



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:47 PM EDT

PDB ID : 3H0R / pdb_00003h0r
Title : Structure of trna-dependent amidotransferase gatcab from aquifex aeolicus
Authors : Wu, J.; Bu, W.; Sheppard, K.; Kitabatake, M.; Soll, D.; Smith, J.L.
Deposited on : 2009-04-10
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

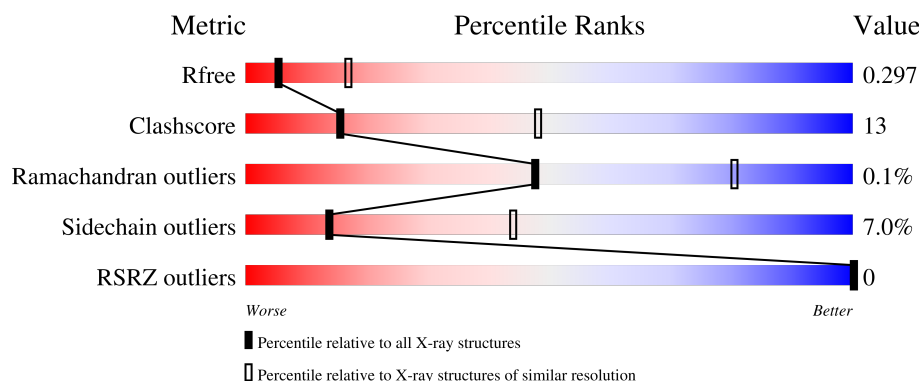
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	478	
1	D	478	
1	G	478	
1	J	478	
1	M	478	

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Mol	Chain	Length	Quality of chain
1	P	478	
1	S	478	
1	V	478	
2	B	478	
2	E	478	
2	H	478	
2	K	478	
2	N	478	
2	Q	478	
2	T	478	
2	W	478	
3	C	94	
3	F	94	
3	I	94	
3	L	94	
3	O	94	
3	R	94	
3	U	94	
3	X	94	

The following table lists non-polymeric compounds, 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	ASN	D	902	-	-	X	-
4	ASN	S	907	-	-	X	-
4	ASN	V	908	-	-	X	-
9	ASP	H	482	-	-	X	-
9	ASP	N	482	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 63243 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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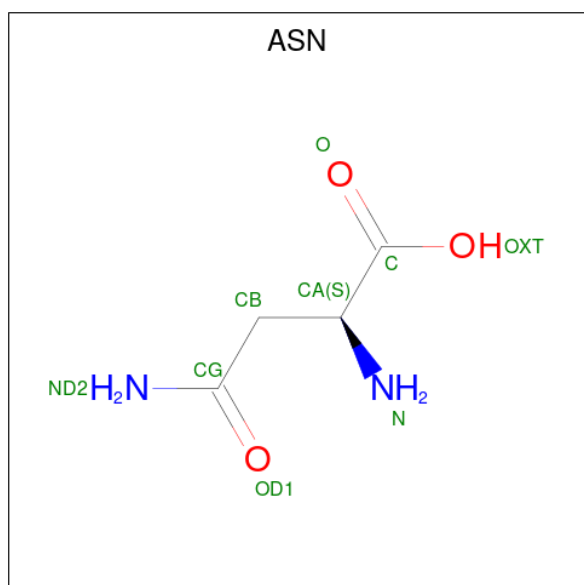
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	W	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			

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

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

- Molecule 4 is ASPARAGINE (CCD ID: ASN) (formula: C₄H₈N₂O₃).

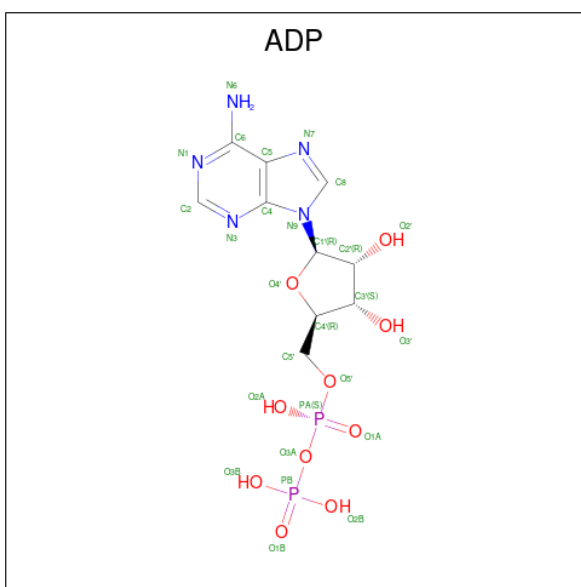


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 4 1 3	0	0
4	D	1	Total C N O 8 4 1 3	0	0
4	G	1	Total C N O 8 4 1 3	0	0
4	J	1	Total C N O 8 4 1 3	0	0
4	M	1	Total C N O 8 4 1 3	0	0
4	P	1	Total C N O 8 4 1 3	0	0
4	S	1	Total C N O 8 4 1 3	0	0
4	V	1	Total C N O 8 4 1 3	0	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

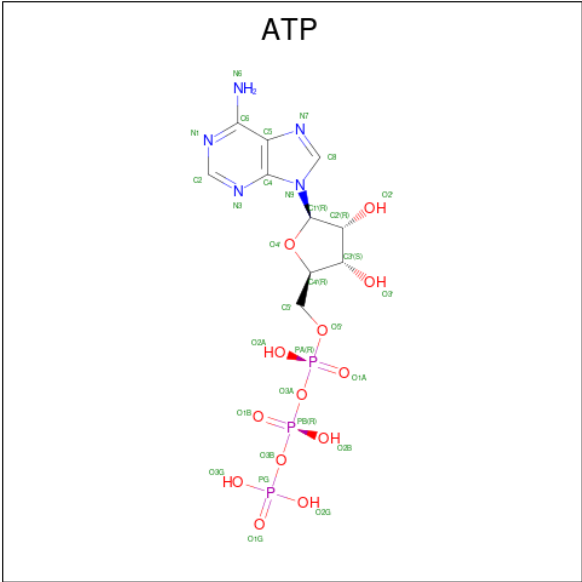


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	
			27	10	5	10	2	0
6	T	1	Total	C	N	O	P	
			27	10	5	10	2	0

- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

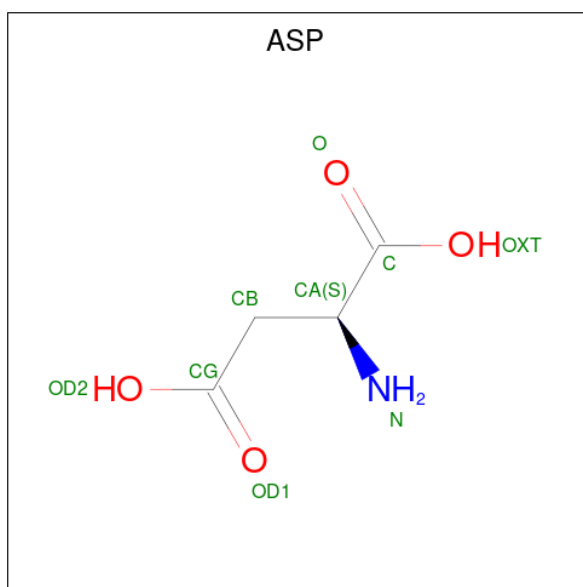
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Mn		
			2	2	0	0
7	E	2	Total	Mn		
			2	2	0	0
7	H	2	Total	Mn		
			2	2	0	0
7	K	2	Total	Mn		
			2	2	0	0
7	N	2	Total	Mn		
			2	2	0	0
7	Q	2	Total	Mn		
			2	2	0	0
7	T	2	Total	Mn		
			2	2	0	0
7	W	2	Total	Mn		
			2	2	0	0

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 9 is ASPARTIC ACID (CCD ID: ASP) (formula: C₄H₇NO₄).



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

- Molecule 10 is water.

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

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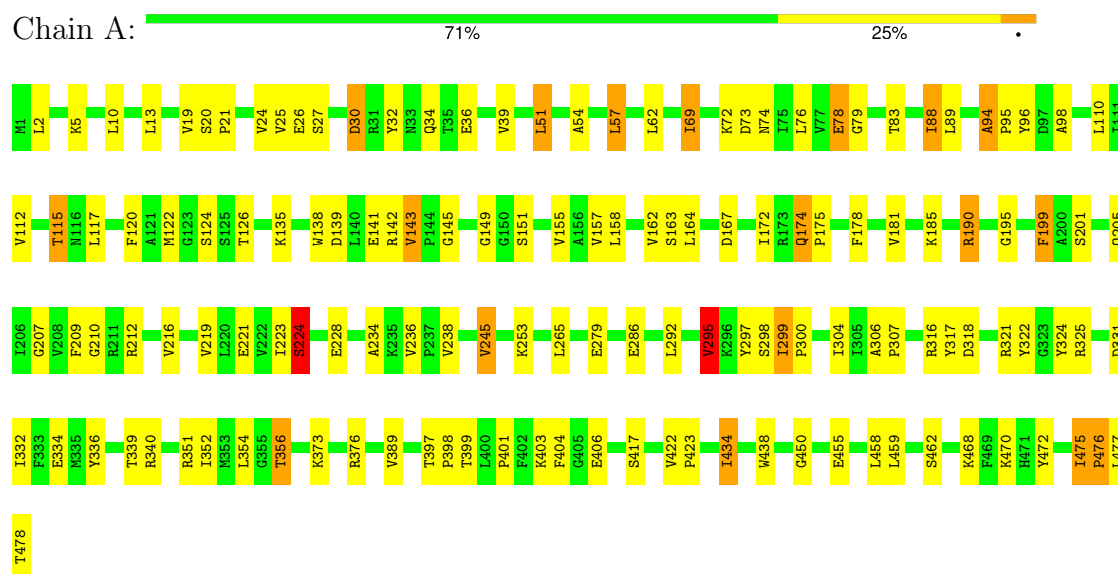
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	Q	7	Total 7	O 7	0	0
10	T	5	Total 5	O 5	0	0
10	V	1	Total 1	O 1	0	0
10	W	6	Total 6	O 6	0	0

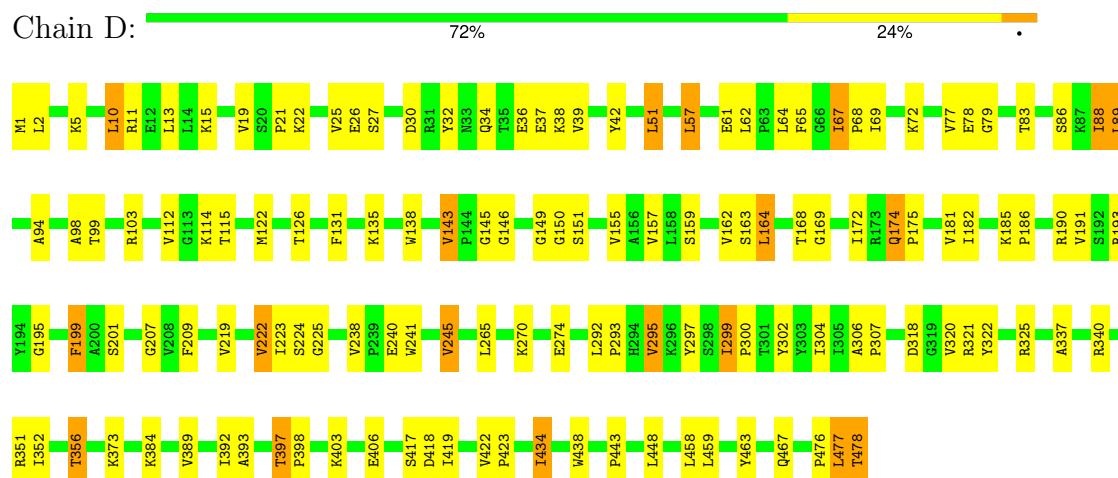
3 Residue-property plots

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

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

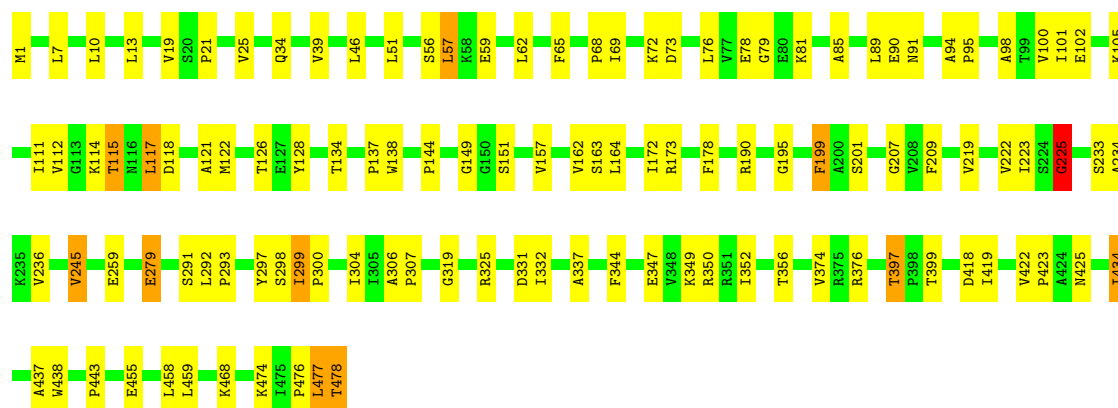


- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



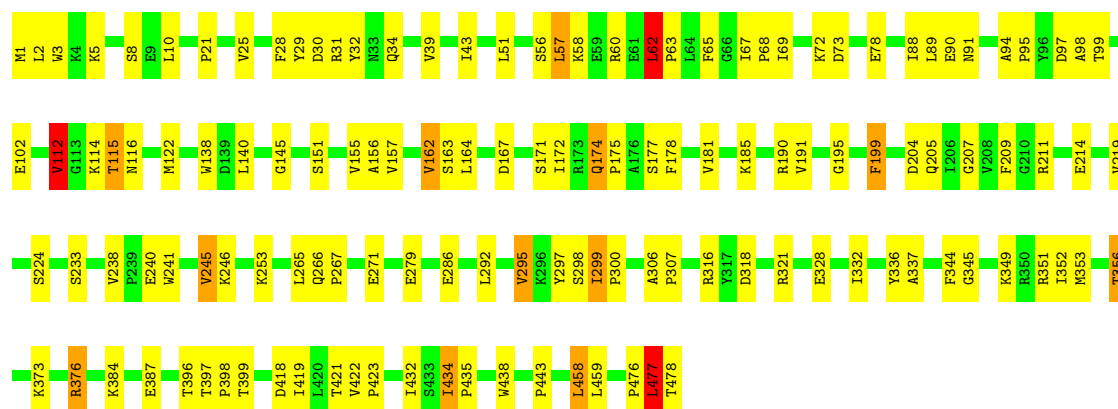
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain G:  76% 22% .



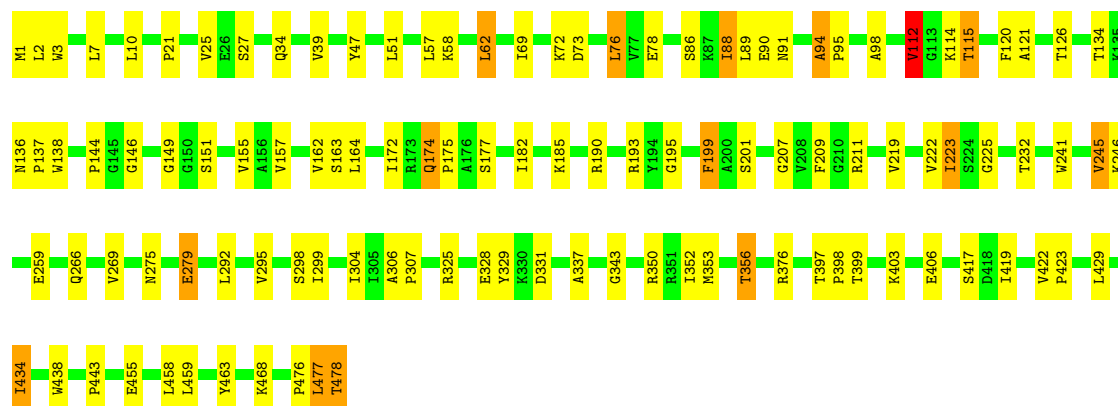
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain J:  72% 25% ..



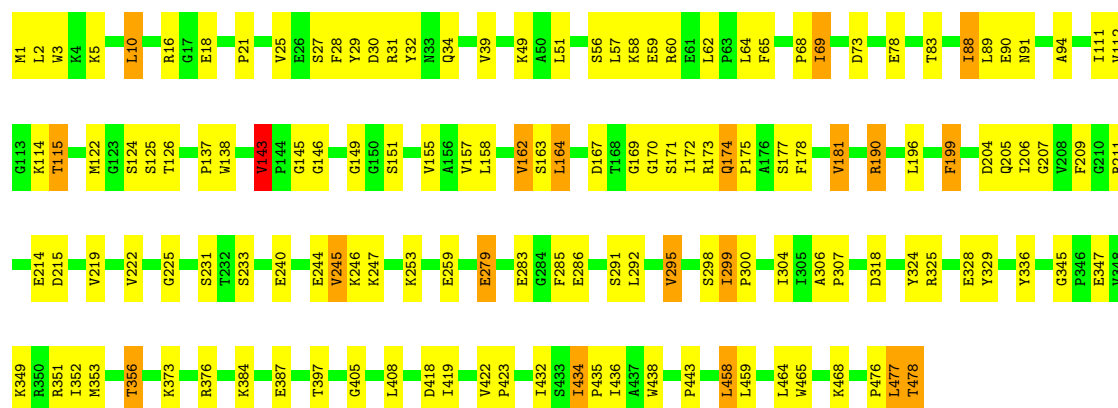
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain M:  76% 21% .



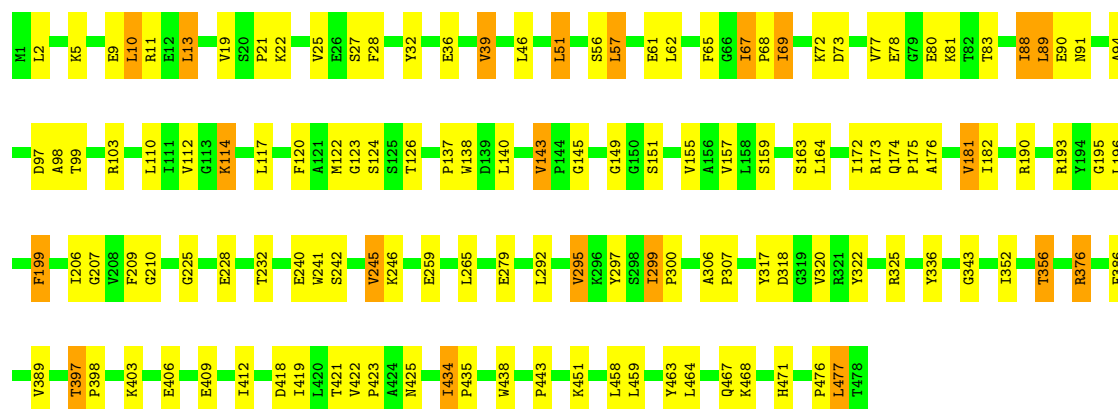
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain P:  70% 26%



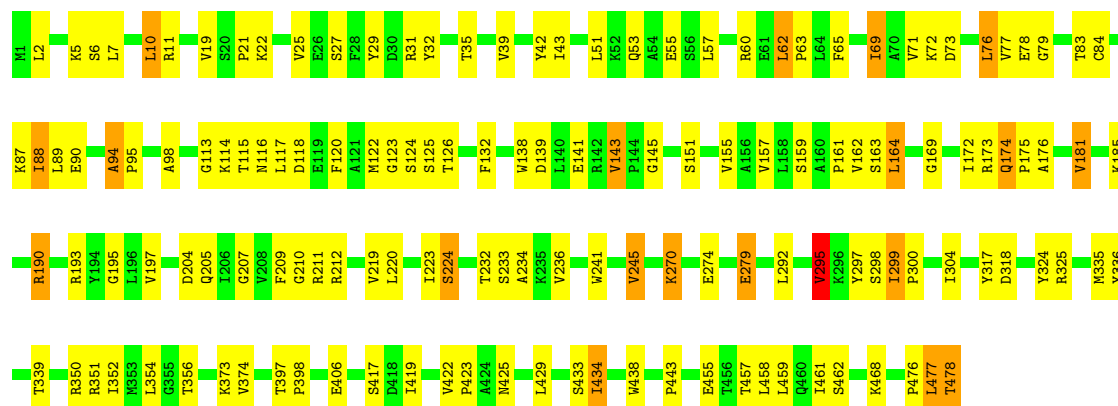
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain S:  72% 24%



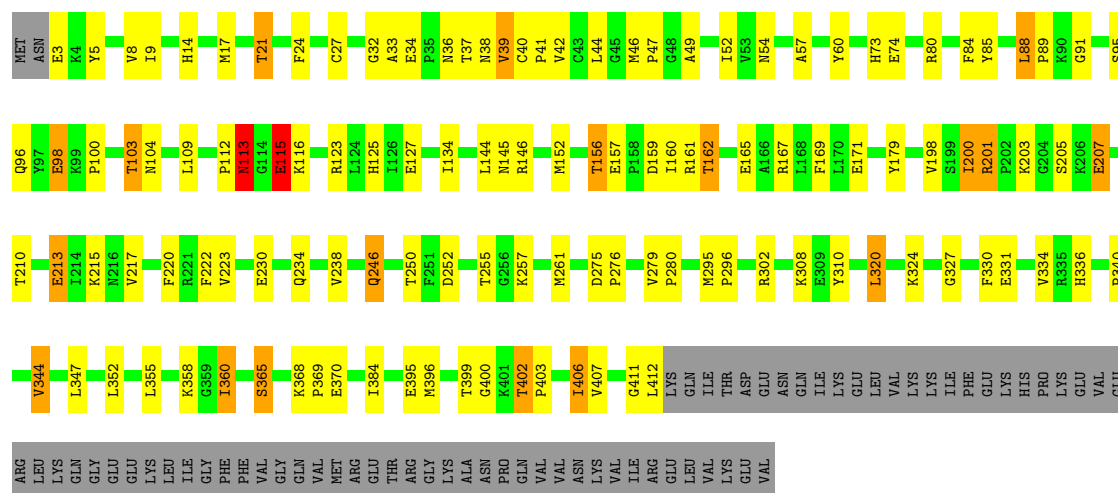
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain V:  70% 26%



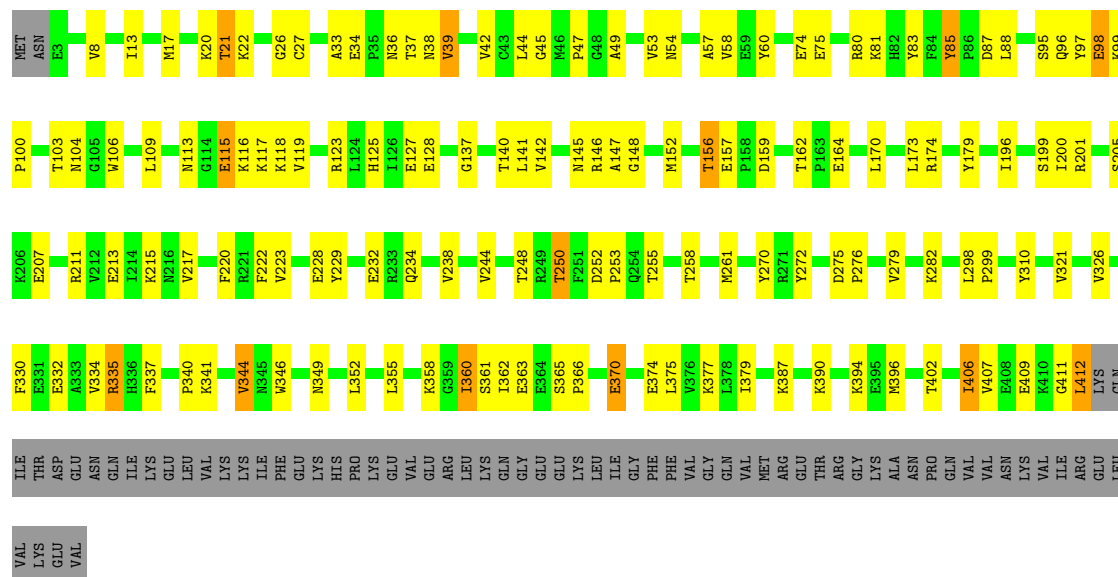
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain B:



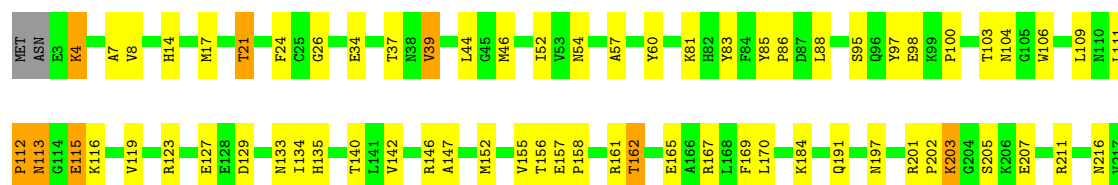
- Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

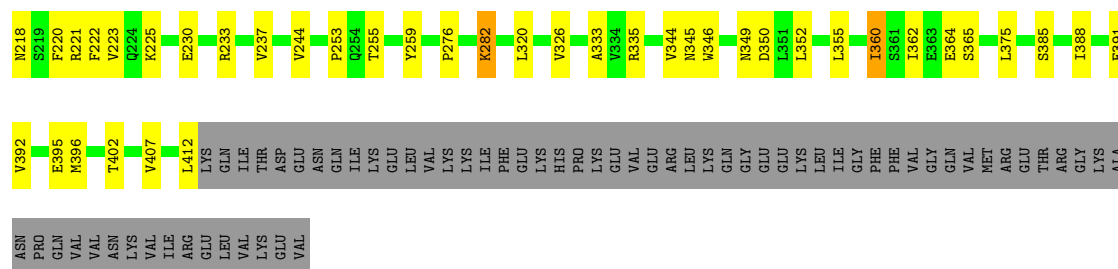
Chain E:



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

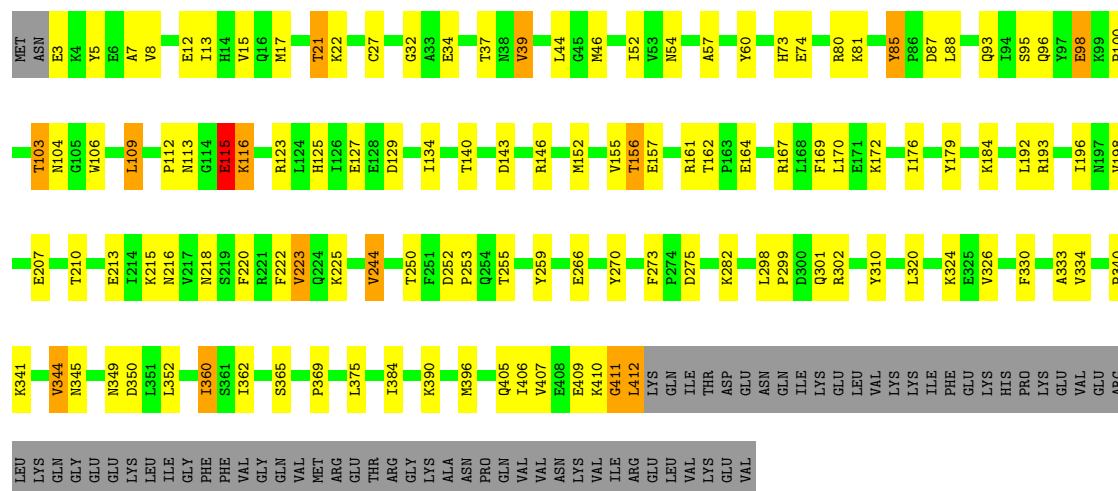
Chain H:





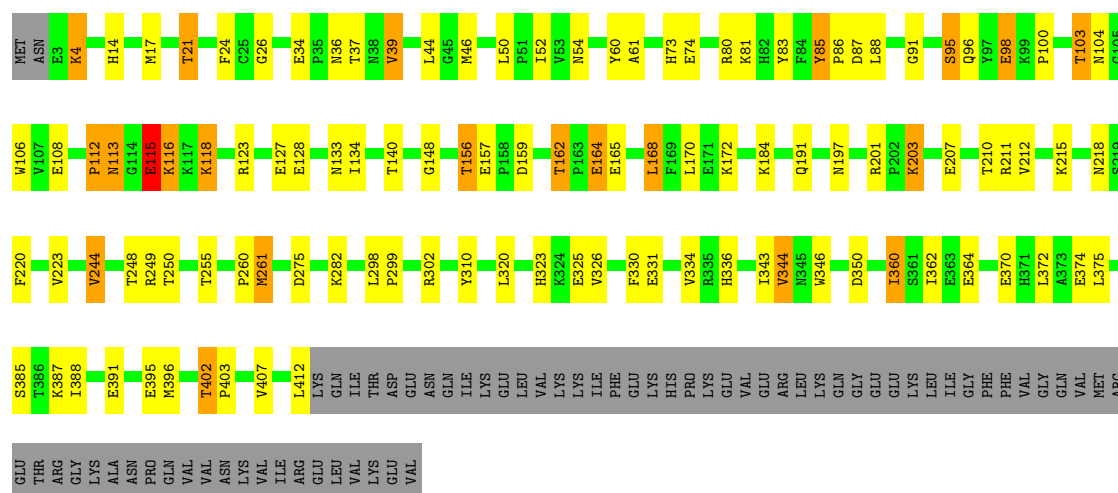
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain K: 60% 22% 14%



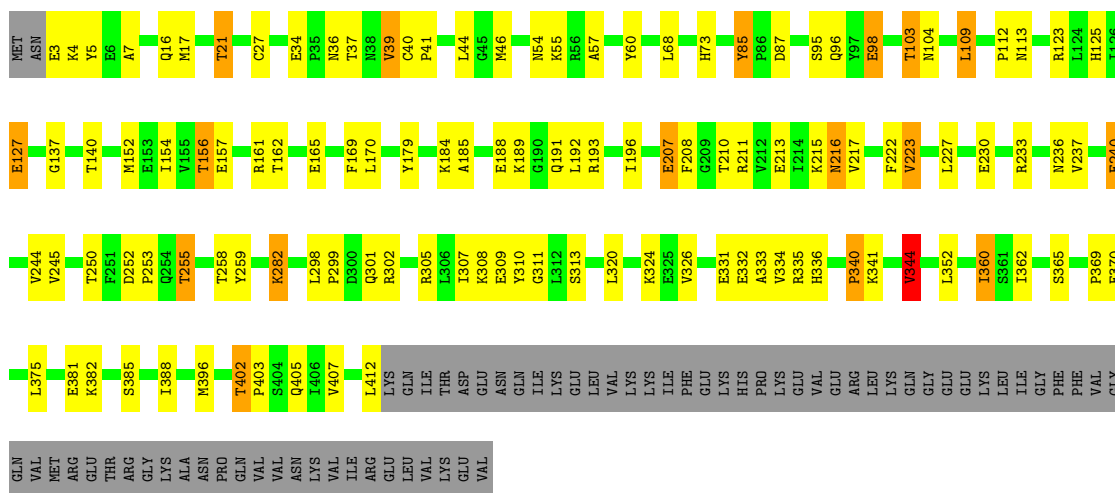
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain N: 63% 19% 14%

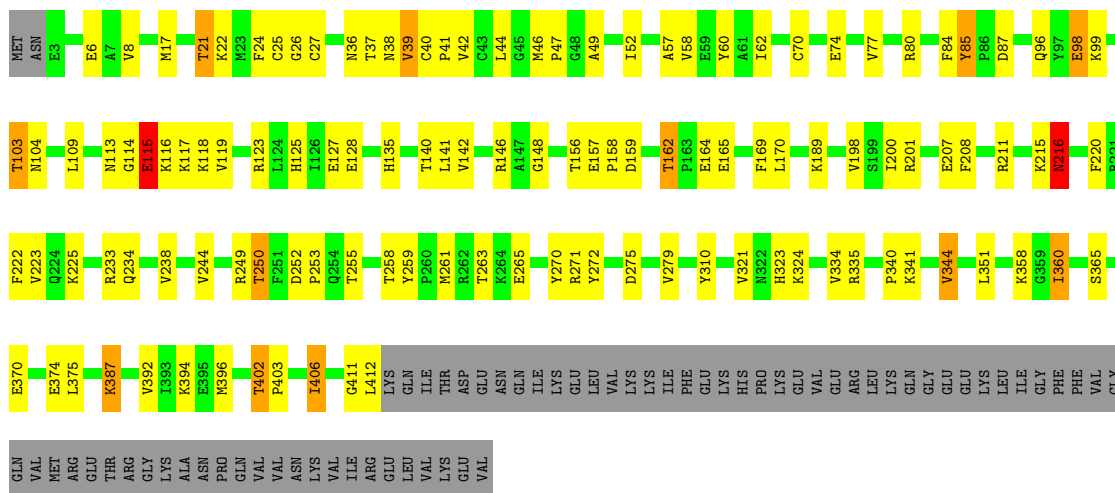


• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

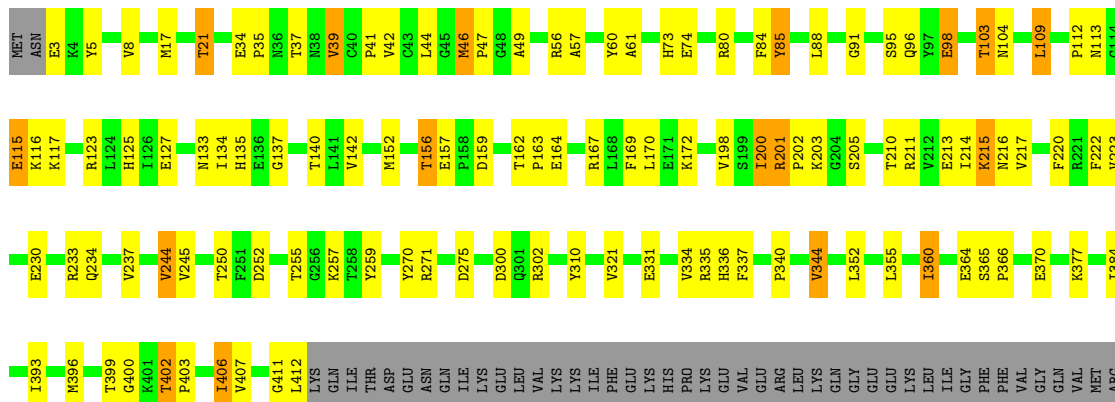
Chain Q: 61% 21% 14%



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



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



GLU
THR
ARG
GLY
LYS
ALA
ASN
PRO
GLN
VAL
VAL
ASN
LYS
VAL
TLE
ARG
GLU
LEU
VAL
LYS
GLU
VAL

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

Chain C:  71% 26%

MET V2 R15 L16 I23 Q27 S31 D32 I33 I37 D38 I33 L43 E46 P50 Y51 I52 F55 E56 P59 M60 E62 D63 E61 E62 D63 D70 R71 E72 K73 M76 G84 V92 GLU VAL

