Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 01:51 PM EDT

PDB ID	:	3H0M
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	:	2009-04-09
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

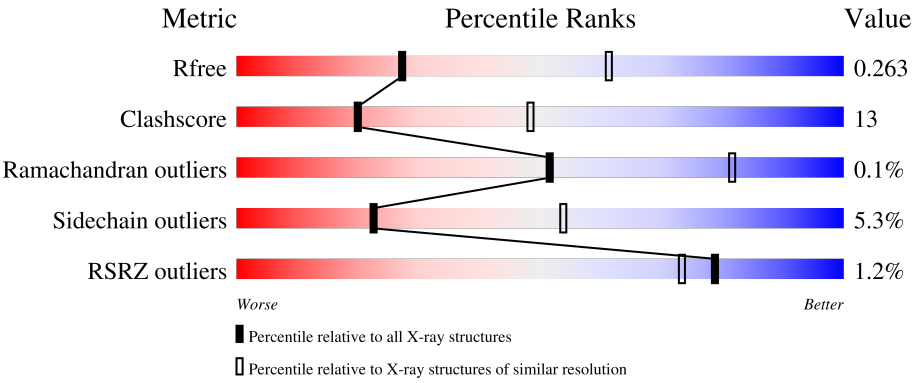
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	478	71% 26%
1	D	478	72% 26%
1	G	478	76% 23%
1	J	478	73% 24%
1	M	478	76% 22%

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Mol	Chain	Length	Quality of chain
1	P	478	71% 26%
1	S	478	72% 25%
1	V	478	71% 26%
2	B	478	66% 17% 14%
2	E	478	64% 21% 14%
2	H	478	64% 20% 14%
2	K	478	64% 19% 14%
2	N	478	63% 20% 14%
2	Q	478	67% 15% 14%
2	T	478	65% 19% 14%
2	W	478	65% 18% 14%
3	C	94	69% 27%
3	F	94	73% 21%
3	I	94	73% 22%
3	L	94	77% 19%
3	O	94	76% 20%
3	R	94	81% 14%
3	U	94	71% 23%
3	X	94	72% 22%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GLN	A	901	-	-	X	-
4	GLN	G	903	-	-	X	-
4	GLN	J	904	-	-	X	-
4	GLN	M	905	-	-	X	-
4	GLN	P	906	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GLN	V	908	-	-	X	-
5	MG	W	479	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 62935 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 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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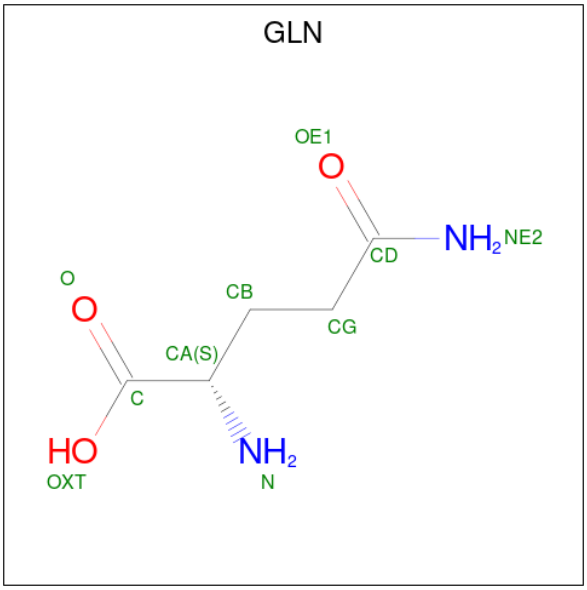
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	W	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			

- 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 GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 9 5 1 3	0	0
4	D	1	Total C N O 9 5 1 3	0	0
4	G	1	Total C N O 9 5 1 3	0	0
4	J	1	Total C N O 9 5 1 3	0	0
4	M	1	Total C N O 9 5 1 3	0	0
4	P	1	Total C N O 9 5 1 3	0	0
4	S	1	Total C N O 9 5 1 3	0	0
4	V	1	Total C N O 9 5 1 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Zn 1 1	0	0
6	E	1	Total Zn 1 1	0	0
6	H	1	Total Zn 1 1	0	0

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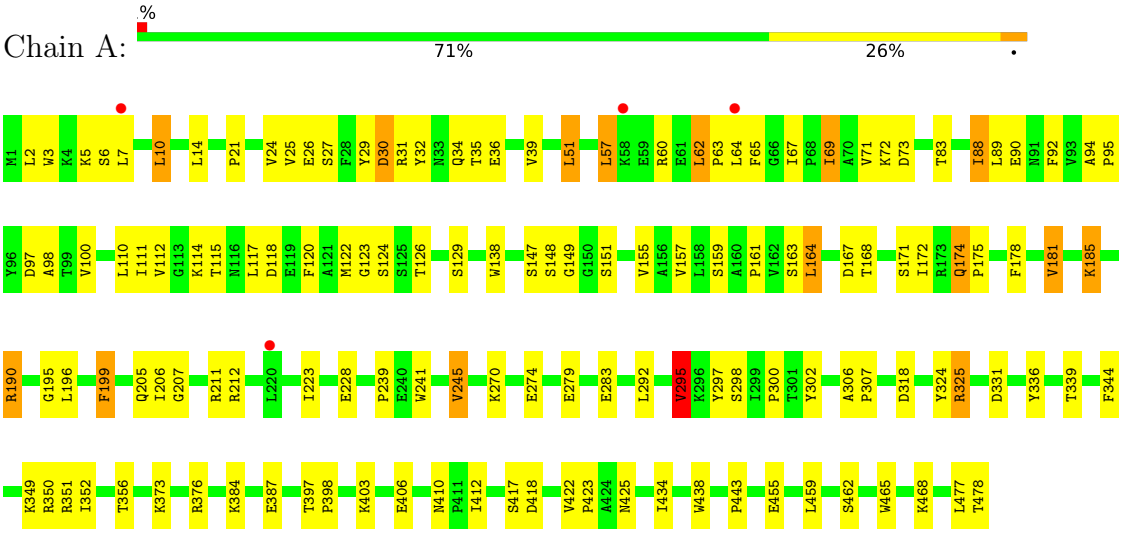
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	K	1	Total Zn 1 1	0	0
6	N	1	Total Zn 1 1	0	0
6	Q	1	Total Zn 1 1	0	0
6	T	1	Total Zn 1 1	0	0
6	W	1	Total Zn 1 1	0	0

3 Residue-property plots (i)

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

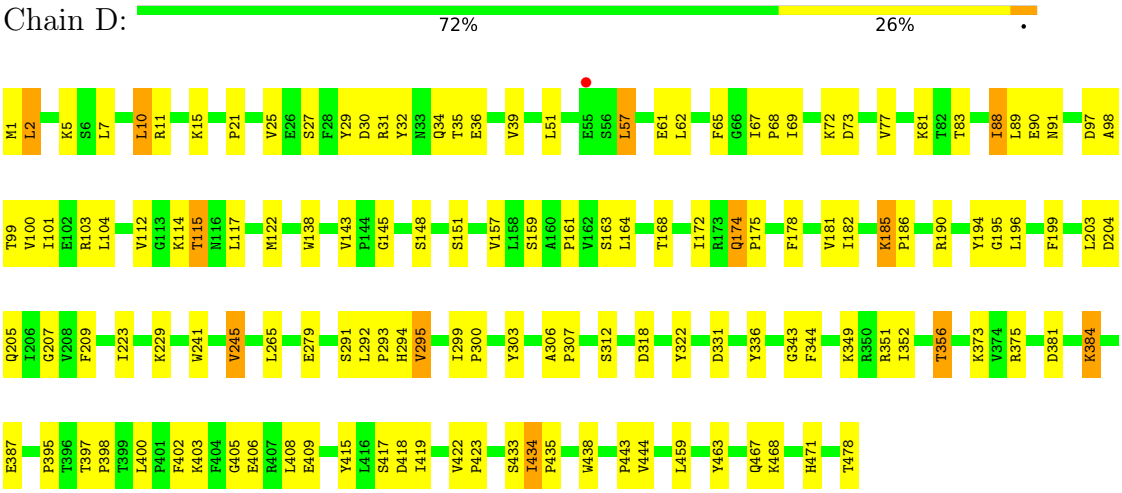
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain A:



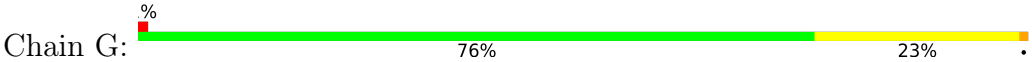
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

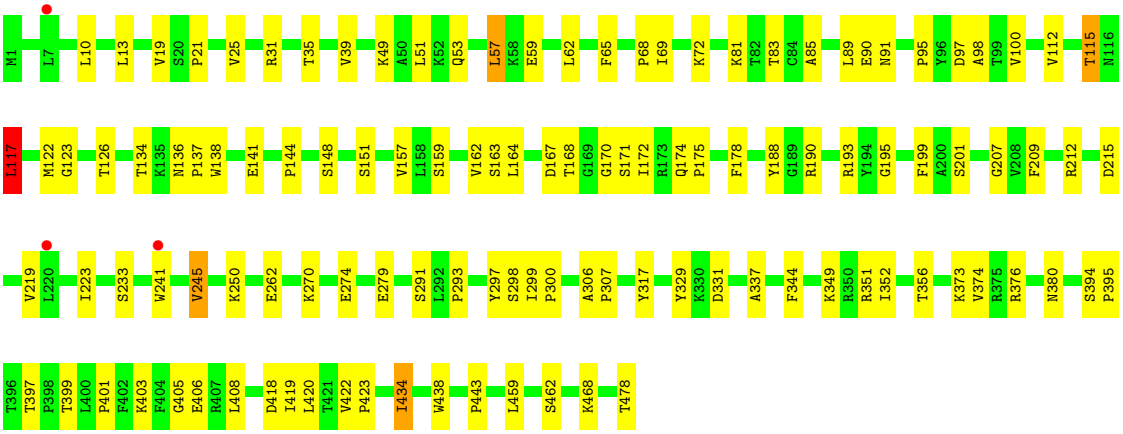
Chain D:



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

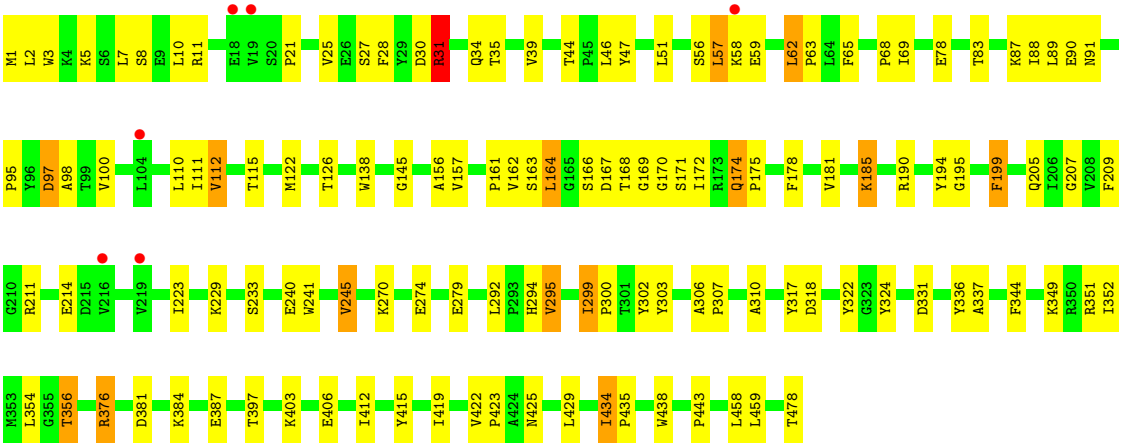
Chain G:





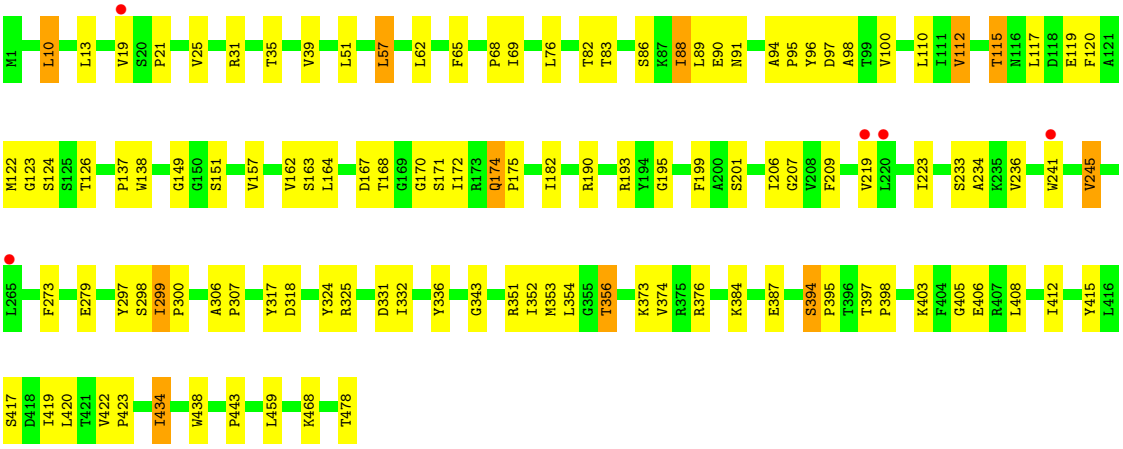
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain J:



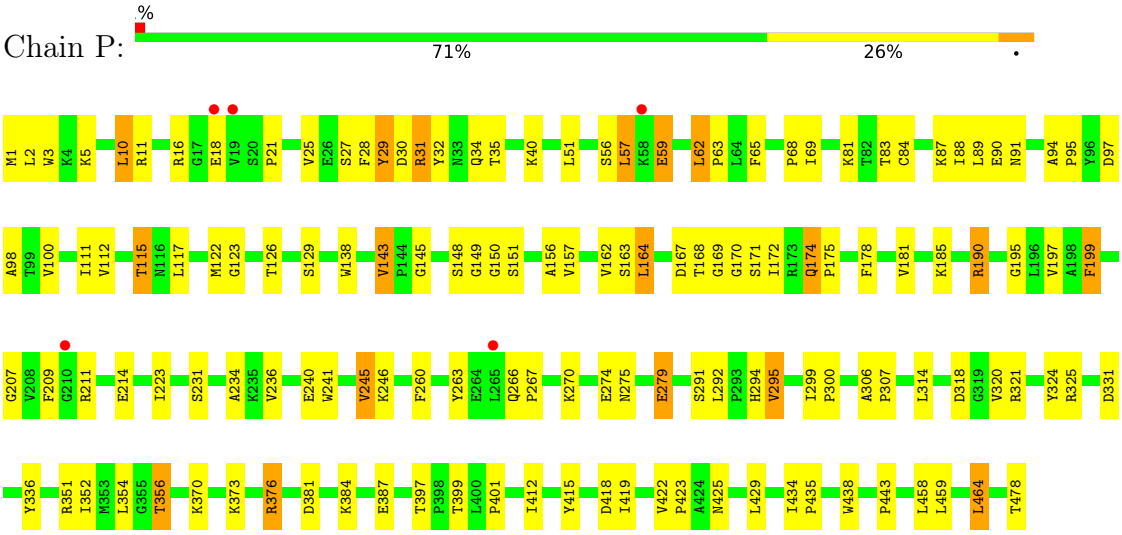
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain M:



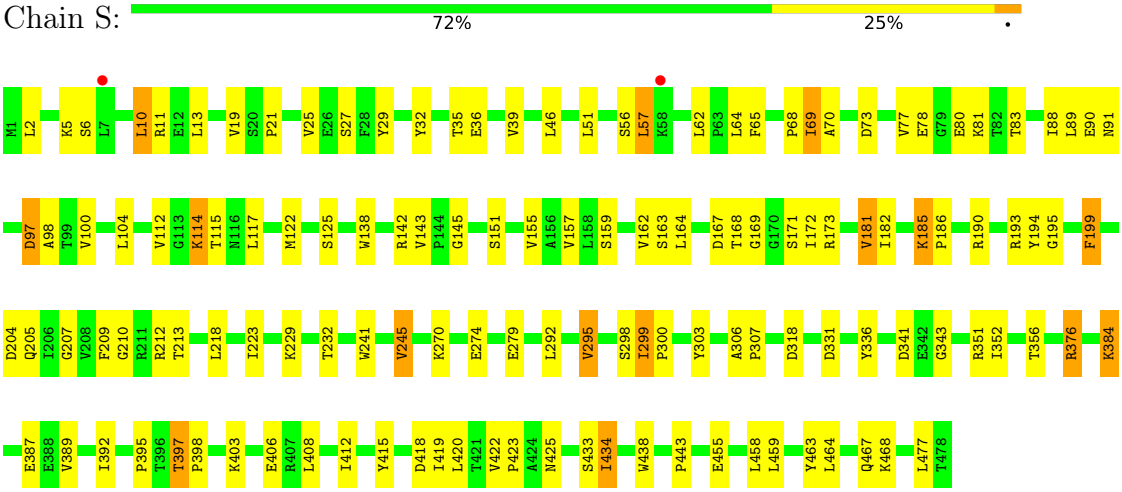
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain P:



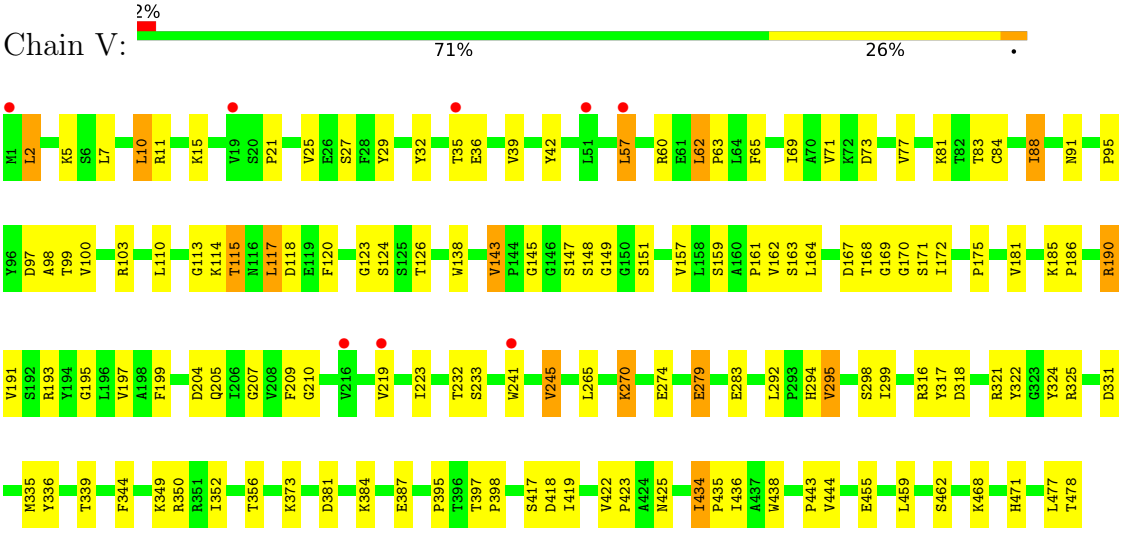
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain S:



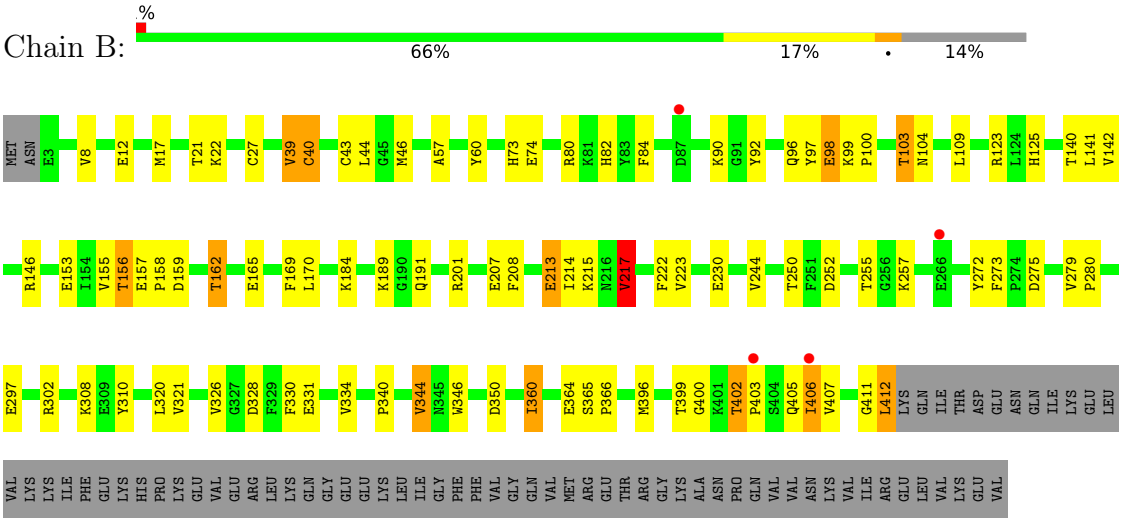
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain V:



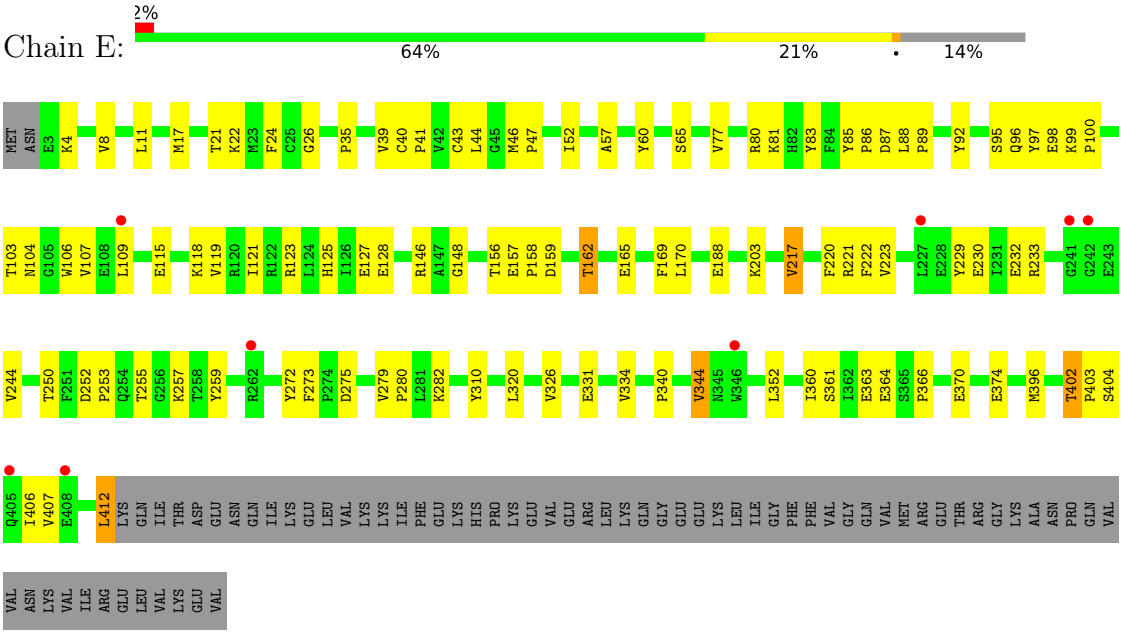
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain B:



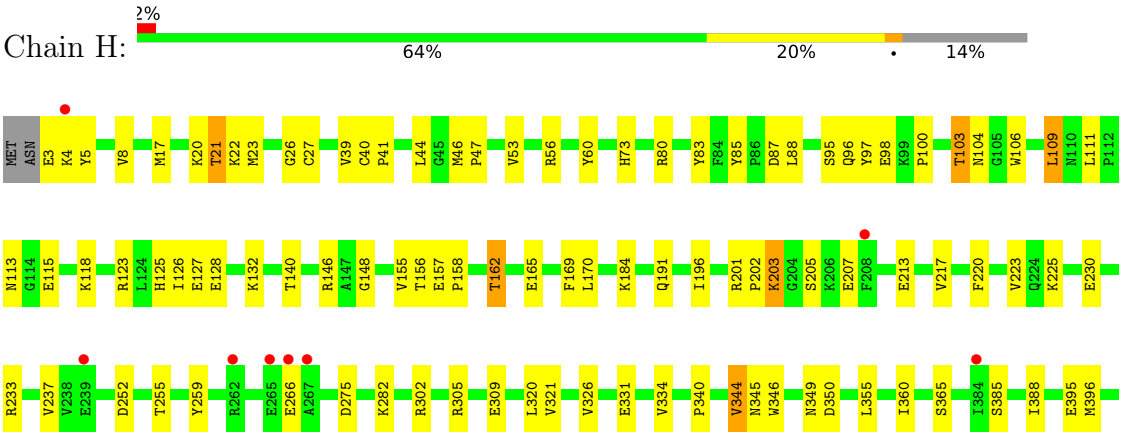
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

