N	232	ASN
1	N	334	GLN
2	n	5	GLN
2	n	41	GLN
2	n	54	ASN
1	O	62	ASN
1	O	105	ASN
1	O	354	GLN
2	o	64	GLN
1	P	30	HIS
1	P	91	GLN
1	P	230	ASN
2	p	56	ASN
2	p	64	GLN
1	Q	124	ASN
2	q	54	ASN
2	q	61	ASN

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Mol	Chain	Res	Type
2	q	149	GLN
2	q	171	GLN
1	R	89	GLN
1	R	197	HIS
1	R	311	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](#)

72 ligands are 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	$\# Z > 2$
3	SO4	O	403	-	4,4,4	0.85	0	6,6,6	0.58	0
4	SPD	L	404	-	9,9,9	0.41	0	8,8,8	1.33	2 (25%)
4	SPD	F	404	-	9,9,9	0.42	0	8,8,8	1.00	0
4	SPD	O	407	-	9,9,9	0.41	0	8,8,8	0.96	0
3	SO4	G	401	-	4,4,4	0.86	0	6,6,6	0.52	0
3	SO4	L	401	-	4,4,4	0.83	0	6,6,6	0.53	0
3	SO4	N	402	-	4,4,4	0.85	0	6,6,6	0.54	0
3	SO4	I	402	-	4,4,4	0.85	0	6,6,6	0.53	0
4	SPD	H	403	-	9,9,9	0.42	0	8,8,8	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	K	401	-	4,4,4	0.83	0	6,6,6	0.56	0
3	SO4	E	402	-	4,4,4	0.86	0	6,6,6	0.52	0
3	SO4	L	402	-	4,4,4	0.87	0	6,6,6	0.63	0
3	SO4	R	402	-	4,4,4	0.85	0	6,6,6	0.54	0
3	SO4	A	402	-	4,4,4	0.85	0	6,6,6	0.59	0
3	SO4	J	401	-	4,4,4	0.86	0	6,6,6	0.53	0
3	SO4	K	402	-	4,4,4	0.81	0	6,6,6	0.55	0
3	SO4	A	403	-	4,4,4	0.86	0	6,6,6	0.57	0
3	SO4	B	403	-	4,4,4	0.86	0	6,6,6	0.51	0
3	SO4	E	404	-	4,4,4	0.85	0	6,6,6	0.58	0
3	SO4	N	403	-	4,4,4	0.85	0	6,6,6	0.53	0
3	SO4	O	401	-	4,4,4	0.82	0	6,6,6	0.62	0
3	SO4	E	403	-	4,4,4	0.84	0	6,6,6	0.50	0
3	SO4	M	402	-	4,4,4	0.86	0	6,6,6	0.56	0
3	SO4	H	402	-	4,4,4	0.87	0	6,6,6	0.53	0
3	SO4	E	401	-	4,4,4	0.85	0	6,6,6	0.59	0
4	SPD	J	404	-	9,9,9	0.43	0	8,8,8	1.03	0
4	SPD	Q	401	-	9,9,9	0.43	0	8,8,8	0.91	0
3	SO4	G	402	-	4,4,4	0.86	0	6,6,6	0.57	0
3	SO4	F	403	-	4,4,4	0.85	0	6,6,6	0.55	0
3	SO4	A	401	-	4,4,4	0.85	0	6,6,6	0.56	0
3	SO4	O	405	-	4,4,4	0.82	0	6,6,6	0.49	0
3	SO4	D	402	-	4,4,4	0.87	0	6,6,6	0.57	0
4	SPD	N	407	-	9,9,9	0.41	0	8,8,8	1.06	0
4	SPD	K	404	-	9,9,9	0.40	0	8,8,8	0.82	0
4	SPD	C	404	-	9,9,9	0.42	0	8,8,8	1.09	0
3	SO4	O	404	-	4,4,4	0.85	0	6,6,6	0.54	0
3	SO4	D	403	-	4,4,4	0.86	0	6,6,6	0.54	0
3	SO4	I	401	-	4,4,4	0.85	0	6,6,6	0.55	0
3	SO4	B	402	-	4,4,4	0.86	0	6,6,6	0.50	0