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

Chain F:  66% 29%

MET V2 D3 R4 V7 L8 A14 E17 Q27 S31 D32 I33 L34 I37 P50 Y51 I52 P59 M60 R61 E62 D63 E64 P65 D70 R71 L75 A78 P79 E80 G84 F85 F86 V87 V88 P89 R90 V91 V92 GLU VAL

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

Chain I:  67% 28%

MET V2 E5 A14 R15 I33 L34 I37 D38 I33 L34 I37 T45 E46 M47 I52 F55 E56 R61 E62 D63 E64 P65 K73 M76 P79 F80 R81 F86 V87 V88 P89 R90 V91 V92 GLU VAL

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

Chain L:  66% 30%

MET V2 D3 V7 A14 E17 S31 D32 I33 L34 I37 E42 T45 E46 M47 I52 F55 E56 T58 R61 E62 D63 P65 R61 R90 R90 V91 V92 GLU VAL

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

Chain O:  78% 18%

MET V2 R15 F26 L34 D38 E46 I52 Q53 E54 F55 T58 R61 E62 D63 P65 R61 G84 P89 R90 R90 V91 V92 GLU VAL

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

Chain R:  69% 28%

MET V2 R4 V7 L8 A14 I33 L34 I37 T45 E46 M47 P50 Y51 I52 F55 E56 E57 T58 P59 M60 R61 E62 D63 H66 R71 R81 P89 R90 V91 V92 GLU VAL

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

Chain U:  69% 27%



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	127.38Å 130.41Å 153.97Å 89.89° 90.21° 89.95°	Depositor
Resolution (Å)	48.97 – 3.00 48.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.97-3.00) 95.5 (48.97-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.263 , 0.306 0.258 , 0.297	Depositor DCC
R_{free} test set	11760 reflections (2.65%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.988	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -k,h,l 0.000 for k,-h,l 0.140 for h,-k,-l 0.439 for -h,k,-l 0.145 for -h,-k,l 0.000 for -k,-h,-l 0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	63243	wwPDB-VP
Average B, all atoms (Å ²)	60.0	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 35.61 % 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 5.6768e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.74	0/3874	0.96	4/5244 (0.1%)
1	D	0.73	1/3874 (0.0%)	0.95	4/5244 (0.1%)
1	G	0.72	1/3874 (0.0%)	0.94	1/5244 (0.0%)
1	J	0.75	1/3874 (0.0%)	1.00	11/5244 (0.2%)
1	M	0.74	0/3874	0.95	4/5244 (0.1%)
1	P	0.73	0/3874	0.96	6/5244 (0.1%)
1	S	0.72	1/3874 (0.0%)	0.96	3/5244 (0.1%)
1	V	0.77	1/3874 (0.0%)	0.98	4/5244 (0.1%)
2	B	0.69	0/3371	0.99	6/4541 (0.1%)
2	E	0.71	0/3371	0.98	8/4541 (0.2%)
2	H	0.74	0/3371	0.99	3/4541 (0.1%)
2	K	0.74	0/3371	1.01	6/4541 (0.1%)
2	N	0.72	0/3371	1.00	7/4541 (0.2%)
2	Q	0.73	0/3371	0.99	7/4541 (0.2%)
2	T	0.75	0/3371	1.01	7/4541 (0.2%)
2	W	0.71	0/3371	1.00	7/4541 (0.2%)
3	C	0.69	0/778	1.03	1/1050 (0.1%)
3	F	0.71	0/778	1.07	3/1050 (0.3%)
3	I	0.74	0/778	1.03	2/1050 (0.2%)
3	L	0.77	0/778	1.13	4/1050 (0.4%)
3	O	0.77	0/778	1.06	2/1050 (0.2%)
3	R	0.73	0/778	1.09	2/1050 (0.2%)
3	U	0.73	0/778	1.09	2/1050 (0.2%)
3	X	0.69	0/778	1.00	0/1050
All	All	0.73	5/64184 (0.0%)	0.99	104/86680 (0.1%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	299	ILE	CA-CB	9.31	1.59	1.54
1	S	299	ILE	CA-CB	8.81	1.59	1.54
1	G	299	ILE	CA-CB	6.77	1.58	1.54
1	D	299	ILE	CA-CB	6.41	1.57	1.54
1	V	299	ILE	CA-CB	5.72	1.57	1.54

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	85	TYR	CA-C-N	8.90	129.80	119.47
2	N	85	TYR	C-N-CA	8.90	129.80	119.47
2	W	85	TYR	CA-C-N	8.71	129.57	119.47
2	W	85	TYR	C-N-CA	8.71	129.57	119.47
2	H	85	TYR	CA-C-N	8.07	128.84	119.47
2	H	85	TYR	C-N-CA	8.07	128.84	119.47
2	B	85	TYR	CA-C-N	8.01	129.85	119.84
2	B	85	TYR	C-N-CA	8.01	129.85	119.84
2	B	88	LEU	CA-C-N	7.56	127.60	119.28
2	B	88	LEU	C-N-CA	7.56	127.60	119.28
2	T	85	TYR	CA-C-N	7.40	127.42	119.28
2	T	85	TYR	C-N-CA	7.40	127.42	119.28
3	R	58	THR	CA-C-N	7.22	128.87	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	58	THR	C-N-CA	7.22	128.87	119.84
2	K	85	TYR	CA-C-N	7.15	127.77	119.47
2	K	85	TYR	C-N-CA	7.15	127.77	119.47
1	D	304	ILE	N-CA-C	-7.07	106.03	111.62
2	B	91	GLY	N-CA-C	-7.04	105.78	114.92
3	L	58	THR	CA-C-N	6.93	128.76	120.23
3	L	58	THR	C-N-CA	6.93	128.76	120.23
2	W	88	LEU	CA-C-N	6.90	127.19	119.32
2	W	88	LEU	C-N-CA	6.90	127.19	119.32
3	C	46	GLU	N-CA-C	-6.87	101.31	110.24
2	T	98	GLU	N-CA-C	-6.83	101.52	110.53
2	B	98	GLU	N-CA-C	-6.81	101.54	110.53
1	M	112	VAL	N-CA-CB	-6.54	105.01	112.21
2	E	85	TYR	CA-C-N	6.46	126.38	119.28
2	E	85	TYR	C-N-CA	6.46	126.38	119.28
1	J	112	VAL	N-CA-CB	-6.44	105.13	112.21
2	W	98	GLU	N-CA-C	-6.37	101.68	110.35
1	A	295	VAL	CB-CA-C	-6.33	103.75	112.04
3	F	3	ASP	N-CA-C	6.28	118.40	110.24
1	J	421	THR	CA-C-N	6.27	124.19	120.24
1	J	421	THR	C-N-CA	6.27	124.19	120.24
1	D	94	ALA	CA-C-N	6.22	126.76	120.04
1	D	94	ALA	C-N-CA	6.22	126.76	120.04
2	W	91	GLY	N-CA-C	-6.04	106.99	115.32
2	N	218	ASN	N-CA-C	6.03	120.64	113.28
2	N	91	GLY	N-CA-C	-6.01	106.95	115.43
2	K	218	ASN	N-CA-C	6.00	120.63	112.88
2	Q	98	GLU	N-CA-C	-5.96	102.25	110.35
1	J	67	ILE	N-CA-C	5.95	113.77	107.76
1	S	94	ALA	CA-C-N	5.91	126.42	120.04
1	S	94	ALA	C-N-CA	5.91	126.42	120.04
1	A	304	ILE	N-CA-C	-5.81	106.56	111.56
1	V	94	ALA	CA-C-N	5.77	126.86	120.45
1	V	94	ALA	C-N-CA	5.77	126.86	120.45
2	N	50	LEU	CA-C-N	5.74	125.50	119.76
2	N	50	LEU	C-N-CA	5.74	125.50	119.76
2	E	298	LEU	CA-C-N	5.73	125.85	119.32
2	E	298	LEU	C-N-CA	5.73	125.85	119.32
3	I	64	GLU	CA-C-N	5.73	125.74	119.90
3	I	64	GLU	C-N-CA	5.73	125.74	119.90
1	M	94	ALA	CA-C-N	5.72	126.21	120.04
1	M	94	ALA	C-N-CA	5.72	126.21	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	58	THR	CA-C-N	5.71	126.98	119.84
3	O	58	THR	C-N-CA	5.71	126.98	119.84
2	Q	344	VAL	CB-CA-C	-5.71	104.56	112.04
1	M	304	ILE	N-CA-C	-5.70	106.66	111.56
2	T	351	LEU	N-CA-C	5.70	117.18	110.97
1	P	39	VAL	N-CA-C	5.63	116.28	110.82
1	S	39	VAL	N-CA-C	5.62	115.70	110.42
3	L	78	ALA	N-CA-C	5.62	116.48	109.57
3	U	35	ASP	N-CA-C	-5.59	105.19	112.23
3	L	46	GLU	N-CA-C	-5.57	102.05	110.24
1	J	345	GLY	CA-C-N	5.56	124.76	118.97
1	J	345	GLY	C-N-CA	5.56	124.76	118.97
1	J	299	ILE	CA-C-N	-5.56	113.30	119.19
1	J	299	ILE	C-N-CA	-5.56	113.30	119.19
1	P	143	VAL	N-CA-CB	-5.53	104.29	109.99
1	P	94	ALA	CA-C-N	5.52	126.00	120.04
1	P	94	ALA	C-N-CA	5.52	126.00	120.04
2	Q	85	TYR	CA-C-N	5.49	125.84	119.47
2	Q	85	TYR	C-N-CA	5.49	125.84	119.47
2	T	127	GLU	N-CA-C	5.49	116.61	108.60
2	T	198	VAL	N-CA-C	5.47	115.77	108.27
2	Q	189	LYS	CA-C-N	5.45	128.34	120.11
2	Q	189	LYS	C-N-CA	5.45	128.34	120.11
1	A	94	ALA	CA-C-N	5.42	126.46	120.45
1	A	94	ALA	C-N-CA	5.42	126.46	120.45
1	J	62	LEU	CA-C-N	5.40	125.47	119.32
1	J	62	LEU	C-N-CA	5.40	125.47	119.32
1	J	112	VAL	CB-CA-C	5.34	117.52	110.84
3	F	78	ALA	CA-C-N	5.33	124.78	119.24
3	F	78	ALA	C-N-CA	5.33	124.78	119.24
2	E	53	VAL	N-CA-C	5.31	115.94	109.30
2	N	98	GLU	N-CA-C	-5.30	103.54	110.53
2	E	142	VAL	N-CA-C	5.29	115.20	107.37
1	P	345	GLY	CA-C-N	5.28	124.46	118.97
1	P	345	GLY	C-N-CA	5.28	124.46	118.97
2	K	98	GLU	N-CA-C	-5.26	102.60	110.23
2	K	273	PHE	CA-C-N	-5.26	114.34	119.76
2	K	273	PHE	C-N-CA	-5.26	114.34	119.76
1	V	43	ILE	N-CA-C	-5.24	106.58	111.45
2	E	326	VAL	N-CA-C	-5.24	105.97	110.74
2	W	115	GLU	CB-CA-C	-5.23	110.12	117.23
3	U	3	ASP	N-CA-C	5.20	117.39	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	218	ASN	N-CA-C	5.20	119.31	112.92
1	V	295	VAL	CB-CA-C	-5.16	104.17	112.16
2	T	142	VAL	N-CA-C	5.14	115.17	107.51
1	G	304	ILE	N-CA-C	-5.12	107.16	111.56
2	Q	127	GLU	N-CA-C	5.07	115.73	108.74
1	D	42	TYR	N-CA-C	5.04	118.03	109.76
2	E	211	ARG	N-CA-C	5.01	116.68	108.52

There are no chirality outliers.

