



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:11 AM GMT

PDB ID : 3H0R  
Title : Structure of trna-dependent amidotransferase gatcab from aquifex aeolicus  
Authors : Wu, J.; Bu, W.; Sheppard, K.; Kitabatake, M.; Soll, D.; Smith, J.L.  
Deposited on : 2009-04-10  
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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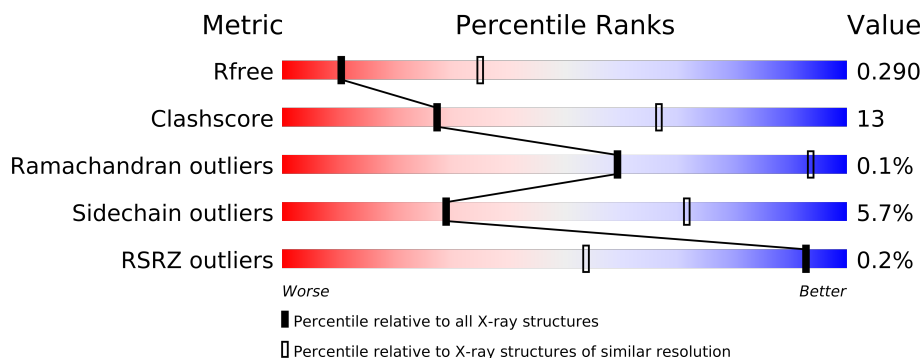
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **FAILED**  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	478	
1	D	478	
1	G	478	
1	J	478	
1	M	478	
1	P	478	
1	S	478	
1	V	478	
2	B	478	
2	E	478	
2	H	478	
2	K	478	
2	N	478	
2	Q	478	

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Mol	Chain	Length	Quality of chain
2	T	478	
2	W	478	
3	C	94	
3	F	94	
3	I	94	
3	L	94	
3	O	94	
3	R	94	
3	U	94	
3	X	94	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	ASN	A	901	-	X
4	ASN	G	903	-	X
4	ASN	M	905	-	X
4	ASN	P	906	-	X
4	ASN	S	907	-	X
4	ASN	V	908	-	X
5	ZN	B	901	-	X
6	ADP	B	479	-	X
7	MN	E	481	-	X
7	MN	N	481	-	X
7	MN	T	481	-	X
7	MN	W	481	-	X
8	ATP	E	479	-	X
8	ATP	K	479	-	X
8	ATP	N	479	-	X
8	ATP	Q	479	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 63243 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Glutamyl-tRNA(Gln) amidotransferase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	D	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	G	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	J	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	M	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	P	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	S	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	V	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			

- Molecule 2 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln)amidotransferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	E	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	H	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	K	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	N	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	Q	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			

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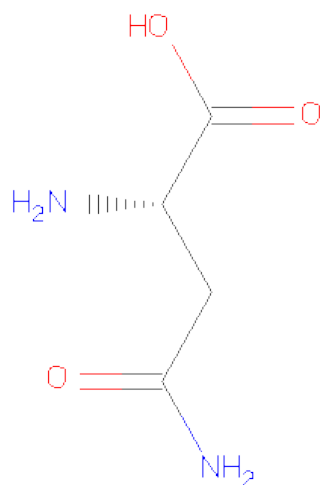
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	W	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			

- Molecule 3 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	F	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	I	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	L	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	O	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	R	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	U	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	X	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			

- Molecule 4 is ASPARAGINE (three-letter code: ASN) (formula: C<sub>4</sub>H<sub>8</sub>N<sub>2</sub>O<sub>3</sub>).

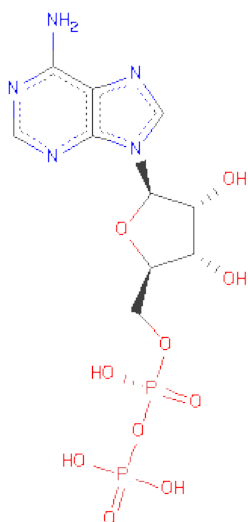


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 4 1 3	0	0
4	D	1	Total C N O 8 4 1 3	0	0
4	G	1	Total C N O 8 4 1 3	0	0
4	J	1	Total C N O 8 4 1 3	0	0
4	M	1	Total C N O 8 4 1 3	0	0
4	P	1	Total C N O 8 4 1 3	0	0
4	S	1	Total C N O 8 4 1 3	0	0
4	V	1	Total C N O 8 4 1 3	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Q	1	Total Zn 1 1	0	0
5	K	1	Total Zn 1 1	0	0
5	E	1	Total Zn 1 1	0	0
5	H	1	Total Zn 1 1	0	0
5	B	1	Total Zn 1 1	0	0
5	W	1	Total Zn 1 1	0	0
5	T	1	Total Zn 1 1	0	0
5	N	1	Total Zn 1 1	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).

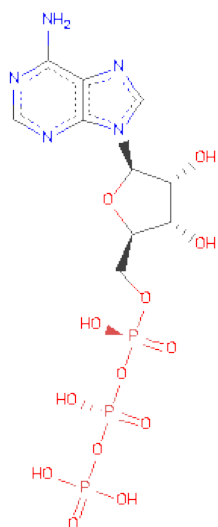


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	T	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	Q	2	Total	Mn	0	0
			2	2		
7	K	2	Total	Mn	0	0
			2	2		
7	E	2	Total	Mn	0	0
			2	2		
7	H	2	Total	Mn	0	0
			2	2		
7	B	2	Total	Mn	0	0
			2	2		
7	W	2	Total	Mn	0	0
			2	2		
7	T	2	Total	Mn	0	0
			2	2		
7	N	2	Total	Mn	0	0
			2	2		

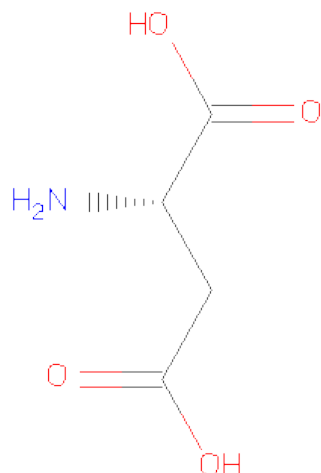
- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
8	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
8	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
8	N	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
8	Q	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
8	W	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 9 is ASPARTIC ACID (three-letter code: ASP) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>4</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	N	O	0	0
			9	4	1	4		
9	N	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	4	Total	O	0	0
			4	4		
10	A	1	Total	O	0	0
			1	1		
10	E	3	Total	O	0	0
			3	3		
10	H	3	Total	O	0	0
			3	3		
10	G	2	Total	O	0	0
			2	2		
10	K	5	Total	O	0	0
			5	5		
10	N	5	Total	O	0	0
			5	5		
10	J	2	Total	O	0	0
			2	2		
10	Q	7	Total	O	0	0
			7	7		
10	M	3	Total	O	0	0
			3	3		

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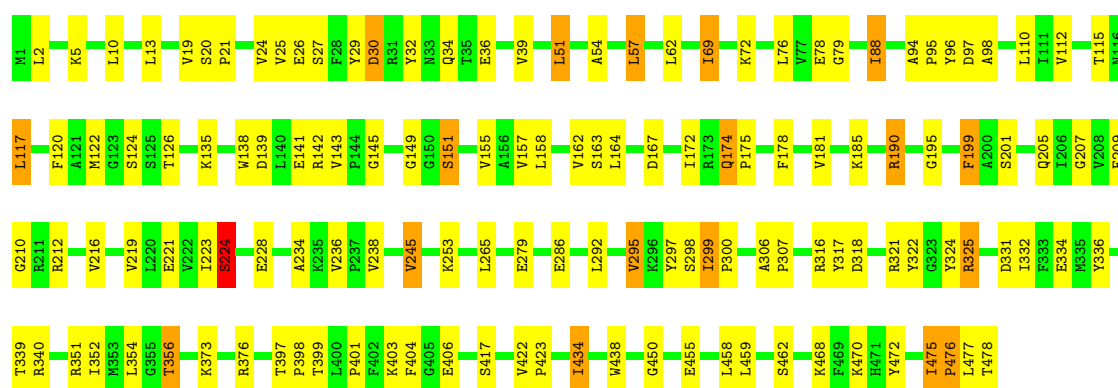
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	T	5	Total 5	O 5	0	0
10	V	1	Total 1	O 1	0	0
10	P	2	Total 2	O 2	0	0
10	W	6	Total 6	O 6	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

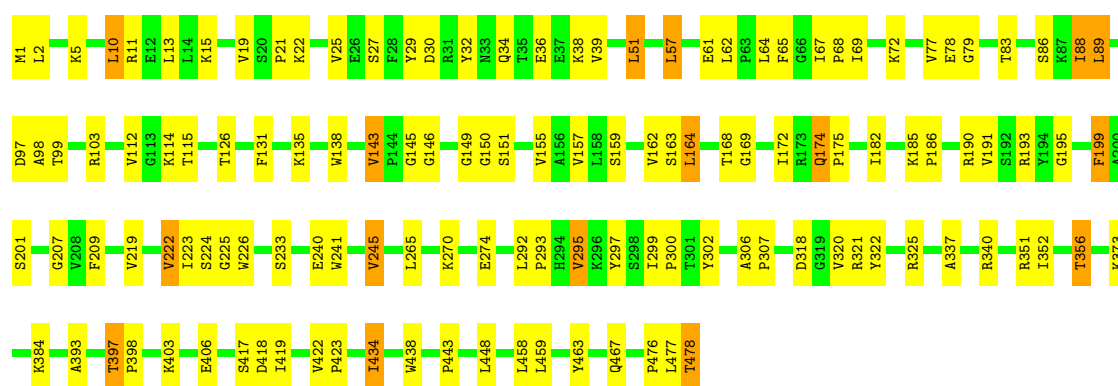
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain A:



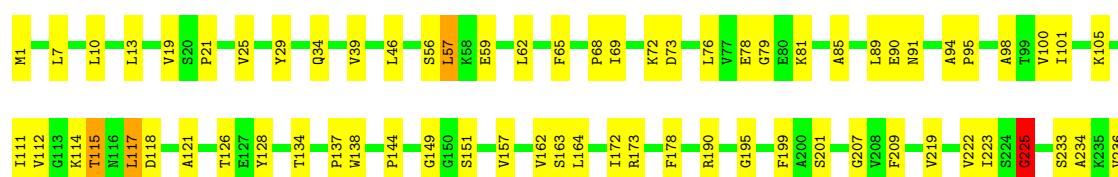
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

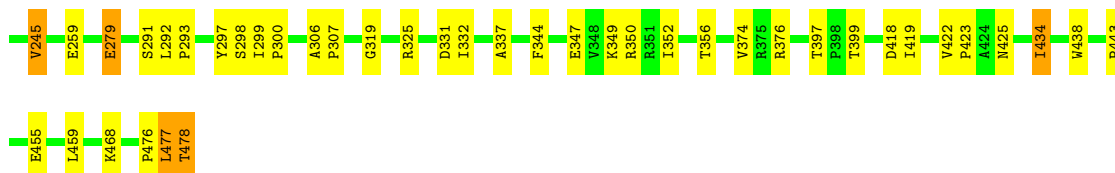
Chain D:



- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

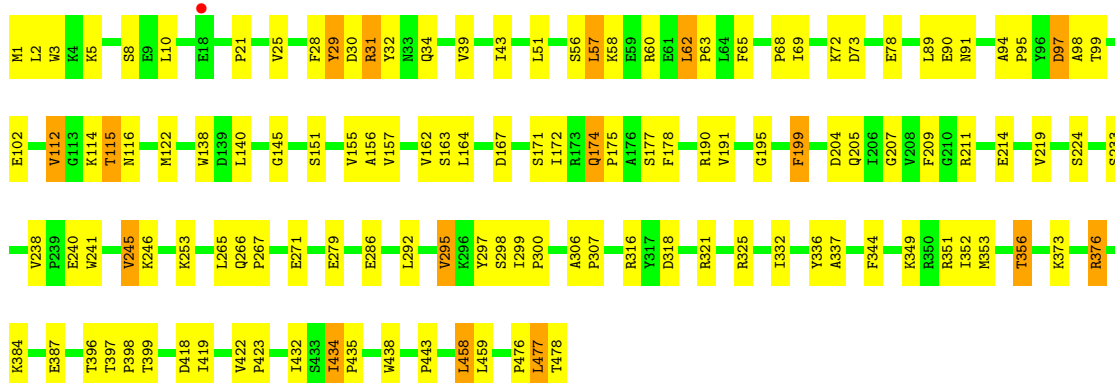
Chain G:





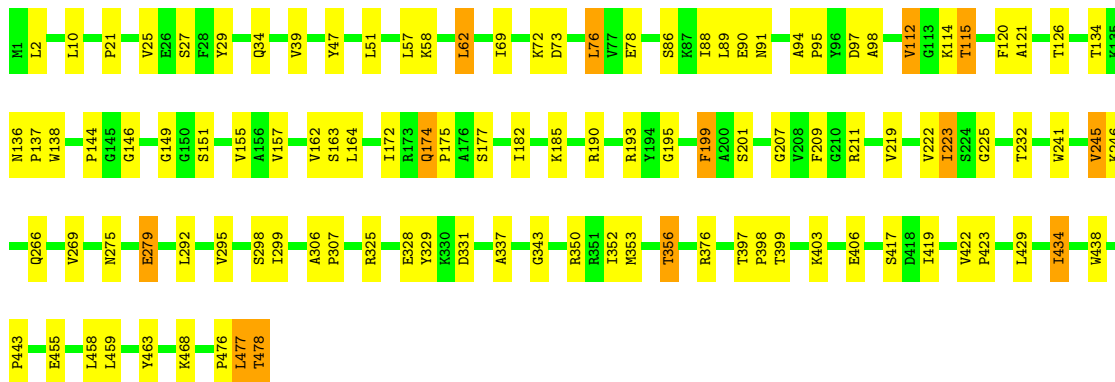
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain J:



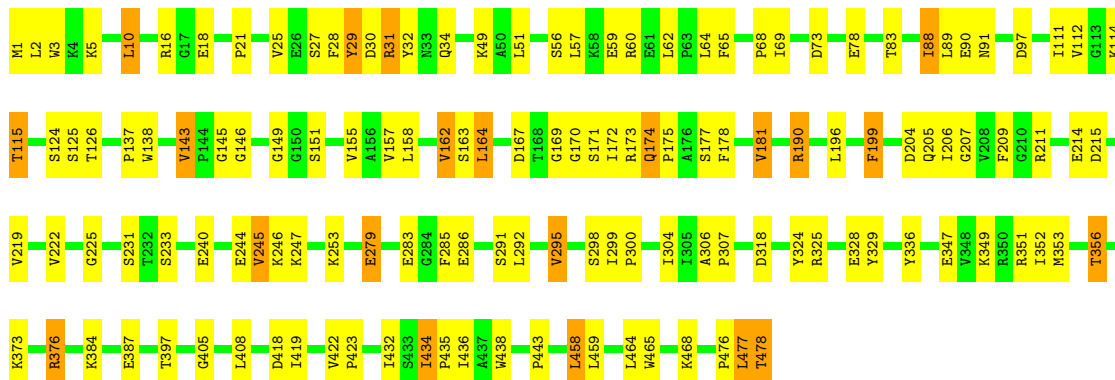
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain M:



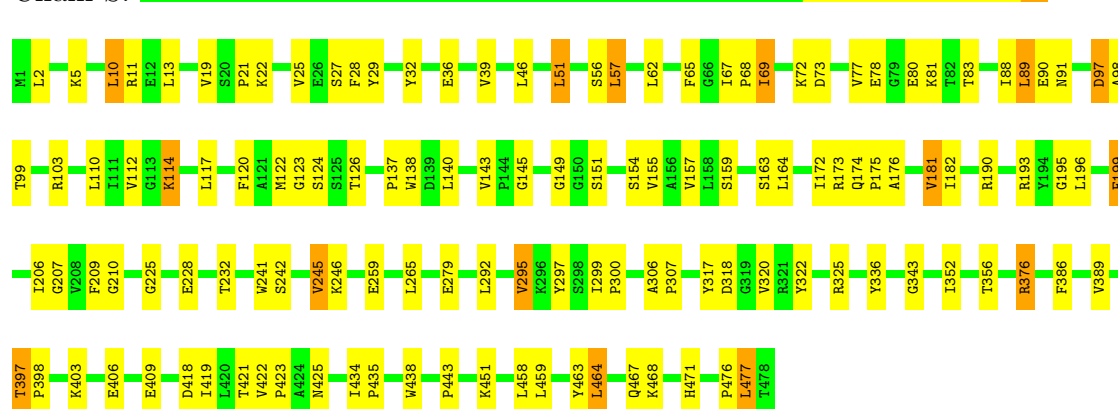
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain P:



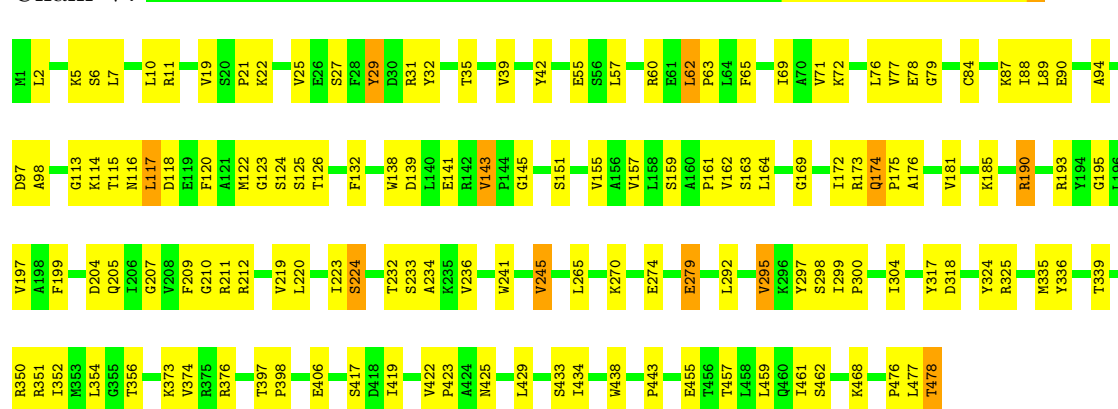
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain S:



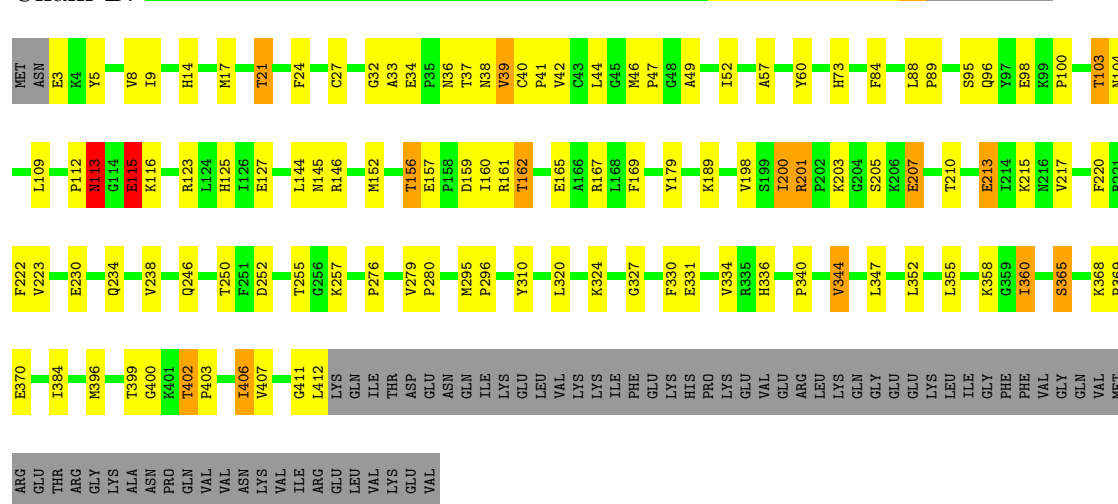
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain V:



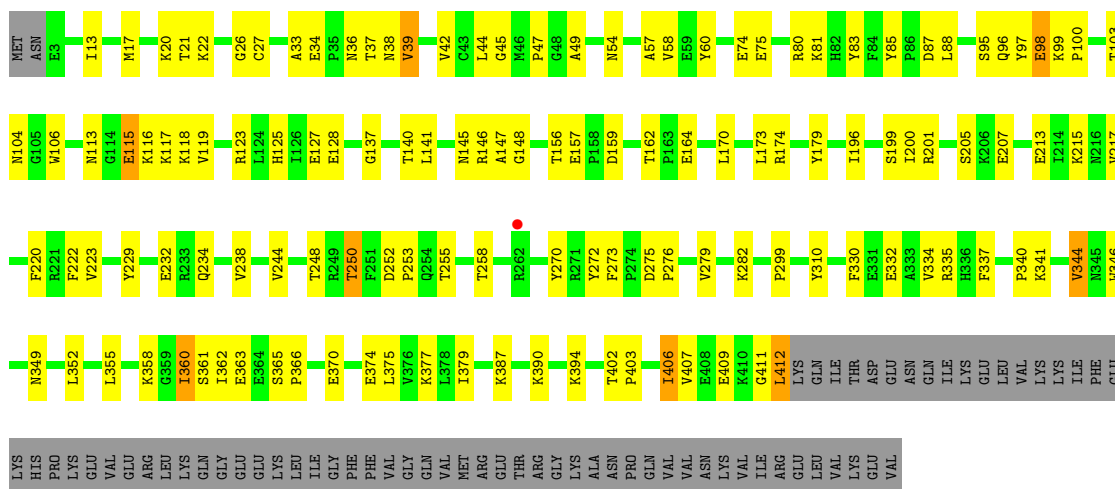
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln)amidotransferase subunit B

Chain B:



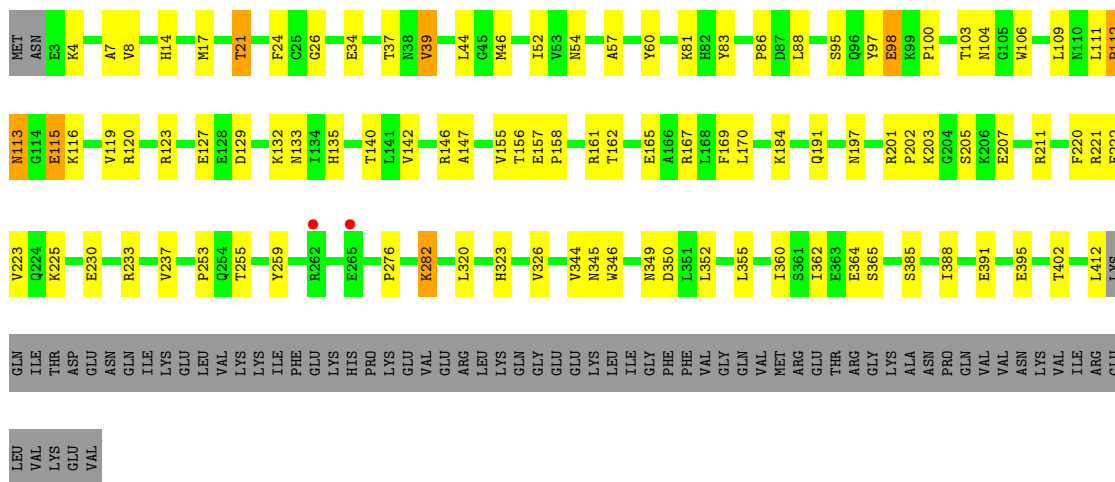
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln)amidotransferase subunit B

Chain E:



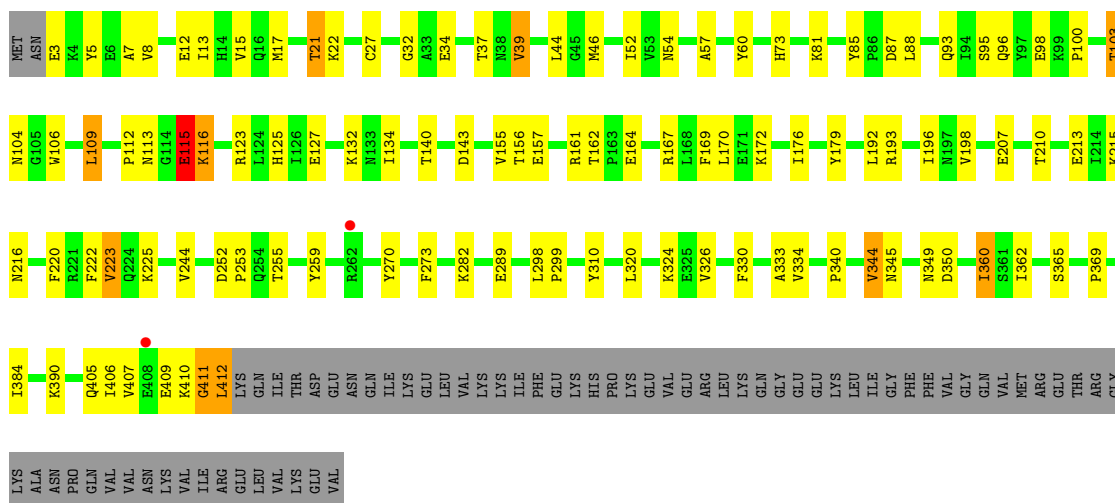
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln)amidotransferase subunit B

Chain H:



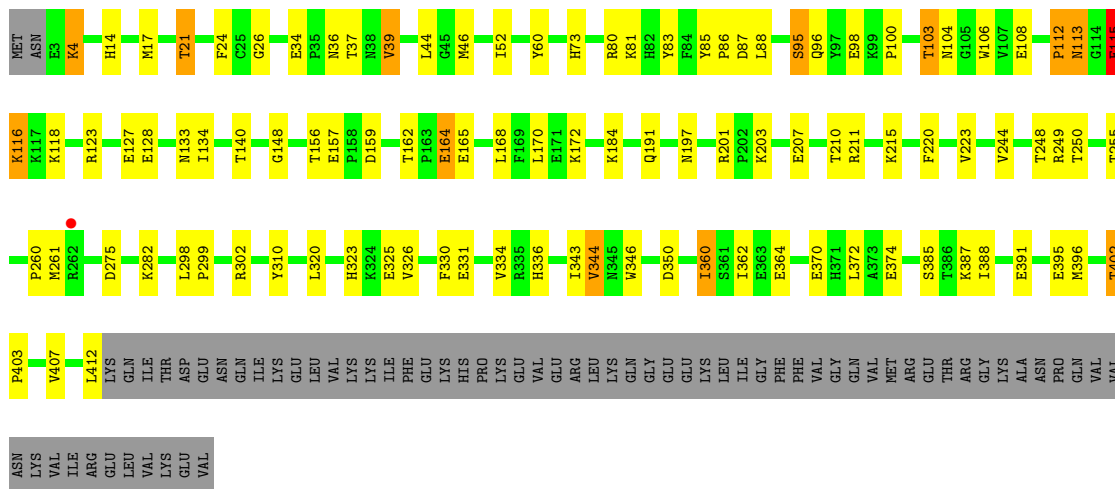
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln)amidotransferase subunit B

