



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:19 PM UTC

PDB ID : 1KYI / pdb_00001kyi
Title : HslUV (H. influenzae)-NLVS Vinyl Sulfone Inhibitor Complex
Authors : Sousa, M.C.; Kessler, B.M.; Overkleeft, H.S.; McKay, D.B.
Deposited on : 2002-02-04
Resolution : 3.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

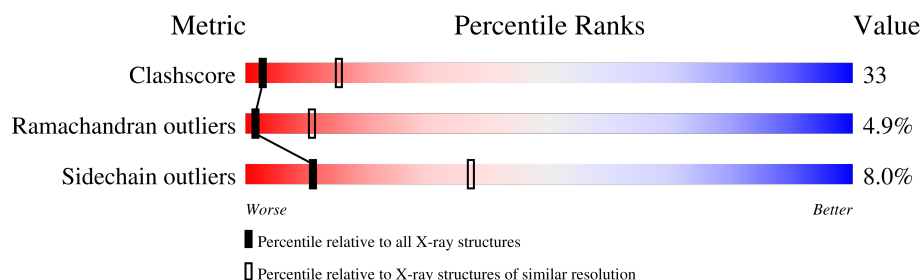
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

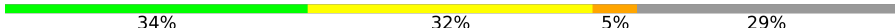
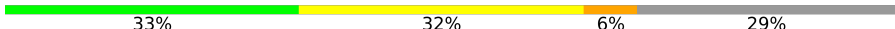
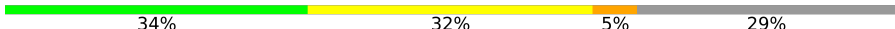
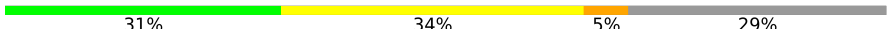
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	444	36% 29% 7% 28%
1	B	444	36% 30% 6% 28%
1	C	444	37% 30% 5% 28%
1	D	444	37% 29% 6% 28%
1	E	444	37% 29% 6% 28%
1	F	444	38% 29% 6% 28%
1	S	444	31% 35% 5% 29%
1	T	444	32% 33% 6% 29%

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Mol	Chain	Length	Quality of chain
1	U	444	
1	V	444	
1	W	444	
1	X	444	
2	G	174	
2	H	174	
2	I	174	
2	J	174	
2	K	174	
2	L	174	
2	M	174	
2	N	174	
2	O	174	
2	P	174	
2	Q	174	
2	R	174	

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	LVS	J	175	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 45756 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 ATP-dependent hsl protease ATP-binding subunit hslU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2488	1557	444	477	10			
1	B	321	Total	C	N	O	S	0	0	0
			2488	1557	444	477	10			
1	C	321	Total	C	N	O	S	0	0	0
			2488	1557	444	477	10			
1	D	321	Total	C	N	O	S	0	0	0
			2488	1557	444	477	10			
1	E	321	Total	C	N	O	S	0	0	0
			2488	1557	444	477	10			
1	F	321	Total	C	N	O	S	0	0	0
			2488	1557	444	477	10			
1	S	317	Total	C	N	O	S	0	0	0
			2469	1543	444	472	10			
1	T	317	Total	C	N	O	S	0	0	0
			2469	1543	444	472	10			
1	U	317	Total	C	N	O	S	0	0	0
			2469	1543	444	472	10			
1	V	317	Total	C	N	O	S	0	0	0
			2469	1543	444	472	10			
1	W	317	Total	C	N	O	S	0	0	0
			2469	1543	444	472	10			
1	X	317	Total	C	N	O	S	0	0	0
			2469	1543	444	472	10			

- Molecule 2 is a protein called ATP-dependent protease hslV.

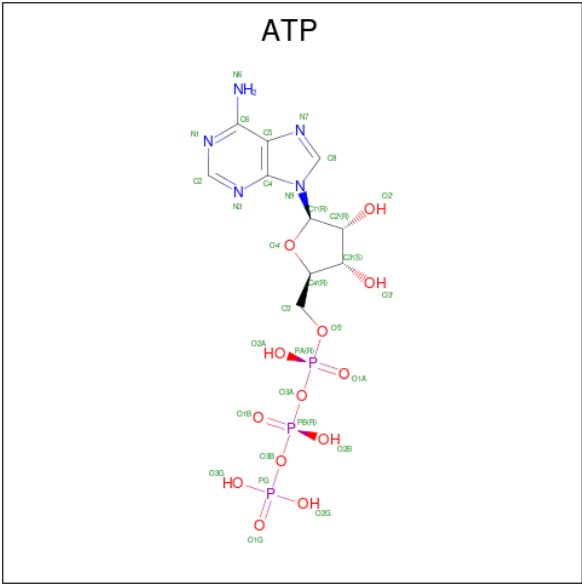
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	173	Total	C	N	O	S	0	0	0
			1290	809	228	249	4			
2	H	173	Total	C	N	O	S	0	0	0
			1290	809	228	249	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	173	Total	C	N	O	S	0	0	0
			1290	809	228	249	4			
2	J	173	Total	C	N	O	S	0	0	0
			1290	809	228	249	4			
2	K	173	Total	C	N	O	S	0	0	0
			1290	809	228	249	4			
2	L	173	Total	C	N	O	S	0	0	0
			1290	809	228	249	4			
2	M	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	N	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	O	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	P	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	Q	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	R	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



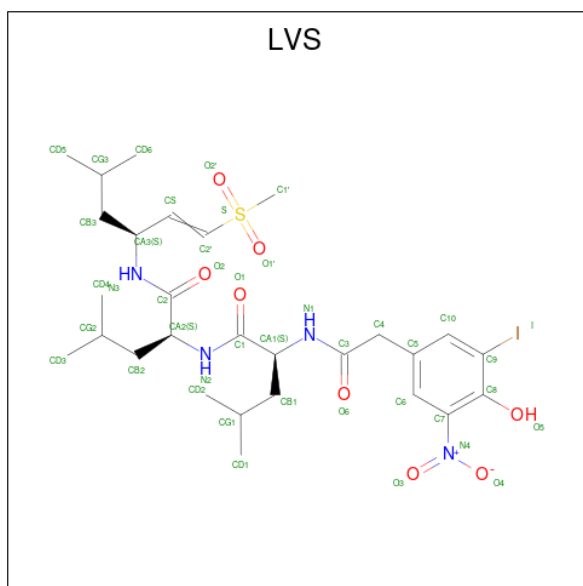
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	S	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	T	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	U	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	V	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	W	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	X	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is 4-iodo-3-nitrophenyl acetyl-leucinyll-leucinyll-leucinyll-vinylsulfone (CCD ID: LVS) (formula: $C_{28}H_{43}IN_4O_8S$).



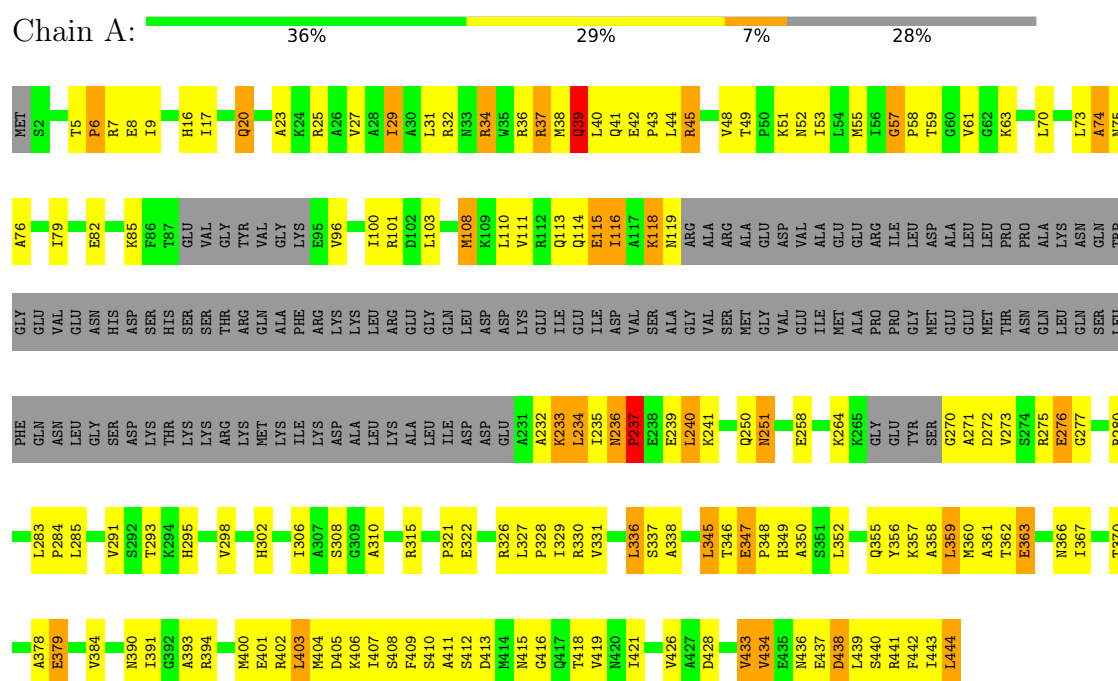
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	N	O	S	0	0
			28	20	3	4	1		
4	H	1	Total	C	N	O	S	0	0
			28	20	3	4	1		
4	I	1	Total	C	N	O	S	0	0
			28	20	3	4	1		
4	J	1	Total	C	N	O	S	0	0
			28	20	3	4	1		
4	K	1	Total	C	N	O	S	0	0
			28	20	3	4	1		
4	L	1	Total	C	N	O	S	0	0
			28	20	3	4	1		
4	M	1	Total	C	N	O	S	0	0
			28	20	3	4	1		
4	N	1	Total	C	N	O	S	0	0
			28	20	3	4	1		
4	O	1	Total	C	N	O	S	0	0
			28	20	3	4	1		
4	P	1	Total	C	N	O	S	0	0
			28	20	3	4	1		
4	Q	1	Total	C	N	O	S	0	0
			28	20	3	4	1		
4	R	1	Total	C	N	O	S	0	0
			28	20	3	4	1		

3 Residue-property plots

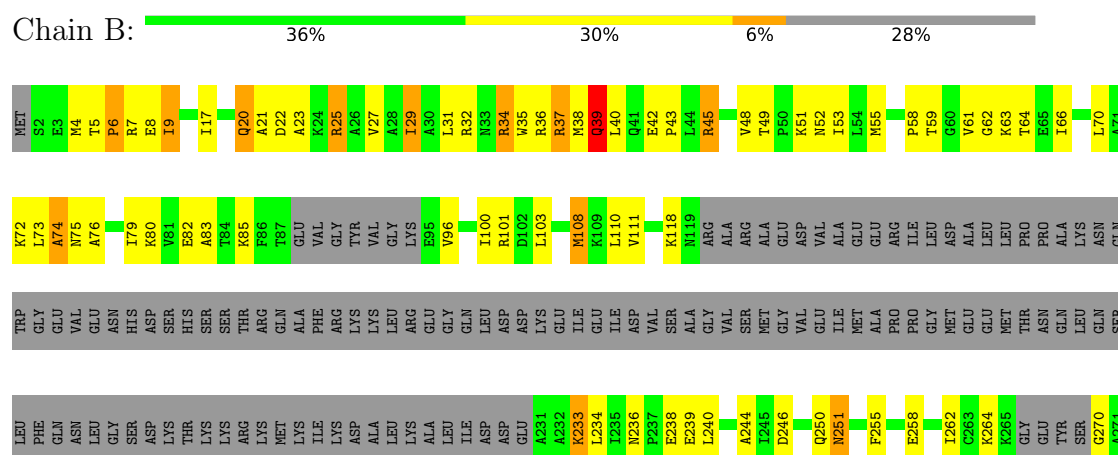
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

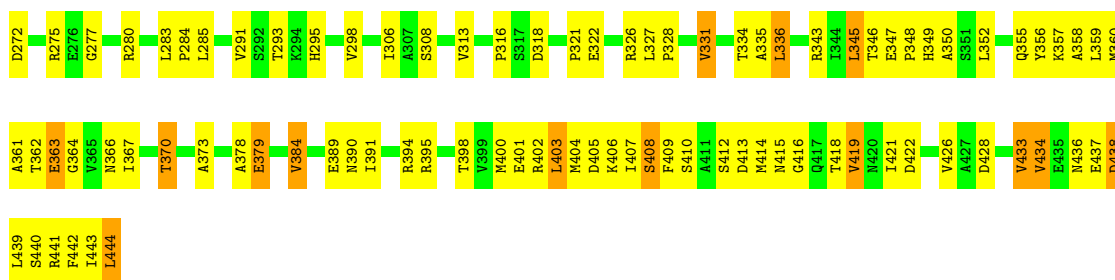
Note EDS was not executed.

- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU



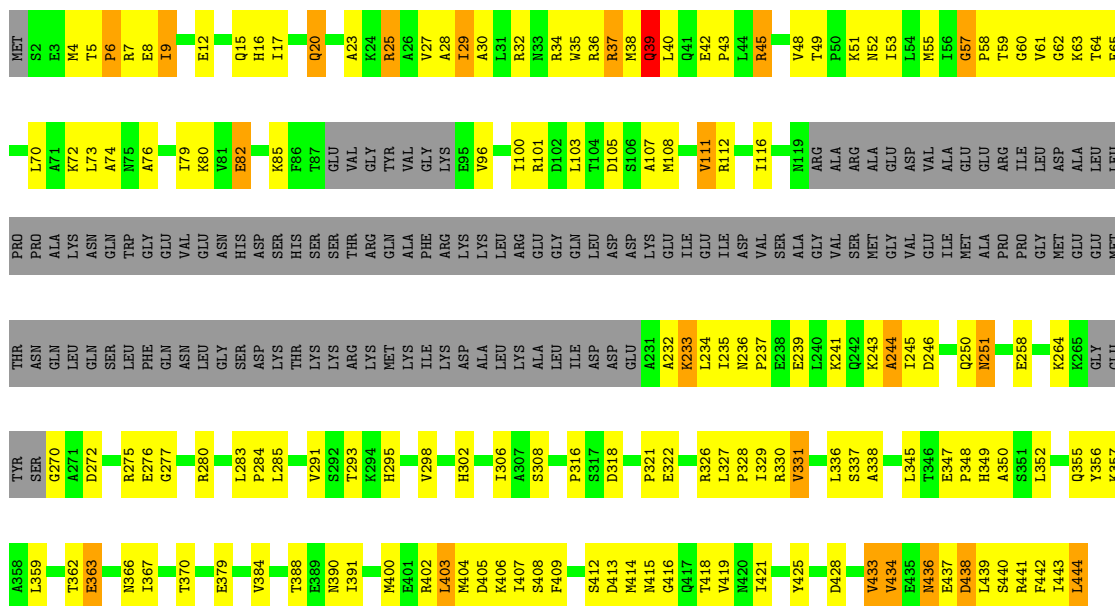
- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU





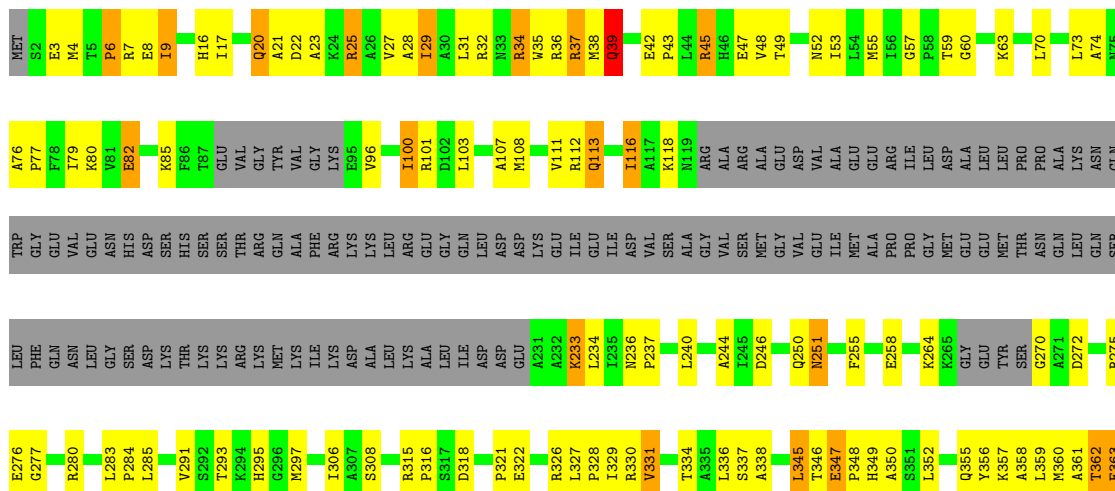
- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU

Chain C: 37% 30% 5% 28%



- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU

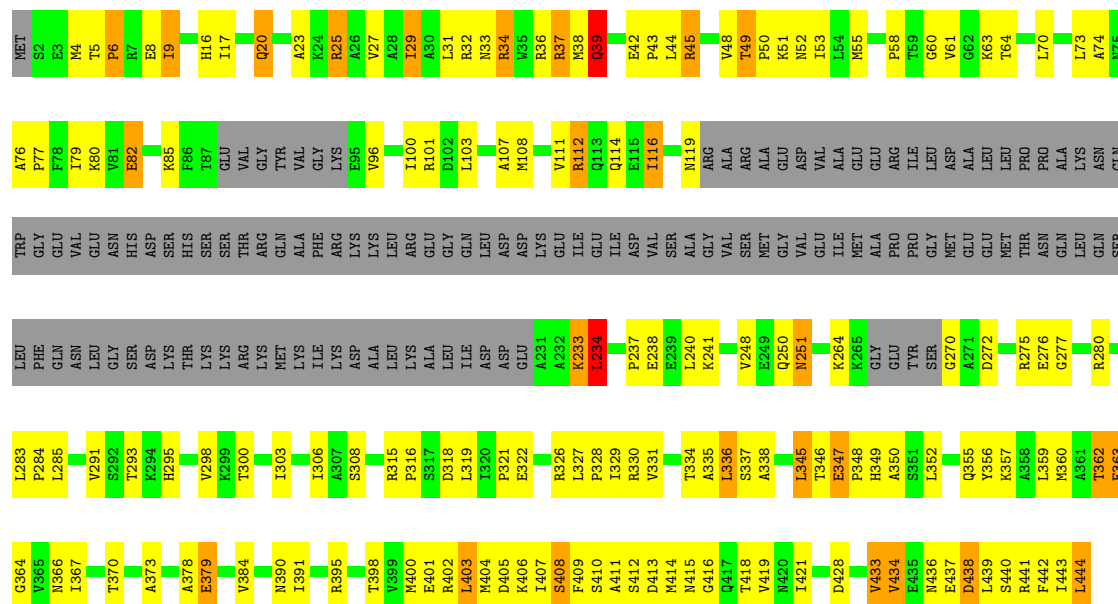
Chain D: 37% 29% 6% 28%





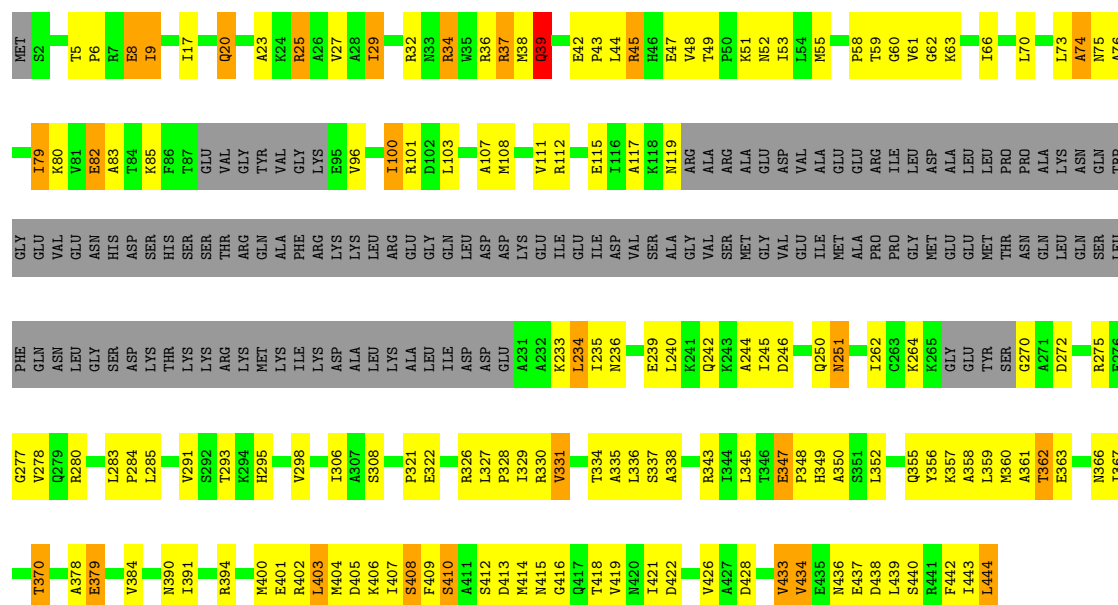
- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU

Chain E: 37% 29% 6% 28%



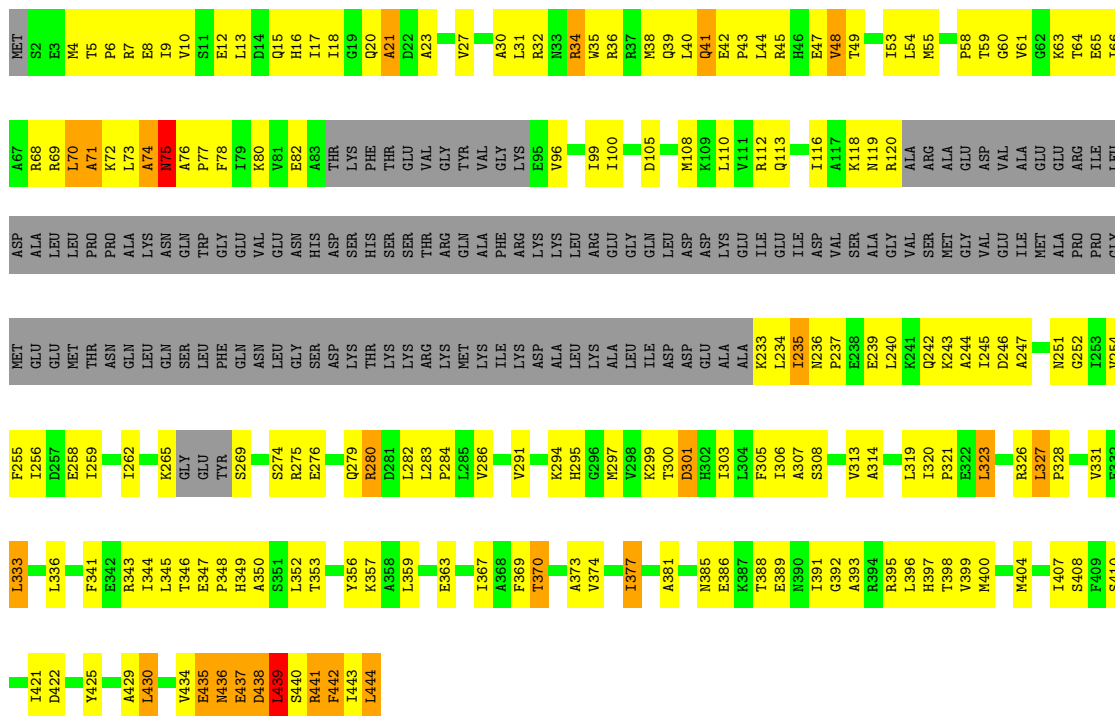
- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU

Chain F: 38% 29% 6% 28%

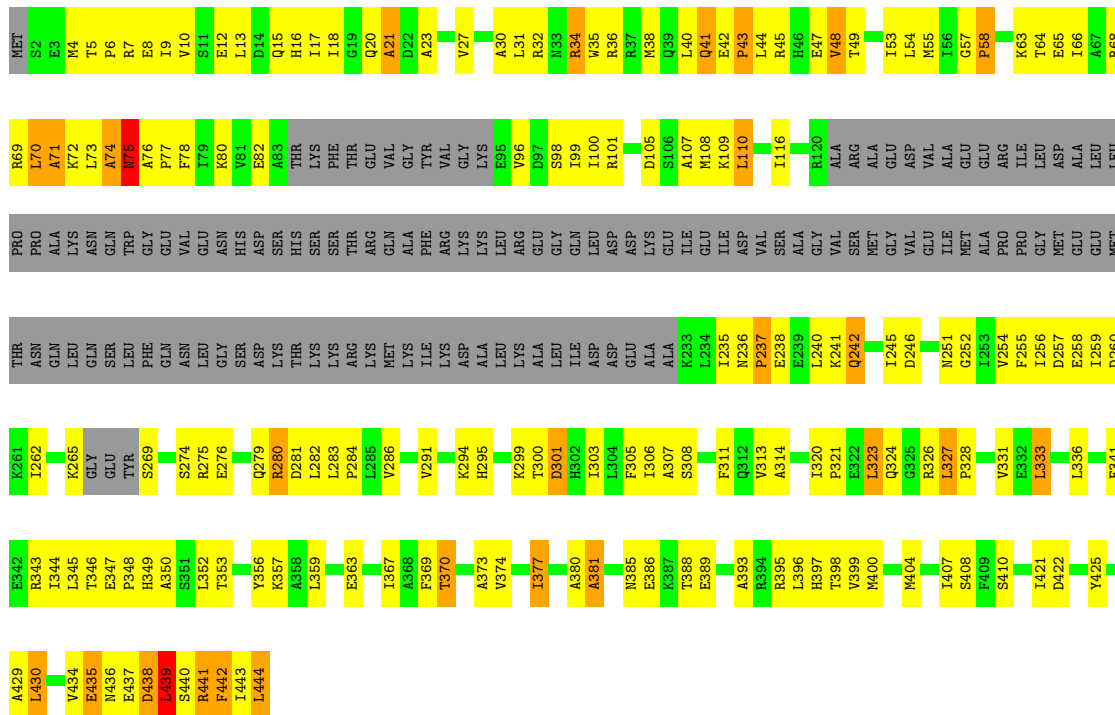


- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU

Chain S: 31% 35% 5% 29%

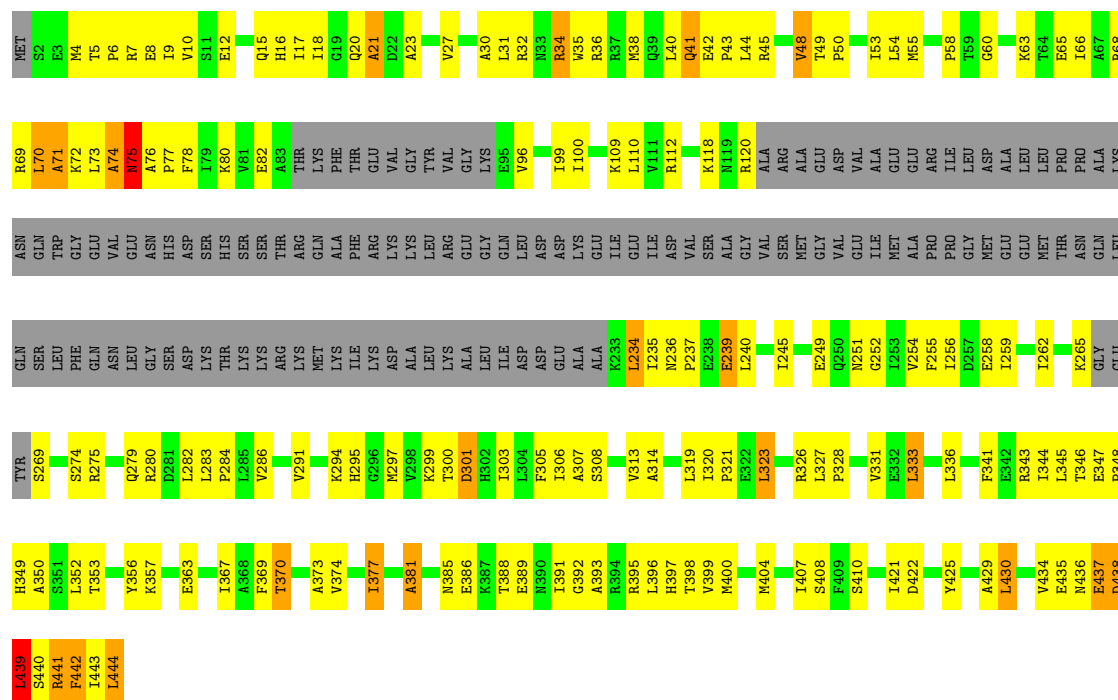


- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU



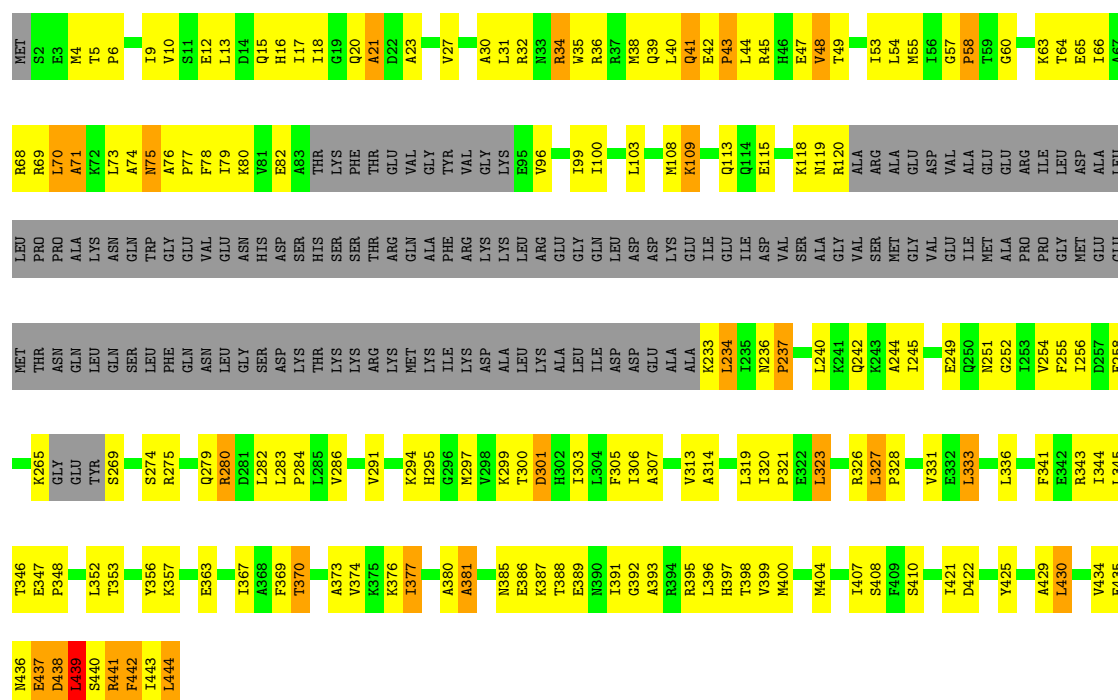
- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU





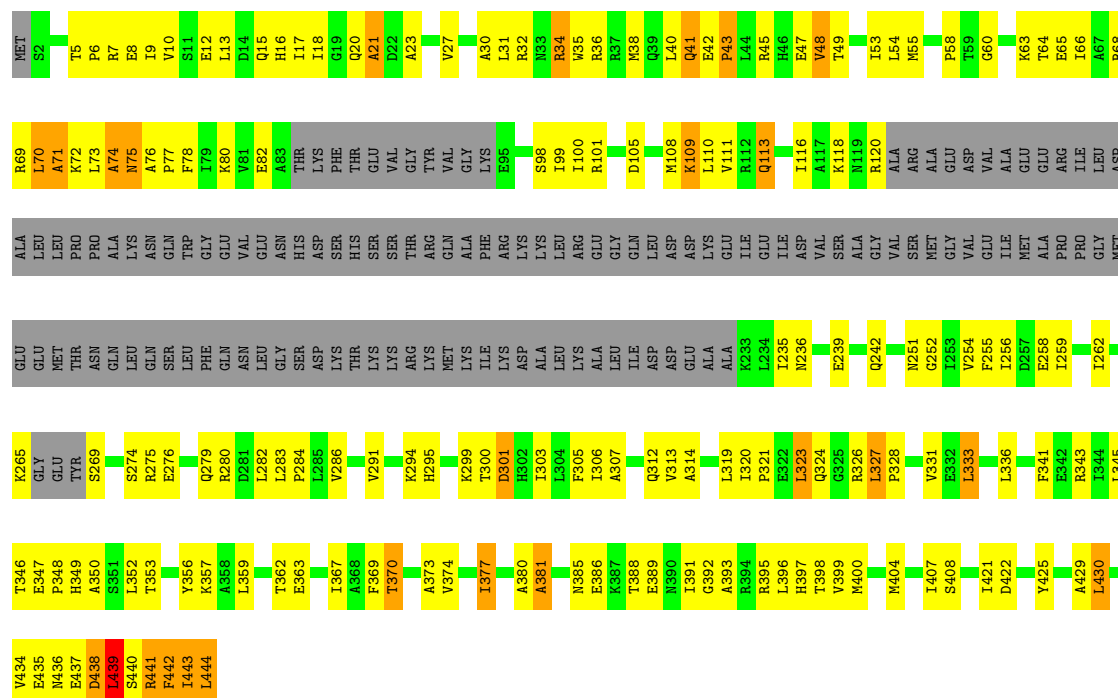
- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU

Chain V: 33% 32% 6% 29%

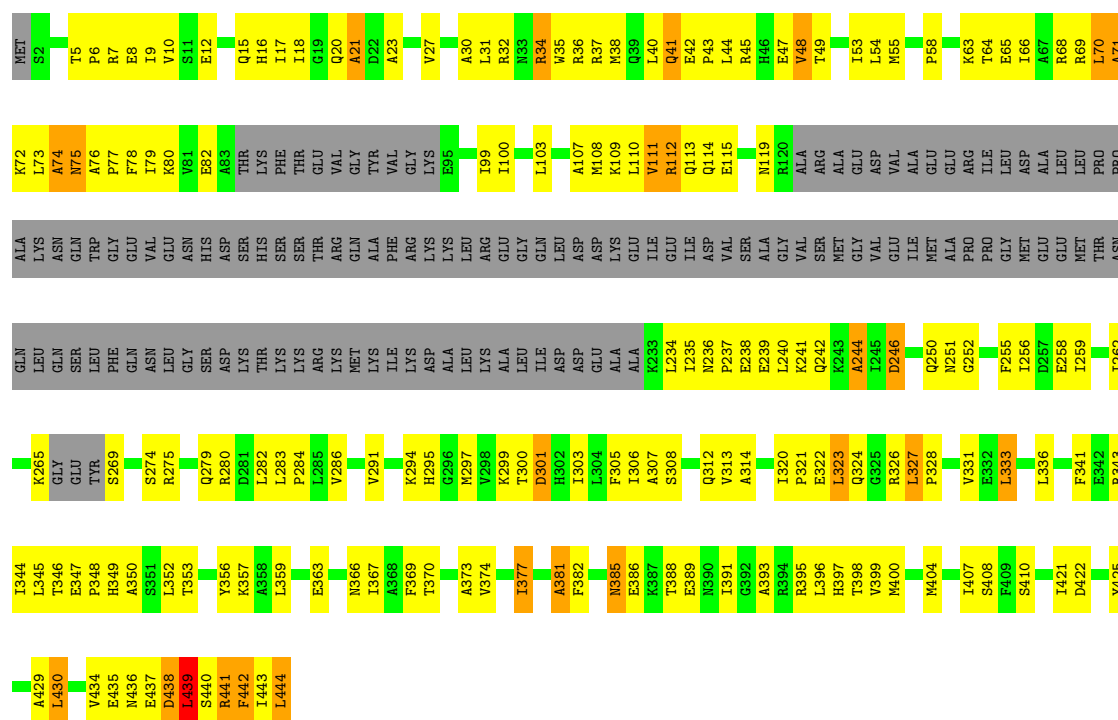


- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU

Chain W: 34% 32% 5% 29%

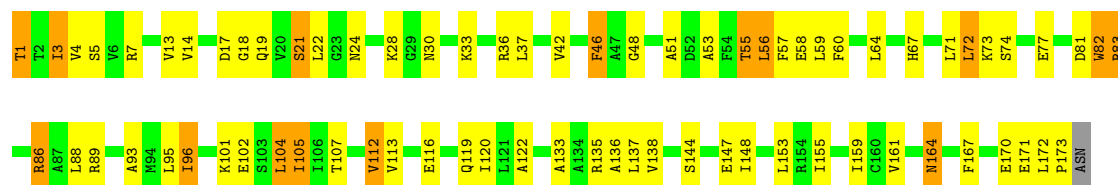


- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU



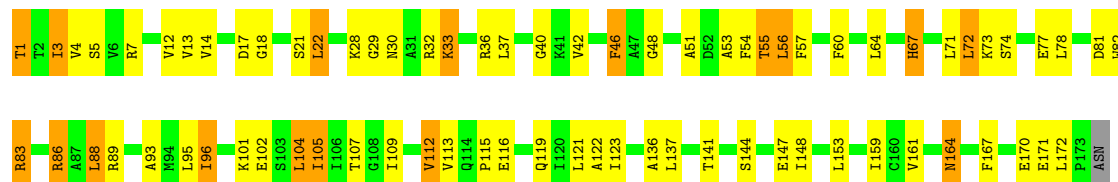
- Molecule 2: ATP-dependent protease hslV





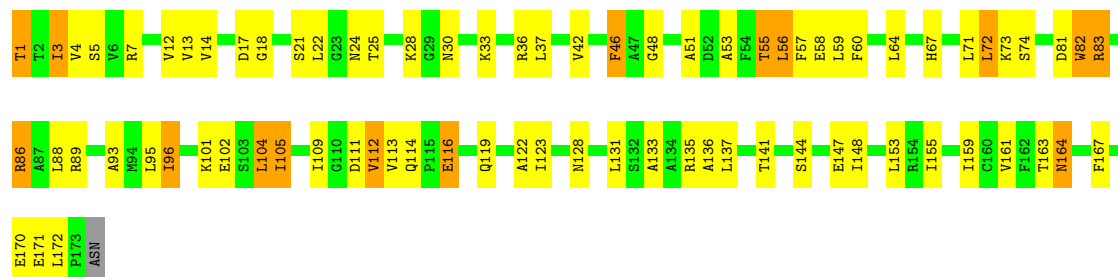
- Molecule 2: ATP-dependent protease hslV

Chain H: 56% 33% 10% .



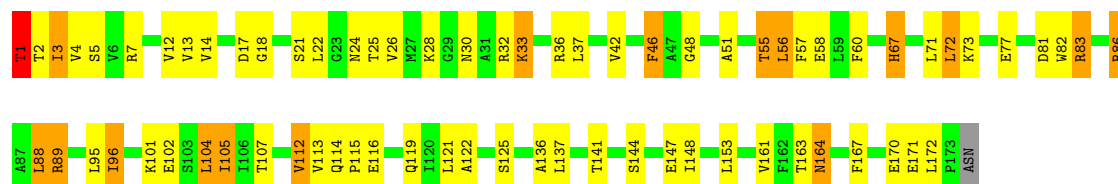
- Molecule 2: ATP-dependent protease hslV

Chain I: 55% 36% 9% .



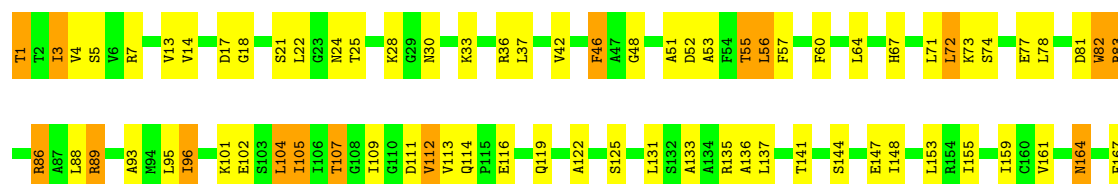
- Molecule 2: ATP-dependent protease hslV

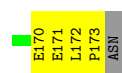
Chain J: 58% 32% 9% ..



- Molecule 2: ATP-dependent protease hslV

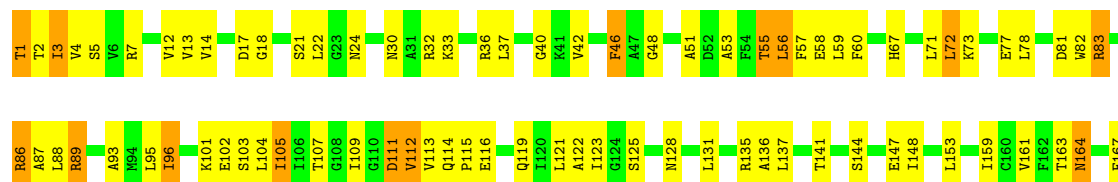
Chain K: 55% 36% 9% .





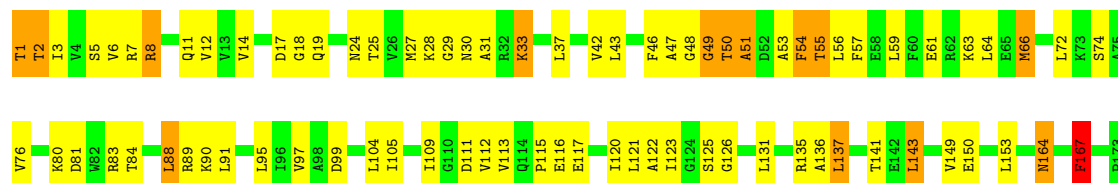
• Molecule 2: ATP-dependent protease hslV

Chain L: 52% 40% 8%



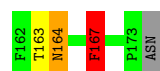
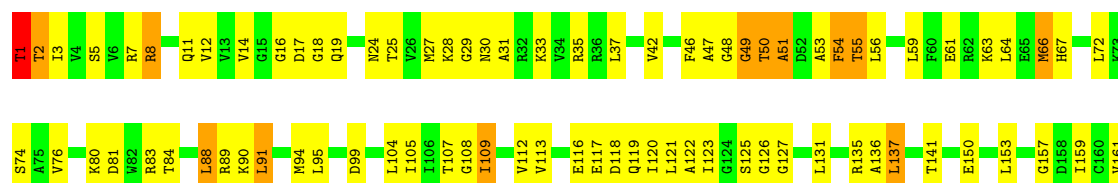
• Molecule 2: ATP-dependent protease hslV

Chain M: 53% 37% 8%



• Molecule 2: ATP-dependent protease hslV

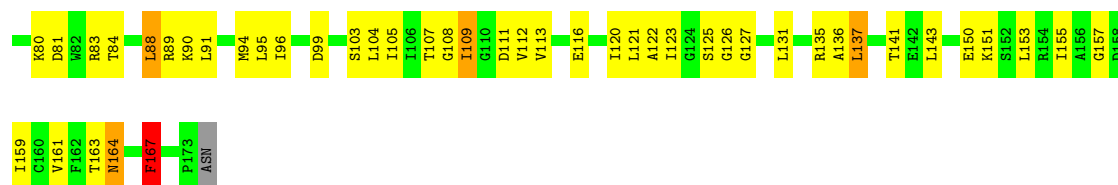
Chain N: 51% 40% 7%



• Molecule 2: ATP-dependent protease hslV

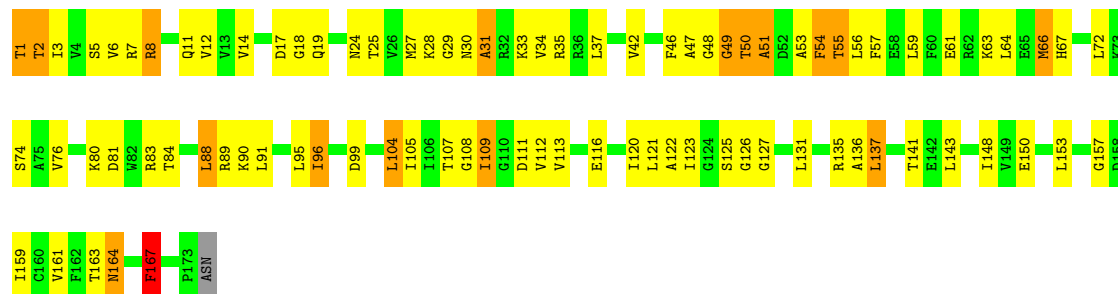
Chain O: 50% 41% 7%





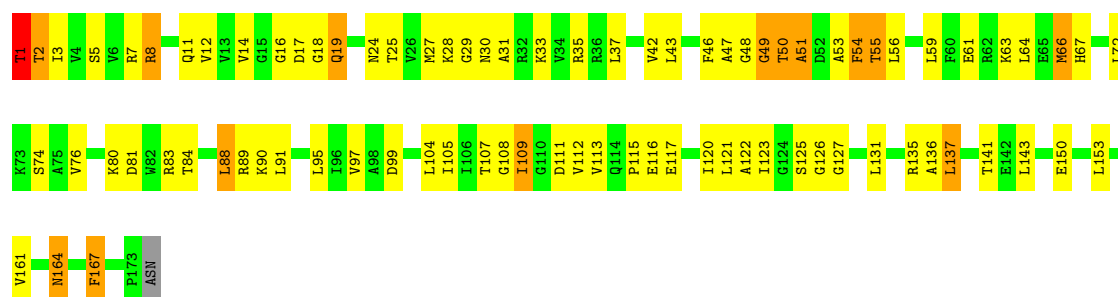
• Molecule 2: ATP-dependent protease hslV

Chain P: 49% 40% 9% ..