3	SO4	N	401	-	4,4,4	0.85	0	6,6,6	0.52	0
3	SO4	H	401	-	4,4,4	0.85	0	6,6,6	0.55	0
3	SO4	N	406	-	4,4,4	0.86	0	6,6,6	0.60	0
3	SO4	O	406	-	4,4,4	0.84	0	6,6,6	0.55	0
4	SPD	G	403	-	9,9,9	0.42	0	8,8,8	0.93	0
4	SPD	P	401	-	9,9,9	0.43	0	8,8,8	1.22	2 (25%)
3	SO4	M	403	-	4,4,4	0.86	0	6,6,6	0.53	0
3	SO4	O	402	-	4,4,4	0.86	0	6,6,6	0.55	0
4	SPD	I	404	-	9,9,9	0.44	0	8,8,8	0.76	0
3	SO4	N	405	-	4,4,4	0.85	0	6,6,6	0.55	0
3	SO4	B	404	-	4,4,4	0.84	0	6,6,6	0.57	0
3	SO4	D	401	-	4,4,4	0.84	0	6,6,6	0.56	0
3	SO4	N	404	-	4,4,4	0.85	0	6,6,6	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SPD	D	404	-	9,9,9	0.42	0	8,8,8	1.10	1 (12%)
4	SPD	E	405	-	9,9,9	0.41	0	8,8,8	0.89	0
3	SO4	C	403	-	4,4,4	0.86	0	6,6,6	0.53	0
3	SO4	B	401	-	4,4,4	0.84	0	6,6,6	0.56	0
4	SPD	M	404	-	9,9,9	0.42	0	8,8,8	0.88	0
3	SO4	M	401	-	4,4,4	0.83	0	6,6,6	0.56	0
3	SO4	R	403	-	4,4,4	0.85	0	6,6,6	0.50	0
4	SPD	A	404	-	9,9,9	0.43	0	8,8,8	0.71	0
4	SPD	B	405	-	9,9,9	0.41	0	8,8,8	0.85	0
4	SPD	R	404	-	9,9,9	0.40	0	8,8,8	1.13	1 (12%)
3	SO4	L	403	-	4,4,4	0.85	0	6,6,6	0.57	0
3	SO4	C	402	-	4,4,4	0.87	0	6,6,6	0.55	0
3	SO4	R	401	-	4,4,4	0.83	0	6,6,6	0.57	0
3	SO4	F	401	-	4,4,4	0.83	0	6,6,6	0.58	0
3	SO4	J	402	-	4,4,4	0.85	0	6,6,6	0.51	0
3	SO4	K	403	-	4,4,4	0.85	0	6,6,6	0.50	0
3	SO4	J	403	-	4,4,4	0.84	0	6,6,6	0.51	0
3	SO4	I	403	-	4,4,4	0.82	0	6,6,6	0.56	0
3	SO4	C	401	-	4,4,4	0.86	0	6,6,6	0.55	0
3	SO4	F	402	-	4,4,4	0.85	0	6,6,6	0.59	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
4	SPD	L	404	-	-	4/7/7/7	-
4	SPD	F	404	-	-	3/7/7/7	-
4	SPD	J	404	-	-	6/7/7/7	-
4	SPD	M	404	-	-	4/7/7/7	-
4	SPD	G	403	-	-	5/7/7/7	-
4	SPD	A	404	-	-	4/7/7/7	-
4	SPD	B	405	-	-	5/7/7/7	-
4	SPD	H	403	-	-	3/7/7/7	-
4	SPD	O	407	-	-	3/7/7/7	-
4	SPD	I	404	-	-	3/7/7/7	-
4	SPD	P	401	-	-	3/7/7/7	-
4	SPD	Q	401	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SPD	R	404	-	-	4/7/7/7	-
4	SPD	N	407	-	-	5/7/7/7	-
4	SPD	D	404	-	-	3/7/7/7	-
4	SPD	K	404	-	-	5/7/7/7	-
4	SPD	C	404	-	-	3/7/7/7	-
4	SPD	E	405	-	-	6/7/7/7	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	404	SPD	C7-C8-C9	-2.41	105.54	114.17
4	R	404	SPD	C4-C5-N6	-2.32	105.84	112.07
4	P	401	SPD	C4-C5-N6	-2.21	106.14	112.07