Chain K:



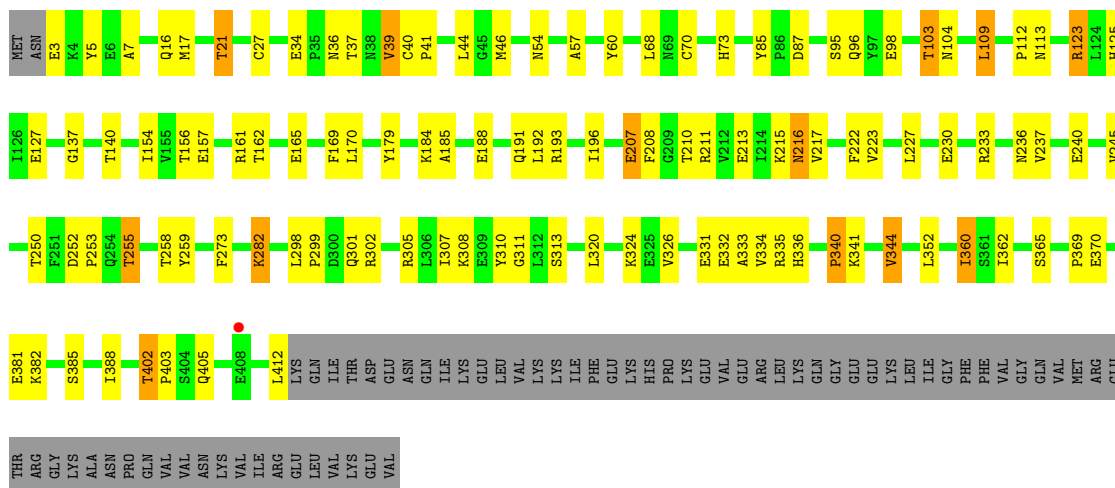
- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln)amidotransferase subunit B

Chain N:



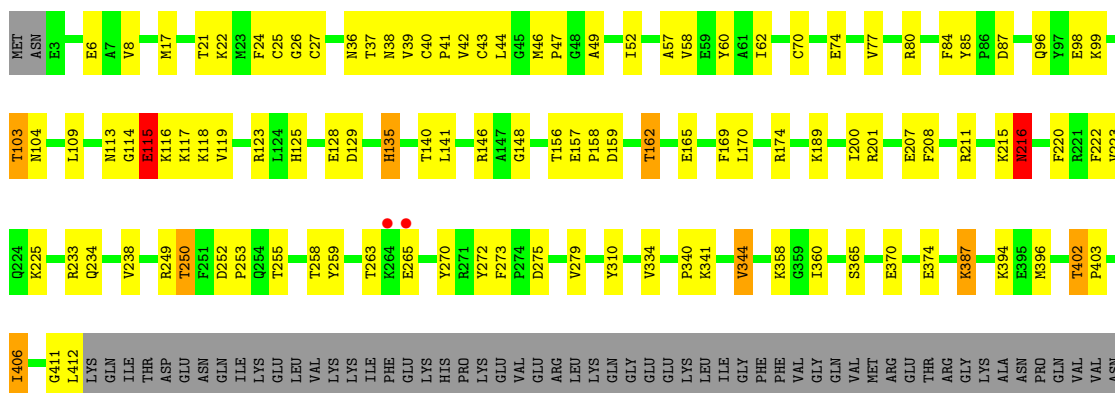
- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln)amidotransferase subunit B

Chain Q:



● Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln)amidotransferase subunit B

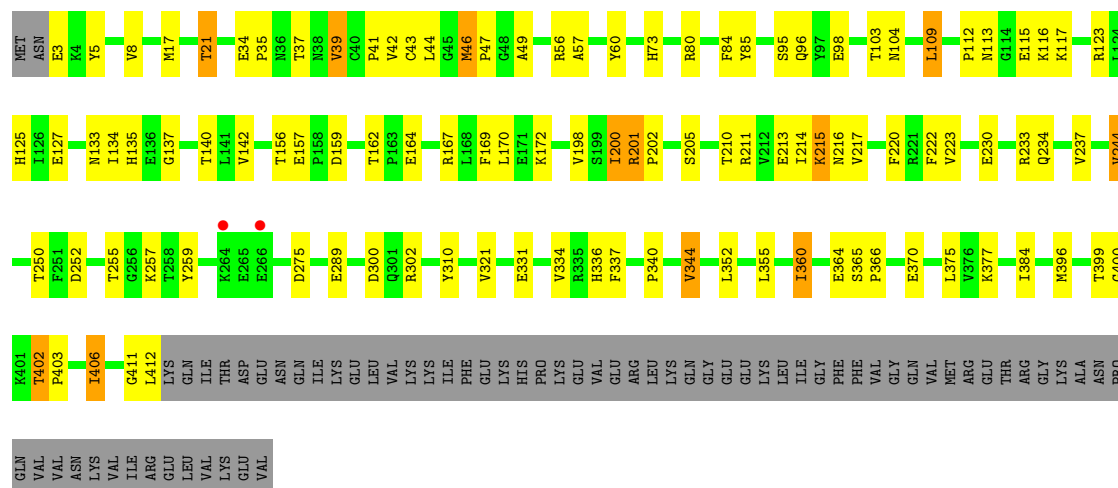
Chain T:



LYS  
VAL  
ILE  
ARG  
GLU  
LEU  
VAL  
LYS  
GLU  
VAL

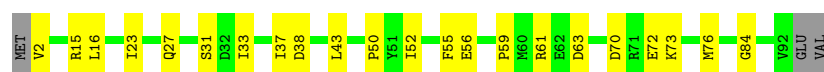
- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln)amidotransferase subunit B

Chain W:



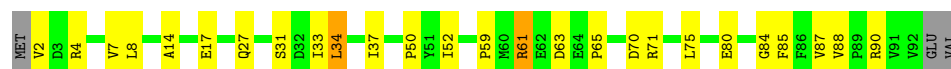
- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain C:



- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain F:



- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain I:



- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain L:



- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain O:





- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain R: 



- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain U: 



- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain X: 



## 4 Data and refinement statistics

Xtriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.38Å 130.41Å 153.97Å 89.89° 90.21° 89.95°	Depositor
Resolution (Å)	48.97 – 3.00 48.98 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.97-3.00) 93.8 (48.98-2.79)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.263 , 0.306 0.268 , 0.290	Depositor DCC
$R_{free}$ test set	11760 reflections (5.34%)	DCC
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 15.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	63243	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MN, ATP, ADP

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	0.66	0/3874	0.71	1/5244 (0.0%)
1	D	0.65	0/3874	0.69	1/5244 (0.0%)
1	G	0.62	0/3874	0.68	0/5244
1	J	0.62	0/3874	0.70	1/5244 (0.0%)
1	M	0.63	0/3874	0.70	1/5244 (0.0%)
1	P	0.62	0/3874	0.67	1/5244 (0.0%)
1	S	0.64	0/3874	0.69	2/5244 (0.0%)
1	V	0.67	0/3874	0.72	2/5244 (0.0%)
2	B	0.60	0/3371	0.66	0/4541
2	E	0.61	0/3371	0.65	0/4541
2	H	0.62	1/3371 (0.0%)	0.70	1/4541 (0.0%)
2	K	0.63	1/3371 (0.0%)	0.69	0/4541
2	N	0.60	0/3371	0.68	0/4541
2	Q	0.62	1/3371 (0.0%)	0.69	0/4541
2	T	0.66	1/3371 (0.0%)	0.68	2/4541 (0.0%)
2	W	0.62	2/3371 (0.1%)	0.69	0/4541
3	C	0.59	0/778	0.74	0/1050
3	F	0.60	0/778	0.75	0/1050
3	I	0.62	0/778	0.69	0/1050
3	L	0.70	1/778 (0.1%)	0.76	0/1050
3	O	0.62	0/778	0.73	0/1050
3	R	0.61	0/778	0.73	0/1050
3	U	0.63	0/778	0.76	0/1050
3	X	0.60	0/778	0.76	0/1050
All	All	0.63	7/64184 (0.0%)	0.69	12/86680 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	D	0	2
1	G	0	3
1	M	0	4
1	P	0	1
1	S	0	1
2	B	0	4
2	E	0	3
2	H	0	2
2	K	0	4
2	N	0	2
2	Q	0	2
2	T	0	2
2	W	0	3
3	I	0	1
3	R	0	1
All	All	0	39