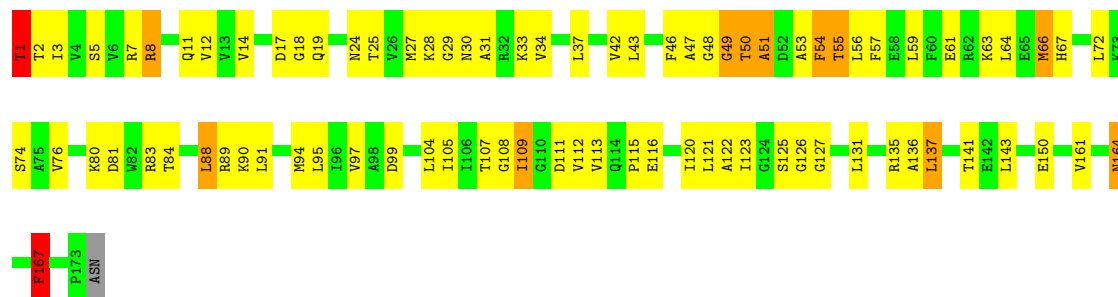
• Molecule 2: ATP-dependent protease hslV

Chain Q: 51% 40% 8% ..



• Molecule 2: ATP-dependent protease hslV

Chain R: 52% 40% 6% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	208.51Å 219.97Å 242.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10	Depositor
% Data completeness (in resolution range)	92.9 (30.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.266 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	45756	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.72	1/2515 (0.0%)	1.26	32/3391 (0.9%)
1	B	0.73	0/2515	1.19	21/3391 (0.6%)
1	C	0.73	0/2515	1.20	24/3391 (0.7%)
1	D	0.76	0/2515	1.18	24/3391 (0.7%)
1	E	0.78	0/2515	1.19	27/3391 (0.8%)
1	F	0.74	0/2515	1.19	21/3391 (0.6%)
1	S	0.36	0/2495	0.99	13/3360 (0.4%)
1	T	0.36	0/2495	0.96	15/3360 (0.4%)
1	U	0.37	0/2495	0.97	8/3360 (0.2%)
1	V	0.37	0/2495	0.99	13/3360 (0.4%)
1	W	0.37	0/2495	0.96	15/3360 (0.4%)
1	X	0.37	0/2495	0.98	18/3360 (0.5%)
2	G	0.72	0/1304	1.08	6/1765 (0.3%)
2	H	0.73	0/1304	1.10	7/1765 (0.4%)
2	I	0.73	0/1304	1.11	7/1765 (0.4%)
2	J	0.78	3/1304 (0.2%)	1.10	8/1765 (0.5%)
2	K	0.71	0/1304	1.10	6/1765 (0.3%)
2	L	0.78	1/1304 (0.1%)	1.13	7/1765 (0.4%)
2	M	0.58	1/1275 (0.1%)	1.02	3/1732 (0.2%)
2	N	0.62	2/1275 (0.2%)	1.04	4/1732 (0.2%)
2	O	0.58	1/1275 (0.1%)	1.01	4/1732 (0.2%)
2	P	0.58	1/1275 (0.1%)	1.01	5/1732 (0.3%)
2	Q	0.59	2/1275 (0.2%)	1.04	3/1732 (0.2%)
2	R	0.69	1/1275 (0.1%)	1.01	3/1732 (0.2%)
All	All	0.62	13/45534 (0.0%)	1.08	294/61488 (0.5%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	1	THR	C-N	14.62	1.52	1.33
2	N	2	THR	N-CA	8.16	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	THR	C-N	7.55	1.43	1.33
2	J	2	THR	CA-C	6.30	1.59	1.52
2	M	2	THR	N-CA	6.16	1.53	1.46
2	P	2	THR	N-CA	6.09	1.53	1.46
2	N	1	THR	C-N	6.02	1.41	1.33
2	J	2	THR	N-CA	5.72	1.53	1.46
2	L	2	THR	N-CA	5.33	1.52	1.46
2	Q	2	THR	N-CA	5.30	1.52	1.46
2	Q	1	THR	C-N	5.22	1.40	1.33
1	A	310	ALA	CA-CB	-5.12	1.45	1.53
2	O	2	THR	N-CA	5.07	1.52	1.46

All (294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	438	ASP	N-CA-C	-12.55	97.07	112.38
1	A	39	GLN	N-CA-C	-11.80	99.58	114.56
1	E	438	ASP	N-CA-C	-11.76	98.03	112.38
1	D	438	ASP	N-CA-C	-11.37	97.56	112.34
1	A	438	ASP	N-CA-C	-11.33	98.56	112.38
1	D	39	GLN	N-CA-C	-11.21	100.32	114.56
1	E	112	ARG	N-CA-C	-10.95	99.42	111.36
1	C	39	GLN	N-CA-C	-10.93	100.68	114.56
1	E	39	GLN	N-CA-C	-10.84	100.79	114.56
1	B	438	ASP	N-CA-C	-10.61	98.55	112.34
1	C	438	ASP	N-CA-C	-10.59	98.20	111.75
1	A	234	LEU	N-CA-C	-10.55	88.32	110.80
1	B	39	GLN	N-CA-C	-10.46	101.28	114.56
1	F	39	GLN	N-CA-C	-9.97	101.89	114.56
2	H	109	ILE	N-CA-C	-9.95	103.28	112.43
1	A	327	LEU	CA-C-N	9.66	129.02	118.97
1	A	327	LEU	C-N-CA	9.66	129.02	118.97
1	B	327	LEU	CA-C-N	9.18	128.51	118.97
1	B	327	LEU	C-N-CA	9.18	128.51	118.97
1	F	327	LEU	CA-C-N	9.08	128.41	118.97
1	F	327	LEU	C-N-CA	9.08	128.41	118.97
1	A	118	LYS	N-CA-C	-8.97	101.07	111.03
2	K	109	ILE	N-CA-C	-8.88	104.26	112.43
2	M	109	ILE	N-CA-C	-8.85	103.78	113.43
1	D	434	VAL	N-CA-C	8.84	127.72	109.34
1	D	327	LEU	CA-C-N	8.76	128.08	118.97
1	D	327	LEU	C-N-CA	8.76	128.08	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	434	VAL	N-CA-C	8.73	127.50	109.34
1	E	37	ARG	N-CA-C	-8.71	99.40	110.19
1	E	434	VAL	N-CA-C	8.63	127.29	109.34
1	A	434	VAL	N-CA-C	8.58	127.19	109.34
1	F	37	ARG	N-CA-C	-8.55	99.59	110.19
1	F	434	VAL	N-CA-C	8.54	127.09	109.34
2	L	109	ILE	N-CA-C	-8.44	104.67	112.43
1	A	37	ARG	N-CA-C	-8.39	99.79	110.19
1	A	436	ASN	N-CA-C	8.37	128.63	110.80
1	V	109	LYS	N-CA-C	-8.36	102.27	114.39
1	A	433	VAL	N-CA-C	8.28	121.15	107.24
2	I	109	ILE	N-CA-C	-8.27	104.82	112.43
1	C	436	ASN	N-CA-C	8.27	128.41	110.80
1	B	436	ASN	N-CA-C	8.01	127.86	110.80
1	B	434	VAL	N-CA-C	7.97	125.92	109.34
1	F	436	ASN	N-CA-C	7.95	127.74	110.80
2	P	109	ILE	N-CA-C	-7.84	104.24	113.42
1	E	436	ASN	N-CA-C	7.83	127.47	110.80
1	W	34	ARG	N-CA-C	-7.82	103.76	113.38
1	F	433	VAL	N-CA-C	7.72	119.56	107.28
1	D	436	ASN	N-CA-C	7.70	127.19	110.80
1	U	34	ARG	N-CA-C	-7.68	103.93	113.38
1	S	34	ARG	N-CA-C	-7.68	103.93	113.38
1	C	49	THR	CA-C-N	7.67	127.73	119.90
1	C	49	THR	C-N-CA	7.67	127.73	119.90
2	Q	109	ILE	N-CA-C	-7.64	105.10	113.43
1	T	34	ARG	N-CA-C	-7.64	103.98	113.38
1	B	433	VAL	N-CA-C	7.62	119.39	107.28
1	V	34	ARG	N-CA-C	-7.59	104.05	113.38
1	D	433	VAL	N-CA-C	7.57	119.96	107.24
1	S	116	ILE	N-CA-C	-7.51	106.17	113.53
2	N	109	ILE	N-CA-C	-7.51	104.64	113.42
1	X	34	ARG	N-CA-C	-7.49	104.17	113.38
1	A	236	ASN	CA-C-N	7.46	127.83	119.32
1	A	236	ASN	C-N-CA	7.46	127.83	119.32
1	C	116	ILE	N-CA-C	-7.41	103.56	110.53
1	X	381	ALA	N-CA-C	-7.37	104.14	113.72
1	C	327	LEU	CA-C-N	7.31	126.57	118.97
1	C	327	LEU	C-N-CA	7.31	126.57	118.97
2	K	82	TRP	N-CA-C	-7.30	103.47	113.18
1	S	381	ALA	N-CA-C	-7.25	104.30	113.72
2	O	109	ILE	N-CA-C	-7.18	105.02	113.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	381	ALA	N-CA-C	-7.17	104.39	113.72
1	V	381	ALA	N-CA-C	-7.17	104.40	113.72
1	C	433	VAL	N-CA-C	7.16	119.26	107.24
1	B	49	THR	CA-C-N	7.11	127.15	119.90
1	B	49	THR	C-N-CA	7.11	127.15	119.90
1	E	433	VAL	N-CA-C	7.07	119.12	107.24
1	T	381	ALA	N-CA-C	-7.02	104.59	113.72
2	L	82	TRP	N-CA-C	-7.02	103.84	113.18
2	L	101	LYS	N-CA-C	7.02	119.96	111.40
1	W	377	ILE	N-CA-C	-6.96	107.10	113.71
1	W	381	ALA	N-CA-C	-6.91	104.73	113.72
1	S	377	ILE	N-CA-C	-6.88	107.18	113.71
1	T	377	ILE	N-CA-C	-6.86	107.19	113.71
1	S	243	LYS	N-CA-C	-6.82	105.24	113.97
2	J	101	LYS	N-CA-C	6.80	119.69	111.40
1	C	433	VAL	CA-C-N	6.79	134.20	121.97
1	C	433	VAL	C-N-CA	6.79	134.20	121.97
1	A	237	PRO	N-CA-C	6.78	123.86	113.75
1	X	377	ILE	N-CA-C	-6.77	107.28	113.71
1	E	49	THR	CA-C-N	6.74	126.77	119.89
1	E	49	THR	C-N-CA	6.74	126.77	119.89
1	V	377	ILE	N-CA-C	-6.70	107.34	113.71
1	A	53	ILE	N-CA-C	6.70	118.12	108.48
2	G	82	TRP	N-CA-C	-6.70	104.28	113.18
2	H	101	LYS	N-CA-C	6.69	119.56	111.40
2	I	82	TRP	N-CA-C	-6.69	104.29	113.18
2	I	102	GLU	N-CA-C	6.68	120.40	109.85
2	R	109	ILE	N-CA-C	-6.66	105.62	113.42
2	J	82	TRP	N-CA-C	-6.65	104.33	113.18
1	F	53	ILE	N-CA-C	6.64	118.04	108.48
2	L	96	ILE	N-CA-C	-6.62	98.08	107.75
1	B	433	VAL	CA-C-N	6.59	133.84	121.97
1	B	433	VAL	C-N-CA	6.59	133.84	121.97
1	A	74	ALA	N-CA-C	-6.57	104.50	113.30
1	F	433	VAL	CA-C-N	6.54	133.74	121.97
1	F	433	VAL	C-N-CA	6.54	133.74	121.97
1	E	433	VAL	CA-C-N	6.52	133.70	121.97
1	E	433	VAL	C-N-CA	6.52	133.70	121.97
1	D	433	VAL	CA-C-N	6.46	133.61	121.97
1	D	433	VAL	C-N-CA	6.46	133.61	121.97
1	T	110	LEU	N-CA-C	-6.45	106.62	114.75
1	U	377	ILE	N-CA-C	-6.44	107.59	113.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	116	GLU	N-CA-C	-6.43	100.94	110.46
1	D	49	THR	CA-C-N	6.42	126.44	119.90
1	D	49	THR	C-N-CA	6.42	126.44	119.90
1	A	433	VAL	CA-C-N	6.41	133.51	121.97
1	A	433	VAL	C-N-CA	6.41	133.51	121.97
2	J	102	GLU	N-CA-C	6.41	119.98	109.85
1	E	327	LEU	CA-C-N	6.41	127.85	119.84
1	E	327	LEU	C-N-CA	6.41	127.85	119.84
1	V	242	GLN	N-CA-C	-6.35	106.49	114.56
1	E	329	ILE	N-CA-C	6.35	116.63	108.12
1	A	234	LEU	CA-CB-CG	6.34	138.48	116.30
2	I	101	LYS	N-CA-C	6.33	119.13	111.40
2	G	101	LYS	N-CA-C	6.33	119.12	111.40
2	I	96	ILE	N-CA-C	-6.31	98.54	107.75
1	C	53	ILE	N-CA-C	6.30	117.56	108.48
2	G	96	ILE	N-CA-C	-6.30	98.45	107.77
1	X	71	ALA	N-CA-C	-6.26	106.24	114.31
2	H	102	GLU	N-CA-C	6.25	119.73	109.85
1	A	233	LYS	N-CA-C	6.25	124.11	110.80
2	G	102	GLU	N-CA-C	6.23	119.70	109.85
1	X	240	LEU	N-CA-C	-6.23	106.05	113.21
1	E	53	ILE	N-CA-C	6.22	117.44	108.48
1	W	71	ALA	N-CA-C	-6.21	106.30	114.31
1	S	71	ALA	N-CA-C	-6.21	106.31	114.31
1	U	71	ALA	N-CA-C	-6.16	106.36	114.31
2	K	96	ILE	N-CA-C	-6.16	98.76	107.75
1	F	335	ALA	N-CA-C	-6.15	101.38	110.48
1	X	244	ALA	N-CA-C	-6.14	105.83	113.38
2	L	46	PHE	N-CA-C	6.13	119.48	109.24
1	E	363	GLU	N-CA-C	-6.13	105.78	113.20
1	E	315	ARG	N-CA-C	-6.12	102.38	110.40
1	T	71	ALA	N-CA-C	-6.12	106.42	114.31
2	H	82	TRP	N-CA-C	-6.10	105.07	113.18
1	X	113	GLN	N-CA-C	-6.08	105.89	113.55
2	J	96	ILE	N-CA-C	-6.08	98.88	107.75
1	C	414	MET	N-CA-C	-6.07	104.71	113.21
2	K	102	GLU	N-CA-C	6.07	119.44	109.85
1	C	234	LEU	N-CA-C	-6.06	103.23	112.99
1	B	74	ALA	N-CA-C	-6.03	105.22	113.30
1	B	238	GLU	N-CA-C	-6.01	105.98	113.38
2	H	46	PHE	N-CA-C	6.00	119.25	109.24
1	T	108	MET	N-CA-C	-5.99	106.02	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	116	ILE	N-CA-C	-5.96	104.70	110.72
2	H	96	ILE	N-CA-C	-5.96	99.06	107.75
2	J	1	THR	CA-C-N	5.95	130.74	121.76
2	J	1	THR	C-N-CA	5.95	130.74	121.76
1	X	246	ASP	N-CA-C	-5.94	105.29	112.54
1	F	49	THR	CA-C-N	5.92	125.94	119.90
1	F	49	THR	C-N-CA	5.92	125.94	119.90
1	B	53	ILE	N-CA-C	5.86	116.92	108.48
1	B	363	GLU	N-CA-C	-5.85	106.12	113.20
2	R	167	PHE	N-CA-C	5.85	119.21	110.14
1	B	108	MET	N-CA-C	-5.81	102.67	111.56
1	V	71	ALA	N-CA-C	-5.80	106.83	114.31
1	D	346	THR	N-CA-C	5.79	120.73	113.43
1	D	53	ILE	N-CA-C	5.75	116.76	108.48
1	D	74	ALA	N-CA-C	-5.73	105.95	113.17
1	E	234	LEU	N-CA-C	-5.72	98.62	110.80
1	A	347	GLU	N-CA-C	5.71	119.93	112.17
1	A	49	THR	CA-C-N	5.68	125.69	119.90
1	A	49	THR	C-N-CA	5.68	125.69	119.90
1	E	414	MET	N-CA-C	-5.66	105.29	113.21
2	R	116	GLU	N-CA-C	-5.66	102.09	110.46
1	X	274	SER	N-CA-C	-5.65	106.43	113.38
1	E	347	GLU	N-CA-C	5.65	120.18	112.55
1	A	240	LEU	N-CA-C	-5.65	105.03	111.07
1	T	274	SER	N-CA-C	-5.64	106.44	113.38
1	E	9	ILE	CB-CA-C	-5.64	104.44	112.22
1	E	74	ALA	N-CA-C	-5.64	105.75	113.30
1	T	363	GLU	N-CA-C	-5.62	106.38	113.18
2	P	116	GLU	N-CA-C	-5.62	102.15	110.46
1	D	315	ARG	N-CA-C	-5.62	103.04	110.40
1	A	329	ILE	N-CA-C	5.61	116.45	107.98
1	B	335	ALA	N-CA-C	-5.59	102.20	110.48
1	W	274	SER	N-CA-C	-5.59	106.50	113.38
1	U	363	GLU	N-CA-C	-5.56	106.45	113.18
1	S	275	ARG	N-CA-C	-5.56	106.34	113.01
1	V	274	SER	N-CA-C	-5.52	106.59	113.38
1	D	347	GLU	N-CA-C	5.51	119.67	112.17
2	K	101	LYS	N-CA-C	5.51	118.12	111.40
1	S	274	SER	N-CA-C	-5.51	106.61	113.38
1	S	363	GLU	N-CA-C	-5.51	106.52	113.18
1	C	57	GLY	CA-C-N	5.50	126.72	119.84
1	C	57	GLY	C-N-CA	5.50	126.72	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	274	SER	N-CA-C	-5.50	106.62	113.38
1	F	9	ILE	CB-CA-C	-5.50	104.64	112.22
1	T	275	ARG	N-CA-C	-5.49	106.42	113.01
1	B	37	ARG	N-CA-C	-5.49	99.11	110.80
1	W	363	GLU	N-CA-C	-5.48	106.55	113.18
1	C	329	ILE	N-CA-C	5.46	116.23	107.98
1	V	99	ILE	N-CA-C	-5.46	105.36	113.39
1	W	99	ILE	N-CA-C	-5.45	105.38	113.39
2	Q	116	GLU	N-CA-C	-5.43	102.43	110.46
1	F	347	GLU	N-CA-C	5.42	119.54	112.17
1	X	363	GLU	N-CA-C	-5.39	106.66	113.18
2	L	103	SER	N-CA-C	-5.39	100.24	109.24
1	D	363	GLU	N-CA-C	-5.38	106.69	113.20
2	L	102	GLU	N-CA-C	5.38	118.36	109.85
2	G	46	PHE	N-CA-C	5.38	118.22	109.24
1	T	99	ILE	N-CA-C	-5.37	105.50	113.39
1	E	346	THR	N-CA-C	5.36	120.19	113.43
1	S	99	ILE	N-CA-C	-5.36	105.51	113.39
1	U	275	ARG	N-CA-C	-5.35	106.59	113.01
1	D	9	ILE	CB-CA-C	-5.35	104.84	112.22
2	I	46	PHE	N-CA-C	5.35	118.17	109.24
2	K	46	PHE	N-CA-C	5.34	118.14	109.06
2	O	116	GLU	N-CA-C	-5.33	102.57	110.46
1	E	319	LEU	N-CA-C	-5.32	103.67	110.53
1	W	275	ARG	N-CA-C	-5.31	106.64	113.01
1	F	47	GLU	N-CA-C	5.31	117.75	111.33
2	O	96	ILE	N-CA-C	-5.31	100.00	107.75
1	C	370	THR	N-CA-C	-5.30	103.53	110.53
2	O	167	PHE	N-CA-C	5.30	118.36	110.14
1	W	443	ILE	N-CA-C	-5.30	101.28	108.06
1	B	9	ILE	CB-CA-C	-5.29	104.91	112.22
1	D	47	GLU	N-CA-C	5.29	117.73	111.33
1	X	275	ARG	N-CA-C	-5.28	106.68	113.01
1	A	57	GLY	CA-C-N	5.27	126.43	119.84
1	A	57	GLY	C-N-CA	5.27	126.43	119.84
1	C	37	ARG	N-CA-C	-5.26	99.60	110.80
2	P	104	LEU	N-CA-C	5.25	116.27	108.86
1	S	327	LEU	CA-C-N	5.25	125.56	119.47
1	S	327	LEU	C-N-CA	5.25	125.56	119.47
1	F	100	ILE	CB-CA-C	-5.25	104.98	112.22
1	A	116	ILE	N-CA-C	-5.24	104.53	111.09
1	X	114	GLN	N-CA-C	-5.24	106.57	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	327	LEU	CA-C-N	5.23	125.54	119.47
1	V	327	LEU	C-N-CA	5.23	125.54	119.47
1	F	74	ALA	N-CA-C	-5.23	106.29	113.30
2	N	167	PHE	N-CA-C	5.23	118.24	110.14
2	P	167	PHE	N-CA-C	5.21	117.80	110.14
1	A	363	GLU	N-CA-C	-5.21	106.90	113.20
1	T	276	GLU	N-CA-C	-5.21	106.71	113.16
2	J	46	PHE	N-CA-C	5.20	117.92	109.24
1	X	324	GLN	N-CA-C	-5.20	106.09	112.90
1	C	363	GLU	N-CA-C	-5.20	106.89	113.18
1	X	99	ILE	N-CA-C	-5.18	105.77	113.39
1	D	276	GLU	N-CA-C	-5.16	105.15	111.75
2	N	91	LEU	N-CA-C	5.16	117.64	109.24
1	U	99	ILE	N-CA-C	-5.15	105.81	113.39
2	I	116	GLU	N-CA-C	-5.15	102.38	110.36
1	A	315	ARG	N-CA-C	-5.15	102.68	110.50
1	C	244	ALA	N-CA-C	-5.14	105.30	112.45
1	W	380	ALA	N-CA-C	-5.14	106.82	114.64
1	X	312	GLN	N-CA-C	-5.14	107.55	113.88
1	V	275	ARG	N-CA-C	-5.14	106.27	112.54
1	A	108	MET	N-CA-C	-5.13	105.14	111.40
1	V	380	ALA	N-CA-C	-5.13	106.83	114.64
1	D	329	ILE	N-CA-C	5.13	115.73	107.98
1	F	329	ILE	N-CA-C	5.12	115.71	107.98
1	W	327	LEU	CA-C-N	5.12	125.41	119.47
1	W	327	LEU	C-N-CA	5.12	125.41	119.47
1	D	37	ARG	N-CA-C	-5.11	99.91	110.80
1	E	335	ALA	N-CA-C	-5.11	102.92	110.48
1	W	324	GLN	N-CA-C	-5.11	106.21	112.90
1	V	363	GLU	N-CA-C	-5.10	107.01	113.18
2	P	96	ILE	N-CA-C	-5.10	100.30	107.75
1	D	100	ILE	CB-CA-C	-5.08	105.43	112.24
1	F	370	THR	N-CA-C	-5.08	103.82	110.53
2	M	116	GLU	N-CA-C	-5.07	102.95	110.46
1	A	310	ALA	N-CA-C	-5.07	105.40	112.45
2	J	67	HIS	N-CA-C	5.07	117.37	110.88
2	M	167	PHE	N-CA-C	5.07	118.00	110.14
1	B	414	MET	N-CA-C	-5.07	104.84	112.99
1	X	327	LEU	CA-C-N	5.06	125.09	119.32
1	X	327	LEU	C-N-CA	5.06	125.09	119.32
1	T	380	ALA	N-CA-C	-5.06	106.95	114.64
1	C	74	ALA	N-CA-C	-5.06	106.52	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	21	SER	N-CA-C	5.05	116.76	108.52
1	W	276	GLU	N-CA-C	-5.05	106.89	113.16
2	H	67	HIS	N-CA-C	5.04	116.49	110.44
1	C	9	ILE	CB-CA-C	-5.04	105.27	112.22
1	B	346	THR	N-CA-C	5.04	121.53	110.80
1	E	116	ILE	N-CA-C	-5.02	107.94	112.96
2	Q	19	GLN	N-CA-C	5.02	116.87	107.99
1	T	324	GLN	N-CA-C	-5.02	106.33	112.90
1	S	276	GLU	N-CA-C	-5.01	106.94	113.16
1	E	248	VAL	CB-CA-C	-5.01	105.41	111.87
1	W	312	GLN	N-CA-C	-5.01	107.72	113.88
1	T	327	LEU	CA-C-N	5.00	125.27	119.47
1	T	327	LEU	C-N-CA	5.00	125.27	119.47
1	X	382	PHE	N-CA-C	-5.00	105.50	112.45
1	A	346	THR	N-CA-C	5.00	119.73	113.43

There are no chirality outliers.