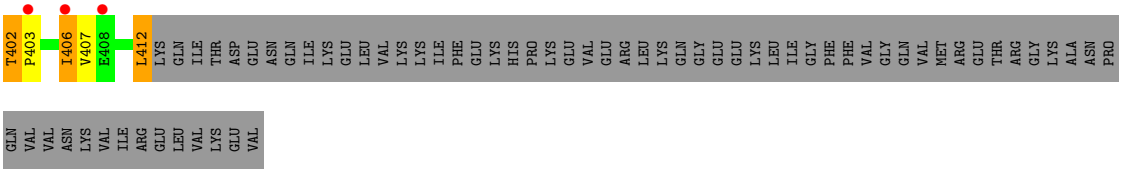
Chain E:



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

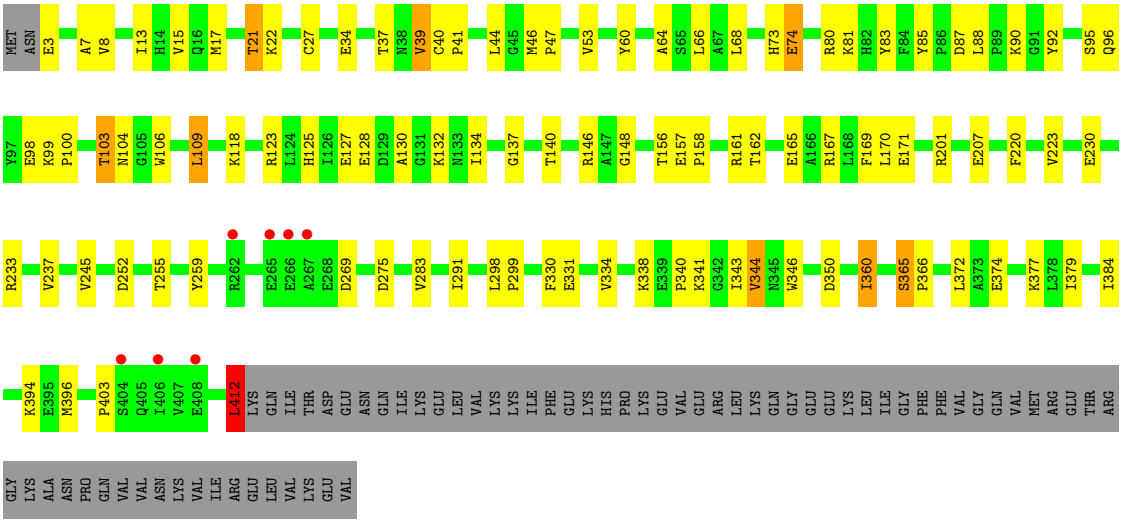
Chain H:





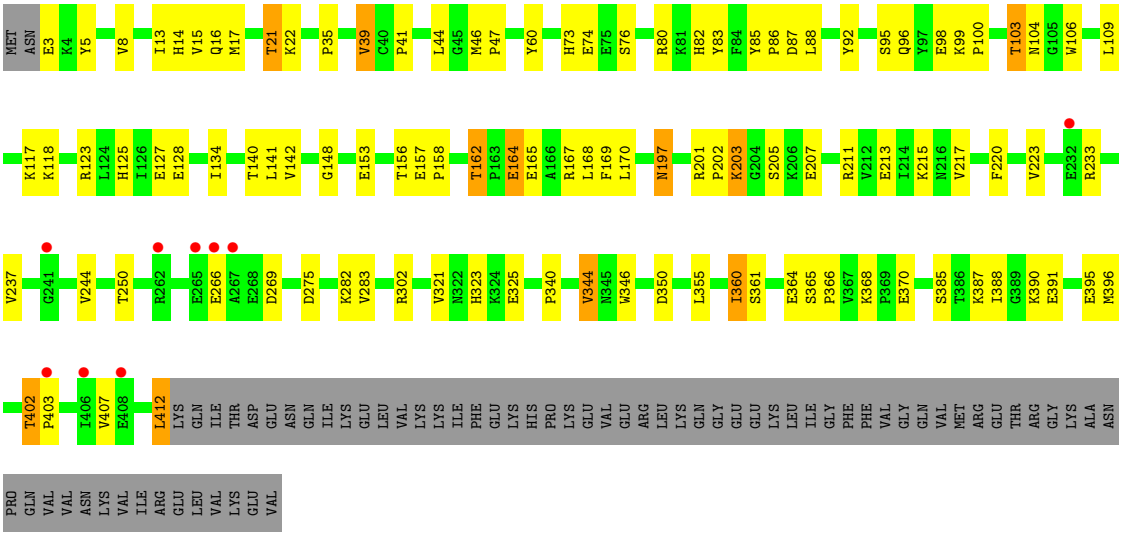
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain K:



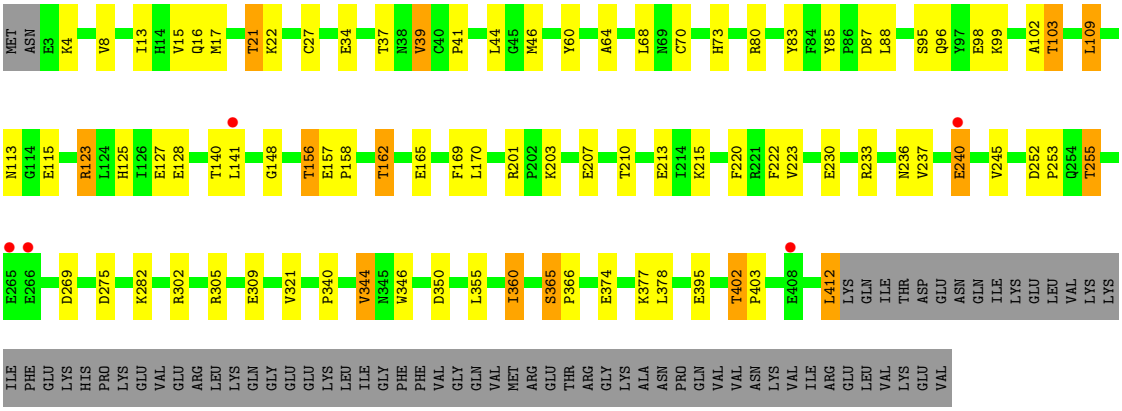
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain N:



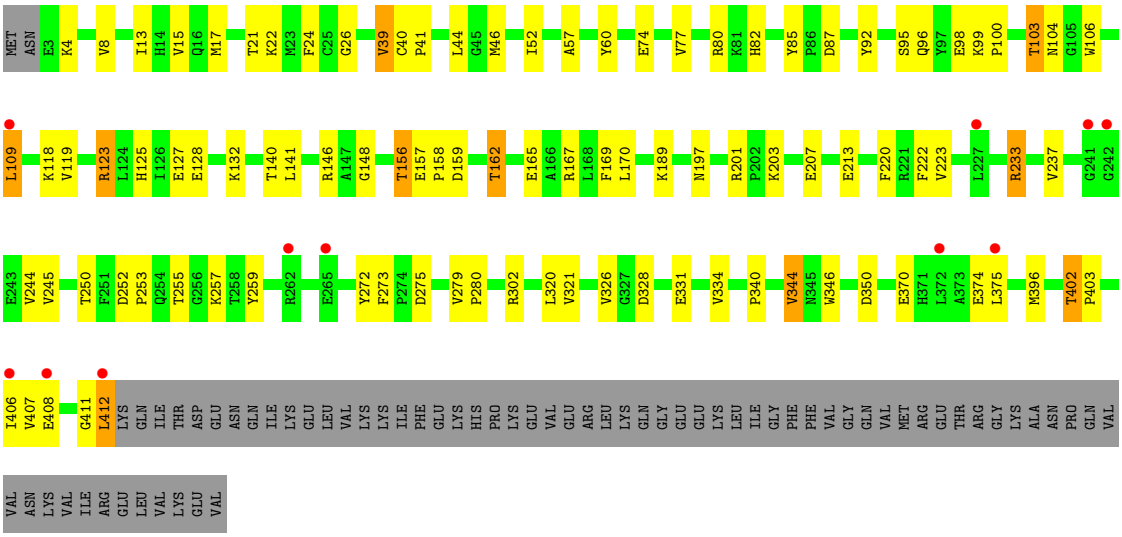
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain Q:



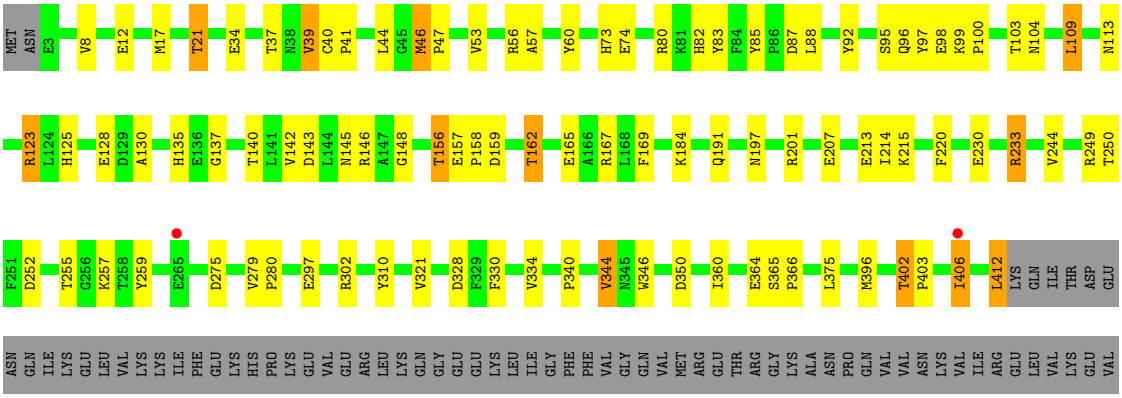
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain T:



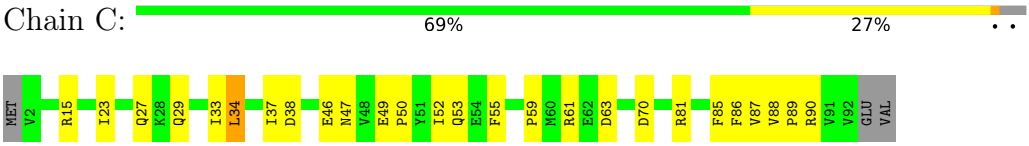
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain W:



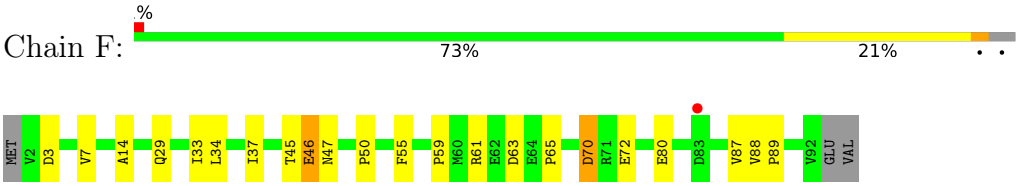
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain C:



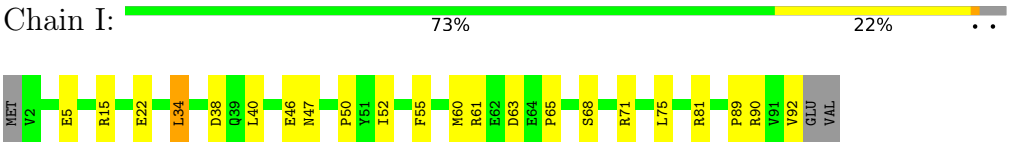
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain F:



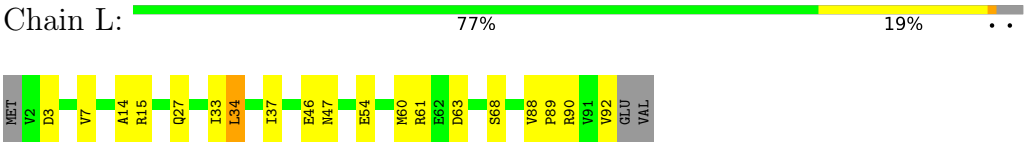
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain I:



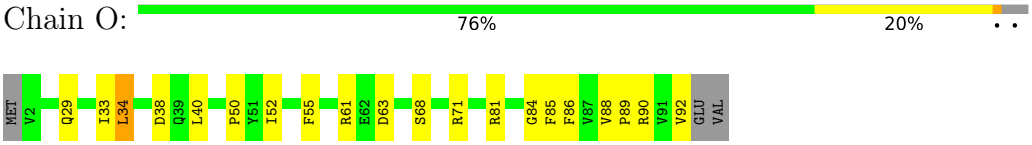
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain L:



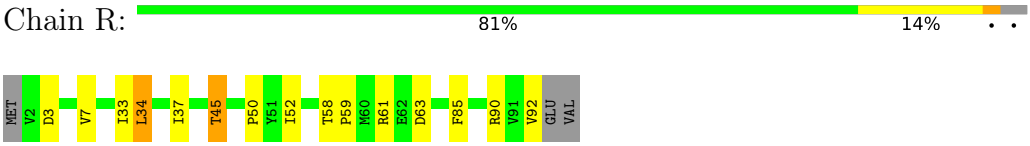
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain O:



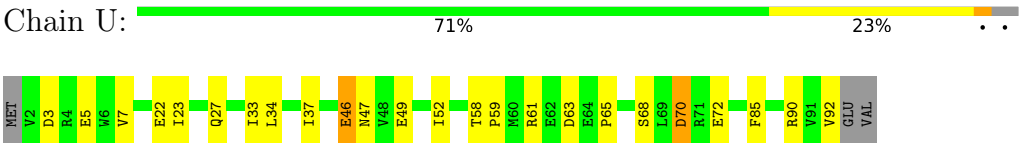
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain R:



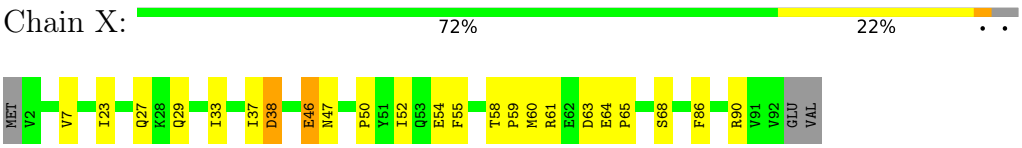
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain U:



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

Chain X:


72%
22%
MET
V2
V7
I23
Q27
K28
Q29
I33
I37
D38
E46
N47
P50
Y51
I52
Q53
E54
F55
T58
P59
M60
R61
E62
D63
E64
P65
S68
F86
R90
V91
V92
GLU
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	128.25Å 129.86Å 155.07Å 90.01° 89.96° 90.11°	Depositor
Resolution (Å)	39.37 – 2.80 39.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.37-2.80) 97.6 (39.36-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.305 0.260 , 0.263	Depositor DCC
R_{free} test set	12256 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	62.9	Xtriage
Anisotropy	0.753	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 15.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -k,h,l 0.000 for k,-h,l 0.185 for h,-k,-l 0.437 for -h,k,-l 0.184 for -h,-k,l 0.000 for -k,-h,-l 0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	62935	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2523e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.64	0/3874	0.72	3/5244 (0.1%)
1	D	0.62	0/3874	0.70	2/5244 (0.0%)
1	G	0.62	0/3874	0.70	3/5244 (0.1%)
1	J	0.63	0/3874	0.70	3/5244 (0.1%)
1	M	0.61	0/3874	0.69	2/5244 (0.0%)
1	P	0.61	0/3874	0.69	2/5244 (0.0%)
1	S	0.63	0/3874	0.71	3/5244 (0.1%)
1	V	0.65	0/3874	0.72	2/5244 (0.0%)
2	B	0.59	0/3371	0.65	0/4541
2	E	0.61	1/3371 (0.0%)	0.64	0/4541
2	H	0.61	0/3371	0.65	1/4541 (0.0%)
2	K	0.61	0/3371	0.67	2/4541 (0.0%)
2	N	0.60	0/3371	0.67	2/4541 (0.0%)
2	Q	0.60	0/3371	0.68	2/4541 (0.0%)
2	T	0.62	0/3371	0.65	0/4541
2	W	0.59	0/3371	0.65	0/4541
3	C	0.58	0/778	0.71	0/1050
3	F	0.58	0/778	0.67	0/1050
3	I	0.56	0/778	0.69	0/1050
3	L	0.56	0/778	0.67	0/1050
3	O	0.56	0/778	0.71	0/1050
3	R	0.58	0/778	0.67	0/1050
3	U	0.60	0/778	0.70	0/1050
3	X	0.60	0/778	0.73	0/1050
All	All	0.61	1/64184 (0.0%)	0.68	27/86680 (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	M	0	1
2	B	0	2
2	E	0	2
2	T	0	1
3	F	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	43	CYS	CB-SG	-5.64	1.72	1.81