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	43	CYS	CB-SG	-5.94	1.72	1.81
2	W	43	CYS	CB-SG	-5.74	1.72	1.81
2	W	289	GLU	CG-CD	5.47	1.60	1.51
2	K	289	GLU	CG-CD	5.19	1.59	1.51
2	H	98	GLU	CG-CD	5.18	1.59	1.51
3	L	46	GLU	CG-CD	5.15	1.59	1.51
2	Q	70	CYS	CB-SG	-5.08	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	174	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	H	120	ARG	NE-CZ-NH2	-5.60	117.50	120.30
2	T	129	ASP	CB-CG-OD1	5.37	123.13	118.30
1	M	97	ASP	CB-CG-OD2	5.23	123.01	118.30
1	V	97	ASP	CB-CG-OD2	5.22	123.00	118.30
1	S	97	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	97	ASP	CB-CG-OD2	5.20	122.98	118.30
1	J	97	ASP	CB-CG-OD2	5.19	122.97	118.30
1	P	97	ASP	CB-CG-OD2	5.17	122.96	118.30
1	S	464	LEU	CA-CB-CG	5.15	127.15	115.30
1	D	97	ASP	CB-CG-OD2	5.15	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	265	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	ILE	Peptide
1	A	224	SER	Peptide
1	A	475	ILE	Peptide
1	A	477	LEU	Peptide
2	B	113	ASN	Peptide
2	B	115	GLU	Peptide
2	B	32	GLY	Peptide
2	B	33	ALA	Peptide
1	D	222	VAL	Peptide
1	D	225	GLY	Peptide
2	E	115	GLU	Peptide
2	E	217	VAL	Peptide
2	E	97	TYR	Peptide
1	G	222	VAL	Peptide
1	G	225	GLY	Peptide
1	G	34	GLN	Peptide
2	H	112	PRO	Peptide
2	H	113	ASN	Peptide
3	I	45	THR	Peptide
2	K	112	PRO	Peptide
2	K	115	GLU	Peptide
2	K	32	GLY	Peptide
2	K	411	GLY	Peptide
1	M	222	VAL	Peptide
1	M	223	ILE	Peptide
1	M	225	GLY	Peptide
1	M	34	GLN	Peptide
2	N	112	PRO	Peptide
2	N	115	GLU	Peptide
1	P	225	GLY	Peptide
2	Q	112	PRO	Peptide
2	Q	113	ASN	Peptide
3	R	45	THR	Peptide
1	S	225	GLY	Peptide
2	T	115	GLU	Peptide
2	T	411	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	W	112	PRO	Peptide
2	W	113	ASN	Peptide
2	W	215	LYS	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3784	0	3816	110	0
1	D	3784	0	3816	116	0
1	G	3784	0	3816	95	0
1	J	3784	0	3816	106	0
1	M	3784	0	3816	88	0
1	P	3784	0	3816	115	0
1	S	3784	0	3816	103	0
1	V	3784	0	3816	107	0
2	B	3308	0	3354	112	0
2	E	3308	0	3353	116	0
2	H	3308	0	3353	91	0
2	K	3308	0	3353	84	0
2	N	3308	0	3353	81	0
2	Q	3308	0	3353	89	0
2	T	3308	0	3353	93	0
2	W	3308	0	3353	92	0
3	C	764	0	755	21	0
3	F	764	0	755	23	0
3	I	764	0	755	30	0
3	L	764	0	755	22	0
3	O	764	0	755	17	0
3	R	764	0	755	17	0
3	U	764	0	755	17	0
3	X	764	0	755	32	0
4	A	8	0	3	1	0
4	D	8	0	3	5	0
4	G	8	0	3	0	0
4	J	8	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	8	0	3	1	0
4	P	8	0	3	1	0
4	S	8	0	3	4	0
4	V	8	0	3	4	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
5	K	1	0	0	0	0
5	N	1	0	0	0	0
5	Q	1	0	0	0	0
5	T	1	0	0	0	0
5	W	1	0	0	0	0
6	B	27	0	12	0	0
6	T	27	0	12	2	0
7	B	2	0	0	0	0
7	E	2	0	0	0	0
7	H	2	0	0	0	0
7	K	2	0	0	0	0
7	N	2	0	0	0	0
7	Q	2	0	0	0	0
7	T	2	0	0	0	0
7	W	2	0	0	0	0
8	E	31	0	12	1	0
8	H	31	0	12	7	0
8	K	31	0	12	1	0
8	N	31	0	12	1	0
8	Q	31	0	12	3	0
8	W	31	0	12	3	0
9	H	9	0	3	5	0
9	N	9	0	3	3	0
10	A	1	0	0	0	0
10	B	4	0	0	0	0
10	E	3	0	0	0	0
10	G	2	0	0	1	0
10	H	3	0	0	2	0
10	J	2	0	0	1	0
10	K	5	0	0	0	0
10	M	3	0	0	2	0
10	N	5	0	0	1	0
10	P	2	0	0	1	0
10	Q	7	0	0	0	0
10	T	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	V	1	0	0	0	0
10	W	6	0	0	0	0
All	All	63243	0	63519	1639	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (1639) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:W:384:ILE:HG22	2:W:412:LEU:CD2	1.62	1.28
1:D:83:THR:HG21	1:D:131:PHE:CZ	1.78	1.19
2:B:280:PRO:HD2	3:C:55:PHE:CZ	1.85	1.12
2:K:115:GLU:OE2	2:K:115:GLU:HA	1.48	1.10
1:V:190:ARG:HH11	1:V:190:ARG:HG3	1.11	1.10
3:X:91:VAL:HG23	3:X:92:VAL:N	1.68	1.09
2:H:81:LYS:NZ	9:H:482:ASP:HA	1.68	1.08
3:I:88:VAL:HB	3:I:89:PRO:HD2	1.34	1.07
1:G:117:LEU:N	1:G:117:LEU:HD12	1.69	1.07
1:J:376:ARG:HG3	1:J:376:ARG:HH11	1.17	1.07
1:D:77:VAL:HG23	1:D:114:LYS:HZ2	1.18	1.07
1:D:13:LEU:HB3	1:D:19:VAL:HG12	1.36	1.07
1:A:190:ARG:HH11	1:A:190:ARG:HG3	1.05	1.06
2:N:115:GLU:HA	2:N:115:GLU:OE2	1.49	1.06
2:B:21:THR:HG21	3:C:61:ARG:HH12	1.20	1.06
3:L:88:VAL:HB	3:L:89:PRO:HD2	1.37	1.06
2:W:384:ILE:HG22	2:W:412:LEU:HD23	1.14	1.05
1:M:88:ILE:HG23	1:M:343:GLY:HA3	1.36	1.05
2:W:384:ILE:CG2	2:W:412:LEU:HD23	1.85	1.04
2:E:360:ILE:HD11	2:E:365:SER:HA	1.35	1.04
1:D:77:VAL:HG23	1:D:114:LYS:NZ	1.73	1.03
2:T:115:GLU:OE2	2:T:115:GLU:HA	1.52	1.03
2:W:360:ILE:HD11	2:W:365:SER:HA	1.38	1.03
1:P:190:ARG:HG3	1:P:190:ARG:HH11	1.24	1.02
1:M:352:ILE:O	1:M:356:THR:HG22	1.57	1.02
1:D:13:LEU:HB3	1:D:19:VAL:CG1	1.89	1.01
2:T:21:THR:HB	3:U:63:ASP:OD1	1.58	1.01
2:H:21:THR:HG21	3:I:61:ARG:HH12	1.25	0.99
2:N:21:THR:HG21	3:O:61:ARG:HH12	1.27	0.99
2:E:21:THR:HG21	3:F:61:ARG:HH12	1.26	0.98
1:M:138:TRP:CZ2	1:M:476:PRO:HD3	1.97	0.98
1:S:422:VAL:CG2	1:S:423:PRO:HD3	1.94	0.98
3:X:91:VAL:HG23	3:X:92:VAL:H	1.23	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:T:21:THR:HG21	3:U:61:ARG:HH12	1.30	0.96
2:K:412:LEU:C	2:K:412:LEU:HD12	1.86	0.96
3:O:91:VAL:O	3:O:92:VAL:HG13	1.65	0.96
2:B:384:ILE:HG22	2:B:412:LEU:HD23	1.44	0.95
1:A:352:ILE:O	1:A:356:THR:HG23	1.66	0.95
1:A:120:PHE:O	1:A:122:MET:HG3	1.65	0.95
1:G:117:LEU:HD12	1:G:117:LEU:H	1.24	0.95
2:Q:156:THR:HG22	2:Q:157:GLU:O	1.67	0.95
1:S:190:ARG:HD3	1:S:241:TRP:HH2	1.33	0.93
1:M:88:ILE:HD11	1:M:120:PHE:CZ	2.05	0.92
2:E:119:VAL:HG13	2:E:159:ASP:HB2	1.52	0.91
2:E:21:THR:HB	3:F:63:ASP:OD1	1.69	0.90
2:H:17:MET:CE	2:H:60:TYR:HB2	2.01	0.90
2:W:384:ILE:HG22	2:W:412:LEU:HD21	1.52	0.90
2:H:17:MET:CE	2:H:60:TYR:CB	2.49	0.90
1:S:422:VAL:HG22	1:S:423:PRO:HD3	1.55	0.89
2:E:39:VAL:HG22	2:E:44:LEU:HG	1.52	0.89
2:E:17:MET:CE	2:E:57:ALA:HA	2.01	0.89
2:H:81:LYS:HZ2	9:H:482:ASP:HA	1.25	0.89
1:D:83:THR:HG21	1:D:131:PHE:HZ	1.30	0.89
1:A:13:LEU:HB3	1:A:19:VAL:HG12	1.53	0.88
1:G:95:PRO:HG2	2:H:46:MET:CE	2.03	0.88
1:D:77:VAL:CG2	1:D:114:LYS:NZ	2.36	0.88
2:Q:95:SER:HB2	2:Q:127:GLU:HB3	1.52	0.88
2:B:103:THR:HG22	2:B:104:ASN:OD1	1.72	0.88
2:E:34:GLU:O	2:E:37:THR:HB	1.71	0.88
2:B:384:ILE:CG2	2:B:412:LEU:HD23	2.03	0.88
2:H:220:PHE:O	2:H:223:VAL:HG22	1.74	0.88
2:B:162:THR:HG22	2:B:165:GLU:H	1.38	0.88
2:W:21:THR:HG21	3:X:61:ARG:HH12	1.37	0.88
1:A:224:SER:HB3	1:A:238:VAL:HG21	1.57	0.87
2:T:115:GLU:HG3	2:T:116:LYS:HE2	1.57	0.87
2:W:39:VAL:HG13	2:W:44:LEU:HD11	1.54	0.87
2:B:347:LEU:O	2:B:352:LEU:HD23	1.76	0.86
1:D:190:ARG:HD3	1:D:241:TRP:HH2	1.40	0.86
2:H:17:MET:HE1	2:H:60:TYR:HB2	1.55	0.86
1:J:72:LYS:HA	1:J:115:THR:HG22	1.58	0.86
2:E:115:GLU:HB3	2:E:116:LYS:HG3	1.57	0.86
2:B:21:THR:CG2	3:C:61:ARG:HH12	1.88	0.85
2:B:40:CYS:O	2:B:44:LEU:HB2	1.75	0.85
2:E:17:MET:HE2	2:E:57:ALA:HA	1.55	0.85
2:W:252:ASP:HB3	2:W:255:THR:HG22	1.58	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:201:ARG:HD2	2:N:207:GLU:O	1.76	0.85
1:S:376:ARG:HH11	1:S:376:ARG:HG3	1.39	0.85
2:B:384:ILE:HG22	2:B:412:LEU:CD2	2.06	0.85
1:V:190:ARG:HG3	1:V:190:ARG:NH1	1.89	0.85
2:N:17:MET:HE1	2:N:60:TYR:CB	2.06	0.85
1:V:279:GLU:HG3	1:V:468:LYS:NZ	1.92	0.85
2:K:21:THR:HG21	3:L:61:ARG:HH12	1.41	0.84
2:E:33:ALA:HB1	2:E:37:THR:HG21	1.59	0.84
2:B:21:THR:HB	3:C:63:ASP:OD1	1.75	0.84
1:A:376:ARG:HG3	1:A:376:ARG:HH11	1.40	0.84
2:Q:207:GLU:HA	2:Q:207:GLU:OE1	1.76	0.84
2:E:39:VAL:HG13	2:E:44:LEU:HD11	1.57	0.84
1:D:83:THR:HG21	1:D:131:PHE:CE2	2.13	0.84
2:T:358:LYS:HB2	2:T:360:ILE:HG22	1.60	0.83
2:N:17:MET:HE1	2:N:60:TYR:HB2	1.59	0.83
1:D:83:THR:HG22	1:D:86:SER:H	1.44	0.83
2:B:100:PRO:HB3	2:B:123:ARG:HH21	1.41	0.83
2:Q:334:VAL:HG21	2:Q:340:PRO:HB3	1.59	0.83
2:E:360:ILE:HD11	2:E:365:SER:CA	2.08	0.83
2:K:412:LEU:O	2:K:412:LEU:HD12	1.80	0.82
2:W:355:LEU:HD22	2:W:360:ILE:CD1	2.10	0.82
1:J:3:TRP:CD2	1:J:31:ARG:HD3	2.14	0.82
2:B:280:PRO:HD2	3:C:55:PHE:HZ	1.38	0.82
2:N:115:GLU:HG3	2:N:116:LYS:HG2	1.60	0.82
1:J:95:PRO:HG2	2:K:46:MET:CE	2.10	0.82
1:G:117:LEU:N	1:G:117:LEU:CD1	2.42	0.81
1:V:163:SER:HB3	1:V:209:PHE:HB2	1.62	0.81
1:P:155:VAL:HG12	1:P:181:VAL:HG21	1.61	0.81
2:B:17:MET:HE2	2:B:57:ALA:HA	1.62	0.81
3:R:46:GLU:O	3:R:47:ASN:HB2	1.81	0.81
2:N:39:VAL:HG13	2:N:44:LEU:HD11	1.62	0.81
1:D:174:GLN:HG3	1:D:175:PRO:HD3	1.64	0.80
1:A:221:GLU:O	1:A:224:SER:HB2	1.81	0.80
3:C:33:ILE:O	3:C:37:ILE:HG12	1.81	0.80
2:W:34:GLU:O	2:W:37:THR:HG22	1.81	0.80
1:J:376:ARG:NH1	1:J:376:ARG:HG3	1.94	0.80
2:H:211:ARG:NH1	8:H:479:ATP:H5'2	1.97	0.80
1:P:177:SER:HA	10:P:907:HOH:O	1.81	0.80
1:M:174:GLN:HG3	1:M:175:PRO:HD3	1.63	0.79
1:V:279:GLU:HG3	1:V:468:LYS:HZ3	1.47	0.79
3:X:33:ILE:O	3:X:37:ILE:HG12	1.82	0.79
2:K:100:PRO:HB3	2:K:123:ARG:HH21	1.45	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:163:SER:HB3	1:D:209:PHE:HB2	1.65	0.79
2:N:81:LYS:HZ1	9:N:482:ASP:HA	1.47	0.79
2:N:81:LYS:NZ	9:N:482:ASP:HA	1.98	0.79
1:G:352:ILE:O	1:G:356:THR:HG23	1.82	0.79
1:D:245:VAL:CG1	1:D:459:LEU:HB3	2.13	0.78
1:A:190:ARG:NH1	1:A:190:ARG:HG3	1.86	0.78
1:D:115:THR:HG21	1:D:151:SER:OG	1.84	0.78
2:T:103:THR:CG2	2:T:104:ASN:OD1	2.32	0.78
2:H:21:THR:CG2	3:I:61:ARG:HH12	1.96	0.78
2:T:207:GLU:HG3	2:T:208:PHE:H	1.49	0.78
2:E:310:TYR:HE1	2:E:334:VAL:HG11	1.48	0.78
2:W:156:THR:HG22	2:W:157:GLU:O	1.84	0.78
1:M:88:ILE:HD11	1:M:120:PHE:HZ	1.48	0.78
2:Q:207:GLU:CA	2:Q:207:GLU:OE1	2.32	0.78
2:H:17:MET:CE	2:H:60:TYR:HB3	2.12	0.77
1:S:477:LEU:N	1:S:477:LEU:HD23	1.99	0.77
1:D:2:LEU:HD23	1:D:27:SER:HB2	1.66	0.77
2:Q:17:MET:CE	2:Q:60:TYR:HB2	2.15	0.77
2:B:252:ASP:HB3	2:B:255:THR:HG22	1.65	0.77
1:J:163:SER:HB3	1:J:209:PHE:HB2	1.65	0.77
1:G:95:PRO:HG2	2:H:46:MET:HE3	1.66	0.77
2:B:200:ILE:HD11	2:B:238:VAL:HG21	1.66	0.77
2:N:220:PHE:O	2:N:223:VAL:HG22	1.85	0.76
1:D:245:VAL:HG12	1:D:459:LEU:HB3	1.66	0.76
2:E:140:THR:OG1	3:F:90:ARG:HA	1.85	0.76
1:J:3:TRP:CE2	1:J:31:ARG:HD3	2.20	0.76
2:B:17:MET:CE	2:B:57:ALA:HA	2.14	0.76
2:T:17:MET:HE2	2:T:57:ALA:HA	1.67	0.76
2:T:115:GLU:OE2	2:T:115:GLU:CA	2.30	0.76
2:W:411:GLY:O	2:W:412:LEU:HB2	1.86	0.76
1:A:434:ILE:HD11	1:A:462:SER:OG	1.85	0.76
1:J:190:ARG:HD3	1:J:241:TRP:HH2	1.51	0.75
2:K:39:VAL:HG13	2:K:44:LEU:HD11	1.67	0.75
1:S:477:LEU:HD23	1:S:477:LEU:H	1.51	0.75
1:J:177:SER:HA	10:J:906:HOH:O	1.85	0.75
2:W:21:THR:CG2	3:X:61:ARG:HH12	2.00	0.75
1:S:245:VAL:HG12	1:S:459:LEU:HB3	1.68	0.75
1:V:138:TRP:CE2	1:V:438:TRP:HH2	2.04	0.75
2:H:103:THR:HG22	2:H:104:ASN:OD1	1.86	0.75
1:D:72:LYS:HA	1:D:115:THR:HG22	1.67	0.75
2:N:95:SER:HB3	2:N:127:GLU:HB3	1.67	0.75
1:A:475:ILE:HG22	1:A:476:PRO:HD2	1.69	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:103:THR:HG22	2:E:104:ASN:OD1	1.86	0.75
2:K:406:ILE:O	2:K:410:LYS:HB2	1.87	0.75
2:E:33:ALA:CB	2:E:37:THR:HG21	2.16	0.74
2:K:115:GLU:OE2	2:K:115:GLU:CA	2.30	0.74
2:W:360:ILE:CD1	2:W:365:SER:HA	2.14	0.74
1:S:422:VAL:HG23	1:S:423:PRO:HD3	1.69	0.74
2:K:34:GLU:O	2:K:37:THR:HG22	1.86	0.74
1:A:450:GLY:HA3	1:A:458:LEU:HD11	1.67	0.74
1:D:138:TRP:CE2	1:D:438:TRP:CH2	2.75	0.74
1:J:174:GLN:HG3	1:J:175:PRO:HD3	1.70	0.74
1:S:190:ARG:HD3	1:S:241:TRP:CH2	2.20	0.74
1:P:356:THR:HG21	3:R:14:ALA:HB2	1.68	0.74
1:M:88:ILE:HG23	1:M:343:GLY:CA	2.16	0.74
1:V:138:TRP:CE2	1:V:438:TRP:CH2	2.76	0.74
2:Q:341:LYS:O	2:Q:344:VAL:HG23	1.88	0.73
2:W:103:THR:HG22	2:W:104:ASN:OD1	1.86	0.73
2:T:220:PHE:O	2:T:223:VAL:HG22	1.89	0.73
2:B:17:MET:HE1	2:B:57:ALA:O	1.88	0.73
1:S:155:VAL:HG12	1:S:181:VAL:HG21	1.70	0.73
2:Q:213:GLU:OE2	2:Q:215:LYS:HE3	1.89	0.73
1:S:397:THR:HG22	1:S:398:PRO:HD2	1.68	0.73
2:B:280:PRO:HD2	3:C:55:PHE:CE1	2.23	0.73
2:Q:39:VAL:HG13	2:Q:44:LEU:HD11	1.70	0.73
2:W:17:MET:CE	2:W:60:TYR:HB2	2.19	0.73
2:B:213:GLU:OE1	2:B:215:LYS:HE2	1.89	0.73
1:P:299:ILE:N	1:P:300:PRO:HD2	2.04	0.72
1:D:138:TRP:CE2	1:D:438:TRP:HH2	2.07	0.72
2:W:213:GLU:OE2	2:W:215:LYS:HE3	1.88	0.72
2:T:39:VAL:HG22	2:T:44:LEU:HG	1.71	0.72
2:E:22:LYS:HD2	2:E:27:CYS:HB2	1.71	0.72
2:N:211:ARG:NH1	8:N:479:ATP:O2A	2.22	0.72
1:S:73:ASP:OD1	1:S:114:LYS:NZ	2.22	0.72
1:M:138:TRP:CE2	1:M:438:TRP:CH2	2.78	0.72
2:N:17:MET:CE	2:N:60:TYR:HB3	2.19	0.72
2:E:360:ILE:CD1	2:E:365:SER:HA	2.16	0.72
1:G:178:PHE:HE1	1:G:397:THR:HG21	1.53	0.72
1:J:3:TRP:CE3	1:J:31:ARG:HD3	2.24	0.72
3:O:91:VAL:O	3:O:92:VAL:CG1	2.37	0.71
2:W:17:MET:HE1	2:W:57:ALA:O	1.89	0.71
1:A:163:SER:HB3	1:A:209:PHE:HB2	1.72	0.71
2:H:17:MET:HE2	2:H:60:TYR:CB	2.19	0.71
2:E:17:MET:CE	2:E:60:TYR:HB2	2.20	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:103:THR:CG2	2:B:104:ASN:OD1	2.38	0.71
2:K:252:ASP:OD2	2:K:255:THR:HG22	1.90	0.71
2:B:17:MET:CE	2:B:60:TYR:HB2	2.20	0.71
3:X:91:VAL:CG2	3:X:92:VAL:N	2.43	0.71
2:T:162:THR:HG22	2:T:165:GLU:HB2	1.73	0.70
2:B:21:THR:HG21	3:C:61:ARG:NH1	2.00	0.70
2:K:156:THR:HG22	2:K:157:GLU:O	1.91	0.70
1:D:138:TRP:CZ2	1:D:438:TRP:CH2	2.80	0.70
1:S:13:LEU:HB3	1:S:19:VAL:HG12	1.74	0.70
2:E:37:THR:HG23	2:E:38:ASN:H	1.55	0.70
1:A:475:ILE:CG2	1:A:476:PRO:HD2	2.21	0.70
1:S:163:SER:HB3	1:S:209:PHE:HB2	1.72	0.70
1:S:397:THR:HG22	1:S:398:PRO:CD	2.20	0.70
1:M:163:SER:HB3	1:M:209:PHE:HB2	1.73	0.70
3:I:46:GLU:O	3:I:47:ASN:HB2	1.92	0.70
2:W:96:GLN:HB2	2:W:125:HIS:HB2	1.74	0.70
1:G:162:VAL:HG21	1:G:219:VAL:HG21	1.72	0.70
1:V:190:ARG:HD2	1:V:455:GLU:OE2	1.91	0.70
2:H:86:PRO:HG2	3:I:91:VAL:HG11	1.72	0.70
2:T:252:ASP:OD2	2:T:255:THR:HG22	1.92	0.70
1:V:84:CYS:SG	1:V:197:VAL:HG21	2.31	0.70
2:N:162:THR:HB	2:N:165:GLU:HG3	1.73	0.69
2:W:21:THR:HB	3:X:63:ASP:OD1	1.92	0.69
2:Q:402:THR:HG22	2:Q:403:PRO:HD2	1.73	0.69
1:M:88:ILE:HD11	1:M:120:PHE:CE2	2.27	0.69
3:L:46:GLU:O	3:L:47:ASN:HB2	1.91	0.69
2:N:103:THR:HG23	2:N:104:ASN:OD1	1.92	0.69
2:E:37:THR:HG23	2:E:38:ASN:N	2.08	0.69
1:P:3:TRP:CZ2	1:P:31:ARG:HD3	2.27	0.69
1:A:306:ALA:HB3	1:A:307:PRO:HD3	1.74	0.69
2:K:17:MET:CE	2:K:60:TYR:HB2	2.22	0.69
3:X:55:PHE:O	3:X:56:GLU:HB3	1.91	0.69
2:E:100:PRO:HG3	2:E:123:ARG:NH1	2.08	0.69
2:B:156:THR:HG23	2:B:157:GLU:O	1.93	0.69
1:J:356:THR:HG21	3:L:14:ALA:HB2	1.75	0.69
1:A:13:LEU:HB3	1:A:19:VAL:CG1	2.23	0.69
2:K:115:GLU:HG3	2:K:116:LYS:HG2	1.75	0.68
1:S:245:VAL:CG1	1:S:459:LEU:HB3	2.24	0.68
1:M:245:VAL:HG12	1:M:459:LEU:HB3	1.74	0.68
2:T:17:MET:CE	2:T:57:ALA:HA	2.24	0.68
2:E:411:GLY:O	2:E:412:LEU:C	2.32	0.68
2:N:17:MET:CE	2:N:60:TYR:CB	2.71	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:163:SER:HB3	1:P:209:PHE:HB2	1.75	0.68
2:N:112:PRO:HG2	2:N:164:GLU:OE1	1.92	0.68
2:E:252:ASP:HB3	2:E:255:THR:HG22	1.76	0.68
1:G:245:VAL:HG12	1:G:459:LEU:HB3	1.76	0.68
2:W:17:MET:HE2	2:W:57:ALA:HA	1.76	0.68
1:V:193:ARG:NH1	1:V:232:THR:OG1	2.26	0.68
2:K:412:LEU:CD1	2:K:412:LEU:O	2.41	0.68
1:P:299:ILE:HG13	1:P:419:ILE:HG22	1.75	0.68
1:D:77:VAL:CG2	1:D:114:LYS:HZ1	2.06	0.68
2:N:21:THR:CG2	3:O:61:ARG:HH12	2.03	0.68
2:Q:95:SER:CB	2:Q:127:GLU:HB3	2.24	0.68
2:T:140:THR:OG1	3:U:90:ARG:HA	1.94	0.67
1:G:344:PHE:O	1:G:349:LYS:HE2	1.94	0.67
2:E:17:MET:HE1	2:E:57:ALA:HA	1.75	0.67
1:G:138:TRP:CE2	1:G:438:TRP:CH2	2.83	0.67
1:P:306:ALA:HB3	1:P:307:PRO:HD3	1.75	0.67
1:P:3:TRP:CH2	1:P:31:ARG:HD3	2.28	0.67
1:G:117:LEU:CD1	1:G:117:LEU:H	2.02	0.67
2:T:17:MET:HE1	2:T:57:ALA:O	1.94	0.67
1:V:292:LEU:HB2	1:V:295:VAL:HG22	1.77	0.67
1:J:438:TRP:CZ3	1:J:443:PRO:HG3	2.29	0.67
2:T:207:GLU:HG3	2:T:208:PHE:N	2.09	0.67
2:E:201:ARG:HD2	2:E:207:GLU:O	1.95	0.67
1:V:69:ILE:HD11	1:V:164:LEU:HD13	1.76	0.67
1:M:306:ALA:HB3	1:M:307:PRO:HD3	1.76	0.67
3:F:33:ILE:O	3:F:37:ILE:HG12	1.95	0.67
1:A:397:THR:HG22	1:A:399:THR:H	1.59	0.67
3:U:33:ILE:O	3:U:37:ILE:HG12	1.95	0.66
2:K:21:THR:HG22	2:K:54:ASN:HD22	1.60	0.66
1:P:190:ARG:HG3	1:P:190:ARG:NH1	1.98	0.66
1:S:422:VAL:HG23	1:S:423:PRO:CD	2.25	0.66
1:J:224:SER:O	1:J:238:VAL:HG21	1.96	0.66
2:B:37:THR:HG23	2:B:38:ASN:N	2.09	0.66
1:G:115:THR:HG21	1:G:151:SER:OG	1.94	0.66
2:W:252:ASP:HB3	2:W:255:THR:CG2	2.25	0.66
1:A:138:TRP:CE2	1:A:438:TRP:HH2	2.13	0.66
2:E:117:LYS:HG2	2:E:118:LYS:N	2.10	0.66
2:K:412:LEU:CD1	2:K:412:LEU:C	2.60	0.66
1:V:352:ILE:O	1:V:356:THR:HG23	1.96	0.66
2:K:3:GLU:HG3	2:K:5:TYR:H	1.61	0.66
1:G:190:ARG:HD2	1:G:455:GLU:OE2	1.95	0.66
1:A:32:TYR:CE1	1:A:36:GLU:HG2	2.31	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:434:ILE:HD11	1:V:462:SER:OG	1.96	0.66
1:M:95:PRO:HG2	2:N:46:MET:CE	2.25	0.66
2:W:355:LEU:HD22	2:W:360:ILE:HD13	1.77	0.66
2:H:135:HIS:CE1	3:I:91:VAL:O	2.48	0.66
1:V:6:SER:HB3	1:V:212:ARG:NH1	2.10	0.66
2:W:411:GLY:O	2:W:412:LEU:CB	2.43	0.66
1:J:138:TRP:CZ2	1:J:476:PRO:HD3	2.30	0.66
2:K:412:LEU:O	2:K:412:LEU:CG	2.44	0.66
1:J:245:VAL:HG12	1:J:459:LEU:HB3	1.77	0.66
2:T:128:GLU:HB2	2:T:148:GLY:HA2	1.78	0.65
8:W:479:ATP:H5'1	8:W:479:ATP:O3B	1.95	0.65
2:T:22:LYS:HD2	2:T:27:CYS:HB2	1.79	0.65
1:P:143:VAL:HG13	1:P:145:GLY:H	1.61	0.65
1:G:85:ALA:HB2	1:G:117:LEU:HD13	1.79	0.65
1:J:95:PRO:HG2	2:K:46:MET:HE1	1.78	0.65
1:G:69:ILE:HD11	1:G:164:LEU:HD13	1.77	0.65
2:N:100:PRO:HB3	2:N:123:ARG:NH2	2.11	0.65
1:A:245:VAL:HG12	1:A:459:LEU:HB3	1.78	0.65
1:J:90:GLU:O	1:J:91:ASN:HB2	1.94	0.65
2:B:34:GLU:O	2:B:37:THR:HB	1.96	0.65
1:V:77:VAL:HG21	1:V:114:LYS:NZ	2.12	0.65
2:E:156:THR:HG22	2:E:157:GLU:O	1.96	0.65
2:Q:156:THR:CG2	2:Q:157:GLU:O	2.41	0.65
2:E:103:THR:HG22	2:E:104:ASN:CG	2.17	0.65
1:V:120:PHE:O	1:V:122:MET:HG3	1.96	0.65
1:S:422:VAL:N	1:S:423:PRO:CD	2.60	0.65
2:T:85:TYR:HD2	2:T:87:ASP:OD1	1.79	0.65
1:V:190:ARG:HH11	1:V:190:ARG:CG	1.99	0.65
8:H:479:ATP:H5'1	8:H:479:ATP:H8	1.62	0.65
1:S:143:VAL:HG12	1:S:145:GLY:H	1.60	0.65
2:N:215:LYS:CD	2:N:248:THR:HG21	2.26	0.65
8:H:479:ATP:O2G	9:H:482:ASP:HB2	1.97	0.65
1:M:422:VAL:CG2	1:M:423:PRO:HD3	2.27	0.65
1:D:83:THR:CG2	1:D:131:PHE:HZ	2.08	0.64
1:J:138:TRP:CE2	1:J:438:TRP:CZ3	2.85	0.64
2:H:95:SER:HB3	2:H:127:GLU:HB3	1.78	0.64
1:V:138:TRP:CZ2	1:V:476:PRO:HD3	2.33	0.64
2:E:252:ASP:HB3	2:E:255:THR:CG2	2.27	0.64
1:V:162:VAL:HG21	1:V:219:VAL:HG21	1.79	0.64
2:E:13:ILE:HG21	2:E:173:LEU:HD21	1.79	0.64
1:J:95:PRO:HG2	2:K:46:MET:HE3	1.78	0.64
1:A:155:VAL:CG2	1:A:163:SER:HB2	2.27	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:220:PHE:O	2:B:223:VAL:HG22	1.98	0.64
1:S:2:LEU:HD23	1:S:27:SER:HB2	1.80	0.64
1:G:374:VAL:HG21	3:I:40:LEU:HD22	1.78	0.64
2:N:21:THR:HB	3:O:63:ASP:OD1	1.96	0.64
1:J:477:LEU:O	1:J:478:THR:C	2.36	0.64
2:N:36:ASN:ND2	3:O:84:GLY:O	2.23	0.64
1:P:438:TRP:CZ3	1:P:443:PRO:HG3	2.33	0.64
1:P:352:ILE:O	1:P:356:THR:HG23	1.98	0.64
2:Q:207:GLU:OE1	2:Q:208:PHE:N	2.31	0.64
1:D:38:LYS:HD2	1:D:477:LEU:HD13	1.80	0.64
2:N:115:GLU:HG3	2:N:116:LYS:CG	2.28	0.64
2:E:17:MET:HE1	2:E:60:TYR:HB2	1.80	0.64
2:K:21:THR:CG2	3:L:61:ARG:HH12	2.09	0.64
1:G:72:LYS:HA	1:G:115:THR:HG22	1.80	0.64
1:P:90:GLU:O	1:P:91:ASN:HB2	1.98	0.64
2:T:115:GLU:HG3	2:T:116:LYS:HG3	1.78	0.63
1:M:138:TRP:CE2	1:M:438:TRP:HH2	2.13	0.63
1:V:397:THR:HG22	1:V:398:PRO:HD2	1.79	0.63
2:H:21:THR:HB	3:I:63:ASP:OD1	1.98	0.63
1:J:190:ARG:HD3	1:J:241:TRP:CH2	2.34	0.63
1:G:306:ALA:HB3	1:G:307:PRO:HD3	1.80	0.63
2:W:255:THR:HG21	2:W:259:TYR:HE1	1.64	0.63
1:G:138:TRP:CZ2	1:G:476:PRO:HD3	2.33	0.63
1:G:422:VAL:CG2	1:G:423:PRO:HD3	2.28	0.63
1:M:299:ILE:HG13	1:M:419:ILE:HG22	1.80	0.63
1:D:83:THR:HG22	1:D:86:SER:N	2.14	0.63
1:M:88:ILE:CG2	1:M:343:GLY:HA3	2.23	0.63
1:A:475:ILE:CG2	1:A:476:PRO:CD	2.76	0.63
1:G:138:TRP:CD2	1:G:438:TRP:HZ3	2.17	0.63
1:V:270:LYS:O	1:V:274:GLU:HG3	1.98	0.63
1:A:2:LEU:HD23	1:A:27:SER:HB2	1.79	0.63
2:T:103:THR:HG23	2:T:104:ASN:OD1	1.97	0.63
1:D:292:LEU:O	1:D:295:VAL:HG22	1.99	0.63
1:S:138:TRP:CE2	1:S:438:TRP:CH2	2.87	0.63
2:N:115:GLU:CA	2:N:115:GLU:OE2	2.32	0.63
1:J:3:TRP:CZ2	1:J:31:ARG:CD	2.82	0.63
1:J:155:VAL:CG2	1:J:163:SER:HB2	2.29	0.63
1:A:78:GLU:HG2	1:A:79:GLY:N	2.14	0.63
1:M:279:GLU:HG3	1:M:468:LYS:NZ	2.14	0.63
2:E:95:SER:HB3	2:E:127:GLU:HB3	1.80	0.63
1:P:64:LEU:HD11	1:P:222:VAL:HG21	1.80	0.62
2:E:215:LYS:HG3	2:E:248:THR:CG2	2.29	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:69:ILE:HD11	1:J:164:LEU:HD13	1.81	0.62
2:B:40:CYS:O	2:B:44:LEU:CB	2.46	0.62
2:B:17:MET:HE1	2:B:60:TYR:HB2	1.81	0.62
1:S:265:LEU:HD23	1:S:398:PRO:HA	1.81	0.62
2:W:17:MET:CE	2:W:57:ALA:HA	2.29	0.62
1:A:138:TRP:CE2	1:A:438:TRP:CH2	2.87	0.62
2:E:17:MET:HE1	2:E:57:ALA:O	2.00	0.62
1:G:422:VAL:HG22	1:G:423:PRO:HD3	1.81	0.62
1:A:190:ARG:CG	1:A:190:ARG:HH11	1.96	0.62
2:W:355:LEU:HD22	2:W:360:ILE:HD11	1.81	0.62
2:H:21:THR:HG21	3:I:61:ARG:NH1	2.08	0.62
1:G:95:PRO:HG2	2:H:46:MET:HE1	1.81	0.62
2:B:39:VAL:HG13	2:B:40:CYS:N	2.14	0.62
1:J:352:ILE:O	1:J:356:THR:HG22	1.99	0.62
1:M:90:GLU:O	1:M:91:ASN:HB2	1.98	0.62
1:S:69:ILE:HD11	1:S:164:LEU:HD13	1.80	0.62
1:S:123:GLY:N	4:S:907:ASN:OXT	2.32	0.62
2:T:200:ILE:HD11	2:T:238:VAL:HG21	1.81	0.62
2:H:346:TRP:O	2:H:350:ASP:HB2	2.00	0.62
1:J:376:ARG:HH11	1:J:376:ARG:CG	2.02	0.62
2:B:37:THR:HG22	2:B:145:ASN:HD21	1.64	0.62
1:J:292:LEU:O	1:J:295:VAL:HG22	1.99	0.62
6:T:479:ADP:PB	6:T:479:ADP:H5'1	2.40	0.62
1:P:190:ARG:CG	1:P:190:ARG:HH11	2.06	0.61
1:S:422:VAL:CG2	1:S:423:PRO:CD	2.73	0.61
1:P:138:TRP:CE2	1:P:438:TRP:CZ3	2.88	0.61
1:D:38:LYS:HD2	1:D:477:LEU:CD1	2.30	0.61
1:G:85:ALA:HB2	1:G:117:LEU:CD1	2.30	0.61
2:W:211:ARG:NH2	8:W:479:ATP:O3A	2.32	0.61
2:T:37:THR:HG23	2:T:38:ASN:N	2.15	0.61
2:T:41:PRO:HB3	2:T:46:MET:HE2	1.83	0.61
1:M:162:VAL:HG21	1:M:219:VAL:HG21	1.83	0.61
2:B:115:GLU:OE2	2:B:116:LYS:HE2	2.00	0.61
2:H:17:MET:HE2	2:H:60:TYR:HB3	1.82	0.61
1:G:90:GLU:O	1:G:91:ASN:HB2	2.01	0.61
3:L:88:VAL:HB	3:L:89:PRO:CD	2.24	0.61
3:L:88:VAL:CB	3:L:89:PRO:HD2	2.21	0.61
2:T:374:GLU:HB3	2:T:403:PRO:HG2	1.83	0.61
1:D:21:PRO:O	1:D:25:VAL:HG23	2.01	0.61
1:J:299:ILE:HG13	1:J:419:ILE:HG22	1.83	0.61
2:E:222:PHE:CZ	2:E:253:PRO:HB3	2.36	0.61
1:V:155:VAL:CG2	1:V:163:SER:HB2	2.30	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:356:THR:HG21	3:I:14:ALA:HB2	1.82	0.61
1:M:422:VAL:HG22	1:M:423:PRO:HD3	1.83	0.61
2:T:201:ARG:HD2	2:T:207:GLU:O	2.00	0.60
1:V:77:VAL:HG23	1:V:114:LYS:HZ2	1.66	0.60
3:R:33:ILE:O	3:R:37:ILE:HG12	2.01	0.60
1:G:279:GLU:HG3	1:G:468:LYS:NZ	2.16	0.60
2:W:331:GLU:O	2:W:334:VAL:HG12	2.00	0.60
1:G:81:LYS:HE2	1:G:91:ASN:HA	1.81	0.60
1:V:77:VAL:CG2	1:V:114:LYS:NZ	2.65	0.60
1:P:68:PRO:HB3	1:P:112:VAL:HG11	1.84	0.60
1:S:68:PRO:HB3	1:S:112:VAL:HG11	1.83	0.60
2:T:21:THR:HG21	3:U:61:ARG:NH1	2.11	0.60
2:K:412:LEU:O	2:K:412:LEU:HG	2.02	0.60
1:S:143:VAL:CG1	1:S:145:GLY:H	2.15	0.60
2:W:360:ILE:CD1	2:W:366:PRO:HD3	2.31	0.60
1:S:81:LYS:HE2	1:S:91:ASN:HA	1.82	0.60
1:V:169:GLY:HA2	1:V:425:ASN:OD1	2.01	0.60
8:W:479:ATP:H5'1	8:W:479:ATP:O3G	2.02	0.60
1:P:138:TRP:CZ2	1:P:476:PRO:HD3	2.37	0.60
2:W:3:GLU:HG3	2:W:5:TYR:H	1.67	0.60
2:B:95:SER:HB3	2:B:127:GLU:HB3	1.84	0.60
1:V:143:VAL:HG13	1:V:145:GLY:H	1.67	0.60
1:S:376:ARG:HG3	1:S:376:ARG:NH1	2.09	0.60
1:S:138:TRP:CZ2	1:S:438:TRP:CH2	2.90	0.60
1:V:422:VAL:CG2	1:V:423:PRO:HD3	2.32	0.60
2:Q:412:LEU:HD12	2:Q:412:LEU:N	2.17	0.60
1:S:151:SER:HB3	1:S:163:SER:OG	2.01	0.60
1:J:397:THR:HG22	1:J:399:THR:H	1.66	0.60
2:B:279:VAL:CG2	3:C:59:PRO:HD2	2.32	0.59
2:T:162:THR:CG2	2:T:165:GLU:H	2.15	0.59
2:N:215:LYS:HD3	2:N:248:THR:HG21	1.82	0.59
1:V:78:GLU:HG2	1:V:79:GLY:N	2.16	0.59
1:G:98:ALA:HA	1:G:195:GLY:HA3	1.83	0.59
2:W:360:ILE:HG12	2:W:360:ILE:O	2.02	0.59
2:N:17:MET:HE2	2:N:60:TYR:HB3	1.84	0.59
2:H:95:SER:CB	2:H:127:GLU:HB3	2.32	0.59
1:S:78:GLU:HB2	1:S:97:ASP:OD1	2.02	0.59
1:P:73:ASP:HA	1:P:114:LYS:HE2	1.83	0.59
2:Q:17:MET:CE	2:Q:60:TYR:CB	2.79	0.59
1:M:2:LEU:HD23	1:M:27:SER:HB2	1.83	0.59
1:D:352:ILE:O	1:D:356:THR:HG23	2.01	0.59
2:H:103:THR:HG22	2:H:104:ASN:CG	2.23	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:297:TYR:O	1:J:300:PRO:HD2	2.02	0.59
2:H:211:ARG:HH11	8:H:479:ATP:H5'2	1.68	0.59
2:E:37:THR:CG2	2:E:38:ASN:H	2.16	0.59
1:D:397:THR:HG22	1:D:398:PRO:HD2	1.85	0.59
1:P:285:PHE:HE1	1:P:464:LEU:CD2	2.16	0.59
2:K:298:LEU:HB3	2:K:299:PRO:CD	2.32	0.59
1:J:306:ALA:HB3	1:J:307:PRO:HD3	1.83	0.59
1:M:86:SER:OG	1:M:88:ILE:HG13	2.03	0.59
2:B:73:HIS:NE2	2:B:103:THR:HB	2.17	0.59
2:W:17:MET:HE1	2:W:60:TYR:HB2	1.84	0.59
2:E:95:SER:CB	2:E:127:GLU:HB3	2.32	0.59
1:S:352:ILE:O	1:S:356:THR:HG23	2.03	0.59
3:F:80:GLU:HG2	3:F:87:VAL:HB	1.84	0.59
1:G:69:ILE:HD12	1:G:162:VAL:HG13	1.84	0.59
1:V:120:PHE:O	1:V:122:MET:CG	2.51	0.59
1:P:292:LEU:O	1:P:295:VAL:HG22	2.02	0.59
2:W:200:ILE:HG23	2:W:234:GLN:OE1	2.02	0.59
1:D:77:VAL:CG2	1:D:114:LYS:HZ2	2.01	0.59
1:J:3:TRP:CH2	1:J:31:ARG:CD	2.86	0.59
3:U:2:VAL:N	3:U:31:SER:HG	2.00	0.59
1:G:121:ALA:HB1	10:G:904:HOH:O	2.01	0.58
8:Q:479:ATP:H5'1	8:Q:479:ATP:O1G	2.03	0.58
1:J:73:ASP:OD1	1:J:114:LYS:HE2	2.03	0.58
2:E:310:TYR:CE1	2:E:334:VAL:HG11	2.36	0.58
2:B:84:PHE:CD2	3:C:15:ARG:HG2	2.37	0.58
2:W:162:THR:HG22	2:W:164:GLU:H	1.67	0.58
1:G:85:ALA:CB	1:G:117:LEU:HD13	2.33	0.58
2:H:133:ASN:ND2	3:I:91:VAL:HG21	2.18	0.58
1:V:422:VAL:HG22	1:V:423:PRO:HD3	1.85	0.58
2:Q:3:GLU:HG3	2:Q:5:TYR:H	1.69	0.58
1:M:115:THR:HG21	1:M:151:SER:OG	2.04	0.58
2:E:39:VAL:CG2	2:E:44:LEU:HG	2.31	0.58
1:G:163:SER:HB3	1:G:209:PHE:HB2	1.86	0.58
1:P:174:GLN:HG3	1:P:175:PRO:HD3	1.85	0.58
1:S:418:ASP:OD2	4:S:907:ASN:N	2.36	0.58
1:G:100:VAL:HG23	1:G:101:ILE:N	2.18	0.58
2:T:96:GLN:HB2	2:T:125:HIS:HB2	1.85	0.58
1:S:22:LYS:HG3	1:S:51:LEU:HD12	1.85	0.58
1:J:253:LYS:HG2	1:J:286:GLU:HB3	1.85	0.58
1:D:306:ALA:HB3	1:D:307:PRO:HD3	1.85	0.58
1:V:317:TYR:HE1	2:W:47:PRO:HG3	1.69	0.58
2:W:360:ILE:HD11	2:W:365:SER:CA	2.22	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:185:LYS:NZ	1:V:429:LEU:O	2.37	0.58
1:G:134:THR:HG22	1:G:144:PRO:HG3	1.86	0.58
1:V:181:VAL:HG13	1:V:210:GLY:O	2.04	0.58
1:P:432:ILE:HG22	1:P:458:LEU:HG	1.86	0.58