There are no planarity outliers.

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	2488	0	2546	164	0
1	B	2488	0	2546	168	0
1	C	2488	0	2546	161	0
1	D	2488	0	2546	155	0
1	E	2488	0	2546	153	0
1	F	2488	0	2546	160	0
1	S	2469	0	2540	175	0
1	T	2469	0	2540	161	0
1	U	2469	0	2540	160	0
1	V	2469	0	2540	160	0
1	W	2469	0	2540	155	0
1	X	2469	0	2540	163	1
2	G	1290	0	1288	98	0
2	H	1290	0	1288	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1290	0	1288	110	0
2	J	1290	0	1288	110	0
2	K	1290	0	1288	101	0
2	L	1290	0	1288	102	0
2	M	1261	0	1239	113	0
2	N	1261	0	1239	117	0
2	O	1261	0	1239	111	0
2	P	1261	0	1239	127	0
2	Q	1261	0	1239	116	0
2	R	1261	0	1239	115	0
3	A	31	0	12	3	0
3	B	31	0	12	5	0
3	C	31	0	12	8	0
3	D	31	0	12	5	0
3	E	31	0	12	6	0
3	F	31	0	12	4	0
3	S	31	0	12	4	0
3	T	31	0	12	4	0
3	U	31	0	12	5	0
3	V	31	0	12	2	0
3	W	31	0	12	4	0
3	X	31	0	12	3	0
4	G	28	0	36	12	0
4	H	28	0	36	14	0
4	I	28	0	36	16	0
4	J	28	0	36	23	0
4	K	28	0	36	16	0
4	L	28	0	36	14	0
4	M	28	0	36	12	0
4	N	28	0	36	19	0
4	O	28	0	36	13	0
4	P	28	0	36	13	0
4	Q	28	0	36	14	0
4	R	28	0	36	13	0
All	All	45756	0	46254	3015	1

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 33.