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	269	ASP	CB-CG-OD1	5.96	123.66	118.30
2	H	412	LEU	CA-CB-CG	5.92	128.92	115.30
1	J	31	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	G	117	LEU	CA-CB-CG	5.56	128.09	115.30
2	K	269	ASP	CB-CG-OD1	5.45	123.21	118.30
2	N	412	LEU	CA-CB-CG	5.44	127.81	115.30
2	Q	412	LEU	CA-CB-CG	5.32	127.53	115.30
1	V	331	ASP	CB-CG-OD2	5.28	123.05	118.30
2	N	269	ASP	CB-CG-OD1	5.28	123.05	118.30
1	P	331	ASP	CB-CG-OD2	5.26	123.03	118.30
2	K	412	LEU	CA-CB-CG	5.24	127.34	115.30
1	M	331	ASP	CB-CG-OD2	5.24	123.01	118.30
1	V	97	ASP	CB-CG-OD2	5.21	122.99	118.30
1	S	331	ASP	CB-CG-OD2	5.20	122.98	118.30
1	J	331	ASP	CB-CG-OD2	5.20	122.97	118.30
1	D	331	ASP	CB-CG-OD2	5.19	122.97	118.30
1	G	97	ASP	CB-CG-OD2	5.19	122.97	118.30
1	S	97	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	97	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	331	ASP	CB-CG-OD2	5.18	122.96	118.30
1	G	331	ASP	CB-CG-OD2	5.18	122.96	118.30
1	M	97	ASP	CB-CG-OD2	5.16	122.95	118.30
1	J	97	ASP	CB-CG-OD2	5.16	122.94	118.30
1	P	97	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	97	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	295	VAL	CB-CA-C	-5.09	101.73	111.40
1	S	408	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	217	VAL	Peptide
2	B	411	GLY	Peptide
2	E	217	VAL	Peptide
2	E	97	TYR	Peptide
3	F	45	THR	Peptide
1	M	394	SER	Peptide
2	T	411	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3784	0	3817	118	0
1	D	3784	0	3816	108	0
1	G	3784	0	3817	100	0
1	J	3784	0	3816	110	0
1	M	3784	0	3817	108	0
1	P	3784	0	3816	118	0
1	S	3784	0	3817	116	0
1	V	3784	0	3817	120	0
2	B	3308	0	3353	95	0
2	E	3308	0	3353	91	0
2	H	3308	0	3353	82	0
2	K	3308	0	3353	77	0
2	N	3308	0	3353	71	0
2	Q	3308	0	3353	66	0
2	T	3308	0	3353	84	0
2	W	3308	0	3353	85	0
3	C	764	0	755	22	0
3	F	764	0	755	20	0
3	I	764	0	755	19	0
3	L	764	0	755	17	0
3	O	764	0	755	21	0
3	R	764	0	755	18	0
3	U	764	0	755	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	764	0	755	22	0
4	A	9	0	5	8	0
4	D	9	0	5	3	0
4	G	9	0	5	12	0
4	J	9	0	5	6	0
4	M	9	0	5	13	0
4	P	9	0	5	7	0
4	S	9	0	5	4	0
4	V	9	0	5	12	0
5	B	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	1	0	0	0	0
6	E	1	0	0	0	0
6	H	1	0	0	0	0
6	K	1	0	0	0	0
6	N	1	0	0	0	0
6	Q	1	0	0	0	0
6	T	1	0	0	0	0
6	W	1	0	0	0	0
All	All	62935	0	63437	1581	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1581) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:LEU:HD22	2:B:412:LEU:O	1.39	1.22
1:P:464:LEU:HD12	1:P:464:LEU:O	1.40	1.20
3:O:88:VAL:HB	3:O:89:PRO:HD2	1.32	1.11
1:D:122:MET:HB3	1:D:351:ARG:NH1	1.63	1.11
2:T:412:LEU:O	2:T:412:LEU:HD22	1.49	1.11
1:V:35:THR:HG22	1:V:39:VAL:CG2	1.78	1.11
1:A:35:THR:HG22	1:A:39:VAL:CG2	1.80	1.10
1:J:122:MET:SD	1:J:351:ARG:HD2	1.91	1.10
1:M:88:ILE:HG23	1:M:343:GLY:HA3	1.15	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:213:GLU:OE2	2:Q:215:LYS:HE3	1.51	1.10
2:W:412:LEU:O	2:W:412:LEU:HD22	1.51	1.09
2:B:21:THR:HG21	3:C:61:ARG:HH12	1.10	1.08
1:G:171:SER:HB2	4:G:903:GLN:OE1	1.54	1.08
1:J:376:ARG:HG3	1:J:376:ARG:HH11	1.19	1.06
2:N:21:THR:HG21	3:O:61:ARG:HH12	1.15	1.06
2:H:21:THR:HG21	3:I:61:ARG:HH12	1.18	1.05
1:V:77:VAL:HG21	1:V:114:LYS:HZ1	1.20	1.03
1:A:190:ARG:HG3	1:A:190:ARG:HH11	1.19	1.03
1:S:35:THR:HG22	1:S:39:VAL:CG2	1.89	1.02
1:A:171:SER:CB	4:A:901:GLN:CD	2.26	1.02
1:V:77:VAL:HG21	1:V:114:LYS:NZ	1.74	1.02
1:V:190:ARG:HG3	1:V:190:ARG:HH11	1.24	1.02
1:A:35:THR:HG22	1:A:39:VAL:HG23	1.41	1.01
2:W:21:THR:HG21	3:X:61:ARG:HH12	1.22	1.01
1:V:35:THR:HG22	1:V:39:VAL:HG23	1.40	1.01
2:T:21:THR:HB	3:U:63:ASP:OD1	1.60	1.00
1:M:88:ILE:HG23	1:M:343:GLY:CA	1.91	1.00
2:B:100:PRO:HB3	2:B:123:ARG:HH21	1.21	1.00
2:E:21:THR:HG21	3:F:61:ARG:HH12	1.26	0.99
1:A:35:THR:HG23	1:A:477:LEU:HD12	1.44	0.99
1:J:174:GLN:HG3	1:J:175:PRO:HD3	1.43	0.98
1:M:174:GLN:HG3	1:M:175:PRO:HD3	1.44	0.97
3:L:88:VAL:HB	3:L:89:PRO:HD2	1.46	0.97
1:S:122:MET:HB3	1:S:351:ARG:NH1	1.80	0.96
2:T:21:THR:HG21	3:U:61:ARG:HH12	1.26	0.96
2:Q:360:ILE:HD11	2:Q:365:SER:HA	1.46	0.96
1:S:376:ARG:HG3	1:S:376:ARG:HH11	1.27	0.96
1:M:88:ILE:CG2	1:M:343:GLY:HA3	1.94	0.96
1:P:31:ARG:O	1:P:35:THR:HG22	1.66	0.96
1:G:171:SER:CB	4:G:903:GLN:CD	2.35	0.95
3:F:88:VAL:HB	3:F:89:PRO:HD2	1.45	0.95
2:N:162:THR:HG22	2:N:165:GLU:H	1.32	0.95
3:C:88:VAL:HB	3:C:89:PRO:HD2	1.47	0.94
1:D:190:ARG:HD3	1:D:241:TRP:HH2	1.32	0.94
1:V:279:GLU:HG3	1:V:468:LYS:NZ	1.82	0.94
1:M:352:ILE:O	1:M:356:THR:HG22	1.68	0.94
1:D:352:ILE:O	1:D:356:THR:HG23	1.66	0.94
2:E:412:LEU:HD22	2:E:412:LEU:O	1.68	0.94
1:P:31:ARG:HH11	1:P:31:ARG:CG	1.80	0.93
2:K:360:ILE:HD11	2:K:365:SER:HA	1.47	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:MET:CB	1:D:351:ARG:NH1	2.31	0.93
1:A:171:SER:HB2	4:A:901:GLN:CD	1.89	0.92
1:S:35:THR:HG22	1:S:39:VAL:HG23	1.49	0.92
1:M:88:ILE:HD11	1:M:120:PHE:CE2	2.05	0.91
1:P:370:LYS:NZ	3:R:45:THR:HB	1.85	0.91
1:A:352:ILE:O	1:A:356:THR:HG23	1.70	0.90
2:K:156:THR:HG22	2:K:157:GLU:O	1.71	0.90
2:W:34:GLU:O	2:W:37:THR:HG22	1.70	0.90
2:Q:17:MET:CE	2:Q:60:TYR:HB2	2.03	0.89
1:V:35:THR:HG22	1:V:39:VAL:HG21	1.51	0.89
1:P:352:ILE:O	1:P:356:THR:HG22	1.72	0.89
1:V:171:SER:CB	4:V:908:GLN:CD	2.41	0.89
2:K:21:THR:HG21	3:L:61:ARG:HH12	1.37	0.89
2:H:17:MET:CE	2:H:60:TYR:HB3	2.02	0.88
1:V:35:THR:HG23	1:V:477:LEU:HD12	1.53	0.88
2:B:21:THR:HG21	3:C:61:ARG:NH1	1.88	0.88
2:H:17:MET:CE	2:H:60:TYR:CB	2.51	0.87
2:B:162:THR:HG22	2:B:165:GLU:H	1.39	0.87
2:E:21:THR:HB	3:F:63:ASP:OD1	1.75	0.87
1:V:35:THR:CG2	1:V:39:VAL:CG2	2.53	0.87
1:J:190:ARG:HD3	1:J:241:TRP:HH2	1.38	0.86
1:A:35:THR:HG22	1:A:39:VAL:HG21	1.53	0.86
1:P:464:LEU:HD12	1:P:464:LEU:C	1.93	0.86
2:H:17:MET:HE1	2:H:60:TYR:HB2	1.59	0.85
2:E:17:MET:CE	2:E:60:TYR:HB2	2.07	0.84
1:J:122:MET:HE2	1:J:199:PHE:CE1	2.12	0.84
2:K:39:VAL:HG13	2:K:44:LEU:HD11	1.57	0.84
2:W:39:VAL:HG13	2:W:44:LEU:HD11	1.58	0.84
1:M:376:ARG:HG3	1:M:376:ARG:HH11	1.42	0.84
2:T:85:TYR:HD2	2:T:87:ASP:OD1	1.60	0.84
2:Q:21:THR:HG21	3:R:61:ARG:HH12	1.40	0.84
1:A:35:THR:CG2	1:A:39:VAL:CG2	2.55	0.84
2:E:39:VAL:HG22	2:E:44:LEU:HG	1.60	0.84
2:E:412:LEU:HD22	2:E:412:LEU:C	1.97	0.83
2:Q:17:MET:HE1	2:Q:60:TYR:HB2	1.59	0.83
1:M:88:ILE:HD11	1:M:120:PHE:CZ	2.13	0.83
2:B:39:VAL:HG13	2:B:44:LEU:HD11	1.60	0.83
1:J:122:MET:SD	1:J:351:ARG:CD	2.66	0.83
2:H:17:MET:HE1	2:H:60:TYR:CB	2.08	0.82
2:E:156:THR:HG22	2:E:157:GLU:O	1.78	0.82
2:W:103:THR:HG22	2:W:104:ASN:OD1	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:HG3	1:A:190:ARG:NH1	1.88	0.82
1:M:90:GLU:O	1:M:91:ASN:HB2	1.79	0.82
3:R:92:VAL:HG12	3:R:92:VAL:O	1.79	0.82
1:V:35:THR:CG2	1:V:39:VAL:HG21	2.08	0.82
1:V:190:ARG:HG3	1:V:190:ARG:NH1	1.92	0.82
1:G:171:SER:CB	4:G:903:GLN:OE1	2.26	0.82
1:J:352:ILE:O	1:J:356:THR:CG2	2.27	0.82
1:P:190:ARG:HH11	1:P:190:ARG:HG3	1.44	0.82
1:V:77:VAL:CG2	1:V:114:LYS:HZ1	1.93	0.82
2:B:21:THR:HB	3:C:63:ASP:OD1	1.80	0.81
1:D:2:LEU:HD23	1:D:27:SER:HB2	1.60	0.81
2:B:21:THR:CG2	3:C:61:ARG:HH12	1.93	0.81
1:D:138:TRP:CE2	1:D:438:TRP:HH2	1.97	0.81
2:N:21:THR:HB	3:O:63:ASP:OD1	1.79	0.81
2:B:40:CYS:O	2:B:44:LEU:HD12	1.79	0.81
1:A:35:THR:CG2	1:A:39:VAL:HG21	2.10	0.81
1:G:270:LYS:HE3	1:G:274:GLU:OE2	1.81	0.80
1:A:190:ARG:HH11	1:A:190:ARG:CG	1.92	0.80
1:P:81:LYS:HE2	1:P:91:ASN:HA	1.61	0.80
1:V:77:VAL:CG2	1:V:114:LYS:NZ	2.43	0.80
1:D:77:VAL:HG23	1:D:114:LYS:NZ	1.96	0.80
1:D:138:TRP:CE2	1:D:438:TRP:CH2	2.70	0.80
2:E:17:MET:HE1	2:E:60:TYR:HB2	1.62	0.80
2:T:17:MET:CE	2:T:60:TYR:HB2	2.12	0.80
2:K:17:MET:CE	2:K:60:TYR:HB2	2.12	0.80
1:S:376:ARG:HG3	1:S:376:ARG:NH1	1.93	0.80
3:O:88:VAL:HB	3:O:89:PRO:CD	2.12	0.80
3:O:88:VAL:CB	3:O:89:PRO:HD2	2.12	0.80
1:V:71:VAL:HB	1:V:114:LYS:HZ3	1.46	0.79
2:E:252:ASP:HB3	2:E:255:THR:HG22	1.64	0.79
1:J:376:ARG:HG3	1:J:376:ARG:NH1	1.92	0.79
2:H:17:MET:HE2	2:H:60:TYR:HB3	1.65	0.79
2:H:220:PHE:O	2:H:223:VAL:HG22	1.83	0.79
1:J:302:TYR:OH	4:J:904:GLN:HA	1.83	0.79
1:J:352:ILE:O	1:J:356:THR:HG22	1.83	0.79
2:K:17:MET:CE	2:K:60:TYR:CB	2.61	0.79
1:A:73:ASP:OD1	1:A:73:ASP:O	2.00	0.79
1:P:370:LYS:HZ2	3:R:45:THR:HB	1.42	0.78
1:G:352:ILE:O	1:G:356:THR:HG23	1.82	0.78
1:V:352:ILE:O	1:V:356:THR:HG23	1.81	0.78
1:G:422:VAL:CG2	1:G:423:PRO:HD3	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:438:TRP:CZ3	1:P:443:PRO:HG3	2.19	0.78
1:S:83:THR:HG22	1:S:90:GLU:HA	1.66	0.78
1:S:35:THR:HG22	1:S:39:VAL:HG21	1.62	0.78
1:V:279:GLU:HG3	1:V:468:LYS:HZ1	1.49	0.78
2:K:100:PRO:HB3	2:K:123:ARG:HH21	1.48	0.78
1:S:35:THR:CG2	1:S:39:VAL:CG2	2.62	0.77
1:D:73:ASP:OD1	1:D:73:ASP:O	2.01	0.77
1:M:245:VAL:HG12	1:M:459:LEU:HB3	1.65	0.77
2:Q:21:THR:CG2	3:R:61:ARG:HH12	1.98	0.77
2:W:280:PRO:HD2	3:X:55:PHE:CZ	2.20	0.77
1:A:279:GLU:HG3	1:A:468:LYS:NZ	2.00	0.77
2:N:109:LEU:HD11	2:N:169:PHE:HA	1.66	0.77
1:S:81:LYS:HE2	1:S:91:ASN:HA	1.66	0.77
1:S:182:ILE:HG12	1:S:434:ILE:HD12	1.66	0.76
2:W:17:MET:CE	2:W:60:TYR:HB2	2.15	0.76
2:B:39:VAL:CG1	2:B:44:LEU:HD11	2.15	0.76
2:W:21:THR:CG2	3:X:61:ARG:HH12	1.96	0.76
1:S:155:VAL:HG12	1:S:181:VAL:HG21	1.69	0.76
2:B:412:LEU:CD1	2:B:412:LEU:H	1.99	0.75
2:Q:39:VAL:HG13	2:Q:44:LEU:HD11	1.68	0.75
1:D:72:LYS:HA	1:D:115:THR:HG22	1.66	0.75
2:N:39:VAL:HG13	2:N:44:LEU:HD11	1.69	0.75
1:M:171:SER:CB	4:M:905:GLN:CD	2.54	0.75
2:E:103:THR:HG22	2:E:104:ASN:OD1	1.85	0.75
1:G:81:LYS:HE2	1:G:91:ASN:HA	1.68	0.75
1:D:182:ILE:HG12	1:D:434:ILE:HD12	1.68	0.75
1:S:35:THR:CG2	1:S:39:VAL:HG21	2.17	0.75
2:W:412:LEU:O	2:W:412:LEU:CD2	2.33	0.75
1:V:73:ASP:OD1	1:V:73:ASP:O	2.04	0.74
1:V:171:SER:HB2	4:V:908:GLN:CD	2.08	0.74
2:B:412:LEU:H	2:B:412:LEU:HD13	1.51	0.74
2:N:17:MET:CE	2:N:60:TYR:CB	2.66	0.74
1:P:31:ARG:HH11	1:P:31:ARG:HG3	1.50	0.74
1:D:122:MET:HB3	1:D:351:ARG:CZ	2.18	0.74
1:P:299:ILE:HG13	1:P:419:ILE:HG22	1.69	0.74
1:M:279:GLU:HG3	1:M:468:LYS:NZ	2.02	0.74
2:H:21:THR:HB	3:I:63:ASP:OD1	1.86	0.74
1:A:138:TRP:CE2	1:A:438:TRP:HH2	2.04	0.74
1:G:85:ALA:CB	1:G:117:LEU:HD13	2.17	0.74
1:A:138:TRP:CE2	1:A:438:TRP:CH2	2.76	0.74
2:Q:17:MET:CE	2:Q:60:TYR:CB	2.64	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:MET:HG2	1:G:351:ARG:HH11	1.53	0.74
1:D:174:GLN:HG3	1:D:175:PRO:HD3	1.70	0.73
1:M:332:ILE:HD13	3:O:88:VAL:HG21	1.70	0.73
2:Q:156:THR:HG22	2:Q:157:GLU:O	1.88	0.73
2:Q:41:PRO:HB3	2:Q:46:MET:HE2	1.70	0.73
1:M:138:TRP:CE2	1:M:438:TRP:CH2	2.77	0.73
2:W:21:THR:HG21	3:X:61:ARG:NH1	2.03	0.73
2:N:17:MET:CE	2:N:60:TYR:HB2	2.18	0.73
2:H:17:MET:CE	2:H:60:TYR:HB2	2.16	0.73
1:J:438:TRP:CZ3	1:J:443:PRO:HG3	2.23	0.73
2:N:8:VAL:HG12	2:N:158:PRO:HB2	1.70	0.73
1:G:85:ALA:HB2	1:G:117:LEU:HD13	1.69	0.72
2:E:17:MET:HE2	2:E:57:ALA:HA	1.69	0.72
1:M:190:ARG:HD3	1:M:241:TRP:HH2	1.55	0.72
1:A:171:SER:N	4:A:901:GLN:OE1	2.21	0.72
1:M:376:ARG:HG3	1:M:376:ARG:NH1	2.01	0.72
1:S:171:SER:CB	4:S:907:GLN:CD	2.57	0.72
1:J:303:TYR:HH	4:J:904:GLN:N	1.87	0.71
1:P:3:TRP:CZ3	1:P:31:ARG:HD2	2.25	0.71
2:W:162:THR:HG22	2:W:165:GLU:H	1.53	0.71
2:N:156:THR:HG22	2:N:157:GLU:O	1.90	0.71
2:W:17:MET:HE1	2:W:60:TYR:HB2	1.71	0.71
2:H:17:MET:HE2	2:H:60:TYR:CB	2.18	0.71
1:G:171:SER:HB2	4:G:903:GLN:CD	2.05	0.71
2:N:17:MET:HE2	2:N:60:TYR:HB2	1.71	0.71
2:N:220:PHE:O	2:N:223:VAL:HG22	1.91	0.71
1:A:438:TRP:CH2	1:A:443:PRO:HG3	2.26	0.71
2:K:17:MET:HE2	2:K:60:TYR:HB2	1.72	0.71
1:S:77:VAL:HG23	1:S:114:LYS:HE3	1.72	0.70
1:S:418:ASP:OD2	4:S:907:GLN:N	2.24	0.70
2:W:17:MET:CE	2:W:57:ALA:HA	2.21	0.70
2:W:21:THR:HB	3:X:63:ASP:OD1	1.91	0.70
1:J:31:ARG:O	1:J:35:THR:HG22	1.91	0.70
1:J:174:GLN:HG3	1:J:175:PRO:CD	2.21	0.70
2:T:17:MET:HE1	2:T:60:TYR:HB2	1.71	0.70
1:P:3:TRP:CE3	1:P:31:ARG:HD2	2.27	0.70
1:S:171:SER:HB2	4:S:907:GLN:OE1	1.91	0.70
2:B:146:ARG:HG2	2:B:146:ARG:HH11	1.57	0.70
1:G:422:VAL:HG22	1:G:423:PRO:HD3	1.73	0.70
2:K:220:PHE:O	2:K:223:VAL:HG22	1.90	0.70
1:A:297:TYR:O	1:A:300:PRO:HD2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:MET:HA	1:D:351:ARG:HH12	1.57	0.70
1:M:138:TRP:CE2	1:M:438:TRP:HH2	2.09	0.70
3:R:92:VAL:O	3:R:92:VAL:CG1	2.40	0.70
1:S:13:LEU:HB3	1:S:19:VAL:HG12	1.74	0.70
1:D:115:THR:HG21	1:D:151:SER:OG	1.92	0.70
2:B:17:MET:CE	2:B:57:ALA:HA	2.22	0.70
3:X:33:ILE:O	3:X:37:ILE:HG12	1.92	0.70
1:G:306:ALA:HB3	1:G:307:PRO:HD3	1.74	0.70
1:G:344:PHE:O	1:G:349:LYS:HE2	1.90	0.70
1:J:122:MET:CE	1:J:199:PHE:CE1	2.75	0.69
1:P:31:ARG:HH11	1:P:31:ARG:HG2	1.57	0.69
2:H:109:LEU:HD11	2:H:169:PHE:HA	1.74	0.69
1:D:100:VAL:HG12	1:D:223:ILE:HB	1.74	0.69
2:T:207:GLU:OE1	2:T:207:GLU:HA	1.91	0.69
2:B:17:MET:CE	2:B:60:TYR:HB2	2.23	0.69
1:P:31:ARG:NE	1:P:157:VAL:O	2.21	0.69
2:B:17:MET:HE1	2:B:60:TYR:HB2	1.74	0.69
3:F:46:GLU:O	3:F:47:ASN:HB2	1.93	0.69
2:B:39:VAL:HG13	2:B:44:LEU:CD1	2.22	0.69
1:G:190:ARG:HD3	1:G:241:TRP:HH2	1.57	0.69
1:M:123:GLY:N	4:M:905:GLN:O	2.26	0.69
2:T:412:LEU:O	2:T:412:LEU:CD2	2.37	0.69
1:V:418:ASP:OD2	4:V:908:GLN:N	2.26	0.69
2:W:213:GLU:OE2	2:W:215:LYS:HE3	1.92	0.69
2:W:252:ASP:HB3	2:W:255:THR:HG22	1.74	0.69
1:G:85:ALA:HB2	1:G:117:LEU:CD1	2.23	0.69
2:N:21:THR:HG21	3:O:61:ARG:NH1	2.00	0.69
1:V:2:LEU:HD23	1:V:27:SER:HB2	1.75	0.69
1:V:190:ARG:HH11	1:V:190:ARG:CG	2.02	0.69
1:D:418:ASP:OD2	4:D:902:GLN:N	2.25	0.68
2:E:220:PHE:O	2:E:223:VAL:HG22	1.93	0.68
2:Q:220:PHE:O	2:Q:223:VAL:HG22	1.91	0.68
2:T:39:VAL:HG22	2:T:44:LEU:HG	1.75	0.68
1:A:185:LYS:HE2	1:A:425:ASN:ND2	2.09	0.68
2:K:3:GLU:HA	2:K:3:GLU:OE1	1.93	0.68
2:T:255:THR:HG21	2:T:259:TYR:OH	1.93	0.68
1:V:138:TRP:CE2	1:V:438:TRP:CH2	2.82	0.68
2:B:280:PRO:HD2	3:C:55:PHE:CZ	2.28	0.68
2:B:17:MET:HE2	2:B:57:ALA:HA	1.75	0.68
2:N:197:ASN:HB3	2:N:211:ARG:HD2	1.75	0.68
1:D:69:ILE:HD11	1:D:164:LEU:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:169:GLY:HA2	1:V:425:ASN:OD1	1.93	0.68
1:P:31:ARG:HG2	1:P:31:ARG:NH1	2.09	0.68
1:J:245:VAL:HG12	1:J:459:LEU:HB3	1.75	0.68
1:M:279:GLU:HG3	1:M:468:LYS:HZ3	1.59	0.68
2:N:17:MET:HE2	2:N:60:TYR:CB	2.24	0.68
1:V:438:TRP:CH2	1:V:443:PRO:HG3	2.29	0.68
2:B:40:CYS:O	2:B:44:LEU:HB2	1.94	0.68
2:H:162:THR:HG22	2:H:165:GLU:H	1.59	0.68
1:J:190:ARG:HD3	1:J:241:TRP:CH2	2.26	0.67
2:K:17:MET:CE	2:K:60:TYR:HB3	2.23	0.67
1:S:78:GLU:HB2	1:S:97:ASP:OD1	1.94	0.67
1:G:178:PHE:HE1	1:G:397:THR:HG21	1.59	0.67
2:H:252:ASP:HB3	2:H:255:THR:CG2	2.24	0.67
1:M:83:THR:HG22	1:M:90:GLU:HA	1.76	0.67
1:D:81:LYS:HE2	1:D:91:ASN:HA	1.75	0.67
1:J:122:MET:HE3	1:J:199:PHE:CD1	2.29	0.67
2:Q:162:THR:HG22	2:Q:165:GLU:H	1.59	0.67
1:A:167:ASP:HB3	1:A:185:LYS:HD2	1.77	0.67
1:A:418:ASP:OD2	4:A:901:GLN:N	2.27	0.67
2:E:17:MET:CE	2:E:57:ALA:HA	2.25	0.67
1:G:376:ARG:HH11	1:G:376:ARG:HG3	1.60	0.67
1:M:68:PRO:HB3	1:M:112:VAL:HG21	1.77	0.67