All (39) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
2	Q	112	PRO	Peptide
2	Q	113	ASN	Peptide
3	R	45	THR	Peptide
1	S	225	GLY	Peptide
2	T	115	GLU	Peptide
2	T	411	GLY	Peptide
2	W	112	PRO	Peptide
2	W	113	ASN	Peptide
2	W	215	LYS	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	3816	113	0
1	D	3784	0	3816	117	0
1	G	3784	0	3816	99	0
1	J	3784	0	3816	108	0
1	M	3784	0	3816	92	0
1	P	3784	0	3816	119	0
1	S	3784	0	3816	104	0
1	V	3784	0	3816	110	0
2	B	3308	0	3354	113	0
2	E	3308	0	3353	122	0
2	H	3308	0	3353	99	0
2	K	3308	0	3353	90	0
2	N	3308	0	3353	88	0
2	Q	3308	0	3353	93	0
2	T	3308	0	3353	101	0
2	W	3308	0	3353	97	0
3	C	764	0	755	21	0
3	F	764	0	755	23	0
3	I	764	0	755	30	0
3	L	764	0	755	24	0
3	O	764	0	755	18	0
3	R	764	0	755	18	0
3	U	764	0	755	18	0
3	X	764	0	755	32	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	N	5	0	0	1	0
10	P	2	0	0	1	0
10	Q	7	0	0	0	0
10	T	5	0	0	0	0
10	V	1	0	0	0	0
10	W	6	0	0	0	0
All	All	63243	0	63519	1701	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 (1701) 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:W:384:ILE:HG22	2:W:412:LEU:CD2	1.62	1.28
1:D:83:THR:HG21	1:D:131:PHE:CZ	1.78	1.19
2:B:280:PRO:HD2	3:C:55:PHE:CZ	1.85	1.12
2:K:115:GLU:HA	2:K:115:GLU:OE2	1.48	1.10
1:V:190:ARG:HH11	1:V:190:ARG:HG3	1.11	1.10
3:X:91:VAL:HG23	3:X:92:VAL:N	1.68	1.09
2:H:81:LYS:NZ	9:H:482:ASP:HA	1.68	1.08
3:I:88:VAL:HB	3:I:89:PRO:HD2	1.34	1.07
1:G:117:LEU:HD12	1:G:117:LEU:N	1.69	1.07
1:J:376:ARG:HH11	1:J:376:ARG:HG3	1.17	1.07
1:D:13:LEU:HB3	1:D:19:VAL:HG12	1.36	1.07
1:D:77:VAL:HG23	1:D:114:LYS:HZ2	1.18	1.07
1:A:190:ARG:HH11	1:A:190:ARG:HG3	1.05	1.06
2:N:115:GLU:HA	2:N:115:GLU:OE2	1.49	1.06
2:B:21:THR:HG21	3:C:61:ARG:HH12	1.20	1.06
3:L:88:VAL:HB	3:L:89:PRO:HD2	1.37	1.06
2:W:384:ILE:HG22	2:W:412:LEU:HD23	1.14	1.05
1:M:88:ILE:HG23	1:M:343:GLY:HA3	1.36	1.05
2:E:360:ILE:HD11	2:E:365:SER:HA	1.35	1.04
2:W:384:ILE:CG2	2:W:412:LEU:HD23	1.85	1.04
2:E:17:MET:HE1	2:E:57:ALA:HA	1.31	1.04
1:D:77:VAL:HG23	1:D:114:LYS:NZ	1.73	1.03
2:T:115:GLU:HA	2:T:115:GLU:OE2	1.52	1.03
2:W:360:ILE:HD11	2:W:365:SER:HA	1.38	1.03
1:P:190:ARG:HH11	1:P:190:ARG:HG3	1.24	1.02
1:M:352:ILE:O	1:M:356:THR:HG22	1.57	1.02
1:D:13:LEU:HB3	1:D:19:VAL:CG1	1.89	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:21:THR:HB	3:U:63:ASP:OD1	1.58	1.01
2:K:412:LEU:C	2:K:412:LEU:HD12	1.86	1.01
1:J:95:PRO:HG2	2:K:46:MET:HE1	1.43	1.00
2:H:21:THR:HG21	3:I:61:ARG:HH12	1.25	0.99
2:N:21:THR:HG21	3:O:61:ARG:HH12	1.27	0.99
2:E:21:THR:HG21	3:F:61:ARG:HH12	1.26	0.98
1:M:138:TRP:CZ2	1:M:476:PRO:HD3	1.97	0.98
1:S:422:VAL:CG2	1:S:423:PRO:HD3	1.94	0.98
2:T:21:THR:HG21	3:U:61:ARG:HH12	1.30	0.96
3:X:91:VAL:HG23	3:X:92:VAL:H	1.23	0.96
3:O:91:VAL:O	3:O:92:VAL:HG13	1.65	0.96
1:A:352:ILE:O	1:A:356:THR:HG23	1.66	0.95
2:B:384:ILE:HG22	2:B:412:LEU:HD23	1.44	0.95
2:B:17:MET:HE1	2:B:57:ALA:HA	1.46	0.95
1:A:120:PHE:O	1:A:122:MET:HG3	1.65	0.95
1:G:117:LEU:HD12	1:G:117:LEU:H	1.24	0.95
2:Q:156:THR:HG22	2:Q:157:GLU:O	1.67	0.95
2:E:17:MET:HE3	2:E:60:TYR:HB2	1.49	0.94
1:S:190:ARG:HD3	1:S:241:TRP:HH2	1.33	0.93
1:M:88:ILE:HD11	1:M:120:PHE:CZ	2.05	0.92
2:E:119:VAL:HG13	2:E:159:ASP:HB2	1.52	0.91
2:E:21:THR:HB	3:F:63:ASP:OD1	1.69	0.90
2:H:17:MET:CE	2:H:60:TYR:HB2	2.01	0.90
2:W:384:ILE:HG22	2:W:412:LEU:HD21	1.52	0.90
2:H:17:MET:CE	2:H:60:TYR:CB	2.49	0.90
2:E:39:VAL:HG22	2:E:44:LEU:HG	1.52	0.89
1:S:422:VAL:HG22	1:S:423:PRO:HD3	1.55	0.89
1:D:83:THR:HG21	1:D:131:PHE:HZ	1.30	0.89
2:E:17:MET:CE	2:E:57:ALA:HA	2.01	0.89
1:A:13:LEU:HB3	1:A:19:VAL:HG12	1.53	0.88
1:G:95:PRO:HG2	2:H:46:MET:CE	2.03	0.88
1:D:77:VAL:CG2	1:D:114:LYS:NZ	2.36	0.88
2:Q:95:SER:HB2	2:Q:127:GLU:HB3	1.52	0.88
2:B:103:THR:HG22	2:B:104:ASN:OD1	1.72	0.88
2:E:34:GLU:O	2:E:37:THR:HB	1.71	0.88
2:B:384:ILE:CG2	2:B:412:LEU:HD23	2.03	0.88
2:H:220:PHE:O	2:H:223:VAL:HG22	1.74	0.88
2:B:162:THR:HG22	2:B:165:GLU:H	1.38	0.88
2:W:21:THR:HG21	3:X:61:ARG:HH12	1.37	0.88
1:A:224:SER:HB3	1:A:238:VAL:HG21	1.57	0.87
2:T:115:GLU:HG3	2:T:116:LYS:HE2	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:39:VAL:HG13	2:W:44:LEU:HD11	1.54	0.87
2:B:347:LEU:O	2:B:352:LEU:HD23	1.76	0.86
2:N:17:MET:HE2	2:N:60:TYR:HB3	1.58	0.86
2:E:17:MET:HE1	2:E:57:ALA:CA	2.04	0.86
1:D:190:ARG:HD3	1:D:241:TRP:HH2	1.40	0.86
2:E:115:GLU:HB3	2:E:116:LYS:HG3	1.57	0.86
1:J:72:LYS:HA	1:J:115:THR:HG22	1.58	0.86
2:B:21:THR:CG2	3:C:61:ARG:HH12	1.88	0.85
2:B:40:CYS:O	2:B:44:LEU:HB2	1.75	0.85
2:W:252:ASP:HB3	2:W:255:THR:HG22	1.58	0.85
2:N:201:ARG:HD2	2:N:207:GLU:O	1.76	0.85
1:S:376:ARG:HG3	1:S:376:ARG:HH11	1.39	0.85
2:B:384:ILE:HG22	2:B:412:LEU:CD2	2.06	0.85
1:V:190:ARG:HG3	1:V:190:ARG:NH1	1.89	0.85
1:V:279:GLU:HG3	1:V:468:LYS:NZ	1.92	0.85
2:K:21:THR:HG21	3:L:61:ARG:HH12	1.41	0.84
2:E:33:ALA:HB1	2:E:37:THR:HG21	1.59	0.84
1:A:376:ARG:HH11	1:A:376:ARG:HG3	1.40	0.84
2:B:21:THR:HB	3:C:63:ASP:OD1	1.75	0.84
2:Q:207:GLU:OE1	2:Q:207:GLU:HA	1.76	0.84
2:E:39:VAL:HG13	2:E:44:LEU:HD11	1.57	0.84
1:D:83:THR:HG21	1:D:131:PHE:CE2	2.13	0.84
2:H:81:LYS:HZ1	9:H:482:ASP:HA	1.41	0.84
2:T:358:LYS:HB2	2:T:360:ILE:HG22	1.60	0.83
2:B:100:PRO:HB3	2:B:123:ARG:HH21	1.41	0.83
1:D:83:THR:HG22	1:D:86:SER:H	1.44	0.83
2:Q:334:VAL:HG21	2:Q:340:PRO:HB3	1.59	0.83
2:E:360:ILE:HD11	2:E:365:SER:CA	2.08	0.83
2:K:412:LEU:HD12	2:K:412:LEU:O	1.80	0.82
2:W:355:LEU:HD22	2:W:360:ILE:CD1	2.10	0.82
1:J:3:TRP:CD2	1:J:31:ARG:HD3	2.14	0.82
2:B:280:PRO:HD2	3:C:55:PHE:HZ	1.38	0.82
1:J:95:PRO:HG2	2:K:46:MET:CE	2.10	0.82
2:N:115:GLU:HG3	2:N:116:LYS:HG2	1.60	0.82
1:G:95:PRO:HG2	2:H:46:MET:HE1	1.60	0.81
1:G:117:LEU:N	1:G:117:LEU:CD1	2.42	0.81
1:V:163:SER:HB3	1:V:209:PHE:HB2	1.62	0.81
1:P:155:VAL:HG12	1:P:181:VAL:HG21	1.61	0.81
2:B:17:MET:HG2	2:B:152:MET:HE3	1.63	0.81
2:N:39:VAL:HG13	2:N:44:LEU:HD11	1.62	0.81
3:R:46:GLU:O	3:R:47:ASN:HB2	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:GLN:HG3	1:D:175:PRO:HD3	1.64	0.80
1:A:221:GLU:O	1:A:224:SER:HB2	1.81	0.80
3:C:33:ILE:O	3:C:37:ILE:HG12	1.81	0.80
2:W:34:GLU:O	2:W:37:THR:HG22	1.81	0.80
1:J:376:ARG:HG3	1:J:376:ARG:NH1	1.94	0.80
2:H:211:ARG:NH1	8:H:479:ATP:H5'2	1.97	0.80
1:P:177:SER:HA	10:P:907:HOH:O	1.81	0.80
1:M:174:GLN:HG3	1:M:175:PRO:HD3	1.63	0.79
2:K:100:PRO:HB3	2:K:123:ARG:HH21	1.45	0.79
3:X:33:ILE:O	3:X:37:ILE:HG12	1.82	0.79
1:D:163:SER:HB3	1:D:209:PHE:HB2	1.65	0.79
2:N:81:LYS:NZ	9:N:482:ASP:HA	1.98	0.79
1:G:352:ILE:O	1:G:356:THR:HG23	1.82	0.79
1:D:245:VAL:CG1	1:D:459:LEU:HB3	2.13	0.78
1:A:190:ARG:HG3	1:A:190:ARG:NH1	1.86	0.78
1:D:115:THR:HG21	1:D:151:SER:OG	1.84	0.78
2:T:103:THR:CG2	2:T:104:ASN:OD1	2.32	0.78
2:H:21:THR:CG2	3:I:61:ARG:HH12	1.96	0.78
2:T:207:GLU:HG3	2:T:208:PHE:H	1.49	0.78
2:E:310:TYR:HE1	2:E:334:VAL:HG11	1.48	0.78
2:H:17:MET:HE1	2:H:60:TYR:HB2	1.63	0.78
2:W:156:THR:HG22	2:W:157:GLU:O	1.84	0.78
1:M:88:ILE:HD11	1:M:120:PHE:HZ	1.48	0.78
2:Q:207:GLU:OE1	2:Q:207:GLU:CA	2.32	0.78
2:H:17:MET:CE	2:H:60:TYR:HB3	2.12	0.77
1:S:477:LEU:N	1:S:477:LEU:HD23	1.99	0.77
1:D:2:LEU:HD23	1:D:27:SER:HB2	1.66	0.77
2:B:252:ASP:HB3	2:B:255:THR:HG22	1.65	0.77
2:Q:17:MET:CE	2:Q:60:TYR:HB2	2.15	0.77
1:J:163:SER:HB3	1:J:209:PHE:HB2	1.65	0.77
2:B:17:MET:HE3	2:B:60:TYR:HB2	1.66	0.77
2:B:17:MET:HE1	2:B:57:ALA:CA	2.15	0.77
2:B:200:ILE:HD11	2:B:238:VAL:HG21	1.66	0.77
2:N:220:PHE:O	2:N:223:VAL:HG22	1.85	0.76
1:D:245:VAL:HG12	1:D:459:LEU:HB3	1.66	0.76
2:E:140:THR:OG1	3:F:90:ARG:HA	1.85	0.76
1:J:3:TRP:CE2	1:J:31:ARG:HD3	2.20	0.76
2:B:17:MET:CE	2:B:57:ALA:HA	2.14	0.76
2:T:115:GLU:OE2	2:T:115:GLU:CA	2.30	0.76
1:A:434:ILE:HD11	1:A:462:SER:OG	1.85	0.76
2:W:411:GLY:O	2:W:412:LEU:HB2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:190:ARG:HD3	1:J:241:TRP:HH2	1.51	0.75
2:T:17:MET:HE1	2:T:57:ALA:HA	1.66	0.75
2:K:39:VAL:HG13	2:K:44:LEU:HD11	1.67	0.75
1:J:177:SER:HA	10:J:906:HOH:O	1.85	0.75
1:S:477:LEU:HD23	1:S:477:LEU:H	1.51	0.75
2:W:21:THR:CG2	3:X:61:ARG:HH12	2.00	0.75
1:S:245:VAL:HG12	1:S:459:LEU:HB3	1.68	0.75
2:H:103:THR:HG22	2:H:104:ASN:OD1	1.86	0.75
1:V:138:TRP:CE2	1:V:438:TRP:HH2	2.04	0.75
1:D:72:LYS:HA	1:D:115:THR:HG22	1.67	0.75
2:N:95:SER:HB3	2:N:127:GLU:HB3	1.67	0.75
1:A:475:ILE:HG22	1:A:476:PRO:HD2	1.69	0.75
2:E:103:THR:HG22	2:E:104:ASN:OD1	1.86	0.75
2:K:406:ILE:O	2:K:410:LYS:HB2	1.87	0.75
2:E:33:ALA:CB	2:E:37:THR:HG21	2.16	0.74
2:N:17:MET:HE2	2:N:60:TYR:CB	2.16	0.74
2:H:17:MET:HE2	2:H:60:TYR:CB	2.16	0.74
2:K:115:GLU:OE2	2:K:115:GLU:CA	2.30	0.74
1:A:450:GLY:HA3	1:A:458:LEU:HD11	1.67	0.74
1:D:138:TRP:CE2	1:D:438:TRP:CH2	2.75	0.74
2:K:34:GLU:O	2:K:37:THR:HG22	1.86	0.74
1:S:422:VAL:HG23	1:S:423:PRO:HD3	1.69	0.74
2:W:360:ILE:CD1	2:W:365:SER:HA	2.14	0.74
1:J:174:GLN:HG3	1:J:175:PRO:HD3	1.70	0.74
1:V:279:GLU:HG3	1:V:468:LYS:HZ1	1.53	0.74
1:P:356:THR:HG21	3:R:14:ALA:HB2	1.68	0.74
1:S:190:ARG:HD3	1:S:241:TRP:CH2	2.20	0.74
1:M:88:ILE:HG23	1:M:343:GLY:CA	2.16	0.74
1:V:138:TRP:CE2	1:V:438:TRP:CH2	2.76	0.74
2:Q:341:LYS:O	2:Q:344:VAL:HG23	1.88	0.73
2:T:220:PHE:O	2:T:223:VAL:HG22	1.89	0.73
2:W:103:THR:HG22	2:W:104:ASN:OD1	1.86	0.73
2:K:17:MET:HE1	2:K:57:ALA:O	1.88	0.73
2:Q:213:GLU:OE2	2:Q:215:LYS:HE3	1.89	0.73
1:S:155:VAL:HG12	1:S:181:VAL:HG21	1.70	0.73
1:S:397:THR:HG22	1:S:398:PRO:HD2	1.68	0.73
2:B:280:PRO:HD2	3:C:55:PHE:CE1	2.23	0.73
2:E:411:GLY:O	2:E:412:LEU:C	2.32	0.73
2:Q:39:VAL:HG13	2:Q:44:LEU:HD11	1.70	0.73
2:W:17:MET:CE	2:W:60:TYR:HB2	2.19	0.73
2:B:213:GLU:OE1	2:B:215:LYS:HE2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:81:LYS:HZ2	9:H:482:ASP:HA	1.51	0.72
2:H:375:LEU:HD13	2:H:396:MET:HE1	1.71	0.72
1:P:299:ILE:N	1:P:300:PRO:HD2	2.04	0.72
2:W:17:MET:HE1	2:W:57:ALA:HA	1.70	0.72
1:D:138:TRP:CE2	1:D:438:TRP:HH2	2.07	0.72
2:T:39:VAL:HG22	2:T:44:LEU:HG	1.71	0.72
2:W:213:GLU:OE2	2:W:215:LYS:HE3	1.88	0.72
2:E:22:LYS:HD2	2:E:27:CYS:HB2	1.71	0.72
2:N:211:ARG:NH1	8:N:479:ATP:O2A	2.22	0.72
1:S:73:ASP:OD1	1:S:114:LYS:NZ	2.22	0.72
1:M:138:TRP:CE2	1:M:438:TRP:CH2	2.78	0.72
2:N:17:MET:CE	2:N:60:TYR:HB3	2.19	0.72
2:W:17:MET:HE1	2:W:57:ALA:O	1.89	0.72
2:E:360:ILE:CD1	2:E:365:SER:HA	2.16	0.72
1:G:178:PHE:HE1	1:G:397:THR:HG21	1.53	0.72
1:J:3:TRP:CE3	1:J:31:ARG:HD3	2.24	0.72
1:J:95:PRO:CG	2:K:46:MET:HE1	2.18	0.71
3:O:91:VAL:O	3:O:92:VAL:CG1	2.37	0.71
1:A:163:SER:HB3	1:A:209:PHE:HB2	1.72	0.71
2:E:17:MET:CE	2:E:60:TYR:HB2	2.20	0.71
2:B:103:THR:CG2	2:B:104:ASN:OD1	2.38	0.71
2:K:252:ASP:OD2	2:K:255:THR:HG22	1.90	0.71
3:X:91:VAL:CG2	3:X:92:VAL:N	2.43	0.71
2:B:17:MET:CE	2:B:60:TYR:HB2	2.20	0.71
2:T:162:THR:HG22	2:T:165:GLU:HB2	1.73	0.70
2:B:21:THR:HG21	3:C:61:ARG:NH1	2.00	0.70
2:K:156:THR:HG22	2:K:157:GLU:O	1.91	0.70
1:D:138:TRP:CZ2	1:D:438:TRP:CH2	2.80	0.70
2:K:412:LEU:C	2:K:412:LEU:CD1	2.60	0.70
1:S:13:LEU:HB3	1:S:19:VAL:HG12	1.74	0.70
1:A:475:ILE:CG2	1:A:476:PRO:HD2	2.21	0.70
2:E:37:THR:HG23	2:E:38:ASN:H	1.55	0.70
1:S:163:SER:HB3	1:S:209:PHE:HB2	1.72	0.70
1:S:397:THR:HG22	1:S:398:PRO:CD	2.20	0.70
1:G:162:VAL:HG21	1:G:219:VAL:HG21	1.72	0.70
3:I:46:GLU:O	3:I:47:ASN:HB2	1.92	0.70
1:M:163:SER:HB3	1:M:209:PHE:HB2	1.73	0.70
2:W:96:GLN:HB2	2:W:125:HIS:HB2	1.74	0.70
2:H:86:PRO:HG2	3:I:91:VAL:HG11	1.72	0.70
2:T:17:MET:HE1	2:T:57:ALA:O	1.92	0.70
2:T:252:ASP:OD2	2:T:255:THR:HG22	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:84:CYS:SG	1:V:197:VAL:HG21	2.31	0.70
1:V:190:ARG:HD2	1:V:455:GLU:OE2	1.91	0.70
2:N:162:THR:HB	2:N:165:GLU:HG3	1.73	0.69
2:E:103:THR:HG22	2:E:104:ASN:CG	2.17	0.69
2:Q:402:THR:HG22	2:Q:403:PRO:HD2	1.73	0.69
2:W:21:THR:HB	3:X:63:ASP:OD1	1.92	0.69
3:L:46:GLU:O	3:L:47:ASN:HB2	1.91	0.69
1:M:88:ILE:HD11	1:M:120:PHE:CE2	2.27	0.69
2:Q:17:MET:HE1	2:Q:57:ALA:O	1.92	0.69
2:N:103:THR:HG23	2:N:104:ASN:OD1	1.92	0.69
1:A:306:ALA:HB3	1:A:307:PRO:HD3	1.74	0.69
2:E:37:THR:HG23	2:E:38:ASN:N	2.08	0.69
2:K:17:MET:CE	2:K:60:TYR:HB2	2.22	0.69
1:P:3:TRP:CZ2	1:P:31:ARG:HD3	2.27	0.69
3:X:55:PHE:O	3:X:56:GLU:HB3	1.91	0.69
2:E:100:PRO:HG3	2:E:123:ARG:NH1	2.08	0.69
2:B:156:THR:HG23	2:B:157:GLU:O	1.93	0.69
1:J:356:THR:HG21	3:L:14:ALA:HB2	1.75	0.69
1:J:477:LEU:O	1:J:478:THR:C	2.36	0.69
1:A:13:LEU:HB3	1:A:19:VAL:CG1	2.23	0.69
2:K:115:GLU:HG3	2:K:116:LYS:HG2	1.75	0.68
1:M:245:VAL:HG12	1:M:459:LEU:HB3	1.74	0.68
1:S:245:VAL:CG1	1:S:459:LEU:HB3	2.24	0.68
2:T:17:MET:CE	2:T:57:ALA:HA	2.24	0.68
2:E:252:ASP:HB3	2:E:255:THR:HG22	1.76	0.68
2:N:17:MET:CE	2:N:60:TYR:CB	2.71	0.68
2:N:112:PRO:HG2	2:N:164:GLU:OE1	1.92	0.68
1:P:163:SER:HB3	1:P:209:PHE:HB2	1.75	0.68
1:G:245:VAL:HG12	1:G:459:LEU:HB3	1.76	0.68
1:V:193:ARG:NH1	1:V:232:THR:OG1	2.26	0.68
2:K:412:LEU:O	2:K:412:LEU:CD1	2.41	0.68
1:P:299:ILE:HG13	1:P:419:ILE:HG22	1.75	0.68
2:B:17:MET:HE1	2:B:57:ALA:O	1.93	0.68
1:D:77:VAL:CG2	1:D:114:LYS:HZ1	2.06	0.68
2:N:21:THR:CG2	3:O:61:ARG:HH12	2.03	0.68
2:Q:95:SER:CB	2:Q:127:GLU:HB3	2.24	0.68
2:E:17:MET:HG2	2:E:152:MET:HE2	1.74	0.68
2:T:140:THR:OG1	3:U:90:ARG:HA	1.94	0.67
2:E:17:MET:HE3	2:E:60:TYR:CB	2.23	0.67
1:G:344:PHE:O	1:G:349:LYS:HE2	1.94	0.67
1:G:138:TRP:CE2	1:G:438:TRP:CH2	2.83	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:306:ALA:HB3	1:P:307:PRO:HD3	1.75	0.67
1:P:3:TRP:CH2	1:P:31:ARG:HD3	2.28	0.67
1:G:117:LEU:H	1:G:117:LEU:CD1	2.02	0.67
1:J:438:TRP:CZ3	1:J:443:PRO:HG3	2.29	0.67
1:V:292:LEU:HB2	1:V:295:VAL:HG22	1.77	0.67
2:E:201:ARG:HD2	2:E:207:GLU:O	1.95	0.67
2:T:207:GLU:HG3	2:T:208:PHE:N	2.09	0.67
1:V:69:ILE:HD11	1:V:164:LEU:HD13	1.76	0.67
1:A:397:THR:HG22	1:A:399:THR:H	1.59	0.67
3:F:33:ILE:O	3:F:37:ILE:HG12	1.95	0.67
1:M:306:ALA:HB3	1:M:307:PRO:HD3	1.76	0.67
3:U:33:ILE:O	3:U:37:ILE:HG12	1.95	0.66
2:K:21:THR:HG22	2:K:54:ASN:HD22	1.60	0.66
2:B:37:THR:HG23	2:B:38:ASN:N	2.09	0.66
1:J:224:SER:O	1:J:238:VAL:HG21	1.96	0.66
1:P:190:ARG:HG3	1:P:190:ARG:NH1	1.98	0.66
1:S:422:VAL:HG23	1:S:423:PRO:CD	2.25	0.66
1:G:115:THR:HG21	1:G:151:SER:OG	1.94	0.66
1:A:138:TRP:CE2	1:A:438:TRP:HH2	2.13	0.66
2:E:117:LYS:HG2	2:E:118:LYS:N	2.10	0.66
2:W:17:MET:HE3	2:W:60:TYR:HB2	1.77	0.66
2:W:252:ASP:HB3	2:W:255:THR:CG2	2.25	0.66
1:A:32:TYR:CE1	1:A:36:GLU:HG2	2.31	0.66
1:G:190:ARG:HD2	1:G:455:GLU:OE2	1.95	0.66
2:K:3:GLU:HG3	2:K:5:TYR:H	1.61	0.66
1:M:95:PRO:HG2	2:N:46:MET:CE	2.25	0.66
2:N:81:LYS:HZ1	9:N:482:ASP:HA	1.59	0.66
1:V:352:ILE:O	1:V:356:THR:HG23	1.96	0.66
1:V:434:ILE:HD11	1:V:462:SER:OG	1.96	0.66
2:B:17:MET:HE3	2:B:60:TYR:CB	2.25	0.66
2:H:135:HIS:CE1	3:I:91:VAL:O	2.48	0.66
1:V:6:SER:HB3	1:V:212:ARG:NH1	2.10	0.66
2:W:355:LEU:HD22	2:W:360:ILE:HD13	1.77	0.66
1:J:138:TRP:CZ2	1:J:476:PRO:HD3	2.30	0.66
2:W:411:GLY:O	2:W:412:LEU:CB	2.43	0.66
2:K:412:LEU:O	2:K:412:LEU:CG	2.44	0.66
1:J:245:VAL:HG12	1:J:459:LEU:HB3	1.77	0.66
2:T:128:GLU:HB2	2:T:148:GLY:HA2	1.78	0.65
1:P:143:VAL:HG13	1:P:145:GLY:H	1.61	0.65
2:T:22:LYS:HD2	2:T:27:CYS:HB2	1.79	0.65
1:G:85:ALA:HB2	1:G:117:LEU:HD13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:ILE:HD11	1:G:164:LEU:HD13	1.77	0.65
1:A:245:VAL:HG12	1:A:459:LEU:HB3	1.78	0.65
1:J:90:GLU:O	1:J:91:ASN:HB2	1.94	0.65
2:N:100:PRO:HB3	2:N:123:ARG:NH2	2.11	0.65
2:T:17:MET:HE3	2:T:60:TYR:HB2	1.78	0.65
2:B:34:GLU:O	2:B:37:THR:HB	1.96	0.65
2:E:156:THR:HG22	2:E:157:GLU:O	1.96	0.65
1:V:77:VAL:HG21	1:V:114:LYS:NZ	2.12	0.65
2:Q:156:THR:CG2	2:Q:157:GLU:O	2.41	0.65
1:V:120:PHE:O	1:V:122:MET:HG3	1.96	0.65
1:S:422:VAL:N	1:S:423:PRO:CD	2.60	0.65
2:T:85:TYR:HD2	2:T:87:ASP:OD1	1.79	0.65
2:N:215:LYS:CD	2:N:248:THR:HG21	2.26	0.65
1:S:143:VAL:HG12	1:S:145:GLY:H	1.60	0.65
1:V:190:ARG:HH11	1:V:190:ARG:CG	1.99	0.65
8:H:479:ATP:O2G	9:H:482:ASP:HB2	1.97	0.65
1:M:422:VAL:CG2	1:M:423:PRO:HD3	2.27	0.65
1:D:83:THR:CG2	1:D:131:PHE:HZ	2.08	0.64
2:H:95:SER:HB3	2:H:127:GLU:HB3	1.78	0.64
1:J:138:TRP:CE2	1:J:438:TRP:CZ3	2.85	0.64
1:V:77:VAL:HG23	1:V:114:LYS:HZ2	1.63	0.64
1:V:138:TRP:CZ2	1:V:476:PRO:HD3	2.33	0.64
2:E:252:ASP:HB3	2:E:255:THR:CG2	2.27	0.64
2:H:17:MET:HE2	2:H:60:TYR:HB2	1.76	0.64
2:E:13:ILE:HG21	2:E:173:LEU:HD21	1.79	0.64
1:V:162:VAL:HG21	1:V:219:VAL:HG21	1.79	0.64
1:A:155:VAL:CG2	1:A:163:SER:HB2	2.27	0.64
2:B:220:PHE:O	2:B:223:VAL:HG22	1.98	0.64
1:G:374:VAL:HG21	3:I:40:LEU:HD22	1.78	0.64
1:S:2:LEU:HD23	1:S:27:SER:HB2	1.80	0.64
2:H:103:THR:HG22	2:H:104:ASN:CG	2.23	0.64
2:N:21:THR:HB	3:O:63:ASP:OD1	1.96	0.64
2:N:36:ASN:ND2	3:O:84:GLY:O	2.23	0.64
1:P:438:TRP:CZ3	1:P:443:PRO:HG3	2.33	0.64
1:P:352:ILE:O	1:P:356:THR:HG23	1.98	0.64
1:D:38:LYS:HD2	1:D:477:LEU:HD13	1.80	0.64
2:Q:207:GLU:OE1	2:Q:208:PHE:N	2.31	0.64
1:G:72:LYS:HA	1:G:115:THR:HG22	1.80	0.64
2:K:21:THR:CG2	3:L:61:ARG:HH12	2.09	0.64
2:N:115:GLU:HG3	2:N:116:LYS:CG	2.28	0.64
1:P:90:GLU:O	1:P:91:ASN:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:17:MET:HG2	2:Q:152:MET:HE2	1.80	0.64
1:M:138:TRP:CE2	1:M:438:TRP:HH2	2.13	0.63
2:T:115:GLU:HG3	2:T:116:LYS:HG3	1.78	0.63
1:V:397:THR:HG22	1:V:398:PRO:HD2	1.79	0.63
1:G:306:ALA:HB3	1:G:307:PRO:HD3	1.80	0.63
2:H:21:THR:HB	3:I:63:ASP:OD1	1.98	0.63
1:J:190:ARG:HD3	1:J:241:TRP:CH2	2.34	0.63
1:G:138:TRP:CZ2	1:G:476:PRO:HD3	2.33	0.63
1:G:422:VAL:CG2	1:G:423:PRO:HD3	2.28	0.63
1:M:299:ILE:HG13	1:M:419:ILE:HG22	1.80	0.63
2:W:255:THR:HG21	2:W:259:TYR:HE1	1.64	0.63
1:A:475:ILE:CG2	1:A:476:PRO:CD	2.76	0.63
1:D:83:THR:HG22	1:D:86:SER:N	2.14	0.63
1:M:88:ILE:CG2	1:M:343:GLY:HA3	2.23	0.63
1:G:138:TRP:CD2	1:G:438:TRP:HZ3	2.17	0.63
1:A:2:LEU:HD23	1:A:27:SER:HB2	1.79	0.63
1:V:270:LYS:O	1:V:274:GLU:HG3	1.98	0.63
1:D:292:LEU:O	1:D:295:VAL:HG22	1.99	0.63
1:S:138:TRP:CE2	1:S:438:TRP:CH2	2.87	0.63
2:T:103:THR:HG23	2:T:104:ASN:OD1	1.97	0.63
1:A:78:GLU:HG2	1:A:79:GLY:N	2.14	0.63
2:E:95:SER:HB3	2:E:127:GLU:HB3	1.80	0.63
1:J:3:TRP:CZ2	1:J:31:ARG:CD	2.82	0.63
1:J:155:VAL:CG2	1:J:163:SER:HB2	2.29	0.63
1:M:279:GLU:HG3	1:M:468:LYS:NZ	2.14	0.63
2:N:115:GLU:OE2	2:N:115:GLU:CA	2.32	0.63
1:P:64:LEU:HD11	1:P:222:VAL:HG21	1.80	0.62
2:E:215:LYS:HG3	2:E:248:THR:CG2	2.29	0.62
1:J:69:ILE:HD11	1:J:164:LEU:HD13	1.81	0.62
2:B:40:CYS:O	2:B:44:LEU:CB	2.46	0.62
1:S:265:LEU:HD23	1:S:398:PRO:HA	1.81	0.62
1:V:77:VAL:CG2	1:V:114:LYS:HZ2	2.13	0.62
2:W:17:MET:CE	2:W:57:ALA:HA	2.29	0.62
1:A:138:TRP:CE2	1:A:438:TRP:CH2	2.87	0.62
1:G:422:VAL:HG22	1:G:423:PRO:HD3	1.81	0.62
1:A:190:ARG:HH11	1:A:190:ARG:CG	1.96	0.62
2:W:355:LEU:HD22	2:W:360:ILE:HD11	1.81	0.62
2:H:21:THR:HG21	3:I:61:ARG:NH1	2.08	0.62
1:J:352:ILE:O	1:J:356:THR:HG22	1.99	0.62
1:M:90:GLU:O	1:M:91:ASN:HB2	1.98	0.62
1:S:69:ILE:HD11	1:S:164:LEU:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:123:GLY:N	4:S:907:ASN:OXT	2.32	0.62
2:H:346:TRP:O	2:H:350:ASP:HB2	2.00	0.62
2:T:200:ILE:HD11	2:T:238:VAL:HG21	1.81	0.62
2:B:37:THR:HG22	2:B:145:ASN:HD21	1.64	0.62
1:J:292:LEU:O	1:J:295:VAL:HG22	1.99	0.62
1:J:376:ARG:HH11	1:J:376:ARG:CG	2.02	0.62
6:T:479:ADP:PB	6:T:479:ADP:H5'1	2.40	0.62
1:D:38:LYS:HD2	1:D:477:LEU:CD1	2.30	0.61
1:P:138:TRP:CE2	1:P:438:TRP:CZ3	2.88	0.61
1:P:190:ARG:HH11	1:P:190:ARG:CG	2.06	0.61
1:S:422:VAL:CG2	1:S:423:PRO:CD	2.73	0.61
1:G:85:ALA:HB2	1:G:117:LEU:CD1	2.30	0.61
2:B:39:VAL:HG13	2:B:40:CYS:N	2.14	0.61
2:B:115:GLU:OE2	2:B:116:LYS:HE2	2.00	0.61
1:M:162:VAL:HG21	1:M:219:VAL:HG21	1.83	0.61
2:T:37:THR:HG23	2:T:38:ASN:N	2.15	0.61
2:T:41:PRO:HB3	2:T:46:MET:HE2	1.83	0.61
2:W:211:ARG:NH2	8:W:479:ATP:O3A	2.32	0.61
1:G:90:GLU:O	1:G:91:ASN:HB2	2.01	0.61
1:D:21:PRO:O	1:D:25:VAL:HG23	2.01	0.61
3:L:88:VAL:HB	3:L:89:PRO:CD	2.24	0.61
3:L:88:VAL:CB	3:L:89:PRO:HD2	2.21	0.61
2:T:374:GLU:HB3	2:T:403:PRO:HG2	1.83	0.61
2:E:222:PHE:CZ	2:E:253:PRO:HB3	2.36	0.61
1:J:299:ILE:HG13	1:J:419:ILE:HG22	1.83	0.61
1:G:356:THR:HG21	3:I:14:ALA:HB2	1.82	0.61
1:V:155:VAL:CG2	1:V:163:SER:HB2	2.30	0.61
1:M:422:VAL:HG22	1:M:423:PRO:HD3	1.83	0.61
1:G:279:GLU:HG3	1:G:468:LYS:NZ	2.16	0.60
3:R:33:ILE:O	3:R:37:ILE:HG12	2.01	0.60
2:T:201:ARG:HD2	2:T:207:GLU:O	2.00	0.60
2:W:331:GLU:O	2:W:334:VAL:HG12	2.00	0.60
1:G:81:LYS:HE2	1:G:91:ASN:HA	1.81	0.60
1:V:77:VAL:CG2	1:V:114:LYS:NZ	2.65	0.60
1:P:68:PRO:HB3	1:P:112:VAL:HG11	1.84	0.60
1:S:68:PRO:HB3	1:S:112:VAL:HG11	1.83	0.60
2:K:412:LEU:O	2:K:412:LEU:HG	2.02	0.60
1:S:143:VAL:CG1	1:S:145:GLY:H	2.15	0.60
2:T:17:MET:HE1	2:T:57:ALA:CA	2.31	0.60
2:T:21:THR:HG21	3:U:61:ARG:NH1	2.11	0.60
1:S:81:LYS:HE2	1:S:91:ASN:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:169:GLY:HA2	1:V:425:ASN:OD1	2.01	0.60
2:W:360:ILE:CD1	2:W:366:PRO:HD3	2.31	0.60
2:B:95:SER:HB3	2:B:127:GLU:HB3	1.84	0.60
1:P:138:TRP:CZ2	1:P:476:PRO:HD3	2.37	0.60
1:V:143:VAL:HG13	1:V:145:GLY:H	1.67	0.60
2:W:3:GLU:HG3	2:W:5:TYR:H	1.67	0.60
2:Q:412:LEU:N	2:Q:412:LEU:HD12	2.17	0.60
1:S:138:TRP:CZ2	1:S:438:TRP:CH2	2.90	0.60
1:S:376:ARG:HG3	1:S:376:ARG:NH1	2.09	0.60
1:V:422:VAL:CG2	1:V:423:PRO:HD3	2.32	0.60
1:J:397:THR:HG22	1:J:399:THR:H	1.66	0.60
1:S:151:SER:HB3	1:S:163:SER:OG	2.01	0.60
2:B:279:VAL:CG2	3:C:59:PRO:HD2	2.32	0.59
1:G:98:ALA:HA	1:G:195:GLY:HA3	1.83	0.59
2:N:215:LYS:HD3	2:N:248:THR:HG21	1.82	0.59
2:T:162:THR:CG2	2:T:165:GLU:H	2.15	0.59
1:V:78:GLU:HG2	1:V:79:GLY:N	2.16	0.59
2:E:17:MET:HE1	2:E:57:ALA:O	2.02	0.59
2:H:95:SER:CB	2:H:127:GLU:HB3	2.32	0.59
1:P:73:ASP:HA	1:P:114:LYS:HE2	1.83	0.59
1:S:78:GLU:HB2	1:S:97:ASP:OD1	2.02	0.59
2:W:360:ILE:O	2:W:360:ILE:HG12	2.02	0.59
1:D:352:ILE:O	1:D:356:THR:HG23	2.01	0.59
1:M:2:LEU:HD23	1:M:27:SER:HB2	1.83	0.59
2:Q:17:MET:CE	2:Q:60:TYR:CB	2.79	0.59
1:J:297:TYR:O	1:J:300:PRO:HD2	2.02	0.59
1:D:397:THR:HG22	1:D:398:PRO:HD2	1.85	0.59
2:E:37:THR:CG2	2:E:38:ASN:H	2.16	0.59
2:H:211:ARG:HH11	8:H:479:ATP:H5'2	1.68	0.59
1:P:285:PHE:HE1	1:P:464:LEU:CD2	2.16	0.59
1:J:306:ALA:HB3	1:J:307:PRO:HD3	1.83	0.59
2:K:298:LEU:HB3	2:K:299:PRO:CD	2.32	0.59
2:B:73:HIS:NE2	2:B:103:THR:HB	2.17	0.59
2:E:95:SER:CB	2:E:127:GLU:HB3	2.32	0.59
3:F:80:GLU:HG2	3:F:87:VAL:HB	1.84	0.59
1:M:86:SER:OG	1:M:88:ILE:HG13	2.03	0.59
1:S:352:ILE:O	1:S:356:THR:HG23	2.03	0.59
1:G:69:ILE:HD12	1:G:162:VAL:HG13	1.84	0.59
1:P:292:LEU:O	1:P:295:VAL:HG22	2.02	0.59
1:V:120:PHE:O	1:V:122:MET:CG	2.51	0.59
2:W:200:ILE:HG23	2:W:234:GLN:OE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:VAL:CG2	1:D:114:LYS:HZ2	2.01	0.59
1:J:3:TRP:CH2	1:J:31:ARG:CD	2.86	0.59
1:G:121:ALA:HB1	10:G:904:HOH:O	2.01	0.58
1:J:73:ASP:OD1	1:J:114:LYS:HE2	2.03	0.58
1:V:22:LYS:NZ	1:V:55:GLU:OE2	2.34	0.58
2:B:84:PHE:CD2	3:C:15:ARG:HG2	2.37	0.58
2:E:310:TYR:CE1	2:E:334:VAL:HG11	2.36	0.58
2:W:162:THR:HG22	2:W:164:GLU:H	1.67	0.58
1:G:85:ALA:CB	1:G:117:LEU:HD13	2.33	0.58
2:H:133:ASN:ND2	3:I:91:VAL:HG21	2.18	0.58
1:M:115:THR:HG21	1:M:151:SER:OG	2.04	0.58
2:Q:3:GLU:HG3	2:Q:5:TYR:H	1.69	0.58
1:V:422:VAL:HG22	1:V:423:PRO:HD3	1.85	0.58
2:E:39:VAL:CG2	2:E:44:LEU:HG	2.31	0.58
1:G:100:VAL:HG23	1:G:101:ILE:N	2.18	0.58
1:G:163:SER:HB3	1:G:209:PHE:HB2	1.86	0.58
1:P:174:GLN:HG3	1:P:175:PRO:HD3	1.85	0.58
1:S:22:LYS:HG3	1:S:51:LEU:HD12	1.85	0.58
1:S:418:ASP:OD2	4:S:907:ASN:N	2.36	0.58
2:T:96:GLN:HB2	2:T:125:HIS:HB2	1.85	0.58
1:D:306:ALA:HB3	1:D:307:PRO:HD3	1.85	0.58
1:J:253:LYS:HG2	1:J:286:GLU:HB3	1.85	0.58
1:V:317:TYR:HE1	2:W:47:PRO:HG3	1.69	0.58
1:G:134:THR:HG22	1:G:144:PRO:HG3	1.86	0.58
1:P:432:ILE:HG22	1:P:458:LEU:HG	1.86	0.58
1:V:181:VAL:HG13	1:V:210:GLY:O	2.04	0.58
1:V:185:LYS:NZ	1:V:429:LEU:O	2.37	0.58
2:W:360:ILE:HD11	2:W:365:SER:CA	2.22	0.58
2:K:156:THR:CG2	2:K:157:GLU:O	2.51	0.58
2:W:233:ARG:O	2:W:237:VAL:HG23	2.04	0.58
2:B:411:GLY:O	2:B:412:LEU:HB2	2.03	0.58
1:M:76:LEU:HD23	1:M:94:ALA:HB1	1.85	0.58
2:N:375:LEU:HD13	2:N:396:MET:HE1	1.84	0.58
2:T:310:TYR:HE1	2:T:334:VAL:HG11	1.69	0.58
1:V:5:LYS:HB2	1:V:10:LEU:CD1	2.33	0.58
1:A:317:TYR:HE1	2:B:47:PRO:HG3	1.69	0.58
1:D:68:PRO:HB3	1:D:112:VAL:HG11	1.86	0.58
2:E:358:LYS:HB2	2:E:360:ILE:HG22	1.84	0.58
1:G:138:TRP:CE2	1:G:438:TRP:CZ3	2.92	0.58
2:N:360:ILE:HD11	2:N:364:GLU:O	2.03	0.58
2:Q:375:LEU:HD13	2:Q:396:MET:HE1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:156:THR:HG22	2:T:157:GLU:O	2.04	0.58
2:T:396:MET:HG3	2:T:406:ILE:HD11	1.86	0.58
2:B:358:LYS:HB2	2:B:360:ILE:HG22	1.86	0.57
2:T:26:GLY:O	3:U:65:PRO:HA	2.04	0.57
1:V:6:SER:HB3	1:V:212:ARG:HH11	1.69	0.57
2:B:252:ASP:HB3	2:B:255:THR:CG2	2.33	0.57
1:J:190:ARG:HG2	1:J:224:SER:HB2	1.86	0.57
2:N:115:GLU:CG	2:N:116:LYS:HG2	2.30	0.57
2:N:282:LYS:HD3	3:O:55:PHE:CE2	2.38	0.57
1:P:28:PHE:CD2	1:P:68:PRO:HG2	2.38	0.57
2:Q:95:SER:HB2	2:Q:127:GLU:OE1	2.05	0.57
1:S:39:VAL:HG21	1:S:157:VAL:HG11	1.87	0.57
2:K:109:LEU:HD11	2:K:169:PHE:HA	1.85	0.57
2:K:167:ARG:HG3	2:K:220:PHE:HB3	1.84	0.57
1:M:397:THR:HG22	1:M:399:THR:H	1.69	0.57
3:U:2:VAL:N	3:U:31:SER:HG	2.02	0.57
1:V:245:VAL:CG1	1:V:459:LEU:HB3	2.34	0.57
2:W:17:MET:HE1	2:W:57:ALA:CA	2.35	0.57
1:M:352:ILE:O	1:M:356:THR:CG2	2.45	0.57
1:D:83:THR:CG2	1:D:131:PHE:CZ	2.71	0.57
2:K:360:ILE:HD11	2:K:365:SER:HA	1.86	0.57
2:B:330:PHE:CE1	2:B:344:VAL:HG13	2.39	0.57
3:I:88:VAL:HG23	3:I:89:PRO:O	2.04	0.57
1:J:3:TRP:CZ3	1:J:31:ARG:HD3	2.40	0.57
1:M:72:LYS:HA	1:M:115:THR:HG22	1.87	0.57
1:D:270:LYS:O	1:D:274:GLU:HG3	2.04	0.57
1:G:138:TRP:CZ2	1:G:438:TRP:CH2	2.93	0.57
2:H:140:THR:OG1	3:I:91:VAL:N	2.33	0.57
2:W:17:MET:HE3	2:W:60:TYR:CB	2.33	0.57
3:X:81:ARG:HG2	3:X:81:ARG:HH11	1.69	0.57
1:M:376:ARG:HH11	1:M:376:ARG:HG3	1.68	0.57
1:P:245:VAL:HG12	1:P:459:LEU:HB3	1.85	0.57
2:T:77:VAL:HG23	2:T:99:LYS:HD2	1.87	0.57
1:V:297:TYR:O	1:V:300:PRO:HD2	2.05	0.57
1:G:190:ARG:O	1:G:225:GLY:N	2.33	0.57
1:M:121:ALA:HB1	10:M:906:HOH:O	2.04	0.57
1:M:245:VAL:CG1	1:M:459:LEU:HB3	2.34	0.57
1:V:298:SER:HB3	1:V:422:VAL:HG23	1.86	0.57
2:B:399:THR:OG1	2:B:400:GLY:N	2.38	0.56
1:G:95:PRO:HG2	2:H:46:MET:HE3	1.86	0.56
2:K:162:THR:HG22	2:K:164:GLU:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:438:TRP:CZ3	1:M:443:PRO:HG3	2.39	0.56
1:A:292:LEU:O	1:A:295:VAL:HG22	2.05	0.56
2:E:85:TYR:HD2	2:E:87:ASP:OD1	1.87	0.56
9:H:482:ASP:N	10:H:485:HOH:O	2.38	0.56
1:J:3:TRP:CZ2	1:J:31:ARG:HD3	2.40	0.56
2:K:362:ILE:O	2:K:362:ILE:HG13	2.05	0.56
2:N:81:LYS:HZ2	9:N:482:ASP:HA	1.71	0.56
1:P:69:ILE:HD11	1:P:164:LEU:HD13	1.87	0.56
2:Q:336:HIS:NE2	2:Q:370:GLU:HG3	2.19	0.56
1:S:182:ILE:HG12	1:S:434:ILE:HD12	1.86	0.56
1:A:373:LYS:HE2	3:C:50:PRO:HD3	1.87	0.56
2:E:103:THR:HG22	2:E:104:ASN:N	2.21	0.56
2:H:103:THR:HG22	2:H:104:ASN:N	2.20	0.56
1:J:138:TRP:CE2	1:J:438:TRP:HZ3	2.23	0.56
2:K:407:VAL:O	2:K:411:GLY:N	2.35	0.56
1:P:155:VAL:CG1	1:P:181:VAL:HG21	2.35	0.56
2:Q:21:THR:HG21	3:R:61:ARG:HH12	1.71	0.56
1:A:279:GLU:HG3	1:A:468:LYS:HZ1	1.70	0.56
1:G:297:TYR:O	1:G:300:PRO:HD2	2.05	0.56
1:P:169:GLY:N	4:P:906:ASN:OD1	2.34	0.56
2:Q:21:THR:HG22	2:Q:54:ASN:ND2	2.20	0.56
2:E:39:VAL:CG1	2:E:44:LEU:HD11	2.33	0.56
2:E:340:PRO:O	2:E:344:VAL:HG22	2.05	0.56
1:P:16:ARG:HB2	1:P:18:GLU:OE2	2.05	0.56
1:P:434:ILE:HD12	1:P:465:TRP:HD1	1.70	0.56
2:Q:21:THR:CG2	3:R:61:ARG:HH12	2.18	0.56
3:U:3:ASP:O	3:U:7:VAL:HG23	2.06	0.56
2:K:12:GLU:OE2	8:K:479:ATP:O1G	2.24	0.56
1:M:138:TRP:CD2	1:M:438:TRP:HZ3	2.23	0.56
3:X:23:ILE:O	3:X:27:GLN:HG3	2.05	0.56
3:I:88:VAL:CB	3:I:89:PRO:HD2	2.05	0.56
1:A:397:THR:CG2	1:A:398:PRO:HD2	2.36	0.56
1:M:155:VAL:CG2	1:M:163:SER:HB2	2.35	0.56
2:N:39:VAL:CG1	2:N:44:LEU:HD11	2.35	0.56
1:P:299:ILE:N	1:P:300:PRO:CD	2.68	0.56
2:E:199:SER:OG	8:E:479:ATP:N1	2.30	0.55
1:G:95:PRO:CG	2:H:46:MET:HE1	2.32	0.55
1:G:122:MET:HE2	1:G:199:PHE:CD1	2.41	0.55
1:D:182:ILE:HG12	1:D:434:ILE:HD12	1.88	0.55
2:E:355:LEU:HD22	2:E:360:ILE:HG12	1.88	0.55
1:G:298:SER:HB3	1:G:422:VAL:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:122:MET:HE2	1:J:199:PHE:CD1	2.40	0.55
2:K:17:MET:CE	2:K:60:TYR:CB	2.84	0.55
1:M:138:TRP:CZ2	1:M:438:TRP:CH2	2.94	0.55
2:Q:55:LYS:HD2	3:R:60:MET:HE3	1.89	0.55
2:E:200:ILE:HD11	2:E:238:VAL:HG21	1.87	0.55
2:K:115:GLU:CG	2:K:116:LYS:HG2	2.37	0.55
2:Q:109:LEU:HD11	2:Q:169:PHE:HA	1.89	0.55
1:S:73:ASP:HA	1:S:114:LYS:HZ3	1.71	0.55
1:J:265:LEU:HD23	1:J:398:PRO:HA	1.87	0.55
2:K:21:THR:HB	3:L:63:ASP:OD1	2.07	0.55
1:S:306:ALA:HB3	1:S:307:PRO:HD3	1.87	0.55
1:A:120:PHE:O	1:A:122:MET:CG	2.48	0.55
1:A:475:ILE:HG22	1:A:476:PRO:CD	2.35	0.55
2:E:103:THR:CG2	2:E:104:ASN:N	2.70	0.55
1:J:422:VAL:CG2	1:J:423:PRO:HD3	2.37	0.55
2:N:156:THR:HG22	2:N:157:GLU:O	2.07	0.55
1:P:83:THR:HG22	1:P:90:GLU:HA	1.88	0.55
2:T:24:PHE:HA	2:T:52:ILE:O	2.05	0.55
1:V:39:VAL:HG21	1:V:157:VAL:HG11	1.88	0.55
1:S:21:PRO:O	1:S:25:VAL:HG23	2.07	0.55
2:W:84:PHE:CD2	3:X:15:ARG:HG2	2.41	0.55
1:A:245:VAL:CG1	1:A:459:LEU:HB3	2.37	0.55
2:B:17:MET:HE1	2:B:57:ALA:C	2.31	0.55
3:I:55:PHE:O	3:I:56:GLU:CB	2.55	0.55
1:A:450:GLY:CA	1:A:458:LEU:HD11	2.35	0.55
2:N:85:TYR:HD2	2:N:87:ASP:OD1	1.89	0.55
2:Q:41:PRO:HB3	2:Q:46:MET:HE2	1.89	0.55
1:G:279:GLU:HG3	1:G:468:LYS:HZ3	1.72	0.55
1:M:138:TRP:CD2	1:M:438:TRP:CZ3	2.95	0.55
1:P:146:GLY:H	1:P:174:GLN:HE21	1.54	0.55
1:D:477:LEU:HD23	1:D:477:LEU:H	1.71	0.54
2:Q:162:THR:HG22	2:Q:165:GLU:HG3	1.88	0.54
2:E:17:MET:HE1	2:E:57:ALA:C	2.32	0.54
1:J:28:PHE:CD2	1:J:68:PRO:HG2	2.42	0.54
1:J:68:PRO:HB3	1:J:112:VAL:HG21	1.89	0.54
1:M:69:ILE:HD11	1:M:164:LEU:HD13	1.89	0.54
1:P:422:VAL:CG2	1:P:423:PRO:HD3	2.37	0.54
3:R:55:PHE:O	3:R:56:GLU:HB3	2.06	0.54
1:A:32:TYR:CE1	1:A:36:GLU:CG	2.90	0.54
1:D:138:TRP:CZ2	1:D:438:TRP:HH2	2.24	0.54
2:Q:17:MET:HE1	2:Q:60:TYR:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:90:GLU:O	1:S:91:ASN:HB2	2.07	0.54
1:S:246:LYS:HG3	1:S:463:TYR:CZ	2.42	0.54
1:V:241:TRP:O	1:V:245:VAL:HG22	2.08	0.54
2:W:39:VAL:CG1	2:W:44:LEU:HD11	2.35	0.54
1:A:397:THR:HG23	1:A:398:PRO:HD2	1.90	0.54
2:B:96:GLN:HB2	2:B:125:HIS:HB2	1.89	0.54
1:J:155:VAL:HG23	1:J:163:SER:HB2	1.88	0.54
1:M:298:SER:HB3	1:M:422:VAL:HG23	1.90	0.54
2:N:39:VAL:HG13	2:N:44:LEU:CD1	2.35	0.54
1:P:214:GLU:OE2	1:P:246:LYS:HE2	2.08	0.54
1:S:438:TRP:CZ3	1:S:443:PRO:HG3	2.43	0.54
2:B:340:PRO:O	2:B:344:VAL:HG22	2.08	0.54
1:J:156:ALA:O	1:J:211:ARG:NH1	2.40	0.54
1:J:292:LEU:HB2	1:J:295:VAL:HG22	1.89	0.54
2:N:197:ASN:HB3	2:N:211:ARG:HD2	1.88	0.54
2:Q:252:ASP:HB3	2:Q:255:THR:CG2	2.38	0.54
2:T:115:GLU:CG	2:T:116:LYS:HG3	2.37	0.54
1:V:220:LEU:O	1:V:224:SER:OG	2.25	0.54
2:H:113:ASN:HA	2:H:115:GLU:H	1.73	0.54
2:H:201:ARG:HD2	2:H:207:GLU:O	2.07	0.54
1:J:422:VAL:HG22	1:J:423:PRO:HD3	1.90	0.54
1:P:3:TRP:CE2	1:P:31:ARG:HD3	2.43	0.54
3:X:81:ARG:HG2	3:X:81:ARG:NH1	2.23	0.54
1:A:21:PRO:O	1:A:25:VAL:HG23	2.08	0.54
1:A:376:ARG:HG3	1:A:376:ARG:NH1	2.14	0.54
1:M:182:ILE:HG12	1:M:434:ILE:HD12	1.90	0.54
2:W:252:ASP:CB	2:W:255:THR:HG22	2.36	0.54
1:A:190:ARG:O	1:A:224:SER:O	2.26	0.54
2:B:37:THR:CG2	2:B:38:ASN:N	2.71	0.54
1:G:178:PHE:CE1	1:G:397:THR:HG21	2.39	0.54
1:P:145:GLY:HA2	1:P:174:GLN:NE2	2.22	0.54
2:T:58:VAL:O	2:T:62:ILE:HG13	2.08	0.54
1:V:124:SER:HG	4:V:908:ASN:N	2.05	0.54
2:H:39:VAL:HG13	2:H:44:LEU:HD11	1.89	0.54
1:A:300:PRO:HA	3:C:37:ILE:HG22	1.89	0.54
1:D:351:ARG:HH12	4:D:902:ASN:C	2.15	0.54
1:G:332:ILE:HD12	3:I:89:PRO:HG2	1.89	0.54
1:J:3:TRP:CE2	1:J:31:ARG:CD	2.91	0.54
1:S:46:LEU:HD11	1:S:80:GLU:HG3	1.89	0.54
2:W:220:PHE:O	2:W:223:VAL:HG22	2.08	0.54
1:J:477:LEU:HD23	1:J:477:LEU:H	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:438:TRP:CZ3	1:G:443:PRO:HG3	2.43	0.53
2:H:162:THR:HG22	2:H:165:GLU:H	1.73	0.53
3:C:73:LYS:O	3:C:76:MET:HG2	2.08	0.53
2:H:100:PRO:HB3	2:H:123:ARG:HH21	1.74	0.53
1:J:73:ASP:HA	1:J:114:LYS:HE2	1.90	0.53
1:M:190:ARG:HD3	1:M:241:TRP:HH2	1.73	0.53
1:V:373:LYS:HE2	3:X:50:PRO:HD3	1.90	0.53
2:B:95:SER:HB3	2:B:127:GLU:CB	2.38	0.53
2:B:156:THR:CG2	2:B:157:GLU:O	2.56	0.53
1:D:190:ARG:HD3	1:D:241:TRP:CH2	2.32	0.53
2:E:100:PRO:HB3	2:E:123:ARG:NH2	2.24	0.53
2:H:360:ILE:HG22	2:H:364:GLU:HB3	1.91	0.53
3:I:88:VAL:HB	3:I:89:PRO:CD	2.23	0.53
2:K:21:THR:HG22	2:K:54:ASN:ND2	2.22	0.53
1:D:322:TYR:CZ	2:E:47:PRO:HD3	2.44	0.53
1:G:299:ILE:HG13	1:G:419:ILE:HG22	1.90	0.53
1:J:162:VAL:HG11	1:J:219:VAL:HG21	1.89	0.53
1:P:138:TRP:CD2	1:P:438:TRP:HZ3	2.27	0.53
1:P:422:VAL:HG22	1:P:423:PRO:HD3	1.89	0.53
1:V:292:LEU:CB	1:V:295:VAL:HG22	2.39	0.53
1:G:245:VAL:CG1	1:G:459:LEU:HB3	2.39	0.53
2:N:86:PRO:HG2	3:O:91:VAL:HG11	1.91	0.53
2:T:80:ARG:HE	2:T:275:ASP:CG	2.16	0.53
2:W:360:ILE:HD12	2:W:366:PRO:HD3	1.88	0.53
1:D:155:VAL:CG2	1:D:163:SER:HB2	2.38	0.53
2:H:17:MET:HE2	2:H:60:TYR:HB3	1.85	0.53
1:A:450:GLY:HA3	1:A:458:LEU:CD1	2.36	0.53
2:E:21:THR:CG2	3:F:61:ARG:HH12	2.09	0.53
2:K:115:GLU:HG3	2:K:116:LYS:CG	2.39	0.53
1:P:31:ARG:HH22	1:P:477:LEU:HB2	1.73	0.53
1:V:204:ASP:O	1:V:205:GLN:HG2	2.09	0.53
2:E:80:ARG:HE	2:E:275:ASP:CG	2.17	0.53
1:M:477:LEU:N	1:M:477:LEU:HD23	2.23	0.53
2:Q:162:THR:HG23	2:Q:165:GLU:H	1.74	0.53
2:B:40:CYS:SG	2:B:41:PRO:HD2	2.49	0.52
2:E:34:GLU:O	2:E:37:THR:CB	2.52	0.52
2:E:37:THR:CG2	2:E:38:ASN:N	2.72	0.52
2:H:385:SER:OG	2:H:388:ILE:HG12	2.08	0.52
1:P:64:LEU:CD1	1:P:222:VAL:HG21	2.38	0.52
1:A:69:ILE:HD11	1:A:164:LEU:HD13	1.91	0.52
1:D:155:VAL:HG23	1:D:163:SER:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:30:ASP:O	1:J:34:GLN:HG3	2.09	0.52
1:J:376:ARG:NH1	1:J:376:ARG:CG	2.67	0.52
1:P:174:GLN:HG3	1:P:175:PRO:CD	2.38	0.52
1:S:297:TYR:O	1:S:300:PRO:HD2	2.09	0.52
1:A:322:TYR:CZ	2:B:47:PRO:HD3	2.44	0.52
1:D:72:LYS:HA	1:D:115:THR:CG2	2.39	0.52
1:J:3:TRP:CZ2	1:J:31:ARG:HD2	2.45	0.52
1:M:376:ARG:HG3	1:M:376:ARG:NH1	2.24	0.52
1:S:138:TRP:CE2	1:S:438:TRP:CZ3	2.96	0.52
2:W:396:MET:HG3	2:W:406:ILE:HD11	1.90	0.52
1:G:1:MET:HG2	1:G:1:MET:O	2.09	0.52
2:N:385:SER:OG	2:N:388:ILE:HG12	2.09	0.52
2:T:279:VAL:CG2	3:U:59:PRO:HD2	2.40	0.52
2:W:336:HIS:NE2	2:W:370:GLU:HG3	2.24	0.52
2:H:133:ASN:HD22	3:I:91:VAL:HG21	1.74	0.52
2:Q:192:LEU:C	2:Q:192:LEU:HD23	2.35	0.52
2:T:310:TYR:CE1	2:T:334:VAL:HG11	2.45	0.52
1:V:124:SER:O	1:V:174:GLN:NE2	2.42	0.52
2:E:360:ILE:HD11	2:E:365:SER:N	2.24	0.52
1:G:138:TRP:CE2	1:G:438:TRP:HH2	2.25	0.52
2:Q:123:ARG:NH1	2:Q:125:HIS:ND1	2.57	0.52
2:Q:332:GLU:HG3	2:Q:335:ARG:HH21	1.74	0.52
2:T:8:VAL:HG12	2:T:158:PRO:HB2	1.90	0.52
1:D:39:VAL:HG21	1:D:157:VAL:HG11	1.92	0.52
2:E:215:LYS:HG3	2:E:248:THR:HG21	1.91	0.52
2:K:17:MET:HE3	2:K:60:TYR:HB3	1.92	0.52
1:M:193:ARG:NH2	1:M:201:SER:HB3	2.25	0.52
2:N:162:THR:HG22	2:N:165:GLU:H	1.73	0.52
1:V:477:LEU:O	1:V:478:THR:C	2.53	0.52
2:W:402:THR:HG22	2:W:403:PRO:HD2	1.92	0.52
2:B:336:HIS:CE1	2:B:370:GLU:HG3	2.44	0.52
2:H:255:THR:HG21	2:H:259:TYR:OH	2.10	0.52
2:N:14:HIS:CD2	2:N:127:GLU:OE2	2.63	0.52
1:P:30:ASP:O	1:P:34:GLN:HG3	2.10	0.52
2:K:34:GLU:O	2:K:37:THR:CG2	2.58	0.52
2:Q:73:HIS:NE2	2:Q:103:THR:HB	2.25	0.52
1:S:32:TYR:CE1	1:S:36:GLU:HG2	2.45	0.52
1:V:72:LYS:HE2	1:V:117:LEU:HD13	1.92	0.52
1:A:167:ASP:HB3	1:A:185:LYS:HG3	1.92	0.52
1:M:39:VAL:HG21	1:M:157:VAL:HG11	1.92	0.52
1:D:22:LYS:HG3	1:D:51:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:109:LEU:HD11	2:H:169:PHE:HA	1.91	0.51
1:D:299:ILE:HG13	1:D:419:ILE:HG22	1.92	0.51
3:I:55:PHE:O	3:I:56:GLU:HB3	2.10	0.51
2:Q:412:LEU:N	2:Q:412:LEU:CD1	2.73	0.51
1:S:122:MET:HE2	1:S:199:PHE:CD1	2.45	0.51
2:T:119:VAL:HG13	2:T:159:ASP:HB2	1.91	0.51
3:U:69:LEU:HD23	3:U:74:ALA:HB2	1.92	0.51
2:E:361:SER:HB2	2:E:363:GLU:OE1	2.10	0.51
1:G:151:SER:HB3	1:G:163:SER:OG	2.10	0.51
1:J:352:ILE:O	1:J:356:THR:CG2	2.59	0.51
2:Q:34:GLU:O	2:Q:37:THR:OG1	2.24	0.51
1:S:13:LEU:HB3	1:S:19:VAL:CG1	2.38	0.51
2:B:9:ILE:HB	2:B:160:ILE:HB	1.91	0.51
1:D:77:VAL:HG21	1:D:114:LYS:NZ	2.22	0.51
1:D:199:PHE:CD1	1:D:199:PHE:C	2.88	0.51
1:D:172:ILE:HD13	1:D:207:GLY:HA3	1.93	0.51
3:F:4:ARG:NH1	3:F:8:LEU:HD11	2.25	0.51
1:G:331:ASP:C	1:G:331:ASP:OD1	2.53	0.51
1:P:285:PHE:CE1	1:P:464:LEU:CD2	2.92	0.51
1:A:30:ASP:O	1:A:34:GLN:HG3	2.10	0.51
1:G:101:ILE:HG22	1:G:105:LYS:HE3	1.92	0.51
1:G:138:TRP:CD2	1:G:438:TRP:CZ3	2.97	0.51
2:H:146:ARG:HG2	2:H:146:ARG:HH11	1.76	0.51
1:J:298:SER:HB3	1:J:422:VAL:HG23	1.93	0.51
2:N:83:TYR:CZ	2:N:88:LEU:HD22	2.45	0.51
1:P:318:ASP:HB2	1:P:336:TYR:CE1	2.45	0.51
1:S:155:VAL:HG23	1:S:163:SER:HB2	1.92	0.51
1:V:397:THR:CG2	1:V:398:PRO:HD2	2.40	0.51
2:E:375:LEU:HD22	2:E:396:MET:HE1	1.93	0.51
2:H:95:SER:HB3	2:H:127:GLU:CB	2.40	0.51
1:J:204:ASP:O	1:J:205:GLN:HG2	2.11	0.51
2:N:17:MET:CE	2:N:60:TYR:HB2	2.39	0.51
2:Q:7:ALA:HB3	2:Q:161:ARG:O	2.10	0.51
2:T:115:GLU:HB3	2:T:116:LYS:HG3	1.92	0.51
2:W:133:ASN:HB3	2:W:140:THR:CG2	2.40	0.51
2:W:340:PRO:O	2:W:344:VAL:HG22	2.11	0.51
1:D:169:GLY:N	4:D:902:ASN:OD1	2.42	0.51
2:E:22:LYS:NZ	2:E:147:ALA:O	2.37	0.51
2:E:95:SER:HB3	2:E:127:GLU:CB	2.41	0.51
1:P:285:PHE:HE1	1:P:464:LEU:HD21	1.76	0.51
1:P:329:TYR:CE2	3:R:89:PRO:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:138:TRP:CD2	1:S:438:TRP:HZ3	2.29	0.51
1:A:340:ARG:HB3	3:C:16:LEU:HD23	1.92	0.51
2:B:17:MET:HG2	2:B:152:MET:CE	2.39	0.51
2:N:17:MET:HE1	2:N:61:ALA:N	2.26	0.51
2:Q:333:ALA:C	2:Q:335:ARG:H	2.17	0.51
2:T:170:LEU:HD12	2:T:223:VAL:HG21	1.93	0.51
2:T:234:GLN:O	2:T:238:VAL:HG23	2.11	0.51
1:G:68:PRO:HB3	1:G:112:VAL:HG11	1.93	0.51
1:G:172:ILE:HD13	1:G:207:GLY:HA3	1.93	0.51
1:G:397:THR:HG22	1:G:399:THR:O	2.11	0.51
2:H:197:ASN:HB3	2:H:211:ARG:HD2	1.91	0.51
1:M:438:TRP:CH2	1:M:443:PRO:HG3	2.46	0.51
2:T:84:PHE:CD2	3:U:15:ARG:HG2	2.46	0.51
1:A:422:VAL:CG2	1:A:423:PRO:HD3	2.41	0.50
2:B:37:THR:HG23	2:B:38:ASN:H	1.75	0.50
2:E:360:ILE:HG13	2:E:361:SER:N	2.26	0.50
2:H:17:MET:HE1	2:H:60:TYR:CB	2.30	0.50
2:N:323:HIS:CD2	2:N:325:GLU:OE1	2.64	0.50
2:T:207:GLU:CG	2:T:208:PHE:H	2.21	0.50
2:W:73:HIS:NE2	2:W:103:THR:HB	2.26	0.50
2:B:37:THR:HG22	2:B:145:ASN:ND2	2.26	0.50
1:J:138:TRP:CD2	1:J:438:TRP:HZ3	2.28	0.50
1:M:21:PRO:O	1:M:25:VAL:HG23	2.11	0.50
1:P:138:TRP:CE2	1:P:438:TRP:CH2	2.98	0.50
1:S:199:PHE:CD1	1:S:199:PHE:C	2.89	0.50
2:T:162:THR:HG22	2:T:165:GLU:CB	2.40	0.50
1:M:73:ASP:HA	1:M:114:LYS:HE2	1.93	0.50
2:N:140:THR:OG1	3:O:90:ARG:HA	2.11	0.50
1:P:477:LEU:HD23	1:P:477:LEU:H	1.74	0.50
2:Q:85:TYR:HD2	2:Q:87:ASP:OD1	1.93	0.50
1:S:182:ILE:HG12	1:S:434:ILE:CD1	2.42	0.50
1:V:118:ASP:CG	1:V:126:THR:HA	2.36	0.50
2:H:17:MET:HG2	2:H:152:MET:HE2	1.93	0.50
1:J:349:LYS:O	1:J:353:MET:HG2	2.12	0.50
1:P:477:LEU:HD23	1:P:477:LEU:N	2.26	0.50
1:S:463:TYR:O	1:S:467:GLN:HG2	2.11	0.50
2:B:3:GLU:HG3	2:B:5:TYR:H	1.76	0.50
1:D:463:TYR:O	1:D:467:GLN:HG2	2.11	0.50
2:K:85:TYR:HD2	2:K:87:ASP:OD1	1.94	0.50
2:K:333:ALA:HB2	2:K:369:PRO:HB3	1.94	0.50
1:M:95:PRO:HG2	2:N:46:MET:HE1	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:80:ARG:HE	2:N:275:ASP:CG	2.20	0.50
1:A:178:PHE:CE1	1:A:397:THR:HG21	2.47	0.50
1:G:78:GLU:HG2	1:G:79:GLY:N	2.25	0.50