All (3015) 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:P:1:THR:HG21	2:P:33:LYS:CD	1.47	1.44
2:G:1:THR:CG2	2:G:33:LYS:CE	1.98	1.41
2:O:1:THR:HG21	2:O:33:LYS:CD	1.50	1.40
2:H:1:THR:HG21	2:H:33:LYS:CE	1.53	1.38
2:G:1:THR:HG21	2:G:33:LYS:CD	1.53	1.38
2:H:1:THR:HG21	2:H:33:LYS:CD	1.52	1.36
2:L:1:THR:HG21	2:L:33:LYS:CD	1.59	1.30
2:M:1:THR:CG2	2:M:33:LYS:HE2	1.62	1.29
2:R:1:THR:HG21	2:R:33:LYS:CD	1.61	1.28
2:O:1:THR:CG2	2:O:33:LYS:CE	2.13	1.27
2:P:1:THR:CG2	2:P:33:LYS:CE	2.12	1.27
2:H:1:THR:HG23	2:H:33:LYS:NZ	1.50	1.26
2:H:1:THR:CG2	2:H:33:LYS:CE	2.15	1.24
2:I:1:THR:HG21	2:I:33:LYS:CD	1.69	1.22
2:K:1:THR:HG21	2:K:33:LYS:CD	1.73	1.17
2:P:1:THR:HG23	2:P:33:LYS:HE2	1.23	1.17
2:Q:1:THR:HG21	2:Q:33:LYS:CD	1.73	1.17
2:G:18:GLY:HA2	2:G:33:LYS:NZ	1.58	1.17
2:O:1:THR:HG21	2:O:33:LYS:HD2	1.16	1.16
2:G:1:THR:HG21	2:G:33:LYS:HD2	1.24	1.15
2:G:1:THR:HG21	2:G:33:LYS:CE	1.64	1.14
2:Q:1:THR:HG21	2:Q:33:LYS:HD2	1.27	1.14
2:P:1:THR:HG21	2:P:33:LYS:HD2	1.14	1.13
2:G:1:THR:HG23	2:G:33:LYS:HE3	1.23	1.13
2:R:1:THR:HG21	2:R:33:LYS:HD2	1.23	1.13
2:M:1:THR:CG2	2:M:33:LYS:CE	2.26	1.12
2:J:1:THR:HG22	2:J:17:ASP:OD1	1.50	1.12
2:M:1:THR:HG21	2:M:33:LYS:HD2	1.23	1.12
2:G:1:THR:CG2	2:G:33:LYS:HE2	1.76	1.11
2:G:56:LEU:CD1	2:G:95:LEU:HG	1.81	1.10
2:N:1:THR:HG21	2:N:33:LYS:CD	1.80	1.10
2:P:1:THR:CG2	2:P:33:LYS:HE2	1.77	1.09
2:R:56:LEU:HD23	2:R:95:LEU:HD13	1.34	1.09
2:L:1:THR:HG23	2:L:33:LYS:HZ2	1.03	1.09
2:L:56:LEU:HD13	2:L:95:LEU:HG	1.34	1.08
2:O:1:THR:CG2	2:O:33:LYS:HE2	1.79	1.08
2:O:1:THR:HG23	2:O:33:LYS:HE2	1.25	1.08
2:J:33:LYS:NZ	4:J:175:LVS:HB32	1.69	1.08
2:H:1:THR:HG21	2:H:33:LYS:HD3	1.31	1.07
2:K:56:LEU:HD13	2:K:95:LEU:HG	1.36	1.07
2:R:1:THR:CG2	2:R:33:LYS:CE	2.33	1.07
1:F:406:LYS:H	1:F:406:LYS:HD2	1.19	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:56:LEU:HD23	2:N:95:LEU:HD13	1.34	1.07
2:M:1:THR:HG21	2:M:33:LYS:CD	1.85	1.06
2:N:1:THR:HG21	2:N:33:LYS:HD2	1.32	1.06
2:P:7:ARG:HE	2:P:12:VAL:HG22	1.21	1.06
2:P:1:THR:CG2	2:P:33:LYS:CD	2.31	1.06
1:B:20:GLN:HA	1:B:20:GLN:HE21	1.16	1.05
2:O:56:LEU:HD23	2:O:95:LEU:HD13	1.36	1.05
1:E:20:GLN:HA	1:E:20:GLN:HE21	1.18	1.05
2:M:1:THR:HG23	2:M:33:LYS:HE2	1.11	1.05
2:O:1:THR:CG2	2:O:33:LYS:CD	2.33	1.05
2:Q:56:LEU:HD23	2:Q:95:LEU:HD13	1.39	1.05
1:B:406:LYS:H	1:B:406:LYS:HD2	1.19	1.04
2:K:1:THR:CG2	2:K:33:LYS:HD3	1.87	1.04
2:L:1:THR:HG23	2:L:33:LYS:NZ	1.72	1.04
2:M:7:ARG:HE	2:M:12:VAL:HG22	1.22	1.04
2:M:56:LEU:HD23	2:M:95:LEU:HD13	1.38	1.04
2:P:1:THR:CG2	2:P:33:LYS:HD2	1.88	1.04
2:G:18:GLY:CA	2:G:33:LYS:HZ1	1.70	1.03
2:H:1:THR:CG2	2:H:33:LYS:CD	2.36	1.03
1:C:20:GLN:HA	1:C:20:GLN:HE21	1.20	1.03
2:G:1:THR:H1	4:G:175:LVS:H1'1	1.23	1.03
2:P:1:THR:HG21	2:P:33:LYS:CE	1.80	1.03
2:R:1:THR:CG2	2:R:33:LYS:CD	2.35	1.03
2:H:1:THR:HG21	2:H:33:LYS:HE2	1.39	1.03
2:J:56:LEU:HD13	2:J:95:LEU:HG	1.40	1.02
1:C:406:LYS:H	1:C:406:LYS:HD2	1.23	1.02
2:Q:7:ARG:HE	2:Q:12:VAL:HG22	1.22	1.02
2:R:1:THR:CG2	2:R:33:LYS:HD2	1.89	1.02
2:L:1:THR:CG2	2:L:33:LYS:CD	2.38	1.02
2:R:7:ARG:HE	2:R:12:VAL:HG22	1.20	1.02
2:H:56:LEU:CD1	2:H:95:LEU:HG	1.90	1.02
2:L:1:THR:CG2	2:L:33:LYS:CE	2.37	1.01
2:K:56:LEU:CD1	2:K:95:LEU:HG	1.90	1.01
2:O:1:THR:CG2	2:O:33:LYS:HD2	1.90	1.01
2:L:1:THR:HG21	2:L:33:LYS:HD3	1.03	1.01
2:N:7:ARG:HE	2:N:12:VAL:HG22	1.23	1.01
1:A:406:LYS:H	1:A:406:LYS:HD2	1.24	1.00
2:G:1:THR:CG2	2:G:33:LYS:HE3	1.75	1.00
2:H:1:THR:CG2	2:H:33:LYS:NZ	2.21	1.00
2:O:7:ARG:HE	2:O:12:VAL:HG22	1.23	1.00
1:F:20:GLN:HA	1:F:20:GLN:HE21	1.25	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:56:LEU:HD23	2:P:95:LEU:HD13	1.43	1.00
2:I:56:LEU:HD13	2:I:95:LEU:HG	1.43	1.00
2:Q:1:THR:CG2	2:Q:33:LYS:HD2	1.93	0.99
2:I:1:THR:CG2	2:I:33:LYS:HD3	1.91	0.99
2:G:18:GLY:CA	2:G:33:LYS:NZ	2.22	0.99
1:D:406:LYS:H	1:D:406:LYS:HD2	1.25	0.98
2:O:49:GLY:HA2	4:O:175:LVS:HA2	1.43	0.98
2:K:1:THR:HG23	2:K:33:LYS:HZ1	1.29	0.98
2:N:49:GLY:HA2	4:N:175:LVS:HA2	1.45	0.98
2:O:1:THR:HG23	2:O:33:LYS:CE	1.86	0.98
2:R:49:GLY:HA2	4:R:175:LVS:HA2	1.45	0.98
2:N:1:THR:HG23	2:N:33:LYS:HE2	1.44	0.98
2:P:49:GLY:HA2	4:P:175:LVS:HA2	1.45	0.98
2:Q:49:GLY:HA2	4:Q:175:LVS:HA2	1.40	0.98
2:I:56:LEU:CD1	2:I:95:LEU:HG	1.91	0.98
1:C:20:GLN:HE21	1:C:20:GLN:CA	1.78	0.97
1:C:79:ILE:HG22	1:C:103:LEU:HD13	1.43	0.97
2:J:56:LEU:CD1	2:J:95:LEU:HG	1.94	0.96
1:A:232:ALA:O	1:A:233:LYS:HB2	1.61	0.96
2:N:1:THR:CG2	2:N:33:LYS:CE	2.43	0.96
2:G:1:THR:N	4:G:175:LVS:H1'1	1.80	0.96
2:H:1:THR:CG2	2:H:33:LYS:HE2	1.93	0.96
2:Q:1:THR:CG2	2:Q:33:LYS:CD	2.43	0.96
2:I:1:THR:HG21	2:I:33:LYS:HD3	0.98	0.96
1:B:391:ILE:HG22	1:C:321:PRO:HB3	1.47	0.96
1:W:120:ARG:H	1:W:120:ARG:HD2	1.26	0.96
1:E:406:LYS:H	1:E:406:LYS:HD2	1.29	0.95
2:L:56:LEU:CD1	2:L:95:LEU:HG	1.97	0.95
2:M:49:GLY:HA2	4:M:175:LVS:HA2	1.48	0.94
2:P:1:THR:HG23	2:P:33:LYS:CE	1.85	0.94
2:H:33:LYS:HE2	4:H:175:LVS:HB32	1.48	0.94
2:G:1:THR:HG22	2:G:33:LYS:HE2	1.48	0.94
1:A:55:MET:HE3	1:A:306:ILE:HG21	1.48	0.94
2:K:1:THR:HG23	2:K:33:LYS:NZ	1.81	0.94
2:O:1:THR:HG21	2:O:33:LYS:CE	1.83	0.94
2:K:1:THR:HG21	2:K:33:LYS:HD3	0.94	0.94
2:Q:1:THR:CG2	2:Q:33:LYS:CE	2.45	0.94
2:K:1:THR:CG2	2:K:33:LYS:NZ	2.31	0.93
1:D:20:GLN:HE21	1:D:20:GLN:HA	1.33	0.93
1:B:20:GLN:HE21	1:B:20:GLN:CA	1.82	0.93
1:E:20:GLN:HE21	1:E:20:GLN:CA	1.80	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:THR:CG2	2:I:33:LYS:NZ	2.32	0.93
1:E:27:VAL:HB	1:E:70:LEU:HD22	1.51	0.92
1:F:79:ILE:HG22	1:F:103:LEU:HD13	1.50	0.92
2:I:1:THR:HG23	2:I:33:LYS:NZ	1.84	0.92
1:B:55:MET:HE3	1:B:306:ILE:HG21	1.49	0.92
2:H:56:LEU:HD13	2:H:95:LEU:HG	1.49	0.92
2:H:1:THR:H1	4:H:175:LVS:H1'1	1.35	0.91
1:A:20:GLN:HE21	1:A:20:GLN:HA	1.35	0.91
2:G:86:ARG:HB3	2:G:86:ARG:HH11	1.34	0.91
2:I:86:ARG:HB3	2:I:86:ARG:HH11	1.33	0.91
2:L:1:THR:CG2	2:L:33:LYS:HZ2	1.84	0.91
2:I:105:ILE:HG23	2:I:113:VAL:HB	1.53	0.91
2:K:1:THR:HG22	2:K:17:ASP:OD1	1.68	0.91
2:L:1:THR:CG2	2:L:33:LYS:NZ	2.33	0.91
2:H:1:THR:HG23	2:H:33:LYS:HZ1	1.35	0.90
1:A:391:ILE:HG22	1:B:321:PRO:HB3	1.51	0.90
1:D:55:MET:HE3	1:D:306:ILE:HG21	1.51	0.90
1:A:409:PHE:CD1	1:B:6:PRO:HB3	2.07	0.90
1:C:55:MET:HE3	1:C:306:ILE:HG21	1.52	0.90
2:K:17:ASP:O	2:K:33:LYS:HD2	1.72	0.90
2:H:86:ARG:HB3	2:H:86:ARG:HH11	1.35	0.89
2:R:1:THR:CG2	2:R:33:LYS:NZ	2.36	0.89
2:Q:17:ASP:O	2:Q:33:LYS:HG3	1.73	0.89
2:J:105:ILE:HG23	2:J:113:VAL:HB	1.53	0.89
1:E:55:MET:HE3	1:E:306:ILE:HG21	1.55	0.89
2:I:1:THR:CG2	2:I:33:LYS:CD	2.49	0.88
2:J:86:ARG:HB3	2:J:86:ARG:HH11	1.37	0.88
1:A:233:LYS:HD3	1:A:235:ILE:HG13	1.54	0.88
1:F:20:GLN:HE21	1:F:20:GLN:CA	1.86	0.88
2:L:86:ARG:HB3	2:L:86:ARG:HH11	1.36	0.88
1:B:409:PHE:CD1	1:C:6:PRO:HB3	2.08	0.88
2:N:1:THR:CG2	2:N:33:LYS:HE2	2.01	0.88
2:M:17:ASP:O	2:M:33:LYS:HG3	1.73	0.88
2:I:1:THR:CG2	2:I:33:LYS:CE	2.52	0.87
1:X:439:LEU:HD23	1:X:439:LEU:H	1.36	0.87
1:A:405:ASP:HB3	1:A:406:LYS:HD2	1.56	0.87
2:K:86:ARG:HB3	2:K:86:ARG:HH11	1.39	0.87
2:R:137:LEU:O	2:R:141:THR:HG22	1.75	0.87
2:M:1:THR:HG21	2:M:33:LYS:CE	2.04	0.87
1:D:79:ILE:HG22	1:D:103:LEU:HD13	1.55	0.86
1:V:439:LEU:HD23	1:V:439:LEU:H	1.38	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1:THR:N	4:G:175:LVS:CS	2.37	0.86
1:B:405:ASP:HB3	1:B:406:LYS:HD2	1.56	0.86
2:L:1:THR:HG21	2:L:33:LYS:CE	2.03	0.86
1:A:235:ILE:HG22	1:A:237:PRO:HD3	1.56	0.86
1:B:443:ILE:HD11	2:H:72:LEU:HD11	1.58	0.86
1:F:55:MET:HE3	1:F:306:ILE:HG21	1.57	0.86
2:I:1:THR:CG2	2:I:33:LYS:HZ2	1.87	0.86
2:K:105:ILE:HG23	2:K:113:VAL:HB	1.56	0.86
2:H:7:ARG:HD2	2:H:119:GLN:HG2	1.58	0.86
2:R:1:THR:HG23	2:R:33:LYS:CE	2.06	0.86
2:H:1:THR:HG23	2:H:33:LYS:HZ3	1.37	0.85
2:K:7:ARG:HD2	2:K:119:GLN:HG2	1.57	0.85
1:C:27:VAL:HB	1:C:70:LEU:HD22	1.56	0.85
2:I:1:THR:HG22	2:I:17:ASP:OD1	1.76	0.85
2:I:7:ARG:HD2	2:I:119:GLN:HG2	1.58	0.85
1:A:27:VAL:HB	1:A:70:LEU:HD22	1.56	0.85
2:G:56:LEU:HD13	2:G:95:LEU:HG	1.57	0.85
2:L:125:SER:H	4:L:175:LVS:H1'2	1.42	0.85
2:J:83:ARG:HG3	2:K:55:THR:HG22	1.58	0.84
1:V:279:GLN:HE21	1:V:320:ILE:HG12	1.42	0.84
1:D:405:ASP:HB3	1:D:406:LYS:HD2	1.59	0.84
1:S:439:LEU:H	1:S:439:LEU:HD23	1.40	0.84
1:T:439:LEU:HD23	1:T:439:LEU:H	1.42	0.84
1:C:391:ILE:HG22	1:D:321:PRO:HB3	1.60	0.84
1:E:367:ILE:HD11	1:E:421:ILE:HD11	1.59	0.84
2:L:1:THR:N	4:L:175:LVS:CS	2.40	0.84
1:A:110:LEU:O	1:A:114:GLN:HB2	1.77	0.84
2:H:105:ILE:HG23	2:H:113:VAL:HB	1.58	0.84
1:W:439:LEU:HD23	1:W:439:LEU:H	1.40	0.84
2:L:1:THR:HG22	2:L:17:ASP:OD1	1.78	0.84
1:U:439:LEU:HD23	1:U:439:LEU:H	1.42	0.84
1:E:402:ARG:HH22	1:E:433:VAL:HG21	1.43	0.84
1:T:279:GLN:HE21	1:T:320:ILE:HG12	1.43	0.84
2:J:7:ARG:HD2	2:J:119:GLN:HG2	1.59	0.83
1:A:20:GLN:HE21	1:A:20:GLN:CA	1.91	0.83
1:C:405:ASP:HB3	1:C:406:LYS:HD2	1.58	0.83
2:O:1:THR:CG2	2:O:33:LYS:NZ	2.40	0.83
2:I:1:THR:H1	4:I:175:LVS:H1'1	1.41	0.83
2:K:125:SER:H	4:K:175:LVS:H1'2	1.42	0.83
2:M:17:ASP:C	2:M:33:LYS:HZ2	1.86	0.83
1:A:6:PRO:HB3	1:F:409:PHE:CD1	2.14	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:279:GLN:HE22	1:U:320:ILE:H	1.27	0.83
1:F:405:ASP:HB3	1:F:406:LYS:HD2	1.61	0.83
2:G:105:ILE:HG23	2:G:113:VAL:HB	1.59	0.83
2:H:1:THR:HG22	2:H:17:ASP:OD1	1.78	0.83
1:C:60:GLY:HA2	3:C:452:ATP:O3A	1.79	0.83
2:J:1:THR:N	4:J:175:LVS:CS	2.41	0.83
2:P:1:THR:CG2	2:P:33:LYS:NZ	2.41	0.82
1:U:279:GLN:HE21	1:U:320:ILE:HG12	1.44	0.82
2:I:1:THR:HG21	2:I:33:LYS:CE	2.10	0.82
2:R:1:THR:HG23	2:R:33:LYS:HE2	1.60	0.82
1:X:279:GLN:HE22	1:X:320:ILE:H	1.27	0.82
2:G:1:THR:HG22	2:G:17:ASP:OD1	1.79	0.82
2:L:7:ARG:HD2	2:L:119:GLN:HG2	1.62	0.82
2:R:1:THR:HG22	2:R:33:LYS:NZ	1.95	0.82
1:S:279:GLN:HE21	1:S:320:ILE:HG12	1.45	0.82
1:D:20:GLN:HE21	1:D:20:GLN:CA	1.92	0.82
1:E:443:ILE:HD11	2:K:72:LEU:HD11	1.61	0.82
2:I:33:LYS:NZ	4:I:175:LVS:HB32	1.95	0.82
2:N:1:THR:CG2	2:N:33:LYS:HD2	2.10	0.81
1:U:279:GLN:NE2	1:U:320:ILE:H	1.78	0.81
1:X:279:GLN:HE21	1:X:320:ILE:HG12	1.44	0.81
2:M:17:ASP:C	2:M:33:LYS:NZ	2.38	0.81
2:R:42:VAL:HG12	2:R:99:ASP:HB3	1.63	0.81
1:S:12:GLU:HG2	1:S:73:LEU:HD23	1.60	0.81
1:B:79:ILE:HG22	1:B:103:LEU:HD13	1.60	0.81
1:W:12:GLU:HG2	1:W:73:LEU:HD23	1.62	0.81
2:H:33:LYS:CE	4:H:175:LVS:HB32	2.10	0.81
1:S:18:ILE:HD11	1:S:343:ARG:NH2	1.95	0.81
1:T:12:GLU:HG2	1:T:73:LEU:HD23	1.63	0.81
2:G:3:ILE:HG22	2:G:96:ILE:HD12	1.62	0.81
2:M:137:LEU:O	2:M:141:THR:HG22	1.79	0.81
1:E:404:MET:O	1:E:408:SER:HB2	1.80	0.81
2:K:1:THR:CG2	2:K:33:LYS:CD	2.51	0.81
1:U:12:GLU:HG2	1:U:73:LEU:HD23	1.63	0.81
1:A:233:LYS:HD3	1:A:235:ILE:CG1	2.10	0.80
1:X:12:GLU:HG2	1:X:73:LEU:HD23	1.62	0.80
2:K:1:THR:CG2	2:K:33:LYS:CE	2.59	0.80
1:V:279:GLN:NE2	1:V:320:ILE:H	1.79	0.80
1:D:402:ARG:HH22	1:D:433:VAL:HG21	1.44	0.80
2:N:1:THR:N	4:N:175:LVS:S	2.55	0.80
1:T:279:GLN:HE22	1:T:320:ILE:H	1.28	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:125:SER:H	4:K:175:LVS:C1'	1.94	0.80
2:K:83:ARG:HG3	2:L:55:THR:HG22	1.64	0.80
2:Q:137:LEU:O	2:Q:141:THR:HG22	1.82	0.80
2:G:17:ASP:O	2:G:33:LYS:NZ	2.15	0.80
1:B:360:MET:HE1	1:C:36:ARG:NH1	1.97	0.80
2:N:1:THR:HG23	2:N:33:LYS:CE	2.10	0.80
2:O:137:LEU:O	2:O:141:THR:HG22	1.82	0.80
2:Q:1:THR:HG23	2:Q:33:LYS:HE2	1.62	0.80
1:T:7:ARG:HH12	1:U:410:SER:HB3	1.45	0.80
1:C:402:ARG:HH22	1:C:433:VAL:HG21	1.47	0.79
1:X:369:PHE:HE2	1:X:421:ILE:HD12	1.47	0.79
1:B:362:THR:CG2	1:C:39:GLN:HG2	2.13	0.79
1:E:367:ILE:HD11	1:E:421:ILE:CD1	2.12	0.79
1:D:391:ILE:HG22	1:E:321:PRO:HB3	1.64	0.79
2:J:33:LYS:HZ3	4:J:175:LVS:HB32	1.47	0.79
2:N:1:THR:CG2	2:N:33:LYS:CD	2.59	0.79
1:D:108:MET:HE1	1:D:240:LEU:HG	1.64	0.79
2:G:7:ARG:HD2	2:G:119:GLN:HG2	1.63	0.79
1:T:279:GLN:NE2	1:T:320:ILE:H	1.81	0.79
1:V:279:GLN:HE22	1:V:320:ILE:H	1.29	0.79
1:W:279:GLN:HE21	1:W:320:ILE:HG12	1.47	0.79
2:O:42:VAL:HG12	2:O:99:ASP:HB3	1.64	0.79
1:S:105:ASP:HB3	1:X:297:MET:HE2	1.63	0.79
1:V:12:GLU:HG2	1:V:73:LEU:HD23	1.63	0.79
1:X:279:GLN:NE2	1:X:320:ILE:H	1.80	0.79
2:J:1:THR:CG2	2:J:33:LYS:NZ	2.45	0.78
2:J:125:SER:H	4:J:175:LVS:C1'	1.97	0.78
2:O:125:SER:H	4:O:175:LVS:C1'	1.96	0.78
2:H:1:THR:N	4:H:175:LVS:CS	2.46	0.78
2:J:1:THR:HG21	2:J:33:LYS:NZ	1.99	0.78
2:I:1:THR:N	4:I:175:LVS:CS	2.45	0.78
1:S:279:GLN:HE22	1:S:320:ILE:H	1.30	0.78
1:A:79:ILE:HG22	1:A:103:LEU:HD13	1.64	0.78
2:J:125:SER:H	4:J:175:LVS:H1'2	1.48	0.78
1:S:279:GLN:NE2	1:S:320:ILE:H	1.80	0.78
1:U:388:THR:HG22	1:U:389:GLU:H	1.47	0.78
1:E:79:ILE:HG22	1:E:103:LEU:HD13	1.65	0.78
2:N:137:LEU:O	2:N:141:THR:HG22	1.81	0.78
2:Q:17:ASP:CG	2:Q:33:LYS:NZ	2.42	0.78
2:H:1:THR:N	4:H:175:LVS:H1'1	1.98	0.78
2:O:125:SER:H	4:O:175:LVS:H1'2	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1:THR:N	4:N:175:LVS:O1'	2.15	0.78
2:L:105:ILE:HG23	2:L:113:VAL:HB	1.66	0.77
2:J:33:LYS:HZ1	4:J:175:LVS:HB32	1.46	0.77
2:P:42:VAL:HG12	2:P:99:ASP:HB3	1.63	0.77
2:K:46:PHE:HB3	2:K:95:LEU:HD23	1.64	0.77
1:V:369:PHE:HE2	1:V:421:ILE:HD12	1.50	0.77
1:E:405:ASP:HB3	1:E:406:LYS:HD2	1.66	0.77
1:S:388:THR:HG22	1:S:389:GLU:H	1.50	0.77
1:E:119:ASN:O	1:E:234:LEU:HD12	1.84	0.77
2:H:83:ARG:HG3	2:I:55:THR:HG22	1.66	0.77
2:L:1:THR:CG2	2:L:33:LYS:HD3	1.99	0.77
1:B:409:PHE:CE1	1:C:6:PRO:HB3	2.19	0.77
2:Q:125:SER:H	4:Q:175:LVS:H1'2	1.50	0.77
1:B:403:LEU:HD23	1:B:404:MET:N	2.00	0.77
1:D:443:ILE:HD11	2:J:72:LEU:HD11	1.66	0.77
2:I:46:PHE:HB3	2:I:95:LEU:HD23	1.67	0.77
1:W:279:GLN:NE2	1:W:320:ILE:H	1.83	0.76
1:A:367:ILE:HD11	1:A:421:ILE:CD1	2.16	0.76
2:K:3:ILE:HG22	2:K:96:ILE:HD12	1.68	0.76
2:Q:42:VAL:HG12	2:Q:99:ASP:HB3	1.66	0.76
2:H:46:PHE:HB3	2:H:95:LEU:HD23	1.68	0.76
2:R:17:ASP:O	2:R:33:LYS:HG3	1.84	0.76
1:W:369:PHE:HE2	1:W:421:ILE:HD12	1.49	0.76
2:M:42:VAL:HG12	2:M:99:ASP:HB3	1.67	0.76
2:P:137:LEU:O	2:P:141:THR:HG22	1.85	0.76
1:E:440:SER:O	1:E:442:PHE:N	2.18	0.76
1:A:402:ARG:HH22	1:A:433:VAL:HG21	1.51	0.76
1:F:406:LYS:HD2	1:F:406:LYS:N	2.00	0.76
2:K:1:THR:N	4:K:175:LVS:CS	2.48	0.76
1:U:323:LEU:O	1:U:323:LEU:HD23	1.85	0.76
2:G:46:PHE:HB3	2:G:95:LEU:HD23	1.67	0.76
2:N:125:SER:H	4:N:175:LVS:H1'2	1.51	0.76
2:P:7:ARG:HH21	2:P:12:VAL:HG21	1.50	0.76
1:E:437:GLU:C	1:E:439:LEU:N	2.41	0.76
2:N:1:THR:HG21	2:N:33:LYS:CE	2.13	0.76
1:U:369:PHE:HE2	1:U:421:ILE:HD12	1.51	0.76