4	L	404	SPD	C4-C5-N6	-2.21	106.15	112.07
4	P	401	SPD	C8-C7-N6	-2.16	106.26	112.07
4	L	404	SPD	C8-C7-N6	-2.07	106.52	112.07

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	405	SPD	N6-C7-C8-C9
4	P	401	SPD	N6-C7-C8-C9
4	J	404	SPD	C3-C4-C5-N6
4	O	407	SPD	C3-C4-C5-N6
4	D	404	SPD	C3-C4-C5-N6
4	P	401	SPD	C3-C4-C5-N6
4	A	404	SPD	C3-C4-C5-N6
4	F	404	SPD	N6-C7-C8-C9
4	B	405	SPD	C3-C4-C5-N6
4	J	404	SPD	N6-C7-C8-C9
4	H	403	SPD	N6-C7-C8-C9
4	K	404	SPD	N6-C7-C8-C9
4	O	407	SPD	N6-C7-C8-C9
4	Q	401	SPD	N6-C7-C8-C9
4	I	404	SPD	C8-C7-N6-C5
4	R	404	SPD	C8-C7-N6-C5
4	L	404	SPD	C3-C4-C5-N6
4	G	403	SPD	C4-C5-N6-C7

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Mol	Chain	Res	Type	Atoms
4	J	404	SPD	C8-C7-N6-C5
4	L	404	SPD	C8-C7-N6-C5
4	G	403	SPD	N6-C7-C8-C9
4	I	404	SPD	C7-C8-C9-N10
4	N	407	SPD	C8-C7-N6-C5
4	K	404	SPD	C3-C4-C5-N6
4	K	404	SPD	N1-C2-C3-C4
4	N	407	SPD	C3-C4-C5-N6
4	G	403	SPD	C3-C4-C5-N6
4	Q	401	SPD	C2-C3-C4-C5
4	R	404	SPD	C3-C4-C5-N6
4	Q	401	SPD	C4-C5-N6-C7
4	M	404	SPD	C3-C4-C5-N6
4	J	404	SPD	C2-C3-C4-C5
4	K	404	SPD	C2-C3-C4-C5
4	H	403	SPD	C7-C8-C9-N10
4	L	404	SPD	C7-C8-C9-N10
4	O	407	SPD	C7-C8-C9-N10
4	R	404	SPD	C7-C8-C9-N10
4	M	404	SPD	C2-C3-C4-C5
4	A	404	SPD	C8-C7-N6-C5
4	B	405	SPD	C8-C7-N6-C5
4	F	404	SPD	C4-C5-N6-C7
4	H	403	SPD	C8-C7-N6-C5
4	L	404	SPD	C4-C5-N6-C7
4	A	404	SPD	N1-C2-C3-C4
4	M	404	SPD	N1-C2-C3-C4
4	R	404	SPD	N1-C2-C3-C4
4	B	405	SPD	C7-C8-C9-N10
4	C	404	SPD	C7-C8-C9-N10
4	E	405	SPD	C8-C7-N6-C5
4	G	403	SPD	C7-C8-C9-N10
4	N	407	SPD	C7-C8-C9-N10
4	P	401	SPD	C7-C8-C9-N10
4	C	404	SPD	N1-C2-C3-C4
4	G	403	SPD	N1-C2-C3-C4
4	N	407	SPD	C4-C5-N6-C7
4	B	405	SPD	N6-C7-C8-C9
4	B	405	SPD	N1-C2-C3-C4
4	D	404	SPD	N1-C2-C3-C4
4	N	407	SPD	N1-C2-C3-C4
4	A	404	SPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	I	404	SPD	C4-C5-N6-C7
4	J	404	SPD	C4-C5-N6-C7
4	K	404	SPD	C8-C7-N6-C5
4	E	405	SPD	N1-C2-C3-C4
4	F	404	SPD	C8-C7-N6-C5
4	D	404	SPD	C4-C5-N6-C7
4	E	405	SPD	C4-C5-N6-C7
4	E	405	SPD	C3-C4-C5-N6
4	E	405	SPD	C7-C8-C9-N10
4	M	404	SPD	C7-C8-C9-N10
4	J	404	SPD	N1-C2-C3-C4
4	C	404	SPD	C3-C4-C5-N6

There are no ring outliers.