1:P:5:LYS:HB2	1:P:10:LEU:HD13	1.94	0.50
2:T:402:THR:HG22	2:T:403:PRO:HD2	1.93	0.50
2:B:8:VAL:HG21	2:B:201:ARG:HE	1.75	0.50
1:J:3:TRP:CH2	1:J:31:ARG:HD3	2.47	0.50
2:Q:236:ASN:O	2:Q:240:GLU:HG2	2.12	0.50
2:Q:305:ARG:HG2	2:Q:305:ARG:HH11	1.77	0.50
1:S:155:VAL:CG2	1:S:163:SER:HB2	2.42	0.50
2:T:340:PRO:O	2:T:344:VAL:HG22	2.12	0.50
1:M:292:LEU:HB3	1:M:295:VAL:HG13	1.92	0.50
1:P:174:GLN:HG3	1:P:175:PRO:N	2.24	0.50
1:S:172:ILE:CD1	1:S:207:GLY:HA3	2.41	0.50
1:S:292:LEU:O	1:S:295:VAL:HG22	2.12	0.50
1:V:356:THR:HG21	3:X:14:ALA:HB2	1.94	0.50
2:W:35:PRO:HG3	3:X:85:PHE:CE2	2.47	0.50
1:G:46:LEU:HD12	1:G:111:ILE:HG22	1.93	0.50
2:H:97:TYR:O	2:H:123:ARG:NH2	2.44	0.50
2:K:17:MET:HE3	2:K:152:MET:HE2	1.93	0.50
2:K:81:LYS:HE3	2:K:270:TYR:CZ	2.47	0.50
2:T:6:GLU:OE1	2:T:201:ARG:NH2	2.42	0.50
1:V:29:TYR:O	1:V:32:TYR:HB3	2.12	0.50
1:A:126:THR:OG1	1:A:149:GLY:HA3	2.11	0.49
1:D:418:ASP:HB3	1:D:422:VAL:HG13	1.94	0.49
2:H:355:LEU:HD21	2:H:365:SER:HB2	1.93	0.49
1:P:122:MET:HE2	1:P:199:PHE:CD1	2.47	0.49
1:V:297:TYR:C	1:V:300:PRO:HD2	2.37	0.49
2:W:41:PRO:HB3	2:W:46:MET:HE2	1.94	0.49
2:B:8:VAL:HG13	2:B:161:ARG:HH12	1.77	0.49
1:D:13:LEU:HB3	1:D:19:VAL:HG11	1.83	0.49
1:D:122:MET:HE2	1:D:199:PHE:CD1	2.47	0.49
2:E:37:THR:HG22	2:E:145:ASN:ND2	2.28	0.49
2:K:340:PRO:O	2:K:344:VAL:HG22	2.12	0.49
2:Q:381:GLU:O	2:Q:382:LYS:HB2	2.13	0.49
1:A:72:LYS:HA	1:A:115:THR:HB	1.94	0.49
1:D:99:THR:O	1:D:103:ARG:HG3	2.12	0.49
2:K:345:ASN:O	2:K:349:ASN:HB2	2.13	0.49
2:N:157:GLU:O	2:N:159:ASP:N	2.44	0.49
2:Q:320:LEU:HD22	2:Q:326:VAL:HG12	1.93	0.49
1:S:421:THR:C	1:S:423:PRO:HD2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:255:THR:HG23	2:W:257:LYS:H	1.77	0.49
3:X:46:GLU:O	3:X:47:ASN:HB2	2.13	0.49
2:B:210:THR:CG2	2:B:246:GLN:HB2	2.42	0.49
2:E:106:TRP:CZ3	1:G:293:PRO:HG3	2.47	0.49
2:E:220:PHE:O	2:E:223:VAL:HG22	2.12	0.49
2:E:279:VAL:CG2	3:F:59:PRO:HD2	2.43	0.49
2:H:282:LYS:HD3	3:I:55:PHE:CE2	2.47	0.49
3:L:55:PHE:O	3:L:56:GLU:HB3	2.13	0.49
1:M:146:GLY:N	1:M:174:GLN:OE1	2.42	0.49
1:A:5:LYS:HB2	1:A:10:LEU:CD1	2.42	0.49
1:D:297:TYR:O	1:D:300:PRO:HD2	2.12	0.49
1:G:297:TYR:C	1:G:300:PRO:HD2	2.38	0.49
1:P:124:SER:O	1:P:174:GLN:NE2	2.46	0.49
1:V:5:LYS:HB2	1:V:10:LEU:HD13	1.93	0.49
1:V:21:PRO:O	1:V:25:VAL:HG23	2.13	0.49
1:A:298:SER:HB3	1:A:422:VAL:HG23	1.94	0.49
1:D:191:VAL:HG22	1:D:224:SER:HB3	1.95	0.49
1:S:297:TYR:C	1:S:300:PRO:HD2	2.38	0.49
1:V:174:GLN:HG3	1:V:175:PRO:N	2.22	0.49
2:B:402:THR:HG22	2:B:403:PRO:HD2	1.95	0.49
1:D:146:GLY:N	1:D:174:GLN:OE1	2.39	0.49
2:E:83:TYR:CZ	2:E:88:LEU:HD22	2.47	0.49
1:G:201:SER:HB2	2:H:276:PRO:HG2	1.94	0.49
1:M:331:ASP:C	1:M:331:ASP:OD1	2.55	0.49
1:P:29:TYR:O	1:P:32:TYR:HB3	2.13	0.49
1:P:298:SER:HB3	1:P:422:VAL:HG23	1.94	0.49
2:Q:103:THR:CG2	2:Q:104:ASN:OD1	2.61	0.49
2:W:85:TYR:OH	3:X:91:VAL:HG21	2.13	0.49
1:A:174:GLN:HG3	1:A:175:PRO:HD3	1.94	0.49
1:A:434:ILE:HD11	1:A:462:SER:HG	1.77	0.49
2:B:95:SER:CB	2:B:127:GLU:HB3	2.43	0.49
2:B:331:GLU:HA	2:B:334:VAL:HG12	1.94	0.49
1:D:477:LEU:HD23	1:D:477:LEU:N	2.27	0.49
2:H:184:LYS:HB2	2:H:191:GLN:OE1	2.13	0.49
2:N:164:GLU:HG3	2:N:168:LEU:HD12	1.95	0.49
2:N:346:TRP:O	2:N:350:ASP:HB2	2.11	0.49
2:T:115:GLU:CB	2:T:116:LYS:HG3	2.42	0.49
2:T:370:GLU:CD	2:T:370:GLU:H	2.21	0.49
2:W:80:ARG:HE	2:W:275:ASP:CG	2.21	0.49
2:W:399:THR:OG1	2:W:400:GLY:N	2.46	0.49
2:E:370:GLU:H	2:E:370:GLU:CD	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:376:ARG:HH11	1:G:376:ARG:HG3	1.78	0.49
2:H:4:LYS:O	2:H:203:LYS:HB2	2.12	0.49
9:N:482:ASP:N	10:N:484:HOH:O	2.45	0.49
2:Q:103:THR:HG23	2:Q:104:ASN:OD1	2.13	0.49
2:Q:207:GLU:OE1	2:Q:207:GLU:C	2.55	0.49
1:D:438:TRP:CZ3	1:D:443:PRO:HG3	2.47	0.49
1:M:190:ARG:HD2	1:M:455:GLU:OE2	2.13	0.49
1:M:246:LYS:HE2	1:M:463:TYR:OH	2.13	0.49
1:P:155:VAL:HG12	1:P:181:VAL:CG2	2.36	0.49
1:P:376:ARG:O	1:P:376:ARG:HG3	2.12	0.49
2:T:37:THR:CG2	2:T:38:ASN:N	2.76	0.49
1:A:20:SER:O	1:A:24:VAL:HG23	2.12	0.48
2:H:119:VAL:CG1	2:H:156:THR:CG2	2.91	0.48
1:A:422:VAL:HG22	1:A:423:PRO:HD3	1.95	0.48
1:D:403:LYS:O	1:D:406:GLU:HB2	2.12	0.48
2:E:170:LEU:HD12	2:E:223:VAL:HG21	1.95	0.48
2:H:39:VAL:CG2	2:H:44:LEU:HD21	2.44	0.48
2:K:384:ILE:HG22	2:K:412:LEU:HD23	1.94	0.48
2:N:4:LYS:O	2:N:203:LYS:HB2	2.13	0.48
1:P:1:MET:O	1:P:1:MET:HG2	2.13	0.48
2:Q:301:GLN:O	2:Q:302:ARG:C	2.56	0.48
1:S:138:TRP:CE2	1:S:438:TRP:HH2	2.30	0.48
1:V:2:LEU:HD23	1:V:27:SER:HB2	1.94	0.48
1:V:292:LEU:HB2	1:V:295:VAL:CG2	2.42	0.48
3:F:2:VAL:N	3:F:31:SER:HG	2.11	0.48
1:G:137:PRO:HB3	1:G:157:VAL:CG1	2.43	0.48
1:J:2:LEU:HA	1:J:5:LYS:HD2	1.95	0.48
2:Q:16:GLN:HB2	2:Q:191:GLN:HA	1.96	0.48
1:S:318:ASP:HB2	1:S:336:TYR:CE1	2.48	0.48
2:T:162:THR:HG23	2:T:165:GLU:H	1.78	0.48
2:W:17:MET:HG2	2:W:152:MET:HE3	1.96	0.48
2:W:142:VAL:HB	3:X:86:PHE:HB2	1.93	0.48
1:A:172:ILE:HD13	1:A:207:GLY:HA3	1.95	0.48
1:D:318:ASP:OD2	1:D:321:ARG:NH1	2.43	0.48
2:E:26:GLY:O	3:F:65:PRO:HA	2.13	0.48
2:E:358:LYS:HB2	2:E:360:ILE:CG2	2.43	0.48
1:G:190:ARG:NH1	1:G:190:ARG:HG3	2.28	0.48
1:P:138:TRP:CE2	1:P:438:TRP:HZ3	2.32	0.48
1:S:81:LYS:CE	1:S:91:ASN:HA	2.43	0.48
2:T:215:LYS:O	2:T:216:ASN:HB2	2.12	0.48
1:A:279:GLU:HG3	1:A:468:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:THR:OG1	1:D:150:GLY:C	2.56	0.48
2:E:21:THR:HG22	2:E:22:LYS:O	2.14	0.48
2:E:137:GLY:O	3:F:90:ARG:NH1	2.43	0.48
1:M:266:GLN:NE2	1:M:399:THR:HB	2.28	0.48
1:M:279:GLU:HG3	1:M:468:LYS:HZ1	1.77	0.48
1:V:123:GLY:O	4:V:908:ASN:HB2	2.13	0.48
1:V:279:GLU:HG3	1:V:468:LYS:HZ3	1.74	0.48
2:W:103:THR:CG2	2:W:104:ASN:OD1	2.59	0.48
2:W:162:THR:HG22	2:W:164:GLU:N	2.28	0.48
2:W:214:ILE:HD11	2:W:230:GLU:HG2	1.96	0.48
1:A:265:LEU:HD23	1:A:398:PRO:HA	1.96	0.48
3:L:55:PHE:O	3:L:56:GLU:CB	2.62	0.48
2:N:170:LEU:HD12	2:N:223:VAL:HG21	1.94	0.48
1:D:320:VAL:HG22	3:F:88:VAL:HG11	1.94	0.48
2:H:140:THR:OG1	3:I:90:ARG:HA	2.13	0.48
1:J:245:VAL:CG1	1:J:459:LEU:HB3	2.43	0.48
1:M:190:ARG:HD3	1:M:241:TRP:CH2	2.48	0.48
2:Q:162:THR:HG22	2:Q:165:GLU:CG	2.44	0.48
1:A:325:ARG:HA	1:A:339:THR:HG23	1.96	0.48
1:G:73:ASP:HA	1:G:114:LYS:HE2	1.94	0.48
1:G:477:LEU:C	1:G:478:THR:HG23	2.39	0.48
2:H:21:THR:HG22	2:H:54:ASN:ND2	2.29	0.48
2:H:26:GLY:O	3:I:65:PRO:HA	2.14	0.48
2:K:330:PHE:CE1	2:K:344:VAL:HG13	2.49	0.48
1:S:477:LEU:N	1:S:477:LEU:CD2	2.71	0.48
2:H:17:MET:HE1	2:H:57:ALA:O	2.13	0.48
2:Q:192:LEU:HD23	2:Q:193:ARG:N	2.29	0.48
2:Q:298:LEU:HB3	2:Q:299:PRO:CD	2.44	0.48
1:J:178:PHE:HE1	1:J:397:THR:HG21	1.78	0.48
2:K:7:ALA:HB3	2:K:161:ARG:O	2.14	0.48
2:K:310:TYR:CE1	2:K:334:VAL:HG11	2.49	0.48
2:N:95:SER:HB2	2:N:96:GLN:H	1.50	0.48
1:P:434:ILE:O	1:P:434:ILE:CG2	2.59	0.48
2:Q:310:TYR:CE1	2:Q:334:VAL:HG11	2.49	0.48
1:S:77:VAL:HG23	1:S:114:LYS:HE2	1.96	0.48
1:V:42:TYR:CE2	1:V:113:GLY:HA3	2.49	0.48
1:G:126:THR:OG1	1:G:149:GLY:HA3	2.13	0.47
2:Q:340:PRO:O	2:Q:344:VAL:HG22	2.14	0.47
1:S:57:LEU:HD12	1:S:110:LEU:HD21	1.96	0.47
1:A:76:LEU:HD22	1:A:96:TYR:CE1	2.49	0.47
1:D:126:THR:OG1	1:D:149:GLY:HA3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:123:ARG:HG2	2:H:155:VAL:HB	1.95	0.47
1:M:403:LYS:O	1:M:406:GLU:HB2	2.14	0.47
1:P:172:ILE:CD1	1:P:207:GLY:HA3	2.44	0.47
1:P:199:PHE:CD1	1:P:199:PHE:C	2.92	0.47
1:V:155:VAL:HG23	1:V:163:SER:HB2	1.96	0.47
2:W:56:ARG:HD2	3:X:63:ASP:OD2	2.14	0.47
2:W:157:GLU:O	2:W:159:ASP:N	2.45	0.47
2:B:37:THR:CG2	2:B:38:ASN:H	2.27	0.47
2:Q:95:SER:CB	2:Q:127:GLU:OE1	2.61	0.47
3:R:3:ASP:O	3:R:7:VAL:HG23	2.14	0.47
2:T:270:TYR:HB2	2:T:272:TYR:CE2	2.49	0.47
1:V:299:ILE:HG13	1:V:419:ILE:HG22	1.95	0.47
1:D:422:VAL:HG22	1:D:423:PRO:HD3	1.97	0.47
2:H:155:VAL:HG21	10:H:483:HOH:O	2.14	0.47
1:P:422:VAL:N	1:P:423:PRO:CD	2.77	0.47
2:Q:308:LYS:C	2:Q:310:TYR:H	2.22	0.47
1:V:351:ARG:HH12	4:V:908:ASN:C	2.23	0.47
2:W:135:HIS:HB3	3:X:90:ARG:CZ	2.44	0.47
1:A:124:SER:O	1:A:174:GLN:NE2	2.48	0.47
2:E:128:GLU:HB2	2:E:148:GLY:HA2	1.96	0.47
2:K:255:THR:HG21	2:K:259:TYR:OH	2.15	0.47
1:M:266:GLN:HG3	1:M:399:THR:HG22	1.97	0.47
1:P:253:LYS:HG2	1:P:286:GLU:HB3	1.97	0.47
2:W:252:ASP:OD2	2:W:255:THR:HG22	2.14	0.47
2:B:157:GLU:O	2:B:159:ASP:N	2.48	0.47
1:D:422:VAL:CG2	1:D:423:PRO:HD3	2.44	0.47
2:H:103:THR:CG2	2:H:104:ASN:N	2.77	0.47
1:A:57:LEU:HD12	1:A:110:LEU:HD21	1.97	0.47
1:A:178:PHE:HE1	1:A:397:THR:HG21	1.80	0.47
2:B:167:ARG:HG3	2:B:220:PHE:HB3	1.96	0.47
2:B:217:VAL:CG1	2:B:222:PHE:HB3	2.44	0.47
1:P:373:LYS:HE2	3:R:50:PRO:HD3	1.96	0.47
1:P:434:ILE:CD1	1:P:465:TRP:HD1	2.27	0.47
1:P:477:LEU:O	1:P:478:THR:C	2.58	0.47
2:Q:222:PHE:CZ	2:Q:253:PRO:HB3	2.50	0.47
1:S:403:LYS:O	1:S:406:GLU:HB2	2.15	0.47
2:T:40:CYS:HB2	2:T:41:PRO:CD	2.44	0.47
2:T:77:VAL:CG2	2:T:99:LYS:HD2	2.44	0.47
2:T:117:LYS:HG2	2:T:118:LYS:N	2.30	0.47
3:U:46:GLU:O	3:U:47:ASN:HB2	2.15	0.47
2:W:167:ARG:HG3	2:W:220:PHE:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:257:LYS:HD2	2:W:259:TYR:OH	2.14	0.47
2:B:384:ILE:HG23	2:B:412:LEU:HD23	1.94	0.47
2:H:111:LEU:HG	2:H:115:GLU:O	2.15	0.47
2:K:17:MET:HE1	2:K:60:TYR:HB2	1.97	0.47
1:A:174:GLN:HG3	1:A:175:PRO:CD	2.44	0.47
1:A:201:SER:HB2	2:B:276:PRO:HG2	1.96	0.47
2:E:21:THR:HG21	3:F:61:ARG:NH1	2.10	0.47
2:E:162:THR:HG22	2:E:164:GLU:H	1.79	0.47
1:G:13:LEU:HB3	1:G:19:VAL:HG12	1.97	0.47
1:M:134:THR:HG22	1:M:144:PRO:HG3	1.96	0.47
2:W:17:MET:HE1	2:W:57:ALA:C	2.39	0.47
2:W:140:THR:OG1	3:X:90:ARG:HA	2.15	0.47
1:G:100:VAL:CG2	1:G:101:ILE:N	2.78	0.47
1:M:477:LEU:HD23	1:M:477:LEU:H	1.79	0.47
2:N:343:ILE:HG23	2:N:372:LEU:HD23	1.97	0.47
2:T:263:THR:C	2:T:265:GLU:H	2.23	0.47
2:W:217:VAL:CG1	2:W:222:PHE:HB3	2.44	0.47
1:D:168:THR:N	4:D:902:ASN:OD1	2.46	0.46
2:E:13:ILE:HG21	2:E:173:LEU:CD2	2.43	0.46
2:E:54:ASN:O	2:E:58:VAL:HG23	2.15	0.46
2:E:375:LEU:HD13	2:E:396:MET:HE1	1.96	0.46
1:G:118:ASP:OD1	1:G:128:TYR:HB2	2.15	0.46
1:J:337:ALA:HB1	3:L:17:GLU:HB2	1.98	0.46
3:L:33:ILE:O	3:L:37:ILE:HG12	2.15	0.46
1:M:329:TYR:CE2	3:O:89:PRO:HG3	2.51	0.46
2:Q:282:LYS:HD2	3:R:55:PHE:CE2	2.51	0.46
1:V:438:TRP:CH2	1:V:443:PRO:HG3	2.50	0.46
1:G:319:GLY:O	3:I:79:PRO:HG2	2.15	0.46
3:I:34:LEU:HD12	3:I:34:LEU:HA	1.74	0.46
2:T:141:LEU:HD23	3:U:85:PHE:CD2	2.50	0.46
1:V:88:ILE:HA	1:V:324:TYR:HB3	1.96	0.46
2:W:156:THR:CG2	2:W:157:GLU:O	2.58	0.46
1:A:307:PRO:HG2	1:A:354:LEU:HD23	1.98	0.46
1:D:1:MET:HG2	1:D:1:MET:O	2.15	0.46
2:H:156:THR:HG22	2:H:157:GLU:O	2.15	0.46
1:P:167:ASP:HA	1:P:171:SER:HB2	1.97	0.46
2:T:21:THR:CG2	3:U:61:ARG:HH12	2.14	0.46
2:B:84:PHE:CE2	3:C:15:ARG:HG2	2.50	0.46
2:B:207:GLU:H	2:B:207:GLU:HG3	1.55	0.46
1:D:83:THR:HG22	1:D:83:THR:O	2.15	0.46
2:H:119:VAL:CG1	2:H:156:THR:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:479:ATP:O2G	9:H:482:ASP:CB	2.64	0.46
1:J:199:PHE:CD1	1:J:199:PHE:C	2.93	0.46
1:P:245:VAL:CG1	1:P:459:LEU:HB3	2.45	0.46
1:V:71:VAL:HB	1:V:114:LYS:NZ	2.31	0.46
2:W:384:ILE:CG2	2:W:412:LEU:CD2	2.54	0.46
2:B:279:VAL:HB	3:C:55:PHE:CE1	2.51	0.46
1:D:69:ILE:HD11	1:D:164:LEU:HD13	1.96	0.46
2:E:75:GLU:HG3	2:E:282:LYS:HG3	1.98	0.46
2:E:332:GLU:HG3	2:E:335:ARG:HH21	1.80	0.46
2:H:119:VAL:HG12	2:H:156:THR:CG2	2.46	0.46
2:K:179:TYR:CE1	2:K:324:LYS:HB2	2.51	0.46
1:P:3:TRP:CZ3	1:P:31:ARG:HD3	2.50	0.46
1:S:124:SER:HG	4:S:907:ASN:N	2.13	0.46
1:V:143:VAL:CG1	1:V:145:GLY:H	2.28	0.46
1:V:335:MET:O	1:V:339:THR:OG1	2.25	0.46
2:B:200:ILE:HG23	2:B:234:GLN:OE1	2.16	0.46
3:C:2:VAL:N	3:C:31:SER:HG	2.14	0.46
1:D:190:ARG:CD	1:D:241:TRP:HH2	2.21	0.46
1:D:297:TYR:C	1:D:300:PRO:HD2	2.40	0.46
2:H:167:ARG:HG3	2:H:220:PHE:HB3	1.96	0.46
2:H:345:ASN:O	2:H:349:ASN:HB2	2.15	0.46
1:P:349:LYS:O	1:P:353:MET:HG2	2.16	0.46
2:Q:170:LEU:CD1	2:Q:223:VAL:HG21	2.45	0.46
2:Q:305:ARG:HG2	2:Q:305:ARG:NH1	2.31	0.46
1:S:259:GLU:OE1	1:S:259:GLU:N	2.49	0.46
1:S:320:VAL:HG22	3:U:88:VAL:HG11	1.97	0.46
1:D:64:LEU:HD11	1:D:222:VAL:HG21	1.98	0.46
1:D:293:PRO:HG3	2:H:106:TRP:CZ3	2.51	0.46
1:P:172:ILE:HD13	1:P:207:GLY:HA3	1.97	0.46
1:P:300:PRO:O	1:P:304:ILE:HG13	2.15	0.46
2:Q:162:THR:CG2	2:Q:165:GLU:H	2.29	0.46
1:S:5:LYS:HB2	1:S:10:LEU:HD13	1.96	0.46
1:V:422:VAL:N	1:V:423:PRO:CD	2.79	0.46
1:D:143:VAL:HG13	1:D:145:GLY:H	1.81	0.46
2:E:96:GLN:HB2	2:E:125:HIS:HB2	1.98	0.46
2:N:249:ARG:NH2	2:N:260:PRO:HD3	2.31	0.46
1:S:2:LEU:HB3	1:S:27:SER:OG	2.14	0.46
1:S:88:ILE:HD13	1:S:317:TYR:HB3	1.98	0.46
2:W:172:LYS:HE3	2:W:300:ASP:OD1	2.16	0.46
2:B:146:ARG:HG2	2:B:146:ARG:HH11	1.81	0.46
1:D:219:VAL:O	1:D:223:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:PRO:O	1:D:477:LEU:C	2.57	0.46
1:D:477:LEU:O	1:D:478:THR:C	2.59	0.46
2:H:115:GLU:HB3	2:H:116:LYS:H	1.54	0.46
2:K:210:THR:HB	2:K:244:VAL:HG13	1.98	0.46
2:N:34:GLU:HB2	2:N:37:THR:HG21	1.98	0.46
1:P:2:LEU:HB3	1:P:27:SER:OG	2.15	0.46
1:P:125:SER:HB2	1:P:143:VAL:HG21	1.98	0.46
2:Q:21:THR:HB	3:R:63:ASP:OD1	2.16	0.46
2:Q:385:SER:OG	2:Q:388:ILE:HG12	2.15	0.46
2:B:8:VAL:HG21	2:B:201:ARG:NE	2.31	0.46
1:J:1:MET:HG2	1:J:1:MET:O	2.15	0.46
1:J:21:PRO:O	1:J:25:VAL:HG23	2.15	0.46
1:M:397:THR:HG23	1:M:398:PRO:HD2	1.98	0.46
2:N:21:THR:HG21	3:O:61:ARG:NH1	2.11	0.46
1:P:178:PHE:HE1	1:P:397:THR:HG21	1.81	0.46
1:S:279:GLU:HG3	1:S:468:LYS:NZ	2.30	0.46
2:T:387:LYS:HG3	1:V:406:GLU:HA	1.98	0.46
2:B:27:CYS:SG	2:B:40:CYS:HB2	2.57	0.45
2:B:112:PRO:O	2:B:113:ASN:HB2	2.15	0.45
1:D:38:LYS:O	1:D:135:LYS:HG3	2.16	0.45
2:E:37:THR:HG22	2:E:145:ASN:HD21	1.81	0.45
2:E:250:THR:O	2:E:258:THR:HA	2.16	0.45
1:J:94:ALA:HA	1:J:95:PRO:HD3	1.78	0.45
1:M:126:THR:OG1	1:M:149:GLY:HA3	2.16	0.45
1:M:477:LEU:O	1:M:478:THR:C	2.58	0.45
2:N:24:PHE:HA	2:N:52:ILE:O	2.16	0.45
1:P:434:ILE:HD12	1:P:465:TRP:CD1	2.50	0.45
1:S:422:VAL:HG23	1:S:423:PRO:N	2.31	0.45
1:A:135:LYS:NZ	2:E:349:ASN:O	2.46	0.45
2:E:234:GLN:O	2:E:238:VAL:HG23	2.16	0.45
2:K:196:ILE:O	2:K:213:GLU:HA	2.16	0.45
1:M:94:ALA:HA	1:M:95:PRO:HD3	1.80	0.45
1:P:88:ILE:HA	1:P:324:TYR:HB3	1.97	0.45
1:P:178:PHE:CE1	1:P:397:THR:HG21	2.51	0.45
1:S:138:TRP:CZ2	1:S:476:PRO:HD3	2.51	0.45
2:W:137:GLY:O	3:X:90:ARG:HD2	2.17	0.45
2:B:14:HIS:CD2	2:B:127:GLU:OE2	2.69	0.45
2:B:146:ARG:HG2	2:B:146:ARG:NH1	2.32	0.45
1:D:30:ASP:O	1:D:34:GLN:HG3	2.16	0.45
1:D:172:ILE:CD1	1:D:207:GLY:HA3	2.46	0.45
1:G:337:ALA:HA	3:I:15:ARG:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:178:PHE:CE1	1:J:397:THR:HG21	2.51	0.45
2:K:22:LYS:HD2	2:K:27:CYS:HB2	1.99	0.45
1:M:172:ILE:HD13	1:M:207:GLY:HA3	1.96	0.45
1:M:185:LYS:NZ	1:M:429:LEU:O	2.49	0.45
2:N:282:LYS:HD3	3:O:55:PHE:CZ	2.52	0.45
1:P:353:MET:HE3	1:P:353:MET:HB3	1.89	0.45
2:B:255:THR:HG23	2:B:257:LYS:H	1.82	0.45
2:E:229:TYR:O	2:E:232:GLU:HB3	2.17	0.45
1:G:39:VAL:HG21	1:G:157:VAL:HG11	1.97	0.45
2:H:230:GLU:OE2	2:H:233:ARG:NH1	2.49	0.45
2:K:17:MET:HE3	2:K:60:TYR:CB	2.45	0.45
2:N:113:ASN:HD21	1:P:49:LYS:HB2	1.80	0.45
1:S:174:GLN:HB3	1:S:175:PRO:HD3	1.98	0.45
2:T:233:ARG:HD2	2:T:249:ARG:NH2	2.31	0.45
1:A:299:ILE:HB	1:A:300:PRO:HD3	1.99	0.45
1:J:62:LEU:HA	1:J:63:PRO:HD3	1.84	0.45
2:K:73:HIS:NE2	2:K:103:THR:HB	2.32	0.45
2:K:95:SER:CB	2:K:127:GLU:HB3	2.46	0.45
2:N:17:MET:HE1	2:N:60:TYR:CB	2.45	0.45
2:N:402:THR:HG22	2:N:403:PRO:HD2	1.99	0.45
1:P:279:GLU:HG3	1:P:468:LYS:NZ	2.30	0.45
1:A:19:VAL:HG22	1:A:20:SER:N	2.31	0.45
1:A:95:PRO:HG2	2:B:46:MET:CE	2.47	0.45
1:A:199:PHE:C	1:A:199:PHE:CD1	2.94	0.45
2:B:8:VAL:HG13	2:B:161:ARG:NH1	2.31	0.45
2:B:368:LYS:O	2:B:369:PRO:C	2.58	0.45
1:G:259:GLU:CD	1:G:292:LEU:H	2.24	0.45
1:G:438:TRP:CH2	1:G:443:PRO:HG3	2.51	0.45
2:H:222:PHE:CZ	2:H:253:PRO:HB3	2.52	0.45
1:M:193:ARG:NH1	1:M:232:THR:OG1	2.49	0.45
1:P:170:GLY:HA2	1:P:173:ARG:NH2	2.31	0.45
2:Q:233:ARG:O	2:Q:237:VAL:HG23	2.17	0.45
1:S:72:LYS:HE2	1:S:117:LEU:HD13	1.98	0.45
1:A:162:VAL:HG21	1:A:219:VAL:HG21	1.98	0.45
2:B:198:VAL:O	2:B:198:VAL:HG13	2.17	0.45
1:D:88:ILE:HG23	1:D:89:LEU:HD13	1.99	0.45
2:H:233:ARG:O	2:H:237:VAL:HG23	2.16	0.45
2:H:320:LEU:CD2	2:H:326:VAL:HG12	2.45	0.45
1:M:353:MET:O	1:M:356:THR:HG23	2.16	0.45
1:P:162:VAL:HG11	1:P:219:VAL:HG21	1.99	0.45
1:S:83:THR:HG22	1:S:90:GLU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:TYR:OH	4:D:902:ASN:HA	2.17	0.45
1:G:476:PRO:O	1:G:477:LEU:C	2.60	0.45
3:I:73:LYS:O	3:I:76:MET:HG2	2.17	0.45
1:J:292:LEU:HB2	1:J:295:VAL:CG2	2.47	0.45
2:K:80:ARG:HE	2:K:275:ASP:CG	2.25	0.45
2:K:123:ARG:HG2	2:K:155:VAL:HB	1.98	0.45
2:K:375:LEU:HD13	2:K:396:MET:HE1	1.97	0.45
2:Q:211:ARG:HD2	8:Q:479:ATP:C8	2.52	0.45
1:S:181:VAL:HG22	1:S:210:GLY:O	2.17	0.45
1:S:317:TYR:HE1	2:T:47:PRO:HG3	1.82	0.45
2:T:114:GLY:O	2:T:115:GLU:OE2	2.35	0.45
2:B:36:ASN:ND2	3:C:84:GLY:O	2.41	0.45
2:H:119:VAL:HG12	2:H:156:THR:HG23	1.98	0.45
1:J:138:TRP:CE2	1:J:438:TRP:CH2	3.05	0.45
1:J:145:GLY:CA	1:J:174:GLN:OE1	2.65	0.45
1:J:422:VAL:N	1:J:423:PRO:CD	2.80	0.45
2:K:96:GLN:HB2	2:K:125:HIS:HB2	1.98	0.45
1:V:138:TRP:NE1	1:V:438:TRP:HH2	2.15	0.45
2:W:21:THR:HG21	3:X:61:ARG:NH1	2.18	0.45
2:W:95:SER:HB3	2:W:127:GLU:OE1	2.17	0.45
1:A:174:GLN:HG3	1:A:175:PRO:N	2.30	0.45
2:B:109:LEU:HD11	2:B:169:PHE:HA	1.99	0.45
2:B:295:MET:HG3	2:B:296:PRO:O	2.16	0.45
1:D:138:TRP:CD2	1:D:438:TRP:CZ3	3.05	0.45
1:G:21:PRO:O	1:G:25:VAL:HG23	2.17	0.45
1:M:47:TYR:CD2	1:M:112:VAL:HG22	2.52	0.45
1:M:98:ALA:HA	1:M:195:GLY:HA3	1.98	0.45
1:P:157:VAL:O	1:P:158:LEU:HB2	2.16	0.45
1:P:384:LYS:O	1:P:387:GLU:HB2	2.16	0.45
1:S:126:THR:OG1	1:S:149:GLY:HA3	2.16	0.45
2:T:17:MET:HE1	2:T:57:ALA:C	2.41	0.45
3:C:23:ILE:O	3:C:27:GLN:HG3	2.17	0.44
2:H:24:PHE:HA	2:H:52:ILE:O	2.16	0.44
2:H:129:ASP:O	2:H:147:ALA:HA	2.17	0.44
1:P:155:VAL:CG2	1:P:163:SER:HB2	2.47	0.44
2:T:156:THR:HG22	2:T:157:GLU:N	2.33	0.44
2:T:360:ILE:HD11	2:T:365:SER:HA	2.00	0.44
2:W:255:THR:HG21	2:W:259:TYR:CE1	2.49	0.44
2:B:42:VAL:HA	2:B:49:ALA:HB1	1.99	0.44
2:B:80:ARG:HE	2:B:275:ASP:CG	2.25	0.44
3:C:72:GLU:OE1	3:C:72:GLU:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:33:ILE:O	3:I:37:ILE:HG12	2.18	0.44
1:J:122:MET:SD	1:J:351:ARG:HD2	2.57	0.44
2:N:95:SER:HB3	2:N:127:GLU:CB	2.43	0.44
2:N:298:LEU:HB3	2:N:299:PRO:CD	2.48	0.44
3:O:91:VAL:C	3:O:92:VAL:HG13	2.38	0.44
2:Q:185:ALA:HB1	2:Q:192:LEU:HD12	1.99	0.44
2:Q:334:VAL:HG21	2:Q:340:PRO:CB	2.41	0.44
2:T:255:THR:HG21	2:T:259:TYR:OH	2.16	0.44
2:W:42:VAL:HA	2:W:49:ALA:HB1	1.99	0.44
2:E:81:LYS:HE2	2:E:270:TYR:CE1	2.53	0.44
1:G:422:VAL:N	1:G:423:PRO:CD	2.81	0.44
2:H:211:ARG:HH12	8:H:479:ATP:H5'2	1.78	0.44
1:J:432:ILE:HG22	1:J:458:LEU:HG	1.99	0.44
1:M:422:VAL:N	1:M:423:PRO:CD	2.81	0.44
2:Q:68:LEU:HD11	2:Q:154:ILE:HD13	1.98	0.44
2:Q:137:GLY:O	3:R:90:ARG:HD2	2.17	0.44
1:S:98:ALA:HA	1:S:195:GLY:HA3	2.00	0.44
1:S:99:THR:O	1:S:103:ARG:HG3	2.17	0.44
1:A:138:TRP:CE2	1:A:476:PRO:HB3	2.53	0.44
1:D:143:VAL:CG1	1:D:145:GLY:H	2.31	0.44
2:K:103:THR:CG2	2:K:104:ASN:OD1	2.66	0.44
1:M:199:PHE:CD1	1:M:199:PHE:C	2.96	0.44
1:P:125:SER:HB2	1:P:143:VAL:CG2	2.48	0.44
1:P:215:ASP:O	1:P:219:VAL:HG23	2.18	0.44
1:V:73:ASP:OD2	1:V:83:THR:OG1	2.33	0.44
1:G:347:GLU:OE1	1:G:350:ARG:NH2	2.44	0.44
1:J:344:PHE:O	1:J:349:LYS:HE2	2.17	0.44
1:P:90:GLU:O	1:P:91:ASN:CB	2.63	0.44
2:Q:332:GLU:HG3	2:Q:335:ARG:NH2	2.33	0.44
2:T:323:HIS:O	2:T:324:LYS:C	2.61	0.44
1:V:76:LEU:HD23	1:V:94:ALA:HB1	1.98	0.44
1:A:115:THR:HG21	1:A:151:SER:N	2.33	0.44
1:A:253:LYS:HG2	1:A:286:GLU:HB3	2.00	0.44
2:H:8:VAL:CG1	2:H:158:PRO:HB2	2.48	0.44
2:T:135:HIS:ND1	2:T:135:HIS:N	2.65	0.44
2:W:8:VAL:HG21	2:W:201:ARG:HE	1.82	0.44
1:A:190:ARG:HD2	1:A:455:GLU:OE2	2.18	0.44
2:B:89:PRO:HG3	2:B:144:LEU:HD13	1.99	0.44
2:B:210:THR:HG22	2:B:246:GLN:HB2	2.00	0.44
2:B:310:TYR:CE1	2:B:334:VAL:HG11	2.52	0.44
1:D:138:TRP:CD2	1:D:438:TRP:HZ3	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:376:ARG:HG3	1:G:376:ARG:NH1	2.31	0.44
2:H:95:SER:HB3	2:H:127:GLU:OE1	2.17	0.44
2:N:156:THR:CG2	2:N:157:GLU:O	2.65	0.44
2:Q:362:ILE:O	2:Q:362:ILE:HG13	2.17	0.44
1:S:67:ILE:HD13	1:S:67:ILE:N	2.33	0.44
1:J:39:VAL:HG21	1:J:157:VAL:HG11	2.00	0.44
2:K:115:GLU:HB3	2:K:116:LYS:H	1.66	0.44
2:K:192:LEU:HD23	2:K:193:ARG:N	2.33	0.44
1:M:350:ARG:HG3	3:O:26:PHE:CE1	2.53	0.44
2:W:210:THR:OG1	2:W:244:VAL:HG13	2.18	0.44
1:D:98:ALA:HA	1:D:195:GLY:HA3	2.00	0.44
2:E:261:MET:HE3	2:E:261:MET:HB2	1.89	0.44
3:F:71:ARG:HG2	3:F:75:LEU:HD23	2.00	0.44
1:J:191:VAL:HG22	1:J:224:SER:HB3	1.99	0.44
2:N:81:LYS:HZ2	9:N:482:ASP:CA	2.31	0.44
2:N:323:HIS:HD2	2:N:325:GLU:OE1	1.99	0.44
1:P:31:ARG:O	1:P:31:ARG:HG3	2.17	0.44
1:S:88:ILE:HG23	1:S:89:LEU:HD13	2.00	0.44
1:S:299:ILE:HG13	1:S:419:ILE:HG22	1.99	0.44
3:X:21:GLU:O	3:X:25:VAL:HG23	2.17	0.44
1:A:36:GLU:OE1	1:A:36:GLU:HA	2.18	0.43
2:B:100:PRO:HB3	2:B:123:ARG:NH2	2.21	0.43
2:E:375:LEU:O	2:E:379:ILE:HG12	2.17	0.43
1:G:173:ARG:NH2	1:G:425:ASN:OD1	2.51	0.43
2:K:88:LEU:HD11	2:K:93:GLN:HB2	2.00	0.43
1:M:137:PRO:HB3	1:M:157:VAL:CG1	2.48	0.43
1:A:434:ILE:HD13	1:A:434:ILE:HA	1.61	0.43
1:A:475:ILE:HG23	1:A:476:PRO:CD	2.47	0.43
2:B:113:ASN:HA	2:B:115:GLU:H	1.83	0.43
2:E:36:ASN:ND2	3:F:84:GLY:O	2.49	0.43
1:G:137:PRO:HB3	1:G:157:VAL:HG13	2.00	0.43
1:M:422:VAL:HG23	1:M:423:PRO:HD3	1.99	0.43
1:P:204:ASP:O	1:P:205:GLN:HG2	2.18	0.43
1:S:28:PHE:CD2	1:S:68:PRO:HG2	2.53	0.43
1:S:120:PHE:O	1:S:122:MET:HG3	2.19	0.43
1:V:155:VAL:HG21	1:V:163:SER:HB2	1.98	0.43
2:W:109:LEU:HD11	2:W:169:PHE:HA	2.00	0.43
1:D:157:VAL:HG23	1:D:159:SER:H	1.83	0.43
2:E:141:LEU:HD23	3:F:85:PHE:CD2	2.54	0.43
2:E:146:ARG:HG2	2:E:146:ARG:HH11	1.82	0.43
2:H:112:PRO:O	2:H:113:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:362:ILE:O	2:H:362:ILE:HG13	2.17	0.43
3:L:80:GLU:CD	3:L:87:VAL:HG11	2.44	0.43
1:P:122:MET:HE2	1:P:199:PHE:CE1	2.54	0.43
2:Q:222:PHE:CE2	2:Q:253:PRO:HB3	2.54	0.43
1:S:196:LEU:HB2	1:S:206:ILE:HD11	1.99	0.43
2:T:40:CYS:HB2	2:T:41:PRO:HD2	2.01	0.43
2:W:5:TYR:HA	2:W:202:PRO:HA	2.00	0.43
1:A:143:VAL:HG23	1:A:145:GLY:H	1.82	0.43
2:B:24:PHE:HA	2:B:52:ILE:O	2.18	0.43
1:D:265:LEU:HD22	1:D:398:PRO:HA	2.00	0.43
2:E:360:ILE:HD13	2:E:366:PRO:HD3	2.00	0.43
1:J:316:ARG:O	1:J:321:ARG:NH2	2.50	0.43
1:J:477:LEU:HD23	1:J:477:LEU:N	2.29	0.43
2:K:375:LEU:HD22	2:K:396:MET:HE1	2.00	0.43
1:M:138:TRP:CE2	1:M:438:TRP:CZ3	3.06	0.43
3:O:34:LEU:HD12	3:O:34:LEU:HA	1.68	0.43
2:Q:230:GLU:OE2	2:Q:233:ARG:NH1	2.52	0.43
2:Q:255:THR:HG21	2:Q:259:TYR:OH	2.19	0.43
3:R:55:PHE:O	3:R:56:GLU:CB	2.66	0.43
1:S:32:TYR:CZ	1:S:36:GLU:HG2	2.53	0.43
2:T:17:MET:CE	2:T:60:TYR:HB2	2.47	0.43
1:A:297:TYR:CD2	3:C:43:LEU:HD11	2.53	0.43
1:J:78:GLU:HB2	1:J:97:ASP:OD1	2.18	0.43
1:J:90:GLU:O	1:J:91:ASN:CB	2.58	0.43
1:J:172:ILE:HD13	1:J:207:GLY:HA3	2.01	0.43
2:K:320:LEU:HD22	2:K:326:VAL:HG12	2.01	0.43
1:M:162:VAL:CG2	1:M:219:VAL:HG21	2.48	0.43
1:P:138:TRP:CZ2	1:P:438:TRP:CH2	3.06	0.43
1:S:386:PHE:CG	1:S:451:LYS:HG2	2.53	0.43
1:V:157:VAL:HG23	1:V:159:SER:H	1.82	0.43
1:A:73:ASP:OD2	1:A:83:THR:OG1	2.25	0.43
1:A:94:ALA:HA	1:A:95:PRO:HD3	1.67	0.43
2:B:88:LEU:HA	2:B:89:PRO:HD3	1.72	0.43
2:E:20:LYS:HE3	3:F:63:ASP:O	2.18	0.43
3:F:7:VAL:HG21	3:F:27:GLN:HG3	1.99	0.43
1:J:60:ARG:HA	1:J:65:PHE:CG	2.54	0.43
2:K:95:SER:HB2	2:K:127:GLU:OE1	2.19	0.43
2:K:222:PHE:CZ	2:K:253:PRO:HB3	2.53	0.43
1:A:88:ILE:HA	1:A:324:TYR:HB3	1.99	0.43
1:D:422:VAL:N	1:D:423:PRO:CD	2.82	0.43
1:G:234:ALA:HB1	1:G:236:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:332:ILE:HD12	3:L:89:PRO:HG2	2.01	0.43
2:K:95:SER:HB2	2:K:127:GLU:HB3	2.00	0.43
1:M:177:SER:HA	10:M:907:HOH:O	2.18	0.43
2:N:106:TRP:CD1	2:N:118:LYS:HE2	2.54	0.43
2:Q:331:GLU:HA	2:Q:334:VAL:HG12	2.00	0.43
1:S:137:PRO:HB3	1:S:157:VAL:HG12	1.99	0.43
2:T:36:ASN:O	3:U:71:ARG:HD3	2.18	0.43
1:V:185:LYS:HE3	1:V:425:ASN:HD22	1.83	0.43
1:V:325:ARG:HA	1:V:339:THR:HG23	2.01	0.43
2:W:302:ARG:HD3	2:W:321:VAL:HG22	2.01	0.43
2:K:170:LEU:HD12	2:K:223:VAL:HG21	2.00	0.43
2:N:108:GLU:O	2:N:172:LYS:NZ	2.51	0.43
2:N:310:TYR:CE1	2:N:334:VAL:HG11	2.53	0.43
1:V:318:ASP:HB2	1:V:336:TYR:CE1	2.54	0.43
1:A:139:ASP:OD1	1:A:141:GLU:HB2	2.18	0.43
2:B:355:LEU:HD21	2:B:365:SER:HB2	1.99	0.43
1:D:322:TYR:OH	2:E:45:GLY:O	2.26	0.43
2:K:129:ASP:CG	2:K:146:ARG:HH11	2.26	0.43
1:M:182:ILE:HG12	1:M:434:ILE:CD1	2.49	0.43
2:N:210:THR:OG1	2:N:244:VAL:HG13	2.19	0.43
1:P:283:GLU:HG3	1:P:468:LYS:HD2	2.01	0.43
2:T:109:LEU:HD11	2:T:169:PHE:HA	2.01	0.43
2:T:222:PHE:CZ	2:T:253:PRO:HB3	2.54	0.43
1:D:57:LEU:HD22	1:D:65:PHE:CE1	2.54	0.43
2:E:156:THR:CG2	2:E:157:GLU:O	2.64	0.43
2:E:196:ILE:O	2:E:213:GLU:HA	2.19	0.43
2:H:202:PRO:O	2:H:205:SER:HB3	2.19	0.43
2:H:320:LEU:HD22	2:H:326:VAL:HG12	2.01	0.43
1:J:57:LEU:HD22	1:J:65:PHE:CE1	2.54	0.43
2:K:282:LYS:HD3	3:L:55:PHE:CE2	2.54	0.43
2:T:146:ARG:HG2	2:T:146:ARG:HH11	1.83	0.43
1:V:77:VAL:HG21	1:V:114:LYS:HZ1	1.84	0.43
1:V:87:LYS:HD3	1:V:90:GLU:OE2	2.19	0.43
1:V:98:ALA:HA	1:V:195:GLY:HA3	2.01	0.43
1:V:300:PRO:HA	3:X:37:ILE:HG22	2.00	0.43
2:W:5:TYR:HB3	2:W:201:ARG:O	2.19	0.43
1:A:26:GLU:HG3	1:A:51:LEU:HD11	2.00	0.42
1:A:72:LYS:HE2	1:A:117:LEU:HD13	2.01	0.42
1:A:406:GLU:HG3	2:E:387:LYS:HD2	2.01	0.42
1:D:67:ILE:HD13	1:D:67:ILE:N	2.34	0.42
1:M:337:ALA:HA	3:O:15:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:196:LEU:HD22	1:P:206:ILE:HG13	2.01	0.42
2:Q:184:LYS:HB2	2:Q:191:GLN:OE1	2.19	0.42
2:T:211:ARG:HD3	6:T:479:ADP:C5	2.54	0.42
2:W:35:PRO:HG3	3:X:85:PHE:CZ	2.54	0.42
2:W:162:THR:O	2:W:163:PRO:C	2.62	0.42
1:A:470:LYS:HG2	1:A:472:TYR:OH	2.18	0.42
2:B:39:VAL:HG13	2:B:44:LEU:HD11	2.01	0.42
2:B:54:ASN:C	2:B:54:ASN:OD1	2.62	0.42
2:B:179:TYR:CE1	2:B:324:LYS:HB2	2.54	0.42
1:D:182:ILE:HG12	1:D:434:ILE:CD1	2.50	0.42
1:D:393:ALA:HB2	1:D:448:LEU:HD23	2.01	0.42
2:E:174:ARG:HD2	2:E:220:PHE:CE2	2.54	0.42
2:H:17:MET:HE3	2:H:60:TYR:HB3	1.95	0.42
2:K:13:ILE:HG22	2:K:15:VAL:HG23	2.00	0.42
2:K:143:ASP:HB2	3:L:85:PHE:CE1	2.55	0.42
2:Q:333:ALA:C	2:Q:335:ARG:N	2.77	0.42
2:T:201:ARG:CD	2:T:207:GLU:O	2.67	0.42
2:T:375:LEU:HD22	2:T:396:MET:HE1	2.01	0.42
1:V:126:THR:HG22	1:V:126:THR:O	2.18	0.42
1:A:403:LYS:O	1:A:406:GLU:HB2	2.19	0.42
2:B:261:MET:HE3	2:B:261:MET:HB2	1.96	0.42
2:E:117:LYS:CG	2:E:118:LYS:N	2.81	0.42
1:G:219:VAL:O	1:G:223:ILE:HG23	2.19	0.42
2:H:360:ILE:H	2:H:360:ILE:HG13	1.67	0.42
1:J:3:TRP:CZ3	1:J:31:ARG:CD	3.02	0.42
2:K:95:SER:CB	2:K:127:GLU:OE1	2.67	0.42
2:K:220:PHE:O	2:K:223:VAL:HG22	2.17	0.42
2:Q:196:ILE:HG21	2:Q:227:LEU:HD21	2.00	0.42
1:S:173:ARG:NH2	1:S:425:ASN:OD1	2.52	0.42
1:D:373:LYS:HE2	3:F:50:PRO:HD3	2.01	0.42
2:E:201:ARG:CD	2:E:207:GLU:O	2.67	0.42
1:G:418:ASP:HB3	1:G:422:VAL:HG13	2.02	0.42
1:J:266:GLN:HA	1:J:267:PRO:HD3	1.93	0.42
2:K:405:GLN:O	2:K:409:GLU:HG3	2.19	0.42
1:P:143:VAL:CG1	1:P:145:GLY:H	2.32	0.42
2:Q:27:CYS:SG	2:Q:40:CYS:HB3	2.59	0.42
2:Q:140:THR:OG1	3:R:91:VAL:HG22	2.20	0.42
1:S:123:GLY:O	4:S:907:ASN:HB2	2.20	0.42
2:T:162:THR:HG22	2:T:165:GLU:H	1.84	0.42
1:V:351:ARG:NH1	4:V:908:ASN:OXT	2.51	0.42
1:V:374:VAL:HG11	3:X:40:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ILE:HG23	1:A:476:PRO:HD2	1.99	0.42
2:E:118:LYS:NZ	1:G:291:SER:HB3	2.35	0.42
2:H:83:TYR:CZ	2:H:88:LEU:HD22	2.55	0.42
1:J:3:TRP:CH2	1:J:31:ARG:NE	2.88	0.42
1:J:318:ASP:HB2	1:J:336:TYR:CE1	2.55	0.42
1:J:476:PRO:O	1:J:477:LEU:C	2.61	0.42
1:P:306:ALA:HB3	1:P:307:PRO:CD	2.46	0.42
1:V:125:SER:O	1:V:126:THR:HB	2.18	0.42
1:A:98:ALA:HA	1:A:195:GLY:HA3	2.02	0.42
1:A:138:TRP:CZ2	1:A:438:TRP:CH2	3.08	0.42
1:D:5:LYS:HB2	1:D:10:LEU:HD13	2.01	0.42
2:H:7:ALA:HB3	2:H:161:ARG:O	2.20	0.42
2:H:392:VAL:C	2:H:396:MET:HE3	2.45	0.42
1:J:438:TRP:CD1	1:J:438:TRP:N	2.87	0.42
1:P:21:PRO:O	1:P:25:VAL:HG23	2.20	0.42
1:P:434:ILE:HA	1:P:435:PRO:HD3	1.93	0.42
1:V:31:ARG:O	1:V:35:THR:HG23	2.20	0.42
2:W:270:TYR:O	2:W:271:ARG:C	2.63	0.42
2:K:8:VAL:O	2:K:198:VAL:HA	2.20	0.42
1:S:157:VAL:HG23	1:S:159:SER:H	1.85	0.42
2:E:39:VAL:HG21	2:E:44:LEU:CD2	2.50	0.42
1:G:57:LEU:HD22	1:G:65:PHE:CE1	2.55	0.42
1:J:98:ALA:HA	1:J:195:GLY:HA3	2.01	0.42
1:M:275:ASN:O	1:M:279:GLU:HB2	2.20	0.42
2:N:362:ILE:O	2:N:362:ILE:HG13	2.20	0.42
1:P:126:THR:O	1:P:126:THR:HG22	2.18	0.42
1:P:418:ASP:HB3	1:P:422:VAL:HG13	2.01	0.42
2:Q:307:ILE:O	2:Q:311:GLY:HA2	2.19	0.42
2:T:140:THR:HB	3:U:88:VAL:HG23	2.02	0.42
2:T:207:GLU:CG	2:T:208:PHE:N	2.79	0.42
1:V:114:LYS:HE2	1:V:114:LYS:HA	2.02	0.42
1:V:219:VAL:O	1:V:223:ILE:HG12	2.19	0.42
2:W:198:VAL:HG11	2:W:230:GLU:HG2	2.02	0.42
1:D:438:TRP:CH2	1:D:443:PRO:HG3	2.55	0.42
1:G:397:THR:HG22	1:G:399:THR:H	1.85	0.42
2:N:54:ASN:C	2:N:54:ASN:OD1	2.63	0.42
2:N:330:PHE:CE1	2:N:344:VAL:HG13	2.54	0.42
1:P:244:GLU:OE2	1:P:247:LYS:HD2	2.20	0.42
1:P:405:GLY:HA2	1:P:408:LEU:HD12	2.02	0.42
1:P:438:TRP:CD1	1:P:438:TRP:N	2.87	0.42
2:Q:250:THR:O	2:Q:258:THR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:322:TYR:CZ	2:T:47:PRO:HD3	2.55	0.42
1:V:62:LEU:HA	1:V:63:PRO:HD3	1.89	0.42
1:V:457:THR:O	1:V:461:ILE:HG13	2.20	0.42
1:A:21:PRO:HB2	1:A:54:ALA:HB1	2.02	0.42
1:D:72:LYS:CA	1:D:115:THR:HG22	2.45	0.42
1:D:138:TRP:CE2	1:D:438:TRP:CZ3	3.08	0.42
2:E:330:PHE:CE1	2:E:344:VAL:HG13	2.54	0.42
2:H:34:GLU:HB2	2:H:37:THR:HG21	2.01	0.42
1:M:136:ASN:HA	1:M:137:PRO:HD2	1.95	0.42
1:M:259:GLU:CD	1:M:292:LEU:H	2.27	0.42
1:P:60:ARG:HA	1:P:65:PHE:CD1	2.54	0.42
1:P:434:ILE:O	1:P:436:ILE:HG23	2.20	0.42
2:Q:252:ASP:HB3	2:Q:255:THR:HG22	2.02	0.42
2:T:270:TYR:O	2:T:271:ARG:C	2.63	0.42
1:V:116:ASN:ND2	1:V:132:PHE:O	2.51	0.42
1:V:300:PRO:O	1:V:304:ILE:HG13	2.20	0.42
1:A:299:ILE:CB	1:A:300:PRO:HD3	2.50	0.41
2:B:320:LEU:HD13	2:B:327:GLY:HA2	2.01	0.41
1:D:168:THR:HB	4:D:902:ASN:OD1	2.20	0.41
1:D:293:PRO:HG3	2:H:106:TRP:CE3	2.54	0.41
2:E:374:GLU:O	2:E:377:LYS:HB3	2.20	0.41
2:E:406:ILE:HA	2:E:409:GLU:HB2	2.01	0.41
2:H:221:ARG:HD3	2:H:221:ARG:HA	1.90	0.41
2:H:333:ALA:C	2:H:335:ARG:N	2.79	0.41
1:J:138:TRP:CZ2	1:J:438:TRP:CH2	3.08	0.41
2:K:172:LYS:O	2:K:176:ILE:HG13	2.19	0.41
2:K:350:ASP:OD1	2:K:390:LYS:NZ	2.52	0.41
3:L:80:GLU:HG2	3:L:87:VAL:HB	2.02	0.41
1:M:95:PRO:HG2	2:N:46:MET:HE3	2.02	0.41
2:T:21:THR:HG23	2:T:25:CYS:O	2.20	0.41
2:B:336:HIS:NE2	2:B:370:GLU:HG3	2.35	0.41
1:D:32:TYR:CE1	1:D:36:GLU:HG2	2.55	0.41
2:E:17:MET:HE2	2:E:17:MET:HB3	1.82	0.41
2:E:179:TYR:CD1	2:E:299:PRO:HG3	2.55	0.41
1:G:90:GLU:O	1:G:91:ASN:CB	2.65	0.41
2:H:333:ALA:C	2:H:335:ARG:H	2.26	0.41
1:J:418:ASP:HB3	1:J:422:VAL:HG13	2.02	0.41
2:K:106:TRP:CD1	2:K:106:TRP:C	2.98	0.41
2:N:26:GLY:O	3:O:65:PRO:HA	2.19	0.41
1:P:347:GLU:O	1:P:351:ARG:HG3	2.20	0.41
1:S:138:TRP:CD2	1:S:438:TRP:CZ3	3.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:392:VAL:C	2:T:396:MET:HE3	2.45	0.41
1:V:176:ALA:HB1	1:V:181:VAL:O	2.20	0.41
2:W:61:ALA:HA	2:W:152:MET:HE2	2.01	0.41
3:X:58:THR:HA	3:X:59:PRO:HD2	1.81	0.41
1:A:234:ALA:HB1	1:A:236:VAL:HG23	2.02	0.41
2:B:198:VAL:HG11	2:B:230:GLU:HG2	2.02	0.41
1:D:356:THR:HG21	3:F:14:ALA:HB2	2.03	0.41
2:E:98:GLU:O	2:E:99:LYS:HB2	2.20	0.41
2:E:362:ILE:O	2:E:362:ILE:HG13	2.19	0.41
1:G:434:ILE:HD13	1:G:434:ILE:HA	1.69	0.41
2:H:142:VAL:HB	3:I:86:PHE:HB2	2.02	0.41
1:J:384:LYS:O	1:J:387:GLU:HB2	2.20	0.41
2:K:213:GLU:OE2	2:K:215:LYS:HE3	2.20	0.41
1:V:42:TYR:O	1:V:132:PHE:HZ	2.02	0.41
1:V:172:ILE:HD13	1:V:207:GLY:HA3	2.01	0.41
1:A:404:PHE:HB3	2:E:390:LYS:HE3	2.02	0.41
1:J:99:THR:O	1:J:102:GLU:HB3	2.20	0.41
1:J:332:ILE:CD1	3:L:89:PRO:HG2	2.50	0.41
1:M:1:MET:HE2	1:M:3:TRP:HE1	1.86	0.41
1:M:219:VAL:O	1:M:223:ILE:HG23	2.21	0.41
2:Q:17:MET:HE2	2:Q:60:TYR:HB2	1.99	0.41
2:Q:179:TYR:CE1	2:Q:324:LYS:HB2	2.56	0.41
2:Q:333:ALA:HB2	2:Q:369:PRO:HB3	2.02	0.41
2:Q:360:ILE:HD11	2:Q:365:SER:HA	2.03	0.41
1:S:88:ILE:HG13	1:S:343:GLY:HA3	2.02	0.41
1:V:350:ARG:HD3	3:X:29:GLN:OE1	2.21	0.41
2:W:393:ILE:HA	2:W:396:MET:HE3	2.02	0.41
3:X:80:GLU:HG2	3:X:87:VAL:HB	2.01	0.41
2:B:252:ASP:CB	2:B:255:THR:HG22	2.44	0.41
1:D:77:VAL:HG21	1:D:114:LYS:HZ1	1.79	0.41
2:H:52:ILE:HG22	3:I:61:ARG:HB2	2.02	0.41
1:J:177:SER:HB2	1:J:396:THR:HG21	2.01	0.41
2:N:128:GLU:HB2	2:N:148:GLY:HA2	2.01	0.41
1:P:259:GLU:CD	1:P:292:LEU:H	2.29	0.41
2:Q:96:GLN:HB2	2:Q:125:HIS:HB2	2.02	0.41
2:Q:215:LYS:O	2:Q:216:ASN:HB2	2.20	0.41
2:T:70:CYS:HB3	2:T:103:THR:H	1.86	0.41
1:A:115:THR:CG2	1:A:151:SER:N	2.84	0.41
2:B:39:VAL:CG1	2:B:44:LEU:HD11	2.50	0.41
2:B:95:SER:HB2	2:B:96:GLN:H	1.68	0.41
2:H:39:VAL:HG21	2:H:44:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:29:TYR:O	1:J:32:TYR:HB3	2.20	0.41
1:J:43:ILE:HG13	1:J:116:ASN:HA	2.02	0.41
1:P:155:VAL:O	1:P:211:ARG:HD2	2.21	0.41
2:Q:217:VAL:HG13	2:Q:222:PHE:HB3	2.03	0.41
1:V:155:VAL:HG21	1:V:163:SER:CB	2.51	0.41
2:W:115:GLU:HB3	2:W:116:LYS:H	1.59	0.41
1:D:201:SER:HB2	2:E:276:PRO:HB2	2.02	0.41
1:G:190:ARG:CG	1:G:190:ARG:HH11	2.34	0.41
2:K:298:LEU:HB3	2:K:299:PRO:HD3	2.02	0.41
3:L:3:ASP:O	3:L:7:VAL:HG23	2.21	0.41
1:M:62:LEU:HD12	1:M:62:LEU:HA	1.96	0.41
1:M:266:GLN:HB2	1:M:269:VAL:HG23	2.03	0.41
1:P:174:GLN:CG	1:P:175:PRO:HD3	2.49	0.41
1:S:57:LEU:HD22	1:S:65:PHE:CE1	2.56	0.41
1:S:193:ARG:NH1	1:S:232:THR:OG1	2.54	0.41
1:A:142:ARG:HD3	1:A:401:PRO:O	2.20	0.41
1:A:331:ASP:O	1:A:334:GLU:N	2.53	0.41
2:B:115:GLU:HB3	2:B:116:LYS:H	1.68	0.41
2:B:252:ASP:OD2	2:B:255:THR:HG22	2.20	0.41
2:E:39:VAL:HG21	2:E:44:LEU:HD21	2.02	0.41
2:E:337:PHE:CE2	2:E:377:LYS:HA	2.55	0.41
2:K:140:THR:OG1	3:L:90:ARG:HA	2.21	0.41
1:P:126:THR:OG1	1:P:149:GLY:HA3	2.20	0.41
1:P:434:ILE:O	1:P:434:ILE:HG22	2.21	0.41
1:S:435:PRO:HG2	1:S:471:HIS:CG	2.55	0.41
2:T:41:PRO:CB	2:T:46:MET:HE2	2.50	0.41
2:T:225:LYS:HD3	2:T:225:LYS:HA	1.87	0.41
2:T:375:LEU:HD13	2:T:396:MET:HE1	2.01	0.41
2:W:310:TYR:CE1	2:W:334:VAL:HG11	2.56	0.41
3:X:53:GLN:O	3:X:55:PHE:HD1	2.03	0.41
1:A:212:ARG:NH2	1:A:472:TYR:CE1	2.89	0.41
1:A:299:ILE:HD13	1:A:299:ILE:HA	1.87	0.41
1:A:318:ASP:HB2	1:A:336:TYR:CE1	2.55	0.41
2:B:14:HIS:HD2	2:B:127:GLU:OE2	2.04	0.41
2:B:396:MET:HG3	2:B:406:ILE:HD11	2.03	0.41
1:D:64:LEU:CD1	1:D:222:VAL:HG21	2.51	0.41
1:D:78:GLU:HG2	1:D:79:GLY:N	2.35	0.41
2:E:42:VAL:HA	2:E:49:ALA:HB1	2.03	0.41
3:F:34:LEU:HD12	3:F:34:LEU:HA	1.93	0.41
2:H:170:LEU:HB3	2:H:220:PHE:CE1	2.56	0.41
1:J:145:GLY:HA2	1:J:174:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:162:THR:HG22	2:N:164:GLU:N	2.35	0.41
1:P:115:THR:HG21	1:P:151:SER:OG	2.21	0.41
1:S:292:LEU:HB2	1:S:295:VAL:HG22	2.02	0.41
1:V:95:PRO:HG2	2:W:46:MET:HE3	2.03	0.41
1:V:234:ALA:HB1	1:V:236:VAL:HG23	2.03	0.41
1:D:193:ARG:NH2	1:D:201:SER:HB3	2.36	0.41
1:D:318:ASP:CG	1:D:321:ARG:HH12	2.26	0.41
2:E:358:LYS:CB	2:E:360:ILE:HG22	2.51	0.41
1:G:190:ARG:HG3	1:G:190:ARG:HH11	1.84	0.41
1:G:300:PRO:HB3	3:I:37:ILE:HA	2.02	0.41
2:K:52:ILE:HG22	3:L:61:ARG:HB2	2.02	0.41
3:L:76:MET:HB2	3:L:76:MET:HE3	1.82	0.41
1:S:299:ILE:HD13	1:S:299:ILE:HA	1.83	0.41
2:T:250:THR:O	2:T:258:THR:HA	2.20	0.41
1:V:374:VAL:HG21	3:X:40:LEU:HD22	2.03	0.41
1:A:151:SER:O	1:A:155:VAL:HG23	2.22	0.40
1:D:299:ILE:HD13	1:D:299:ILE:HA	1.99	0.40
1:G:98:ALA:HB3	1:G:101:ILE:HG12	2.03	0.40
1:G:437:ALA:C	1:G:438:TRP:CD1	2.99	0.40
1:J:373:LYS:HD3	3:L:45:THR:HB	2.03	0.40
1:M:90:GLU:O	1:M:91:ASN:CB	2.62	0.40
2:N:331:GLU:HA	2:N:334:VAL:HG12	2.03	0.40
1:V:7:LEU:HD21	1:V:161:PRO:HB2	2.03	0.40
1:V:60:ARG:HA	1:V:65:PHE:CG	2.56	0.40
1:V:139:ASP:OD1	1:V:141:GLU:HB2	2.20	0.40
2:W:337:PHE:CE2	2:W:377:LYS:HA	2.56	0.40
2:E:270:TYR:HB2	2:E:272:TYR:CE2	2.57	0.40
2:E:346:TRP:CH2	2:E:390:LYS:HG3	2.56	0.40
1:G:76:LEU:HD23	1:G:94:ALA:HB1	2.03	0.40
1:J:58:LYS:HG2	2:Q:240:GLU:HB3	2.03	0.40
2:K:225:LYS:HA	2:K:225:LYS:HD3	1.91	0.40
2:N:73:HIS:NE2	2:N:103:THR:HB	2.36	0.40
1:P:137:PRO:HB3	1:P:157:VAL:CG1	2.51	0.40
2:Q:36:ASN:O	3:R:71:ARG:CD	2.69	0.40
1:S:176:ALA:HA	1:S:181:VAL:HG12	2.03	0.40
2:T:42:VAL:HA	2:T:49:ALA:HB1	2.03	0.40
1:V:155:VAL:O	1:V:211:ARG:HD2	2.21	0.40
1:A:74:ASN:OD1	1:A:74:ASN:C	2.65	0.40
1:D:185:LYS:HA	1:D:186:PRO:HD3	1.90	0.40
2:H:14:HIS:CD2	2:H:127:GLU:OE2	2.74	0.40
2:K:301:GLN:O	2:K:302:ARG:C	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:52:ILE:HG22	3:O:61:ARG:HB2	2.03	0.40
2:N:215:LYS:HD2	2:N:248:THR:HG21	2.03	0.40
2:N:374:GLU:HB3	2:N:403:PRO:HG2	2.04	0.40
3:R:4:ARG:NH1	3:R:8:LEU:HD11	2.36	0.40
2:T:37:THR:HG23	2:T:38:ASN:H	1.85	0.40
2:T:261:MET:HE3	2:T:261:MET:HB2	1.81	0.40
3:U:88:VAL:O	3:U:89:PRO:C	2.64	0.40
1:V:173:ARG:HB3	1:V:433:SER:HB2	2.02	0.40
1:A:210:GLY:HA3	1:A:216:VAL:HG23	2.03	0.40
1:A:475:ILE:HA	1:A:476:PRO:HD3	1.82	0.40
1:D:162:VAL:HG21	1:D:219:VAL:HG21	2.04	0.40
1:D:337:ALA:HB1	3:F:17:GLU:N	2.36	0.40
1:G:477:LEU:O	1:G:478:THR:C	2.63	0.40
1:J:434:ILE:HA	1:J:435:PRO:HD3	1.91	0.40
3:L:2:VAL:N	3:L:31:SER:HG	2.19	0.40
1:M:155:VAL:O	1:M:211:ARG:HD2	2.20	0.40
1:M:199:PHE:HE2	4:M:905:ASN:HB3	1.87	0.40
2:N:87:ASP:HB3	2:N:133:ASN:OD1	2.21	0.40
2:N:184:LYS:HB2	2:N:191:GLN:OE1	2.21	0.40
2:N:261:MET:HE3	2:N:261:MET:HB2	1.91	0.40
2:N:320:LEU:CD2	2:N:326:VAL:HG12	2.51	0.40
2:N:336:HIS:NE2	2:N:370:GLU:HG3	2.36	0.40
1:P:111:ILE:HD12	1:P:111:ILE:H	1.85	0.40
2:Q:140:THR:OG1	3:R:90:ARG:HA	2.21	0.40
2:W:170:LEU:HD12	2:W:223:VAL:HG21	2.04	0.40
1:A:39:VAL:HG21	1:A:157:VAL:HG11	2.03	0.40
1:A:57:LEU:CD1	1:A:110:LEU:HD21	2.51	0.40
1:A:316:ARG:O	1:A:321:ARG:NH2	2.51	0.40
1:A:351:ARG:NH1	4:A:901:ASN:O	2.50	0.40
1:D:241:TRP:O	1:D:245:VAL:HG22	2.22	0.40
1:D:340:ARG:NH2	3:F:14:ALA:O	2.54	0.40
1:J:167:ASP:HA	1:J:171:SER:HB2	2.04	0.40
2:T:117:LYS:CG	2:T:118:LYS:N	2.84	0.40
2:W:170:LEU:HB3	2:W:220:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/478 (100%)	455 (96%)	20 (4%)	1 (0%)	43	76
1	D	476/478 (100%)	457 (96%)	19 (4%)	0	100	100
1	G	476/478 (100%)	454 (95%)	21 (4%)	1 (0%)	43	76
1	J	476/478 (100%)	458 (96%)	17 (4%)	1 (0%)	43	76
1	M	476/478 (100%)	454 (95%)	22 (5%)	0	100	100
1	P	476/478 (100%)	455 (96%)	21 (4%)	0	100	100
1	S	476/478 (100%)	458 (96%)	18 (4%)	0	100	100
1	V	476/478 (100%)	458 (96%)	18 (4%)	0	100	100
2	B	408/478 (85%)	388 (95%)	19 (5%)	1 (0%)	43	76
2	E	408/478 (85%)	381 (93%)	27 (7%)	0	100	100
2	H	408/478 (85%)	385 (94%)	23 (6%)	0	100	100
2	K	408/478 (85%)	381 (93%)	27 (7%)	0	100	100
2	N	408/478 (85%)	388 (95%)	20 (5%)	0	100	100
2	Q	408/478 (85%)	383 (94%)	24 (6%)	1 (0%)	43	76
2	T	408/478 (85%)	375 (92%)	32 (8%)	1 (0%)	43	76
2	W	408/478 (85%)	388 (95%)	19 (5%)	1 (0%)	43	76
3	C	89/94 (95%)	82 (92%)	7 (8%)	0	100	100
3	F	89/94 (95%)	84 (94%)	5 (6%)	0	100	100
3	I	89/94 (95%)	80 (90%)	8 (9%)	1 (1%)	11	43
3	L	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	O	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	R	89/94 (95%)	82 (92%)	7 (8%)	0	100	100
3	U	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
3	X	89/94 (95%)	78 (88%)	10 (11%)	1 (1%)	11	43
All	All	7784/8400 (93%)	7379 (95%)	396 (5%)	9 (0%)	48	80