1:V:388:THR:HG22	1:V:389:GLU:H	1.51	0.76
2:L:46:PHE:HB3	2:L:95:LEU:HD23	1.68	0.76
1:A:39:GLN:HG2	1:F:362:THR:CG2	2.16	0.76
3:E:454:ATP:C8	3:E:454:ATP:H5'1	2.21	0.75
1:X:388:THR:HG22	1:X:389:GLU:H	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1:THR:HG21	2:J:33:LYS:HZ2	1.49	0.75
1:B:402:ARG:HH22	1:B:433:VAL:HG21	1.48	0.75
1:E:38:MET:HA	1:E:45:ARG:HD2	1.69	0.75
2:K:37:LEU:HD21	2:K:57:PHE:CZ	2.21	0.75
1:V:441:ARG:HB3	1:V:442:PHE:CD1	2.20	0.75
2:M:18:GLY:H	2:M:164:ASN:HD21	1.35	0.75
1:T:241:LYS:HE3	1:T:295:HIS:HA	1.66	0.75
1:A:108:MET:HE3	1:A:240:LEU:HG	1.69	0.75
2:Q:64:LEU:HD23	2:Q:74:SER:OG	1.85	0.75
1:W:279:GLN:HE22	1:W:320:ILE:H	1.32	0.75
1:W:388:THR:HG22	1:W:389:GLU:H	1.52	0.75
2:P:64:LEU:HD23	2:P:74:SER:OG	1.86	0.75
1:D:402:ARG:NH2	1:D:433:VAL:HG21	2.00	0.75
1:F:443:ILE:HD11	2:L:72:LEU:HD11	1.66	0.75
1:F:27:VAL:HB	1:F:70:LEU:HD22	1.69	0.74
1:F:119:ASN:ND2	1:F:234:LEU:HD12	2.01	0.74
2:K:13:VAL:HG22	2:K:171:GLU:HB3	1.67	0.74
2:L:164:ASN:HD22	2:L:164:ASN:C	1.95	0.74
1:X:20:GLN:OE1	1:X:333:LEU:HB3	1.87	0.74
1:C:108:MET:HE1	1:C:241:LYS:HG2	1.67	0.74
2:L:13:VAL:HG22	2:L:171:GLU:HB3	1.68	0.74
2:M:7:ARG:HH21	2:M:12:VAL:HG21	1.51	0.74
1:S:15:GLN:O	1:S:348:PRO:HA	1.87	0.74
1:S:369:PHE:HE2	1:S:421:ILE:HD12	1.50	0.74
1:A:406:LYS:HD2	1:A:406:LYS:N	2.02	0.74
2:R:1:THR:HG21	2:R:33:LYS:HD3	1.66	0.74
1:U:20:GLN:OE1	1:U:333:LEU:HB3	1.86	0.74
1:C:38:MET:HA	1:C:45:ARG:HD2	1.68	0.74
2:O:18:GLY:H	2:O:164:ASN:HD21	1.35	0.74
1:T:388:THR:HG22	1:T:389:GLU:H	1.51	0.74
1:A:6:PRO:HB3	1:F:409:PHE:CE1	2.23	0.74
2:J:1:THR:H3	4:J:175:LVS:C2'	1.99	0.74
2:K:1:THR:HG23	2:K:33:LYS:CE	2.17	0.74
2:N:7:ARG:NE	2:N:12:VAL:HG22	2.02	0.74
2:N:42:VAL:HG12	2:N:99:ASP:HB3	1.68	0.74
1:W:439:LEU:O	1:W:441:ARG:N	2.21	0.74
1:A:270:GLY:C	1:A:272:ASP:H	1.93	0.74
2:L:1:THR:H3	4:L:175:LVS:C2'	2.00	0.74
1:T:323:LEU:HD23	1:T:323:LEU:O	1.86	0.74
1:D:60:GLY:HA2	3:D:453:ATP:O3A	1.88	0.74
2:I:83:ARG:HG3	2:J:55:THR:HG22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:48:GLY:H	4:G:175:LVS:H2'	1.52	0.74
2:J:83:ARG:CG	2:K:55:THR:HG22	2.17	0.74
2:M:64:LEU:HD23	2:M:74:SER:OG	1.88	0.73
1:S:410:SER:HB3	1:X:7:ARG:HH12	1.53	0.73
1:V:20:GLN:OE1	1:V:333:LEU:HB3	1.87	0.73
1:C:403:LEU:HD23	1:C:404:MET:N	2.02	0.73
1:E:391:ILE:HG22	1:F:321:PRO:HB3	1.70	0.73
2:J:46:PHE:HB3	2:J:95:LEU:HD23	1.68	0.73
1:C:443:ILE:HD11	2:I:72:LEU:HD11	1.70	0.73
2:I:1:THR:N	4:I:175:LVS:H1'1	2.02	0.73
2:R:1:THR:CG2	2:R:33:LYS:HE2	2.18	0.73
1:S:20:GLN:OE1	1:S:333:LEU:HB3	1.89	0.73
1:S:323:LEU:O	1:S:323:LEU:HD23	1.87	0.73
1:A:403:LEU:HD23	1:A:404:MET:N	2.01	0.73
2:G:83:ARG:HG3	2:H:55:THR:HG22	1.68	0.73
1:A:55:MET:HE3	1:A:306:ILE:CG2	2.17	0.73
1:B:406:LYS:HD2	1:B:406:LYS:N	2.00	0.73
1:D:38:MET:HA	1:D:45:ARG:HD2	1.70	0.73
2:I:1:THR:HG21	2:I:33:LYS:HZ2	1.50	0.73
1:A:437:GLU:C	1:A:439:LEU:N	2.45	0.73
2:L:1:THR:HG23	2:L:33:LYS:CE	2.10	0.73
1:F:23:ALA:HA	1:F:331:VAL:HG21	1.71	0.73
1:B:23:ALA:HA	1:B:331:VAL:HG21	1.70	0.73
2:J:48:GLY:H	4:J:175:LVS:H2'	1.54	0.73
2:Q:7:ARG:HH21	2:Q:12:VAL:HG21	1.52	0.73
1:T:20:GLN:OE1	1:T:333:LEU:HB3	1.88	0.73
1:W:441:ARG:HB3	1:W:442:PHE:CD1	2.24	0.73
1:F:437:GLU:C	1:F:439:LEU:N	2.41	0.72
1:T:369:PHE:HE2	1:T:421:ILE:HD12	1.52	0.72
1:D:367:ILE:HD11	1:D:421:ILE:CD1	2.18	0.72
2:I:1:THR:H1	4:I:175:LVS:CS	2.02	0.72
1:B:437:GLU:C	1:B:439:LEU:N	2.38	0.72
1:D:406:LYS:HD2	1:D:406:LYS:N	2.03	0.72
2:P:7:ARG:NE	2:P:12:VAL:HG22	2.02	0.72
1:T:328:PRO:HA	1:U:398:THR:HG22	1.70	0.72
1:B:38:MET:HA	1:B:45:ARG:HD2	1.70	0.72
1:E:402:ARG:NH2	1:E:433:VAL:HG21	2.04	0.72
2:J:1:THR:N	4:J:175:LVS:S	2.62	0.72
2:J:105:ILE:CG2	2:J:113:VAL:HB	2.19	0.72
2:I:33:LYS:HZ2	4:I:175:LVS:HB32	1.53	0.72
2:K:105:ILE:CG2	2:K:113:VAL:HB	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:18:GLY:N	2:Q:33:LYS:HZ1	1.88	0.72
1:W:323:LEU:HD23	1:W:323:LEU:O	1.88	0.72
1:A:38:MET:HA	1:A:45:ARG:HD2	1.71	0.72
1:C:403:LEU:HD23	1:C:403:LEU:C	2.15	0.72
1:C:437:GLU:C	1:C:439:LEU:N	2.43	0.72
2:N:125:SER:H	4:N:175:LVS:C1'	2.01	0.72
1:T:441:ARG:HB3	1:T:442:PHE:CD1	2.24	0.72
2:N:64:LEU:HD23	2:N:74:SER:OG	1.89	0.72
2:P:125:SER:H	4:P:175:LVS:H1'2	1.53	0.72
2:G:1:THR:H3	4:G:175:LVS:C2'	2.02	0.71
2:N:7:ARG:HH21	2:N:12:VAL:HG21	1.53	0.71
1:U:395:ARG:O	1:U:399:VAL:HG23	1.90	0.71
1:V:18:ILE:HD11	1:V:343:ARG:NH2	2.05	0.71
2:H:13:VAL:HG22	2:H:171:GLU:HB3	1.72	0.71
1:B:111:VAL:HG21	1:B:244:ALA:HA	1.72	0.71
2:Q:18:GLY:H	2:Q:164:ASN:HD21	1.36	0.71
1:A:403:LEU:HD23	1:A:403:LEU:C	2.14	0.71
1:B:55:MET:HE3	1:B:306:ILE:CG2	2.20	0.71
1:B:402:ARG:NH2	1:B:433:VAL:HG21	2.05	0.71
2:G:18:GLY:HA2	2:G:33:LYS:HZ3	1.50	0.71
2:G:55:THR:HG22	2:L:83:ARG:HG3	1.71	0.71
2:G:1:THR:H1	4:G:175:LVS:C1'	2.03	0.71
2:G:18:GLY:N	2:G:33:LYS:HZ1	1.87	0.71
3:B:451:ATP:C8	3:B:451:ATP:H5'1	2.25	0.71
1:F:406:LYS:H	1:F:406:LYS:CD	2.02	0.71
2:J:17:ASP:O	2:J:33:LYS:CD	2.39	0.71
2:R:125:SER:H	4:R:175:LVS:H1'2	1.54	0.71
1:S:441:ARG:HB3	1:S:442:PHE:CD1	2.26	0.71
1:A:58:PRO:HG2	1:A:61:VAL:HG11	1.73	0.71
1:B:37:ARG:HD2	1:B:48:VAL:HG13	1.72	0.71
3:E:454:ATP:H5'1	3:E:454:ATP:H8	1.53	0.71
2:I:13:VAL:HG22	2:I:171:GLU:HB3	1.72	0.71
1:D:409:PHE:CD1	1:E:6:PRO:HB3	2.25	0.71
2:R:7:ARG:HH21	2:R:12:VAL:HG21	1.53	0.71
2:I:1:THR:HG21	2:I:33:LYS:NZ	2.05	0.71
1:S:75:ASN:HD21	1:S:110:LEU:HD21	1.56	0.71
2:J:13:VAL:HG22	2:J:171:GLU:HB3	1.73	0.70
2:P:131:LEU:HD11	2:P:135:ARG:NE	2.06	0.70
2:R:18:GLY:H	2:R:164:ASN:HD21	1.37	0.70
1:X:439:LEU:O	1:X:441:ARG:N	2.24	0.70
1:A:367:ILE:HD11	1:A:421:ILE:HD11	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:VAL:HB	1:B:70:LEU:HD22	1.72	0.70
1:D:270:GLY:C	1:D:272:ASP:H	1.99	0.70
2:K:48:GLY:H	4:K:175:LVS:H2'	1.56	0.70
2:K:83:ARG:CG	2:L:55:THR:HG22	2.19	0.70
1:U:441:ARG:HB3	1:U:442:PHE:CD1	2.26	0.70
1:W:15:GLN:O	1:W:348:PRO:HA	1.90	0.70
1:A:321:PRO:HB3	1:F:391:ILE:HG22	1.72	0.70
2:M:125:SER:H	4:M:175:LVS:H1'2	1.56	0.70
2:P:18:GLY:H	2:P:164:ASN:HD21	1.38	0.70
2:R:125:SER:H	4:R:175:LVS:C1'	2.05	0.70
1:X:441:ARG:HB3	1:X:442:PHE:CD1	2.26	0.70
2:R:7:ARG:NE	2:R:12:VAL:HG22	2.02	0.70
2:G:13:VAL:HG22	2:G:171:GLU:HB3	1.73	0.70
1:T:279:GLN:NE2	1:T:320:ILE:HG12	2.06	0.70
1:D:403:LEU:HD23	1:D:404:MET:N	2.06	0.70
2:M:125:SER:H	4:M:175:LVS:C1'	2.04	0.70
1:T:327:LEU:N	1:T:328:PRO:HD3	2.07	0.70
1:X:369:PHE:CE2	1:X:421:ILE:HD12	2.26	0.70
2:J:1:THR:HG21	2:J:33:LYS:CE	2.22	0.70
2:L:4:VAL:HG23	2:L:122:ALA:HB2	1.73	0.70
2:Q:125:SER:H	4:Q:175:LVS:C1'	2.03	0.70
2:R:1:THR:HG21	2:R:33:LYS:CE	2.11	0.70
1:C:20:GLN:HA	1:C:20:GLN:NE2	2.01	0.70
2:G:1:THR:N	4:G:175:LVS:C1'	2.55	0.70
1:D:27:VAL:HB	1:D:70:LEU:HD22	1.73	0.70
1:A:280:ARG:HD3	1:F:82:GLU:OE2	1.92	0.70
1:E:363:GLU:OE1	1:E:412:SER:HA	1.92	0.70
2:G:17:ASP:C	2:G:33:LYS:NZ	2.50	0.70
2:J:17:ASP:O	2:J:33:LYS:HD2	1.92	0.70
1:V:395:ARG:O	1:V:399:VAL:HG23	1.91	0.70
2:R:64:LEU:HD23	2:R:74:SER:OG	1.92	0.69
1:W:20:GLN:OE1	1:W:333:LEU:HB3	1.92	0.69
1:B:406:LYS:H	1:B:406:LYS:CD	2.02	0.69
1:F:38:MET:HA	1:F:45:ARG:HD2	1.74	0.69
1:S:100:ILE:HG13	1:S:291:VAL:HG21	1.74	0.69
1:W:369:PHE:CE2	1:W:421:ILE:HD12	2.27	0.69
2:G:164:ASN:HD22	2:G:164:ASN:C	1.98	0.69
2:I:164:ASN:C	2:I:164:ASN:HD22	1.99	0.69
2:J:1:THR:CG2	2:J:33:LYS:CE	2.71	0.69
2:Q:7:ARG:NE	2:Q:12:VAL:HG22	2.04	0.69
2:R:1:THR:HG22	2:R:33:LYS:HZ2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:100:ILE:HG13	1:U:291:VAL:HG21	1.73	0.69
2:K:33:LYS:NZ	4:K:175:LVS:HB32	2.07	0.69
2:Q:131:LEU:HD11	2:Q:135:ARG:NE	2.07	0.69
1:T:395:ARG:O	1:T:399:VAL:HG23	1.93	0.69
1:W:327:LEU:N	1:W:328:PRO:HD3	2.07	0.69
1:B:404:MET:O	1:B:408:SER:HB2	1.92	0.69
1:D:55:MET:HE3	1:D:306:ILE:CG2	2.21	0.69
2:O:37:LEU:HB2	2:O:42:VAL:HG23	1.73	0.69
1:T:356:TYR:HB3	1:T:404:MET:HE2	1.75	0.69
1:E:270:GLY:C	1:E:272:ASP:H	2.00	0.69
2:K:1:THR:HG21	2:K:33:LYS:CE	2.21	0.69
2:P:125:SER:H	4:P:175:LVS:C1'	2.06	0.69
1:S:327:LEU:N	1:S:328:PRO:HD3	2.08	0.69
1:B:437:GLU:C	1:B:439:LEU:H	2.00	0.69
2:I:3:ILE:HG22	2:I:96:ILE:HD12	1.75	0.69
1:U:327:LEU:N	1:U:328:PRO:HD3	2.07	0.69
1:V:369:PHE:CE2	1:V:421:ILE:HD12	2.28	0.69
1:X:100:ILE:HG13	1:X:291:VAL:HG21	1.75	0.69
1:B:403:LEU:HD23	1:B:403:LEU:C	2.17	0.69
2:H:22:LEU:HB2	4:H:175:LVS:HD13	1.75	0.69
2:M:37:LEU:HB2	2:M:42:VAL:HG23	1.75	0.69
2:R:1:THR:N	4:R:175:LVS:CS	2.56	0.69
1:S:118:LYS:C	1:S:118:LYS:HD3	2.18	0.69
1:U:328:PRO:HA	1:V:398:THR:HG22	1.75	0.69
2:I:48:GLY:H	4:I:175:LVS:H2'	1.57	0.68
1:B:363:GLU:OE1	1:B:412:SER:HA	1.94	0.68
2:M:131:LEU:HD11	2:M:135:ARG:NE	2.08	0.68
2:O:64:LEU:HD23	2:O:74:SER:OG	1.92	0.68
1:F:444:LEU:OXT	2:L:113:VAL:HA	1.92	0.68
1:C:443:ILE:HG21	2:I:114:GLN:HG3	1.75	0.68
2:O:7:ARG:HH21	2:O:12:VAL:HG21	1.58	0.68
2:Q:17:ASP:HA	2:Q:167:PHE:HB3	1.76	0.68
1:S:439:LEU:O	1:S:441:ARG:N	2.27	0.68
2:I:22:LEU:HB2	4:I:175:LVS:HD13	1.75	0.68
2:J:1:THR:CG2	2:J:33:LYS:HE3	2.24	0.68
1:T:18:ILE:HD11	1:T:343:ARG:NH2	2.08	0.68
2:J:3:ILE:HG22	2:J:96:ILE:HD12	1.76	0.68
1:S:369:PHE:CE2	1:S:421:ILE:HD12	2.28	0.68
1:T:100:ILE:HG13	1:T:291:VAL:HG21	1.75	0.68
2:G:1:THR:H1	4:G:175:LVS:CS	2.04	0.68
2:I:18:GLY:H	2:I:164:ASN:HD21	1.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:344:ILE:HG23	3:U:458:ATP:C2	2.29	0.68
1:X:279:GLN:NE2	1:X:320:ILE:HG12	2.08	0.68
1:X:323:LEU:O	1:X:323:LEU:HD23	1.92	0.68
1:B:349:HIS:O	1:B:350:ALA:HB3	1.94	0.68
1:C:402:ARG:NH2	1:C:433:VAL:HG21	2.08	0.68
1:D:437:GLU:C	1:D:439:LEU:N	2.44	0.68
2:J:22:LEU:HB2	4:J:175:LVS:HD13	1.75	0.68
2:K:1:THR:CG2	2:K:33:LYS:HZ1	2.03	0.68
1:V:323:LEU:O	1:V:323:LEU:HD23	1.94	0.68
1:D:352:LEU:HD13	1:D:400:MET:HG3	1.75	0.67
1:E:280:ARG:HH11	1:E:280:ARG:HG3	1.57	0.67
2:N:37:LEU:HB2	2:N:42:VAL:HG23	1.74	0.67
1:T:369:PHE:CE2	1:T:421:ILE:HD12	2.29	0.67
1:A:235:ILE:O	1:A:236:ASN:HB3	1.93	0.67
1:A:264:LYS:HA	1:A:272:ASP:OD1	1.94	0.67
2:K:56:LEU:HD13	2:K:95:LEU:CG	2.20	0.67
1:V:54:LEU:HD21	1:V:327:LEU:HD13	1.76	0.67
1:V:100:ILE:HG13	1:V:291:VAL:HG21	1.75	0.67
1:D:404:MET:O	1:D:408:SER:HB2	1.94	0.67
2:K:46:PHE:HB3	2:K:95:LEU:CD2	2.24	0.67
2:L:1:THR:H1	4:L:175:LVS:CS	2.07	0.67
1:S:77:PRO:HD2	1:S:251:ASN:O	1.95	0.67
1:X:395:ARG:O	1:X:399:VAL:HG23	1.95	0.67
1:B:20:GLN:HA	1:B:20:GLN:NE2	1.99	0.67
1:W:345:LEU:HD23	1:W:374:VAL:HG13	1.76	0.67
2:M:18:GLY:HA2	2:M:33:LYS:HZ2	1.59	0.67
2:P:19:GLN:H	2:P:33:LYS:HZ1	1.41	0.67
2:R:37:LEU:HB2	2:R:42:VAL:HG23	1.76	0.67
1:U:369:PHE:CE2	1:U:421:ILE:HD12	2.29	0.67
1:W:100:ILE:HG13	1:W:291:VAL:HG21	1.76	0.67
2:L:33:LYS:HZ3	4:L:175:LVS:HB32	1.58	0.67
1:V:279:GLN:NE2	1:V:320:ILE:HG12	2.09	0.67
1:A:37:ARG:HD2	1:A:48:VAL:HG13	1.75	0.67
1:E:403:LEU:HD23	1:E:404:MET:N	2.09	0.67
1:F:280:ARG:HH11	1:F:280:ARG:HG3	1.60	0.67
2:Q:37:LEU:HB2	2:Q:42:VAL:HG23	1.77	0.67
1:W:395:ARG:O	1:W:399:VAL:HG23	1.95	0.67
2:Q:105:ILE:HG23	2:Q:113:VAL:HB	1.76	0.67
1:S:75:ASN:HD21	1:S:110:LEU:CD2	2.07	0.67
1:S:326:ARG:HA	1:S:326:ARG:HH11	1.60	0.67
1:V:327:LEU:N	1:V:328:PRO:HD3	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:17:ASP:O	2:I:33:LYS:HD2	1.94	0.67
2:N:131:LEU:HD11	2:N:135:ARG:NE	2.10	0.67
2:P:1:THR:H3	4:P:175:LVS:CS	2.08	0.67
1:U:54:LEU:HD21	1:U:327:LEU:HD13	1.77	0.67
1:W:356:TYR:HB3	1:W:404:MET:HE2	1.76	0.67
1:X:327:LEU:N	1:X:328:PRO:HD3	2.07	0.67
2:G:144:SER:OG	2:G:147:GLU:HG3	1.95	0.66
2:K:33:LYS:HZ2	4:K:175:LVS:HB32	1.59	0.66
2:Q:1:THR:HG23	2:Q:33:LYS:CE	2.21	0.66
1:V:356:TYR:HB3	1:V:404:MET:HE2	1.76	0.66
1:C:440:SER:O	1:C:442:PHE:N	2.28	0.66
2:P:1:THR:N	4:P:175:LVS:CS	2.58	0.66
2:P:19:GLN:N	2:P:33:LYS:HZ1	1.93	0.66
1:V:297:MET:HE2	1:W:105:ASP:HB3	1.77	0.66
1:V:439:LEU:O	1:V:441:ARG:N	2.27	0.66
1:X:345:LEU:HD23	1:X:374:VAL:HG13	1.77	0.66
1:D:440:SER:O	1:D:442:PHE:N	2.28	0.66
2:R:17:ASP:HA	2:R:167:PHE:HB3	1.77	0.66
1:V:42:GLU:HB3	1:V:43:PRO:HD3	1.78	0.66
1:V:326:ARG:HA	1:V:326:ARG:HH11	1.61	0.66
1:E:20:GLN:HA	1:E:20:GLN:NE2	2.02	0.66
1:U:42:GLU:HB3	1:U:43:PRO:HD3	1.78	0.66
2:O:17:ASP:HB2	2:O:164:ASN:ND2	2.10	0.66
1:A:440:SER:HB3	2:H:32:ARG:HH22	1.60	0.66
1:D:443:ILE:HG21	2:J:114:GLN:HG3	1.77	0.66
1:E:55:MET:HE3	1:E:306:ILE:CG2	2.25	0.66
2:L:3:ILE:HG22	2:L:96:ILE:HD12	1.76	0.66
1:T:345:LEU:HD23	1:T:374:VAL:HG13	1.77	0.66
1:U:356:TYR:HB3	1:U:404:MET:HE2	1.76	0.66
1:X:42:GLU:HB3	1:X:43:PRO:HD3	1.77	0.66
2:H:48:GLY:H	4:H:175:LVS:H2'	1.61	0.66
2:N:105:ILE:HG23	2:N:113:VAL:HB	1.77	0.66
1:S:395:ARG:O	1:S:399:VAL:HG23	1.96	0.66
1:U:279:GLN:NE2	1:U:320:ILE:HG12	2.09	0.66
1:B:5:THR:O	1:B:9:ILE:HG13	1.96	0.66
1:C:79:ILE:CG2	1:C:103:LEU:HD13	2.23	0.66
1:E:403:LEU:HD23	1:E:403:LEU:C	2.21	0.66
2:L:1:THR:CG2	2:L:33:LYS:HE3	2.26	0.66
1:U:345:LEU:HD23	1:U:374:VAL:HG13	1.78	0.66
2:H:18:GLY:H	2:H:164:ASN:HD21	1.41	0.65
2:J:164:ASN:HD22	2:J:164:ASN:C	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:7:ARG:NE	2:O:12:VAL:HG22	2.06	0.65
1:S:279:GLN:NE2	1:S:320:ILE:HG12	2.11	0.65
1:U:265:LYS:HA	1:U:269:SER:HB3	1.78	0.65
1:F:349:HIS:O	1:F:350:ALA:HB3	1.96	0.65
1:T:7:ARG:NH1	1:U:410:SER:HB3	2.11	0.65
1:U:385:ASN:ND2	1:U:395:ARG:HE	1.94	0.65
3:D:453:ATP:C8	3:D:453:ATP:H5'1	2.32	0.65
1:F:367:ILE:HD11	1:F:421:ILE:HD11	1.77	0.65
1:X:18:ILE:HD11	1:X:343:ARG:NH2	2.11	0.65
2:G:1:THR:CG2	2:G:33:LYS:CD	2.42	0.65
2:J:1:THR:H1	4:J:175:LVS:CS	2.09	0.65
1:T:75:ASN:HD21	1:T:110:LEU:HD22	1.61	0.65
1:A:402:ARG:NH2	1:A:433:VAL:HG21	2.11	0.65
1:C:55:MET:HE3	1:C:306:ILE:CG2	2.26	0.65
1:F:55:MET:HE3	1:F:306:ILE:CG2	2.27	0.65
2:J:1:THR:H3	4:J:175:LVS:CS	2.10	0.65
2:N:18:GLY:H	2:N:164:ASN:HD21	1.42	0.65
1:X:326:ARG:HA	1:X:326:ARG:HH11	1.60	0.65
2:M:1:THR:N	4:M:175:LVS:CS	2.60	0.65
2:M:7:ARG:NE	2:M:12:VAL:HG22	2.03	0.65
2:P:37:LEU:HB2	2:P:42:VAL:HG23	1.76	0.65
1:T:326:ARG:HH11	1:T:326:ARG:HA	1.60	0.65
1:X:77:PRO:HD2	1:X:251:ASN:O	1.97	0.65
1:E:443:ILE:HG23	2:K:112:VAL:HG23	1.78	0.65
2:G:1:THR:H3	4:G:175:LVS:CS	2.07	0.65
2:H:46:PHE:HB3	2:H:95:LEU:CD2	2.27	0.65
2:R:19:GLN:H	2:R:33:LYS:HZ1	1.43	0.65
1:T:77:PRO:HD2	1:T:251:ASN:O	1.97	0.65
1:X:356:TYR:HB3	1:X:404:MET:HE2	1.77	0.65
1:A:280:ARG:HH11	1:A:280:ARG:HG3	1.61	0.65