1:M:299:ILE:N	1:M:300:PRO:HD2	2.10	0.67
1:S:143:VAL:HG12	1:S:145:GLY:H	1.60	0.67
1:V:171:SER:HG	4:V:908:GLN:CD	1.95	0.67
1:A:376:ARG:HG3	1:A:376:ARG:HH11	1.60	0.67
1:S:122:MET:CB	1:S:351:ARG:NH1	2.57	0.67
1:D:77:VAL:HG23	1:D:114:LYS:HZ2	1.57	0.66
1:J:344:PHE:O	1:J:349:LYS:HE2	1.95	0.66
2:E:8:VAL:HG12	2:E:158:PRO:HB2	1.76	0.66
1:M:124:SER:HG	4:M:905:GLN:N	1.94	0.66
1:M:115:THR:HG21	1:M:151:SER:OG	1.96	0.66
2:N:21:THR:CG2	3:O:61:ARG:HH12	2.00	0.66
2:B:40:CYS:HB2	2:B:43:CYS:SG	2.34	0.66
1:D:83:THR:HG22	1:D:90:GLU:HA	1.78	0.66
1:P:83:THR:HG22	1:P:90:GLU:HA	1.76	0.66
1:S:138:TRP:CE2	1:S:438:TRP:CH2	2.84	0.66
1:V:138:TRP:CE2	1:V:438:TRP:HH2	2.13	0.66
2:K:85:TYR:HD2	2:K:87:ASP:OD1	1.79	0.66
1:S:190:ARG:HD3	1:S:241:TRP:HH2	1.60	0.66
1:G:299:ILE:HG13	1:G:419:ILE:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:46:GLU:O	3:L:47:ASN:HB2	1.95	0.66
1:D:245:VAL:HG12	1:D:459:LEU:HB3	1.77	0.65
1:J:163:SER:HB3	1:J:209:PHE:HB2	1.78	0.65
1:S:73:ASP:OD1	1:S:114:LYS:NZ	2.29	0.65
2:N:17:MET:CE	2:N:60:TYR:HB3	2.27	0.65
2:T:8:VAL:HG12	2:T:158:PRO:HB2	1.78	0.65
2:K:162:THR:HG22	2:K:165:GLU:H	1.61	0.65
2:N:100:PRO:HB3	2:N:123:ARG:NH2	2.12	0.65
2:B:412:LEU:O	2:B:412:LEU:CD2	2.31	0.65
1:P:318:ASP:HB2	1:P:336:TYR:CE1	2.32	0.65
2:B:297:GLU:OE2	2:B:302:ARG:HA	1.97	0.65
1:J:322:TYR:CZ	2:K:47:PRO:HD3	2.31	0.65
2:N:103:THR:HG23	2:N:104:ASN:OD1	1.97	0.65
1:J:292:LEU:HB2	1:J:295:VAL:HG22	1.78	0.65
1:V:193:ARG:NH1	1:V:232:THR:OG1	2.29	0.65
2:W:402:THR:HG22	2:W:403:PRO:HD2	1.79	0.65
2:H:146:ARG:HH11	2:H:146:ARG:HG2	1.63	0.64
1:J:122:MET:CE	1:J:199:PHE:CD1	2.81	0.64
2:K:95:SER:HB2	2:K:127:GLU:HB3	1.80	0.64
2:B:302:ARG:HD3	2:B:321:VAL:HG22	1.79	0.64
1:G:49:LYS:HE2	1:G:53:GLN:NE2	2.13	0.64
2:H:355:LEU:HD21	2:H:365:SER:HB2	1.80	0.64
2:Q:213:GLU:OE2	2:Q:215:LYS:CE	2.39	0.64
2:W:252:ASP:OD2	2:W:255:THR:HG22	1.96	0.64
1:D:356:THR:HG21	3:F:14:ALA:HB2	1.80	0.64
2:Q:21:THR:HG21	3:R:61:ARG:NH1	2.12	0.64
1:V:279:GLU:HG3	1:V:468:LYS:HZ3	1.59	0.64
2:B:412:LEU:HD13	2:B:412:LEU:N	2.11	0.64
2:E:412:LEU:O	2:E:412:LEU:CD2	2.44	0.64
2:N:360:ILE:HD11	2:N:364:GLU:O	1.97	0.64
1:P:190:ARG:HG3	1:P:190:ARG:NH1	2.09	0.64
1:V:265:LEU:HD11	1:V:395:PRO:HG2	1.79	0.64
2:B:252:ASP:HB3	2:B:255:THR:HG22	1.80	0.64
1:D:151:SER:HB3	1:D:163:SER:OG	1.98	0.64
1:P:373:LYS:HE2	3:R:50:PRO:HD3	1.78	0.64
1:D:21:PRO:O	1:D:25:VAL:HG23	1.98	0.64
2:K:8:VAL:HG12	2:K:158:PRO:HB2	1.79	0.64
2:Q:252:ASP:HB3	2:Q:255:THR:HG23	1.80	0.64
1:S:306:ALA:HB3	1:S:307:PRO:HD3	1.79	0.64
1:P:370:LYS:HZ3	3:R:45:THR:HB	1.63	0.63
1:D:138:TRP:CZ2	1:D:438:TRP:CH2	2.87	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:THR:HG21	1:G:151:SER:OG	1.97	0.63
2:H:346:TRP:O	2:H:350:ASP:HB2	1.98	0.63
1:P:115:THR:HG21	1:P:151:SER:N	2.13	0.63
2:Q:236:ASN:O	2:Q:240:GLU:HG2	1.98	0.63
1:S:35:THR:CG2	1:S:39:VAL:HG23	2.26	0.63
1:S:352:ILE:O	1:S:356:THR:HG23	1.98	0.63
2:N:85:TYR:HD2	2:N:87:ASP:OD1	1.81	0.63
1:D:31:ARG:O	1:D:35:THR:HG22	1.99	0.63
1:P:31:ARG:CG	1:P:31:ARG:NH1	2.48	0.63
2:T:252:ASP:HB3	2:T:255:THR:HG22	1.81	0.63
2:T:220:PHE:O	2:T:223:VAL:HG22	1.99	0.63
1:V:204:ASP:O	1:V:205:GLN:HG2	1.99	0.63
1:A:2:LEU:HD23	1:A:27:SER:HB2	1.80	0.63
3:C:29:GLN:O	3:C:33:ILE:HG13	1.98	0.63
1:J:185:LYS:NZ	1:J:429:LEU:O	2.32	0.63
1:S:2:LEU:HD23	1:S:27:SER:HB2	1.80	0.63
2:T:156:THR:HG22	2:T:157:GLU:O	1.98	0.63
2:W:109:LEU:HD11	2:W:169:PHE:HA	1.79	0.63
2:H:80:ARG:HE	2:H:275:ASP:CG	2.02	0.63
1:A:171:SER:HB2	4:A:901:GLN:OE1	1.98	0.63
1:M:306:ALA:HB3	1:M:307:PRO:HD3	1.81	0.63
1:P:174:GLN:HG3	1:P:175:PRO:N	2.14	0.63
1:J:21:PRO:O	1:J:25:VAL:HG23	1.99	0.62
1:M:88:ILE:HD11	1:M:120:PHE:HE2	1.62	0.62
2:Q:156:THR:CG2	2:Q:157:GLU:O	2.46	0.62
1:D:190:ARG:HD3	1:D:241:TRP:CH2	2.24	0.62
2:K:109:LEU:HD11	2:K:169:PHE:HA	1.79	0.62
1:G:100:VAL:HG12	1:G:223:ILE:HB	1.81	0.62
2:H:201:ARG:HD2	2:H:207:GLU:O	1.99	0.62
1:S:171:SER:CB	4:S:907:GLN:OE1	2.48	0.62
2:B:73:HIS:NE2	2:B:103:THR:HB	2.14	0.62
2:H:21:THR:CG2	3:I:61:ARG:HH12	2.04	0.62
1:M:395:PRO:O	1:M:420:LEU:HD13	2.00	0.62
1:M:245:VAL:CG1	1:M:459:LEU:HB3	2.29	0.62
1:P:68:PRO:HB3	1:P:112:VAL:HG11	1.81	0.62
2:T:233:ARG:O	2:T:237:VAL:HG23	1.98	0.62
1:A:73:ASP:OD1	1:A:83:THR:N	2.33	0.62
2:B:201:ARG:HD2	2:B:207:GLU:O	1.99	0.62
2:E:21:THR:HG21	3:F:61:ARG:NH1	2.08	0.62
1:S:35:THR:HG21	1:S:157:VAL:HG11	1.82	0.62
2:Q:170:LEU:HD12	2:Q:223:VAL:HG21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLY:N	4:A:901:GLN:O	2.30	0.62
1:D:73:ASP:OD1	1:D:83:THR:N	2.33	0.62
2:T:17:MET:CE	2:T:57:ALA:HA	2.30	0.62
1:V:171:SER:HB2	4:V:908:GLN:OE1	2.00	0.62
1:V:344:PHE:O	1:V:349:LYS:HE2	2.00	0.62
1:S:279:GLU:HG3	1:S:468:LYS:NZ	2.15	0.61
1:V:438:TRP:CZ3	1:V:443:PRO:HG3	2.35	0.61
1:G:21:PRO:O	1:G:25:VAL:HG23	2.00	0.61
1:G:168:THR:HB	4:G:903:GLN:HG3	1.82	0.61
1:S:21:PRO:O	1:S:25:VAL:HG23	2.00	0.61
2:T:146:ARG:HH11	2:T:146:ARG:HG2	1.63	0.61
1:D:77:VAL:CG2	1:D:114:LYS:NZ	2.62	0.61
1:M:31:ARG:O	1:M:35:THR:HG22	2.00	0.61
1:M:174:GLN:HG3	1:M:175:PRO:CD	2.26	0.61
2:Q:85:TYR:HD2	2:Q:87:ASP:OD1	1.83	0.61
1:S:151:SER:HB3	1:S:163:SER:OG	2.01	0.61
1:V:35:THR:CG2	1:V:39:VAL:HG23	2.22	0.61
2:H:95:SER:HB3	2:H:127:GLU:HB3	1.83	0.61
2:N:80:ARG:HE	2:N:275:ASP:CG	2.02	0.61
1:P:214:GLU:OE2	1:P:246:LYS:HE3	2.00	0.61
3:U:46:GLU:O	3:U:47:ASN:HB2	1.99	0.61
1:G:376:ARG:HG3	1:G:376:ARG:NH1	2.14	0.61
2:H:73:HIS:NE2	2:H:103:THR:HB	2.15	0.61
2:H:85:TYR:HD2	2:H:87:ASP:OD1	1.83	0.61
1:P:169:GLY:N	4:P:906:GLN:OE1	2.21	0.61
1:V:292:LEU:HB2	1:V:295:VAL:HG22	1.82	0.61
3:U:33:ILE:O	3:U:37:ILE:HG12	2.01	0.61
1:G:68:PRO:HB3	1:G:112:VAL:HG11	1.82	0.61
2:T:162:THR:HG22	2:T:165:GLU:H	1.65	0.61
1:V:21:PRO:O	1:V:25:VAL:HG23	2.01	0.61
2:K:21:THR:CG2	3:L:61:ARG:HH12	2.11	0.61
1:S:397:THR:HG22	1:S:398:PRO:HD2	1.82	0.61
2:T:41:PRO:HB3	2:T:46:MET:HE2	1.83	0.61
1:P:306:ALA:HB3	1:P:307:PRO:HD3	1.82	0.60
2:T:140:THR:OG1	3:U:90:ARG:HA	2.01	0.60
1:G:297:TYR:O	1:G:300:PRO:HD2	2.02	0.60
2:N:360:ILE:HD11	2:N:364:GLU:C	2.22	0.60
1:D:291:SER:HB3	2:H:118:LYS:NZ	2.16	0.60
2:T:141:LEU:HD23	3:U:85:PHE:CD2	2.37	0.60
3:X:23:ILE:O	3:X:27:GLN:HG3	2.01	0.60
1:D:168:THR:N	4:D:902:GLN:OE1	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:8:VAL:HG12	2:Q:158:PRO:HB2	1.82	0.60
2:E:217:VAL:CG1	2:E:222:PHE:HB3	2.32	0.60
1:G:72:LYS:HA	1:G:115:THR:HG22	1.82	0.60
1:S:422:VAL:CG2	1:S:423:PRO:HD3	2.31	0.60
1:V:115:THR:HG21	1:V:151:SER:OG	2.02	0.60
1:M:86:SER:OG	1:M:88:ILE:HG13	2.02	0.60
1:D:299:ILE:HB	1:D:300:PRO:HD3	1.83	0.60
1:P:122:MET:HG2	1:P:351:ARG:HH11	1.66	0.60
1:P:143:VAL:HG13	1:P:145:GLY:H	1.65	0.60
2:W:412:LEU:C	2:W:412:LEU:HD13	2.22	0.60
2:T:17:MET:HE3	2:T:60:TYR:HB2	1.82	0.60
2:T:412:LEU:H	2:T:412:LEU:CD1	2.14	0.60
1:V:73:ASP:OD1	1:V:83:THR:N	2.34	0.60
2:W:8:VAL:HG12	2:W:158:PRO:HB2	1.83	0.60
2:E:4:LYS:O	2:E:203:LYS:HB2	2.01	0.60
1:G:31:ARG:O	1:G:35:THR:HG22	2.01	0.60
2:E:340:PRO:O	2:E:344:VAL:HG22	2.01	0.60
1:A:35:THR:HG23	1:A:477:LEU:CD1	2.27	0.59
1:J:167:ASP:OD1	1:J:170:GLY:N	2.32	0.59
1:J:299:ILE:HG13	1:J:419:ILE:HG22	1.84	0.59
1:J:422:VAL:CG2	1:J:423:PRO:HD3	2.32	0.59
1:G:394:SER:HB2	1:G:395:PRO:HD2	1.84	0.59
1:P:190:ARG:HH11	1:P:190:ARG:CG	2.14	0.59
1:D:77:VAL:HG23	1:D:114:LYS:HZ1	1.66	0.59
1:D:306:ALA:HB3	1:D:307:PRO:HD3	1.83	0.59
1:G:90:GLU:O	1:G:91:ASN:HB2	2.02	0.59
2:N:83:TYR:CZ	2:N:88:LEU:HD22	2.37	0.59
1:P:464:LEU:C	1:P:464:LEU:CD1	2.67	0.59
1:S:163:SER:HB3	1:S:209:PHE:HB2	1.84	0.59
1:A:434:ILE:HD12	1:A:465:TRP:CD1	2.38	0.59
2:K:170:LEU:HD12	2:K:223:VAL:HG21	1.84	0.59
2:Q:17:MET:HE1	2:Q:60:TYR:CB	2.27	0.59
2:W:98:GLU:O	2:W:99:LYS:HB2	2.02	0.59
1:D:163:SER:HB3	1:D:209:PHE:HB2	1.84	0.59
2:K:156:THR:CG2	2:K:157:GLU:O	2.47	0.59
3:U:46:GLU:CD	3:U:46:GLU:H	2.05	0.59
1:A:185:LYS:CE	1:A:425:ASN:ND2	2.66	0.59
3:C:23:ILE:O	3:C:27:GLN:HG3	2.03	0.59
1:G:83:THR:HG22	1:G:90:GLU:HA	1.85	0.59
2:H:95:SER:HB3	2:H:127:GLU:CB	2.33	0.59
1:S:245:VAL:CG1	1:S:459:LEU:HB3	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:VAL:CG1	1:D:459:LEU:HB3	2.33	0.59
1:P:122:MET:HB3	1:P:351:ARG:NH1	2.18	0.59
1:P:185:LYS:NZ	1:P:429:LEU:O	2.35	0.59
2:Q:233:ARG:O	2:Q:237:VAL:HG23	2.03	0.59
2:T:17:MET:HE2	2:T:57:ALA:HA	1.85	0.59
1:V:168:THR:N	4:V:908:GLN:OE1	2.33	0.59
1:V:422:VAL:CG2	1:V:423:PRO:HD3	2.33	0.59
1:M:163:SER:HB3	1:M:209:PHE:HB2	1.85	0.59
2:B:8:VAL:HG12	2:B:158:PRO:HB2	1.86	0.58
1:D:194:TYR:CD1	1:D:229:LYS:HB3	2.38	0.58
1:J:352:ILE:O	1:J:356:THR:HG23	2.02	0.58
2:E:98:GLU:O	2:E:99:LYS:HB2	2.02	0.58
1:J:83:THR:HA	1:J:89:LEU:O	2.03	0.58
1:A:35:THR:HG21	1:A:157:VAL:HG11	1.85	0.58
1:D:122:MET:HB3	1:D:351:ARG:HH11	1.64	0.58
1:J:318:ASP:HB2	1:J:336:TYR:CE1	2.37	0.58
1:A:5:LYS:HB2	1:A:10:LEU:HD13	1.85	0.58
2:E:17:MET:HE3	2:E:60:TYR:HB2	1.83	0.58
1:P:168:THR:H	4:P:906:GLN:CD	2.06	0.58
1:P:245:VAL:HG12	1:P:459:LEU:HB3	1.86	0.58
1:G:245:VAL:HG12	1:G:459:LEU:HB3	1.85	0.58
1:G:422:VAL:HG23	1:G:423:PRO:HD3	1.84	0.58
1:P:21:PRO:O	1:P:25:VAL:HG23	2.03	0.58
2:E:21:THR:CG2	2:E:22:LYS:N	2.66	0.58
1:V:81:LYS:HE2	1:V:91:ASN:HA	1.84	0.58
1:A:124:SER:O	1:A:174:GLN:NE2	2.36	0.58
2:E:106:TRP:CZ3	1:G:293:PRO:HG3	2.38	0.58
1:M:171:SER:CB	4:M:905:GLN:OE1	2.52	0.58
2:Q:340:PRO:O	2:Q:344:VAL:HG22	2.04	0.58
2:T:412:LEU:HD22	2:T:412:LEU:C	2.23	0.58
1:G:122:MET:HG2	1:G:351:ARG:NH1	2.18	0.58
1:M:90:GLU:O	1:M:91:ASN:CB	2.48	0.58
2:Q:230:GLU:OE2	2:Q:233:ARG:NH1	2.37	0.58
1:V:270:LYS:O	1:V:274:GLU:HG3	2.03	0.58
1:M:190:ARG:HD3	1:M:241:TRP:CH2	2.38	0.57
2:W:17:MET:HE2	2:W:57:ALA:HA	1.85	0.57
2:N:201:ARG:HD2	2:N:207:GLU:O	2.03	0.57
3:L:7:VAL:HG21	3:L:27:GLN:HG3	1.86	0.57
2:Q:73:HIS:NE2	2:Q:103:THR:HB	2.19	0.57
2:W:297:GLU:OE2	2:W:302:ARG:HA	2.05	0.57
2:H:8:VAL:HG12	2:H:158:PRO:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:103:THR:HG22	2:T:104:ASN:OD1	2.05	0.57
2:E:21:THR:HG22	2:E:22:LYS:O	2.04	0.57
1:M:405:GLY:HA2	1:M:408:LEU:HD12	1.87	0.57
2:W:135:HIS:HB3	3:X:90:ARG:NH1	2.19	0.57
1:A:21:PRO:O	1:A:25:VAL:HG23	2.05	0.57
1:D:168:THR:HB	4:D:902:GLN:HG3	1.85	0.57
2:E:252:ASP:HB3	2:E:255:THR:CG2	2.34	0.57
2:H:140:THR:OG1	3:I:90:ARG:HA	2.05	0.57
1:J:31:ARG:CG	1:J:31:ARG:HH11	2.16	0.57
2:N:39:VAL:CG1	2:N:44:LEU:HD11	2.35	0.57
1:S:35:THR:HG23	1:S:477:LEU:HD12	1.85	0.57
1:A:118:ASP:OD2	1:A:147:SER:HA	2.05	0.57
1:D:435:PRO:HG2	1:D:471:HIS:CG	2.39	0.57
2:E:95:SER:HB3	2:E:127:GLU:HB2	1.87	0.57
2:H:39:VAL:HG13	2:H:44:LEU:HD11	1.87	0.57
1:P:168:THR:N	4:P:906:GLN:OE1	2.38	0.57
2:Q:162:THR:CG2	2:Q:165:GLU:H	2.16	0.57
2:T:162:THR:HG22	2:T:165:GLU:HB2	1.86	0.57
2:W:201:ARG:HD2	2:W:207:GLU:O	2.05	0.57
1:M:138:TRP:CZ2	1:M:438:TRP:CH2	2.93	0.57
1:P:31:ARG:O	1:P:35:THR:CG2	2.49	0.57
1:J:422:VAL:HG22	1:J:423:PRO:HD3	1.87	0.57
1:P:412:ILE:HA	1:P:415:TYR:CD2	2.39	0.57
2:W:97:TYR:O	2:W:123:ARG:NH2	2.28	0.57
2:W:252:ASP:HB3	2:W:255:THR:CG2	2.35	0.57
1:J:412:ILE:HA	1:J:415:TYR:CD2	2.40	0.56
1:S:193:ARG:NH1	1:S:232:THR:OG1	2.36	0.56
2:W:103:THR:CG2	2:W:104:ASN:OD1	2.52	0.56
2:B:412:LEU:CD1	2:B:412:LEU:N	2.69	0.56
1:M:76:LEU:HD12	1:M:96:TYR:CZ	2.40	0.56
1:S:299:ILE:HG13	1:S:419:ILE:HG22	1.86	0.56
2:T:279:VAL:CG2	3:U:59:PRO:HD2	2.35	0.56
1:A:245:VAL:HG12	1:A:459:LEU:HB3	1.86	0.56
1:A:350:ARG:HD3	3:C:29:GLN:OE1	2.06	0.56
2:B:17:MET:HE1	2:B:57:ALA:O	2.04	0.56
2:B:100:PRO:HB3	2:B:123:ARG:NH2	2.06	0.56
1:D:122:MET:CA	1:D:351:ARG:NH1	2.68	0.56
1:D:373:LYS:HE2	3:F:50:PRO:HD3	1.87	0.56
2:H:340:PRO:O	2:H:344:VAL:HG22	2.05	0.56
1:M:171:SER:N	4:M:905:GLN:OE1	2.34	0.56
1:P:178:PHE:HE1	1:P:397:THR:HG21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:384:LYS:O	1:P:387:GLU:HB2	2.06	0.56
1:S:100:VAL:HG12	1:S:223:ILE:HB	1.86	0.56
2:T:402:THR:HG22	2:T:403:PRO:HD2	1.87	0.56
3:U:46:GLU:CD	3:U:46:GLU:N	2.59	0.56
1:V:77:VAL:HG21	1:V:114:LYS:CE	2.34	0.56
2:E:80:ARG:HE	2:E:275:ASP:CG	2.08	0.56
1:P:83:THR:HA	1:P:89:LEU:O	2.04	0.56
1:P:117:LEU:O	1:P:129:SER:HB2	2.05	0.56
1:S:138:TRP:CZ2	1:S:438:TRP:CH2	2.93	0.56
1:A:30:ASP:O	1:A:34:GLN:HG3	2.06	0.56
1:M:138:TRP:CD2	1:M:438:TRP:HZ3	2.23	0.56
1:M:167:ASP:OD1	1:M:170:GLY:N	2.37	0.56
1:M:422:VAL:CG2	1:M:423:PRO:HD3	2.35	0.56
2:Q:95:SER:HB3	2:Q:127:GLU:CB	2.36	0.56
2:T:340:PRO:O	2:T:344:VAL:HG22	2.05	0.56
1:P:163:SER:HB3	1:P:209:PHE:HB2	1.87	0.56
2:E:21:THR:HG22	2:E:22:LYS:N	2.21	0.56
2:K:330:PHE:CE1	2:K:344:VAL:HG13	2.41	0.56
1:V:325:ARG:HA	1:V:339:THR:HG23	1.88	0.56
1:A:306:ALA:HB3	1:A:307:PRO:HD3	1.87	0.56
1:P:100:VAL:HG12	1:P:223:ILE:HB	1.87	0.56
1:V:143:VAL:HG13	1:V:145:GLY:H	1.71	0.56
2:H:156:THR:HG22	2:H:157:GLU:O	2.06	0.56
1:J:306:ALA:HB3	1:J:307:PRO:HD3	1.88	0.56
2:T:320:LEU:HD22	2:T:326:VAL:HG12	1.88	0.56
1:A:171:SER:CB	4:A:901:GLN:OE1	2.52	0.56
2:B:156:THR:HG23	2:B:157:GLU:O	2.05	0.56
2:H:53:VAL:HG12	3:I:60:MET:HG2	1.87	0.56
1:V:163:SER:HB3	1:V:209:PHE:HB2	1.88	0.56
1:J:156:ALA:O	1:J:211:ARG:NH1	2.38	0.55
1:M:21:PRO:O	1:M:25:VAL:HG23	2.05	0.55
2:Q:95:SER:CB	2:Q:127:GLU:HB3	2.36	0.55
1:S:376:ARG:HD2	3:U:49:GLU:O	2.07	0.55
1:V:384:LYS:O	1:V:387:GLU:HB2	2.06	0.55
1:D:172:ILE:CD1	1:D:207:GLY:HA3	2.36	0.55
1:G:171:SER:OG	4:G:903:GLN:CB	2.53	0.55
1:G:178:PHE:CE1	1:G:397:THR:HG21	2.41	0.55
1:S:433:SER:O	1:S:434:ILE:HD13	2.06	0.55
2:W:17:MET:HE1	2:W:57:ALA:HA	1.87	0.55
1:G:190:ARG:HD3	1:G:241:TRP:CH2	2.39	0.55
1:J:90:GLU:O	1:J:91:ASN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:340:PRO:O	2:N:344:VAL:HG22	2.06	0.55
1:S:138:TRP:CE2	1:S:438:TRP:HH2	2.22	0.55
3:I:46:GLU:O	3:I:47:ASN:HB2	2.07	0.55
1:J:167:ASP:HB3	1:J:185:LYS:HG3	1.88	0.55
2:K:21:THR:HB	3:L:63:ASP:OD1	2.07	0.55
1:M:76:LEU:CD1	1:M:96:TYR:CZ	2.89	0.55
1:M:100:VAL:HG12	1:M:223:ILE:HB	1.88	0.55
2:Q:402:THR:HG22	2:Q:403:PRO:HD2	1.88	0.55
1:V:422:VAL:HG22	1:V:423:PRO:HD3	1.88	0.55
2:W:340:PRO:O	2:W:344:VAL:HG22	2.05	0.55
1:D:143:VAL:CG1	1:D:145:GLY:H	2.20	0.55
2:H:331:GLU:HA	2:H:334:VAL:HG12	1.87	0.55
2:N:41:PRO:HB3	2:N:46:MET:HE2	1.87	0.55
1:S:190:ARG:HD3	1:S:241:TRP:CH2	2.40	0.55
1:V:299:ILE:HG13	1:V:419:ILE:HG22	1.88	0.55
1:D:57:LEU:HD22	1:D:65:PHE:CE1	2.41	0.55
1:G:245:VAL:CG1	1:G:459:LEU:HB3	2.37	0.55
1:S:69:ILE:HD12	1:S:162:VAL:HG13	1.88	0.55
1:V:172:ILE:CD1	1:V:207:GLY:HA3	2.37	0.55
1:A:35:THR:CG2	1:A:39:VAL:HG23	2.23	0.55
1:D:68:PRO:HB3	1:D:112:VAL:HG11	1.89	0.55
2:T:170:LEU:CD1	2:T:223:VAL:HG21	2.37	0.55
1:V:123:GLY:N	4:V:908:GLN:O	2.40	0.55
2:B:98:GLU:O	2:B:99:LYS:HB2	2.07	0.55
2:H:252:ASP:HB3	2:H:255:THR:HG22	1.89	0.55
1:M:88:ILE:HA	1:M:324:TYR:HB3	1.88	0.55
1:M:122:MET:HB3	1:M:351:ARG:NH1	2.22	0.55
2:B:21:THR:HG22	2:B:22:LYS:O	2.07	0.55