All (9) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/406 (100%)	378 (93%)	28 (7%)	14	45
1	D	406/406 (100%)	374 (92%)	32 (8%)	11	39
1	G	406/406 (100%)	384 (95%)	22 (5%)	20	53
1	J	406/406 (100%)	375 (92%)	31 (8%)	12	41
1	M	406/406 (100%)	382 (94%)	24 (6%)	18	50
1	P	406/406 (100%)	372 (92%)	34 (8%)	10	37
1	S	406/406 (100%)	372 (92%)	34 (8%)	10	37
1	V	406/406 (100%)	376 (93%)	30 (7%)	13	42
2	B	364/427 (85%)	335 (92%)	29 (8%)	11	38
2	E	364/427 (85%)	340 (93%)	24 (7%)	15	46
2	H	364/427 (85%)	344 (94%)	20 (6%)	19	53
2	K	364/427 (85%)	341 (94%)	23 (6%)	16	48
2	N	364/427 (85%)	333 (92%)	31 (8%)	10	36
2	Q	364/427 (85%)	339 (93%)	25 (7%)	14	45
2	T	364/427 (85%)	340 (93%)	24 (7%)	15	46
2	W	364/427 (85%)	338 (93%)	26 (7%)	13	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	86/89 (97%)	81 (94%)	5 (6%)	18	51
3	F	86/89 (97%)	81 (94%)	5 (6%)	18	51
3	I	86/89 (97%)	80 (93%)	6 (7%)	14	44
3	L	86/89 (97%)	81 (94%)	5 (6%)	18	51
3	O	86/89 (97%)	80 (93%)	6 (7%)	14	44
3	R	86/89 (97%)	81 (94%)	5 (6%)	18	51
3	U	86/89 (97%)	81 (94%)	5 (6%)	18	51
3	X	86/89 (97%)	80 (93%)	6 (7%)	14	44
All	All	6848/7376 (93%)	6368 (93%)	480 (7%)	14	44