2:P:112:VAL:HB	1:V:443:ILE:HD12	1.79	0.65
2:Q:72:LEU:HG	1:W:438:ASP:OD2	1.97	0.65
2:I:116:GLU:HG2	2:J:30:ASN:HD21	1.61	0.65
1:U:77:PRO:HD2	1:U:251:ASN:O	1.97	0.65
1:V:77:PRO:HD2	1:V:251:ASN:O	1.96	0.65
2:Q:1:THR:HG22	2:Q:33:LYS:NZ	2.12	0.65
1:B:362:THR:HG21	1:C:39:GLN:HG2	1.78	0.64
2:N:1:THR:N	4:N:175:LVS:CS	2.60	0.64
2:Q:17:ASP:C	2:Q:33:LYS:HZ1	2.04	0.64
1:V:265:LYS:HA	1:V:269:SER:HB3	1.80	0.64
1:X:54:LEU:HD21	1:X:327:LEU:HD13	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:265:LYS:HA	1:X:269:SER:HB3	1.79	0.64
1:D:17:ILE:N	1:D:17:ILE:HD12	2.12	0.64
1:E:63:LYS:HD2	1:E:308:SER:HB2	1.78	0.64
2:M:18:GLY:CA	2:M:33:LYS:HZ2	2.11	0.64
1:B:440:SER:O	1:B:442:PHE:N	2.29	0.64
1:D:403:LEU:HD23	1:D:403:LEU:C	2.21	0.64
1:T:245:ILE:HD11	1:T:295:HIS:O	1.97	0.64
1:U:326:ARG:HA	1:U:326:ARG:HH11	1.61	0.64
1:C:52:ASN:O	1:C:328:PRO:HD2	1.98	0.64
2:R:27:MET:HE1	4:R:175:LVS:HD21	1.79	0.64
1:W:42:GLU:HB3	1:W:43:PRO:HD3	1.79	0.64
2:O:131:LEU:HD11	2:O:135:ARG:NE	2.11	0.64
2:Q:1:THR:N	4:Q:175:LVS:CS	2.60	0.64
1:W:328:PRO:HA	1:X:398:THR:HG22	1.80	0.64
1:B:270:GLY:C	1:B:272:ASP:H	2.05	0.64
2:H:164:ASN:C	2:H:164:ASN:HD22	2.05	0.64
2:K:81:ASP:O	2:K:88:LEU:HB2	1.97	0.64
1:W:54:LEU:HD21	1:W:327:LEU:HD13	1.78	0.64
1:C:232:ALA:C	1:C:233:LYS:HD3	2.23	0.64
1:E:60:GLY:HA2	3:E:454:ATP:O3A	1.98	0.64
1:F:402:ARG:HH22	1:F:433:VAL:HG21	1.61	0.64
1:F:443:ILE:HG21	2:L:114:GLN:HG3	1.79	0.64
2:M:105:ILE:HG23	2:M:113:VAL:HB	1.80	0.64
1:S:265:LYS:HA	1:S:269:SER:HB3	1.80	0.64
1:U:279:GLN:HE22	1:U:320:ILE:N	1.95	0.64
1:X:239:GLU:C	1:X:241:LYS:H	2.05	0.64
2:H:86:ARG:HB3	2:H:86:ARG:NH1	2.11	0.64
2:I:86:ARG:HB3	2:I:86:ARG:NH1	2.10	0.64
2:P:17:ASP:HB2	2:P:164:ASN:ND2	2.13	0.64
1:S:42:GLU:HB3	1:S:43:PRO:HD3	1.80	0.64
1:T:42:GLU:HB3	1:T:43:PRO:HD3	1.79	0.64
1:V:370:THR:CG2	1:V:422:ASP:HA	2.28	0.64
1:X:256:ILE:HD13	1:X:282:LEU:HD21	1.80	0.64
1:C:406:LYS:HD2	1:C:406:LYS:N	2.03	0.64
1:F:440:SER:O	1:F:442:PHE:N	2.31	0.64
2:I:116:GLU:HG2	2:J:30:ASN:ND2	2.13	0.64
1:T:54:LEU:HD21	1:T:327:LEU:HD13	1.79	0.64
1:T:64:THR:HB	3:T:457:ATP:O1A	1.97	0.64
1:W:326:ARG:HH11	1:W:326:ARG:HA	1.62	0.64
1:D:233:LYS:HB2	1:D:233:LYS:NZ	2.13	0.64
2:H:37:LEU:HD21	2:H:57:PHE:CZ	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:THR:HG23	2:I:33:LYS:HZ1	1.62	0.64
2:K:164:ASN:C	2:K:164:ASN:HD22	2.04	0.64
1:U:439:LEU:O	1:U:441:ARG:N	2.30	0.64
1:A:440:SER:O	1:A:442:PHE:N	2.31	0.63
1:F:37:ARG:HD2	1:F:48:VAL:HG13	1.79	0.63
1:F:367:ILE:HD11	1:F:421:ILE:CD1	2.28	0.63
2:H:1:THR:H1	4:H:175:LVS:CS	2.11	0.63
2:L:56:LEU:HD13	2:L:95:LEU:CG	2.21	0.63
2:R:131:LEU:HD11	2:R:135:ARG:NE	2.13	0.63
1:W:265:LYS:HA	1:W:269:SER:HB3	1.80	0.63
1:W:279:GLN:NE2	1:W:320:ILE:HG12	2.12	0.63
1:A:409:PHE:CE1	1:B:6:PRO:HB3	2.33	0.63
1:D:406:LYS:H	1:D:406:LYS:CD	2.05	0.63
1:F:60:GLY:HA2	3:F:455:ATP:O3A	1.98	0.63
2:K:18:GLY:H	2:K:164:ASN:HD21	1.43	0.63
2:N:7:ARG:HH21	2:N:12:VAL:CG2	2.11	0.63
2:O:105:ILE:HG23	2:O:113:VAL:HB	1.79	0.63
2:Q:17:ASP:HB2	2:Q:164:ASN:ND2	2.14	0.63
2:R:17:ASP:CG	2:R:33:LYS:NZ	2.56	0.63
1:E:37:ARG:HD2	1:E:48:VAL:HG13	1.80	0.63
1:F:403:LEU:HD23	1:F:404:MET:N	2.13	0.63
2:L:125:SER:H	4:L:175:LVS:C1'	2.11	0.63
2:P:3:ILE:O	2:P:122:ALA:HA	1.98	0.63
1:T:265:LYS:HA	1:T:269:SER:HB3	1.80	0.63
1:V:5:THR:OG1	1:V:6:PRO:HD2	1.97	0.63
1:C:280:ARG:HH11	1:C:280:ARG:HG3	1.63	0.63
2:J:7:ARG:HD2	2:J:119:GLN:CG	2.27	0.63
2:L:48:GLY:H	4:L:175:LVS:H2'	1.64	0.63
2:R:105:ILE:HG23	2:R:113:VAL:HB	1.80	0.63
1:S:356:TYR:HB3	1:S:404:MET:HE2	1.79	0.63
1:S:54:LEU:HD21	1:S:327:LEU:HD13	1.80	0.63
1:D:367:ILE:HD11	1:D:421:ILE:HD11	1.81	0.63
1:F:403:LEU:HD23	1:F:403:LEU:C	2.24	0.63
2:N:17:ASP:O	2:N:33:LYS:HG3	1.97	0.63
1:X:279:GLN:HE22	1:X:320:ILE:N	1.95	0.63
1:A:408:SER:O	1:B:36:ARG:NH2	2.30	0.63
2:L:37:LEU:HD21	2:L:57:PHE:CZ	2.33	0.63
2:H:3:ILE:HG22	2:H:96:ILE:HD12	1.81	0.63
2:M:17:ASP:O	2:M:33:LYS:NZ	2.30	0.63
1:B:352:LEU:HD13	1:B:400:MET:HG3	1.81	0.63
1:F:20:GLN:HA	1:F:20:GLN:NE2	2.06	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:1:THR:HG21	2:O:33:LYS:HD3	1.72	0.63
1:T:15:GLN:O	1:T:348:PRO:HA	1.99	0.63
2:L:46:PHE:HB3	2:L:95:LEU:CD2	2.28	0.62
2:P:5:SER:HB2	2:P:14:VAL:HG22	1.81	0.62
1:T:279:GLN:HE22	1:T:320:ILE:N	1.97	0.62
1:V:385:ASN:ND2	1:V:395:ARG:HE	1.97	0.62
2:P:3:ILE:HB	2:P:123:ILE:HG13	1.81	0.62
1:E:409:PHE:CD1	1:F:6:PRO:HB3	2.34	0.62
2:H:116:GLU:HG2	2:I:30:ASN:ND2	2.14	0.62
2:H:137:LEU:CD1	2:N:136:ALA:HB1	2.29	0.62
2:O:1:THR:N	4:O:175:LVS:CS	2.61	0.62
2:Q:1:THR:HG21	2:Q:33:LYS:HD3	1.76	0.62
1:T:345:LEU:HD13	1:T:396:LEU:HD22	1.81	0.62
1:V:345:LEU:HD23	1:V:374:VAL:HG13	1.80	0.62
2:Q:1:THR:CG2	2:Q:33:LYS:HE2	2.19	0.62
2:R:8:ARG:O	2:R:11:GLN:HB2	1.99	0.62
1:U:18:ILE:HD11	1:U:343:ARG:NH2	2.14	0.62
1:U:370:THR:CG2	1:U:422:ASP:HA	2.30	0.62
1:X:115:GLU:HG2	1:X:119:ASN:ND2	2.14	0.62
2:I:1:THR:HG23	2:I:33:LYS:CE	2.24	0.62
2:K:1:THR:H3	4:K:175:LVS:C2'	2.12	0.62
2:M:83:ARG:HG2	2:R:55:THR:HG22	1.80	0.62
2:O:17:ASP:HA	2:O:167:PHE:HB3	1.81	0.62
2:P:55:THR:HG22	2:Q:83:ARG:HG2	1.82	0.62
1:W:444:LEU:HD22	1:W:444:LEU:OXT	1.99	0.62
1:B:73:LEU:C	1:B:73:LEU:HD12	2.24	0.62
1:C:270:GLY:C	1:C:272:ASP:H	2.06	0.62
2:G:46:PHE:HB3	2:G:95:LEU:CD2	2.29	0.62
2:J:46:PHE:HB3	2:J:95:LEU:CD2	2.29	0.62
2:L:1:THR:H3	4:L:175:LVS:CS	2.11	0.62
2:O:112:VAL:HB	1:U:443:ILE:HD12	1.80	0.62
2:R:47:ALA:HB3	2:R:123:ILE:HD12	1.81	0.62
2:M:72:LEU:HG	1:S:438:ASP:OD2	2.00	0.62
2:M:112:VAL:HB	1:S:443:ILE:HD12	1.79	0.62
1:S:244:ALA:O	1:S:247:ALA:HB3	1.99	0.62
2:I:67:HIS:CD2	2:I:73:LYS:HE3	2.35	0.62
2:N:2:THR:OG1	2:N:126:GLY:HA3	1.99	0.62
2:P:2:THR:OG1	2:P:126:GLY:HA3	2.00	0.62
1:D:280:ARG:HH11	1:D:280:ARG:HG3	1.64	0.62
1:F:5:THR:O	1:F:9:ILE:HG13	1.99	0.62
2:K:4:VAL:HG23	2:K:122:ALA:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:22:LEU:HB2	4:K:175:LVS:HD13	1.81	0.62
2:O:1:THR:HG22	2:O:33:LYS:NZ	2.14	0.62
2:P:112:VAL:HB	1:V:443:ILE:CD1	2.30	0.62
1:S:5:THR:OG1	1:S:6:PRO:HD2	1.99	0.62
1:S:345:LEU:HD23	1:S:374:VAL:HG13	1.80	0.62
1:T:439:LEU:O	1:T:441:ARG:N	2.33	0.62
1:B:83:ALA:HB1	1:B:262:ILE:HD13	1.82	0.62
1:D:409:PHE:CE1	1:E:6:PRO:HB3	2.34	0.62
1:F:270:GLY:C	1:F:272:ASP:H	2.07	0.62
2:H:81:ASP:O	2:H:88:LEU:HB2	2.00	0.62
2:I:37:LEU:HD21	2:I:57:PHE:CZ	2.35	0.62
2:Q:17:ASP:C	2:Q:33:LYS:NZ	2.58	0.62
1:T:5:THR:OG1	1:T:6:PRO:HD2	2.00	0.62
1:A:407:ILE:HD11	1:A:419:VAL:HG11	1.81	0.61
1:C:64:THR:HB	3:C:452:ATP:O1A	2.00	0.61
1:E:360:MET:HE1	1:F:36:ARG:NH1	2.15	0.61
2:K:1:THR:H1	4:K:175:LVS:CS	2.13	0.61
2:M:17:ASP:HB2	2:M:164:ASN:ND2	2.15	0.61
1:F:52:ASN:O	1:F:328:PRO:HD2	2.00	0.61
2:I:105:ILE:CG2	2:I:113:VAL:HB	2.27	0.61
2:P:7:ARG:HH21	2:P:12:VAL:CG2	2.14	0.61
1:S:370:THR:CG2	1:S:422:ASP:HA	2.29	0.61
1:T:370:THR:CG2	1:T:422:ASP:HA	2.31	0.61
1:W:18:ILE:HD11	1:W:343:ARG:NH2	2.15	0.61
2:G:86:ARG:HB3	2:G:86:ARG:NH1	2.10	0.61
2:I:137:LEU:CD1	2:O:136:ALA:HB1	2.31	0.61
2:R:19:GLN:H	2:R:33:LYS:NZ	1.98	0.61
1:T:385:ASN:ND2	1:T:395:ARG:HE	1.98	0.61
1:A:39:GLN:HG2	1:F:362:THR:HG23	1.81	0.61
1:C:349:HIS:O	1:C:350:ALA:HB3	1.98	0.61
1:C:363:GLU:OE1	1:C:412:SER:HA	2.01	0.61
2:I:81:ASP:O	2:I:88:LEU:HB2	2.01	0.61
2:P:27:MET:HE1	4:P:175:LVS:HD21	1.81	0.61
1:U:23:ALA:O	1:U:27:VAL:HG23	2.01	0.61
2:K:1:THR:CG2	2:K:17:ASP:OD1	2.46	0.61
2:Q:17:ASP:OD2	2:Q:33:LYS:NZ	2.34	0.61
1:C:23:ALA:HA	1:C:331:VAL:HG21	1.81	0.61
1:F:444:LEU:HD23	2:L:113:VAL:HG22	1.83	0.61
2:G:83:ARG:CG	2:H:55:THR:HG22	2.31	0.61
1:V:80:LYS:HG3	1:V:255:PHE:HD2	1.64	0.61
1:F:63:LYS:HD2	1:F:308:SER:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:30:ASN:ND2	2:L:116:GLU:HG2	2.16	0.61
1:T:256:ILE:HD13	1:T:282:LEU:HD21	1.83	0.61
1:D:37:ARG:HD2	1:D:48:VAL:HG13	1.82	0.61
2:J:137:LEU:CD1	2:P:136:ALA:HB1	2.31	0.61
1:U:5:THR:OG1	1:U:6:PRO:HD2	2.00	0.61
1:X:370:THR:CG2	1:X:422:ASP:HA	2.30	0.61
1:D:73:LEU:C	1:D:73:LEU:HD12	2.26	0.61
1:F:58:PRO:HG2	1:F:61:VAL:HG11	1.82	0.61
2:G:60:PHE:HZ	2:G:71:LEU:HD22	1.66	0.61
2:L:86:ARG:HB3	2:L:86:ARG:NH1	2.13	0.61
1:W:256:ILE:HD13	1:W:282:LEU:HD21	1.83	0.61
1:W:385:ASN:ND2	1:W:395:ARG:HE	1.99	0.61
3:B:451:ATP:H5'1	3:B:451:ATP:H8	1.65	0.60
2:M:1:THR:H3	4:M:175:LVS:CS	2.14	0.60
2:N:72:LEU:HG	1:T:438:ASP:OD2	2.00	0.60
2:P:81:ASP:HB3	2:P:88:LEU:HD12	1.83	0.60
1:T:63:LYS:HG2	1:T:333:LEU:CD1	2.31	0.60
1:W:5:THR:OG1	1:W:6:PRO:HD2	2.02	0.60
1:E:233:LYS:HA	1:E:233:LYS:HZ2	1.66	0.60
2:N:46:PHE:HB3	2:N:95:LEU:HD12	1.84	0.60
2:P:19:GLN:H	2:P:33:LYS:NZ	1.99	0.60
2:Q:1:THR:CG2	2:Q:33:LYS:NZ	2.63	0.60
1:C:444:LEU:OXT	2:I:113:VAL:HA	2.02	0.60
2:I:1:THR:H3	4:I:175:LVS:C2'	2.14	0.60
2:K:7:ARG:HD2	2:K:119:GLN:CG	2.31	0.60
1:S:279:GLN:HE22	1:S:320:ILE:N	1.98	0.60
1:W:77:PRO:HD2	1:W:251:ASN:O	2.00	0.60
1:C:352:LEU:HD13	1:C:400:MET:HG3	1.82	0.60
1:E:264:LYS:HA	1:E:272:ASP:OD1	2.00	0.60
2:J:136:ALA:HB1	2:P:137:LEU:HD13	1.84	0.60
2:M:7:ARG:HH21	2:M:12:VAL:CG2	2.14	0.60
2:O:17:ASP:HB2	2:O:164:ASN:HD22	1.66	0.60
1:A:73:LEU:C	1:A:73:LEU:HD12	2.26	0.60
1:D:20:GLN:HA	1:D:20:GLN:NE2	2.11	0.60
2:H:4:VAL:HG23	2:H:122:ALA:HB2	1.84	0.60
2:I:33:LYS:NZ	4:I:175:LVS:CB3	2.64	0.60
2:M:8:ARG:O	2:M:11:GLN:HB2	2.01	0.60
2:N:104:LEU:HD13	2:N:112:VAL:CG1	2.32	0.60
2:O:27:MET:HE1	4:O:175:LVS:HD21	1.82	0.60
2:P:17:ASP:HA	2:P:167:PHE:HB3	1.82	0.60
2:Q:7:ARG:HH21	2:Q:12:VAL:CG2	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:80:LYS:HG3	1:S:255:PHE:HD2	1.66	0.60
1:V:279:GLN:HE22	1:V:320:ILE:N	1.97	0.60
1:A:404:MET:O	1:A:408:SER:HB2	2.01	0.60
1:E:406:LYS:HD2	1:E:406:LYS:N	2.11	0.60
2:G:56:LEU:HD13	2:G:95:LEU:CG	2.30	0.60
2:J:60:PHE:HZ	2:J:71:LEU:HD22	1.67	0.60
2:K:67:HIS:CD2	2:K:73:LYS:HE3	2.37	0.60
2:M:17:ASP:HA	2:M:167:PHE:HB3	1.83	0.60
2:N:3:ILE:O	2:N:122:ALA:HA	2.01	0.60
2:O:17:ASP:O	2:O:33:LYS:HG3	2.01	0.60
1:W:63:LYS:HG2	1:W:333:LEU:CD1	2.31	0.60
1:X:5:THR:OG1	1:X:6:PRO:HD2	2.01	0.60
1:B:264:LYS:HA	1:B:272:ASP:OD1	2.01	0.60
1:C:367:ILE:HD11	1:C:421:ILE:CD1	2.32	0.60
1:D:349:HIS:O	1:D:350:ALA:HB3	2.02	0.60
1:E:349:HIS:O	1:E:350:ALA:HB3	2.02	0.60
2:N:19:GLN:H	2:N:33:LYS:HZ1	1.50	0.60
1:A:403:LEU:CD1	1:A:426:VAL:HG22	2.32	0.60
2:M:112:VAL:HB	1:S:443:ILE:CD1	2.32	0.60
1:A:20:GLN:HA	1:A:20:GLN:NE2	2.14	0.60
1:B:443:ILE:CD1	2:H:72:LEU:HD11	2.32	0.60
1:C:264:LYS:HA	1:C:272:ASP:OD1	2.02	0.60
2:I:46:PHE:HB3	2:I:95:LEU:CD2	2.31	0.60
2:J:116:GLU:HG2	2:K:30:ASN:ND2	2.17	0.60
2:K:67:HIS:HD2	2:K:73:LYS:HE3	1.67	0.60
2:O:5:SER:HB2	2:O:14:VAL:HG22	1.83	0.60
2:Q:81:ASP:HB3	2:Q:88:LEU:HD12	1.83	0.60
1:X:15:GLN:O	1:X:348:PRO:HA	2.02	0.60
1:X:345:LEU:HD13	1:X:396:LEU:HD22	1.84	0.60
1:B:62:GLY:O	1:B:66:ILE:HG13	2.01	0.60
1:D:264:LYS:HA	1:D:272:ASP:OD1	2.02	0.60
2:H:60:PHE:HZ	2:H:71:LEU:HD22	1.67	0.60
2:O:81:ASP:HB3	2:O:88:LEU:HD12	1.84	0.60
1:X:344:ILE:HG23	3:X:461:ATP:C2	2.37	0.60
1:C:37:ARG:HD2	1:C:48:VAL:HG13	1.84	0.59
1:D:63:LYS:HD2	1:D:308:SER:HB2	1.83	0.59
1:E:5:THR:O	1:E:9:ILE:HG13	2.02	0.59
1:E:17:ILE:HD12	1:E:17:ILE:N	2.17	0.59
2:K:137:LEU:CD1	2:Q:136:ALA:HB1	2.31	0.59
1:V:23:ALA:O	1:V:27:VAL:HG23	2.02	0.59
1:W:80:LYS:HG3	1:W:255:PHE:HD2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:370:THR:CG2	1:W:422:ASP:HA	2.30	0.59
1:A:443:ILE:HG23	2:G:112:VAL:HG23	1.84	0.59
2:G:88:LEU:O	2:G:89:ARG:CB	2.50	0.59
1:U:7:ARG:HH12	1:V:410:SER:HB3	1.67	0.59
1:V:108:MET:SD	1:V:244:ALA:HB1	2.42	0.59
3:E:454:ATP:H8	3:E:454:ATP:C5'	2.15	0.59
2:G:55:THR:HG22	2:L:83:ARG:CG	2.31	0.59
2:G:81:ASP:O	2:G:88:LEU:HB2	2.01	0.59
2:H:105:ILE:CG2	2:H:113:VAL:HB	2.29	0.59
2:J:81:ASP:O	2:J:88:LEU:HB2	2.01	0.59
2:L:88:LEU:O	2:L:89:ARG:CB	2.50	0.59
2:P:46:PHE:HB3	2:P:95:LEU:HD12	1.83	0.59
2:P:105:ILE:HG23	2:P:113:VAL:HB	1.82	0.59
2:Q:55:THR:HG22	2:R:83:ARG:HG2	1.85	0.59
1:S:385:ASN:ND2	1:S:395:ARG:HE	1.99	0.59
1:B:408:SER:O	1:C:36:ARG:NH2	2.34	0.59
2:N:1:THR:H3	4:N:175:LVS:H1'2	1.67	0.59
1:S:256:ILE:HD13	1:S:282:LEU:HD21	1.84	0.59
1:U:256:ILE:HD13	1:U:282:LEU:HD21	1.83	0.59
2:G:30:ASN:HD21	2:L:116:GLU:HG2	1.67	0.59
2:G:56:LEU:HD12	2:G:95:LEU:HG	1.80	0.59
2:M:46:PHE:HB3	2:M:95:LEU:HD12	1.85	0.59
1:S:345:LEU:HD13	1:S:396:LEU:HD22	1.84	0.59
1:A:5:THR:O	1:A:9:ILE:HG13	2.02	0.59
2:N:17:ASP:HB2	2:N:164:ASN:ND2	2.17	0.59
2:N:81:ASP:HB3	2:N:88:LEU:HD12	1.84	0.59
1:A:443:ILE:HD11	2:G:72:LEU:HD11	1.85	0.59
1:E:362:THR:CG2	1:F:39:GLN:HG2	2.32	0.59
1:F:83:ALA:HB1	1:F:262:ILE:HD13	1.83	0.59
2:G:18:GLY:H	2:G:164:ASN:HD21	1.50	0.59
2:O:47:ALA:HB3	2:O:123:ILE:HD12	1.82	0.59
2:R:17:ASP:HB2	2:R:164:ASN:ND2	2.18	0.59
1:T:80:LYS:HG3	1:T:255:PHE:HD2	1.67	0.59
1:W:64:THR:HB	3:W:460:ATP:O1A	2.02	0.59
1:F:246:ASP:O	1:F:250:GLN:HG2	2.03	0.59
2:H:7:ARG:HD2	2:H:119:GLN:CG	2.32	0.59
1:W:120:ARG:HD2	1:W:120:ARG:N	2.10	0.59
1:W:346:THR:HG22	1:W:353:THR:HG21	1.85	0.59
1:A:363:GLU:OE1	1:A:412:SER:HA	2.03	0.59
1:C:58:PRO:HG2	1:C:61:VAL:HG11	1.85	0.59
3:D:453:ATP:H5'1	3:D:453:ATP:H8	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:ARG:CG	2:I:55:THR:HG22	2.33	0.59
1:C:5:THR:O	1:C:9:ILE:HG13	2.02	0.59
1:D:402:ARG:NH2	1:D:433:VAL:CG2	2.66	0.59
2:H:1:THR:H3	4:H:175:LVS:C2'	2.15	0.59
2:L:60:PHE:HZ	2:L:71:LEU:HD22	1.68	0.59
2:P:17:ASP:HB2	2:P:164:ASN:HD22	1.68	0.59
2:R:81:ASP:HB3	2:R:88:LEU:HD12	1.83	0.59
1:A:403:LEU:CD2	1:A:404:MET:SD	2.91	0.58
2:I:88:LEU:O	2:I:89:ARG:CB	2.51	0.58
2:M:105:ILE:CG2	2:M:113:VAL:HB	2.33	0.58
2:O:19:GLN:H	2:O:33:LYS:NZ	1.99	0.58
2:P:105:ILE:CG2	2:P:113:VAL:HB	2.33	0.58
2:Q:27:MET:HE1	4:Q:175:LVS:HD21	1.85	0.58
2:R:17:ASP:OD2	2:R:33:LYS:NZ	2.36	0.58
2:N:17:ASP:HA	2:N:167:PHE:HB3	1.85	0.58
1:S:410:SER:HB3	1:X:7:ARG:NH1	2.17	0.58
2:K:86:ARG:HB3	2:K:86:ARG:NH1	2.15	0.58
2:O:1:THR:HG23	2:O:33:LYS:NZ	2.13	0.58
1:S:23:ALA:O	1:S:27:VAL:HG23	2.03	0.58
1:S:328:PRO:HA	1:T:398:THR:HG22	1.86	0.58
1:V:297:MET:CE	1:W:105:ASP:HB3	2.33	0.58
1:W:63:LYS:HB2	3:W:460:ATP:O2B	2.03	0.58
1:C:111:VAL:HG12	1:C:112:ARG:N	2.19	0.58
2:K:161:VAL:HG13	2:P:24:ASN:O	2.04	0.58
1:X:23:ALA:O	1:X:27:VAL:HG23	2.04	0.58
2:G:18:GLY:HA2	2:G:33:LYS:HZ2	1.63	0.58