1:M:394:SER:HB2	1:M:395:PRO:HD2	1.86	0.55
1:D:39:VAL:HG21	1:D:157:VAL:HG11	1.89	0.55
2:H:100:PRO:HB3	2:H:123:ARG:HH21	1.71	0.55
1:J:3:TRP:CE3	1:J:31:ARG:HD2	2.42	0.55
1:J:245:VAL:CG1	1:J:459:LEU:HB3	2.37	0.55
1:P:30:ASP:O	1:P:34:GLN:HG3	2.07	0.55
1:P:169:GLY:H	4:P:906:GLN:CD	2.09	0.55
2:E:17:MET:HE1	2:E:57:ALA:O	2.07	0.54
2:H:21:THR:HG21	3:I:61:ARG:NH1	2.03	0.54
1:S:438:TRP:CZ3	1:S:443:PRO:HG3	2.42	0.54
1:A:100:VAL:HG12	1:A:223:ILE:HB	1.88	0.54
1:G:168:THR:N	4:G:903:GLN:OE1	2.24	0.54
1:G:422:VAL:N	1:G:423:PRO:CD	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:292:LEU:HB2	1:P:295:VAL:HG22	1.89	0.54
2:W:96:GLN:HB2	2:W:125:HIS:HB2	1.88	0.54
1:M:88:ILE:CD1	1:M:120:PHE:CZ	2.90	0.54
2:T:21:THR:CG2	2:T:22:LYS:N	2.70	0.54
1:V:350:ARG:HD3	3:X:29:GLN:OE1	2.07	0.54
1:M:162:VAL:HG21	1:M:219:VAL:HG21	1.89	0.54
1:S:279:GLU:HG3	1:S:468:LYS:HZ3	1.72	0.54
1:G:138:TRP:CE2	1:G:438:TRP:CH2	2.96	0.54
2:N:346:TRP:O	2:N:350:ASP:HB2	2.06	0.54
1:A:168:THR:HG22	1:A:302:TYR:OH	2.08	0.54
1:D:182:ILE:HG12	1:D:434:ILE:CD1	2.38	0.54
1:P:190:ARG:HD3	1:P:241:TRP:HH2	1.72	0.54
1:S:245:VAL:HG12	1:S:459:LEU:HB3	1.89	0.54
1:S:81:LYS:CE	1:S:91:ASN:HA	2.35	0.54
1:V:157:VAL:HG23	1:V:159:SER:H	1.72	0.54
1:D:299:ILE:CB	1:D:300:PRO:HD3	2.37	0.54
1:D:299:ILE:HG13	1:D:419:ILE:HG22	1.89	0.54
2:E:255:THR:HG23	2:E:257:LYS:H	1.72	0.54
1:P:122:MET:CB	1:P:351:ARG:NH1	2.71	0.54
1:P:438:TRP:CH2	1:P:443:PRO:HG3	2.42	0.54
2:T:80:ARG:HE	2:T:275:ASP:CG	2.11	0.54
2:W:56:ARG:HD2	3:X:63:ASP:OD2	2.06	0.54
1:A:422:VAL:CG2	1:A:423:PRO:HD3	2.38	0.54
2:B:103:THR:CG2	2:B:104:ASN:OD1	2.56	0.54
2:K:21:THR:HG21	3:L:61:ARG:NH1	2.16	0.54
1:J:384:LYS:O	1:J:387:GLU:HB2	2.08	0.54
1:S:143:VAL:CG1	1:S:145:GLY:H	2.21	0.54
2:W:17:MET:HE3	2:W:60:TYR:HB2	1.89	0.54
1:A:120:PHE:CE2	1:A:344:PHE:HE1	2.26	0.53
1:A:151:SER:HB3	1:A:163:SER:OG	2.08	0.53
2:T:252:ASP:OD2	2:T:255:THR:HG22	2.09	0.53
1:D:265:LEU:HD11	1:D:395:PRO:HG2	1.90	0.53
1:J:294:HIS:HB2	1:J:381:ASP:OD2	2.08	0.53
1:P:29:TYR:O	1:P:32:TYR:HB3	2.09	0.53
2:Q:113:ASN:HD21	2:Q:115:GLU:CD	2.12	0.53
1:V:168:THR:H	4:V:908:GLN:CD	2.10	0.53
2:W:130:ALA:O	2:W:146:ARG:HG2	2.08	0.53
2:W:140:THR:OG1	3:X:90:ARG:HA	2.08	0.53
2:W:156:THR:HG22	2:W:157:GLU:O	2.09	0.53
1:D:405:GLY:HA2	1:D:408:LEU:HD12	1.90	0.53
1:G:329:TYR:CE2	3:I:89:PRO:HG3	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:98:GLU:O	2:K:99:LYS:HB2	2.09	0.53
1:V:171:SER:CB	4:V:908:GLN:OE1	2.55	0.53
2:W:157:GLU:O	2:W:159:ASP:N	2.38	0.53
1:A:279:GLU:HG3	1:A:468:LYS:CE	2.38	0.53
2:B:320:LEU:HD22	2:B:326:VAL:HG12	1.90	0.53
1:D:292:LEU:O	1:D:295:VAL:HG22	2.09	0.53
1:G:171:SER:OG	4:G:903:GLN:HB3	2.08	0.53
1:S:77:VAL:CG2	1:S:114:LYS:HE3	2.37	0.53
1:G:373:LYS:CE	3:I:50:PRO:HD3	2.39	0.53
2:K:95:SER:CB	2:K:127:GLU:HB3	2.37	0.53
1:P:172:ILE:CD1	1:P:207:GLY:HA3	2.38	0.53
2:Q:95:SER:HB3	2:Q:127:GLU:HB2	1.90	0.53
1:A:64:LEU:HD23	1:A:67:ILE:HG13	1.90	0.53
1:A:376:ARG:HG3	1:A:376:ARG:NH1	2.24	0.53
2:B:40:CYS:O	2:B:44:LEU:CD1	2.56	0.53
2:B:402:THR:HG22	2:B:403:PRO:HD2	1.90	0.53
2:Q:109:LEU:HD11	2:Q:169:PHE:HA	1.90	0.53
1:A:373:LYS:HE2	3:C:50:PRO:HD3	1.89	0.53
2:H:282:LYS:HD3	3:I:55:PHE:CE2	2.44	0.53
1:S:69:ILE:HD11	1:S:164:LEU:HD13	1.90	0.53
1:S:77:VAL:HG23	1:S:114:LYS:CE	2.38	0.53
1:S:299:ILE:HB	1:S:300:PRO:HD3	1.91	0.53
1:M:138:TRP:CD2	1:M:438:TRP:CZ3	2.97	0.53
3:O:71:ARG:NH1	3:O:84:GLY:HA3	2.23	0.53
1:P:299:ILE:N	1:P:300:PRO:HD2	2.24	0.53
1:P:318:ASP:HB2	1:P:336:TYR:HE1	1.74	0.53
2:T:21:THR:HG21	3:U:61:ARG:NH1	2.09	0.53
2:T:128:GLU:HB2	2:T:148:GLY:HA2	1.89	0.53
1:A:157:VAL:HG23	1:A:159:SER:H	1.74	0.53
1:V:190:ARG:HD3	1:V:241:TRP:HH2	1.74	0.53
2:E:17:MET:HE3	2:E:60:TYR:CB	2.39	0.53
1:G:138:TRP:CD2	1:G:438:TRP:HZ3	2.27	0.53
2:H:230:GLU:OE2	2:H:233:ARG:NH1	2.41	0.53
1:J:58:LYS:HG2	2:Q:240:GLU:HB3	1.91	0.53
2:T:21:THR:HG22	2:T:22:LYS:O	2.09	0.53
2:T:106:TRP:CD1	2:T:118:LYS:HE2	2.44	0.53
1:D:322:TYR:CZ	2:E:47:PRO:HD3	2.43	0.52
1:G:126:THR:O	1:G:126:THR:HG22	2.08	0.52
1:G:374:VAL:HG21	3:I:40:LEU:HD22	1.91	0.52
2:T:201:ARG:HD2	2:T:207:GLU:O	2.09	0.52
2:B:141:LEU:HD23	3:C:85:PHE:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:TRP:CZ2	1:G:438:TRP:CH2	2.97	0.52
1:G:438:TRP:CZ3	1:G:443:PRO:HG3	2.45	0.52
2:H:184:LYS:HB2	2:H:191:GLN:OE1	2.09	0.52
2:Q:21:THR:HB	3:R:63:ASP:OD1	2.10	0.52
2:T:162:THR:CG2	2:T:165:GLU:H	2.22	0.52
2:T:370:GLU:CD	2:T:370:GLU:H	2.13	0.52
1:A:318:ASP:HB2	1:A:336:TYR:HE1	1.73	0.52
1:D:294:HIS:HB2	1:D:381:ASP:OD2	2.09	0.52
2:E:85:TYR:HD2	2:E:87:ASP:OD1	1.93	0.52
3:F:80:GLU:HG2	3:F:87:VAL:HB	1.90	0.52
2:K:103:THR:CG2	2:K:104:ASN:OD1	2.58	0.52
2:K:252:ASP:OD2	2:K:255:THR:HG22	2.08	0.52
1:P:90:GLU:O	1:P:91:ASN:HB2	2.08	0.52
1:V:172:ILE:C	1:V:175:PRO:HD2	2.29	0.52
1:J:270:LYS:HE3	1:J:274:GLU:OE2	2.09	0.52
2:K:233:ARG:O	2:K:237:VAL:HG23	2.10	0.52
2:K:252:ASP:HB3	2:K:255:THR:HG22	1.91	0.52
1:M:299:ILE:N	1:M:300:PRO:CD	2.72	0.52
1:A:115:THR:HG21	1:A:151:SER:OG	2.09	0.52
2:K:17:MET:HE1	2:K:60:TYR:CB	2.39	0.52
2:K:74:GLU:HG2	2:K:283:VAL:O	2.09	0.52
2:E:118:LYS:NZ	1:G:291:SER:HB3	2.24	0.52
2:H:39:VAL:CG1	2:H:44:LEU:HD11	2.40	0.52
1:M:373:LYS:HE2	3:O:50:PRO:HD3	1.92	0.52
1:S:73:ASP:OD2	1:S:83:THR:OG1	2.23	0.52
1:A:172:ILE:O	1:A:175:PRO:HD2	2.10	0.52
1:D:279:GLU:HG3	1:D:468:LYS:NZ	2.24	0.52
2:E:162:THR:HG22	2:E:165:GLU:H	1.74	0.52
1:J:31:ARG:NE	1:J:157:VAL:O	2.35	0.52
3:L:88:VAL:CB	3:L:89:PRO:HD2	2.29	0.52
2:N:39:VAL:HG13	2:N:44:LEU:CD1	2.37	0.52
1:S:422:VAL:HG22	1:S:423:PRO:HD3	1.91	0.52
2:B:310:TYR:CE1	2:B:334:VAL:HG11	2.45	0.52
2:B:330:PHE:CE1	2:B:344:VAL:HG13	2.45	0.52
2:B:412:LEU:HD22	2:B:412:LEU:C	2.23	0.52
1:D:7:LEU:HD21	1:D:161:PRO:HB2	1.92	0.52
1:M:332:ILE:CD1	3:O:88:VAL:HG21	2.38	0.52
1:V:434:ILE:HD11	1:V:462:SER:OG	2.09	0.52
2:B:146:ARG:HG2	2:B:146:ARG:NH1	2.24	0.52
2:H:233:ARG:O	2:H:237:VAL:HG23	2.10	0.52
2:K:340:PRO:O	2:K:344:VAL:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:88:ILE:HG23	1:M:343:GLY:C	2.29	0.52
1:M:171:SER:HB2	4:M:905:GLN:CD	2.30	0.52
2:Q:22:LYS:HE3	2:Q:27:CYS:HB2	1.92	0.52
2:T:302:ARG:HD3	2:T:321:VAL:HG22	1.92	0.52
1:A:292:LEU:O	1:A:295:VAL:HG22	2.10	0.52
1:D:30:ASP:O	1:D:34:GLN:HG3	2.10	0.52
2:N:355:LEU:HD21	2:N:365:SER:HB2	1.91	0.52
2:Q:17:MET:HE3	2:Q:60:TYR:HB3	1.91	0.52
1:S:299:ILE:CB	1:S:300:PRO:HD3	2.40	0.52
2:K:13:ILE:HG22	2:K:15:VAL:HG23	1.91	0.51
1:M:76:LEU:HD23	1:M:82:THR:HG21	1.93	0.51
1:M:168:THR:H	4:M:905:GLN:CD	2.12	0.51
1:P:5:LYS:HB2	1:P:10:LEU:HD13	1.93	0.51
2:Q:140:THR:OG1	3:R:90:ARG:HA	2.10	0.51
2:T:331:GLU:HA	2:T:334:VAL:HG12	1.91	0.51
1:V:77:VAL:CG2	1:V:114:LYS:HZ2	2.23	0.51
2:E:217:VAL:HG12	2:E:222:PHE:HB3	1.92	0.51
1:G:39:VAL:HG21	1:G:157:VAL:HG11	1.92	0.51
1:M:86:SER:HB2	1:M:119:GLU:HG3	1.91	0.51
1:P:234:ALA:HB1	1:P:236:VAL:HG23	1.91	0.51
1:P:397:THR:HG22	1:P:399:THR:H	1.73	0.51
1:V:350:ARG:NH1	3:X:29:GLN:OE1	2.40	0.51
2:B:156:THR:CG2	2:B:157:GLU:O	2.59	0.51
2:T:100:PRO:HB3	2:T:123:ARG:NH1	2.25	0.51
1:V:69:ILE:HD11	1:V:164:LEU:HD13	1.91	0.51
1:A:57:LEU:HD12	1:A:110:LEU:HD21	1.93	0.51
2:B:96:GLN:HB2	2:B:125:HIS:HB2	1.91	0.51
2:B:279:VAL:HG21	3:C:59:PRO:HD2	1.92	0.51
2:E:170:LEU:HD12	2:E:223:VAL:HG21	1.93	0.51
1:J:95:PRO:HG2	2:K:46:MET:CE	2.41	0.51
1:J:302:TYR:HH	4:J:904:GLN:HA	1.75	0.51
1:M:438:TRP:CZ3	1:M:443:PRO:HG3	2.45	0.51
1:S:403:LYS:O	1:S:406:GLU:HB2	2.10	0.51
2:T:103:THR:CG2	2:T:104:ASN:OD1	2.59	0.51
2:W:302:ARG:HD3	2:W:321:VAL:HG22	1.91	0.51
1:A:122:MET:HB3	1:A:351:ARG:NH1	2.26	0.51
2:B:340:PRO:O	2:B:344:VAL:HG22	2.10	0.51
3:C:88:VAL:CB	3:C:89:PRO:HD2	2.24	0.51
2:K:374:GLU:O	2:K:377:LYS:HB3	2.11	0.51
1:M:299:ILE:HG13	1:M:419:ILE:HG22	1.93	0.51
3:R:45:THR:O	3:R:45:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ALA:HA	1:A:195:GLY:HA3	1.92	0.51
2:E:412:LEU:C	2:E:412:LEU:CD2	2.71	0.51
2:H:103:THR:CG2	2:H:104:ASN:OD1	2.58	0.51
1:J:87:LYS:C	1:J:89:LEU:H	2.14	0.51
2:K:22:LYS:HE3	2:K:27:CYS:HB2	1.92	0.51
1:P:314:LEU:HD23	1:P:352:ILE:HD11	1.93	0.51
1:S:168:THR:HG21	1:S:199:PHE:CD2	2.46	0.51
1:S:190:ARG:HG3	1:S:190:ARG:HH11	1.74	0.51
1:A:434:ILE:HG21	1:A:462:SER:OG	2.11	0.51
2:B:399:THR:OG1	2:B:400:GLY:N	2.43	0.51
1:D:384:LYS:O	1:D:387:GLU:HB2	2.10	0.51
2:E:109:LEU:HD11	2:E:169:PHE:HA	1.93	0.51
1:M:438:TRP:CH2	1:M:443:PRO:HG3	2.46	0.51
2:Q:17:MET:CE	2:Q:60:TYR:HB3	2.41	0.51
2:Q:222:PHE:CZ	2:Q:253:PRO:HB3	2.46	0.51
1:V:100:VAL:HG12	1:V:223:ILE:HB	1.93	0.51
2:B:255:THR:HG23	2:B:257:LYS:H	1.76	0.51
2:E:128:GLU:HB2	2:E:148:GLY:HA2	1.92	0.51
2:E:170:LEU:CD1	2:E:223:VAL:HG21	2.41	0.51
1:J:318:ASP:HB2	1:J:336:TYR:HE1	1.74	0.51
2:N:14:HIS:CD2	2:N:127:GLU:OE2	2.62	0.51
1:A:185:LYS:O	1:A:185:LYS:HG2	2.11	0.51
1:J:168:THR:HB	4:J:904:GLN:HG3	1.93	0.51
1:J:169:GLY:HA2	1:J:425:ASN:OD1	2.10	0.51
1:V:185:LYS:NZ	1:V:186:PRO:O	2.40	0.51
1:V:373:LYS:HE2	3:X:50:PRO:HD3	1.93	0.51
2:E:402:THR:HG22	2:E:403:PRO:HD2	1.93	0.51
2:N:128:GLU:HB2	2:N:148:GLY:HA2	1.91	0.51
2:E:252:ASP:CB	2:E:255:THR:HG22	2.39	0.50
1:G:171:SER:OG	4:G:903:GLN:CG	2.58	0.50
2:Q:305:ARG:O	2:Q:309:GLU:HB2	2.11	0.50
2:W:83:TYR:CZ	2:W:88:LEU:HD22	2.47	0.50
2:W:302:ARG:NH2	2:W:328:ASP:OD1	2.45	0.50
2:B:279:VAL:CG2	3:C:59:PRO:HD2	2.41	0.50
1:M:90:GLU:O	1:M:90:GLU:HG3	2.11	0.50
1:M:332:ILE:HD13	3:O:88:VAL:CG2	2.40	0.50
1:M:422:VAL:HG22	1:M:423:PRO:HD3	1.92	0.50
1:P:464:LEU:O	1:P:464:LEU:CD1	2.34	0.50
1:A:60:ARG:HA	1:A:65:PHE:CD1	2.45	0.50
1:A:95:PRO:HG2	2:B:46:MET:CE	2.42	0.50
2:H:123:ARG:HG2	2:H:155:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:190:ARG:HD2	1:S:455:GLU:OE2	2.11	0.50
1:S:463:TYR:O	1:S:467:GLN:HG2	2.12	0.50
2:E:39:VAL:HG22	2:E:44:LEU:CG	2.37	0.50
2:K:17:MET:HE1	2:K:60:TYR:HB2	1.91	0.50
2:K:39:VAL:CG1	2:K:44:LEU:HD11	2.37	0.50
2:K:73:HIS:NE2	2:K:103:THR:HB	2.26	0.50
1:S:157:VAL:HG23	1:S:159:SER:H	1.77	0.50
1:S:190:ARG:HG3	1:S:190:ARG:NH1	2.26	0.50
2:T:26:GLY:O	3:U:65:PRO:HA	2.12	0.50
2:T:109:LEU:HD11	2:T:169:PHE:HA	1.93	0.50
1:V:60:ARG:HA	1:V:65:PHE:CD1	2.46	0.50
1:A:32:TYR:CE1	1:A:36:GLU:HG2	2.47	0.50
2:E:40:CYS:HB2	2:E:41:PRO:CD	2.42	0.50
1:J:194:TYR:CE2	1:J:229:LYS:HD2	2.47	0.50
1:S:172:ILE:HD13	1:S:207:GLY:HA3	1.93	0.50
1:S:438:TRP:CH2	1:S:443:PRO:HG3	2.46	0.50
1:V:298:SER:HB3	1:V:422:VAL:HG23	1.94	0.50
2:N:17:MET:HE1	2:N:60:TYR:HB2	1.93	0.50
3:O:88:VAL:CB	3:O:89:PRO:CD	2.77	0.50
1:P:270:LYS:HE3	1:P:274:GLU:OE2	2.11	0.50
1:D:403:LYS:O	1:D:406:GLU:HB2	2.12	0.50
2:E:103:THR:HG22	2:E:104:ASN:CG	2.32	0.50
1:J:83:THR:HG22	1:J:90:GLU:HA	1.93	0.50
2:K:396:MET:HE1	2:K:403:PRO:HB3	1.94	0.50
2:T:412:LEU:CD1	2:T:412:LEU:N	2.75	0.50
2:E:222:PHE:CZ	2:E:253:PRO:HB3	2.46	0.50
3:F:3:ASP:O	3:F:7:VAL:HG23	2.11	0.50
1:M:403:LYS:O	1:M:406:GLU:HB2	2.12	0.50
1:P:3:TRP:CZ2	1:P:31:ARG:HG3	2.47	0.50
1:S:5:LYS:HB2	1:S:10:LEU:HD13	1.92	0.50
1:S:181:VAL:HG22	1:S:210:GLY:O	2.11	0.50
1:V:190:ARG:HD2	1:V:455:GLU:OE2	2.11	0.50
1:A:298:SER:HB3	1:A:422:VAL:HG23	1.94	0.50
1:D:2:LEU:HB3	1:D:27:SER:OG	2.12	0.50
2:K:17:MET:HE3	2:K:60:TYR:HB3	1.93	0.50
1:S:2:LEU:HB3	1:S:27:SER:OG	2.12	0.50
1:V:5:LYS:HB2	1:V:10:LEU:HD13	1.93	0.50
1:V:98:ALA:HA	1:V:195:GLY:HA3	1.93	0.50
2:E:119:VAL:HG13	2:E:159:ASP:HB2	1.93	0.49
1:G:13:LEU:HB3	1:G:19:VAL:HG12	1.94	0.49
2:K:106:TRP:CD1	2:K:118:LYS:HD3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:190:ARG:HD3	1:P:241:TRP:CH2	2.46	0.49
1:V:126:THR:OG1	1:V:149:GLY:HA3	2.12	0.49
1:A:26:GLU:HG3	1:A:51:LEU:HD11	1.93	0.49
1:G:403:LYS:O	1:G:406:GLU:HB2	2.12	0.49
1:J:58:LYS:HE2	2:Q:240:GLU:O	2.12	0.49
2:T:85:TYR:CD2	2:T:87:ASP:OD1	2.52	0.49
2:T:412:LEU:N	2:T:412:LEU:HD13	2.26	0.49
1:V:167:ASP:OD1	1:V:170:GLY:N	2.43	0.49
1:D:1:MET:O	1:D:1:MET:HG2	2.11	0.49
1:G:85:ALA:HB3	1:G:117:LEU:HD13	1.91	0.49
2:H:97:TYR:O	2:H:123:ARG:NH2	2.45	0.49
2:H:255:THR:HG21	2:H:259:TYR:OH	2.12	0.49
2:N:8:VAL:CG1	2:N:158:PRO:HB2	2.39	0.49
2:N:202:PRO:O	2:N:205:SER:HB3	2.12	0.49
1:P:294:HIS:HB2	1:P:381:ASP:OD2	2.12	0.49
1:S:395:PRO:O	1:S:420:LEU:HD13	2.12	0.49
2:B:17:MET:HE1	2:B:57:ALA:HA	1.94	0.49
2:E:106:TRP:CD1	2:E:118:LYS:HE2	2.48	0.49
1:A:297:TYR:C	1:A:300:PRO:HD2	2.33	0.49
1:A:351:ARG:NH1	4:A:901:GLN:OXT	2.37	0.49
3:F:33:ILE:O	3:F:37:ILE:HG12	2.12	0.49
2:K:90:LYS:NZ	2:K:128:GLU:OE2	2.42	0.49
1:S:167:ASP:HB2	1:S:172:ILE:HD12	1.93	0.49
1:A:318:ASP:HB2	1:A:336:TYR:CE1	2.47	0.49
1:D:157:VAL:HG23	1:D:159:SER:H	1.77	0.49
1:D:438:TRP:CH2	1:D:443:PRO:HG3	2.48	0.49
2:E:98:GLU:O	2:E:98:GLU:HG3	2.13	0.49
2:N:13:ILE:HG22	2:N:15:VAL:HG23	1.94	0.49
1:P:138:TRP:CE2	1:P:438:TRP:CH2	3.00	0.49
1:V:120:PHE:CE2	1:V:344:PHE:HE1	2.31	0.49
1:G:122:MET:HB3	1:G:351:ARG:NH1	2.27	0.49
1:G:134:THR:HG22	1:G:144:PRO:HG3	1.95	0.49
2:H:22:LYS:HE3	2:H:27:CYS:HB2	1.94	0.49
2:K:167:ARG:O	2:K:171:GLU:HG3	2.13	0.49
3:L:33:ILE:O	3:L:37:ILE:HG12	2.13	0.49
2:N:125:HIS:NE2	2:N:153:GLU:OE1	2.45	0.49
2:W:128:GLU:HB2	2:W:148:GLY:HA2	1.95	0.49
1:A:422:VAL:HG22	1:A:423:PRO:HD3	1.95	0.49
2:B:331:GLU:O	2:B:334:VAL:HG12	2.12	0.49
1:J:100:VAL:HG12	1:J:223:ILE:HB	1.94	0.49
1:P:87:LYS:C	1:P:89:LEU:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:118:ASP:OD2	1:V:147:SER:HA	2.12	0.49
1:D:77:VAL:CG2	1:D:114:LYS:HZ1	2.23	0.49
2:E:40:CYS:O	2:E:44:LEU:HB2	2.12	0.49
1:M:318:ASP:HB2	1:M:336:TYR:CE1	2.48	0.49
2:W:184:LYS:HB2	2:W:191:GLN:OE1	2.13	0.49
1:D:293:PRO:HG3	2:H:106:TRP:CE3	2.47	0.49
2:H:302:ARG:HD3	2:H:321:VAL:HG22	1.95	0.49
2:K:17:MET:HE2	2:K:60:TYR:CB	2.38	0.49
2:K:331:GLU:HA	2:K:334:VAL:HG12	1.94	0.49
1:S:98:ALA:HA	1:S:195:GLY:HA3	1.94	0.49
2:T:132:LYS:HE2	2:T:146:ARG:HH21	1.78	0.49
2:W:255:THR:HG23	2:W:257:LYS:H	1.77	0.49
1:A:172:ILE:CD1	1:A:207:GLY:HA3	2.43	0.48
1:D:88:ILE:HG13	1:D:343:GLY:HA3	1.94	0.48
1:D:122:MET:HA	1:D:351:ARG:NH1	2.26	0.48
1:D:303:TYR:CE2	1:D:415:TYR:HB3	2.48	0.48
2:H:320:LEU:HD22	2:H:326:VAL:HG12	1.95	0.48
2:T:4:LYS:O	2:T:203:LYS:HB2	2.12	0.48
2:H:103:THR:HG22	2:H:104:ASN:OD1	2.13	0.48
1:J:57:LEU:HD22	1:J:65:PHE:CE1	2.48	0.48
1:V:245:VAL:CG1	1:V:459:LEU:HB3	2.43	0.48
1:J:90:GLU:O	1:J:91:ASN:CB	2.61	0.48
1:M:317:TYR:HE1	2:N:47:PRO:HG3	1.77	0.48
1:P:418:ASP:OD2	4:P:906:GLN:N	2.46	0.48
2:T:96:GLN:HB2	2:T:125:HIS:HB2	1.95	0.48
1:V:171:SER:O	1:V:175:PRO:HG2	2.13	0.48
1:G:98:ALA:HA	1:G:195:GLY:HA3	1.95	0.48
1:G:172:ILE:HD13	1:G:207:GLY:HA3	1.95	0.48
2:K:298:LEU:HB3	2:K:299:PRO:CD	2.44	0.48
1:A:71:VAL:HG12	1:A:114:LYS:HE3	1.94	0.48
1:G:122:MET:CB	1:G:351:ARG:NH1	2.77	0.48
1:G:395:PRO:O	1:G:420:LEU:HD13	2.12	0.48
1:M:171:SER:HB2	4:M:905:GLN:OE1	2.14	0.48