2:B:411:GLY:O	2:B:412:LEU:HB2	2.03	0.58
2:K:156:THR:CG2	2:K:157:GLU:O	2.51	0.58
2:W:233:ARG:O	2:W:237:VAL:HG23	2.04	0.58
1:M:76:LEU:HD23	1:M:94:ALA:HB1	1.85	0.58
2:T:310:TYR:HE1	2:T:334:VAL:HG11	1.69	0.58
1:V:5:LYS:HB2	1:V:10:LEU:CD1	2.33	0.58
2:E:358:LYS:HB2	2:E:360:ILE:HG22	1.84	0.58
2:K:17:MET:HE2	2:K:57:ALA:HA	1.86	0.58
1:G:138:TRP:CE2	1:G:438:TRP:CZ3	2.92	0.58
2:T:396:MET:HG3	2:T:406:ILE:HD11	1.86	0.58
2:T:156:THR:HG22	2:T:157:GLU:O	2.04	0.58
1:D:68:PRO:HB3	1:D:112:VAL:HG11	1.86	0.58
2:N:360:ILE:HD11	2:N:364:GLU:O	2.03	0.58
1:A:317:TYR:HE1	2:B:47:PRO:HG3	1.69	0.58
1:V:6:SER:HB3	1:V:212:ARG:HH11	1.69	0.57
2:T:26:GLY:O	3:U:65:PRO:HA	2.04	0.57
2:B:358:LYS:HB2	2:B:360:ILE:HG22	1.86	0.57
2:N:115:GLU:CG	2:N:116:LYS:HG2	2.30	0.57
2:Q:95:SER:HB2	2:Q:127:GLU:OE1	2.05	0.57
2:B:252:ASP:HB3	2:B:255:THR:CG2	2.33	0.57
1:J:190:ARG:HG2	1:J:224:SER:HB2	1.86	0.57
1:P:28:PHE:CD2	1:P:68:PRO:HG2	2.38	0.57
1:S:39:VAL:HG21	1:S:157:VAL:HG11	1.87	0.57
2:N:282:LYS:HD3	3:O:55:PHE:CE2	2.38	0.57
2:K:109:LEU:HD11	2:K:169:PHE:HA	1.85	0.57
1:V:245:VAL:CG1	1:V:459:LEU:HB3	2.34	0.57
2:K:167:ARG:HG3	2:K:220:PHE:HB3	1.84	0.57
1:M:397:THR:HG22	1:M:399:THR:H	1.69	0.57
1:M:352:ILE:O	1:M:356:THR:CG2	2.45	0.57
1:D:83:THR:CG2	1:D:131:PHE:CZ	2.71	0.57
2:K:360:ILE:HD11	2:K:365:SER:HA	1.86	0.57
8:H:479:ATP:H5'1	8:H:479:ATP:C8	2.40	0.57
3:I:88:VAL:HG23	3:I:89:PRO:O	2.04	0.57
1:J:3:TRP:CZ3	1:J:31:ARG:HD3	2.40	0.57
1:M:72:LYS:HA	1:M:115:THR:HG22	1.87	0.57
2:B:330:PHE:CE1	2:B:344:VAL:HG13	2.39	0.57
2:H:140:THR:OG1	3:I:91:VAL:N	2.33	0.57
1:G:138:TRP:CZ2	1:G:438:TRP:CH2	2.93	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:77:VAL:CG2	1:V:114:LYS:HZ2	2.18	0.57
3:X:81:ARG:HG2	3:X:81:ARG:HH11	1.69	0.57
1:D:270:LYS:O	1:D:274:GLU:HG3	2.04	0.57
2:H:17:MET:HE1	2:H:60:TYR:CB	2.26	0.57
1:V:297:TYR:O	1:V:300:PRO:HD2	2.05	0.57
1:V:124:SER:HG	4:V:908:ASN:N	2.03	0.57
1:P:245:VAL:HG12	1:P:459:LEU:HB3	1.85	0.57
1:M:376:ARG:HH11	1:M:376:ARG:HG3	1.68	0.57
2:T:77:VAL:HG23	2:T:99:LYS:HD2	1.87	0.57
2:E:17:MET:HE3	2:E:60:TYR:HB2	1.86	0.57
1:M:245:VAL:CG1	1:M:459:LEU:HB3	2.34	0.57
1:G:190:ARG:O	1:G:225:GLY:N	2.33	0.57
1:V:298:SER:HB3	1:V:422:VAL:HG23	1.86	0.57
1:M:121:ALA:HB1	10:M:906:HOH:O	2.04	0.57
2:B:399:THR:OG1	2:B:400:GLY:N	2.38	0.56
1:M:438:TRP:CZ3	1:M:443:PRO:HG3	2.39	0.56
2:Q:41:PRO:HB3	2:Q:46:MET:HE2	1.87	0.56
2:K:162:THR:HG22	2:K:164:GLU:N	2.20	0.56
9:H:482:ASP:N	10:H:485:HOH:O	2.38	0.56
1:J:3:TRP:CZ2	1:J:31:ARG:HD3	2.40	0.56
2:Q:336:HIS:NE2	2:Q:370:GLU:HG3	2.19	0.56
1:P:69:ILE:HD11	1:P:164:LEU:HD13	1.87	0.56
1:S:182:ILE:HG12	1:S:434:ILE:HD12	1.86	0.56
2:E:85:TYR:HD2	2:E:87:ASP:OD1	1.87	0.56
2:K:362:ILE:HG13	2:K:362:ILE:O	2.05	0.56
1:A:292:LEU:O	1:A:295:VAL:HG22	2.05	0.56
1:P:155:VAL:CG1	1:P:181:VAL:HG21	2.35	0.56
2:H:103:THR:HG22	2:H:104:ASN:N	2.20	0.56
2:E:103:THR:HG22	2:E:104:ASN:N	2.21	0.56
1:J:138:TRP:CE2	1:J:438:TRP:HZ3	2.23	0.56
2:Q:21:THR:HG21	3:R:61:ARG:HH12	1.71	0.56
1:A:373:LYS:HE2	3:C:50:PRO:HD3	1.87	0.56
2:K:407:VAL:O	2:K:411:GLY:N	2.35	0.56
1:P:169:GLY:N	4:P:906:ASN:OD1	2.34	0.56
1:G:297:TYR:O	1:G:300:PRO:HD2	2.05	0.56
2:K:17:MET:HE1	2:K:57:ALA:O	2.05	0.56
2:Q:21:THR:HG22	2:Q:54:ASN:ND2	2.20	0.56
2:E:39:VAL:CG1	2:E:44:LEU:HD11	2.33	0.56
2:Q:21:THR:CG2	3:R:61:ARG:HH12	2.18	0.56
1:P:434:ILE:HD12	1:P:465:TRP:HD1	1.70	0.56
2:E:340:PRO:O	2:E:344:VAL:HG22	2.05	0.56
1:P:16:ARG:HB2	1:P:18:GLU:OE2	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:U:3:ASP:O	3:U:7:VAL:HG23	2.06	0.56
1:M:138:TRP:CD2	1:M:438:TRP:HZ3	2.23	0.56
1:V:22:LYS:NZ	1:V:55:GLU:OE2	2.34	0.56
3:X:23:ILE:O	3:X:27:GLN:HG3	2.05	0.56
2:K:12:GLU:OE2	8:K:479:ATP:O1G	2.24	0.56
3:I:88:VAL:CB	3:I:89:PRO:HD2	2.05	0.56
2:N:39:VAL:CG1	2:N:44:LEU:HD11	2.35	0.56
1:P:299:ILE:N	1:P:300:PRO:CD	2.68	0.56
1:M:155:VAL:CG2	1:M:163:SER:HB2	2.35	0.56
1:A:397:THR:CG2	1:A:398:PRO:HD2	2.36	0.56
2:E:199:SER:OG	8:E:479:ATP:N1	2.30	0.55
2:E:355:LEU:HD22	2:E:360:ILE:HG12	1.88	0.55
1:M:138:TRP:CZ2	1:M:438:TRP:CH2	2.94	0.55
2:K:17:MET:CE	2:K:60:TYR:CB	2.84	0.55
1:G:298:SER:HB3	1:G:422:VAL:HG23	1.87	0.55
1:D:182:ILE:HG12	1:D:434:ILE:HD12	1.88	0.55
2:K:115:GLU:CG	2:K:116:LYS:HG2	2.37	0.55
2:Q:109:LEU:HD11	2:Q:169:PHE:HA	1.89	0.55
2:E:200:ILE:HD11	2:E:238:VAL:HG21	1.87	0.55
2:K:21:THR:HB	3:L:63:ASP:OD1	2.07	0.55
1:S:306:ALA:HB3	1:S:307:PRO:HD3	1.87	0.55
1:J:265:LEU:HD23	1:J:398:PRO:HA	1.87	0.55
1:A:120:PHE:O	1:A:122:MET:CG	2.48	0.55
1:A:475:ILE:HG22	1:A:476:PRO:CD	2.35	0.55
2:E:103:THR:CG2	2:E:104:ASN:N	2.70	0.55
1:P:83:THR:HG22	1:P:90:GLU:HA	1.88	0.55
2:N:156:THR:HG22	2:N:157:GLU:O	2.07	0.55
2:T:24:PHE:HA	2:T:52:ILE:O	2.05	0.55
1:V:39:VAL:HG21	1:V:157:VAL:HG11	1.88	0.55
1:J:422:VAL:CG2	1:J:423:PRO:HD3	2.37	0.55
2:W:84:PHE:CD2	3:X:15:ARG:HG2	2.41	0.55
1:S:21:PRO:O	1:S:25:VAL:HG23	2.07	0.55
1:A:245:VAL:CG1	1:A:459:LEU:HB3	2.37	0.55
3:I:55:PHE:O	3:I:56:GLU:CB	2.55	0.55
1:A:450:GLY:CA	1:A:458:LEU:HD11	2.35	0.55
2:N:85:TYR:HD2	2:N:87:ASP:OD1	1.89	0.55
2:B:17:MET:HG2	2:B:152:MET:HE3	1.88	0.55
1:M:138:TRP:CD2	1:M:438:TRP:CZ3	2.95	0.55
1:P:146:GLY:H	1:P:174:GLN:HE21	1.54	0.55
1:G:279:GLU:HG3	1:G:468:LYS:HZ3	1.72	0.55
1:D:477:LEU:HD23	1:D:477:LEU:H	1.71	0.54
2:Q:162:THR:HG22	2:Q:165:GLU:HG3	1.88	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:28:PHE:CD2	1:J:68:PRO:HG2	2.42	0.54
1:J:68:PRO:HB3	1:J:112:VAL:HG21	1.89	0.54
1:M:69:ILE:HD11	1:M:164:LEU:HD13	1.89	0.54
3:R:55:PHE:O	3:R:56:GLU:HB3	2.06	0.54
1:P:422:VAL:CG2	1:P:423:PRO:HD3	2.37	0.54
2:W:39:VAL:CG1	2:W:44:LEU:HD11	2.35	0.54
1:D:138:TRP:CZ2	1:D:438:TRP:HH2	2.24	0.54
1:A:32:TYR:CE1	1:A:36:GLU:CG	2.90	0.54
1:S:90:GLU:O	1:S:91:ASN:HB2	2.07	0.54
1:V:241:TRP:O	1:V:245:VAL:HG22	2.08	0.54
1:S:246:LYS:HG3	1:S:463:TYR:CZ	2.42	0.54
2:N:39:VAL:HG13	2:N:44:LEU:CD1	2.35	0.54
1:J:155:VAL:HG23	1:J:163:SER:HB2	1.88	0.54
1:A:397:THR:HG23	1:A:398:PRO:HD2	1.90	0.54
1:M:298:SER:HB3	1:M:422:VAL:HG23	1.90	0.54
1:S:438:TRP:CZ3	1:S:443:PRO:HG3	2.43	0.54
2:B:96:GLN:HB2	2:B:125:HIS:HB2	1.89	0.54
1:P:214:GLU:OE2	1:P:246:LYS:HE2	2.08	0.54
2:T:115:GLU:CG	2:T:116:LYS:HG3	2.37	0.54
2:N:197:ASN:HB3	2:N:211:ARG:HD2	1.88	0.54
1:J:292:LEU:HB2	1:J:295:VAL:HG22	1.89	0.54
2:B:340:PRO:O	2:B:344:VAL:HG22	2.08	0.54
2:Q:252:ASP:HB3	2:Q:255:THR:CG2	2.38	0.54
1:J:156:ALA:O	1:J:211:ARG:NH1	2.40	0.54
1:V:220:LEU:O	1:V:224:SER:OG	2.25	0.54
1:P:3:TRP:CE2	1:P:31:ARG:HD3	2.43	0.54
3:X:81:ARG:HG2	3:X:81:ARG:NH1	2.23	0.54
1:J:422:VAL:HG22	1:J:423:PRO:HD3	1.90	0.54
2:H:201:ARG:HD2	2:H:207:GLU:O	2.07	0.54
2:H:113:ASN:HA	2:H:115:GLU:H	1.73	0.54
2:H:17:MET:HE2	2:H:60:TYR:HB2	1.84	0.54
2:W:252:ASP:CB	2:W:255:THR:HG22	2.36	0.54
1:A:376:ARG:NH1	1:A:376:ARG:HG3	2.14	0.54
1:M:182:ILE:HG12	1:M:434:ILE:HD12	1.90	0.54
1:A:21:PRO:O	1:A:25:VAL:HG23	2.08	0.54
1:A:190:ARG:O	1:A:224:SER:O	2.26	0.54
1:G:178:PHE:CE1	1:G:397:THR:HG21	2.39	0.54
2:B:37:THR:CG2	2:B:38:ASN:N	2.71	0.54
1:M:95:PRO:HG2	2:N:46:MET:HE1	1.88	0.54
1:P:145:GLY:HA2	1:P:174:GLN:NE2	2.22	0.54
2:T:58:VAL:O	2:T:62:ILE:HG13	2.08	0.54
2:H:39:VAL:HG13	2:H:44:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:332:ILE:HD12	3:I:89:PRO:HG2	1.89	0.54
1:J:3:TRP:CE2	1:J:31:ARG:CD	2.91	0.54
1:A:300:PRO:HA	3:C:37:ILE:HG22	1.89	0.54
1:S:46:LEU:HD11	1:S:80:GLU:HG3	1.89	0.54
2:W:220:PHE:O	2:W:223:VAL:HG22	2.08	0.54
2:Q:17:MET:HE2	2:Q:60:TYR:HB2	1.90	0.53
1:J:477:LEU:H	1:J:477:LEU:HD23	1.71	0.53
1:G:438:TRP:CZ3	1:G:443:PRO:HG3	2.43	0.53
2:H:162:THR:HG22	2:H:165:GLU:H	1.73	0.53
3:C:73:LYS:O	3:C:76:MET:HG2	2.08	0.53
1:J:73:ASP:HA	1:J:114:LYS:HE2	1.90	0.53
2:H:100:PRO:HB3	2:H:123:ARG:HH21	1.74	0.53
1:V:373:LYS:HE2	3:X:50:PRO:HD3	1.90	0.53
1:M:190:ARG:HD3	1:M:241:TRP:HH2	1.73	0.53
3:I:88:VAL:HB	3:I:89:PRO:CD	2.23	0.53
1:D:190:ARG:HD3	1:D:241:TRP:CH2	2.32	0.53
2:K:21:THR:HG22	2:K:54:ASN:ND2	2.22	0.53
1:S:73:ASP:HA	1:S:114:LYS:HZ3	1.73	0.53
2:E:100:PRO:HB3	2:E:123:ARG:NH2	2.24	0.53
2:B:156:THR:CG2	2:B:157:GLU:O	2.56	0.53
2:B:95:SER:HB3	2:B:127:GLU:CB	2.38	0.53
2:H:360:ILE:HG22	2:H:364:GLU:HB3	1.91	0.53
1:V:292:LEU:CB	1:V:295:VAL:HG22	2.39	0.53
1:P:138:TRP:CD2	1:P:438:TRP:HZ3	2.27	0.53
1:P:422:VAL:HG22	1:P:423:PRO:HD3	1.89	0.53
1:D:322:TYR:CZ	2:E:47:PRO:HD3	2.44	0.53
1:J:162:VAL:HG11	1:J:219:VAL:HG21	1.89	0.53
1:G:299:ILE:HG13	1:G:419:ILE:HG22	1.90	0.53
2:W:360:ILE:HD12	2:W:366:PRO:HD3	1.88	0.53
2:N:86:PRO:HG2	3:O:91:VAL:HG11	1.91	0.53
1:G:245:VAL:CG1	1:G:459:LEU:HB3	2.39	0.53
2:B:17:MET:HG2	2:B:152:MET:CE	2.39	0.53
1:D:155:VAL:CG2	1:D:163:SER:HB2	2.38	0.53
2:K:115:GLU:HG3	2:K:116:LYS:CG	2.39	0.53
2:E:21:THR:CG2	3:F:61:ARG:HH12	2.09	0.53
1:A:450:GLY:HA3	1:A:458:LEU:CD1	2.36	0.53
1:P:31:ARG:HH22	1:P:477:LEU:HB2	1.73	0.53
1:V:204:ASP:O	1:V:205:GLN:HG2	2.09	0.53
2:Q:162:THR:HG23	2:Q:165:GLU:H	1.74	0.53
1:M:477:LEU:HD23	1:M:477:LEU:N	2.23	0.53
2:E:34:GLU:O	2:E:37:THR:CB	2.52	0.52
2:E:37:THR:CG2	2:E:38:ASN:N	2.72	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:40:CYS:SG	2:B:41:PRO:HD2	2.49	0.52
1:P:64:LEU:CD1	1:P:222:VAL:HG21	2.38	0.52
2:H:385:SER:OG	2:H:388:ILE:HG12	2.08	0.52
1:J:376:ARG:NH1	1:J:376:ARG:CG	2.67	0.52
1:D:155:VAL:HG23	1:D:163:SER:HB2	1.91	0.52
1:P:174:GLN:HG3	1:P:175:PRO:CD	2.38	0.52
2:W:41:PRO:HB3	2:W:46:MET:HE2	1.92	0.52
1:A:69:ILE:HD11	1:A:164:LEU:HD13	1.91	0.52
1:S:297:TYR:O	1:S:300:PRO:HD2	2.09	0.52
1:J:30:ASP:O	1:J:34:GLN:HG3	2.09	0.52
1:J:3:TRP:CZ2	1:J:31:ARG:HD2	2.45	0.52
1:D:72:LYS:HA	1:D:115:THR:CG2	2.39	0.52
1:S:138:TRP:CE2	1:S:438:TRP:CZ3	2.96	0.52
1:A:322:TYR:CZ	2:B:47:PRO:HD3	2.44	0.52
1:M:376:ARG:NH1	1:M:376:ARG:HG3	2.24	0.52
2:W:396:MET:HG3	2:W:406:ILE:HD11	1.90	0.52
2:W:336:HIS:NE2	2:W:370:GLU:HG3	2.24	0.52
2:N:385:SER:OG	2:N:388:ILE:HG12	2.09	0.52
2:T:279:VAL:CG2	3:U:59:PRO:HD2	2.40	0.52
1:G:1:MET:O	1:G:1:MET:HG2	2.09	0.52
2:H:133:ASN:HD22	3:I:91:VAL:HG21	1.74	0.52
2:T:310:TYR:CE1	2:T:334:VAL:HG11	2.45	0.52
1:V:124:SER:O	1:V:174:GLN:NE2	2.42	0.52
2:E:360:ILE:HD11	2:E:365:SER:N	2.24	0.52
1:G:138:TRP:CE2	1:G:438:TRP:HH2	2.25	0.52
2:T:8:VAL:HG12	2:T:158:PRO:HB2	1.90	0.52
2:Q:123:ARG:NH1	2:Q:125:HIS:ND1	2.57	0.52
2:Q:332:GLU:HG3	2:Q:335:ARG:HH21	1.74	0.52
2:N:162:THR:HG22	2:N:165:GLU:H	1.73	0.52
2:E:215:LYS:HG3	2:E:248:THR:HG21	1.91	0.52
1:D:39:VAL:HG21	1:D:157:VAL:HG11	1.92	0.52
2:W:402:THR:HG22	2:W:403:PRO:HD2	1.92	0.52
1:M:193:ARG:NH2	1:M:201:SER:HB3	2.25	0.52
2:N:14:HIS:CD2	2:N:127:GLU:OE2	2.63	0.52
2:B:336:HIS:CE1	2:B:370:GLU:HG3	2.44	0.52
2:H:255:THR:HG21	2:H:259:TYR:OH	2.10	0.52
1:P:30:ASP:O	1:P:34:GLN:HG3	2.10	0.52
2:K:34:GLU:O	2:K:37:THR:CG2	2.58	0.52
1:V:72:LYS:HE2	1:V:117:LEU:HD13	1.92	0.52
2:Q:73:HIS:NE2	2:Q:103:THR:HB	2.25	0.52
1:S:32:TYR:CE1	1:S:36:GLU:HG2	2.45	0.52
2:Q:17:MET:HE1	2:Q:57:ALA:O	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:39:VAL:HG21	1:M:157:VAL:HG11	1.92	0.52
1:A:167:ASP:HB3	1:A:185:LYS:HG3	1.92	0.52
2:H:109:LEU:HD11	2:H:169:PHE:HA	1.91	0.51
1:D:22:LYS:HG3	1:D:51:LEU:HD12	1.93	0.51
2:Q:412:LEU:N	2:Q:412:LEU:CD1	2.73	0.51
3:I:55:PHE:O	3:I:56:GLU:HB3	2.10	0.51
3:U:69:LEU:HD23	3:U:74:ALA:HB2	1.92	0.51
1:D:299:ILE:HG13	1:D:419:ILE:HG22	1.92	0.51
2:T:119:VAL:HG13	2:T:159:ASP:HB2	1.91	0.51
2:E:361:SER:HB2	2:E:363:GLU:OE1	2.10	0.51
1:S:13:LEU:HB3	1:S:19:VAL:CG1	2.38	0.51
1:J:352:ILE:O	1:J:356:THR:CG2	2.59	0.51
1:G:151:SER:HB3	1:G:163:SER:OG	2.10	0.51
2:Q:34:GLU:O	2:Q:37:THR:OG1	2.24	0.51
1:D:77:VAL:HG21	1:D:114:LYS:NZ	2.22	0.51
2:B:9:ILE:HB	2:B:160:ILE:HB	1.91	0.51
1:P:285:PHE:CE1	1:P:464:LEU:CD2	2.92	0.51
1:D:172:ILE:HD13	1:D:207:GLY:HA3	1.93	0.51
3:F:4:ARG:NH1	3:F:8:LEU:HD11	2.25	0.51
1:S:155:VAL:HG23	1:S:163:SER:HB2	1.92	0.51
1:G:138:TRP:CD2	1:G:438:TRP:CZ3	2.97	0.51
1:V:397:THR:CG2	1:V:398:PRO:HD2	2.40	0.51
1:G:101:ILE:HG22	1:G:105:LYS:HE3	1.92	0.51
1:J:298:SER:HB3	1:J:422:VAL:HG23	1.93	0.51
2:N:83:TYR:CZ	2:N:88:LEU:HD22	2.45	0.51
1:A:30:ASP:O	1:A:34:GLN:HG3	2.10	0.51
1:P:318:ASP:HB2	1:P:336:TYR:CE1	2.45	0.51
2:H:146:ARG:HG2	2:H:146:ARG:HH11	1.76	0.51
2:T:115:GLU:HB3	2:T:116:LYS:HG3	1.92	0.51
2:H:95:SER:HB3	2:H:127:GLU:CB	2.40	0.51
2:Q:7:ALA:HB3	2:Q:161:ARG:O	2.10	0.51
1:J:204:ASP:O	1:J:205:GLN:HG2	2.11	0.51
2:W:340:PRO:O	2:W:344:VAL:HG22	2.11	0.51
2:W:133:ASN:HB3	2:W:140:THR:CG2	2.40	0.51
1:P:174:GLN:HG3	1:P:175:PRO:N	2.24	0.51
1:S:138:TRP:CD2	1:S:438:TRP:HZ3	2.29	0.51
2:E:95:SER:HB3	2:E:127:GLU:CB	2.41	0.51
1:P:285:PHE:HE1	1:P:464:LEU:HD21	1.76	0.51
1:P:329:TYR:CE2	3:R:89:PRO:HG3	2.46	0.51
1:D:169:GLY:N	4:D:902:ASN:OD1	2.42	0.51
2:T:170:LEU:HD12	2:T:223:VAL:HG21	1.93	0.51
2:T:234:GLN:O	2:T:238:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:340:ARG:HB3	3:C:16:LEU:HD23	1.92	0.51
2:H:197:ASN:HB3	2:H:211:ARG:HD2	1.91	0.51
1:M:438:TRP:CH2	1:M:443:PRO:HG3	2.46	0.51
1:G:397:THR:HG22	1:G:399:THR:O	2.11	0.51
1:G:172:ILE:HD13	1:G:207:GLY:HA3	1.93	0.51
2:T:84:PHE:CD2	3:U:15:ARG:HG2	2.46	0.51
1:G:68:PRO:HB3	1:G:112:VAL:HG11	1.93	0.51
2:E:360:ILE:HG13	2:E:361:SER:N	2.26	0.50
2:B:17:MET:HE3	2:B:60:TYR:HB2	1.93	0.50
2:T:207:GLU:CG	2:T:208:PHE:H	2.21	0.50
2:W:73:HIS:NE2	2:W:103:THR:HB	2.26	0.50
2:B:37:THR:HG23	2:B:38:ASN:H	1.75	0.50
1:A:422:VAL:CG2	1:A:423:PRO:HD3	2.41	0.50
2:N:323:HIS:CD2	2:N:325:GLU:OE1	2.64	0.50
2:T:162:THR:HG22	2:T:165:GLU:CB	2.40	0.50
1:J:138:TRP:CD2	1:J:438:TRP:HZ3	2.28	0.50
2:B:37:THR:HG22	2:B:145:ASN:ND2	2.26	0.50
1:P:138:TRP:CE2	1:P:438:TRP:CH2	2.98	0.50
1:M:21:PRO:O	1:M:25:VAL:HG23	2.11	0.50
1:P:477:LEU:H	1:P:477:LEU:HD23	1.74	0.50
1:S:182:ILE:HG12	1:S:434:ILE:CD1	2.42	0.50
2:N:140:THR:OG1	3:O:90:ARG:HA	2.11	0.50
2:Q:85:TYR:HD2	2:Q:87:ASP:OD1	1.93	0.50
1:M:73:ASP:HA	1:M:114:LYS:HE2	1.93	0.50
1:P:477:LEU:N	1:P:477:LEU:HD23	2.26	0.50
1:S:463:TYR:O	1:S:467:GLN:HG2	2.11	0.50
1:J:349:LYS:O	1:J:353:MET:HG2	2.12	0.50
1:P:434:ILE:O	1:P:434:ILE:CG2	2.59	0.50
1:D:463:TYR:O	1:D:467:GLN:HG2	2.11	0.50
2:K:85:TYR:HD2	2:K:87:ASP:OD1	1.94	0.50
2:K:333:ALA:HB2	2:K:369:PRO:HB3	1.94	0.50
2:B:3:GLU:HG3	2:B:5:TYR:H	1.76	0.50
1:A:178:PHE:CE1	1:A:397:THR:HG21	2.47	0.50
2:T:402:THR:HG22	2:T:403:PRO:HD2	1.93	0.50
1:G:78:GLU:HG2	1:G:79:GLY:N	2.25	0.50
1:P:5:LYS:HB2	1:P:10:LEU:HD13	1.94	0.50
1:J:3:TRP:CH2	1:J:31:ARG:HD3	2.47	0.50
1:S:155:VAL:CG2	1:S:163:SER:HB2	2.42	0.50
2:Q:236:ASN:O	2:Q:240:GLU:HG2	2.12	0.50
2:T:340:PRO:O	2:T:344:VAL:HG22	2.12	0.50
2:B:8:VAL:HG21	2:B:201:ARG:HE	1.75	0.50
2:Q:305:ARG:HG2	2:Q:305:ARG:HH11	1.77	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:356:THR:HG21	3:X:14:ALA:HB2	1.94	0.50
2:W:35:PRO:HG3	3:X:85:PHE:CE2	2.47	0.50
1:S:172:ILE:CD1	1:S:207:GLY:HA3	2.41	0.50
1:S:292:LEU:O	1:S:295:VAL:HG22	2.12	0.50
1:M:292:LEU:HB3	1:M:295:VAL:HG13	1.92	0.50
2:T:6:GLU:OE1	2:T:201:ARG:NH2	2.42	0.50
2:H:97:TYR:O	2:H:123:ARG:NH2	2.44	0.50
2:K:81:LYS:HE3	2:K:270:TYR:CZ	2.47	0.50
1:G:46:LEU:HD12	1:G:111:ILE:HG22	1.93	0.50
1:V:29:TYR:O	1:V:32:TYR:HB3	2.12	0.50
1:A:126:THR:OG1	1:A:149:GLY:HA3	2.11	0.49
2:H:355:LEU:HD21	2:H:365:SER:HB2	1.93	0.49
1:D:418:ASP:HB3	1:D:422:VAL:HG13	1.94	0.49
1:D:13:LEU:HB3	1:D:19:VAL:HG11	1.83	0.49
2:E:37:THR:HG22	2:E:145:ASN:ND2	2.28	0.49
2:B:8:VAL:HG13	2:B:161:ARG:HH12	1.77	0.49
2:Q:381:GLU:O	2:Q:382:LYS:HB2	2.13	0.49
2:K:340:PRO:O	2:K:344:VAL:HG22	2.12	0.49
2:W:255:THR:HG23	2:W:257:LYS:H	1.77	0.49
1:A:72:LYS:HA	1:A:115:THR:HB	1.94	0.49
2:N:157:GLU:O	2:N:159:ASP:N	2.44	0.49
1:D:99:THR:O	1:D:103:ARG:HG3	2.12	0.49
3:X:46:GLU:O	3:X:47:ASN:HB2	2.13	0.49
2:K:345:ASN:O	2:K:349:ASN:HB2	2.13	0.49
2:Q:320:LEU:HD22	2:Q:326:VAL:HG12	1.93	0.49
1:M:146:GLY:N	1:M:174:GLN:OE1	2.42	0.49
2:W:17:MET:HE3	2:W:60:TYR:HB2	1.95	0.49
2:H:282:LYS:HD3	3:I:55:PHE:CE2	2.47	0.49
2:B:210:THR:CG2	2:B:246:GLN:HB2	2.42	0.49
3:L:55:PHE:O	3:L:56:GLU:HB3	2.13	0.49
2:E:279:VAL:CG2	3:F:59:PRO:HD2	2.43	0.49
2:E:106:TRP:CZ3	1:G:293:PRO:HG3	2.47	0.49
2:E:220:PHE:O	2:E:223:VAL:HG22	2.12	0.49
1:P:124:SER:O	1:P:174:GLN:NE2	2.46	0.49
1:V:5:LYS:HB2	1:V:10:LEU:HD13	1.93	0.49
1:A:5:LYS:HB2	1:A:10:LEU:CD1	2.42	0.49
1:D:297:TYR:O	1:D:300:PRO:HD2	2.12	0.49
1:V:21:PRO:O	1:V:25:VAL:HG23	2.13	0.49
1:V:174:GLN:HG3	1:V:175:PRO:N	2.22	0.49
1:A:298:SER:HB3	1:A:422:VAL:HG23	1.94	0.49
1:D:191:VAL:HG22	1:D:224:SER:HB3	1.95	0.49
2:W:85:TYR:OH	3:X:91:VAL:HG21	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:146:GLY:N	1:D:174:GLN:OE1	2.39	0.49
1:P:298:SER:HB3	1:P:422:VAL:HG23	1.94	0.49
2:Q:103:THR:CG2	2:Q:104:ASN:OD1	2.61	0.49
2:B:402:THR:HG22	2:B:403:PRO:HD2	1.95	0.49
2:E:83:TYR:CZ	2:E:88:LEU:HD22	2.47	0.49
1:G:201:SER:HB2	2:H:276:PRO:HG2	1.94	0.49
1:P:29:TYR:O	1:P:32:TYR:HB3	2.13	0.49
2:T:115:GLU:CB	2:T:116:LYS:HG3	2.42	0.49
2:N:164:GLU:HG3	2:N:168:LEU:HD12	1.95	0.49
1:D:477:LEU:N	1:D:477:LEU:HD23	2.27	0.49
2:B:95:SER:CB	2:B:127:GLU:HB3	2.43	0.49
1:D:351:ARG:HH12	4:D:902:ASN:C	2.15	0.49
2:B:331:GLU:HA	2:B:334:VAL:HG12	1.94	0.49
2:N:346:TRP:O	2:N:350:ASP:HB2	2.11	0.49
1:A:174:GLN:HG3	1:A:175:PRO:HD3	1.94	0.49
2:W:399:THR:OG1	2:W:400:GLY:N	2.46	0.49
2:H:184:LYS:HB2	2:H:191:GLN:OE1	2.13	0.49
9:N:482:ASP:N	10:N:484:HOH:O	2.45	0.49
2:Q:103:THR:HG23	2:Q:104:ASN:OD1	2.13	0.49
2:H:4:LYS:O	2:H:203:LYS:HB2	2.12	0.49
1:G:376:ARG:HG3	1:G:376:ARG:HH11	1.78	0.49
1:P:155:VAL:HG12	1:P:181:VAL:CG2	2.36	0.49
1:D:438:TRP:CZ3	1:D:443:PRO:HG3	2.47	0.49
2:T:37:THR:CG2	2:T:38:ASN:N	2.76	0.49
1:M:190:ARG:HD2	1:M:455:GLU:OE2	2.13	0.49
1:M:246:LYS:HE2	1:M:463:TYR:OH	2.13	0.49
1:P:376:ARG:HG3	1:P:376:ARG:O	2.12	0.49
1:A:20:SER:O	1:A:24:VAL:HG23	2.12	0.48
2:H:119:VAL:CG1	2:H:156:THR:CG2	2.91	0.48
2:K:384:ILE:HG22	2:K:412:LEU:HD23	1.94	0.48
1:V:292:LEU:HB2	1:V:295:VAL:CG2	2.42	0.48
1:S:138:TRP:CE2	1:S:438:TRP:HH2	2.30	0.48
2:H:39:VAL:CG2	2:H:44:LEU:HD21	2.44	0.48
1:A:422:VAL:HG22	1:A:423:PRO:HD3	1.95	0.48
2:E:170:LEU:HD12	2:E:223:VAL:HG21	1.95	0.48
2:N:396:MET:HE1	2:N:403:PRO:HB3	1.96	0.48
1:D:403:LYS:O	1:D:406:GLU:HB2	2.12	0.48
2:N:4:LYS:O	2:N:203:LYS:HB2	2.13	0.48
1:V:2:LEU:HD23	1:V:27:SER:HB2	1.94	0.48
1:P:1:MET:O	1:P:1:MET:HG2	2.13	0.48
2:T:162:THR:HG23	2:T:165:GLU:H	1.78	0.48
8:Q:479:ATP:O1A	8:Q:479:ATP:O2B	2.31	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:137:PRO:HB3	1:G:157:VAL:CG1	2.43	0.48
1:S:318:ASP:HB2	1:S:336:TYR:CE1	2.48	0.48
1:J:2:LEU:HA	1:J:5:LYS:HD2	1.95	0.48
2:Q:16:GLN:HB2	2:Q:191:GLN:HA	1.96	0.48
2:W:142:VAL:HB	3:X:86:PHE:HB2	1.93	0.48
2:E:358:LYS:HB2	2:E:360:ILE:CG2	2.43	0.48
1:G:190:ARG:NH1	1:G:190:ARG:HG3	2.28	0.48
1:P:138:TRP:CE2	1:P:438:TRP:HZ3	2.32	0.48
1:S:81:LYS:CE	1:S:91:ASN:HA	2.43	0.48
2:T:215:LYS:O	2:T:216:ASN:HB2	2.12	0.48
2:E:26:GLY:O	3:F:65:PRO:HA	2.13	0.48
3:F:2:VAL:N	3:F:31:SER:HG	2.11	0.48
1:D:318:ASP:OD2	1:D:321:ARG:NH1	2.43	0.48
1:A:172:ILE:HD13	1:A:207:GLY:HA3	1.95	0.48
2:E:21:THR:HG22	2:E:22:LYS:O	2.14	0.48
2:E:137:GLY:O	3:F:90:ARG:NH1	2.43	0.48
2:W:103:THR:CG2	2:W:104:ASN:OD1	2.59	0.48
1:V:77:VAL:HG21	1:V:114:LYS:HZ1	1.78	0.48
2:W:162:THR:HG22	2:W:164:GLU:N	2.28	0.48
1:M:266:GLN:NE2	1:M:399:THR:HB	2.28	0.48
1:V:123:GLY:O	4:V:908:ASN:HB2	2.13	0.48
1:A:279:GLU:HG3	1:A:468:LYS:NZ	2.28	0.48
2:T:80:ARG:HE	2:T:275:ASP:CG	2.16	0.48
2:W:214:ILE:HD11	2:W:230:GLU:HG2	1.96	0.48
2:N:170:LEU:HD12	2:N:223:VAL:HG21	1.94	0.48
1:A:265:LEU:HD23	1:A:398:PRO:HA	1.96	0.48
3:L:55:PHE:O	3:L:56:GLU:CB	2.62	0.48
2:H:140:THR:OG1	3:I:90:ARG:HA	2.13	0.48
1:J:245:VAL:CG1	1:J:459:LEU:HB3	2.43	0.48
2:Q:162:THR:HG22	2:Q:165:GLU:CG	2.44	0.48
1:M:190:ARG:HD3	1:M:241:TRP:CH2	2.48	0.48
1:D:320:VAL:HG22	3:F:88:VAL:HG11	1.94	0.48
2:H:21:THR:HG22	2:H:54:ASN:ND2	2.29	0.48
1:S:477:LEU:CD2	1:S:477:LEU:N	2.71	0.48
2:K:330:PHE:CE1	2:K:344:VAL:HG13	2.49	0.48
1:A:325:ARG:HA	1:A:339:THR:HG23	1.96	0.48
2:H:26:GLY:O	3:I:65:PRO:HA	2.14	0.48
1:G:73:ASP:HA	1:G:114:LYS:HE2	1.94	0.48
2:Q:192:LEU:HD23	2:Q:193:ARG:N	2.29	0.48
2:Q:298:LEU:HB3	2:Q:299:PRO:CD	2.44	0.48
2:Q:310:TYR:CE1	2:Q:334:VAL:HG11	2.49	0.48
2:N:95:SER:HB2	2:N:96:GLN:H	1.50	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:77:VAL:HG23	1:S:114:LYS:HE2	1.96	0.48
1:J:178:PHE:HE1	1:J:397:THR:HG21	1.78	0.48
1:V:42:TYR:CE2	1:V:113:GLY:HA3	2.49	0.48
2:K:7:ALA:HB3	2:K:161:ARG:O	2.14	0.48
2:K:310:TYR:CE1	2:K:334:VAL:HG11	2.49	0.48
2:Q:340:PRO:O	2:Q:344:VAL:HG22	2.14	0.47
1:G:126:THR:OG1	1:G:149:GLY:HA3	2.13	0.47
1:S:57:LEU:HD12	1:S:110:LEU:HD21	1.96	0.47
2:W:56:ARG:HD2	3:X:63:ASP:OD2	2.14	0.47
1:V:155:VAL:HG23	1:V:163:SER:HB2	1.96	0.47
2:W:157:GLU:O	2:W:159:ASP:N	2.45	0.47
2:H:123:ARG:HG2	2:H:155:VAL:HB	1.95	0.47
1:A:76:LEU:HD22	1:A:96:TYR:CE1	2.49	0.47
1:D:126:THR:OG1	1:D:149:GLY:HA3	2.14	0.47
1:P:172:ILE:CD1	1:P:207:GLY:HA3	2.44	0.47
1:M:403:LYS:O	1:M:406:GLU:HB2	2.14	0.47
2:Q:95:SER:CB	2:Q:127:GLU:OE1	2.61	0.47
2:B:37:THR:CG2	2:B:38:ASN:H	2.27	0.47
1:V:299:ILE:HG13	1:V:419:ILE:HG22	1.95	0.47
3:R:3:ASP:O	3:R:7:VAL:HG23	2.14	0.47
2:T:270:TYR:HB2	2:T:272:TYR:CE2	2.49	0.47
1:S:124:SER:HG	4:S:907:ASN:N	2.12	0.47
1:P:422:VAL:N	1:P:423:PRO:CD	2.77	0.47
2:H:155:VAL:HG21	10:H:483:HOH:O	2.14	0.47
2:W:135:HIS:HB3	3:X:90:ARG:CZ	2.44	0.47
1:D:422:VAL:HG22	1:D:423:PRO:HD3	1.97	0.47
2:Q:192:LEU:HD23	2:Q:192:LEU:C	2.35	0.47
2:W:252:ASP:OD2	2:W:255:THR:HG22	2.14	0.47
2:K:255:THR:HG21	2:K:259:TYR:OH	2.15	0.47
1:M:266:GLN:HG3	1:M:399:THR:HG22	1.97	0.47
1:A:124:SER:O	1:A:174:GLN:NE2	2.48	0.47
1:P:253:LYS:HG2	1:P:286:GLU:HB3	1.97	0.47
1:V:477:LEU:O	1:V:478:THR:C	2.53	0.47
2:E:128:GLU:HB2	2:E:148:GLY:HA2	1.96	0.47
2:H:103:THR:CG2	2:H:104:ASN:N	2.77	0.47
2:B:157:GLU:O	2:B:159:ASP:N	2.48	0.47
1:D:422:VAL:CG2	1:D:423:PRO:HD3	2.44	0.47
2:W:257:LYS:HD2	2:W:259:TYR:OH	2.14	0.47
1:A:178:PHE:HE1	1:A:397:THR:HG21	1.80	0.47
2:B:167:ARG:HG3	2:B:220:PHE:HB3	1.96	0.47
2:T:40:CYS:HB2	2:T:41:PRO:CD	2.44	0.47
2:T:77:VAL:CG2	2:T:99:LYS:HD2	2.44	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:434:ILE:CD1	1:P:465:TRP:HD1	2.27	0.47
2:W:167:ARG:HG3	2:W:220:PHE:HB3	1.96	0.47
2:B:217:VAL:CG1	2:B:222:PHE:HB3	2.44	0.47
2:E:80:ARG:HE	2:E:275:ASP:CG	2.17	0.47
2:T:117:LYS:HG2	2:T:118:LYS:N	2.30	0.47
2:Q:222:PHE:CZ	2:Q:253:PRO:HB3	2.50	0.47
1:P:373:LYS:HE2	3:R:50:PRO:HD3	1.96	0.47
1:S:403:LYS:O	1:S:406:GLU:HB2	2.15	0.47
1:A:57:LEU:HD12	1:A:110:LEU:HD21	1.97	0.47
3:U:46:GLU:O	3:U:47:ASN:HB2	2.15	0.47
2:B:384:ILE:HG23	2:B:412:LEU:HD23	1.94	0.47
2:H:111:LEU:HG	2:H:115:GLU:O	2.15	0.47
2:Q:333:ALA:C	2:Q:335:ARG:H	2.17	0.47
2:E:21:THR:HG21	3:F:61:ARG:NH1	2.10	0.47
2:W:140:THR:OG1	3:X:90:ARG:HA	2.15	0.47
1:A:174:GLN:HG3	1:A:175:PRO:CD	2.44	0.47
1:G:13:LEU:HB3	1:G:19:VAL:HG12	1.97	0.47
1:A:201:SER:HB2	2:B:276:PRO:HG2	1.96	0.47
2:E:162:THR:HG22	2:E:164:GLU:H	1.79	0.47
1:M:134:THR:HG22	1:M:144:PRO:HG3	1.96	0.47
1:G:100:VAL:CG2	1:G:101:ILE:N	2.78	0.47
1:M:477:LEU:HD23	1:M:477:LEU:H	1.79	0.47
2:W:217:VAL:CG1	2:W:222:PHE:HB3	2.44	0.47
2:N:343:ILE:HG23	2:N:372:LEU:HD23	1.97	0.47
2:H:17:MET:HE1	2:H:57:ALA:O	2.14	0.46
1:V:438:TRP:CH2	1:V:443:PRO:HG3	2.50	0.46
2:E:13:ILE:HG21	2:E:173:LEU:CD2	2.43	0.46
2:Q:282:LYS:HD2	3:R:55:PHE:CE2	2.51	0.46
1:D:168:THR:N	4:D:902:ASN:OD1	2.46	0.46
1:J:337:ALA:HB1	3:L:17:GLU:HB2	1.98	0.46
1:M:329:TYR:CE2	3:O:89:PRO:HG3	2.51	0.46
3:L:33:ILE:O	3:L:37:ILE:HG12	2.15	0.46
1:G:118:ASP:OD1	1:G:128:TYR:HB2	2.15	0.46
2:E:54:ASN:O	2:E:58:VAL:HG23	2.15	0.46
2:W:156:THR:CG2	2:W:157:GLU:O	2.58	0.46
1:G:319:GLY:O	3:I:79:PRO:HG2	2.15	0.46
2:T:141:LEU:HD23	3:U:85:PHE:CD2	2.50	0.46
1:V:88:ILE:HA	1:V:324:TYR:HB3	1.96	0.46
1:G:331:ASP:C	1:G:331:ASP:OD1	2.53	0.46
3:I:34:LEU:HA	3:I:34:LEU:HD12	1.74	0.46
2:T:21:THR:CG2	3:U:61:ARG:HH12	2.14	0.46
1:A:307:PRO:HG2	1:A:354:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:156:THR:HG22	2:H:157:GLU:O	2.15	0.46
1:P:167:ASP:HA	1:P:171:SER:HB2	1.97	0.46
1:D:1:MET:HG2	1:D:1:MET:O	2.15	0.46
2:W:384:ILE:CG2	2:W:412:LEU:CD2	2.54	0.46
1:D:83:THR:O	1:D:83:THR:HG22	2.15	0.46
8:H:479:ATP:O2G	9:H:482:ASP:CB	2.64	0.46
2:K:46:MET:HE2	2:K:46:MET:HB3	1.66	0.46
1:V:71:VAL:HB	1:V:114:LYS:NZ	2.31	0.46
2:B:84:PHE:CE2	3:C:15:ARG:HG2	2.50	0.46
1:P:245:VAL:CG1	1:P:459:LEU:HB3	2.45	0.46
2:H:119:VAL:CG1	2:H:156:THR:HG21	2.46	0.46
2:B:207:GLU:H	2:B:207:GLU:HG3	1.55	0.46
1:D:199:PHE:C	1:D:199:PHE:CD1	2.88	0.46
2:B:279:VAL:HB	3:C:55:PHE:CE1	2.51	0.46
1:P:3:TRP:CZ3	1:P:31:ARG:HD3	2.50	0.46
1:V:143:VAL:CG1	1:V:145:GLY:H	2.28	0.46
2:H:119:VAL:HG12	2:H:156:THR:CG2	2.46	0.46
3:C:2:VAL:N	3:C:31:SER:HG	2.14	0.46
1:D:69:ILE:HD11	1:D:164:LEU:HD13	1.96	0.46
2:E:75:GLU:HG3	2:E:282:LYS:HG3	1.98	0.46
1:V:335:MET:O	1:V:339:THR:OG1	2.25	0.46
2:K:179:TYR:CE1	2:K:324:LYS:HB2	2.51	0.46
2:E:332:GLU:HG3	2:E:335:ARG:HH21	1.80	0.46
2:H:167:ARG:HG3	2:H:220:PHE:HB3	1.96	0.46
1:D:190:ARG:CD	1:D:241:TRP:HH2	2.21	0.46
2:B:200:ILE:HG23	2:B:234:GLN:OE1	2.16	0.46
1:S:320:VAL:HG22	3:U:88:VAL:HG11	1.97	0.46
2:Q:305:ARG:NH1	2:Q:305:ARG:HG2	2.31	0.46
2:Q:170:LEU:CD1	2:Q:223:VAL:HG21	2.45	0.46
2:H:345:ASN:O	2:H:349:ASN:HB2	2.15	0.46
1:P:349:LYS:O	1:P:353:MET:HG2	2.16	0.46
1:S:259:GLU:OE1	1:S:259:GLU:N	2.49	0.46
1:S:199:PHE:C	1:S:199:PHE:CD1	2.89	0.46
1:P:300:PRO:O	1:P:304:ILE:HG13	2.15	0.46
1:V:422:VAL:N	1:V:423:PRO:CD	2.79	0.46
2:Q:162:THR:CG2	2:Q:165:GLU:H	2.29	0.46