All (480) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	51	LEU
1	A	57	LEU
1	A	62	LEU
1	A	69	ILE
1	A	78	GLU
1	A	88	ILE
1	A	89	LEU
1	A	112	VAL
1	A	115	THR
1	A	143	VAL
1	A	158	LEU
1	A	174	GLN
1	A	181	VAL
1	A	190	ARG
1	A	199	PHE
1	A	205	GLN
1	A	224	SER
1	A	228	GLU
1	A	245	VAL
1	A	295	VAL
1	A	299	ILE
1	A	332	ILE
1	A	356	THR
1	A	389	VAL
1	A	417	SER

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Mol	Chain	Res	Type
1	A	434	ILE
1	A	478	THR
2	B	21	THR
2	B	39	VAL
2	B	74	GLU
2	B	98	GLU
2	B	103	THR
2	B	113	ASN
2	B	115	GLU
2	B	134	ILE
2	B	156	THR
2	B	162	THR
2	B	171	GLU
2	B	200	ILE
2	B	201	ARG
2	B	203	LYS
2	B	205	SER
2	B	207	GLU
2	B	213	GLU
2	B	246	GLN
2	B	250	THR
2	B	302	ARG
2	B	308	LYS
2	B	320	LEU
2	B	344	VAL
2	B	360	ILE
2	B	365	SER
2	B	395	GLU
2	B	402	THR
2	B	406	ILE
2	B	407	VAL
3	C	38	ASP
3	C	52	ILE
3	C	56	GLU
3	C	70	ASP
3	C	92	VAL
1	D	10	LEU
1	D	11	ARG
1	D	15	LYS
1	D	26	GLU
1	D	37	GLU
1	D	51	LEU

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Mol	Chain	Res	Type
1	D	57	LEU
1	D	61	GLU
1	D	62	LEU
1	D	67	ILE
1	D	88	ILE
1	D	89	LEU
1	D	143	VAL
1	D	164	LEU
1	D	174	GLN
1	D	181	VAL
1	D	199	PHE
1	D	238	VAL
1	D	240	GLU
1	D	245	VAL
1	D	295	VAL
1	D	325	ARG
1	D	356	THR
1	D	384	LYS
1	D	389	VAL
1	D	392	ILE
1	D	397	THR
1	D	417	SER
1	D	434	ILE
1	D	458	LEU
1	D	477	LEU
1	D	478	THR
2	E	8	VAL
2	E	21	THR
2	E	39	VAL
2	E	74	GLU
2	E	98	GLU
2	E	109	LEU
2	E	113	ASN
2	E	156	THR
2	E	205	SER
2	E	228	GLU
2	E	244	VAL
2	E	250	THR
2	E	321	VAL
2	E	335	ARG
2	E	341	LYS
2	E	344	VAL

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Mol	Chain	Res	Type
2	E	352	LEU
2	E	360	ILE
2	E	370	GLU
2	E	394	LYS
2	E	402	THR
2	E	406	ILE
2	E	407	VAL
2	E	412	LEU
3	F	34	LEU
3	F	52	ILE
3	F	61	ARG
3	F	70	ASP
3	F	92	VAL
1	G	7	LEU
1	G	10	LEU
1	G	51	LEU
1	G	56	SER
1	G	57	LEU
1	G	59	GLU
1	G	62	LEU
1	G	89	LEU
1	G	102	GLU
1	G	115	THR
1	G	117	LEU
1	G	199	PHE
1	G	233	SER
1	G	245	VAL
1	G	279	GLU
1	G	325	ARG
1	G	397	THR
1	G	434	ILE
1	G	458	LEU
1	G	474	LYS
1	G	477	LEU
1	G	478	THR
2	H	4	LYS
2	H	21	THR
2	H	39	VAL
2	H	98	GLU
2	H	115	GLU
2	H	134	ILE
2	H	162	THR

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Mol	Chain	Res	Type
2	H	203	LYS
2	H	216	ASN
2	H	225	LYS
2	H	244	VAL
2	H	282	LYS
2	H	344	VAL
2	H	352	LEU
2	H	360	ILE
2	H	391	GLU
2	H	395	GLU
2	H	402	THR
2	H	407	VAL
2	H	412	LEU
3	I	5	GLU
3	I	34	LEU
3	I	38	ASP
3	I	52	ILE
3	I	81	ARG
3	I	92	VAL
1	J	8	SER
1	J	10	LEU
1	J	51	LEU
1	J	56	SER
1	J	57	LEU
1	J	62	LEU
1	J	88	ILE
1	J	89	LEU
1	J	112	VAL
1	J	115	THR
1	J	140	LEU
1	J	151	SER
1	J	162	VAL
1	J	174	GLN
1	J	181	VAL
1	J	185	LYS
1	J	199	PHE
1	J	214	GLU
1	J	233	SER
1	J	240	GLU
1	J	245	VAL
1	J	246	LYS
1	J	271	GLU

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Mol	Chain	Res	Type
1	J	279	GLU
1	J	295	VAL
1	J	328	GLU
1	J	356	THR
1	J	376	ARG
1	J	434	ILE
1	J	458	LEU
1	J	477	LEU
2	K	21	THR
2	K	39	VAL
2	K	74	GLU
2	K	98	GLU
2	K	103	THR
2	K	109	LEU
2	K	113	ASN
2	K	115	GLU
2	K	116	LYS
2	K	134	ILE
2	K	156	THR
2	K	184	LYS
2	K	207	GLU
2	K	216	ASN
2	K	223	VAL
2	K	244	VAL
2	K	250	THR
2	K	266	GLU
2	K	341	LYS
2	K	344	VAL
2	K	352	LEU
2	K	360	ILE
2	K	412	LEU
3	L	34	LEU
3	L	42	GLU
3	L	52	ILE
3	L	70	ASP
3	L	92	VAL
1	M	7	LEU
1	M	10	LEU
1	M	51	LEU
1	M	57	LEU
1	M	58	LYS
1	M	62	LEU

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Mol	Chain	Res	Type
1	M	76	LEU
1	M	78	GLU
1	M	88	ILE
1	M	89	LEU
1	M	112	VAL
1	M	115	THR
1	M	174	GLN
1	M	199	PHE
1	M	245	VAL
1	M	279	GLU
1	M	325	ARG
1	M	328	GLU
1	M	356	THR
1	M	417	SER
1	M	434	ILE
1	M	458	LEU
1	M	477	LEU
1	M	478	THR
2	N	4	LYS
2	N	21	THR
2	N	39	VAL
2	N	74	GLU
2	N	95	SER
2	N	98	GLU
2	N	103	THR
2	N	113	ASN
2	N	115	GLU
2	N	116	LYS
2	N	118	LYS
2	N	134	ILE
2	N	156	THR
2	N	162	THR
2	N	164	GLU
2	N	168	LEU
2	N	203	LYS
2	N	212	VAL
2	N	244	VAL
2	N	250	THR
2	N	255	THR
2	N	261	MET
2	N	302	ARG
2	N	344	VAL

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Mol	Chain	Res	Type
2	N	360	ILE
2	N	387	LYS
2	N	391	GLU
2	N	395	GLU
2	N	402	THR
2	N	407	VAL
2	N	412	LEU
3	O	34	LEU
3	O	38	ASP
3	O	46	GLU
3	O	52	ILE
3	O	53	GLN
3	O	81	ARG
1	P	10	LEU
1	P	51	LEU
1	P	56	SER
1	P	57	LEU
1	P	58	LYS
1	P	59	GLU
1	P	62	LEU
1	P	69	ILE
1	P	78	GLU
1	P	88	ILE
1	P	89	LEU
1	P	115	THR
1	P	143	VAL
1	P	162	VAL
1	P	164	LEU
1	P	174	GLN
1	P	181	VAL
1	P	190	ARG
1	P	199	PHE
1	P	231	SER
1	P	233	SER
1	P	240	GLU
1	P	245	VAL
1	P	279	GLU
1	P	291	SER
1	P	295	VAL
1	P	299	ILE
1	P	325	ARG
1	P	328	GLU

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Mol	Chain	Res	Type
1	P	356	THR
1	P	434	ILE
1	P	458	LEU
1	P	477	LEU
1	P	478	THR
2	Q	4	LYS
2	Q	21	THR
2	Q	39	VAL
2	Q	98	GLU
2	Q	103	THR
2	Q	109	LEU
2	Q	156	THR
2	Q	188	GLU
2	Q	207	GLU
2	Q	210	THR
2	Q	216	ASN
2	Q	223	VAL
2	Q	240	GLU
2	Q	244	VAL
2	Q	245	VAL
2	Q	255	THR
2	Q	282	LYS
2	Q	309	GLU
2	Q	313	SER
2	Q	344	VAL
2	Q	352	LEU
2	Q	360	ILE
2	Q	402	THR
2	Q	405	GLN
2	Q	407	VAL
3	R	34	LEU
3	R	52	ILE
3	R	66	HIS
3	R	81	ARG
3	R	92	VAL
1	S	9	GLU
1	S	10	LEU
1	S	11	ARG
1	S	13	LEU
1	S	51	LEU
1	S	56	SER
1	S	57	LEU

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Mol	Chain	Res	Type
1	S	61	GLU
1	S	62	LEU
1	S	67	ILE
1	S	69	ILE
1	S	88	ILE
1	S	89	LEU
1	S	114	LYS
1	S	140	LEU
1	S	143	VAL
1	S	181	VAL
1	S	199	PHE
1	S	228	GLU
1	S	240	GLU
1	S	242	SER
1	S	245	VAL
1	S	295	VAL
1	S	325	ARG
1	S	356	THR
1	S	376	ARG
1	S	389	VAL
1	S	397	THR
1	S	409	GLU
1	S	412	ILE
1	S	434	ILE
1	S	458	LEU
1	S	464	LEU
1	S	477	LEU
2	T	21	THR
2	T	39	VAL
2	T	74	GLU
2	T	98	GLU
2	T	103	THR
2	T	113	ASN
2	T	115	GLU
2	T	123	ARG
2	T	162	THR
2	T	164	GLU
2	T	189	LYS
2	T	216	ASN
2	T	244	VAL
2	T	250	THR
2	T	321	VAL

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Mol	Chain	Res	Type
2	T	335	ARG
2	T	341	LYS
2	T	344	VAL
2	T	360	ILE
2	T	387	LYS
2	T	394	LYS
2	T	402	THR
2	T	406	ILE
2	T	412	LEU
3	U	5	GLU
3	U	34	LEU
3	U	56	GLU
3	U	70	ASP
3	U	81	ARG
1	V	10	LEU
1	V	11	ARG
1	V	19	VAL
1	V	51	LEU
1	V	53	GLN
1	V	57	LEU
1	V	62	LEU
1	V	69	ILE
1	V	76	LEU
1	V	88	ILE
1	V	89	LEU
1	V	115	THR
1	V	143	VAL
1	V	151	SER
1	V	164	LEU
1	V	174	GLN
1	V	181	VAL
1	V	190	ARG
1	V	224	SER
1	V	233	SER
1	V	245	VAL
1	V	270	LYS
1	V	279	GLU
1	V	295	VAL
1	V	354	LEU
1	V	417	SER
1	V	434	ILE
1	V	458	LEU

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Mol	Chain	Res	Type
1	V	477	LEU
1	V	478	THR
2	W	21	THR
2	W	39	VAL
2	W	46	MET
2	W	74	GLU
2	W	98	GLU
2	W	103	THR
2	W	109	LEU
2	W	117	LYS
2	W	123	ARG
2	W	134	ILE
2	W	156	THR
2	W	200	ILE
2	W	201	ARG
2	W	203	LYS
2	W	205	SER
2	W	244	VAL
2	W	245	VAL
2	W	250	THR
2	W	335	ARG
2	W	344	VAL
2	W	352	LEU
2	W	360	ILE
2	W	364	GLU
2	W	402	THR
2	W	406	ILE
2	W	407	VAL
3	X	38	ASP
3	X	52	ILE
3	X	54	GLU
3	X	56	GLU
3	X	91	VAL
3	X	92	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
2	B	216	ASN
2	B	371	HIS
1	D	467	GLN