42 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	403	SO4	1	0
4	L	404	SPD	2	0
4	F	404	SPD	3	0
4	O	407	SPD	6	0
3	G	401	SO4	2	0
3	L	401	SO4	1	0
3	I	402	SO4	2	0
4	H	403	SPD	4	0
3	K	401	SO4	1	0
3	E	402	SO4	1	0
3	R	402	SO4	1	0
3	A	403	SO4	2	0
3	E	404	SO4	1	0
3	M	402	SO4	2	0
4	J	404	SPD	3	0
4	Q	401	SPD	7	0
3	G	402	SO4	1	0
3	F	403	SO4	1	0
3	A	401	SO4	1	0
4	N	407	SPD	6	0
4	K	404	SPD	3	0
4	C	404	SPD	3	0
3	H	401	SO4	1	0
3	N	406	SO4	3	0
3	O	406	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	403	SPD	2	0
4	P	401	SPD	5	0
4	I	404	SPD	1	0
3	D	401	SO4	1	0
3	N	404	SO4	3	0
4	D	404	SPD	5	0
4	E	405	SPD	5	0
4	M	404	SPD	3	0
3	M	401	SO4	2	0
4	A	404	SPD	5	0
4	B	405	SPD	2	0
4	R	404	SPD	3	0
3	R	401	SO4	2	0
3	J	402	SO4	1	0
3	I	403	SO4	1	0
3	C	401	SO4	1	0
3	F	402	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	335/340 (98%)	-1.13	0	100	100	35, 45, 60, 64	0
1	B	335/340 (98%)	-1.08	0	100	100	33, 47, 62, 71	0
1	C	335/340 (98%)	-1.09	0	100	100	34, 45, 58, 62	0
1	D	335/340 (98%)	-1.13	0	100	100	33, 45, 58, 65	0
1	E	335/340 (98%)	-1.11	0	100	100	35, 47, 60, 65	0
1	F	335/340 (98%)	-1.12	0	100	100	35, 47, 61, 71	0
1	G	335/340 (98%)	-1.13	0	100	100	34, 43, 51, 59	0
1	H	335/340 (98%)	-1.15	0	100	100	34, 44, 52, 59	0
1	I	335/340 (98%)	-1.08	0	100	100	37, 50, 72, 78	0
1	J	335/340 (98%)	-1.03	0	100	100	38, 52, 73, 77	0
1	K	335/340 (98%)	-1.03	0	100	100	36, 52, 72, 78	0
1	L	335/340 (98%)	-0.95	0	100	100	63, 73, 84, 87	0
1	M	335/340 (98%)	-1.09	0	100	100	34, 44, 52, 63	0
1	N	335/340 (98%)	-1.00	0	100	100	62, 74, 82, 86	0
1	O	335/340 (98%)	-0.91	1 (0%)	90	84	62, 72, 82, 86	0
1	P	335/340 (98%)	-0.98	0	100	100	62, 72, 82, 88	0
1	Q	335/340 (98%)	-0.94	0	100	100	62, 74, 84, 89	0
1	R	335/340 (98%)	-0.91	0	100	100	61, 73, 84, 90	0
2	a	225/258 (87%)	-1.10	0	100	100	44, 56, 64, 75	0
2	b	225/258 (87%)	-1.11	0	100	100	38, 45, 59, 89	0
2	c	225/258 (87%)	-1.09	0	100	100	42, 52, 61, 82	0
2	d	225/258 (87%)	-1.10	0	100	100	42, 52, 61, 74	0
2	e	225/258 (87%)	-1.12	0	100	100	38, 45, 59, 102	0