1:P:172:ILE:HD13	1:P:207:GLY:HA3	1.97	0.46
1:D:293:PRO:HG3	2:H:106:TRP:CZ3	2.51	0.46
1:S:5:LYS:HB2	1:S:10:LEU:HD13	1.96	0.46
1:D:64:LEU:HD11	1:D:222:VAL:HG21	1.98	0.46
1:S:2:LEU:HB3	1:S:27:SER:OG	2.14	0.46
2:N:249:ARG:NH2	2:N:260:PRO:HD3	2.31	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:88:ILE:HD13	1:S:317:TYR:HB3	1.98	0.46
2:W:172:LYS:HE3	2:W:300:ASP:OD1	2.16	0.46
2:E:96:GLN:HB2	2:E:125:HIS:HB2	1.98	0.46
1:D:143:VAL:HG13	1:D:145:GLY:H	1.81	0.46
1:P:125:SER:HB2	1:P:143:VAL:HG21	1.98	0.46
2:Q:21:THR:HB	3:R:63:ASP:OD1	2.16	0.46
2:H:115:GLU:HB3	2:H:116:LYS:H	1.54	0.46
2:Q:385:SER:OG	2:Q:388:ILE:HG12	2.15	0.46
1:D:219:VAL:O	1:D:223:ILE:HG12	2.16	0.46
2:N:34:GLU:HB2	2:N:37:THR:HG21	1.98	0.46
2:K:210:THR:HB	2:K:244:VAL:HG13	1.98	0.46
1:P:2:LEU:HB3	1:P:27:SER:OG	2.15	0.46
2:B:146:ARG:HH11	2:B:146:ARG:HG2	1.81	0.46
2:N:21:THR:HG21	3:O:61:ARG:NH1	2.11	0.46
1:M:397:THR:HG23	1:M:398:PRO:HD2	1.98	0.46
2:B:8:VAL:HG21	2:B:201:ARG:NE	2.31	0.46
1:V:118:ASP:CG	1:V:126:THR:HA	2.36	0.46
1:J:21:PRO:O	1:J:25:VAL:HG23	2.15	0.46
2:T:387:LYS:HG3	1:V:406:GLU:HA	1.98	0.46
1:S:279:GLU:HG3	1:S:468:LYS:NZ	2.30	0.46
1:P:178:PHE:HE1	1:P:397:THR:HG21	1.81	0.46
1:J:1:MET:O	1:J:1:MET:HG2	2.15	0.46
2:N:24:PHE:HA	2:N:52:ILE:O	2.16	0.45
1:S:422:VAL:HG23	1:S:423:PRO:N	2.31	0.45
2:E:37:THR:HG22	2:E:145:ASN:HD21	1.81	0.45
2:B:27:CYS:SG	2:B:40:CYS:HB2	2.57	0.45
1:J:94:ALA:HA	1:J:95:PRO:HD3	1.78	0.45
2:K:17:MET:HE1	2:K:60:TYR:HB2	1.98	0.45
1:D:38:LYS:O	1:D:135:LYS:HG3	2.16	0.45
2:B:112:PRO:O	2:B:113:ASN:HB2	2.15	0.45
1:P:434:ILE:HD12	1:P:465:TRP:CD1	2.50	0.45
1:M:126:THR:OG1	1:M:149:GLY:HA3	2.16	0.45
2:E:250:THR:O	2:E:258:THR:HA	2.16	0.45
1:M:94:ALA:HA	1:M:95:PRO:HD3	1.80	0.45
1:S:138:TRP:CZ2	1:S:476:PRO:HD3	2.51	0.45
2:E:234:GLN:O	2:E:238:VAL:HG23	2.16	0.45
2:W:137:GLY:O	3:X:90:ARG:HD2	2.17	0.45
1:A:279:GLU:HG3	1:A:468:LYS:HZ1	1.81	0.45
1:P:178:PHE:CE1	1:P:397:THR:HG21	2.51	0.45
2:K:196:ILE:O	2:K:213:GLU:HA	2.16	0.45
1:P:88:ILE:HA	1:P:324:TYR:HB3	1.97	0.45
1:A:135:LYS:NZ	2:E:349:ASN:O	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:14:HIS:CD2	2:B:127:GLU:OE2	2.69	0.45
1:J:178:PHE:CE1	1:J:397:THR:HG21	2.51	0.45
2:N:282:LYS:HD3	3:O:55:PHE:CZ	2.52	0.45
1:D:172:ILE:CD1	1:D:207:GLY:HA3	2.46	0.45
2:B:146:ARG:HG2	2:B:146:ARG:NH1	2.32	0.45
2:K:22:LYS:HD2	2:K:27:CYS:HB2	1.99	0.45
1:M:185:LYS:NZ	1:M:429:LEU:O	2.49	0.45
1:G:337:ALA:HA	3:I:15:ARG:O	2.15	0.45
1:M:172:ILE:HD13	1:M:207:GLY:HA3	1.96	0.45
1:D:30:ASP:O	1:D:34:GLN:HG3	2.16	0.45
2:B:255:THR:HG23	2:B:257:LYS:H	1.82	0.45
1:G:39:VAL:HG21	1:G:157:VAL:HG11	1.97	0.45
2:H:230:GLU:OE2	2:H:233:ARG:NH1	2.49	0.45
2:T:233:ARG:HD2	2:T:249:ARG:NH2	2.31	0.45
1:S:174:GLN:HB3	1:S:175:PRO:HD3	1.98	0.45
2:N:113:ASN:HD21	1:P:49:LYS:HB2	1.80	0.45
2:E:229:TYR:O	2:E:232:GLU:HB3	2.17	0.45
1:A:299:ILE:HB	1:A:300:PRO:HD3	1.99	0.45
2:N:402:THR:HG22	2:N:403:PRO:HD2	1.99	0.45
1:J:62:LEU:HA	1:J:63:PRO:HD3	1.84	0.45
2:K:73:HIS:NE2	2:K:103:THR:HB	2.32	0.45
1:P:279:GLU:HG3	1:P:468:LYS:NZ	2.30	0.45
2:K:95:SER:CB	2:K:127:GLU:HB3	2.46	0.45
1:A:19:VAL:HG22	1:A:20:SER:N	2.31	0.45
1:G:438:TRP:CH2	1:G:443:PRO:HG3	2.51	0.45
1:M:279:GLU:HG3	1:M:468:LYS:HZ3	1.81	0.45
1:M:193:ARG:NH1	1:M:232:THR:OG1	2.49	0.45
2:B:8:VAL:HG13	2:B:161:ARG:NH1	2.31	0.45
1:A:95:PRO:HG2	2:B:46:MET:CE	2.47	0.45
2:H:222:PHE:CZ	2:H:253:PRO:HB3	2.52	0.45
2:Q:233:ARG:O	2:Q:237:VAL:HG23	2.17	0.45
1:S:72:LYS:HE2	1:S:117:LEU:HD13	1.98	0.45
1:P:170:GLY:HA2	1:P:173:ARG:NH2	2.31	0.45
1:M:353:MET:O	1:M:356:THR:HG23	2.16	0.45
1:S:83:THR:HG22	1:S:90:GLU:HA	1.98	0.45
2:H:233:ARG:O	2:H:237:VAL:HG23	2.16	0.45
2:H:320:LEU:CD2	2:H:326:VAL:HG12	2.45	0.45
2:B:198:VAL:O	2:B:198:VAL:HG13	2.17	0.45
1:A:162:VAL:HG21	1:A:219:VAL:HG21	1.98	0.45
1:P:162:VAL:HG11	1:P:219:VAL:HG21	1.99	0.45
1:D:88:ILE:HG23	1:D:89:LEU:HD13	1.99	0.45
2:T:114:GLY:O	2:T:115:GLU:OE2	2.35	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:V:297:TYR:C	1:V:300:PRO:HD2	2.37	0.45
2:K:123:ARG:HG2	2:K:155:VAL:HB	1.98	0.45
1:S:181:VAL:HG22	1:S:210:GLY:O	2.17	0.45
1:J:292:LEU:HB2	1:J:295:VAL:CG2	2.47	0.45
2:Q:211:ARG:HD2	8:Q:479:ATP:C8	2.52	0.45
1:D:302:TYR:OH	4:D:902:ASN:HA	2.17	0.45
1:S:317:TYR:HE1	2:T:47:PRO:HG3	1.82	0.45
3:I:73:LYS:O	3:I:76:MET:HG2	2.17	0.45
1:S:421:THR:C	1:S:423:PRO:HD2	2.38	0.45
2:W:21:THR:HG21	3:X:61:ARG:NH1	2.18	0.45
1:V:138:TRP:NE1	1:V:438:TRP:HH2	2.15	0.45
1:J:145:GLY:CA	1:J:174:GLN:OE1	2.65	0.45
1:J:138:TRP:CE2	1:J:438:TRP:CH2	3.05	0.45
1:J:422:VAL:N	1:J:423:PRO:CD	2.80	0.45
2:H:119:VAL:HG12	2:H:156:THR:HG23	1.98	0.45
2:B:36:ASN:ND2	3:C:84:GLY:O	2.41	0.45
2:W:95:SER:HB3	2:W:127:GLU:OE1	2.17	0.45
2:K:96:GLN:HB2	2:K:125:HIS:HB2	1.98	0.45
1:D:138:TRP:CD2	1:D:438:TRP:CZ3	3.05	0.45
1:A:174:GLN:HG3	1:A:175:PRO:N	2.30	0.45
1:M:98:ALA:HA	1:M:195:GLY:HA3	1.98	0.45
1:S:126:THR:OG1	1:S:149:GLY:HA3	2.16	0.45
1:P:384:LYS:O	1:P:387:GLU:HB2	2.16	0.45
2:B:109:LEU:HD11	2:B:169:PHE:HA	1.99	0.45
1:G:21:PRO:O	1:G:25:VAL:HG23	2.17	0.45
1:M:47:TYR:CD2	1:M:112:VAL:HG22	2.52	0.45
2:N:80:ARG:HE	2:N:275:ASP:CG	2.20	0.45
1:P:157:VAL:O	1:P:158:LEU:HB2	2.16	0.45
2:B:295:MET:HG3	2:B:296:PRO:O	2.16	0.45
1:M:331:ASP:OD1	1:M:331:ASP:C	2.55	0.45
2:H:24:PHE:HA	2:H:52:ILE:O	2.16	0.44
2:W:255:THR:HG21	2:W:259:TYR:CE1	2.49	0.44
2:T:360:ILE:HD11	2:T:365:SER:HA	2.00	0.44
1:P:155:VAL:CG2	1:P:163:SER:HB2	2.47	0.44
2:Q:17:MET:HE1	2:Q:60:TYR:HB2	1.97	0.44
2:T:156:THR:HG22	2:T:157:GLU:N	2.33	0.44
2:H:129:ASP:O	2:H:147:ALA:HA	2.17	0.44
3:C:23:ILE:O	3:C:27:GLN:HG3	2.17	0.44
2:Q:334:VAL:HG21	2:Q:340:PRO:CB	2.41	0.44
2:N:95:SER:HB3	2:N:127:GLU:CB	2.43	0.44
2:T:255:THR:HG21	2:T:259:TYR:OH	2.16	0.44
1:G:297:TYR:C	1:G:300:PRO:HD2	2.38	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:33:ILE:O	3:I:37:ILE:HG12	2.18	0.44
1:S:297:TYR:C	1:S:300:PRO:HD2	2.38	0.44
2:Q:185:ALA:HB1	2:Q:192:LEU:HD12	1.99	0.44
2:W:42:VAL:HA	2:W:49:ALA:HB1	1.99	0.44
2:B:42:VAL:HA	2:B:49:ALA:HB1	1.99	0.44
2:N:298:LEU:HB3	2:N:299:PRO:CD	2.48	0.44
1:J:122:MET:SD	1:J:351:ARG:HD2	2.57	0.44
3:C:72:GLU:OE1	3:C:72:GLU:HA	2.16	0.44
2:H:211:ARG:HH12	8:H:479:ATP:H5'2	1.78	0.44
2:Q:207:GLU:OE1	2:Q:207:GLU:C	2.55	0.44
1:M:422:VAL:N	1:M:423:PRO:CD	2.81	0.44
1:G:422:VAL:N	1:G:423:PRO:CD	2.81	0.44
2:W:41:PRO:CB	2:W:46:MET:HE2	2.47	0.44
2:E:81:LYS:HE2	2:E:270:TYR:CE1	2.53	0.44
2:Q:68:LEU:HD11	2:Q:154:ILE:HD13	1.98	0.44
1:S:98:ALA:HA	1:S:195:GLY:HA3	2.00	0.44
1:S:99:THR:O	1:S:103:ARG:HG3	2.17	0.44
1:J:432:ILE:HG22	1:J:458:LEU:HG	1.99	0.44
2:Q:137:GLY:O	3:R:90:ARG:HD2	2.17	0.44
2:T:370:GLU:CD	2:T:370:GLU:H	2.21	0.44
2:T:17:MET:CE	2:T:60:TYR:HB2	2.47	0.44
1:A:138:TRP:CE2	1:A:476:PRO:HB3	2.53	0.44
1:P:125:SER:HB2	1:P:143:VAL:CG2	2.48	0.44
1:D:143:VAL:CG1	1:D:145:GLY:H	2.31	0.44
2:K:103:THR:CG2	2:K:104:ASN:OD1	2.66	0.44
1:P:215:ASP:O	1:P:219:VAL:HG23	2.18	0.44
2:K:17:MET:HE3	2:K:60:TYR:HB3	1.99	0.44
1:P:90:GLU:O	1:P:91:ASN:CB	2.63	0.44
2:Q:332:GLU:HG3	2:Q:335:ARG:NH2	2.33	0.44
1:J:344:PHE:O	1:J:349:LYS:HE2	2.17	0.44
1:G:347:GLU:OE1	1:G:350:ARG:NH2	2.44	0.44
1:V:76:LEU:HD23	1:V:94:ALA:HB1	1.98	0.44
2:E:370:GLU:CD	2:E:370:GLU:H	2.20	0.44
1:A:115:THR:HG21	1:A:151:SER:N	2.33	0.44
2:W:8:VAL:HG21	2:W:201:ARG:HE	1.82	0.44
1:A:253:LYS:HG2	1:A:286:GLU:HB3	2.00	0.44
2:H:8:VAL:CG1	2:H:158:PRO:HB2	2.48	0.44
2:T:135:HIS:N	2:T:135:HIS:ND1	2.65	0.44
1:A:190:ARG:HD2	1:A:455:GLU:OE2	2.18	0.44
1:D:138:TRP:CD2	1:D:438:TRP:HZ3	2.35	0.44
2:H:95:SER:HB3	2:H:127:GLU:OE1	2.17	0.44
2:N:156:THR:CG2	2:N:157:GLU:O	2.65	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:210:THR:HG22	2:B:246:GLN:HB2	2.00	0.44
2:B:396:MET:HE1	2:B:403:PRO:HB3	1.99	0.44
2:B:310:TYR:CE1	2:B:334:VAL:HG11	2.52	0.44
1:G:376:ARG:HG3	1:G:376:ARG:NH1	2.31	0.44
2:B:89:PRO:HG3	2:B:144:LEU:HD13	1.99	0.44
2:Q:362:ILE:O	2:Q:362:ILE:HG13	2.17	0.44
1:S:67:ILE:HD13	1:S:67:ILE:N	2.33	0.44
2:K:115:GLU:HB3	2:K:116:LYS:H	1.66	0.44
2:K:192:LEU:HD23	2:K:193:ARG:N	2.33	0.44
2:Q:301:GLN:O	2:Q:302:ARG:C	2.56	0.44
1:J:39:VAL:HG21	1:J:157:VAL:HG11	2.00	0.44
1:M:350:ARG:HG3	3:O:26:PHE:CE1	2.53	0.44
2:W:210:THR:OG1	2:W:244:VAL:HG13	2.18	0.44
1:J:191:VAL:HG22	1:J:224:SER:HB3	1.99	0.44
1:P:31:ARG:O	1:P:31:ARG:HG3	2.17	0.44
2:N:323:HIS:HD2	2:N:325:GLU:OE1	1.99	0.44
1:S:88:ILE:HG23	1:S:89:LEU:HD13	2.00	0.44
1:D:98:ALA:HA	1:D:195:GLY:HA3	2.00	0.44
3:X:21:GLU:O	3:X:25:VAL:HG23	2.17	0.44
1:S:299:ILE:HG13	1:S:419:ILE:HG22	1.99	0.44
3:F:71:ARG:HG2	3:F:75:LEU:HD23	2.00	0.44
2:B:100:PRO:HB3	2:B:123:ARG:NH2	2.21	0.43
1:A:36:GLU:OE1	1:A:36:GLU:HA	2.18	0.43
1:M:137:PRO:HB3	1:M:157:VAL:CG1	2.48	0.43
2:E:375:LEU:O	2:E:379:ILE:HG12	2.17	0.43
1:G:173:ARG:NH2	1:G:425:ASN:OD1	2.51	0.43
2:K:88:LEU:HD11	2:K:93:GLN:HB2	2.00	0.43
1:V:155:VAL:HG21	1:V:163:SER:HB2	1.98	0.43
2:B:17:MET:HE1	2:B:57:ALA:HA	1.94	0.43
1:D:115:THR:OG1	1:D:150:GLY:C	2.56	0.43
1:A:434:ILE:HD13	1:A:434:ILE:HA	1.61	0.43
1:A:475:ILE:HG23	1:A:476:PRO:CD	2.47	0.43
1:M:422:VAL:HG23	1:M:423:PRO:HD3	1.99	0.43
2:B:113:ASN:HA	2:B:115:GLU:H	1.83	0.43
1:S:28:PHE:CD2	1:S:68:PRO:HG2	2.53	0.43
1:G:137:PRO:HB3	1:G:157:VAL:HG13	2.00	0.43
1:P:204:ASP:O	1:P:205:GLN:HG2	2.18	0.43
2:W:109:LEU:HD11	2:W:169:PHE:HA	2.00	0.43
2:E:36:ASN:ND2	3:F:84:GLY:O	2.49	0.43
1:S:120:PHE:O	1:S:122:MET:HG3	2.19	0.43
2:T:40:CYS:HB2	2:T:41:PRO:HD2	2.01	0.43
2:W:5:TYR:HA	2:W:202:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:112:PRO:O	2:H:113:ASN:HB2	2.18	0.43
1:D:157:VAL:HG23	1:D:159:SER:H	1.83	0.43
2:Q:222:PHE:CE2	2:Q:253:PRO:HB3	2.54	0.43
2:W:80:ARG:HE	2:W:275:ASP:CG	2.21	0.43
1:S:196:LEU:HB2	1:S:206:ILE:HD11	1.99	0.43
2:E:141:LEU:HD23	3:F:85:PHE:CD2	2.54	0.43
2:H:362:ILE:O	2:H:362:ILE:HG13	2.17	0.43
2:E:146:ARG:HH11	2:E:146:ARG:HG2	1.82	0.43
2:E:360:ILE:HD13	2:E:366:PRO:HD3	2.00	0.43
1:M:138:TRP:CE2	1:M:438:TRP:CZ3	3.06	0.43
1:J:477:LEU:HD23	1:J:477:LEU:N	2.29	0.43
1:D:265:LEU:HD22	1:D:398:PRO:HA	2.00	0.43
3:R:55:PHE:O	3:R:56:GLU:CB	2.66	0.43
2:Q:255:THR:HG21	2:Q:259:TYR:OH	2.19	0.43
1:S:32:TYR:CZ	1:S:36:GLU:HG2	2.53	0.43
2:Q:230:GLU:OE2	2:Q:233:ARG:NH1	2.52	0.43
1:A:143:VAL:HG23	1:A:145:GLY:H	1.82	0.43
1:J:316:ARG:O	1:J:321:ARG:NH2	2.50	0.43
2:B:24:PHE:HA	2:B:52:ILE:O	2.18	0.43
3:O:34:LEU:HA	3:O:34:LEU:HD12	1.68	0.43
1:G:477:LEU:C	1:G:478:THR:HG23	2.39	0.43
1:J:90:GLU:O	1:J:91:ASN:CB	2.58	0.43
1:P:138:TRP:CZ2	1:P:438:TRP:CH2	3.06	0.43
1:M:162:VAL:CG2	1:M:219:VAL:HG21	2.48	0.43
1:V:157:VAL:HG23	1:V:159:SER:H	1.82	0.43
1:J:172:ILE:HD13	1:J:207:GLY:HA3	2.01	0.43
1:J:78:GLU:HB2	1:J:97:ASP:OD1	2.18	0.43
1:S:386:PHE:CG	1:S:451:LYS:HG2	2.53	0.43
1:A:297:TYR:CD2	3:C:43:LEU:HD11	2.53	0.43
2:K:320:LEU:HD22	2:K:326:VAL:HG12	2.01	0.43
2:E:20:LYS:HE3	3:F:63:ASP:O	2.18	0.43
2:K:95:SER:HB2	2:K:127:GLU:OE1	2.19	0.43
1:A:94:ALA:HA	1:A:95:PRO:HD3	1.67	0.43
2:B:88:LEU:HA	2:B:89:PRO:HD3	1.72	0.43
1:J:60:ARG:HA	1:J:65:PHE:CG	2.54	0.43
2:K:222:PHE:CZ	2:K:253:PRO:HB3	2.53	0.43
3:F:7:VAL:HG21	3:F:27:GLN:HG3	1.99	0.43
1:P:199:PHE:CD1	1:P:199:PHE:C	2.92	0.43
1:J:332:ILE:HD12	3:L:89:PRO:HG2	2.01	0.43
2:Q:331:GLU:HA	2:Q:334:VAL:HG12	2.00	0.43
1:V:185:LYS:HE3	1:V:425:ASN:HD22	1.83	0.43
1:S:137:PRO:HB3	1:S:157:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:422:VAL:N	1:D:423:PRO:CD	2.82	0.43
1:V:325:ARG:HA	1:V:339:THR:HG23	2.01	0.43
2:K:95:SER:HB2	2:K:127:GLU:HB3	2.00	0.43
1:G:234:ALA:HB1	1:G:236:VAL:HG23	2.01	0.43
1:A:88:ILE:HA	1:A:324:TYR:HB3	1.99	0.43
1:M:177:SER:HA	10:M:907:HOH:O	2.18	0.43
2:W:302:ARG:HD3	2:W:321:VAL:HG22	2.01	0.43
2:T:36:ASN:O	3:U:71:ARG:HD3	2.18	0.43
2:N:106:TRP:CD1	2:N:118:LYS:HE2	2.54	0.43
2:K:170:LEU:HD12	2:K:223:VAL:HG21	2.00	0.43
2:N:310:TYR:CE1	2:N:334:VAL:HG11	2.53	0.43
1:V:318:ASP:HB2	1:V:336:TYR:CE1	2.54	0.43
1:M:182:ILE:HG12	1:M:434:ILE:CD1	2.49	0.43
1:D:322:TYR:OH	2:E:45:GLY:O	2.26	0.43
1:P:283:GLU:HG3	1:P:468:LYS:HD2	2.01	0.43
2:N:210:THR:OG1	2:N:244:VAL:HG13	2.19	0.43
1:A:139:ASP:OD1	1:A:141:GLU:HB2	2.18	0.43
2:T:222:PHE:CZ	2:T:253:PRO:HB3	2.54	0.43
2:B:355:LEU:HD21	2:B:365:SER:HB2	1.99	0.43
2:T:109:LEU:HD11	2:T:169:PHE:HA	2.01	0.43
1:V:300:PRO:HA	3:X:37:ILE:HG22	2.00	0.43
2:E:156:THR:CG2	2:E:157:GLU:O	2.64	0.43
2:W:5:TYR:HB3	2:W:201:ARG:O	2.19	0.43
2:K:282:LYS:HD3	3:L:55:PHE:CE2	2.54	0.43
2:H:320:LEU:HD22	2:H:326:VAL:HG12	2.01	0.43
1:J:57:LEU:HD22	1:J:65:PHE:CE1	2.54	0.43
1:D:57:LEU:HD22	1:D:65:PHE:CE1	2.54	0.43
1:V:87:LYS:HD3	1:V:90:GLU:OE2	2.19	0.43
1:V:98:ALA:HA	1:V:195:GLY:HA3	2.01	0.43
2:E:196:ILE:O	2:E:213:GLU:HA	2.19	0.43
2:T:146:ARG:HH11	2:T:146:ARG:HG2	1.83	0.43
2:H:202:PRO:O	2:H:205:SER:HB3	2.19	0.43
2:Q:308:LYS:C	2:Q:310:TYR:H	2.22	0.42
1:A:72:LYS:HE2	1:A:117:LEU:HD13	2.01	0.42
2:T:211:ARG:HD3	6:T:479:ADP:C5	2.54	0.42
1:V:351:ARG:HH12	4:V:908:ASN:C	2.23	0.42
2:W:35:PRO:HG3	3:X:85:PHE:CZ	2.54	0.42
2:Q:184:LYS:HB2	2:Q:191:GLN:OE1	2.19	0.42
1:P:196:LEU:HD22	1:P:206:ILE:HG13	2.01	0.42
1:M:337:ALA:HA	3:O:15:ARG:O	2.19	0.42
1:A:406:GLU:HG3	2:E:387:LYS:HD2	2.01	0.42
1:A:26:GLU:HG3	1:A:51:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:67:ILE:HD13	1:D:67:ILE:N	2.34	0.42
2:B:39:VAL:HG13	2:B:44:LEU:HD11	2.01	0.42
2:T:201:ARG:CD	2:T:207:GLU:O	2.67	0.42
2:T:17:MET:HE3	2:T:60:TYR:HB2	2.02	0.42
1:D:182:ILE:HG12	1:D:434:ILE:CD1	2.50	0.42
2:E:174:ARG:HD2	2:E:220:PHE:CE2	2.54	0.42
1:V:126:THR:O	1:V:126:THR:HG22	2.18	0.42
1:D:393:ALA:HB2	1:D:448:LEU:HD23	2.01	0.42
2:B:179:TYR:CE1	2:B:324:LYS:HB2	2.54	0.42
1:A:470:LYS:HG2	1:A:472:TYR:OH	2.18	0.42
2:K:13:ILE:HG22	2:K:15:VAL:HG23	2.00	0.42
2:K:143:ASP:HB2	3:L:85:PHE:CE1	2.55	0.42
1:J:3:TRP:CZ3	1:J:31:ARG:CD	3.02	0.42
1:G:219:VAL:O	1:G:223:ILE:HG23	2.19	0.42
2:E:117:LYS:CG	2:E:118:LYS:N	2.81	0.42
2:K:220:PHE:O	2:K:223:VAL:HG22	2.17	0.42
2:H:360:ILE:H	2:H:360:ILE:HG13	1.67	0.42
2:K:95:SER:CB	2:K:127:GLU:OE1	2.67	0.42
1:A:403:LYS:O	1:A:406:GLU:HB2	2.19	0.42
1:S:173:ARG:NH2	1:S:425:ASN:OD1	2.52	0.42
2:Q:196:ILE:HG21	2:Q:227:LEU:HD21	2.00	0.42
2:T:162:THR:HG22	2:T:165:GLU:H	1.84	0.42
2:E:201:ARG:CD	2:E:207:GLU:O	2.67	0.42
1:P:143:VAL:CG1	1:P:145:GLY:H	2.32	0.42
1:G:418:ASP:HB3	1:G:422:VAL:HG13	2.02	0.42
1:S:123:GLY:O	4:S:907:ASN:HB2	2.20	0.42
1:V:351:ARG:NH1	4:V:908:ASN:OXT	2.51	0.42
2:W:375:LEU:HD13	2:W:396:MET:HE1	2.01	0.42
2:Q:140:THR:OG1	3:R:91:VAL:HG22	2.20	0.42
2:Q:27:CYS:SG	2:Q:40:CYS:HB3	2.59	0.42
1:D:373:LYS:HE2	3:F:50:PRO:HD3	2.01	0.42
2:K:405:GLN:O	2:K:409:GLU:HG3	2.19	0.42
1:J:266:GLN:HA	1:J:267:PRO:HD3	1.93	0.42
1:V:374:VAL:HG11	3:X:40:LEU:HD22	2.01	0.42
1:J:3:TRP:CH2	1:J:31:ARG:NE	2.88	0.42
1:A:475:ILE:HG23	1:A:476:PRO:HD2	1.99	0.42
1:P:477:LEU:O	1:P:478:THR:C	2.58	0.42
1:P:306:ALA:HB3	1:P:307:PRO:CD	2.46	0.42
2:E:118:LYS:NZ	1:G:291:SER:HB3	2.35	0.42
1:V:125:SER:O	1:V:126:THR:HB	2.18	0.42
2:H:83:TYR:CZ	2:H:88:LEU:HD22	2.55	0.42
1:J:318:ASP:HB2	1:J:336:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:138:TRP:CZ2	1:A:438:TRP:CH2	3.08	0.42
1:J:438:TRP:CD1	1:J:438:TRP:N	2.87	0.42
1:P:434:ILE:HA	1:P:435:PRO:HD3	1.93	0.42
1:A:98:ALA:HA	1:A:195:GLY:HA3	2.02	0.42
1:V:31:ARG:O	1:V:35:THR:HG23	2.20	0.42
2:H:7:ALA:HB3	2:H:161:ARG:O	2.20	0.42
1:D:5:LYS:HB2	1:D:10:LEU:HD13	2.01	0.42
1:P:21:PRO:O	1:P:25:VAL:HG23	2.20	0.42
1:S:157:VAL:HG23	1:S:159:SER:H	1.85	0.42
2:B:46:MET:HB3	2:B:46:MET:HE2	1.71	0.42
2:K:8:VAL:O	2:K:198:VAL:HA	2.20	0.42
2:E:39:VAL:HG21	2:E:44:LEU:CD2	2.50	0.42
2:T:207:GLU:CG	2:T:208:PHE:N	2.79	0.42
2:T:140:THR:HB	3:U:88:VAL:HG23	2.02	0.42
1:V:114:LYS:HE2	1:V:114:LYS:HA	2.02	0.42
1:V:219:VAL:O	1:V:223:ILE:HG12	2.19	0.42
1:M:275:ASN:O	1:M:279:GLU:HB2	2.20	0.42
1:P:418:ASP:HB3	1:P:422:VAL:HG13	2.01	0.42
2:W:198:VAL:HG11	2:W:230:GLU:HG2	2.02	0.42
1:P:126:THR:O	1:P:126:THR:HG22	2.18	0.42
2:T:263:THR:C	2:T:265:GLU:H	2.23	0.42
2:Q:307:ILE:O	2:Q:311:GLY:HA2	2.19	0.42
1:J:98:ALA:HA	1:J:195:GLY:HA3	2.01	0.42
1:G:57:LEU:HD22	1:G:65:PHE:CE1	2.55	0.42
2:N:362:ILE:O	2:N:362:ILE:HG13	2.20	0.42
1:D:438:TRP:CH2	1:D:443:PRO:HG3	2.55	0.42
1:G:397:THR:HG22	1:G:399:THR:H	1.85	0.42
1:P:438:TRP:N	1:P:438:TRP:CD1	2.87	0.42
1:S:322:TYR:CZ	2:T:47:PRO:HD3	2.55	0.42
1:V:457:THR:O	1:V:461:ILE:HG13	2.20	0.42
1:V:62:LEU:HA	1:V:63:PRO:HD3	1.89	0.42
2:Q:250:THR:O	2:Q:258:THR:HA	2.19	0.42
2:N:330:PHE:CE1	2:N:344:VAL:HG13	2.54	0.42
1:P:405:GLY:HA2	1:P:408:LEU:HD12	2.02	0.42
1:P:244:GLU:OE2	1:P:247:LYS:HD2	2.20	0.42
1:V:300:PRO:O	1:V:304:ILE:HG13	2.20	0.42
1:D:72:LYS:CA	1:D:115:THR:HG22	2.45	0.42
1:D:138:TRP:CE2	1:D:438:TRP:CZ3	3.08	0.42
1:P:434:ILE:O	1:P:436:ILE:HG23	2.20	0.42
2:E:330:PHE:CE1	2:E:344:VAL:HG13	2.54	0.42
2:Q:252:ASP:HB3	2:Q:255:THR:HG22	2.02	0.42
1:A:21:PRO:HB2	1:A:54:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:136:ASN:HA	1:M:137:PRO:HD2	1.95	0.42
1:V:116:ASN:ND2	1:V:132:PHE:O	2.51	0.42
1:P:60:ARG:HA	1:P:65:PHE:CD1	2.54	0.42
1:D:226:TRP:HD1	1:D:233:SER:HG	1.66	0.42
2:H:34:GLU:HB2	2:H:37:THR:HG21	2.01	0.42
2:B:368:LYS:O	2:B:369:PRO:C	2.58	0.42
2:N:108:GLU:O	2:N:172:LYS:NZ	2.51	0.42
2:T:21:THR:HG23	2:T:25:CYS:O	2.20	0.41
2:B:17:MET:HE3	2:B:60:TYR:CB	2.50	0.41
1:A:299:ILE:CB	1:A:300:PRO:HD3	2.50	0.41
1:J:138:TRP:CZ2	1:J:438:TRP:CH2	3.08	0.41
1:D:168:THR:HB	4:D:902:ASN:OD1	2.20	0.41
1:D:293:PRO:HG3	2:H:106:TRP:CE3	2.54	0.41
2:K:172:LYS:O	2:K:176:ILE:HG13	2.19	0.41
2:E:374:GLU:O	2:E:377:LYS:HB3	2.20	0.41
2:B:320:LEU:HD13	2:B:327:GLY:HA2	2.01	0.41
2:K:350:ASP:OD1	2:K:390:LYS:NZ	2.52	0.41
2:E:406:ILE:HA	2:E:409:GLU:HB2	2.01	0.41
3:L:80:GLU:HG2	3:L:87:VAL:HB	2.02	0.41
2:H:221:ARG:HA	2:H:221:ARG:HD3	1.90	0.41
1:S:138:TRP:CD2	1:S:438:TRP:CZ3	3.07	0.41
1:G:90:GLU:O	1:G:91:ASN:CB	2.65	0.41
1:V:176:ALA:HB1	1:V:181:VAL:O	2.20	0.41
1:J:418:ASP:HB3	1:J:422:VAL:HG13	2.02	0.41
2:B:336:HIS:NE2	2:B:370:GLU:HG3	2.35	0.41
2:E:179:TYR:CD1	2:E:299:PRO:HG3	2.55	0.41
3:X:58:THR:HA	3:X:59:PRO:HD2	1.81	0.41
2:N:26:GLY:O	3:O:65:PRO:HA	2.19	0.41
1:P:347:GLU:O	1:P:351:ARG:HG3	2.20	0.41
1:D:32:TYR:CE1	1:D:36:GLU:HG2	2.55	0.41
1:D:356:THR:HG21	3:F:14:ALA:HB2	2.03	0.41
1:V:42:TYR:O	1:V:132:PHE:HZ	2.02	0.41
2:K:213:GLU:OE2	2:K:215:LYS:HE3	2.20	0.41
2:B:198:VAL:HG11	2:B:230:GLU:HG2	2.02	0.41
1:A:234:ALA:HB1	1:A:236:VAL:HG23	2.02	0.41
1:J:384:LYS:O	1:J:387:GLU:HB2	2.20	0.41
2:H:142:VAL:HB	3:I:86:PHE:HB2	2.02	0.41
2:E:98:GLU:O	2:E:99:LYS:HB2	2.20	0.41
1:V:172:ILE:HD13	1:V:207:GLY:HA3	2.01	0.41
2:E:362:ILE:HG13	2:E:362:ILE:O	2.19	0.41
1:G:434:ILE:HA	1:G:434:ILE:HD13	1.69	0.41
1:J:332:ILE:CD1	3:L:89:PRO:HG2	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:219:VAL:O	1:M:223:ILE:HG23	2.21	0.41
2:Q:333:ALA:HB2	2:Q:369:PRO:HB3	2.02	0.41
1:D:297:TYR:C	1:D:300:PRO:HD2	2.40	0.41
1:S:88:ILE:HG13	1:S:343:GLY:HA3	2.02	0.41
2:Q:179:TYR:CE1	2:Q:324:LYS:HB2	2.56	0.41
2:Q:360:ILE:HD11	2:Q:365:SER:HA	2.03	0.41
1:J:99:THR:O	1:J:102:GLU:HB3	2.20	0.41
1:A:404:PHE:HB3	2:E:390:LYS:HE3	2.02	0.41
3:X:80:GLU:HG2	3:X:87:VAL:HB	2.01	0.41
1:V:350:ARG:HD3	3:X:29:GLN:OE1	2.21	0.41
1:D:77:VAL:HG21	1:D:114:LYS:HZ1	1.79	0.41
2:H:52:ILE:HG22	3:I:61:ARG:HB2	2.02	0.41
2:T:70:CYS:HB3	2:T:103:THR:H	1.86	0.41
2:B:252:ASP:CB	2:B:255:THR:HG22	2.44	0.41
1:J:177:SER:HB2	1:J:396:THR:HG21	2.01	0.41
2:Q:215:LYS:O	2:Q:216:ASN:HB2	2.20	0.41
2:W:17:MET:HE3	2:W:60:TYR:CB	2.49	0.41
2:Q:96:GLN:HB2	2:Q:125:HIS:HB2	2.02	0.41
2:N:128:GLU:HB2	2:N:148:GLY:HA2	2.01	0.41
2:E:22:LYS:NZ	2:E:147:ALA:O	2.37	0.41
2:B:39:VAL:CG1	2:B:44:LEU:HD11	2.50	0.41
1:V:155:VAL:HG21	1:V:163:SER:CB	2.51	0.41
1:P:155:VAL:O	1:P:211:ARG:HD2	2.21	0.41
1:A:115:THR:CG2	1:A:151:SER:N	2.84	0.41
2:B:95:SER:HB2	2:B:96:GLN:H	1.68	0.41
2:H:39:VAL:HG21	2:H:44:LEU:HD21	2.02	0.41
2:Q:217:VAL:HG13	2:Q:222:PHE:HB3	2.03	0.41
1:J:43:ILE:HG13	1:J:116:ASN:HA	2.02	0.41
2:W:115:GLU:HB3	2:W:116:LYS:H	1.59	0.41
1:J:29:TYR:O	1:J:32:TYR:HB3	2.20	0.41
1:G:190:ARG:HH11	1:G:190:ARG:CG	2.34	0.41
1:P:174:GLN:CG	1:P:175:PRO:HD3	2.49	0.41
1:D:477:LEU:O	1:D:478:THR:C	2.59	0.41
2:K:298:LEU:HB3	2:K:299:PRO:HD3	2.02	0.41
1:M:266:GLN:HB2	1:M:269:VAL:HG23	2.03	0.41
1:S:57:LEU:HD22	1:S:65:PHE:CE1	2.56	0.41
1:S:193:ARG:NH1	1:S:232:THR:OG1	2.54	0.41
1:D:201:SER:HB2	2:E:276:PRO:HB2	2.02	0.41
3:L:3:ASP:O	3:L:7:VAL:HG23	2.21	0.41
1:M:62:LEU:HD12	1:M:62:LEU:HA	1.96	0.41
2:E:39:VAL:HG21	2:E:44:LEU:HD21	2.02	0.41
2:B:252:ASP:OD2	2:B:255:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:X:53:GLN:O	3:X:55:PHE:HD1	2.03	0.41
1:D:476:PRO:O	1:D:477:LEU:C	2.57	0.41
2:T:41:PRO:CB	2:T:46:MET:HE2	2.50	0.41
2:B:115:GLU:HB3	2:B:116:LYS:H	1.68	0.41
2:W:310:TYR:CE1	2:W:334:VAL:HG11	2.56	0.41
1:P:434:ILE:O	1:P:434:ILE:HG22	2.21	0.41
1:P:126:THR:OG1	1:P:149:GLY:HA3	2.20	0.41
2:E:337:PHE:CE2	2:E:377:LYS:HA	2.55	0.41
1:A:142:ARG:HD3	1:A:401:PRO:O	2.20	0.41
1:A:331:ASP:O	1:A:334:GLU:N	2.53	0.41
1:S:435:PRO:HG2	1:S:471:HIS:CG	2.55	0.41
2:K:140:THR:OG1	3:L:90:ARG:HA	2.21	0.41
2:T:225:LYS:HA	2:T:225:LYS:HD3	1.87	0.41
2:H:170:LEU:HB3	2:H:220:PHE:CE1	2.56	0.41
1:A:299:ILE:HD13	1:A:299:ILE:HA	1.87	0.41
1:J:145:GLY:HA2	1:J:174:GLN:OE1	2.21	0.41
2:N:162:THR:HG22	2:N:164:GLU:N	2.35	0.41
2:B:14:HIS:HD2	2:B:127:GLU:OE2	2.04	0.41
1:M:477:LEU:O	1:M:478:THR:C	2.58	0.41
1:S:292:LEU:HB2	1:S:295:VAL:HG22	2.02	0.41
2:B:396:MET:HG3	2:B:406:ILE:HD11	2.03	0.41
1:D:64:LEU:CD1	1:D:222:VAL:HG21	2.51	0.41
1:A:212:ARG:NH2	1:A:472:TYR:CE1	2.89	0.41
2:E:42:VAL:HA	2:E:49:ALA:HB1	2.03	0.41
1:V:234:ALA:HB1	1:V:236:VAL:HG23	2.03	0.41
1:P:115:THR:HG21	1:P:151:SER:OG	2.21	0.41
1:J:199:PHE:C	1:J:199:PHE:CD1	2.93	0.41
1:A:318:ASP:HB2	1:A:336:TYR:CE1	2.55	0.41
1:D:78:GLU:HG2	1:D:79:GLY:N	2.35	0.41
3:F:34:LEU:HA	3:F:34:LEU:HD12	1.93	0.41
2:E:358:LYS:CB	2:E:360:ILE:HG22	2.51	0.41
2:K:52:ILE:HG22	3:L:61:ARG:HB2	2.02	0.41
1:G:190:ARG:HH11	1:G:190:ARG:HG3	1.84	0.41
1:G:300:PRO:HB3	3:I:37:ILE:HA	2.02	0.41
1:S:299:ILE:HD13	1:S:299:ILE:HA	1.83	0.41
1:V:374:VAL:HG21	3:X:40:LEU:HD22	2.03	0.41
1:D:193:ARG:NH2	1:D:201:SER:HB3	2.36	0.41
2:T:250:THR:O	2:T:258:THR:HA	2.20	0.41
1:A:199:PHE:CD1	1:A:199:PHE:C	2.94	0.41
1:A:151:SER:O	1:A:155:VAL:HG23	2.22	0.40
1:M:90:GLU:O	1:M:91:ASN:CB	2.62	0.40
1:G:98:ALA:HB3	1:G:101:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:299:ILE:HA	1:D:299:ILE:HD13	1.99	0.40
2:N:331:GLU:HA	2:N:334:VAL:HG12	2.03	0.40
1:J:373:LYS:HD3	3:L:45:THR:HB	2.03	0.40
1:V:7:LEU:HD21	1:V:161:PRO:HB2	2.03	0.40
2:W:337:PHE:CE2	2:W:377:LYS:HA	2.56	0.40
1:V:60:ARG:HA	1:V:65:PHE:CG	2.56	0.40
1:V:139:ASP:OD1	1:V:141:GLU:HB2	2.20	0.40
1:V:155:VAL:O	1:V:211:ARG:HD2	2.21	0.40
1:S:176:ALA:HA	1:S:181:VAL:HG12	2.03	0.40
2:N:73:HIS:NE2	2:N:103:THR:HB	2.36	0.40
1:J:58:LYS:HG2	2:Q:240:GLU:HB3	2.03	0.40
1:P:137:PRO:HB3	1:P:157:VAL:CG1	2.51	0.40
2:E:270:TYR:HB2	2:E:272:TYR:CE2	2.57	0.40
2:E:346:TRP:CH2	2:E:390:LYS:HG3	2.56	0.40
2:Q:36:ASN:O	3:R:71:ARG:CD	2.69	0.40
2:T:42:VAL:HA	2:T:49:ALA:HB1	2.03	0.40
1:G:76:LEU:HD23	1:G:94:ALA:HB1	2.03	0.40
2:K:225:LYS:HA	2:K:225:LYS:HD3	1.91	0.40
2:N:52:ILE:HG22	3:O:61:ARG:HB2	2.03	0.40
2:N:215:LYS:HD2	2:N:248:THR:HG21	2.03	0.40
2:H:14:HIS:CD2	2:H:127:GLU:OE2	2.74	0.40
2:T:37:THR:HG23	2:T:38:ASN:H	1.85	0.40
2:N:374:GLU:HB3	2:N:403:PRO:HG2	2.04	0.40
3:R:4:ARG:NH1	3:R:8:LEU:HD11	2.36	0.40
1:V:173:ARG:HB3	1:V:433:SER:HB2	2.02	0.40
1:D:185:LYS:HA	1:D:186:PRO:HD3	1.90	0.40
1:A:475:ILE:HA	1:A:476:PRO:HD3	1.82	0.40
1:M:155:VAL:O	1:M:211:ARG:HD2	2.20	0.40
2:N:87:ASP:HB3	2:N:133:ASN:OD1	2.21	0.40
2:W:170:LEU:HD12	2:W:223:VAL:HG21	2.04	0.40
1:D:162:VAL:HG21	1:D:219:VAL:HG21	2.04	0.40
2:Q:140:THR:OG1	3:R:90:ARG:HA	2.21	0.40
1:D:337:ALA:HB1	3:F:17:GLU:N	2.36	0.40
2:N:320:LEU:CD2	2:N:326:VAL:HG12	2.51	0.40
1:A:210:GLY:HA3	1:A:216:VAL:HG23	2.03	0.40
1:M:199:PHE:HE2	4:M:905:ASN:HB3	1.87	0.40
2:N:184:LYS:HB2	2:N:191:GLN:OE1	2.21	0.40
1:G:259:GLU:CD	1:G:292:LEU:H	2.24	0.40
2:N:336:HIS:NE2	2:N:370:GLU:HG3	2.36	0.40
1:J:434:ILE:HA	1:J:435:PRO:HD3	1.91	0.40
1:P:111:ILE:H	1:P:111:ILE:HD12	1.85	0.40
1:D:241:TRP:O	1:D:245:VAL:HG22	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:476:PRO:O	1:G:477:LEU:C	2.60	0.40
1:D:340:ARG:NH2	3:F:14:ALA:O	2.54	0.40
2:W:170:LEU:HB3	2:W:220:PHE:CE1	2.57	0.40
2:T:117:LYS:CG	2:T:118:LYS:N	2.84	0.40
1:A:57:LEU:CD1	1:A:110:LEU:HD21	2.51	0.40
1:A:316:ARG:O	1:A:321:ARG:NH2	2.51	0.40
1:A:39:VAL:HG21	1:A:157:VAL:HG11	2.03	0.40
3:L:2:VAL:N	3:L:31:SER:HG	2.19	0.40
1:A:351:ARG:NH1	4:A:901:ASN:O	2.50	0.40
1:J:167:ASP:HA	1:J:171:SER:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/478 (100%)	455 (96%)	20 (4%)	1 (0%)	56	92
1	D	476/478 (100%)	457 (96%)	19 (4%)	0	100	100
1	G	476/478 (100%)	454 (95%)	21 (4%)	1 (0%)	56	92
1	J	476/478 (100%)	458 (96%)	17 (4%)	1 (0%)	56	92
1	M	476/478 (100%)	454 (95%)	22 (5%)	0	100	100
1	P	476/478 (100%)	455 (96%)	21 (4%)	0	100	100
1	S	476/478 (100%)	458 (96%)	18 (4%)	0	100	100
1	V	476/478 (100%)	458 (96%)	18 (4%)	0	100	100
2	B	408/478 (85%)	388 (95%)	19 (5%)	1 (0%)	56	92
2	E	408/478 (85%)	381 (93%)	27 (7%)	0	100	100
2	H	408/478 (85%)	385 (94%)	23 (6%)	0	100	100
2	K	408/478 (85%)	381 (93%)	27 (7%)	0	100	100
2	N	408/478 (85%)	388 (95%)	20 (5%)	0	100	100
2	Q	408/478 (85%)	383 (94%)	24 (6%)	1 (0%)	56	92