1:P:28:PHE:CD2	1:P:68:PRO:HG2	2.48	0.48
1:S:57:LEU:HD22	1:S:65:PHE:CE1	2.48	0.48
1:V:316:ARG:O	1:V:321:ARG:NH2	2.47	0.48
2:B:142:VAL:HB	3:C:86:PHE:HB2	1.94	0.48
2:B:170:LEU:HD12	2:B:223:VAL:HG21	1.96	0.48
1:M:172:ILE:HD13	1:M:207:GLY:HA3	1.96	0.48
2:N:170:LEU:HD12	2:N:223:VAL:HG21	1.95	0.48
1:V:335:MET:O	1:V:339:THR:OG1	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:40:CYS:HB2	2:W:41:PRO:HD2	1.95	0.48
1:D:122:MET:CA	1:D:351:ARG:HH12	2.23	0.48
2:N:140:THR:OG1	3:O:90:ARG:HA	2.14	0.48
1:V:57:LEU:HD12	1:V:110:LEU:HD21	1.96	0.48
2:W:123:ARG:NH1	2:W:125:HIS:ND1	2.57	0.48
1:M:57:LEU:HD12	1:M:110:LEU:HD21	1.95	0.48
1:V:143:VAL:CG1	1:V:145:GLY:H	2.26	0.48
1:V:190:ARG:HD3	1:V:241:TRP:CH2	2.49	0.48
2:W:17:MET:HE3	2:W:60:TYR:CB	2.44	0.48
2:H:20:LYS:HE2	2:H:56:ARG:HH12	1.79	0.48
2:K:128:GLU:HB2	2:K:148:GLY:HA2	1.94	0.48
2:K:360:ILE:CD1	2:K:366:PRO:HD3	2.44	0.48
1:M:279:GLU:HG3	1:M:468:LYS:HZ1	1.79	0.48
2:N:167:ARG:HG3	2:N:220:PHE:HB3	1.96	0.48
2:N:282:LYS:HD3	3:O:55:PHE:CE2	2.49	0.48
1:S:81:LYS:HE2	1:S:91:ASN:CA	2.40	0.48
1:S:318:ASP:HB2	1:S:336:TYR:CE1	2.49	0.48
2:W:85:TYR:HD2	2:W:87:ASP:OD1	1.96	0.48
2:B:396:MET:HG3	2:B:406:ILE:HD11	1.96	0.48
2:K:201:ARG:HD2	2:K:207:GLU:O	2.14	0.48
1:M:373:LYS:CE	3:O:50:PRO:HD3	2.44	0.48
1:V:322:TYR:CZ	2:W:47:PRO:HD3	2.49	0.48
2:W:360:ILE:CD1	2:W:366:PRO:HD3	2.44	0.48
1:A:32:TYR:CE1	1:A:36:GLU:CG	2.96	0.47
2:B:360:ILE:HD11	2:B:364:GLU:O	2.13	0.47
2:E:41:PRO:HB3	2:E:46:MET:HE2	1.95	0.47
1:J:138:TRP:CE2	1:J:438:TRP:CH2	3.02	0.47
1:M:39:VAL:HG21	1:M:157:VAL:HG11	1.96	0.47
1:V:171:SER:OG	4:V:908:GLN:CG	2.61	0.47
2:W:39:VAL:HG13	2:W:44:LEU:CD1	2.39	0.47
1:D:463:TYR:O	1:D:467:GLN:HG2	2.14	0.47
1:G:279:GLU:HG3	1:G:468:LYS:NZ	2.29	0.47
1:G:397:THR:HG22	1:G:399:THR:H	1.76	0.47
2:H:39:VAL:HG13	2:H:44:LEU:CD1	2.44	0.47
1:S:70:ALA:HB1	1:S:115:THR:CG2	2.44	0.47
1:S:88:ILE:HG23	1:S:89:LEU:HD13	1.96	0.47
3:C:34:LEU:HD12	3:C:37:ILE:HD11	1.96	0.47
2:E:310:TYR:CE1	2:E:334:VAL:HG11	2.49	0.47
3:F:70:ASP:OD2	3:F:72:GLU:HB3	2.14	0.47
1:G:90:GLU:O	1:G:91:ASN:CB	2.62	0.47
2:W:39:VAL:CG1	2:W:44:LEU:HD11	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:ARG:NH2	2:B:328:ASP:OD1	2.48	0.47
2:H:385:SER:OG	2:H:388:ILE:HG12	2.15	0.47
1:J:356:THR:HG21	3:L:14:ALA:HB2	1.95	0.47
1:M:353:MET:O	1:M:356:THR:HG23	2.14	0.47
2:T:156:THR:CG2	2:T:157:GLU:O	2.62	0.47
1:V:181:VAL:HG13	1:V:210:GLY:O	2.15	0.47
2:W:142:VAL:HB	3:X:86:PHE:HB2	1.96	0.47
2:E:106:TRP:CE3	1:G:293:PRO:HG3	2.50	0.47
2:E:252:ASP:OD2	2:E:255:THR:HG22	2.14	0.47
1:J:138:TRP:CE2	1:J:438:TRP:CZ3	3.02	0.47
1:J:172:ILE:CD1	1:J:207:GLY:HA3	2.44	0.47
2:N:35:PRO:HG3	3:O:85:PHE:CE2	2.50	0.47
1:V:172:ILE:O	1:V:175:PRO:HD2	2.14	0.47
2:B:213:GLU:OE1	2:B:215:LYS:HE2	2.14	0.47
1:G:123:GLY:N	4:G:903:GLN:O	2.48	0.47
2:H:402:THR:HG22	2:H:403:PRO:HD2	1.95	0.47
1:P:57:LEU:HD22	1:P:65:PHE:CE1	2.49	0.47
2:T:21:THR:CG2	3:U:61:ARG:HH12	2.12	0.47
1:V:292:LEU:O	1:V:295:VAL:HG22	2.14	0.47
2:W:53:VAL:HG12	3:X:60:MET:HG2	1.97	0.47
2:W:73:HIS:NE2	2:W:103:THR:HB	2.30	0.47
1:A:384:LYS:O	1:A:387:GLU:HB2	2.14	0.47
2:B:109:LEU:HD11	2:B:169:PHE:HA	1.96	0.47
2:E:146:ARG:HH11	2:E:146:ARG:HG2	1.80	0.47
2:E:320:LEU:HD22	2:E:326:VAL:HG12	1.94	0.47
1:J:1:MET:O	1:J:1:MET:HG2	2.15	0.47
1:J:31:ARG:HH11	1:J:31:ARG:HG2	1.80	0.47
1:J:299:ILE:CB	1:J:300:PRO:HD3	2.44	0.47
2:N:3:GLU:HG3	2:N:5:TYR:H	1.79	0.47
1:P:422:VAL:N	1:P:423:PRO:CD	2.78	0.47
1:S:46:LEU:HD11	1:S:80:GLU:HG3	1.96	0.47
1:S:194:TYR:CD1	1:S:229:LYS:HB3	2.50	0.47
2:T:40:CYS:HB2	2:T:41:PRO:CD	2.45	0.47
2:T:255:THR:HG23	2:T:257:LYS:H	1.79	0.47
2:T:374:GLU:HB3	2:T:403:PRO:HG2	1.95	0.47
1:D:88:ILE:HG23	1:D:89:LEU:HD13	1.97	0.47
1:D:293:PRO:HG3	2:H:106:TRP:CZ3	2.50	0.47
1:G:298:SER:HB3	1:G:422:VAL:HG23	1.97	0.47
2:Q:34:GLU:O	2:Q:37:THR:HG23	2.15	0.47
2:T:119:VAL:HG13	2:T:159:ASP:HB2	1.96	0.47
1:D:98:ALA:HA	1:D:195:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:272:TYR:O	2:E:273:PHE:HB3	2.14	0.47
1:P:174:GLN:HE21	1:P:174:GLN:HB2	1.51	0.47
2:T:201:ARG:CD	2:T:207:GLU:O	2.63	0.47
1:V:71:VAL:CB	1:V:114:LYS:HZ3	2.21	0.47
1:A:155:VAL:HG21	1:A:163:SER:HB3	1.97	0.47
2:B:252:ASP:OD2	2:B:255:THR:HG22	2.15	0.47
1:G:138:TRP:CE2	1:G:438:TRP:CZ3	3.03	0.47
2:N:117:LYS:HG2	2:N:118:LYS:N	2.29	0.47
2:N:302:ARG:HD3	2:N:321:VAL:HG22	1.97	0.47
3:X:46:GLU:O	3:X:47:ASN:HB2	2.14	0.47
1:A:245:VAL:CG1	1:A:459:LEU:HB3	2.45	0.46
2:E:24:PHE:HA	2:E:52:ILE:O	2.15	0.46
1:J:126:THR:O	1:J:126:THR:HG22	2.14	0.46
2:K:40:CYS:HB2	2:K:41:PRO:CD	2.45	0.46
2:K:412:LEU:O	2:K:412:LEU:HD22	2.15	0.46
2:Q:201:ARG:HD2	2:Q:207:GLU:O	2.15	0.46
1:S:292:LEU:O	1:S:295:VAL:HG22	2.15	0.46
2:T:82:HIS:CD2	2:T:92:TYR:HB3	2.50	0.46
2:W:17:MET:HE1	2:W:57:ALA:O	2.15	0.46
2:E:83:TYR:CZ	2:E:88:LEU:HD22	2.49	0.46
2:E:100:PRO:HB3	2:E:123:ARG:NH2	2.30	0.46
2:E:279:VAL:CG2	3:F:59:PRO:HD2	2.45	0.46
2:E:360:ILE:HD12	2:E:366:PRO:HD3	1.97	0.46
2:N:96:GLN:HB2	2:N:125:HIS:HB2	1.97	0.46
1:S:13:LEU:HB3	1:S:19:VAL:CG1	2.41	0.46
1:V:318:ASP:HB2	1:V:336:TYR:HE1	1.80	0.46
1:A:279:GLU:HG3	1:A:468:LYS:HZ3	1.75	0.46
1:J:3:TRP:CZ3	1:J:31:ARG:HD2	2.51	0.46
1:M:171:SER:OG	4:M:905:GLN:CB	2.63	0.46
1:M:422:VAL:N	1:M:423:PRO:CD	2.79	0.46
1:P:169:GLY:HA2	1:P:425:ASN:OD1	2.15	0.46
1:V:2:LEU:HB3	1:V:27:SER:OG	2.15	0.46
1:D:77:VAL:HG22	1:D:101:ILE:HG13	1.97	0.46
1:D:422:VAL:N	1:D:423:PRO:CD	2.79	0.46
3:L:88:VAL:HB	3:L:89:PRO:CD	2.31	0.46
1:P:16:ARG:HB2	1:P:18:GLU:OE2	2.15	0.46
1:P:123:GLY:N	4:P:906:GLN:O	2.48	0.46
2:Q:170:LEU:CD1	2:Q:223:VAL:HG21	2.45	0.46
1:S:73:ASP:HA	1:S:114:LYS:HZ3	1.80	0.46
2:B:184:LYS:HB2	2:B:191:GLN:OE1	2.15	0.46
1:G:212:ARG:O	1:G:215:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:373:LYS:HE2	3:I:50:PRO:HD3	1.96	0.46
1:S:88:ILE:HG13	1:S:343:GLY:HA3	1.98	0.46
1:S:204:ASP:O	1:S:205:GLN:HG2	2.14	0.46
1:A:95:PRO:HG2	2:B:46:MET:HE3	1.96	0.46
1:A:190:ARG:NH1	1:A:190:ARG:CG	2.61	0.46
1:D:185:LYS:NZ	1:D:186:PRO:O	2.49	0.46
1:J:168:THR:N	4:J:904:GLN:OE1	2.41	0.46
1:J:292:LEU:O	1:J:295:VAL:HG22	2.16	0.46
1:J:299:ILE:HB	1:J:300:PRO:HD3	1.96	0.46
1:M:69:ILE:HD11	1:M:164:LEU:HD13	1.98	0.46
3:U:3:ASP:O	3:U:7:VAL:HG23	2.15	0.46
1:J:292:LEU:HB2	1:J:295:VAL:CG2	2.44	0.46
1:V:99:THR:O	1:V:103:ARG:HG3	2.15	0.46
1:V:245:VAL:HG12	1:V:459:LEU:HB3	1.97	0.46
1:V:436:ILE:HD11	1:V:444:VAL:HG12	1.98	0.46
2:B:360:ILE:HD11	2:B:365:SER:HA	1.97	0.46
2:K:53:VAL:HG12	3:L:60:MET:HG2	1.98	0.46
1:M:94:ALA:HA	1:M:95:PRO:HD3	1.80	0.46
3:R:33:ILE:O	3:R:37:ILE:HG12	2.16	0.46
2:T:77:VAL:HG23	2:T:99:LYS:HD2	1.97	0.46
1:A:83:THR:HG22	1:A:90:GLU:HA	1.96	0.46
1:G:95:PRO:HG2	2:H:46:MET:CE	2.45	0.46
2:N:82:HIS:CD2	2:N:92:TYR:HB3	2.51	0.46
1:A:88:ILE:HA	1:A:324:TYR:HB3	1.97	0.46
1:A:279:GLU:HG3	1:A:468:LYS:HE2	1.97	0.46
2:E:22:LYS:HB3	2:E:148:GLY:O	2.17	0.46
2:Q:83:TYR:CZ	2:Q:88:LEU:HD22	2.51	0.46
1:A:174:GLN:HG3	1:A:175:PRO:N	2.30	0.45
2:E:88:LEU:HA	2:E:89:PRO:HD2	1.87	0.45
1:M:384:LYS:O	1:M:387:GLU:HB2	2.15	0.45
1:P:111:ILE:N	1:P:111:ILE:HD12	2.31	0.45
1:D:143:VAL:HG12	1:D:145:GLY:H	1.80	0.45
3:F:88:VAL:HB	3:F:89:PRO:CD	2.32	0.45
2:H:202:PRO:O	2:H:205:SER:HB3	2.16	0.45
1:J:145:GLY:CA	1:J:174:GLN:OE1	2.65	0.45
1:J:317:TYR:OH	2:K:47:PRO:HB3	2.16	0.45
1:A:138:TRP:NE1	1:A:438:TRP:HH2	2.15	0.45
2:E:361:SER:HB2	2:E:363:GLU:OE1	2.17	0.45
1:G:188:TYR:OH	1:G:201:SER:O	2.31	0.45
1:J:3:TRP:CZ2	1:J:31:ARG:HG3	2.51	0.45
1:J:403:LYS:O	1:J:406:GLU:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:257:LYS:HD2	2:W:259:TYR:OH	2.15	0.45
2:B:217:VAL:HG12	2:B:222:PHE:HB3	1.98	0.45
2:E:280:PRO:HD2	3:F:55:PHE:CZ	2.51	0.45
1:J:199:PHE:CE2	4:J:904:GLN:OXT	2.70	0.45
1:P:143:VAL:CG1	1:P:145:GLY:H	2.27	0.45
1:P:171:SER:N	4:P:906:GLN:OE1	2.50	0.45
2:Q:4:LYS:O	2:Q:203:LYS:HB2	2.15	0.45
2:Q:95:SER:HB2	2:Q:127:GLU:HB3	1.98	0.45
1:S:169:GLY:HA2	1:S:425:ASN:OD1	2.15	0.45
1:V:435:PRO:HG2	1:V:471:HIS:CG	2.51	0.45
2:B:46:MET:HB3	2:B:46:MET:HE2	1.61	0.45
3:C:81:ARG:HA	3:C:87:VAL:HG23	1.98	0.45
1:G:394:SER:HB2	1:G:395:PRO:CD	2.45	0.45
2:N:217:VAL:HG11	2:N:223:VAL:HA	1.99	0.45
1:P:373:LYS:HD3	3:R:45:THR:HG23	1.98	0.45
3:X:7:VAL:HG21	3:X:27:GLN:HG2	1.97	0.45
2:H:95:SER:CB	2:H:127:GLU:HB3	2.47	0.45
2:H:396:MET:HE1	2:H:403:PRO:HB3	1.99	0.45
2:K:40:CYS:HB2	2:K:41:PRO:HD2	1.98	0.45
2:N:76:SER:HB2	2:N:99:LYS:O	2.16	0.45
2:N:106:TRP:CD1	2:N:118:LYS:HE2	2.52	0.45
2:N:385:SER:OG	2:N:388:ILE:HG12	2.16	0.45
1:G:57:LEU:HD22	1:G:65:PHE:CE1	2.51	0.45
1:G:69:ILE:HD11	1:G:164:LEU:HD13	1.98	0.45
1:M:171:SER:HG	4:M:905:GLN:CD	2.13	0.45
3:O:29:GLN:O	3:O:33:ILE:HG13	2.16	0.45
2:Q:360:ILE:CD1	2:Q:366:PRO:HD3	2.47	0.45
2:W:167:ARG:HG3	2:W:220:PHE:HB3	1.98	0.45
1:A:403:LYS:O	1:A:406:GLU:HB2	2.17	0.45
2:E:99:LYS:N	2:E:100:PRO:CD	2.80	0.45
1:J:39:VAL:HG21	1:J:157:VAL:HG11	1.97	0.45
2:K:81:LYS:O	2:K:92:TYR:HA	2.17	0.45
2:K:96:GLN:HB2	2:K:125:HIS:HB2	1.98	0.45
2:K:360:ILE:HD11	2:K:366:PRO:HD3	1.98	0.45
1:M:88:ILE:CD1	1:M:120:PHE:HZ	2.29	0.45
1:M:126:THR:HG22	1:M:126:THR:O	2.16	0.45
2:N:162:THR:HG22	2:N:165:GLU:N	2.14	0.45
2:Q:141:LEU:HD23	3:R:85:PHE:CD2	2.51	0.45
1:S:422:VAL:HG23	1:S:423:PRO:HD3	1.97	0.45
1:V:265:LEU:HD22	1:V:398:PRO:HA	1.99	0.45
2:W:99:LYS:N	2:W:100:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:MET:CB	1:D:351:ARG:HH11	2.23	0.45
1:P:266:GLN:HA	1:P:267:PRO:HD3	1.85	0.45
2:Q:13:ILE:HG22	2:Q:15:VAL:HG23	1.98	0.45
1:V:35:THR:HG21	1:V:39:VAL:HG21	1.97	0.45
1:A:190:ARG:HD2	1:A:455:GLU:OE2	2.17	0.45
1:J:62:LEU:HA	1:J:63:PRO:HD3	1.87	0.45
2:N:73:HIS:NE2	2:N:103:THR:HB	2.32	0.45
2:N:213:GLU:OE2	2:N:215:LYS:HE3	2.17	0.45
1:P:88:ILE:HA	1:P:324:TYR:HB3	1.99	0.45
1:S:168:THR:HG21	1:S:199:PHE:CE2	2.52	0.45
2:W:40:CYS:HB2	2:W:41:PRO:CD	2.47	0.45
1:A:69:ILE:HD11	1:A:164:LEU:HD13	1.99	0.44
2:B:39:VAL:HG11	2:B:44:LEU:HD11	1.98	0.44
2:B:84:PHE:CD2	3:C:15:ARG:HG2	2.52	0.44
2:H:26:GLY:O	3:I:65:PRO:HA	2.17	0.44
1:J:122:MET:HE1	1:J:310:ALA:HB1	2.00	0.44
1:M:298:SER:HB3	1:M:422:VAL:HG23	1.99	0.44
2:N:368:LYS:HB3	2:N:370:GLU:OE2	2.16	0.44
2:N:402:THR:HG22	2:N:403:PRO:HD2	1.99	0.44
1:P:84:CYS:SG	1:P:197:VAL:HG21	2.56	0.44
2:Q:80:ARG:HE	2:Q:275:ASP:CG	2.20	0.44
2:T:17:MET:HE3	2:T:60:TYR:CB	2.47	0.44
2:T:162:THR:HG22	2:T:165:GLU:CB	2.47	0.44
2:W:375:LEU:HD13	2:W:396:MET:HE1	1.99	0.44
2:B:97:TYR:O	2:B:123:ARG:NH2	2.50	0.44
2:B:310:TYR:HE1	2:B:334:VAL:HG11	1.82	0.44
1:J:2:LEU:HA	1:J:5:LYS:HD2	1.99	0.44
2:N:21:THR:CG2	2:N:22:LYS:N	2.80	0.44
1:P:138:TRP:CE2	1:P:438:TRP:CZ3	3.05	0.44
2:Q:8:VAL:CG1	2:Q:158:PRO:HB2	2.46	0.44
2:Q:355:LEU:HD21	2:Q:365:SER:HB2	1.99	0.44
1:S:303:TYR:CE2	1:S:415:TYR:HB3	2.52	0.44
1:S:384:LYS:O	1:S:387:GLU:HB2	2.17	0.44
1:D:2:LEU:HD23	1:D:27:SER:CB	2.40	0.44
1:D:265:LEU:HD22	1:D:398:PRO:HA	1.99	0.44
1:G:49:LYS:HE2	1:G:53:GLN:HE22	1.80	0.44
2:H:217:VAL:HG11	2:H:223:VAL:HA	1.97	0.44
2:H:396:MET:HG3	2:H:406:ILE:HD11	2.00	0.44
1:J:299:ILE:HG22	1:J:300:PRO:HD3	2.00	0.44
2:N:85:TYR:HA	2:N:86:PRO:HD3	1.89	0.44
1:S:68:PRO:HB3	1:S:112:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:317:TYR:HE1	2:W:47:PRO:HG3	1.82	0.44
1:A:410:ASN:HD21	1:A:412:ILE:HD12	1.82	0.44
1:A:422:VAL:N	1:A:423:PRO:CD	2.81	0.44
1:J:69:ILE:HD11	1:J:164:LEU:HD13	1.99	0.44
2:N:323:HIS:HD2	2:N:325:GLU:OE1	2.00	0.44
1:D:99:THR:O	1:D:103:ARG:HG3	2.16	0.44
2:E:21:THR:CG2	3:F:61:ARG:HH12	2.13	0.44
2:H:170:LEU:HD12	2:H:223:VAL:HG21	2.00	0.44
1:M:98:ALA:HA	1:M:195:GLY:HA3	1.98	0.44
1:P:90:GLU:O	1:P:91:ASN:CB	2.66	0.44
1:P:307:PRO:HG2	1:P:354:LEU:HD23	1.99	0.44
1:V:88:ILE:HA	1:V:324:TYR:HB3	1.98	0.44
1:V:422:VAL:N	1:V:423:PRO:CD	2.81	0.44
2:W:310:TYR:CE1	2:W:334:VAL:HG11	2.52	0.44
1:D:115:THR:CG2	1:D:151:SER:OG	2.63	0.44
2:H:111:LEU:HB2	2:H:115:GLU:O	2.18	0.44
2:H:128:GLU:HB2	2:H:148:GLY:HA2	1.99	0.44
2:K:34:GLU:O	2:K:37:THR:HG23	2.17	0.44
2:N:164:GLU:HG3	2:N:168:LEU:HD12	2.00	0.44
2:N:365:SER:HA	2:N:366:PRO:HD3	1.86	0.44
1:P:94:ALA:HA	1:P:95:PRO:HD3	1.83	0.44
1:P:174:GLN:HG3	1:P:175:PRO:CD	2.48	0.44
1:V:95:PRO:HG2	2:W:46:MET:HE3	1.98	0.44
1:A:117:LEU:O	1:A:129:SER:HB2	2.17	0.44
1:A:178:PHE:CE1	1:A:397:THR:HG21	2.53	0.44
1:A:199:PHE:CD1	1:A:199:PHE:C	2.90	0.44
1:G:262:GLU:OE1	1:G:262:GLU:HA	2.18	0.44
1:P:115:THR:HG23	1:P:150:GLY:HA3	1.99	0.44
1:P:126:THR:OG1	1:P:149:GLY:HA3	2.17	0.44
1:P:376:ARG:O	1:P:376:ARG:HG3	2.18	0.44
1:S:69:ILE:HG13	1:S:70:ALA:O	2.17	0.44
2:T:167:ARG:HG3	2:T:220:PHE:HB3	2.00	0.44
1:V:117:LEU:HD12	1:V:118:ASP:O	2.18	0.44
2:W:252:ASP:CB	2:W:255:THR:HG22	2.43	0.44
2:B:17:MET:HE3	2:B:60:TYR:HB2	1.99	0.44
1:J:95:PRO:HG2	2:K:46:MET:HE1	2.00	0.44
1:P:88:ILE:O	1:P:88:ILE:HG23	2.18	0.44
1:P:178:PHE:CE1	1:P:397:THR:HG21	2.52	0.44
2:T:170:LEU:HD12	2:T:223:VAL:HG21	2.00	0.44
2:W:82:HIS:CD2	2:W:92:TYR:HB3	2.53	0.44
2:W:143:ASP:OD1	2:W:145:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:95:SER:HB3	2:E:127:GLU:CB	2.47	0.44
2:K:8:VAL:CG1	2:K:158:PRO:HB2	2.46	0.44
1:M:126:THR:OG1	1:M:149:GLY:HA3	2.18	0.44
2:Q:96:GLN:HB2	2:Q:125:HIS:HB2	1.98	0.44
1:S:299:ILE:HG22	1:S:300:PRO:HD3	1.98	0.44
1:V:171:SER:OG	4:V:908:GLN:HB3	2.18	0.44
2:W:201:ARG:CD	2:W:207:GLU:O	2.66	0.44
1:A:7:LEU:HD21	1:A:161:PRO:HB2	2.00	0.43
2:B:40:CYS:O	2:B:44:LEU:CB	2.66	0.43
1:G:376:ARG:HG2	1:G:380:ASN:ND2	2.33	0.43
1:M:83:THR:HA	1:M:89:LEU:O	2.18	0.43
1:S:298:SER:HB3	1:S:422:VAL:HG23	2.00	0.43
3:X:29:GLN:O	3:X:33:ILE:HG13	2.16	0.43
2:B:80:ARG:HE	2:B:275:ASP:CG	2.22	0.43
1:J:3:TRP:CE2	1:J:31:ARG:HG3	2.53	0.43
1:J:422:VAL:N	1:J:423:PRO:CD	2.82	0.43
2:K:170:LEU:CD1	2:K:223:VAL:HG21	2.48	0.43
1:P:1:MET:O	1:P:1:MET:HG2	2.18	0.43
1:P:98:ALA:HA	1:P:195:GLY:HA3	2.00	0.43
1:S:412:ILE:HA	1:S:415:TYR:CD2	2.53	0.43
2:W:83:TYR:CE1	2:W:88:LEU:HD22	2.53	0.43
1:A:185:LYS:O	1:A:185:LYS:CG	2.65	0.43
2:E:40:CYS:HB2	2:E:41:PRO:HD2	2.00	0.43
1:M:297:TYR:O	1:M:300:PRO:HD2	2.17	0.43
1:S:190:ARG:HH11	1:S:190:ARG:CG	2.31	0.43
2:B:217:VAL:HG12	2:B:222:PHE:CB	2.48	0.43
3:I:71:ARG:HG3	3:I:75:LEU:HD23	2.01	0.43
1:J:438:TRP:CD1	1:J:438:TRP:N	2.86	0.43
2:K:137:GLY:O	3:L:90:ARG:HD2	2.18	0.43
1:M:13:LEU:HB3	1:M:19:VAL:HG12	2.00	0.43
1:M:171:SER:OG	4:M:905:GLN:CG	2.63	0.43
1:P:69:ILE:HD11	1:P:164:LEU:HD13	2.00	0.43
2:Q:39:VAL:CG1	2:Q:44:LEU:HD11	2.46	0.43
1:S:6:SER:HB2	1:S:212:ARG:HD2	1.99	0.43
2:W:330:PHE:CE1	2:W:344:VAL:HG13	2.54	0.43
1:D:172:ILE:CD1	1:D:207:GLY:CA	2.96	0.43
1:G:422:VAL:N	1:G:423:PRO:HD2	2.33	0.43
2:H:3:GLU:HG3	2:H:5:TYR:H	1.82	0.43
2:H:4:LYS:O	2:H:203:LYS:HB2	2.18	0.43
1:M:137:PRO:HB3	1:M:157:VAL:CG1	2.48	0.43