2	f	225/258 (87%)	-1.16	0	100	100	39, 46, 61, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	g	225/258 (87%)	-1.05	0 100 100	46, 53, 66, 79	0
2	h	225/258 (87%)	-1.03	0 100 100	46, 55, 67, 85	0
2	i	225/258 (87%)	-1.10	0 100 100	40, 49, 68, 102	0
2	j	225/258 (87%)	-1.03	0 100 100	43, 50, 70, 106	0
2	k	225/258 (87%)	-1.02	0 100 100	42, 49, 69, 103	0
2	l	225/258 (87%)	-0.71	0 100 100	80, 102, 121, 126	0
2	m	225/258 (87%)	-1.07	0 100 100	46, 53, 65, 79	0
2	n	225/258 (87%)	-0.88	0 100 100	59, 72, 84, 102	0
2	o	225/258 (87%)	-0.89	0 100 100	44, 56, 64, 75	0
2	p	225/258 (87%)	-0.92	0 100 100	44, 56, 64, 75	0
2	q	225/258 (87%)	-0.84	1 (0%) 88 81	58, 73, 85, 102	0
2	r	225/258 (87%)	-0.80	0 100 100	56, 72, 83, 103	0
All	All	10080/10764 (93%)	-1.03	2 (0%) 100 100	33, 53, 81, 126	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	217	SER	2.7
2	q	191	GLY	2.4

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
3	SO4	O	404	5/5	0.96	0.09	92,92,92,92	0
4	SPD	O	407	10/10	0.96	0.10	67,67,67,67	0
3	SO4	L	402	5/5	0.97	0.12	93,93,93,93	0
4	SPD	G	403	10/10	0.97	0.09	37,37,37,37	0
4	SPD	L	404	10/10	0.97	0.11	67,67,67,68	0
3	SO4	N	401	5/5	0.97	0.06	88,88,88,88	0
3	SO4	N	402	5/5	0.98	0.05	87,87,87,87	0
3	SO4	N	404	5/5	0.98	0.08	93,93,94,94	0
3	SO4	O	402	5/5	0.98	0.06	92,92,93,93	0
3	SO4	K	401	5/5	0.98	0.06	79,79,80,80	0
3	SO4	R	402	5/5	0.98	0.07	90,90,90,91	0
3	SO4	R	403	5/5	0.98	0.07	85,86,86,86	0
4	SPD	A	404	10/10	0.98	0.08	38,38,38,38	0
4	SPD	B	405	10/10	0.98	0.07	39,40,40,40	0
4	SPD	D	404	10/10	0.98	0.08	38,38,39,39	0
3	SO4	L	401	5/5	0.98	0.05	83,83,83,84	0
4	SPD	H	403	10/10	0.98	0.08	37,37,37,37	0
4	SPD	I	404	10/10	0.98	0.07	45,45,46,46	0
3	SO4	E	402	5/5	0.98	0.11	60,60,60,60	0
4	SPD	M	404	10/10	0.98	0.07	36,36,36,37	0
3	SO4	I	401	5/5	0.98	0.08	76,76,76,76	0
4	SPD	P	401	10/10	0.98	0.08	65,65,65,65	0
4	SPD	Q	401	10/10	0.98	0.08	64,65,66,66	0
4	SPD	R	404	10/10	0.98	0.08	67,68,68,68	0
3	SO4	J	403	5/5	0.99	0.06	54,55,55,55	0