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	408/478 (85%)	375 (92%)	32 (8%)	1 (0%)	56	92
2	W	408/478 (85%)	388 (95%)	19 (5%)	1 (0%)	56	92
3	C	89/94 (95%)	82 (92%)	7 (8%)	0	100	100
3	F	89/94 (95%)	84 (94%)	5 (6%)	0	100	100
3	I	89/94 (95%)	80 (90%)	8 (9%)	1 (1%)	21	67
3	L	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	O	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	R	89/94 (95%)	82 (92%)	7 (8%)	0	100	100
3	U	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	X	89/94 (95%)	78 (88%)	10 (11%)	1 (1%)	21	67
All	All	7784/8400 (93%)	7379 (95%)	396 (5%)	9 (0%)	59	93

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	56	GLU
2	B	113	ASN
2	T	216	ASN
2	W	216	ASN
1	J	477	LEU
1	G	225	GLY
3	X	91	VAL
1	A	476	PRO
2	Q	340	PRO

### 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	406/406 (100%)	379 (93%)	27 (7%)	23	64
1	D	406/406 (100%)	381 (94%)	25 (6%)	26	67
1	G	406/406 (100%)	388 (96%)	18 (4%)	39	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	406/406 (100%)	378 (93%)	28 (7%)	22	62
1	M	406/406 (100%)	383 (94%)	23 (6%)	29	71
1	P	406/406 (100%)	372 (92%)	34 (8%)	16	51
1	S	406/406 (100%)	380 (94%)	26 (6%)	25	66
1	V	406/406 (100%)	384 (95%)	22 (5%)	31	74
2	B	364/427 (85%)	342 (94%)	22 (6%)	27	69
2	E	364/427 (85%)	346 (95%)	18 (5%)	35	78
2	H	364/427 (85%)	350 (96%)	14 (4%)	44	85
2	K	364/427 (85%)	346 (95%)	18 (5%)	35	78
2	N	364/427 (85%)	341 (94%)	23 (6%)	25	66
2	Q	364/427 (85%)	344 (94%)	20 (6%)	30	73
2	T	364/427 (85%)	345 (95%)	19 (5%)	32	75
2	W	364/427 (85%)	345 (95%)	19 (5%)	32	75
3	C	86/89 (97%)	82 (95%)	4 (5%)	36	80
3	F	86/89 (97%)	82 (95%)	4 (5%)	36	80
3	I	86/89 (97%)	81 (94%)	5 (6%)	28	71
3	L	86/89 (97%)	81 (94%)	5 (6%)	28	71
3	O	86/89 (97%)	81 (94%)	5 (6%)	28	71
3	R	86/89 (97%)	83 (96%)	3 (4%)	48	87
3	U	86/89 (97%)	81 (94%)	5 (6%)	28	71
3	X	86/89 (97%)	79 (92%)	7 (8%)	17	53
All	All	6848/7376 (93%)	6454 (94%)	394 (6%)	29	71