2:N:233:ARG:O	2:N:237:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:62:LEU:HA	1:P:63:PRO:HD3	1.87	0.43
1:P:292:LEU:O	1:P:295:VAL:HG22	2.18	0.43
2:T:346:TRP:O	2:T:350:ASP:HB2	2.18	0.43
2:W:40:CYS:O	2:W:44:LEU:HB2	2.18	0.43
1:A:71:VAL:CG1	1:A:114:LYS:HE3	2.49	0.43
1:A:270:LYS:HE3	1:A:274:GLU:OE2	2.19	0.43
1:D:143:VAL:HG13	1:D:145:GLY:H	1.83	0.43
2:E:230:GLU:OE2	2:E:233:ARG:NH1	2.52	0.43
1:G:349:LYS:NZ	3:I:22:GLU:OE2	2.41	0.43
1:J:88:ILE:O	1:J:88:ILE:HG23	2.18	0.43
1:J:122:MET:HE2	1:J:199:PHE:HE1	1.78	0.43
1:J:292:LEU:CB	1:J:295:VAL:HG22	2.47	0.43
1:M:234:ALA:HB1	1:M:236:VAL:HG23	2.01	0.43
1:M:376:ARG:HH11	1:M:376:ARG:CG	2.20	0.43
1:M:412:ILE:HA	1:M:415:TYR:CD2	2.54	0.43
1:P:31:ARG:HA	1:P:34:GLN:HG3	2.00	0.43
3:R:58:THR:HA	3:R:59:PRO:HD3	1.80	0.43
1:S:418:ASP:HB3	1:S:422:VAL:HG13	2.01	0.43
2:T:39:VAL:HG13	2:T:44:LEU:HD11	1.99	0.43
3:U:23:ILE:O	3:U:27:GLN:HG3	2.18	0.43
2:B:90:LYS:HB2	2:B:90:LYS:HE2	1.80	0.43
2:B:346:TRP:O	2:B:350:ASP:HB2	2.19	0.43
1:J:138:TRP:CD2	1:J:438:TRP:HZ3	2.36	0.43
2:Q:70:CYS:HB3	2:Q:102:ALA:HB1	1.99	0.43
2:Q:346:TRP:O	2:Q:350:ASP:HB2	2.18	0.43
2:W:95:SER:HB2	2:W:96:GLN:H	1.62	0.43
1:A:397:THR:CG2	1:A:398:PRO:HD2	2.48	0.43
1:D:5:LYS:HB2	1:D:10:LEU:HD13	2.00	0.43
1:D:32:TYR:CE1	1:D:36:GLU:HG2	2.53	0.43
1:G:138:TRP:CE2	1:G:438:TRP:HH2	2.35	0.43
2:H:40:CYS:HB2	2:H:41:PRO:CD	2.48	0.43
1:J:438:TRP:CH2	1:J:443:PRO:HG3	2.54	0.43
2:K:130:ALA:O	2:K:146:ARG:HG2	2.19	0.43
1:V:397:THR:HG22	1:V:398:PRO:HD2	2.01	0.43
2:W:12:GLU:HG3	2:W:197:ASN:HD21	1.84	0.43
2:W:412:LEU:O	2:W:412:LEU:CG	2.65	0.43
2:E:217:VAL:HG12	2:E:222:PHE:CB	2.49	0.43
1:M:193:ARG:NH2	1:M:201:SER:HB3	2.34	0.43
3:R:3:ASP:O	3:R:7:VAL:HG23	2.18	0.43
1:D:422:VAL:CG2	1:D:423:PRO:HD3	2.49	0.43
1:G:438:TRP:CD1	1:G:438:TRP:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:7:LEU:HD21	1:J:161:PRO:HB2	2.01	0.43
1:M:182:ILE:HG12	1:M:434:ILE:HD12	2.00	0.43
2:Q:98:GLU:O	2:Q:99:LYS:HB2	2.19	0.43
3:R:34:LEU:HD12	3:R:34:LEU:HA	1.82	0.43
2:T:272:TYR:O	2:T:273:PHE:HB3	2.19	0.43
3:X:58:THR:HA	3:X:59:PRO:HD2	1.86	0.43
1:A:6:SER:HB2	1:A:212:ARG:HD2	2.01	0.42
2:H:96:GLN:HB2	2:H:125:HIS:HB2	1.99	0.42
1:J:28:PHE:CD2	1:J:68:PRO:HG2	2.54	0.42
2:T:222:PHE:CZ	2:T:253:PRO:HB3	2.54	0.42
2:N:323:HIS:CD2	2:N:325:GLU:OE1	2.72	0.42
1:P:11:ARG:HE	1:P:11:ARG:HB3	1.51	0.42
1:S:270:LYS:HE3	1:S:274:GLU:OE2	2.19	0.42
1:V:84:CYS:SG	1:V:197:VAL:HG21	2.58	0.42
2:W:34:GLU:O	2:W:37:THR:CG2	2.55	0.42
2:W:412:LEU:O	2:W:412:LEU:HD13	2.20	0.42
2:B:22:LYS:HE3	2:B:27:CYS:HB2	2.01	0.42
2:B:125:HIS:NE2	2:B:153:GLU:OE1	2.53	0.42
2:B:407:VAL:HG13	2:B:412:LEU:HA	2.01	0.42
1:D:291:SER:HB3	2:H:118:LYS:HZ1	1.84	0.42
1:D:318:ASP:HB2	1:D:336:TYR:CE1	2.54	0.42
2:H:83:TYR:CZ	2:H:88:LEU:HD22	2.55	0.42
3:I:34:LEU:HD12	3:I:34:LEU:HA	1.86	0.42
1:J:2:LEU:HB3	1:J:27:SER:OG	2.19	0.42
2:K:255:THR:HG21	2:K:259:TYR:OH	2.19	0.42
1:M:57:LEU:HD22	1:M:65:PHE:CE1	2.54	0.42
1:M:138:TRP:CE2	1:M:438:TRP:CZ3	3.07	0.42
2:N:211:ARG:HE	2:N:211:ARG:HB3	1.65	0.42
1:S:213:THR:HG22	1:S:245:VAL:HG11	2.01	0.42
1:S:422:VAL:N	1:S:423:PRO:CD	2.82	0.42
1:V:318:ASP:HB2	1:V:336:TYR:CE1	2.55	0.42
2:W:233:ARG:HD2	2:W:249:ARG:NH2	2.34	0.42
1:A:94:ALA:HA	1:A:95:PRO:HD3	1.70	0.42
1:A:376:ARG:HD2	3:C:49:GLU:O	2.19	0.42
1:D:67:ILE:HD13	1:D:67:ILE:N	2.35	0.42
2:E:40:CYS:CB	2:E:41:PRO:CD	2.98	0.42
2:E:85:TYR:HA	2:E:86:PRO:HD3	1.91	0.42
1:G:337:ALA:HA	3:I:15:ARG:O	2.19	0.42
1:G:418:ASP:OD2	4:G:903:GLN:N	2.52	0.42
2:H:146:ARG:HG2	2:H:146:ARG:NH1	2.31	0.42
1:J:434:ILE:HA	1:J:435:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:100:VAL:HG21	1:M:206:ILE:HD13	2.01	0.42
2:N:5:TYR:O	2:N:203:LYS:HG3	2.20	0.42
2:Q:252:ASP:HB3	2:Q:255:THR:CG2	2.49	0.42
2:W:279:VAL:CG2	3:X:59:PRO:HD2	2.49	0.42
1:A:14:LEU:HD11	1:A:24:VAL:HG21	2.00	0.42
2:B:140:THR:OG1	3:C:90:ARG:HA	2.19	0.42
2:K:83:TYR:CZ	2:K:88:LEU:HD22	2.53	0.42
2:N:396:MET:HE1	2:N:403:PRO:HB3	2.01	0.42
2:Q:128:GLU:HB2	2:Q:148:GLY:HA2	2.00	0.42
1:S:185:LYS:NZ	1:S:186:PRO:O	2.52	0.42
1:V:35:THR:HG21	1:V:157:VAL:HG11	2.01	0.42
1:A:325:ARG:HA	1:A:339:THR:HG23	2.02	0.42
1:D:204:ASP:O	1:D:205:GLN:HG2	2.19	0.42
2:E:370:GLU:CD	2:E:370:GLU:H	2.23	0.42
1:G:171:SER:HG	4:G:903:GLN:HB3	1.85	0.42
2:K:140:THR:OG1	3:L:90:ARG:HA	2.18	0.42
1:M:10:LEU:HD12	1:M:10:LEU:HA	1.90	0.42
1:P:320:VAL:HG12	1:P:321:ARG:HG3	2.02	0.42
2:Q:302:ARG:HD3	2:Q:321:VAL:HG22	2.02	0.42
2:T:39:VAL:HG22	2:T:44:LEU:CG	2.44	0.42
2:T:95:SER:HB3	2:T:127:GLU:OE1	2.20	0.42
1:V:32:TYR:CE1	1:V:36:GLU:CG	3.03	0.42
1:V:162:VAL:HG21	1:V:219:VAL:HG21	2.00	0.42
1:A:438:TRP:CZ3	1:A:443:PRO:HG3	2.55	0.42
1:G:157:VAL:HG23	1:G:159:SER:H	1.83	0.42
2:H:305:ARG:O	2:H:309:GLU:HB2	2.18	0.42
1:J:337:ALA:HA	3:L:15:ARG:O	2.19	0.42
1:M:374:VAL:HG21	3:O:40:LEU:HD22	2.00	0.42
1:P:434:ILE:HA	1:P:435:PRO:HD3	1.87	0.42
1:V:42:TYR:CE2	1:V:113:GLY:HA3	2.54	0.42
1:A:181:VAL:HG22	1:A:211:ARG:HG2	2.01	0.42
1:D:318:ASP:HB2	1:D:336:TYR:HE1	1.84	0.42
1:G:163:SER:HB3	1:G:209:PHE:HB2	2.01	0.42
1:J:166:SER:O	1:J:171:SER:HB2	2.20	0.42
2:T:13:ILE:HG22	2:T:15:VAL:HG23	2.01	0.42
2:T:17:MET:HE1	2:T:57:ALA:O	2.19	0.42
2:T:17:MET:HE1	2:T:57:ALA:HA	2.01	0.42
2:T:280:PRO:O	3:U:58:THR:OG1	2.34	0.42
3:U:70:ASP:OD2	3:U:72:GLU:HB3	2.20	0.42
1:V:283:GLU:OE2	1:V:468:LYS:HD2	2.20	0.42
1:A:2:LEU:HB3	1:A:27:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:TRP:NE1	1:D:438:TRP:HH2	2.15	0.42
3:O:34:LEU:HD12	3:O:34:LEU:HA	1.96	0.42
2:Q:123:ARG:NH1	2:Q:125:HIS:ND1	2.67	0.42
1:J:47:TYR:CD2	1:J:112:VAL:HG22	2.55	0.42
1:J:57:LEU:HD12	1:J:110:LEU:HD21	2.02	0.42
2:K:379:ILE:HD13	2:K:384:ILE:HG13	2.02	0.42
2:N:17:MET:HE1	2:N:60:TYR:CB	2.45	0.42
1:P:126:THR:HG22	1:P:126:THR:O	2.20	0.42
2:Q:374:GLU:O	2:Q:377:LYS:HB3	2.20	0.42
1:V:172:ILE:CD1	1:V:207:GLY:CA	2.98	0.42
1:V:294:HIS:HB2	1:V:381:ASP:OD2	2.20	0.42
1:A:126:THR:OG1	1:A:149:GLY:HA3	2.19	0.41
1:A:172:ILE:C	1:A:175:PRO:HD2	2.40	0.41
2:B:8:VAL:HG11	2:B:208:PHE:HE1	1.85	0.41
2:B:214:ILE:HD11	2:B:230:GLU:HG2	2.02	0.41
2:E:26:GLY:O	3:F:65:PRO:HA	2.20	0.41
1:J:111:ILE:HD12	1:J:111:ILE:N	2.34	0.41
2:K:343:ILE:HG23	2:K:372:LEU:HD23	2.02	0.41
1:M:318:ASP:HB2	1:M:336:TYR:CD1	2.55	0.41
1:P:199:PHE:CD1	1:P:199:PHE:C	2.92	0.41
1:S:125:SER:HB2	1:S:143:VAL:HG11	2.01	0.41
1:V:292:LEU:HB2	1:V:295:VAL:CG2	2.48	0.41
2:B:8:VAL:HG11	2:B:208:PHE:CE1	2.55	0.41
1:D:138:TRP:CD2	1:D:438:TRP:CZ3	3.07	0.41
1:D:196:LEU:HD21	1:D:204:ASP:HB3	2.02	0.41
1:D:418:ASP:HB3	1:D:422:VAL:HG13	2.02	0.41
2:E:107:VAL:HG23	2:E:121:ILE:HD11	2.02	0.41
2:H:95:SER:HB3	2:H:127:GLU:HB2	2.02	0.41
2:H:345:ASN:O	2:H:349:ASN:HB2	2.20	0.41
1:J:68:PRO:HB3	1:J:112:VAL:HG21	2.02	0.41
2:K:40:CYS:CB	2:K:41:PRO:CD	2.98	0.41
1:G:141:GLU:OE2	2:K:394:LYS:HD3	2.20	0.41
1:G:317:TYR:HE1	2:H:47:PRO:HG3	1.84	0.41
1:M:171:SER:OG	4:M:905:GLN:HB3	2.20	0.41
1:P:275:ASN:O	1:P:279:GLU:HB2	2.20	0.41
1:S:138:TRP:CE2	1:S:438:TRP:CZ3	3.08	0.41
1:V:292:LEU:CB	1:V:295:VAL:HG22	2.49	0.41
2:W:156:THR:CG2	2:W:157:GLU:O	2.67	0.41
2:W:346:TRP:O	2:W:350:ASP:HB2	2.19	0.41
1:A:92:PHE:CZ	1:A:95:PRO:HD3	2.55	0.41
2:E:331:GLU:HA	2:E:334:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:88:VAL:CB	3:F:89:PRO:CD	2.97	0.41
2:H:23:MET:CE	2:H:126:ILE:HG21	2.49	0.41
3:I:5:GLU:OE1	2:T:408:GLU:OE2	2.38	0.41
1:J:307:PRO:HG2	1:J:354:LEU:HD23	2.02	0.41
1:P:172:ILE:O	1:P:175:PRO:HD2	2.20	0.41
2:Q:64:ALA:O	2:Q:68:LEU:HG	2.20	0.41
1:S:90:GLU:O	1:S:91:ASN:HB2	2.20	0.41
2:T:302:ARG:NH2	2:T:328:ASP:OD1	2.53	0.41
1:V:418:ASP:HB3	1:V:422:VAL:HG13	2.02	0.41
2:W:80:ARG:HE	2:W:275:ASP:CG	2.23	0.41
1:A:3:TRP:CZ2	1:A:31:ARG:HD3	2.56	0.41
2:B:17:MET:HE3	2:B:17:MET:HB3	1.91	0.41
2:B:82:HIS:CD2	2:B:92:TYR:HB3	2.56	0.41
3:C:46:GLU:O	3:C:47:ASN:HB2	2.20	0.41
1:G:162:VAL:HG21	1:G:219:VAL:HG21	2.02	0.41
2:H:196:ILE:O	2:H:213:GLU:HA	2.20	0.41
1:J:44:THR:HG22	1:J:46:LEU:HD21	2.03	0.41
1:M:168:THR:N	4:M:905:GLN:OE1	2.51	0.41
1:P:245:VAL:CG1	1:P:459:LEU:HB3	2.49	0.41
2:T:24:PHE:HA	2:T:52:ILE:O	2.20	0.41
2:T:197:ASN:OD1	2:T:213:GLU:HG3	2.20	0.41
2:W:396:MET:HG3	2:W:406:ILE:HD11	2.02	0.41
2:W:412:LEU:N	2:W:412:LEU:CD1	2.84	0.41
2:B:157:GLU:O	2:B:159:ASP:N	2.50	0.41
1:D:312:SER:OG	2:E:80:ARG:NH1	2.38	0.41
1:D:402:PHE:CD2	1:D:402:PHE:N	2.89	0.41
2:E:77:VAL:HG22	2:E:280:PRO:HB3	2.02	0.41
2:E:81:LYS:O	2:E:92:TYR:HA	2.20	0.41
2:E:255:THR:HG21	2:E:259:TYR:OH	2.20	0.41
1:J:122:MET:CE	1:J:310:ALA:HB1	2.50	0.41
3:L:3:ASP:O	3:L:7:VAL:HG23	2.21	0.41
2:N:360:ILE:HG13	2:N:361:SER:N	2.34	0.41
2:E:11:LEU:H	2:E:156:THR:HB	1.86	0.41
2:E:374:GLU:OE2	2:E:404:SER:HB3	2.21	0.41
1:J:88:ILE:HA	1:J:324:TYR:HB3	2.03	0.41
2:K:346:TRP:O	2:K:350:ASP:HB2	2.20	0.41
1:S:104:LEU:HD11	1:S:164:LEU:CD2	2.51	0.41
1:S:172:ILE:HG22	1:S:173:ARG:N	2.35	0.41
1:S:376:ARG:HH11	1:S:376:ARG:CG	2.09	0.41
1:V:32:TYR:CE1	1:V:36:GLU:HG2	2.55	0.41
1:A:72:LYS:HA	1:A:115:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLU:OE2	1:A:468:LYS:HD2	2.20	0.41
1:D:122:MET:CG	1:D:351:ARG:HH11	2.34	0.41
1:D:400:LEU:CD2	1:D:444:VAL:HG22	2.50	0.41
3:F:88:VAL:CB	3:F:89:PRO:HD2	2.25	0.41
1:G:136:ASN:HA	1:G:137:PRO:HD2	1.90	0.41
1:G:418:ASP:HB3	1:G:422:VAL:HG13	2.03	0.41
2:H:355:LEU:CD2	2:H:365:SER:HB2	2.48	0.41
2:K:64:ALA:O	2:K:68:LEU:HG	2.21	0.41
1:S:142:ARG:NH2	1:S:403:LYS:HE3	2.34	0.41
1:A:196:LEU:HB2	1:A:206:ILE:HD11	2.03	0.41
1:A:344:PHE:O	1:A:349:LYS:HE2	2.21	0.41
2:B:360:ILE:HD13	2:B:366:PRO:HD3	2.03	0.41
1:D:203:LEU:HD23	1:D:375:ARG:NH2	2.36	0.41
1:D:433:SER:O	1:D:434:ILE:HD13	2.20	0.41
2:E:96:GLN:HB2	2:E:125:HIS:HB2	2.03	0.41
2:E:221:ARG:HD3	2:E:221:ARG:HA	1.93	0.41
2:H:40:CYS:O	2:H:44:LEU:HB2	2.21	0.41
2:H:100:PRO:HB3	2:H:123:ARG:NH2	2.36	0.41
2:H:156:THR:HG22	2:H:157:GLU:N	2.35	0.41
2:H:170:LEU:HB3	2:H:220:PHE:CE1	2.56	0.41
2:K:80:ARG:HE	2:K:275:ASP:CG	2.25	0.41
1:M:88:ILE:HA	1:M:324:TYR:CB	2.51	0.41
2:N:74:GLU:HG2	2:N:283:VAL:O	2.20	0.41
1:P:31:ARG:HA	1:P:34:GLN:CG	2.51	0.41
1:P:122:MET:HG2	1:P:351:ARG:NH1	2.33	0.41
1:P:318:ASP:HB2	1:P:336:TYR:CD1	2.56	0.41
2:Q:374:GLU:O	2:Q:378:LEU:HG	2.21	0.41
1:S:32:TYR:CE1	1:S:36:GLU:HG2	2.56	0.41
1:S:64:LEU:HD21	1:S:218:LEU:HG	2.03	0.41
2:T:146:ARG:HG2	2:T:146:ARG:NH1	2.34	0.41
1:A:39:VAL:HG21	1:A:157:VAL:HG11	2.02	0.41
1:A:418:ASP:HB3	1:A:422:VAL:HG13	2.03	0.41
2:B:162:THR:HG22	2:B:165:GLU:N	2.21	0.41
2:B:280:PRO:HD2	3:C:55:PHE:CE1	2.54	0.41
1:D:104:LEU:HD11	1:D:164:LEU:CD2	2.51	0.41
3:F:29:GLN:O	3:F:33:ILE:HG13	2.21	0.41
2:K:66:LEU:HD12	2:K:291:ILE:HG22	2.02	0.41
2:K:230:GLU:OE2	2:K:233:ARG:NH1	2.54	0.41
1:M:122:MET:CB	1:M:351:ARG:NH1	2.84	0.41
1:P:59:GLU:O	1:P:65:PHE:CD1	2.74	0.41
2:T:40:CYS:CB	2:T:41:PRO:CD	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:GLU:O	2:B:98:GLU:HG3	2.20	0.40
2:B:272:TYR:O	2:B:273:PHE:HB3	2.21	0.40
2:E:396:MET:HG3	2:E:406:ILE:HD11	2.02	0.40
1:G:167:ASP:OD1	1:G:170:GLY:N	2.46	0.40
3:L:34:LEU:HD12	3:L:34:LEU:HA	1.92	0.40
1:P:156:ALA:O	1:P:211:ARG:NH1	2.54	0.40
1:S:39:VAL:HG21	1:S:157:VAL:HG11	2.03	0.40
1:V:191:VAL:HG11	1:V:223:ILE:HD12	2.02	0.40
1:A:239:PRO:HD2	1:A:241:TRP:CZ2	2.56	0.40
2:B:252:ASP:HB3	2:B:255:THR:CG2	2.48	0.40
1:D:178:PHE:HE2	1:D:402:PHE:CE2	2.40	0.40
2:E:282:LYS:HD3	3:F:55:PHE:CE2	2.57	0.40
1:G:174:GLN:HB3	1:G:175:PRO:HD3	2.03	0.40
1:P:260:PHE:CD1	1:P:263:TYR:CE2	3.10	0.40
1:P:299:ILE:N	1:P:300:PRO:CD	2.84	0.40
1:S:35:THR:HG23	1:S:477:LEU:CD1	2.51	0.40
1:S:341:ASP:OD1	3:U:22:GLU:OE1	2.39	0.40
2:T:375:LEU:HD22	2:T:396:MET:HE3	2.03	0.40
2:W:214:ILE:HD11	2:W:230:GLU:HG2	2.03	0.40
1:A:111:ILE:N	1:A:111:ILE:HD12	2.36	0.40
2:B:12:GLU:HG2	2:B:155:VAL:HG22	2.04	0.40
1:G:373:LYS:HE3	3:I:50:PRO:HD3	2.02	0.40
2:H:406:ILE:H	2:H:406:ILE:HG12	1.72	0.40
1:J:98:ALA:HA	1:J:195:GLY:HA3	2.02	0.40
1:M:397:THR:CG2	1:M:398:PRO:HD2	2.50	0.40
2:N:142:VAL:HB	3:O:86:PHE:HB2	2.02	0.40
1:P:2:LEU:HB3	1:P:27:SER:OG	2.21	0.40
1:P:178:PHE:CE2	1:P:401:PRO:HA	2.57	0.40
2:Q:17:MET:HE3	2:Q:60:TYR:CB	2.45	0.40
1:S:193:ARG:HD2	1:S:204:ASP:HB2	2.03	0.40
1:V:7:LEU:HD21	1:V:161:PRO:HB2	2.02	0.40
1:V:138:TRP:CZ2	1:V:438:TRP:CH2	3.09	0.40
1:V:171:SER:OG	4:V:908:GLN:CB	2.69	0.40
1:D:344:PHE:O	1:D:349:LYS:HE2	2.21	0.40
1:G:193:ARG:NH2	1:G:201:SER:HB3	2.36	0.40
1:G:434:ILE:HD11	1:G:462:SER:OG	2.21	0.40
1:J:78:GLU:HB2	1:J:97:ASP:OD1	2.20	0.40
1:J:167:ASP:HB3	1:J:185:LYS:CG	2.50	0.40
2:K:7:ALA:O	2:K:161:ARG:HD3	2.21	0.40
1:A:62:LEU:HA	1:A:63:PRO:HD3	1.94	0.40
1:A:138:TRP:CD2	1:A:438:TRP:CH2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:ARG:CD	2:B:207:GLU:O	2.69	0.40
1:D:422:VAL:HG22	1:D:423:PRO:HD3	2.04	0.40
2:E:157:GLU:O	2:E:159:ASP:N	2.50	0.40
2:E:229:TYR:O	2:E:232:GLU:HB3	2.22	0.40
1:G:405:GLY:HA2	1:G:408:LEU:HD12	2.04	0.40
1:J:30:ASP:O	1:J:34:GLN:HG3	2.22	0.40
1:J:122:MET:HG2	1:J:199:PHE:CZ	2.56	0.40
1:J:178:PHE:CE1	1:J:397:THR:HG21	2.57	0.40
1:M:273:PHE:CG	1:M:395:PRO:HD3	2.57	0.40
1:P:167:ASP:OD1	1:P:170:GLY:N	2.51	0.40
1:S:433:SER:C	1:S:434:ILE:HD13	2.42	0.40
1:V:62:LEU:HA	1:V:63:PRO:HD3	1.95	0.40
2:W:137:GLY:O	3:X:90:ARG:HD2	2.22	0.40
3:X:64:GLU:HA	3:X:65:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	476/478 (100%)	455 (96%)	20 (4%)	1 (0%)	47 78
1	D	476/478 (100%)	456 (96%)	18 (4%)	2 (0%)	34 66
1	G	476/478 (100%)	452 (95%)	23 (5%)	1 (0%)	47 78
1	J	476/478 (100%)	453 (95%)	23 (5%)	0	100 100
1	M	476/478 (100%)	453 (95%)	23 (5%)	0	100 100
1	P	476/478 (100%)	451 (95%)	24 (5%)	1 (0%)	47 78
1	S	476/478 (100%)	456 (96%)	20 (4%)	0	100 100
1	V	476/478 (100%)	456 (96%)	18 (4%)	2 (0%)	34 66
2	B	408/478 (85%)	396 (97%)	12 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	408/478 (85%)	390 (96%)	18 (4%)	0	100	100
2	H	408/478 (85%)	395 (97%)	13 (3%)	0	100	100
2	K	408/478 (85%)	392 (96%)	16 (4%)	0	100	100
2	N	408/478 (85%)	395 (97%)	13 (3%)	0	100	100
2	Q	408/478 (85%)	393 (96%)	15 (4%)	0	100	100
2	T	408/478 (85%)	388 (95%)	20 (5%)	0	100	100
2	W	408/478 (85%)	396 (97%)	12 (3%)	0	100	100
3	C	89/94 (95%)	86 (97%)	3 (3%)	0	100	100
3	F	89/94 (95%)	83 (93%)	6 (7%)	0	100	100
3	I	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	L	89/94 (95%)	86 (97%)	3 (3%)	0	100	100
3	O	89/94 (95%)	82 (92%)	7 (8%)	0	100	100
3	R	89/94 (95%)	83 (93%)	6 (7%)	0	100	100
3	U	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	X	89/94 (95%)	84 (94%)	4 (4%)	1 (1%)	14	41
All	All	7784/8400 (93%)	7451 (96%)	325 (4%)	8 (0%)	51	81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	148	SER
1	A	148	SER
1	V	148	SER
1	D	2	LEU
1	D	148	SER
1	G	148	SER
1	V	2	LEU
3	X	38	ASP