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Mol	Chain	Res	Type
2	E	38	ASN
2	E	216	ASN
2	H	133	ASN
2	H	135	HIS
3	I	53	GLN
2	K	216	ASN
2	K	322	ASN
2	K	405	GLN
1	M	53	GLN
1	M	275	ASN
1	M	467	GLN
2	N	113	ASN
2	N	216	ASN
2	N	294	ASN
2	N	323	HIS
2	N	349	ASN
2	N	405	GLN
3	O	53	GLN
1	P	53	GLN
1	P	174	GLN
2	Q	216	ASN
2	Q	301	GLN
3	R	27	GLN
3	R	53	GLN
2	T	110	ASN
2	T	216	ASN
2	T	218	ASN
2	T	405	GLN
1	V	34	GLN
1	V	91	ASN
1	V	460	GLN
2	W	216	ASN
2	W	218	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	ADP	B	479	-	28,29,29	1.46	6 (21%)	43,45,45	2.00	12 (27%)
8	ATP	N	479	-	32,33,33	1.54	7 (21%)	48,52,52	1.73	10 (20%)
4	ASN	J	904	1	6,7,8	1.06	0	3,8,10	2.82	1 (33%)
4	ASN	G	903	1	6,7,8	1.26	1 (16%)	3,8,10	2.36	1 (33%)
9	ASP	H	482	7	7,8,8	1.10	1 (14%)	6,10,10	1.89	1 (16%)
8	ATP	K	479	-	32,33,33	1.45	5 (15%)	48,52,52	1.72	8 (16%)
6	ADP	T	479	-	28,29,29	1.44	7 (25%)	43,45,45	1.90	10 (23%)
4	ASN	D	902	1	6,7,8	1.24	1 (16%)	3,8,10	2.81	2 (66%)
4	ASN	V	908	1	6,7,8	1.25	1 (16%)	3,8,10	2.69	2 (66%)
8	ATP	W	479	-	32,33,33	1.60	6 (18%)	48,52,52	2.29	17 (35%)
8	ATP	H	479	-	32,33,33	1.66	7 (21%)	48,52,52	1.81	9 (18%)
4	ASN	P	906	1	6,7,8	1.07	1 (16%)	3,8,10	1.92	1 (33%)
4	ASN	S	907	1	6,7,8	1.22	1 (16%)	3,8,10	2.31	1 (33%)
8	ATP	E	479	-	32,33,33	1.50	8 (25%)	48,52,52	1.88	9 (18%)
9	ASP	N	482	-	7,8,8	1.43	1 (14%)	6,10,10	1.25	1 (16%)
8	ATP	Q	479	-	32,33,33	1.44	5 (15%)	48,52,52	1.88	8 (16%)
4	ASN	A	901	1	6,7,8	1.35	1 (16%)	3,8,10	2.43	2 (66%)
4	ASN	M	905	1	6,7,8	1.16	1 (16%)	3,8,10	2.21	2 (66%)

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
6	ADP	B	479	-	-	0/16/32/32	0/3/3/3
8	ATP	N	479	-	-	8/22/38/38	0/3/3/3
4	ASN	J	904	1	-	1/7/7/8	-
4	ASN	G	903	1	-	0/7/7/8	-
9	ASP	H	482	7	-	6/8/8/8	-
8	ATP	K	479	-	-	4/22/38/38	0/3/3/3
6	ADP	T	479	-	-	5/16/32/32	0/3/3/3
4	ASN	D	902	1	-	3/7/7/8	-
4	ASN	V	908	1	-	4/7/7/8	-
8	ATP	W	479	-	-	6/22/38/38	0/3/3/3
8	ATP	H	479	-	-	5/22/38/38	0/3/3/3
4	ASN	P	906	1	-	1/7/7/8	-
4	ASN	S	907	1	-	4/7/7/8	-
8	ATP	E	479	-	-	5/22/38/38	0/3/3/3
9	ASP	N	482	-	-	3/8/8/8	-
8	ATP	Q	479	-	-	4/22/38/38	0/3/3/3
4	ASN	A	901	1	-	2/7/7/8	-
4	ASN	M	905	1	-	1/7/7/8	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	479	ATP	C5-C4	4.91	1.47	1.39
8	H	479	ATP	C5-C4	4.47	1.47	1.39
8	K	479	ATP	C5-C4	4.36	1.46	1.39
6	T	479	ADP	C5-C4	4.08	1.46	1.39
8	E	479	ATP	C5-C4	4.05	1.46	1.39
6	B	479	ADP	C5-C4	4.00	1.46	1.39
8	W	479	ATP	C5-C4	3.98	1.46	1.39
8	H	479	ATP	PA-O3A	3.97	1.63	1.59
8	Q	479	ATP	C5-C4	3.92	1.46	1.39
8	K	479	ATP	C5-N7	-3.32	1.33	1.39
8	H	479	ATP	PB-O3A	3.25	1.63	1.59
8	H	479	ATP	C5-N7	-3.24	1.33	1.39
8	Q	479	ATP	C5-N7	-3.20	1.33	1.39
8	W	479	ATP	PA-O3A	3.15	1.62	1.59
6	T	479	ADP	C5-N7	-3.06	1.33	1.39
8	W	479	ATP	C5-N7	-2.96	1.33	1.39
8	K	479	ATP	PB-O3B	2.93	1.62	1.59
8	E	479	ATP	C5-N7	-2.91	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	479	ATP	PA-O3A	2.90	1.62	1.59
8	K	479	ATP	C8-N7	2.87	1.37	1.31
4	G	903	ASN	OXT-C	-2.85	1.21	1.30
4	A	901	ASN	OXT-C	-2.83	1.21	1.30
4	V	908	ASN	OXT-C	-2.83	1.21	1.30
4	S	907	ASN	OXT-C	-2.81	1.21	1.30
6	B	479	ADP	C5-N7	-2.77	1.34	1.39
8	E	479	ATP	PB-O3A	2.75	1.62	1.59
8	N	479	ATP	PB-O3A	2.74	1.62	1.59
4	D	902	ASN	OXT-C	-2.67	1.22	1.30
6	B	479	ADP	C4-N9	-2.64	1.32	1.37
8	N	479	ATP	C5-N7	-2.63	1.34	1.39
8	N	479	ATP	C4-N9	-2.62	1.32	1.37
8	W	479	ATP	C5-C6	2.62	1.48	1.41
8	Q	479	ATP	PB-O3B	2.61	1.62	1.59
8	W	479	ATP	PB-O3B	2.61	1.62	1.59
6	B	479	ADP	C5-C6	2.59	1.48	1.41
4	M	905	ASN	OXT-C	-2.54	1.22	1.30
8	E	479	ATP	C5-C6	2.48	1.47	1.41
8	H	479	ATP	C5-C6	2.47	1.47	1.41
6	T	479	ADP	C5-C6	2.47	1.47	1.41
8	N	479	ATP	C5-C6	2.43	1.47	1.41
6	T	479	ADP	PA-O3A	2.37	1.62	1.59
8	N	479	ATP	C8-N7	2.36	1.36	1.31
4	P	906	ASN	OXT-C	-2.35	1.23	1.30
6	B	479	ADP	C8-N9	-2.34	1.33	1.37
8	Q	479	ATP	C4-N9	-2.32	1.32	1.37
8	K	479	ATP	C4-N9	-2.32	1.32	1.37
6	T	479	ADP	C4-N9	-2.30	1.32	1.37
8	H	479	ATP	C8-N7	2.25	1.36	1.31
9	N	482	ASP	OXT-C	-2.25	1.23	1.30
8	Q	479	ATP	C8-N7	2.21	1.35	1.31
8	E	479	ATP	PB-O3B	2.14	1.61	1.59
6	T	479	ADP	C8-N7	2.12	1.35	1.31
9	H	482	ASP	OXT-C	-2.12	1.23	1.30
8	E	479	ATP	C8-N7	2.11	1.35	1.31
8	N	479	ATP	PB-O3B	2.10	1.61	1.59
8	E	479	ATP	C8-N9	-2.09	1.34	1.37
8	W	479	ATP	C4-N9	-2.09	1.33	1.37
6	T	479	ADP	C8-N9	-2.06	1.34	1.37
8	H	479	ATP	C4-N9	-2.04	1.33	1.37
6	B	479	ADP	PA-O3A	2.01	1.61	1.59

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	479	ATP	C5-C4-N3	-6.83	117.31	126.72
8	E	479	ATP	C5-C4-N3	-6.79	117.37	126.72
6	T	479	ADP	C5-C4-N3	-6.21	118.17	126.72
8	H	479	ATP	C5-C4-N3	-5.86	118.65	126.72
8	K	479	ATP	C5-C4-N3	-5.76	118.79	126.72
8	Q	479	ATP	C5-C4-N3	-5.75	118.80	126.72
6	B	479	ADP	C5-C4-N3	-5.51	119.12	126.72
8	W	479	ATP	N3-C4-N9	5.15	135.93	127.17
8	N	479	ATP	C5-C4-N3	-5.12	119.67	126.72
8	E	479	ATP	N3-C4-N9	4.93	135.54	127.17
4	J	904	ASN	OXT-C-O	-4.53	113.81	124.08
6	T	479	ADP	N3-C4-N9	4.50	134.81	127.17
6	B	479	ADP	N3-C4-N9	4.46	134.76	127.17
8	Q	479	ATP	N3-C4-N9	4.45	134.73	127.17
8	W	479	ATP	O3'-C3'-C4'	-4.40	98.44	111.08
8	Q	479	ATP	N3-C2-N1	-4.34	122.01	128.58
8	Q	479	ATP	O4'-C1'-N9	4.28	116.31	108.09
8	E	479	ATP	C4-C5-N7	-4.28	105.69	110.58
8	Q	479	ATP	C2-N3-C4	4.26	122.23	111.83
8	H	479	ATP	N3-C4-N9	4.13	134.19	127.17
8	N	479	ATP	N3-C4-N9	4.06	134.07	127.17
8	E	479	ATP	C2-N3-C4	4.06	121.73	111.83
6	B	479	ADP	C4-C5-N7	-4.05	105.95	110.58
8	W	479	ATP	C2-N3-C4	4.05	121.72	111.83
8	K	479	ATP	N3-C4-N9	4.05	134.06	127.17
6	T	479	ADP	C4-C5-N7	-3.96	106.05	110.58
4	D	902	ASN	OXT-C-O	-3.96	115.10	124.08
8	W	479	ATP	C4-C5-N7	-3.94	106.07	110.58
6	T	479	ADP	C2-N3-C4	3.79	121.10	111.83
8	K	479	ATP	C2-N3-C4	3.76	121.01	111.83
6	B	479	ADP	C4-N9-C8	3.70	109.63	105.74
8	H	479	ATP	C2-N3-C4	3.70	120.87	111.83
8	W	479	ATP	O3G-PG-O3B	-3.70	92.23	104.64
9	H	482	ASP	OXT-C-O	-3.70	115.69	124.08
4	G	903	ASN	OXT-C-O	-3.65	115.80	124.08
8	K	479	ATP	N3-C2-N1	-3.59	123.15	128.58
4	S	907	ASN	OXT-C-O	-3.53	116.06	124.08
4	A	901	ASN	OXT-C-O	-3.49	116.17	124.08
6	B	479	ADP	C2-N3-C4	3.49	120.34	111.83
4	V	908	ASN	OXT-C-O	-3.47	116.22	124.08
8	H	479	ATP	O3G-PG-O2G	3.42	120.64	107.80
8	W	479	ATP	O3'-C3'-C2'	-3.37	101.02	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	479	ATP	N3-C2-N1	-3.31	123.56	128.58
8	N	479	ATP	C2-N3-C4	3.31	119.92	111.83
8	H	479	ATP	N3-C2-N1	-3.23	123.69	128.58
6	T	479	ADP	N3-C2-N1	-3.21	123.72	128.58
8	K	479	ATP	C4-C5-N7	-3.20	106.92	110.58
8	E	479	ATP	C5-N7-C8	3.19	108.46	103.45
6	B	479	ADP	C5-N7-C8	3.16	108.41	103.45
6	B	479	ADP	N3-C2-N1	-3.11	123.87	128.58
8	W	479	ATP	C5-N7-C8	3.06	108.26	103.45
4	V	908	ASN	OD1-CG-CB	-3.06	116.47	125.38
8	H	479	ATP	C4-C5-N7	-3.03	107.12	110.58
8	N	479	ATP	N3-C2-N1	-2.99	124.06	128.58
8	W	479	ATP	N3-C2-N1	-2.96	124.10	128.58
4	M	905	ASN	OXT-C-O	-2.94	117.42	124.08
6	T	479	ADP	C5-N7-C8	2.85	107.94	103.45
8	N	479	ATP	C4-C5-N7	-2.85	107.32	110.58
9	N	482	ASP	OXT-C-O	-2.85	117.61	124.08
6	B	479	ADP	N9-C8-N7	-2.85	109.89	113.94
4	D	902	ASN	OD1-CG-CB	-2.83	117.15	125.38
4	P	906	ASN	OXT-C-O	-2.83	117.67	124.08
8	W	479	ATP	O2'-C2'-C1'	-2.82	100.40	110.10
8	W	479	ATP	C2'-C3'-C4'	2.70	107.83	102.61
8	H	479	ATP	O3A-PA-O1A	-2.68	102.66	110.70
8	W	479	ATP	O4'-C1'-N9	2.59	113.06	108.09
8	N	479	ATP	O3'-C3'-C4'	-2.57	103.69	111.08
8	Q	479	ATP	C4-C5-N7	-2.51	107.71	110.58
8	N	479	ATP	C4-N9-C8	2.45	108.31	105.74
8	W	479	ATP	C4-N9-C8	2.44	108.31	105.74
6	T	479	ADP	C5'-C4'-C3'	-2.38	106.63	115.21
6	B	479	ADP	O3'-C3'-C4'	-2.38	104.25	111.08
8	W	479	ATP	O2B-PB-O1B	2.37	123.49	112.44
8	W	479	ATP	N9-C8-N7	-2.36	110.59	113.94
8	K	479	ATP	C2'-C3'-C4'	2.35	107.15	102.61
8	E	479	ATP	N9-C8-N7	-2.33	110.63	113.94
4	M	905	ASN	OD1-CG-CB	-2.33	118.59	125.38
4	A	901	ASN	OD1-CG-CB	-2.32	118.61	125.38
6	B	479	ADP	C6-C5-N7	2.32	136.56	132.09
8	W	479	ATP	O3G-PG-O1G	2.31	119.85	110.83
8	E	479	ATP	C4-N9-C8	2.29	108.14	105.74
6	T	479	ADP	C4-N9-C8	2.24	108.09	105.74
8	W	479	ATP	O3G-PG-O2G	2.22	116.11	107.80
6	B	479	ADP	O3'-C3'-C2'	-2.21	104.75	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	479	ADP	O3B-PB-O2B	2.18	115.97	107.80
8	K	479	ATP	C5-N7-C8	2.17	106.86	103.45
8	N	479	ATP	O4'-C1'-N9	2.15	112.21	108.09
6	T	479	ADP	N9-C8-N7	-2.14	110.89	113.94
8	K	479	ATP	C2-N1-C6	2.12	122.21	118.73
6	T	479	ADP	O3B-PB-O2B	2.11	115.71	107.80
8	H	479	ATP	O2A-PA-O1A	2.10	122.23	112.44
8	Q	479	ATP	C2'-C1'-N9	-2.09	108.11	113.30
8	N	479	ATP	C6-C5-N7	2.09	136.12	132.09
8	E	479	ATP	O3G-PG-O2G	2.06	115.54	107.80
8	N	479	ATP	O3B-PB-O1B	-2.05	104.53	110.70
8	H	479	ATP	C5-N7-C8	2.04	106.65	103.45
8	Q	479	ATP	C2-N1-C6	2.04	122.07	118.73

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	902	ASN	O-C-CA-N
4	S	907	ASN	O-C-CA-N
4	S	907	ASN	C-CA-CB-CG
4	V	908	ASN	O-C-CA-N
4	V	908	ASN	C-CA-CB-CG
6	T	479	ADP	C5'-O5'-PA-O1A
6	T	479	ADP	C5'-O5'-PA-O2A
6	T	479	ADP	O4'-C4'-C5'-O5'
8	K	479	ATP	C5'-O5'-PA-O2A
8	N	479	ATP	PB-O3B-PG-O2G
8	N	479	ATP	PB-O3B-PG-O3G
8	N	479	ATP	PB-O3A-PA-O5'
8	N	479	ATP	O4'-C4'-C5'-O5'
8	W	479	ATP	PB-O3B-PG-O2G
8	W	479	ATP	PB-O3B-PG-O3G
8	W	479	ATP	O4'-C4'-C5'-O5'
9	H	482	ASP	O-C-CA-N
6	T	479	ADP	C3'-C4'-C5'-O5'
8	N	479	ATP	C3'-C4'-C5'-O5'
4	D	902	ASN	OXT-C-CA-N
4	S	907	ASN	OXT-C-CA-N
4	V	908	ASN	OXT-C-CA-N
9	H	482	ASP	OXT-C-CA-N
8	W	479	ATP	C3'-C4'-C5'-O5'

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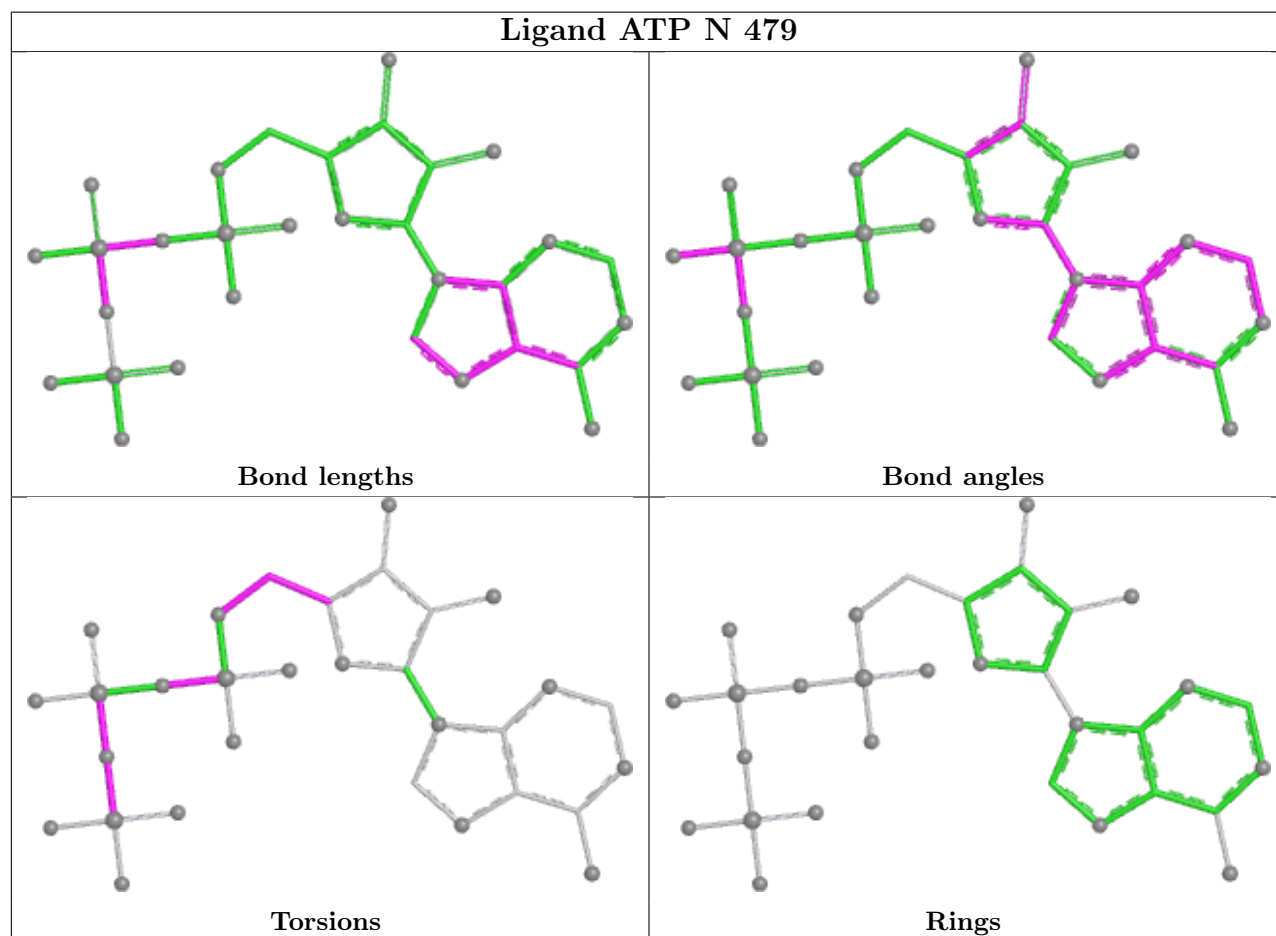
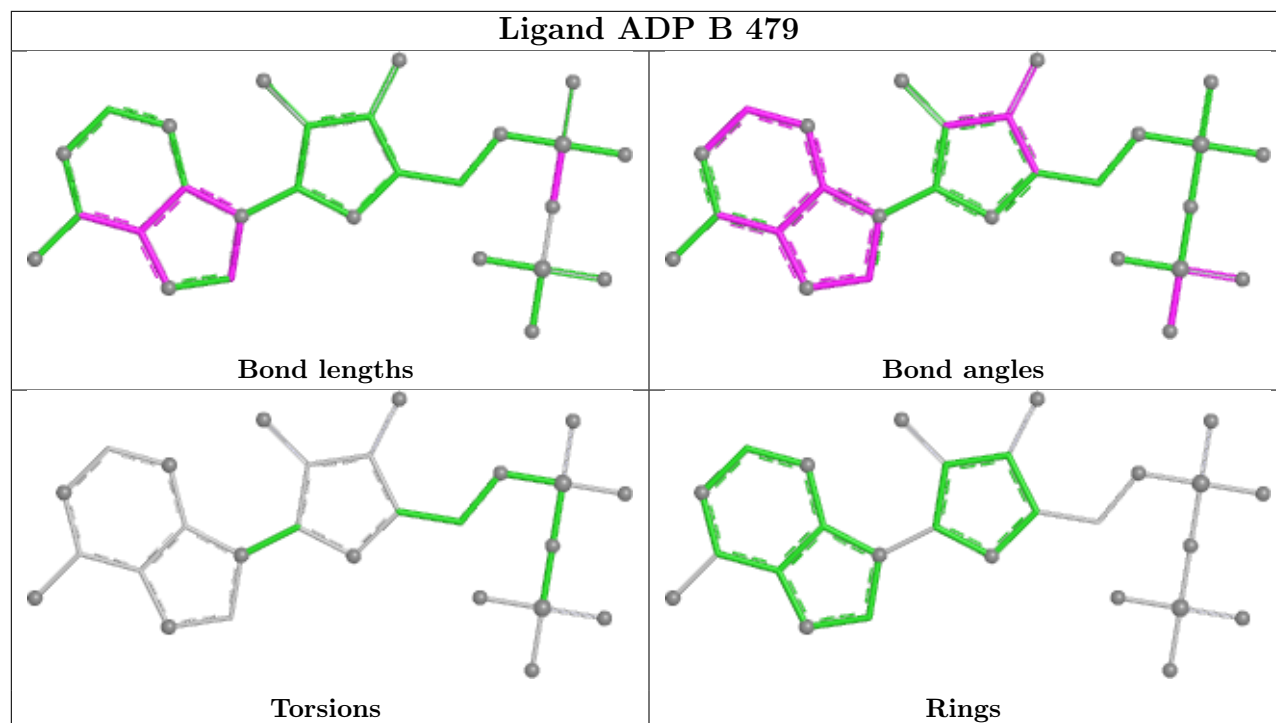
Mol	Chain	Res	Type	Atoms
9	H	482	ASP	CA-CB-CG-OD1
9	H	482	ASP	CA-CB-CG-OD2
4	S	907	ASN	N-CA-CB-CG
4	V	908	ASN	N-CA-CB-CG
8	K	479	ATP	O4'-C4'-C5'-O5'
8	H	479	ATP	PB-O3B-PG-O1G
8	E	479	ATP	PG-O3B-PB-O1B
8	W	479	ATP	PB-O3A-PA-O2A
4	A	901	ASN	O-C-CA-CB
9	H	482	ASP	OXT-C-CA-CB
4	D	902	ASN	CA-CB-CG-OD1
4	J	904	ASN	CA-CB-CG-OD1
4	M	905	ASN	CA-CB-CG-OD1
6	T	479	ADP	C5'-O5'-PA-O3A
8	E	479	ATP	C5'-O5'-PA-O1A
8	K	479	ATP	C5'-O5'-PA-O1A
8	K	479	ATP	C5'-O5'-PA-O3A
8	Q	479	ATP	C5'-O5'-PA-O1A
8	Q	479	ATP	C5'-O5'-PA-O2A
8	Q	479	ATP	C5'-O5'-PA-O3A
9	H	482	ASP	O-C-CA-CB
9	N	482	ASP	C-CA-CB-CG
4	A	901	ASN	OXT-C-CA-CB
8	H	479	ATP	PB-O3A-PA-O2A
8	N	479	ATP	C4'-C5'-O5'-PA
8	E	479	ATP	PA-O3A-PB-O3B
8	H	479	ATP	PB-O3B-PG-O2G
8	Q	479	ATP	PB-O3B-PG-O3G
8	E	479	ATP	PG-O3B-PB-O2B
8	E	479	ATP	PA-O3A-PB-O1B
8	H	479	ATP	PB-O3A-PA-O1A
8	N	479	ATP	PB-O3B-PG-O1G
8	H	479	ATP	O4'-C4'-C5'-O5'
4	P	906	ASN	OXT-C-CA-N
9	N	482	ASP	OXT-C-CA-N
9	N	482	ASP	O-C-CA-N
8	N	479	ATP	PG-O3B-PB-O1B
8	W	479	ATP	PB-O3A-PA-O1A

There are no ring outliers.

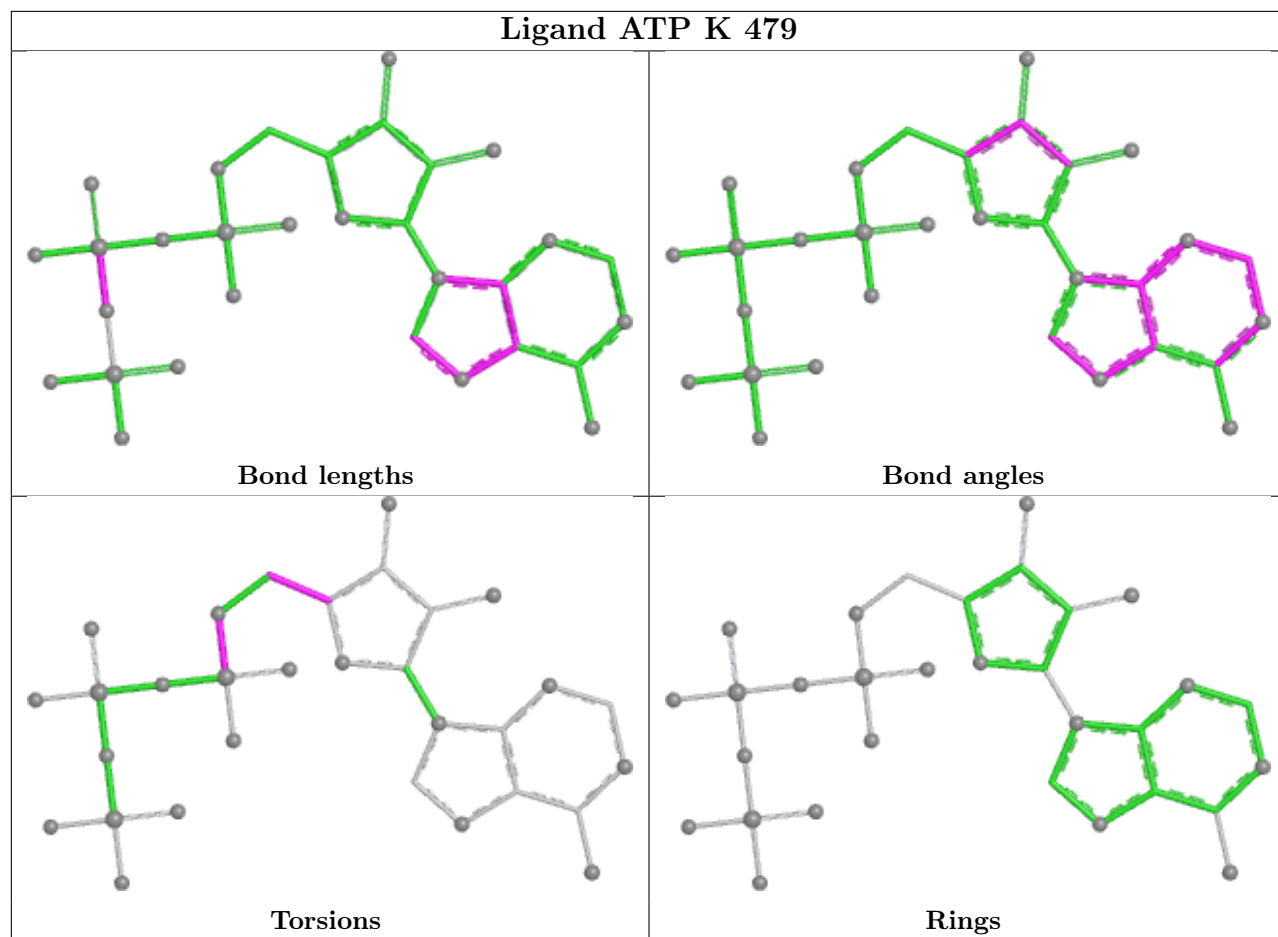
15 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	479	ATP	1	0
9	H	482	ASP	6	0
8	K	479	ATP	1	0
6	T	479	ADP	2	0
4	D	902	ASN	5	0
4	V	908	ASN	4	0
8	W	479	ATP	1	0
8	H	479	ATP	5	0
4	P	906	ASN	1	0
4	S	907	ASN	4	0
8	E	479	ATP	1	0
9	N	482	ASP	5	0
8	Q	479	ATP	1	0
4	A	901	ASN	1	0
4	M	905	ASN	1	0

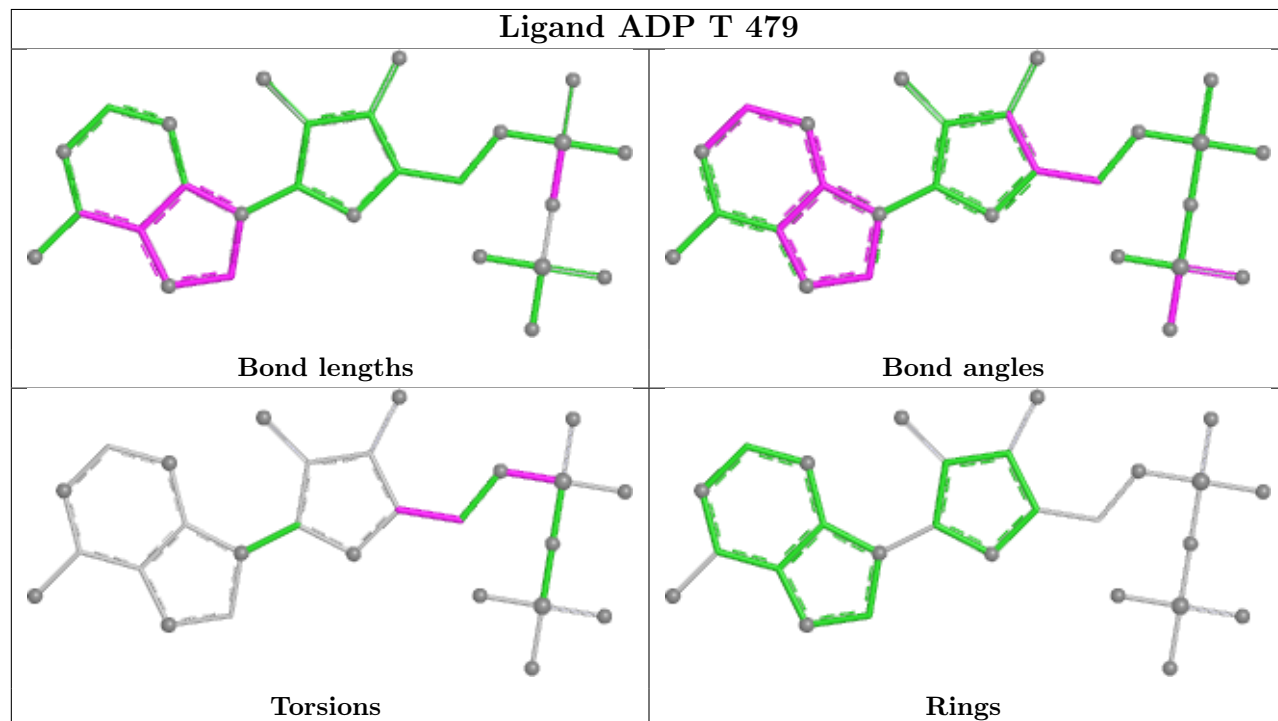
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