All (394) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	TYR
1	A	30	ASP
1	A	51	LEU
1	A	57	LEU
1	A	62	LEU
1	A	69	ILE
1	A	88	ILE
1	A	112	VAL
1	A	117	LEU

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Mol	Chain	Res	Type
1	A	151	SER
1	A	158	LEU
1	A	174	GLN
1	A	181	VAL
1	A	190	ARG
1	A	199	PHE
1	A	205	GLN
1	A	224	SER
1	A	228	GLU
1	A	245	VAL
1	A	295	VAL
1	A	299	ILE
1	A	325	ARG
1	A	332	ILE
1	A	356	THR
1	A	417	SER
1	A	434	ILE
1	A	478	THR
2	B	21	THR
2	B	39	VAL
2	B	98	GLU
2	B	103	THR
2	B	113	ASN
2	B	115	GLU
2	B	156	THR
2	B	162	THR
2	B	189	LYS
2	B	200	ILE
2	B	201	ARG
2	B	203	LYS
2	B	205	SER
2	B	207	GLU
2	B	213	GLU
2	B	250	THR
2	B	344	VAL
2	B	360	ILE
2	B	365	SER
2	B	402	THR
2	B	406	ILE
2	B	407	VAL
3	C	38	ASP
3	C	52	ILE

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Mol	Chain	Res	Type
3	C	56	GLU
3	C	70	ASP
1	D	10	LEU
1	D	11	ARG
1	D	15	LYS
1	D	29	TYR
1	D	51	LEU
1	D	57	LEU
1	D	61	GLU
1	D	62	LEU
1	D	88	ILE
1	D	89	LEU
1	D	143	VAL
1	D	164	LEU
1	D	174	GLN
1	D	199	PHE
1	D	240	GLU
1	D	245	VAL
1	D	295	VAL
1	D	325	ARG
1	D	356	THR
1	D	384	LYS
1	D	397	THR
1	D	417	SER
1	D	434	ILE
1	D	458	LEU
1	D	478	THR
2	E	39	VAL
2	E	74	GLU
2	E	98	GLU
2	E	113	ASN
2	E	205	SER
2	E	244	VAL
2	E	250	THR
2	E	273	PHE
2	E	341	LYS
2	E	344	VAL
2	E	352	LEU
2	E	360	ILE
2	E	394	LYS
2	E	402	THR
2	E	403	PRO

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Mol	Chain	Res	Type
2	E	406	ILE
2	E	407	VAL
2	E	412	LEU
3	F	34	LEU
3	F	52	ILE
3	F	61	ARG
3	F	70	ASP
1	G	7	LEU
1	G	10	LEU
1	G	29	TYR
1	G	56	SER
1	G	57	LEU
1	G	59	GLU
1	G	62	LEU
1	G	89	LEU
1	G	115	THR
1	G	117	LEU
1	G	199	PHE
1	G	233	SER
1	G	245	VAL
1	G	279	GLU
1	G	325	ARG
1	G	434	ILE
1	G	477	LEU
1	G	478	THR
2	H	21	THR
2	H	39	VAL
2	H	98	GLU
2	H	115	GLU
2	H	132	LYS
2	H	225	LYS
2	H	282	LYS
2	H	323	HIS
2	H	344	VAL
2	H	352	LEU
2	H	391	GLU
2	H	395	GLU
2	H	402	THR
2	H	412	LEU
3	I	5	GLU
3	I	34	LEU
3	I	38	ASP

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Mol	Chain	Res	Type
3	I	52	ILE
3	I	81	ARG
1	J	8	SER
1	J	10	LEU
1	J	29	TYR
1	J	31	ARG
1	J	51	LEU
1	J	56	SER
1	J	57	LEU
1	J	62	LEU
1	J	89	LEU
1	J	112	VAL
1	J	115	THR
1	J	140	LEU
1	J	151	SER
1	J	174	GLN
1	J	199	PHE
1	J	214	GLU
1	J	233	SER
1	J	240	GLU
1	J	245	VAL
1	J	246	LYS
1	J	271	GLU
1	J	279	GLU
1	J	295	VAL
1	J	325	ARG
1	J	356	THR
1	J	376	ARG
1	J	434	ILE
1	J	458	LEU
2	K	21	THR
2	K	39	VAL
2	K	98	GLU
2	K	103	THR
2	K	106	TRP
2	K	109	LEU
2	K	113	ASN
2	K	115	GLU
2	K	116	LYS
2	K	132	LYS
2	K	134	ILE
2	K	207	GLU