3	SO4	B	401	5/5	0.99	0.03	54,54,54,54	0
3	SO4	K	402	5/5	0.99	0.04	63,63,63,64	0
3	SO4	B	402	5/5	0.99	0.03	64,64,64,64	0
3	SO4	C	401	5/5	0.99	0.04	60,60,60,61	0
3	SO4	L	403	5/5	0.99	0.03	84,84,84,84	0
3	SO4	M	401	5/5	0.99	0.07	47,47,47,47	0
3	SO4	M	402	5/5	0.99	0.04	51,51,51,51	0
3	SO4	M	403	5/5	0.99	0.05	53,53,54,54	0
3	SO4	C	402	5/5	0.99	0.06	53,53,53,53	0
3	SO4	C	403	5/5	0.99	0.03	52,52,52,52	0
3	SO4	N	403	5/5	0.99	0.03	83,83,83,83	0
3	SO4	D	401	5/5	0.99	0.06	57,57,57,57	0
3	SO4	N	405	5/5	0.99	0.05	86,86,86,86	0
3	SO4	N	406	5/5	0.99	0.04	90,90,90,90	0
3	SO4	O	401	5/5	0.99	0.04	95,95,95,95	0
3	SO4	D	402	5/5	0.99	0.06	55,55,55,55	0
3	SO4	O	403	5/5	0.99	0.07	88,88,88,88	0
3	SO4	D	403	5/5	0.99	0.03	50,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	O	405	5/5	0.99	0.09	85,85,85,85	0
3	SO4	O	406	5/5	0.99	0.04	85,85,86,86	0
3	SO4	R	401	5/5	0.99	0.05	89,89,89,89	0
3	SO4	E	401	5/5	0.99	0.03	52,52,52,52	0
3	SO4	A	402	5/5	0.99	0.05	54,54,54,54	0
3	SO4	E	403	5/5	0.99	0.03	51,51,51,51	0
3	SO4	E	404	5/5	0.99	0.05	56,56,56,56	0
4	SPD	C	404	10/10	0.99	0.05	39,40,40,40	0
3	SO4	F	401	5/5	0.99	0.03	53,53,53,54	0
4	SPD	E	405	10/10	0.99	0.06	39,39,39,39	0
4	SPD	F	404	10/10	0.99	0.06	39,39,39,39	0
3	SO4	F	402	5/5	0.99	0.10	65,65,66,66	0
3	SO4	G	401	5/5	0.99	0.07	50,50,50,50	0
3	SO4	G	402	5/5	0.99	0.03	49,49,50,50	0
4	SPD	J	404	10/10	0.99	0.06	45,45,46,46	0
4	SPD	K	404	10/10	0.99	0.06	45,45,45,45	0
3	SO4	H	401	5/5	0.99	0.05	49,49,50,50	0
3	SO4	H	402	5/5	0.99	0.03	52,52,52,52	0
4	SPD	N	407	10/10	0.99	0.06	67,67,67,67	0
3	SO4	A	403	5/5	0.99	0.04	54,55,55,55	0
3	SO4	I	402	5/5	0.99	0.04	66,66,66,66	0
3	SO4	J	401	5/5	0.99	0.03	76,76,76,76	0
3	SO4	J	402	5/5	0.99	0.06	66,66,66,66	0
3	SO4	B	403	5/5	1.00	0.03	52,52,52,52	0
3	SO4	I	403	5/5	1.00	0.04	51,51,51,51	0
3	SO4	K	403	5/5	1.00	0.03	56,56,56,56	0
3	SO4	B	404	5/5	1.00	0.02	54,54,54,54	0
3	SO4	F	403	5/5	1.00	0.03	56,56,56,56	0
3	SO4	A	401	5/5	1.00	0.04	56,57,57,57	0

6.5 Other polymers

There are no such residues in this entry.