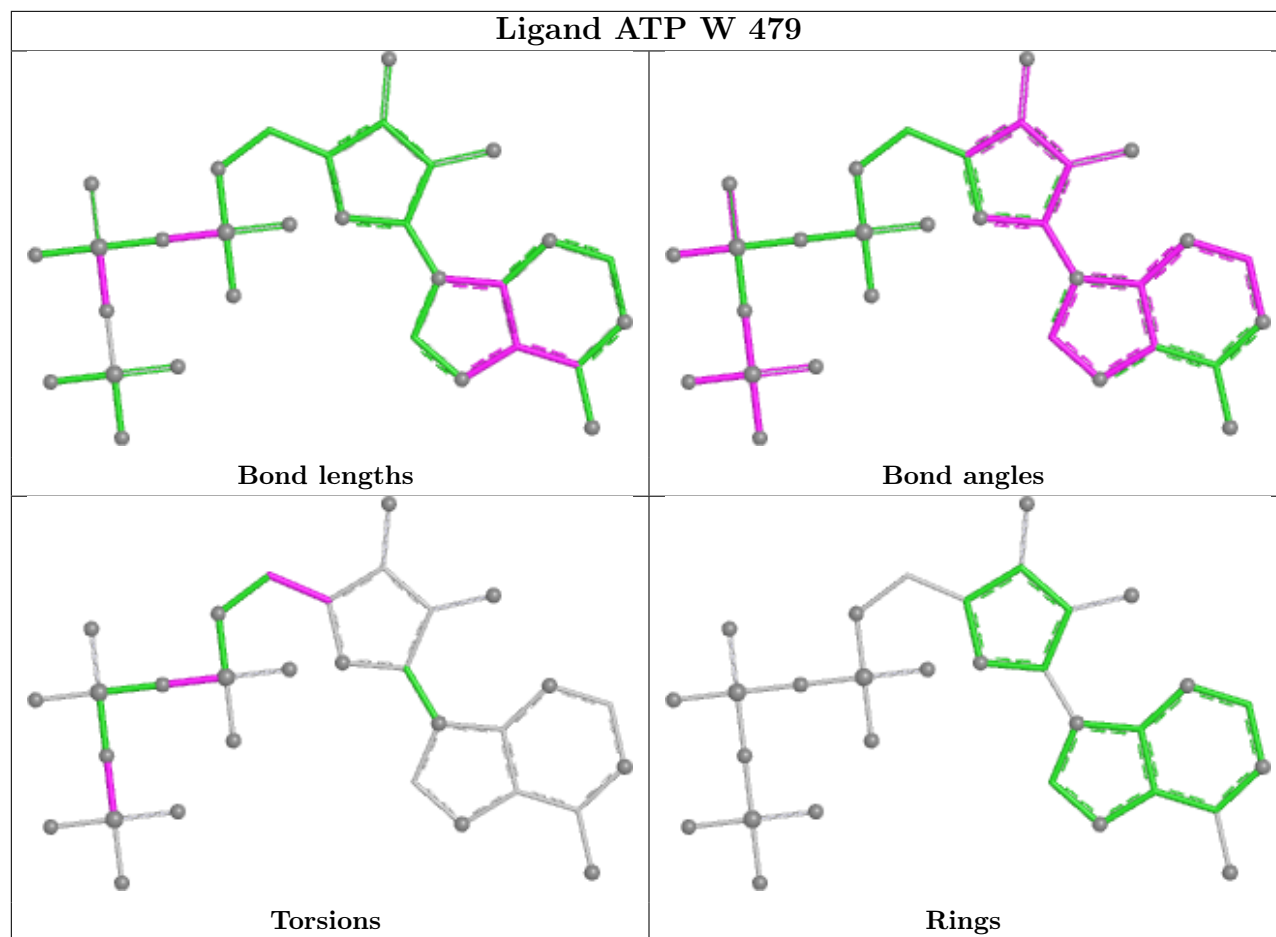


Ligand ATP K 479

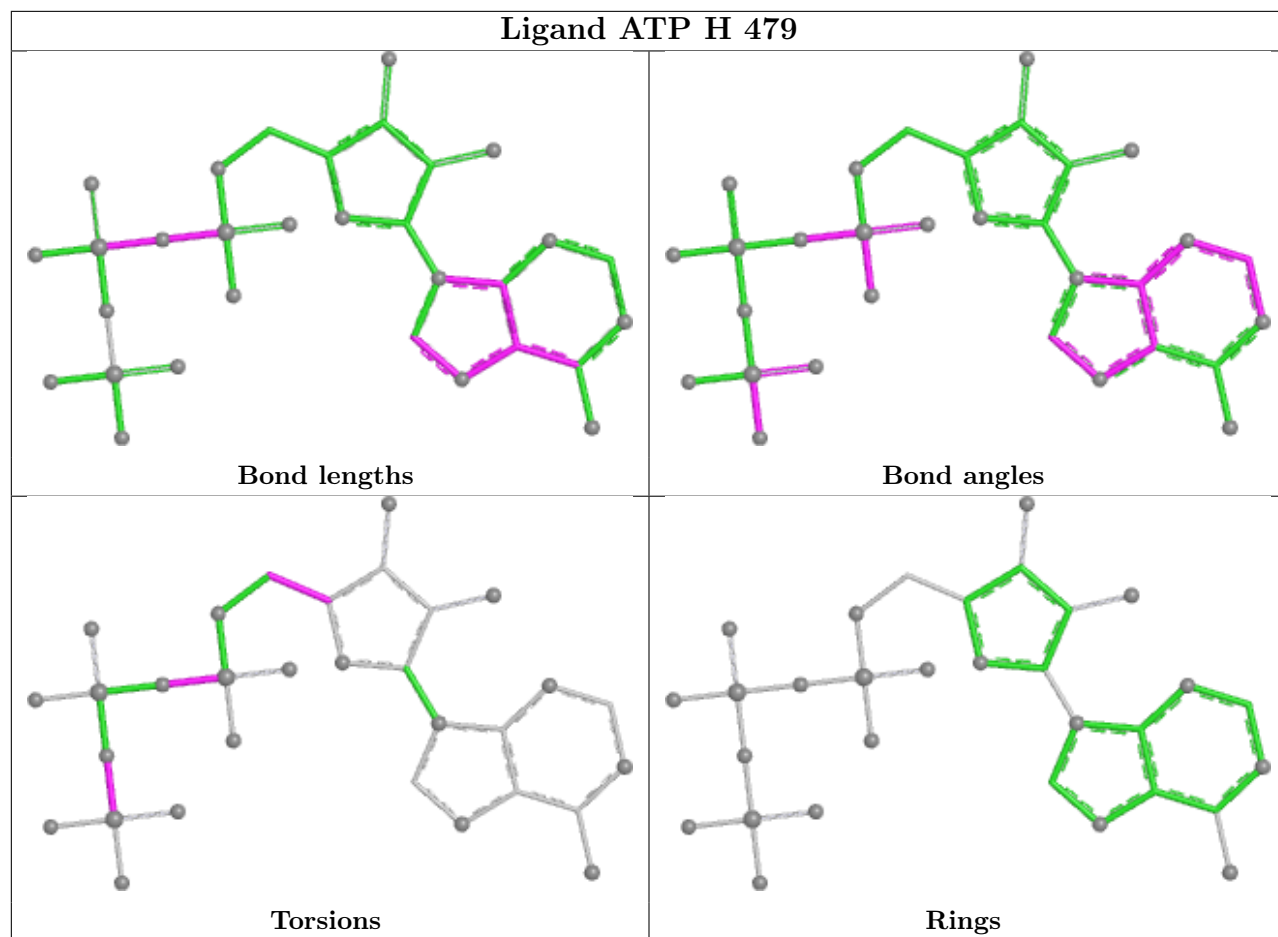


Ligand ADP T 479

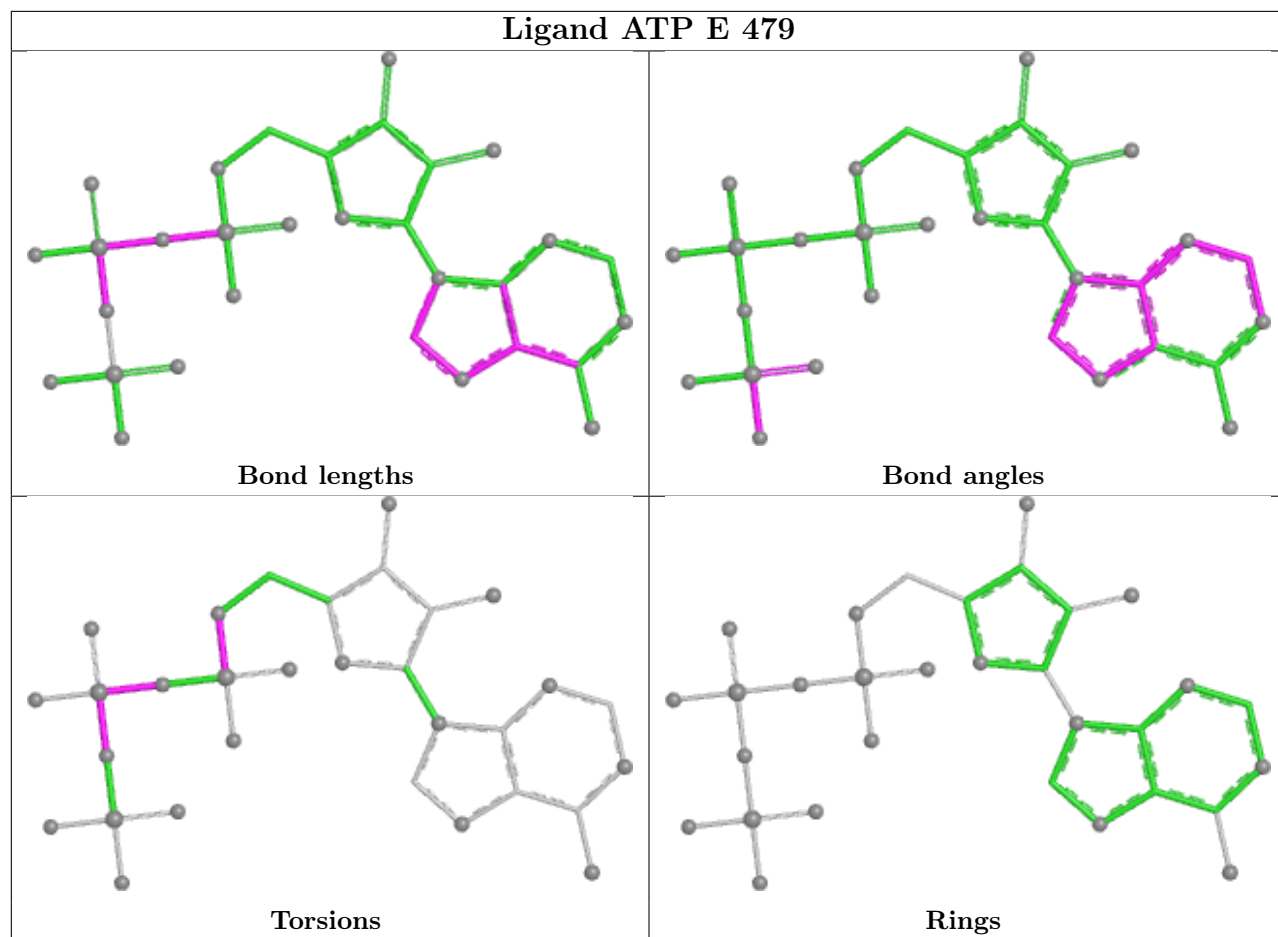


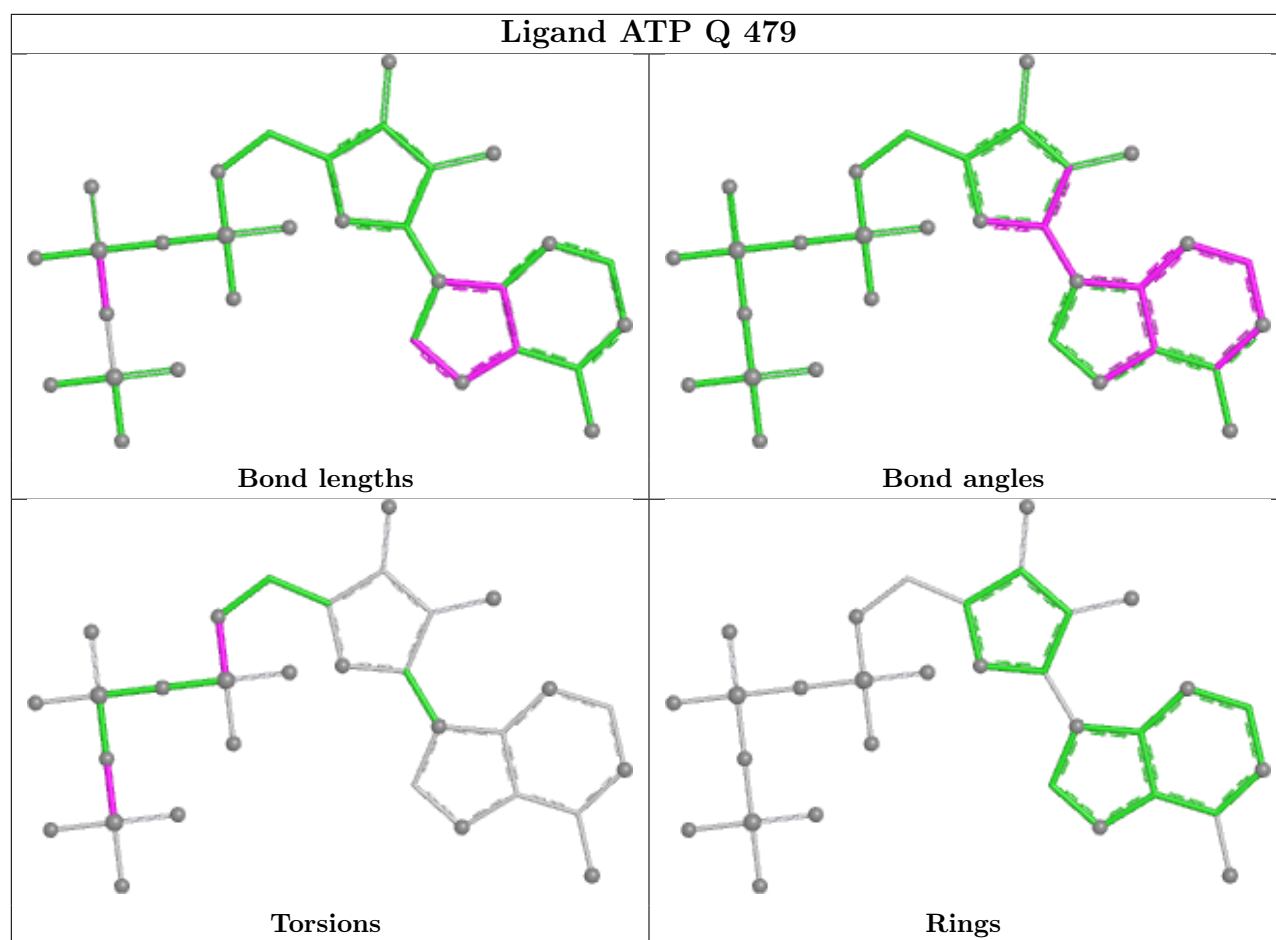


Ligand ATP H 479



Ligand ATP E 479





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	478/478 (100%)	-1.50	0 100 100	23, 53, 79, 88	0
1	D	478/478 (100%)	-1.52	0 100 100	23, 53, 79, 88	0
1	G	478/478 (100%)	-1.50	0 100 100	23, 53, 78, 88	0
1	J	478/478 (100%)	-1.49	0 100 100	23, 53, 78, 88	0
1	M	478/478 (100%)	-1.52	0 100 100	23, 53, 79, 88	0
1	P	478/478 (100%)	-1.52	0 100 100	23, 53, 78, 88	0
1	S	478/478 (100%)	-1.52	0 100 100	23, 53, 79, 88	0
1	V	478/478 (100%)	-1.52	0 100 100	23, 53, 79, 88	0
2	B	410/478 (85%)	-1.51	0 100 100	31, 63, 93, 112	0
2	E	410/478 (85%)	-1.46	0 100 100	31, 63, 94, 112	0
2	H	410/478 (85%)	-1.50	0 100 100	31, 63, 93, 112	0
2	K	410/478 (85%)	-1.48	0 100 100	31, 63, 93, 112	0
2	N	410/478 (85%)	-1.51	0 100 100	31, 63, 93, 112	0
2	Q	410/478 (85%)	-1.51	0 100 100	31, 63, 93, 112	0
2	T	410/478 (85%)	-1.47	0 100 100	31, 63, 93, 112	0
2	W	410/478 (85%)	-1.49	0 100 100	31, 63, 93, 112	0
3	C	91/94 (96%)	-1.50	0 100 100	25, 60, 72, 76	0
3	F	91/94 (96%)	-1.53	0 100 100	25, 60, 72, 76	0
3	I	91/94 (96%)	-1.54	0 100 100	25, 59, 72, 76	0
3	L	91/94 (96%)	-1.51	0 100 100	25, 59, 71, 76	0
3	O	91/94 (96%)	-1.51	0 100 100	25, 59, 71, 76	0
3	R	91/94 (96%)	-1.54	0 100 100	25, 59, 71, 76	0
3	U	91/94 (96%)	-1.43	0 100 100	25, 60, 72, 76	0
3	X	91/94 (96%)	-1.54	0 100 100	25, 59, 72, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7832/8400 (93%)	-1.50	0 100 100	23, 56, 88, 112	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	ASP	N	482	9/9	0.97	0.08	71,79,81,82	0
4	ASN	M	905	8/9	0.98	0.13	31,31,32,32	8
4	ASN	S	907	8/9	0.98	0.05	53,53,55,57	0
7	MN	B	481	1/1	0.98	0.10	56,56,56,56	1
7	MN	E	481	1/1	0.98	0.09	85,85,85,85	1
7	MN	N	481	1/1	0.98	0.04	86,86,86,86	1
8	ATP	E	479	31/31	0.98	0.04	34,40,85,85	31
8	ATP	K	479	31/31	0.98	0.06	24,35,57,58	31
9	ASP	H	482	9/9	0.98	0.06	71,79,81,82	0
4	ASN	A	901	8/9	0.98	0.13	31,32,34,35	8
4	ASN	J	904	8/9	0.99	0.03	52,53,54,54	0
4	ASN	D	902	8/9	0.99	0.05	62,62,62,62	0
7	MN	H	481	1/1	0.99	0.03	75,75,75,75	1
7	MN	K	481	1/1	0.99	0.05	63,63,63,63	1
4	ASN	P	906	8/9	0.99	0.12	28,28,29,29	8
7	MN	Q	481	1/1	0.99	0.03	64,64,64,64	1
7	MN	T	481	1/1	0.99	0.04	75,75,75,75	0
7	MN	W	481	1/1	0.99	0.06	82,82,82,82	1
4	ASN	G	903	8/9	0.99	0.07	27,29,30,31	8

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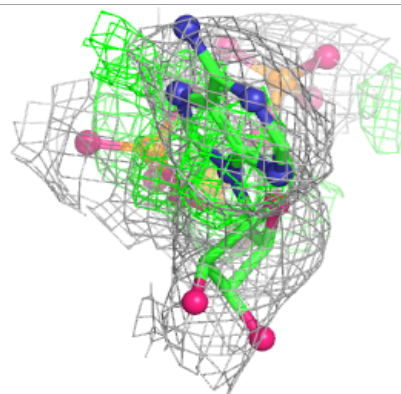
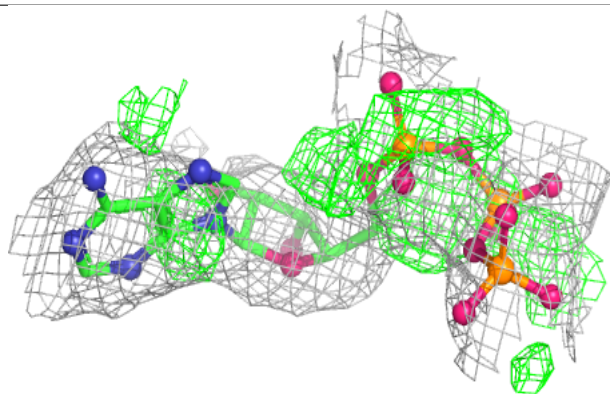
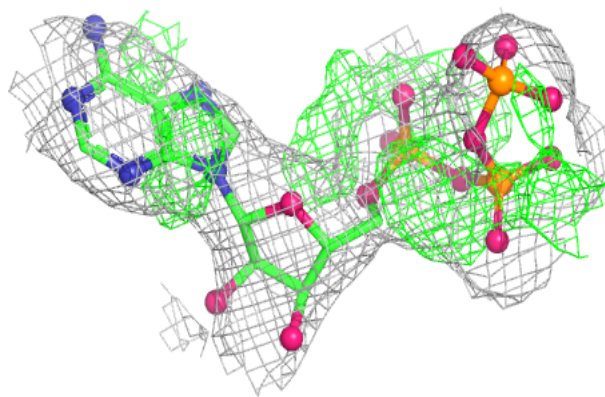
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	ATP	H	479	31/31	0.99	0.03	21,28,49,51	31
4	ASN	V	908	8/9	0.99	0.09	28,29,29,30	8
8	ATP	N	479	31/31	0.99	0.04	35,39,66,66	31
8	ATP	Q	479	31/31	0.99	0.04	30,37,49,50	31
8	ATP	W	479	31/31	0.99	0.03	14,21,28,32	31
6	ADP	B	479	27/27	0.99	0.04	70,71,82,82	27
6	ADP	T	479	27/27	0.99	0.05	75,76,87,88	27
7	MN	N	480	1/1	1.00	0.01	49,49,49,49	0
5	ZN	T	907	1/1	1.00	0.01	55,55,55,55	0
7	MN	Q	480	1/1	1.00	0.01	51,51,51,51	0
5	ZN	W	908	1/1	1.00	0.01	55,55,55,55	0
7	MN	T	480	1/1	1.00	0.01	55,55,55,55	0
5	ZN	B	901	1/1	1.00	0.01	57,57,57,57	0
7	MN	W	480	1/1	1.00	0.02	52,52,52,52	0
5	ZN	E	902	1/1	1.00	0.01	59,59,59,59	0
7	MN	B	480	1/1	1.00	0.02	44,44,44,44	0
5	ZN	H	903	1/1	1.00	0.01	53,53,53,53	0
7	MN	E	480	1/1	1.00	0.01	53,53,53,53	0
5	ZN	K	904	1/1	1.00	0.01	50,50,50,50	0
7	MN	H	480	1/1	1.00	0.01	50,50,50,50	0
5	ZN	N	905	1/1	1.00	0.01	53,53,53,53	0
7	MN	K	480	1/1	1.00	0.01	45,45,45,45	0
5	ZN	Q	906	1/1	1.00	0.01	51,51,51,51	0

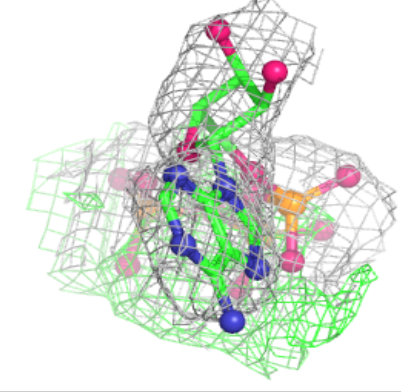
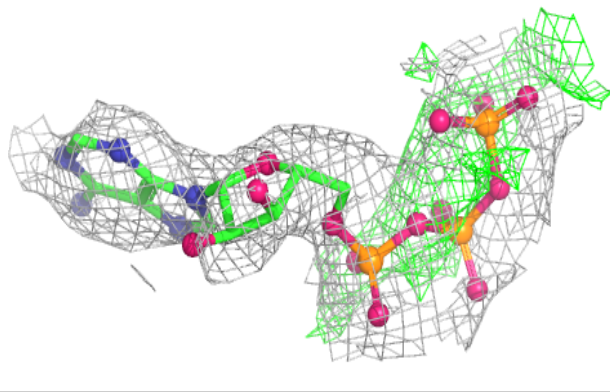
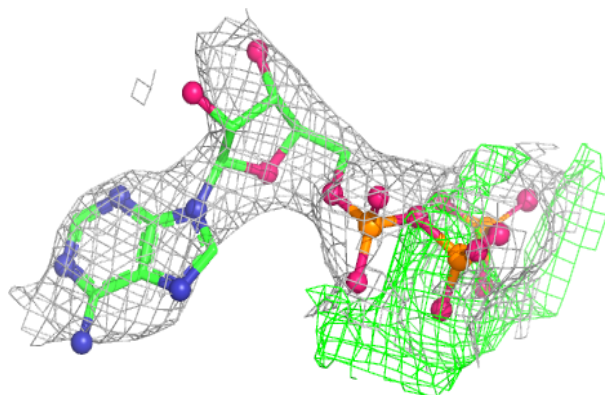
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP E 479:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

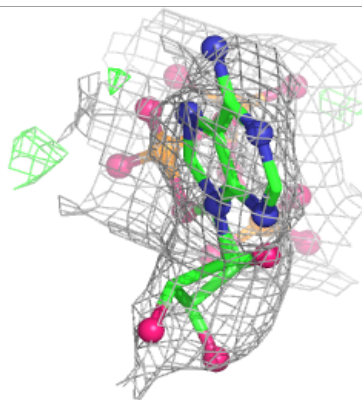
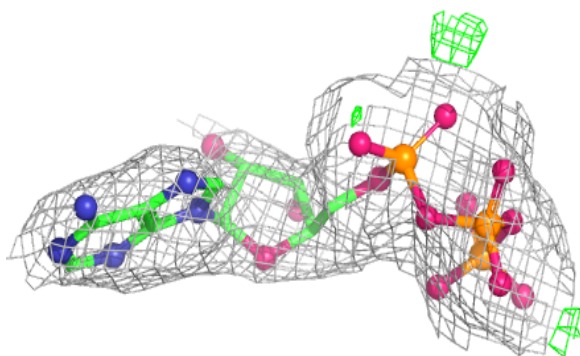
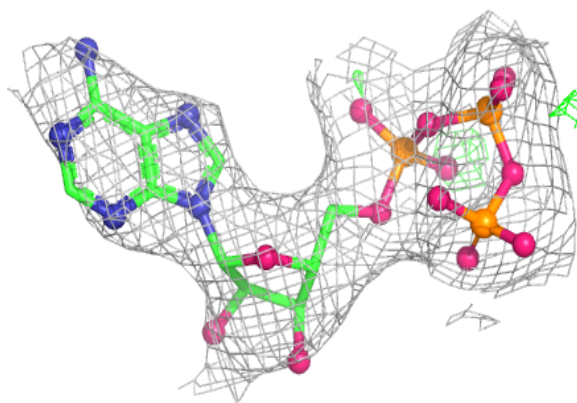
**Electron density around ATP K 479:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

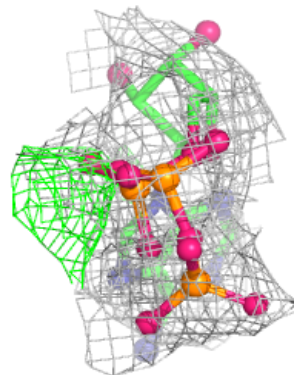
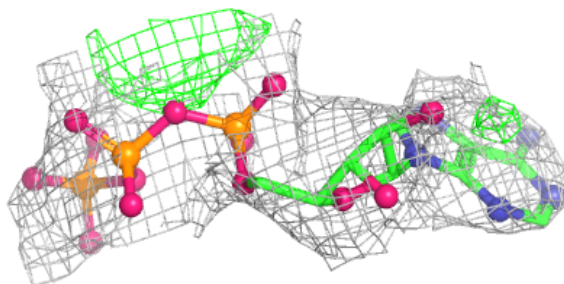
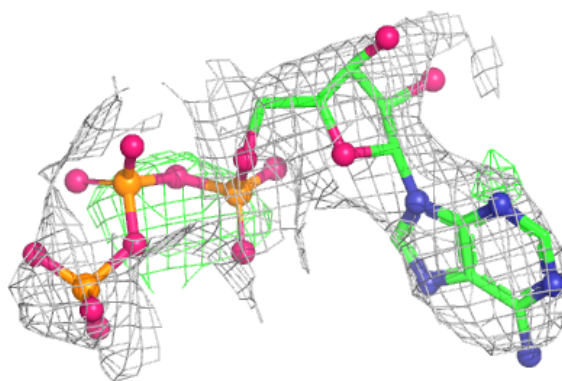


Electron density around ATP H 479:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

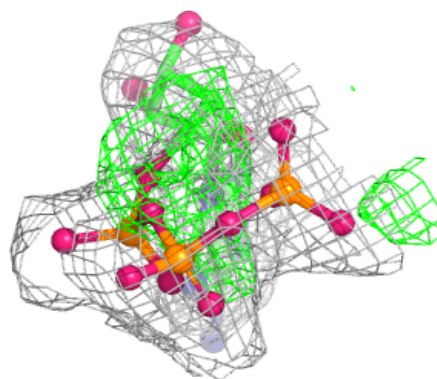
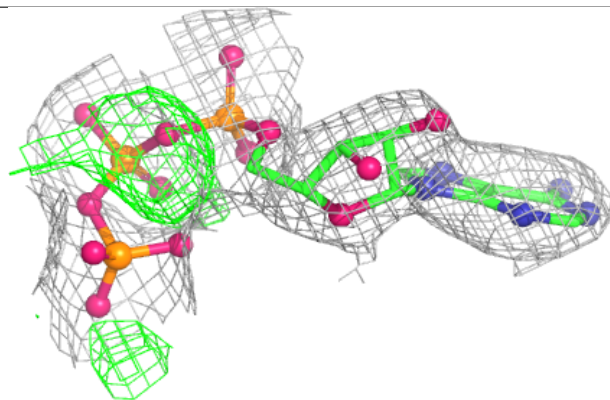
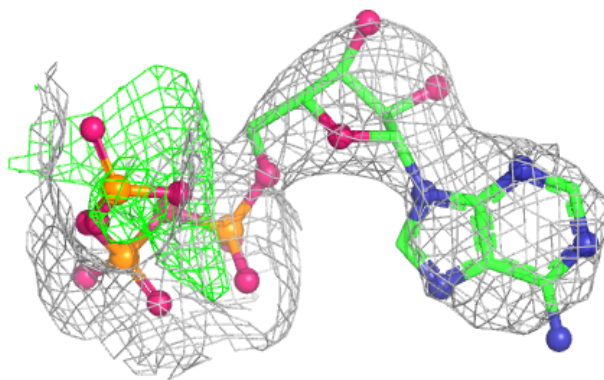
**Electron density around ATP N 479:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

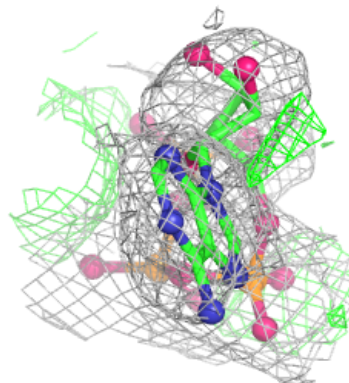
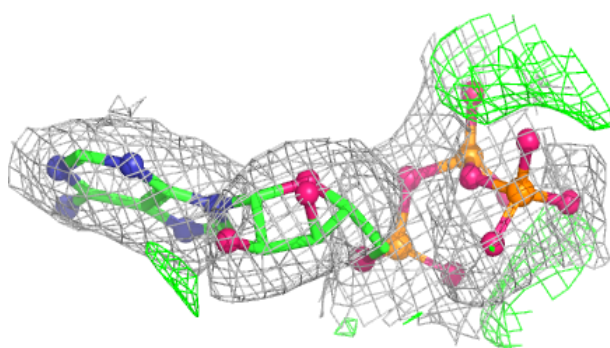
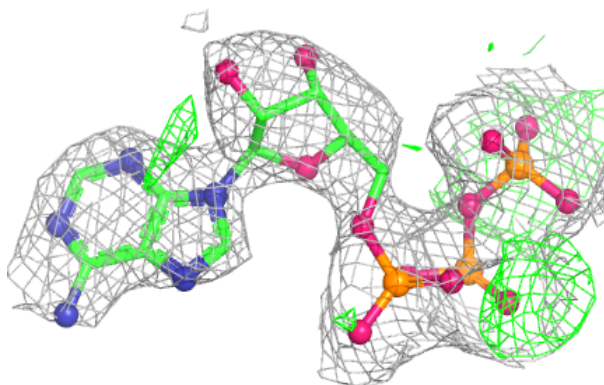


Electron density around ATP Q 479:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

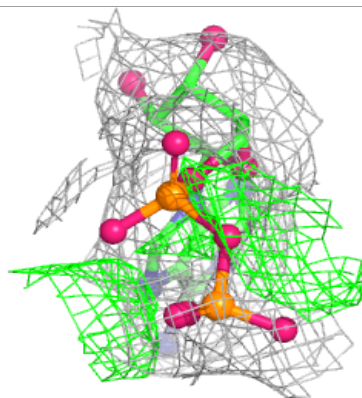
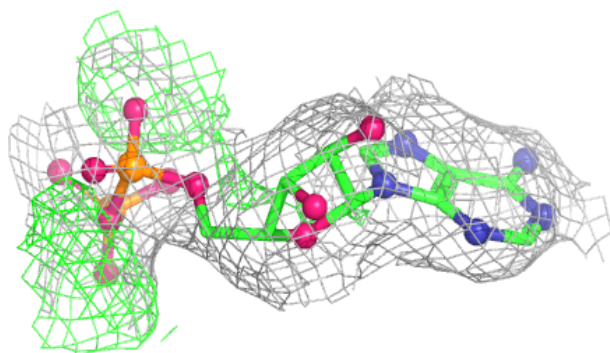
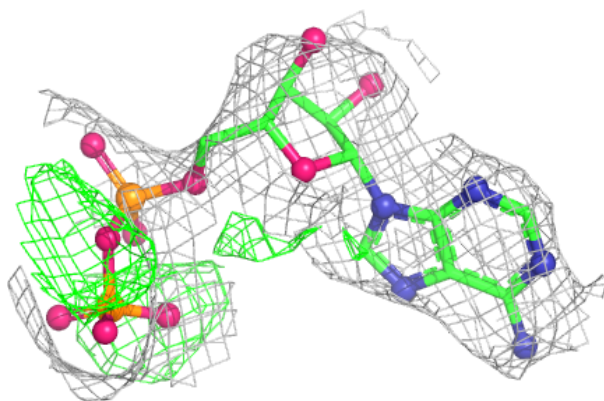
**Electron density around ATP W 479:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

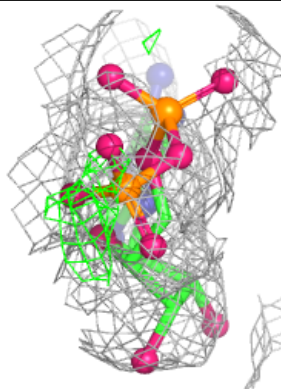
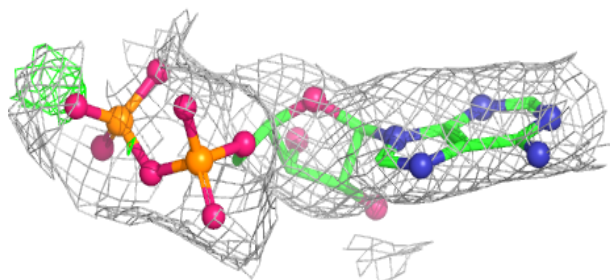
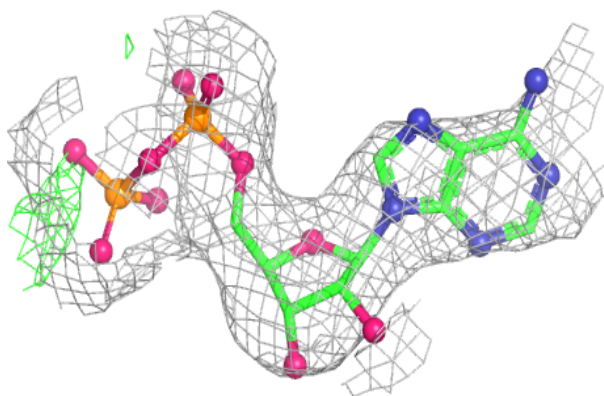


Electron density around ADP B 479:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP T 479:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.