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Mol	Chain	Res	Type
2	K	216	ASN
2	K	223	VAL
2	K	273	PHE
2	K	344	VAL
2	K	360	ILE
2	K	412	LEU
3	L	34	LEU
3	L	52	ILE
3	L	70	ASP
3	L	81	ARG
3	L	92	VAL
1	M	10	LEU
1	M	29	TYR
1	M	51	LEU
1	M	57	LEU
1	M	58	LYS
1	M	62	LEU
1	M	76	LEU
1	M	78	GLU
1	M	89	LEU
1	M	112	VAL
1	M	115	THR
1	M	174	GLN
1	M	199	PHE
1	M	245	VAL
1	M	279	GLU
1	M	325	ARG
1	M	328	GLU
1	M	356	THR
1	M	417	SER
1	M	434	ILE
1	M	458	LEU
1	M	477	LEU
1	M	478	THR
2	N	4	LYS
2	N	21	THR
2	N	39	VAL
2	N	95	SER
2	N	98	GLU
2	N	103	THR
2	N	113	ASN
2	N	115	GLU

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Mol	Chain	Res	Type
2	N	116	LYS
2	N	134	ILE
2	N	164	GLU
2	N	250	THR
2	N	255	THR
2	N	261	MET
2	N	302	ARG
2	N	344	VAL
2	N	360	ILE
2	N	387	LYS
2	N	391	GLU
2	N	395	GLU
2	N	402	THR
2	N	407	VAL
2	N	412	LEU
3	O	34	LEU
3	O	38	ASP
3	O	52	ILE
3	O	53	GLN
3	O	81	ARG
1	P	10	LEU
1	P	29	TYR
1	P	31	ARG
1	P	51	LEU
1	P	56	SER
1	P	57	LEU
1	P	59	GLU
1	P	62	LEU
1	P	78	GLU
1	P	88	ILE
1	P	89	LEU
1	P	115	THR
1	P	143	VAL
1	P	162	VAL
1	P	164	LEU
1	P	174	GLN
1	P	181	VAL
1	P	190	ARG
1	P	199	PHE
1	P	231	SER
1	P	233	SER
1	P	240	GLU

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Mol	Chain	Res	Type
1	P	245	VAL
1	P	279	GLU
1	P	291	SER
1	P	295	VAL
1	P	325	ARG
1	P	328	GLU
1	P	356	THR
1	P	376	ARG
1	P	434	ILE
1	P	458	LEU
1	P	477	LEU
1	P	478	THR
2	Q	21	THR
2	Q	39	VAL
2	Q	98	GLU
2	Q	103	THR
2	Q	109	LEU
2	Q	123	ARG
2	Q	188	GLU
2	Q	207	GLU
2	Q	210	THR
2	Q	216	ASN
2	Q	245	VAL
2	Q	255	THR
2	Q	273	PHE
2	Q	282	LYS
2	Q	313	SER
2	Q	344	VAL
2	Q	352	LEU
2	Q	360	ILE
2	Q	402	THR
2	Q	405	GLN
3	R	34	LEU
3	R	52	ILE
3	R	81	ARG
1	S	10	LEU
1	S	11	ARG
1	S	29	TYR
1	S	51	LEU
1	S	56	SER
1	S	57	LEU
1	S	62	LEU

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Mol	Chain	Res	Type
1	S	69	ILE
1	S	89	LEU
1	S	114	LYS
1	S	140	LEU
1	S	154	SER
1	S	181	VAL
1	S	199	PHE
1	S	228	GLU
1	S	242	SER
1	S	245	VAL
1	S	295	VAL
1	S	325	ARG
1	S	376	ARG
1	S	389	VAL
1	S	397	THR
1	S	409	GLU
1	S	458	LEU
1	S	464	LEU
1	S	477	LEU
2	T	74	GLU
2	T	98	GLU
2	T	103	THR
2	T	113	ASN
2	T	115	GLU
2	T	123	ARG
2	T	135	HIS
2	T	162	THR
2	T	189	LYS
2	T	216	ASN
2	T	250	THR
2	T	273	PHE
2	T	341	LYS
2	T	344	VAL
2	T	387	LYS
2	T	394	LYS
2	T	402	THR
2	T	406	ILE
2	T	412	LEU
3	U	5	GLU
3	U	34	LEU
3	U	56	GLU
3	U	70	ASP

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Mol	Chain	Res	Type
3	U	81	ARG
1	V	11	ARG
1	V	19	VAL
1	V	29	TYR
1	V	57	LEU
1	V	62	LEU
1	V	89	LEU
1	V	115	THR
1	V	117	LEU
1	V	143	VAL
1	V	151	SER
1	V	174	GLN
1	V	190	ARG
1	V	199	PHE
1	V	224	SER
1	V	233	SER
1	V	245	VAL
1	V	279	GLU
1	V	295	VAL
1	V	354	LEU
1	V	376	ARG
1	V	417	SER
1	V	478	THR
2	W	21	THR
2	W	39	VAL
2	W	46	MET
2	W	98	GLU
2	W	109	LEU
2	W	117	LYS
2	W	123	ARG
2	W	134	ILE
2	W	200	ILE
2	W	201	ARG
2	W	205	SER
2	W	244	VAL
2	W	250	THR
2	W	344	VAL
2	W	352	LEU
2	W	360	ILE
2	W	364	GLU
2	W	402	THR
2	W	406	ILE

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Mol	Chain	Res	Type
3	X	38	ASP
3	X	52	ILE
3	X	54	GLU
3	X	56	GLU
3	X	81	ARG
3	X	91	VAL
3	X	92	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	216	ASN
2	E	216	ASN
3	F	27	GLN
2	H	135	HIS
2	K	216	ASN
2	K	322	ASN
2	N	216	ASN
2	N	323	HIS
3	O	53	GLN
1	P	174	GLN
2	Q	216	ASN
2	T	216	ASN
2	W	216	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 42 ligands modelled in this entry, 24 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ASN	A	901	1	7,7,8	7.42	3 (42%)	6,8,10	1.85	2 (33%)
6	ADP	B	479	-	29,29,29	1.26	4 (13%)	45,45,45	2.01	11 (24%)
4	ASN	D	902	1	7,7,8	5.94	3 (42%)	6,8,10	2.63	2 (33%)
8	ATP	E	479	-	33,33,33	1.09	2 (6%)	52,52,52	1.76	7 (13%)
4	ASN	G	903	1	7,7,8	6.99	3 (42%)	6,8,10	2.37	2 (33%)
8	ATP	H	479	-	33,33,33	1.17	3 (9%)	52,52,52	1.86	10 (19%)
9	ASP	H	482	7	8,8,8	0.92	0	10,10,10	2.02	2 (20%)
4	ASN	J	904	1	7,7,8	7.59	2 (28%)	6,8,10	2.89	3 (50%)
8	ATP	K	479	-	33,33,33	1.16	3 (9%)	52,52,52	1.80	8 (15%)
4	ASN	M	905	1	7,7,8	6.95	3 (42%)	6,8,10	2.63	3 (50%)
8	ATP	N	479	-	33,33,33	1.20	2 (6%)	52,52,52	1.78	11 (21%)
9	ASP	N	482	-	8,8,8	1.21	0	10,10,10	1.15	1 (10%)
4	ASN	P	906	1	7,7,8	6.89	2 (28%)	6,8,10	1.62	2 (33%)
8	ATP	Q	479	-	33,33,33	1.22	3 (9%)	52,52,52	2.25	10 (19%)
4	ASN	S	907	1	7,7,8	6.17	2 (28%)	6,8,10	1.84	2 (33%)
6	ADP	T	479	-	29,29,29	1.16	2 (6%)	45,45,45	1.83	8 (17%)
4	ASN	V	908	1	7,7,8	6.83	3 (42%)	6,8,10	1.80	2 (33%)
8	ATP	W	479	-	33,33,33	1.34	4 (12%)	52,52,52	2.34	17 (32%)

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	ASN	A	901	1	-	0/6/7/8	0/0/0/0
6	ADP	B	479	-	-	0/16/32/32	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ASN	D	902	1	-	0/6/7/8	0/0/0/0
8	ATP	E	479	-	-	0/22/38/38	0/1/3/3
4	ASN	G	903	1	-	0/6/7/8	0/0/0/0
8	ATP	H	479	-	-	0/22/38/38	0/1/3/3
9	ASP	H	482	7	-	0/8/8/8	0/0/0/0
4	ASN	J	904	1	-	0/6/7/8	0/0/0/0
8	ATP	K	479	-	-	0/22/38/38	0/1/3/3
4	ASN	M	905	1	-	0/6/7/8	0/0/0/0
8	ATP	N	479	-	-	0/22/38/38	0/1/3/3
9	ASP	N	482	-	-	0/8/8/8	0/0/0/0
4	ASN	P	906	1	-	0/6/7/8	0/0/0/0
8	ATP	Q	479	-	-	0/22/38/38	0/1/3/3
4	ASN	S	907	1	-	0/6/7/8	0/0/0/0
6	ADP	T	479	-	-	0/16/32/32	0/1/3/3
4	ASN	V	908	1	-	0/6/7/8	0/0/0/0
8	ATP	W	479	-	-	0/22/38/38	0/1/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	904	ASN	OD1-CG	19.73	1.25	1.11
4	A	901	ASN	OD1-CG	19.15	1.24	1.11
4	G	903	ASN	OD1-CG	18.11	1.23	1.11
4	M	905	ASN	OD1-CG	18.00	1.23	1.11
4	P	906	ASN	OD1-CG	17.85	1.23	1.11
4	V	908	ASN	OD1-CG	17.69	1.23	1.11
4	S	907	ASN	OD1-CG	16.07	1.22	1.11
4	D	902	ASN	OD1-CG	15.26	1.21	1.11
6	B	479	ADP	C4-N9	-3.80	1.32	1.37
8	N	479	ATP	C4-N9	-3.77	1.32	1.37
8	Q	479	ATP	C4-N9	-3.35	1.32	1.37
8	K	479	ATP	C4-N9	-3.34	1.32	1.37
6	T	479	ADP	C4-N9	-3.32	1.32	1.37
8	W	479	ATP	C2'-C1'	-3.30	1.48	1.53
8	N	479	ATP	C5-C4	3.26	1.47	1.40
4	A	901	ASN	CB-CA	-3.26	1.50	1.54
8	Q	479	ATP	C2'-C1'	-3.14	1.49	1.53
8	W	479	ATP	C4-N9	-3.01	1.33	1.37
4	M	905	ASN	CB-CA	-2.99	1.51	1.54
8	H	479	ATP	C4-N9	-2.95	1.33	1.37
8	H	479	ATP	C5-C4	2.91	1.47	1.40
4	P	906	ASN	CB-CA	-2.91	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	479	ATP	C4-N9	-2.84	1.33	1.37
8	K	479	ATP	C5-C4	2.83	1.46	1.40
4	J	904	ASN	CB-CA	-2.71	1.51	1.54
6	T	479	ADP	C5-C4	2.60	1.46	1.40
8	E	479	ATP	C5-C4	2.58	1.46	1.40
6	B	479	ADP	C5-C4	2.54	1.46	1.40
8	W	479	ATP	C5-C4	2.52	1.46	1.40
4	D	902	ASN	CB-CA	2.52	1.57	1.54
4	V	908	ASN	CB-CA	-2.51	1.51	1.54
8	Q	479	ATP	C5-C4	2.47	1.46	1.40
4	G	903	ASN	OXT-C	-2.44	1.21	1.30
4	A	901	ASN	OXT-C	-2.42	1.21	1.30
4	V	908	ASN	OXT-C	-2.42	1.21	1.30
4	S	907	ASN	OXT-C	-2.40	1.21	1.30
6	B	479	ADP	C2'-C1'	-2.40	1.50	1.53
4	G	903	ASN	CB-CA	-2.39	1.51	1.54
4	D	902	ASN	OXT-C	-2.27	1.22	1.30
4	M	905	ASN	OXT-C	-2.16	1.22	1.30
8	H	479	ATP	PA-O3A	2.16	1.63	1.59
8	W	479	ATP	O4'-C1'	2.10	1.44	1.41
6	B	479	ADP	C8-N9	-2.05	1.33	1.36
8	K	479	ATP	C2'-C1'	-2.04	1.50	1.53

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Q	479	ATP	O4'-C1'-N9	8.46	116.31	108.44
8	Q	479	ATP	N3-C2-N1	-8.01	122.01	128.71
8	K	479	ATP	N3-C2-N1	-6.65	123.15	128.71
8	E	479	ATP	N3-C2-N1	-6.15	123.56	128.71
8	H	479	ATP	N3-C2-N1	-6.00	123.69	128.71
6	T	479	ADP	N3-C2-N1	-5.97	123.72	128.71
8	W	479	ATP	N3-C4-N9	5.81	135.93	125.43
6	B	479	ADP	N3-C2-N1	-5.79	123.87	128.71
8	E	479	ATP	N3-C4-N9	5.60	135.54	125.43
8	N	479	ATP	N3-C2-N1	-5.56	124.06	128.71
8	W	479	ATP	N3-C2-N1	-5.51	124.10	128.71
6	T	479	ADP	N3-C4-N9	5.20	134.81	125.43
6	B	479	ADP	N3-C4-N9	5.16	134.76	125.43
8	Q	479	ATP	N3-C4-N9	5.15	134.73	125.43
8	W	479	ATP	O3A-PB-O3B	-5.11	91.27	101.66
8	W	479	ATP	O4'-C1'-N9	4.96	113.06	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	905	ASN	C-CA-N	4.96	117.58	109.36
8	H	479	ATP	N3-C4-N9	4.85	134.19	125.43
8	Q	479	ATP	PA-O3A-PB	-4.80	117.60	131.68
8	N	479	ATP	N3-C4-N9	4.78	134.07	125.43
8	K	479	ATP	PA-O3A-PB	-4.78	117.68	131.68
8	K	479	ATP	N3-C4-N9	4.78	134.06	125.43
8	W	479	ATP	PA-O3A-PB	-4.70	117.90	131.68
4	J	904	ASN	OXT-C-O	-4.54	113.81	124.07
8	H	479	ATP	PB-O3B-PG	-4.53	118.41	131.68
8	E	479	ATP	C4-C5-N7	-4.47	105.69	109.52
6	B	479	ADP	PA-O3A-PB	-4.40	118.79	131.68
8	W	479	ATP	O3'-C3'-C4'	-4.29	98.44	111.08
6	B	479	ADP	C4-C5-N7	-4.18	105.95	109.52
4	J	904	ASN	C-CA-N	4.10	116.16	109.36
8	N	479	ATP	O4'-C1'-N9	4.06	112.21	108.44
6	T	479	ADP	C4-C5-N7	-4.05	106.05	109.52
8	W	479	ATP	C4-C5-N7	-4.03	106.07	109.52
4	D	902	ASN	C-CA-N	-3.98	102.77	109.36
4	D	902	ASN	OXT-C-O	-3.97	115.10	124.07
9	H	482	ASP	C-CA-N	3.86	115.75	109.36
8	W	479	ATP	C5-C4-N3	-3.86	117.31	125.70
8	E	479	ATP	C5-C4-N3	-3.83	117.37	125.70
9	H	482	ASP	OXT-C-O	-3.70	115.69	124.07
4	G	903	ASN	OXT-C-O	-3.66	115.80	124.07
8	K	479	ATP	PB-O3B-PG	-3.61	121.09	131.68
8	W	479	ATP	O2'-C2'-C1'	-3.58	100.40	111.23
4	G	903	ASN	C-CA-N	3.58	115.29	109.36
6	B	479	ADP	C8-N9-C4	3.57	109.63	106.90
4	S	907	ASN	OXT-C-O	-3.54	116.06	124.07
4	A	901	ASN	OXT-C-O	-3.49	116.17	124.07
4	V	908	ASN	OXT-C-O	-3.47	116.22	124.07
6	T	479	ADP	C5-C4-N3	-3.46	118.17	125.70
8	H	479	ATP	O3G-PG-O2G	3.35	120.64	107.61
8	W	479	ATP	O3'-C3'-C2'	-3.32	101.02	111.83
8	H	479	ATP	C5-C4-N3	-3.24	118.65	125.70
8	K	479	ATP	C5-C4-N3	-3.17	118.79	125.70
8	Q	479	ATP	C5-C4-N3	-3.17	118.80	125.70
6	T	479	ADP	PA-O3A-PB	-3.17	122.40	131.68
8	H	479	ATP	C4'-O4'-C1'	3.11	113.13	109.75
8	H	479	ATP	PA-O3A-PB	-3.10	122.59	131.68
8	K	479	ATP	C4-C5-N7	-3.03	106.92	109.52
8	N	479	ATP	PA-O3A-PB	-3.03	122.79	131.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	479	ADP	C5-C4-N3	-3.02	119.12	125.70
4	M	905	ASN	OXT-C-O	-2.94	117.42	124.07
8	Q	479	ATP	C2-N3-C4	2.89	122.23	114.01
8	W	479	ATP	O3G-PG-O1G	2.88	119.85	110.44
9	N	482	ASP	OXT-C-O	-2.86	117.61	124.07
4	J	904	ASN	OXT-C-CA	2.84	123.25	116.88
4	P	906	ASN	OXT-C-O	-2.83	117.67	124.07
8	N	479	ATP	PB-O3B-PG	-2.82	123.42	131.68
8	H	479	ATP	C4-C5-N7	-2.80	107.12	109.52
8	Q	479	ATP	PB-O3B-PG	-2.81	123.46	131.68
8	N	479	ATP	C5-C4-N3	-2.77	119.67	125.70
8	W	479	ATP	O3G-PG-O3B	-2.72	92.23	105.14
8	E	479	ATP	C2-N3-C4	2.71	121.73	114.01
8	W	479	ATP	C2-N3-C4	2.71	121.72	114.01
8	E	479	ATP	PB-O3B-PG	-2.65	123.92	131.68
8	W	479	ATP	C2'-C3'-C4'	2.60	107.83	102.65
8	N	479	ATP	C4-C5-N7	-2.57	107.32	109.52
8	H	479	ATP	C3'-C2'-C1'	2.55	104.89	100.91
4	A	901	ASN	O-C-CA	2.54	125.70	118.36
8	N	479	ATP	O3'-C3'-C4'	-2.51	103.69	111.08
6	T	479	ADP	C2-N3-C4	2.49	121.10	114.01
8	K	479	ATP	C2-N3-C4	2.46	121.01	114.01
8	N	479	ATP	O4'-C1'-C2'	-2.44	103.03	106.77
8	H	479	ATP	C2-N3-C4	2.41	120.87	114.01
8	W	479	ATP	C4'-O4'-C1'	2.36	112.32	109.75
4	M	905	ASN	OXT-C-CA	2.36	122.17	116.88
6	B	479	ADP	O3'-C3'-C4'	-2.32	104.25	111.08
8	N	479	ATP	C1'-N9-C4	-2.27	122.70	126.64
8	K	479	ATP	C2'-C3'-C4'	2.26	107.15	102.65
6	B	479	ADP	O4'-C1'-C2'	-2.23	103.35	106.77
6	B	479	ADP	C2-N3-C4	2.23	120.34	114.01
8	Q	479	ATP	C4'-O4'-C1'	2.20	112.13	109.75
4	S	907	ASN	O-C-CA	2.19	124.68	118.36
8	W	479	ATP	O3G-PG-O2G	2.18	116.11	107.61
6	B	479	ADP	O3'-C3'-C2'	-2.18	104.75	111.83
6	B	479	ADP	O3B-PB-O2B	2.15	115.97	107.61
6	T	479	ADP	C5'-C4'-C3'	-2.14	106.63	115.21
8	Q	479	ATP	C4-C5-N7	-2.12	107.71	109.52
4	V	908	ASN	O-C-CA	2.11	124.46	118.36
6	T	479	ADP	O3B-PB-O2B	2.08	115.71	107.61
8	N	479	ATP	C2-N3-C4	2.08	119.92	114.01
4	P	906	ASN	OXT-C-CA	2.05	121.47	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	479	ATP	O3G-PG-O2G	2.04	115.54	107.61
8	W	479	ATP	O2B-PB-O1B	2.02	123.49	112.21
8	Q	479	ATP	C2'-C1'-N9	-2.01	108.11	113.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	478/478 (100%)	-0.18	0 100 100	23, 53, 79, 88	0
1	D	478/478 (100%)	-0.19	0 100 100	23, 53, 79, 88	0
1	G	478/478 (100%)	-0.20	0 100 100	23, 53, 78, 88	0
1	J	478/478 (100%)	-0.19	1 (0%) 93 54	23, 53, 78, 88	0
1	M	478/478 (100%)	-0.20	0 100 100	23, 53, 79, 88	0
1	P	478/478 (100%)	-0.19	0 100 100	23, 53, 78, 88	0
1	S	478/478 (100%)	-0.19	0 100 100	23, 53, 79, 88	0
1	V	478/478 (100%)	-0.19	0 100 100	23, 53, 79, 88	0
2	B	410/478 (85%)	-0.17	0 100 100	31, 63, 93, 112	0
2	E	410/478 (85%)	-0.13	1 (0%) 93 54	31, 63, 94, 112	0
2	H	410/478 (85%)	-0.14	2 (0%) 88 36	31, 63, 93, 112	0
2	K	410/478 (85%)	-0.15	2 (0%) 88 36	31, 63, 93, 112	0
2	N	410/478 (85%)	-0.16	1 (0%) 93 54	31, 63, 93, 112	0
2	Q	410/478 (85%)	-0.15	1 (0%) 93 54	31, 63, 93, 112	0
2	T	410/478 (85%)	-0.13	2 (0%) 88 36	31, 63, 93, 112	0
2	W	410/478 (85%)	-0.14	2 (0%) 88 36	31, 63, 93, 112	0
3	C	91/94 (96%)	-0.17	0 100 100	25, 60, 72, 76	0
3	F	91/94 (96%)	-0.18	0 100 100	25, 60, 72, 76	0
3	I	91/94 (96%)	-0.19	0 100 100	25, 59, 72, 76	0
3	L	91/94 (96%)	-0.18	0 100 100	25, 59, 71, 76	0
3	O	91/94 (96%)	-0.19	0 100 100	25, 59, 71, 76	0
3	R	91/94 (96%)	-0.13	0 100 100	25, 59, 71, 76	0
3	U	91/94 (96%)	-0.17	0 100 100	25, 60, 72, 76	0
3	X	91/94 (96%)	-0.18	0 100 100	25, 59, 72, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
All	All	7832/8400 (93%)	-0.17	12 (0%)	93 54	23, 56, 88, 112	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	262	ARG	3.6
2	H	262	ARG	3.2
2	N	262	ARG	2.9
1	J	18	GLU	2.6
2	T	265	GLU	2.6
2	W	266	GLU	2.4
2	H	265	GLU	2.4
2	Q	408	GLU	2.3
2	T	264	LYS	2.3
2	K	262	ARG	2.3
2	W	264	LYS	2.2
2	K	408	GLU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	ASN	M	905	8/9	0.36	5.52	31,31,32,32	8
4	ASN	A	901	8/9	0.49	5.06	31,32,34,35	8
4	ASN	P	906	8/9	0.35	4.66	28,28,29,29	8

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ASN	V	908	8/9	0.39	4.47	28,29,29,30	8
5	ZN	B	901	1/1	0.24	4.00	57,57,57,57	0
7	MN	T	481	1/1	0.23	3.63	75,75,75,75	0
7	MN	E	481	1/1	0.30	3.50	85,85,85,85	1
7	MN	N	481	1/1	0.28	3.48	86,86,86,86	1
4	ASN	G	903	8/9	0.39	3.04	27,29,30,31	8
8	ATP	N	479	31/31	0.32	2.82	35,39,66,66	31
8	ATP	Q	479	31/31	0.38	2.58	30,37,49,50	31
8	ATP	K	479	31/31	0.35	2.53	24,35,57,58	31
7	MN	W	481	1/1	0.29	2.38	82,82,82,82	1
6	ADP	B	479	27/27	0.30	2.28	70,71,82,82	27
8	ATP	E	479	31/31	0.35	2.07	34,40,85,85	31
4	ASN	S	907	8/9	0.24	2.01	53,53,55,57	0
8	ATP	H	479	31/31	0.31	1.41	21,28,49,51	31
4	ASN	D	902	8/9	0.20	1.37	62,62,62,62	0
4	ASN	J	904	8/9	0.23	1.17	52,53,54,54	0
7	MN	K	481	1/1	0.29	1.07	63,63,63,63	1
6	ADP	T	479	27/27	0.30	1.05	75,76,87,88	27
8	ATP	W	479	31/31	0.30	1.05	14,21,28,32	31
5	ZN	E	902	1/1	0.20	0.79	59,59,59,59	0
7	MN	B	480	1/1	0.22	0.71	44,44,44,44	0
5	ZN	N	905	1/1	0.20	0.66	53,53,53,53	0
5	ZN	Q	906	1/1	0.21	0.53	51,51,51,51	0
9	ASP	N	482	9/9	0.19	0.47	71,79,81,82	0
5	ZN	K	904	1/1	0.21	0.45	50,50,50,50	0
5	ZN	W	908	1/1	0.21	0.40	55,55,55,55	0
5	ZN	T	907	1/1	0.18	0.24	55,55,55,55	0
7	MN	H	481	1/1	0.24	0.12	75,75,75,75	1
9	ASP	H	482	9/9	0.20	0.01	71,79,81,82	0
7	MN	Q	481	1/1	0.23	0.00	64,64,64,64	1
5	ZN	H	903	1/1	0.18	-0.10	53,53,53,53	0
7	MN	W	480	1/1	0.17	-0.48	52,52,52,52	0
7	MN	H	480	1/1	0.15	-1.28	50,50,50,50	0
7	MN	Q	480	1/1	0.17	-1.83	51,51,51,51	0
7	MN	K	480	1/1	0.15	-2.10	45,45,45,45	0
7	MN	T	480	1/1	0.07	-3.29	55,55,55,55	0
7	MN	B	481	1/1	0.13	-3.42	56,56,56,56	1
7	MN	N	480	1/1	0.13	-3.46	49,49,49,49	0
7	MN	E	480	1/1	0.12	-4.42	53,53,53,53	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.