5.3.2 Protein sidechains (i)

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%)	383 (94%)	23 (6%)	20	50
1	D	406/406 (100%)	382 (94%)	24 (6%)	19	49
1	G	406/406 (100%)	391 (96%)	15 (4%)	34	68
1	J	406/406 (100%)	376 (93%)	30 (7%)	13	37
1	M	406/406 (100%)	387 (95%)	19 (5%)	26	59
1	P	406/406 (100%)	377 (93%)	29 (7%)	14	39
1	S	406/406 (100%)	382 (94%)	24 (6%)	19	49
1	V	406/406 (100%)	385 (95%)	21 (5%)	23	55
2	B	364/427 (85%)	345 (95%)	19 (5%)	23	55
2	E	364/427 (85%)	351 (96%)	13 (4%)	35	69
2	H	364/427 (85%)	347 (95%)	17 (5%)	26	59
2	K	364/427 (85%)	350 (96%)	14 (4%)	33	67
2	N	364/427 (85%)	340 (93%)	24 (7%)	16	44
2	Q	364/427 (85%)	345 (95%)	19 (5%)	23	55
2	T	364/427 (85%)	346 (95%)	18 (5%)	25	57
2	W	364/427 (85%)	346 (95%)	18 (5%)	25	57
3	C	86/89 (97%)	81 (94%)	5 (6%)	20	50
3	F	86/89 (97%)	83 (96%)	3 (4%)	36	70
3	I	86/89 (97%)	80 (93%)	6 (7%)	15	40
3	L	86/89 (97%)	82 (95%)	4 (5%)	26	59
3	O	86/89 (97%)	80 (93%)	6 (7%)	15	40
3	R	86/89 (97%)	83 (96%)	3 (4%)	36	70
3	U	86/89 (97%)	79 (92%)	7 (8%)	11	33
3	X	86/89 (97%)	81 (94%)	5 (6%)	20	50
All	All	6848/7376 (93%)	6482 (95%)	366 (5%)	22	54

All (366) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	29	TYR
1	A	30	ASP
1	A	51	LEU
1	A	57	LEU
1	A	62	LEU

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Mol	Chain	Res	Type
1	A	69	ILE
1	A	88	ILE
1	A	89	LEU
1	A	112	VAL
1	A	164	LEU
1	A	174	GLN
1	A	181	VAL
1	A	185	LYS
1	A	190	ARG
1	A	199	PHE
1	A	205	GLN
1	A	228	GLU
1	A	245	VAL
1	A	295	VAL
1	A	325	ARG
1	A	417	SER
1	A	478	THR
2	B	39	VAL
2	B	40	CYS
2	B	74	GLU
2	B	98	GLU
2	B	103	THR
2	B	156	THR
2	B	162	THR
2	B	189	LYS
2	B	213	GLU
2	B	217	VAL
2	B	244	VAL
2	B	250	THR
2	B	308	LYS
2	B	344	VAL
2	B	360	ILE
2	B	402	THR
2	B	405	GLN
2	B	406	ILE
2	B	412	LEU
3	C	34	LEU
3	C	38	ASP
3	C	52	ILE
3	C	53	GLN
3	C	70	ASP
1	D	10	LEU

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Mol	Chain	Res	Type
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	115	THR
1	D	117	LEU
1	D	174	GLN
1	D	181	VAL
1	D	185	LYS
1	D	199	PHE
1	D	245	VAL
1	D	295	VAL
1	D	356	THR
1	D	384	LYS
1	D	397	THR
1	D	409	GLU
1	D	417	SER
1	D	434	ILE
1	D	478	THR
2	E	35	PRO
2	E	65	SER
2	E	115	GLU
2	E	162	THR
2	E	188	GLU
2	E	244	VAL
2	E	250	THR
2	E	344	VAL
2	E	352	LEU
2	E	364	GLU
2	E	402	THR
2	E	407	VAL
2	E	412	LEU
3	F	34	LEU
3	F	46	GLU
3	F	70	ASP
1	G	10	LEU
1	G	51	LEU
1	G	57	LEU

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Mol	Chain	Res	Type
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	250	LYS
1	G	401	PRO
1	G	434	ILE
1	G	478	THR
2	H	21	THR
2	H	98	GLU
2	H	103	THR
2	H	109	LEU
2	H	113	ASN
2	H	132	LYS
2	H	162	THR
2	H	203	LYS
2	H	225	LYS
2	H	266	GLU
2	H	344	VAL
2	H	360	ILE
2	H	395	GLU
2	H	402	THR
2	H	406	ILE
2	H	407	VAL
2	H	412	LEU
3	I	34	LEU
3	I	38	ASP
3	I	52	ILE
3	I	68	SER
3	I	81	ARG
3	I	92	VAL
1	J	8	SER
1	J	10	LEU
1	J	11	ARG
1	J	31	ARG
1	J	51	LEU
1	J	56	SER
1	J	57	LEU

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Mol	Chain	Res	Type
1	J	59	GLU
1	J	62	LEU
1	J	112	VAL
1	J	115	THR
1	J	162	VAL
1	J	164	LEU
1	J	174	GLN
1	J	181	VAL
1	J	185	LYS
1	J	199	PHE
1	J	205	GLN
1	J	214	GLU
1	J	233	SER
1	J	240	GLU
1	J	245	VAL
1	J	279	GLU
1	J	295	VAL
1	J	299	ILE
1	J	356	THR
1	J	376	ARG
1	J	434	ILE
1	J	458	LEU
1	J	478	THR
2	K	21	THR
2	K	39	VAL
2	K	74	GLU
2	K	103	THR
2	K	109	LEU
2	K	132	LYS
2	K	134	ILE
2	K	245	VAL
2	K	338	LYS
2	K	341	LYS
2	K	344	VAL
2	K	360	ILE
2	K	365	SER
2	K	412	LEU
3	L	34	LEU
3	L	54	GLU
3	L	68	SER
3	L	92	VAL
1	M	10	LEU

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Mol	Chain	Res	Type
1	M	51	LEU
1	M	57	LEU
1	M	62	LEU
1	M	88	ILE
1	M	112	VAL
1	M	115	THR
1	M	117	LEU
1	M	174	GLN
1	M	199	PHE
1	M	233	SER
1	M	245	VAL
1	M	299	ILE
1	M	325	ARG
1	M	354	LEU
1	M	356	THR
1	M	417	SER
1	M	434	ILE
1	M	478	THR
2	N	16	GLN
2	N	21	THR
2	N	39	VAL
2	N	95	SER
2	N	98	GLU
2	N	103	THR
2	N	134	ILE
2	N	141	LEU
2	N	162	THR
2	N	164	GLU
2	N	197	ASN
2	N	203	LYS
2	N	244	VAL
2	N	250	THR
2	N	266	GLU
2	N	344	VAL
2	N	360	ILE
2	N	387	LYS
2	N	390	LYS
2	N	391	GLU
2	N	395	GLU
2	N	402	THR
2	N	407	VAL
2	N	412	LEU

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Mol	Chain	Res	Type
3	O	34	LEU
3	O	38	ASP
3	O	52	ILE
3	O	68	SER
3	O	81	ARG
3	O	92	VAL
1	P	10	LEU
1	P	29	TYR
1	P	31	ARG
1	P	40	LYS
1	P	51	LEU
1	P	56	SER
1	P	57	LEU
1	P	59	GLU
1	P	62	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	240	GLU
1	P	245	VAL
1	P	279	GLU
1	P	291	SER
1	P	295	VAL
1	P	325	ARG
1	P	356	THR
1	P	376	ARG
1	P	458	LEU
1	P	464	LEU
1	P	478	THR
2	Q	16	GLN
2	Q	21	THR
2	Q	39	VAL
2	Q	103	THR
2	Q	109	LEU
2	Q	123	ARG
2	Q	156	THR

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Mol	Chain	Res	Type
2	Q	162	THR
2	Q	210	THR
2	Q	240	GLU
2	Q	245	VAL
2	Q	255	THR
2	Q	282	LYS
2	Q	344	VAL
2	Q	360	ILE
2	Q	365	SER
2	Q	395	GLU
2	Q	402	THR
2	Q	412	LEU
3	R	34	LEU
3	R	45	THR
3	R	52	ILE
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
1	S	69	ILE
1	S	114	LYS
1	S	117	LEU
1	S	181	VAL
1	S	185	LYS
1	S	199	PHE
1	S	245	VAL
1	S	295	VAL
1	S	299	ILE
1	S	376	ARG
1	S	384	LYS
1	S	389	VAL
1	S	392	ILE
1	S	397	THR
1	S	434	ILE
1	S	458	LEU
1	S	464	LEU
2	T	39	VAL
2	T	74	GLU
2	T	98	GLU

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Mol	Chain	Res	Type
2	T	103	THR
2	T	109	LEU
2	T	123	ARG
2	T	156	THR
2	T	162	THR
2	T	189	LYS
2	T	233	ARG
2	T	244	VAL
2	T	245	VAL
2	T	250	THR
2	T	344	VAL
2	T	402	THR
2	T	406	ILE
2	T	407	VAL
2	T	412	LEU
3	U	5	GLU
3	U	34	LEU
3	U	46	GLU
3	U	52	ILE
3	U	68	SER
3	U	70	ASP
3	U	92	VAL
1	V	10	LEU
1	V	11	ARG
1	V	15	LYS
1	V	29	TYR
1	V	57	LEU
1	V	62	LEU
1	V	88	ILE
1	V	115	THR
1	V	117	LEU
1	V	124	SER
1	V	143	VAL
1	V	190	ARG
1	V	199	PHE
1	V	233	SER
1	V	245	VAL
1	V	270	LYS
1	V	279	GLU
1	V	295	VAL
1	V	417	SER
1	V	434	ILE

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Mol	Chain	Res	Type
1	V	478	THR
2	W	21	THR
2	W	39	VAL
2	W	46	MET
2	W	74	GLU
2	W	109	LEU
2	W	113	ASN
2	W	123	ARG
2	W	156	THR
2	W	162	THR
2	W	233	ARG
2	W	244	VAL
2	W	250	THR
2	W	344	VAL
2	W	364	GLU
2	W	365	SER
2	W	402	THR
2	W	406	ILE
2	W	412	LEU
3	X	38	ASP
3	X	46	GLU
3	X	52	ILE
3	X	54	GLU
3	X	68	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	216	ASN
3	C	53	GLN
2	E	110	ASN
2	E	323	HIS
1	G	53	GLN
1	G	380	ASN
2	H	322	ASN
1	J	275	ASN
2	K	323	HIS
2	N	323	HIS
3	O	53	GLN
2	T	110	ASN
1	V	460	GLN
2	W	345	ASN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 15 are monoatomic - leaving 8 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	GLN	S	907	1	7,8,9	0.89	0	7,9,11	1.49	2 (28%)
4	GLN	A	901	1	7,8,9	1.08	1 (14%)	7,9,11	1.56	2 (28%)
4	GLN	M	905	1	7,8,9	0.93	0	7,9,11	1.70	2 (28%)
4	GLN	G	903	1	7,8,9	1.07	0	7,9,11	1.54	2 (28%)
4	GLN	D	902	1	7,8,9	0.96	0	7,9,11	1.19	2 (28%)
4	GLN	J	904	1	7,8,9	0.91	1 (14%)	7,9,11	1.35	2 (28%)
4	GLN	P	906	1	7,8,9	1.08	1 (14%)	7,9,11	1.47	2 (28%)
4	GLN	V	908	1	7,8,9	1.14	1 (14%)	7,9,11	1.33	1 (14%)

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	GLN	S	907	1	-	0/7/8/9	-
4	GLN	A	901	1	-	0/7/8/9	-
4	GLN	M	905	1	-	0/7/8/9	-
4	GLN	G	903	1	-	0/7/8/9	-
4	GLN	D	902	1	-	0/7/8/9	-
4	GLN	J	904	1	-	0/7/8/9	-
4	GLN	P	906	1	-	1/7/8/9	-
4	GLN	V	908	1	-	0/7/8/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	906	GLN	OXT-C	-2.37	1.22	1.30
4	V	908	GLN	OXT-C	-2.25	1.23	1.30
4	A	901	GLN	OXT-C	-2.24	1.23	1.30
4	J	904	GLN	OXT-C	-2.05	1.23	1.30

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	905	GLN	OXT-C-O	-3.61	115.89	124.09
4	P	906	GLN	OXT-C-O	-2.92	117.47	124.09
4	G	903	GLN	OXT-C-CA	2.84	123.07	113.38
4	S	907	GLN	OXT-C-O	-2.79	117.76	124.09
4	A	901	GLN	OXT-C-CA	2.68	122.50	113.38
4	A	901	GLN	OXT-C-O	-2.67	118.03	124.09
4	S	907	GLN	OXT-C-CA	2.49	121.87	113.38
4	J	904	GLN	OXT-C-O	-2.43	118.56	124.09
4	M	905	GLN	OXT-C-CA	2.41	121.60	113.38
4	V	908	GLN	OXT-C-CA	2.38	121.48	113.38
4	J	904	GLN	OXT-C-CA	2.37	121.45	113.38
4	G	903	GLN	OXT-C-O	-2.29	118.88	124.09
4	P	906	GLN	OXT-C-CA	2.23	120.98	113.38
4	D	902	GLN	OXT-C-O	-2.11	119.30	124.09
4	D	902	GLN	OXT-C-CA	2.01	120.23	113.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	906	GLN	OXT-C-CA-N

There are no ring outliers.

8 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	907	GLN	4	0
4	A	901	GLN	8	0
4	M	905	GLN	13	0
4	G	903	GLN	12	0
4	D	902	GLN	3	0
4	J	904	GLN	6	0
4	P	906	GLN	7	0
4	V	908	GLN	12	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	478/478 (100%)	-0.04	4 (0%)	86	81	23, 52, 78, 87	0
1	D	478/478 (100%)	-0.02	1 (0%)	95	94	23, 52, 78, 87	0
1	G	478/478 (100%)	0.07	3 (0%)	89	86	23, 51, 77, 87	0
1	J	478/478 (100%)	0.04	6 (1%)	77	72	23, 51, 77, 87	0
1	M	478/478 (100%)	0.10	5 (1%)	82	77	23, 51, 77, 87	0
1	P	478/478 (100%)	0.04	5 (1%)	82	77	23, 51, 77, 87	0
1	S	478/478 (100%)	-0.05	2 (0%)	92	91	23, 52, 78, 87	0
1	V	478/478 (100%)	-0.01	8 (1%)	70	63	23, 52, 78, 87	0
2	B	410/478 (85%)	0.12	4 (0%)	82	77	31, 61, 92, 111	0
2	E	410/478 (85%)	0.07	8 (1%)	65	56	31, 62, 92, 111	0
2	H	410/478 (85%)	0.12	11 (2%)	54	44	31, 61, 92, 111	0
2	K	410/478 (85%)	0.09	7 (1%)	70	63	31, 61, 92, 111	0
2	N	410/478 (85%)	0.09	9 (2%)	62	52	31, 62, 92, 111	0
2	Q	410/478 (85%)	0.09	5 (1%)	79	73	31, 61, 92, 111	0
2	T	410/478 (85%)	0.06	11 (2%)	54	44	31, 61, 92, 111	0
2	W	410/478 (85%)	0.09	2 (0%)	91	88	31, 61, 92, 111	0
3	C	91/94 (96%)	0.09	0	100	100	25, 58, 71, 75	0
3	F	91/94 (96%)	0.09	1 (1%)	80	75	25, 58, 70, 75	0
3	I	91/94 (96%)	-0.04	0	100	100	25, 58, 71, 75	0
3	L	91/94 (96%)	0.02	0	100	100	25, 58, 71, 75	0
3	O	91/94 (96%)	0.06	0	100	100	25, 58, 71, 75	0
3	R	91/94 (96%)	0.00	0	100	100	25, 58, 70, 75	0
3	U	91/94 (96%)	0.10	0	100	100	25, 58, 71, 75	0
3	X	91/94 (96%)	0.14	0	100	100	25, 58, 71, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	7832/8400 (93%)	0.05	92 (1%)	79	73	23, 55, 87, 111	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	266	GLU	4.4
2	T	408	GLU	4.3
2	H	262	ARG	4.2
2	N	262	ARG	4.1
2	E	262	ARG	4.1
2	K	266	GLU	4.1
2	H	267	ALA	4.0
2	N	241	GLY	4.0
2	K	408	GLU	4.0
2	H	408	GLU	3.8
1	G	220	LEU	3.6
1	P	210	GLY	3.6
2	N	267	ALA	3.5
2	E	408	GLU	3.5
1	J	18	GLU	3.4
1	P	18	GLU	3.4
2	W	406	ILE	3.3
2	E	346	TRP	3.2
2	B	406	ILE	3.2
2	T	242	GLY	3.2
2	T	262	ARG	3.2
2	T	412	LEU	3.0
2	E	405	GLN	3.0
2	N	232	GLU	2.9
1	J	58	LYS	2.9
1	J	19	VAL	2.9
2	H	406	ILE	2.8
1	J	219	VAL	2.8
2	H	265	GLU	2.8
1	M	219	VAL	2.8
2	N	408	GLU	2.8
2	W	265	GLU	2.6
2	E	109	LEU	2.6
2	K	406	ILE	2.6
2	H	4	LYS	2.6
2	E	241	GLY	2.6
2	N	403	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	Q	266	GLU	2.5
2	Q	240	GLU	2.5
1	G	241	TRP	2.5
1	J	216	VAL	2.5
1	V	19	VAL	2.5
2	E	242	GLY	2.5
1	P	19	VAL	2.4
2	T	406	ILE	2.4
1	V	35	THR	2.4
2	N	406	ILE	2.4
1	M	19	VAL	2.3
2	T	265	GLU	2.3
2	N	265	GLU	2.3
1	M	241	TRP	2.3
2	H	208	PHE	2.3
2	H	403	PRO	2.3
1	A	7	LEU	2.3
1	S	7	LEU	2.3
1	V	1	MET	2.3
2	T	109	LEU	2.3
2	T	227	LEU	2.3
1	A	220	LEU	2.3
2	B	266	GLU	2.3
1	D	55	GLU	2.3
1	A	58	LYS	2.2
1	V	241	TRP	2.2
3	F	83	ASP	2.2
1	G	7	LEU	2.2
2	K	265	GLU	2.2
2	Q	265	GLU	2.2
2	N	266	GLU	2.2
1	S	58	LYS	2.2
2	Q	408	GLU	2.2
1	A	64	LEU	2.2
1	J	104	LEU	2.2
1	P	265	LEU	2.2
2	K	267	ALA	2.1
1	M	265	LEU	2.1
2	T	372	LEU	2.1
1	V	219	VAL	2.1
1	V	216	VAL	2.1
2	E	227	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	K	404	SER	2.1
2	H	239	GLU	2.1
2	T	375	LEU	2.1
1	P	58	LYS	2.1
2	B	403	PRO	2.1
2	H	384	ILE	2.1
1	V	57	LEU	2.1
2	T	241	GLY	2.1
2	K	262	ARG	2.1
2	Q	141	LEU	2.0
2	B	87	ASP	2.0
1	M	220	LEU	2.0
1	V	51	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	H	479	1/1	0.28	0.34	61,61,61,61	1
5	MG	B	479	1/1	0.35	0.29	57,57,57,57	1
5	MG	W	479	1/1	0.53	0.41	75,75,75,75	1
5	MG	K	479	1/1	0.63	0.28	53,53,53,53	1
4	GLN	A	901	9/10	0.64	0.31	48,49,55,59	0
4	GLN	J	904	9/10	0.69	0.37	59,59,60,63	0
4	GLN	P	906	9/10	0.69	0.34	52,53,54,56	0
5	MG	Q	479	1/1	0.72	0.24	61,61,61,61	1
4	GLN	V	908	9/10	0.72	0.32	49,51,54,59	0
4	GLN	M	905	9/10	0.73	0.30	47,48,53,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GLN	G	903	9/10	0.74	0.23	51,52,60,65	0
4	GLN	S	907	9/10	0.76	0.24	55,56,57,62	0
5	MG	N	479	1/1	0.76	0.32	86,86,86,86	1
4	GLN	D	902	9/10	0.82	0.33	55,56,57,61	0
5	MG	T	479	1/1	0.84	0.25	60,60,60,60	1
6	ZN	T	907	1/1	0.95	0.19	49,49,49,49	0
6	ZN	W	908	1/1	0.95	0.19	50,50,50,50	0
6	ZN	B	901	1/1	0.97	0.22	49,49,49,49	0
6	ZN	E	902	1/1	0.98	0.18	59,59,59,59	0
6	ZN	N	905	1/1	0.99	0.18	47,47,47,47	0
6	ZN	Q	906	1/1	0.99	0.17	44,44,44,44	0
6	ZN	H	903	1/1	0.99	0.17	51,51,51,51	0
6	ZN	K	904	1/1	0.99	0.16	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.