2:J:18:GLY:H	2:J:164:ASN:HD21	1.51	0.58
2:L:81:ASP:O	2:L:88:LEU:HB2	2.02	0.58
1:V:15:GLN:O	1:V:348:PRO:HA	2.04	0.58
1:V:240:LEU:O	1:V:244:ALA:HB3	2.03	0.58
1:V:346:THR:HG22	1:V:353:THR:HG21	1.86	0.58
1:A:119:ASN:HB2	1:A:234:LEU:HD11	1.85	0.58
1:D:355:GLN:O	1:D:359:LEU:HD23	2.03	0.58
1:F:119:ASN:HD21	1:F:234:LEU:HD12	1.67	0.58
2:J:1:THR:HG23	2:J:33:LYS:HE3	1.85	0.58
2:N:28:LYS:HE2	2:N:30:ASN:OD1	2.03	0.58
2:Q:105:ILE:CG2	2:Q:113:VAL:HB	2.33	0.58
1:S:7:ARG:HH12	1:T:410:SER:HB3	1.69	0.58
1:X:352:LEU:HD13	1:X:400:MET:HG3	1.86	0.58
1:A:37:ARG:HD2	1:A:48:VAL:CG1	2.33	0.58
1:B:73:LEU:HD12	1:B:73:LEU:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:GLU:HG3	3:C:452:ATP:O2'	2.04	0.58
2:M:3:ILE:HB	2:M:123:ILE:HG13	1.85	0.58
2:P:1:THR:HG23	2:P:33:LYS:NZ	2.13	0.58
1:S:23:ALA:HA	1:S:331:VAL:HG21	1.86	0.58
1:V:64:THR:HB	3:V:459:ATP:O1A	2.04	0.58
1:V:280:ARG:HG3	1:W:82:GLU:OE1	2.02	0.58
1:V:439:LEU:H	1:V:439:LEU:CD2	2.14	0.58
1:A:352:LEU:HD13	1:A:400:MET:HG3	1.85	0.58
2:H:67:HIS:HD2	2:H:73:LYS:HE3	1.69	0.58
2:R:137:LEU:C	2:R:141:THR:HG22	2.28	0.58
1:U:15:GLN:O	1:U:348:PRO:HA	2.04	0.58
1:A:100:ILE:HB	1:A:291:VAL:HG21	1.85	0.58
1:A:403:LEU:C	1:A:405:ASP:H	2.11	0.58
1:D:9:ILE:HD13	1:D:31:LEU:HD23	1.86	0.58
2:G:4:VAL:HG23	2:G:122:ALA:HB2	1.85	0.58
2:H:88:LEU:O	2:H:89:ARG:CB	2.51	0.58
2:L:67:HIS:CD2	2:L:73:LYS:HE3	2.38	0.58
1:X:385:ASN:ND2	1:X:395:ARG:HE	2.00	0.58
1:A:362:THR:CG2	1:B:39:GLN:HG2	2.33	0.58
1:D:23:ALA:HA	1:D:331:VAL:HG21	1.85	0.58
1:E:100:ILE:HB	1:E:291:VAL:HG21	1.85	0.58
2:P:1:THR:HG21	2:P:33:LYS:HD3	1.70	0.58
2:R:2:THR:OG1	2:R:126:GLY:HA3	2.03	0.58
1:F:264:LYS:HA	1:F:272:ASP:OD1	2.04	0.57
2:G:22:LEU:HB2	4:G:175:LVS:HD13	1.86	0.57
2:H:67:HIS:CD2	2:H:73:LYS:HE3	2.39	0.57
2:K:1:THR:HG21	2:K:33:LYS:NZ	2.15	0.57
2:K:88:LEU:O	2:K:89:ARG:CB	2.52	0.57
2:Q:8:ARG:HB3	2:Q:8:ARG:HH11	1.69	0.57
1:W:279:GLN:HE22	1:W:320:ILE:N	2.00	0.57
1:B:437:GLU:HG3	1:B:439:LEU:HD12	1.84	0.57
1:B:444:LEU:OXT	2:H:113:VAL:HA	2.03	0.57
1:E:437:GLU:C	1:E:439:LEU:H	2.02	0.57
1:F:73:LEU:C	1:F:73:LEU:HD12	2.29	0.57
1:F:119:ASN:CG	1:F:234:LEU:HD12	2.30	0.57
2:I:4:VAL:HG23	2:I:122:ALA:HB2	1.86	0.57
2:L:67:HIS:HD2	2:L:73:LYS:HE3	1.69	0.57
2:M:27:MET:HE1	4:M:175:LVS:HD21	1.86	0.57
2:M:81:ASP:HB3	2:M:88:LEU:HD12	1.85	0.57
2:N:19:GLN:H	2:N:33:LYS:NZ	2.01	0.57
2:Q:164:ASN:ND2	2:Q:164:ASN:H	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:7:ARG:HH21	2:R:12:VAL:CG2	2.17	0.57
1:S:346:THR:HG22	1:S:353:THR:HG21	1.86	0.57
1:T:23:ALA:HA	1:T:331:VAL:HG21	1.86	0.57
1:W:23:ALA:O	1:W:27:VAL:HG23	2.04	0.57
1:A:20:GLN:CA	1:A:20:GLN:NE2	2.65	0.57
1:B:234:LEU:O	1:B:234:LEU:HD23	2.04	0.57
2:J:1:THR:N	4:J:175:LVS:C2'	2.66	0.57
2:J:86:ARG:HB3	2:J:86:ARG:NH1	2.13	0.57
2:N:27:MET:HE1	4:N:175:LVS:HD21	1.86	0.57
2:Q:18:GLY:CA	2:Q:33:LYS:HZ1	2.17	0.57
2:Q:66:MET:O	2:Q:67:HIS:ND1	2.37	0.57
2:R:7:ARG:HE	2:R:12:VAL:CG2	2.06	0.57
1:S:236:ASN:HB3	1:S:239:GLU:HB2	1.86	0.57
1:A:236:ASN:N	1:A:237:PRO:HD3	2.19	0.57
2:I:83:ARG:CG	2:J:55:THR:HG22	2.34	0.57
2:J:17:ASP:O	2:J:33:LYS:HD3	2.04	0.57
2:M:3:ILE:O	2:M:122:ALA:HA	2.04	0.57
1:V:385:ASN:HD21	1:V:395:ARG:HE	1.53	0.57
2:P:7:ARG:NH2	2:P:12:VAL:HG21	2.19	0.57
1:U:352:LEU:HD13	1:U:400:MET:HG3	1.86	0.57
1:V:256:ILE:HD13	1:V:282:LEU:HD21	1.85	0.57
1:B:403:LEU:CD1	1:B:426:VAL:HG22	2.34	0.57
1:C:406:LYS:H	1:C:406:LYS:CD	2.05	0.57
1:D:367:ILE:HD11	1:D:421:ILE:HD12	1.84	0.57
1:E:73:LEU:C	1:E:73:LEU:HD12	2.29	0.57
2:I:56:LEU:HD13	2:I:95:LEU:CG	2.26	0.57
2:O:28:LYS:HE2	2:O:30:ASN:OD1	2.05	0.57
1:D:52:ASN:O	1:D:328:PRO:HD2	2.05	0.57
1:E:402:ARG:NH2	1:E:433:VAL:CG2	2.68	0.57
1:S:63:LYS:HG2	1:S:333:LEU:CD1	2.35	0.57
1:C:73:LEU:C	1:C:73:LEU:HD12	2.29	0.57
2:I:1:THR:N	4:I:175:LVS:S	2.78	0.57
2:M:7:ARG:NH2	2:M:12:VAL:HG21	2.19	0.57
1:U:385:ASN:HD21	1:U:395:ARG:HE	1.51	0.57
1:F:100:ILE:HB	1:F:291:VAL:HG21	1.87	0.57
2:M:17:ASP:HB2	2:M:164:ASN:HD22	1.70	0.57
2:O:19:GLN:H	2:O:33:LYS:HZ1	1.53	0.57
1:A:437:GLU:C	1:A:439:LEU:H	2.09	0.56
1:B:63:LYS:HD2	1:B:308:SER:HB2	1.87	0.56
2:J:1:THR:HG23	2:J:33:LYS:NZ	2.20	0.56
2:K:1:THR:H3	4:K:175:LVS:CS	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:8:ARG:O	2:N:11:GLN:HB2	2.05	0.56
2:Q:3:ILE:O	2:Q:122:ALA:HA	2.04	0.56
2:R:1:THR:HG23	2:R:33:LYS:NZ	2.16	0.56
1:X:23:ALA:HA	1:X:331:VAL:HG21	1.86	0.56
1:B:37:ARG:HD2	1:B:48:VAL:CG1	2.33	0.56
2:H:1:THR:H3	4:H:175:LVS:CS	2.18	0.56
2:I:67:HIS:HD2	2:I:73:LYS:HE3	1.70	0.56
2:O:19:GLN:N	2:O:33:LYS:HZ1	2.01	0.56
2:P:72:LEU:HG	1:V:438:ASP:OD2	2.05	0.56
2:Q:164:ASN:H	2:Q:164:ASN:HD22	1.52	0.56
1:S:352:LEU:HD13	1:S:400:MET:HG3	1.87	0.56
1:T:346:THR:HG22	1:T:353:THR:HG21	1.87	0.56
1:W:109:LYS:C	1:W:110:LEU:HD12	2.30	0.56
1:A:17:ILE:N	1:A:17:ILE:HD12	2.19	0.56
1:A:360:MET:HE1	1:B:36:ARG:NH1	2.20	0.56
1:B:401:GLU:OE1	1:C:51:LYS:HG3	2.05	0.56
1:D:362:THR:CG2	1:E:39:GLN:HG2	2.35	0.56
2:J:1:THR:N	4:J:175:LVS:OI'	2.37	0.56
2:L:137:LEU:CD1	2:R:136:ALA:HB1	2.35	0.56
2:O:1:THR:N	4:O:175:LVS:OI'	2.38	0.56
2:P:8:ARG:HB3	2:P:8:ARG:HH11	1.71	0.56
2:Q:17:ASP:HB2	2:Q:164:ASN:HD22	1.71	0.56
1:U:63:LYS:HG2	1:U:333:LEU:CD1	2.35	0.56
1:W:23:ALA:HA	1:W:331:VAL:HG21	1.87	0.56
1:W:352:LEU:HD13	1:W:400:MET:HG3	1.87	0.56
1:B:403:LEU:C	1:B:405:ASP:H	2.13	0.56
1:F:111:VAL:HG21	1:F:244:ALA:HA	1.87	0.56
2:I:144:SER:OG	2:I:147:GLU:HG3	2.06	0.56
2:J:88:LEU:O	2:J:89:ARG:CB	2.53	0.56
2:K:1:THR:CG2	2:K:33:LYS:HZ2	2.16	0.56
2:K:17:ASP:HB2	2:K:164:ASN:ND2	2.20	0.56
2:L:1:THR:N	4:L:175:LVS:C2'	2.67	0.56
2:N:1:THR:CG2	2:N:33:LYS:NZ	2.68	0.56
2:P:1:THR:HG22	2:P:33:LYS:NZ	2.18	0.56
2:P:17:ASP:O	2:P:33:LYS:HG3	2.06	0.56
1:S:297:MET:HG3	1:T:109:LYS:NZ	2.21	0.56
1:U:23:ALA:HA	1:U:331:VAL:HG21	1.88	0.56
1:X:439:LEU:H	1:X:439:LEU:CD2	2.13	0.56
1:D:360:MET:HE1	1:E:36:ARG:NH1	2.19	0.56
2:H:116:GLU:HG2	2:I:30:ASN:HD21	1.70	0.56
2:J:161:VAL:HG13	2:O:24:ASN:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:46:PHE:HB3	2:P:95:LEU:CD1	2.35	0.56
2:Q:8:ARG:O	2:Q:11:GLN:HB2	2.05	0.56
1:S:385:ASN:HD21	1:S:395:ARG:HE	1.53	0.56
1:U:75:ASN:HD21	1:U:110:LEU:HD21	1.69	0.56
1:U:345:LEU:HD13	1:U:396:LEU:HD22	1.88	0.56
1:E:403:LEU:CD2	1:E:404:MET:SD	2.93	0.56
2:O:8:ARG:HB3	2:O:8:ARG:HH11	1.71	0.56
1:V:63:LYS:HG2	1:V:333:LEU:CD1	2.36	0.56
2:H:56:LEU:HD13	2:H:95:LEU:CG	2.29	0.56
2:I:153:LEU:HB3	2:I:167:PHE:CE2	2.41	0.56
2:Q:1:THR:N	4:Q:175:LVS:O1'	2.39	0.56
2:Q:131:LEU:HD11	2:Q:135:ARG:CZ	2.36	0.56
1:V:23:ALA:HA	1:V:331:VAL:HG21	1.88	0.56
1:X:357:LYS:HA	1:X:367:ILE:HD11	1.88	0.56
1:A:85:LYS:HG2	1:A:85:LYS:O	2.05	0.56
1:D:443:ILE:CG2	2:J:114:GLN:HG3	2.35	0.56
2:K:144:SER:O	2:K:148:ILE:HG13	2.06	0.56
2:Q:95:LEU:O	2:Q:105:ILE:HA	2.06	0.56
2:R:112:VAL:HB	1:X:443:ILE:CD1	2.35	0.56
1:T:23:ALA:O	1:T:27:VAL:HG23	2.05	0.56
1:B:367:ILE:HD11	1:B:421:ILE:CD1	2.35	0.56
2:L:22:LEU:HB2	4:L:175:LVS:HD13	1.87	0.56
2:Q:28:LYS:HE2	2:Q:30:ASN:OD1	2.06	0.56
1:T:16:HIS:CD2	1:T:69:ARG:HE	2.24	0.56
1:X:16:HIS:CD2	1:X:69:ARG:HE	2.24	0.56
2:K:60:PHE:HZ	2:K:71:LEU:HD22	1.69	0.56
2:M:5:SER:HB2	2:M:14:VAL:HG22	1.88	0.56
2:R:46:PHE:HB3	2:R:95:LEU:HD12	1.87	0.56
2:R:105:ILE:CG2	2:R:113:VAL:HB	2.35	0.56
1:S:120:ARG:HD2	1:S:120:ARG:C	2.30	0.56
1:V:68:ARG:HH11	1:V:68:ARG:HG3	1.70	0.56
1:V:345:LEU:HD13	1:V:396:LEU:HD22	1.88	0.56
1:C:108:MET:HE2	1:C:295:HIS:CE1	2.40	0.55
2:I:144:SER:O	2:I:148:ILE:HG13	2.07	0.55
2:L:88:LEU:O	2:L:89:ARG:HB3	2.06	0.55
1:X:346:THR:HG22	1:X:353:THR:HG21	1.88	0.55
1:X:352:LEU:HD11	1:X:397:HIS:HD2	1.71	0.55
2:G:137:LEU:CD1	2:M:136:ALA:HB1	2.37	0.55
2:M:1:THR:N	4:M:175:LVS:O1'	2.39	0.55
2:P:8:ARG:O	2:P:11:GLN:HB2	2.06	0.55
2:Q:112:VAL:HB	1:W:443:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:5:SER:HB2	2:R:14:VAL:HG22	1.87	0.55
1:A:63:LYS:HD2	1:A:308:SER:HB2	1.87	0.55
1:F:407:ILE:HD11	1:F:419:VAL:HG11	1.89	0.55
2:H:137:LEU:HD11	2:N:136:ALA:HB1	1.87	0.55
2:Q:46:PHE:HB3	2:Q:95:LEU:HD12	1.86	0.55
1:S:398:THR:HG22	1:X:328:PRO:HA	1.88	0.55
1:T:65:GLU:HG2	3:T:457:ATP:H5'2	1.88	0.55
1:T:444:LEU:OXT	1:T:444:LEU:HD22	2.06	0.55
1:U:80:LYS:HG3	1:U:255:PHE:HD2	1.71	0.55
2:J:56:LEU:HD13	2:J:95:LEU:CG	2.24	0.55
2:N:1:THR:H1	4:N:175:LVS:CS	2.19	0.55
1:S:16:HIS:CD2	1:S:69:ARG:HE	2.24	0.55
2:J:36:ARG:NH1	2:J:170:GLU:OE2	2.40	0.55
2:M:18:GLY:N	2:M:33:LYS:HZ2	2.04	0.55
2:O:1:THR:H3	4:O:175:LVS:CS	2.19	0.55
2:O:105:ILE:CG2	2:O:113:VAL:HB	2.36	0.55
1:S:68:ARG:HG3	1:S:68:ARG:HH11	1.71	0.55
1:T:280:ARG:HG3	1:U:82:GLU:OE1	2.07	0.55
1:U:16:HIS:CD2	1:U:69:ARG:HE	2.25	0.55
1:U:442:PHE:O	1:U:443:ILE:HD13	2.07	0.55
1:V:352:LEU:HD13	1:V:400:MET:HG3	1.89	0.55
1:X:64:THR:HB	3:X:461:ATP:O1A	2.06	0.55
3:A:450:ATP:C8	3:A:450:ATP:H5'1	2.42	0.55
1:B:34:ARG:O	1:B:38:MET:HE3	2.07	0.55
1:B:402:ARG:NH2	1:B:433:VAL:CG2	2.69	0.55
1:C:443:ILE:HG23	2:I:112:VAL:HG23	1.89	0.55
2:Q:104:LEU:HD13	2:Q:112:VAL:CG1	2.37	0.55
1:W:352:LEU:HD11	1:W:397:HIS:HD2	1.71	0.55
1:W:439:LEU:H	1:W:439:LEU:CD2	2.15	0.55
1:F:63:LYS:HB2	3:F:455:ATP:O2B	2.07	0.55
2:G:1:THR:N	4:G:175:LVS:S	2.79	0.55
2:J:18:GLY:HA2	2:J:33:LYS:HD2	1.89	0.55
1:W:439:LEU:C	1:W:441:ARG:H	2.15	0.55
1:B:64:THR:HB	3:B:451:ATP:O1A	2.07	0.55
2:I:17:ASP:HB2	2:I:164:ASN:ND2	2.22	0.55
2:J:144:SER:OG	2:J:147:GLU:HG3	2.07	0.55
2:N:8:ARG:HB3	2:N:8:ARG:HH11	1.71	0.55
2:O:46:PHE:HB3	2:O:95:LEU:HD12	1.87	0.55
2:O:104:LEU:HD13	2:O:112:VAL:CG1	2.37	0.55
2:O:137:LEU:C	2:O:141:THR:HG22	2.32	0.55
1:T:352:LEU:HD11	1:T:397:HIS:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:346:THR:HG22	1:U:353:THR:HG21	1.89	0.55
1:A:366:ASN:HB3	1:A:418:THR:HG22	1.88	0.55
2:I:161:VAL:HG13	2:N:24:ASN:O	2.06	0.55
2:K:137:LEU:HD11	2:Q:136:ALA:HB1	1.89	0.55
2:L:161:VAL:HG13	2:Q:24:ASN:O	2.06	0.55
2:N:19:GLN:N	2:N:33:LYS:HZ1	2.03	0.55
2:P:1:THR:N	4:P:175:LVS:O1'	2.39	0.55
1:T:352:LEU:HD13	1:T:400:MET:HG3	1.88	0.55
1:U:344:ILE:HG23	3:U:458:ATP:H2	1.71	0.55
1:U:439:LEU:H	1:U:439:LEU:CD2	2.18	0.55
1:B:280:ARG:HG3	1:B:280:ARG:HH11	1.71	0.55
1:B:366:ASN:HB3	1:B:418:THR:HG22	1.88	0.55
1:F:79:ILE:CG2	1:F:103:LEU:HD13	2.30	0.55
2:N:17:ASP:HB2	2:N:164:ASN:HD22	1.72	0.55
2:R:1:THR:CG2	2:R:33:LYS:HZ3	2.19	0.55
2:R:28:LYS:HE2	2:R:30:ASN:OD1	2.07	0.55
1:A:23:ALA:HA	1:A:331:VAL:HG21	1.88	0.54
1:B:108:MET:HA	1:B:108:MET:HE3	1.89	0.54
1:C:443:ILE:HG12	2:I:112:VAL:CG2	2.37	0.54
2:L:18:GLY:H	2:L:164:ASN:HD21	1.56	0.54
2:M:120:ILE:O	2:M:121:LEU:HD23	2.06	0.54
2:O:8:ARG:O	2:O:11:GLN:HB2	2.07	0.54
2:R:8:ARG:HB3	2:R:8:ARG:HH11	1.71	0.54
2:R:112:VAL:HB	1:X:443:ILE:HD12	1.88	0.54
1:S:352:LEU:HD11	1:S:397:HIS:HD2	1.72	0.54
1:U:71:ALA:HB1	1:U:78:PHE:HB2	1.89	0.54
1:W:345:LEU:HD13	1:W:396:LEU:HD22	1.88	0.54
2:H:161:VAL:HG13	2:M:24:ASN:O	2.07	0.54
2:N:55:THR:HG22	2:O:83:ARG:HG2	1.88	0.54
1:A:113:GLN:OE1	1:A:113:GLN:HA	2.06	0.54
1:D:100:ILE:HB	1:D:291:VAL:HG21	1.89	0.54
1:E:366:ASN:HB3	1:E:418:THR:HG22	1.88	0.54
1:F:37:ARG:HD2	1:F:48:VAL:CG1	2.37	0.54
1:F:402:ARG:NH2	1:F:433:VAL:HG21	2.22	0.54
2:H:1:THR:CG2	2:H:33:LYS:HZ3	2.01	0.54
2:J:67:HIS:CD2	2:J:73:LYS:HE3	2.42	0.54
2:P:28:LYS:HE2	2:P:30:ASN:OD1	2.08	0.54
2:P:164:ASN:HD22	2:P:164:ASN:H	1.56	0.54
2:Q:3:ILE:HB	2:Q:123:ILE:HG13	1.89	0.54
1:U:313:VAL:HG23	1:U:314:ALA:N	2.23	0.54
1:A:356:TYR:O	1:A:357:LYS:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:H	1:A:406:LYS:CD	2.04	0.54
1:C:63:LYS:HD2	1:C:308:SER:HB2	1.89	0.54
1:F:437:GLU:C	1:F:439:LEU:H	2.05	0.54
2:G:18:GLY:C	2:G:33:LYS:HZ1	2.13	0.54
1:W:16:HIS:CD2	1:W:69:ARG:HE	2.26	0.54
1:B:100:ILE:HB	1:B:291:VAL:HG21	1.89	0.54
1:C:409:PHE:CE1	1:D:6:PRO:HB3	2.43	0.54
1:D:37:ARG:HD2	1:D:48:VAL:CG1	2.38	0.54
2:G:133:ALA:HB1	2:G:155:ILE:HD12	1.89	0.54
2:H:56:LEU:HD12	2:H:95:LEU:HG	1.86	0.54
2:I:136:ALA:HB1	2:O:137:LEU:HD13	1.90	0.54
2:K:72:LEU:HD22	2:K:104:LEU:HD21	1.89	0.54
2:M:8:ARG:HB3	2:M:8:ARG:HH11	1.73	0.54
1:X:108:MET:C	1:X:110:LEU:H	2.16	0.54
1:D:437:GLU:C	1:D:439:LEU:H	2.12	0.54
2:M:1:THR:HG21	2:M:33:LYS:HE2	1.68	0.54
2:Q:5:SER:HB2	2:Q:14:VAL:HG22	1.90	0.54
1:T:313:VAL:HG23	1:T:314:ALA:N	2.23	0.54
1:U:357:LYS:HA	1:U:367:ILE:HD11	1.89	0.54
1:W:68:ARG:HH11	1:W:68:ARG:HG3	1.73	0.54
2:K:5:SER:HB2	2:K:14:VAL:HG22	1.88	0.54
2:L:24:ASN:O	2:Q:161:VAL:HG13	2.08	0.54
2:R:7:ARG:NH2	2:R:12:VAL:HG21	2.22	0.54
1:V:352:LEU:HD11	1:V:397:HIS:HD2	1.71	0.54
1:A:75:ASN:HD21	1:A:114:GLN:HE22	1.56	0.54
1:C:36:ARG:C	1:C:37:ARG:O	2.46	0.54
1:C:100:ILE:CG2	1:C:298:VAL:HG21	2.37	0.54
2:J:116:GLU:HG2	2:K:30:ASN:HD21	1.72	0.54
2:O:2:THR:OG1	2:O:126:GLY:HA3	2.08	0.54
2:O:76:VAL:HG22	1:U:443:ILE:HD11	1.90	0.54
2:Q:46:PHE:HB3	2:Q:95:LEU:CD1	2.37	0.54
1:S:233:LYS:C	1:S:235:ILE:H	2.16	0.54
1:S:279:GLN:NE2	1:S:320:ILE:N	2.54	0.54
1:S:370:THR:HG22	1:S:421:ILE:O	2.08	0.54
1:T:75:ASN:ND2	1:T:110:LEU:HD22	2.23	0.54
1:X:68:ARG:HG3	1:X:68:ARG:HH11	1.73	0.54
1:A:32:ARG:C	1:A:34:ARG:N	2.65	0.54
2:I:60:PHE:HZ	2:I:71:LEU:HD22	1.72	0.54
2:N:55:THR:O	2:N:59:LEU:HD13	2.07	0.54
2:O:3:ILE:O	2:O:122:ALA:HA	2.08	0.54
2:Q:47:ALA:HB3	2:Q:123:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LEU:OXT	2:G:113:VAL:HA	2.09	0.54
1:D:85:LYS:O	1:D:85:LYS:HG2	2.08	0.54
1:F:404:MET:O	1:F:408:SER:HB2	2.08	0.54
2:K:144:SER:OG	2:K:147:GLU:HG3	2.08	0.54
2:N:5:SER:HB2	2:N:14:VAL:HG22	1.90	0.54
2:N:7:ARG:NH2	2:N:12:VAL:HG21	2.21	0.54
1:S:313:VAL:HG23	1:S:314:ALA:N	2.23	0.54
1:X:279:GLN:NE2	1:X:320:ILE:N	2.53	0.54
2:H:136:ALA:HB1	2:N:137:LEU:HD13	1.90	0.53
1:U:300:THR:O	1:U:303:ILE:HG13	2.08	0.53
1:W:32:ARG:NH1	1:W:35:TRP:HZ3	2.06	0.53
1:B:355:GLN:O	1:B:359:LEU:HD23	2.08	0.53
1:C:100:ILE:HB	1:C:291:VAL:HG21	1.89	0.53
1:D:443:ILE:HG12	2:J:112:VAL:CG2	2.38	0.53
4:J:175:LVS:HD33	4:J:175:LVS:C1	2.38	0.53
2:K:116:GLU:HG2	2:L:30:ASN:ND2	2.23	0.53
2:P:164:ASN:ND2	2:P:164:ASN:H	2.06	0.53
1:W:71:ALA:HB1	1:W:78:PHE:HB2	1.89	0.53
1:B:389:GLU:CD	1:C:321:PRO:HG3	2.33	0.53
1:C:407:ILE:HD11	1:C:419:VAL:HG11	1.90	0.53
1:D:55:MET:CE	1:D:306:ILE:HG21	2.33	0.53
1:D:111:VAL:HG21	1:D:244:ALA:HA	1.91	0.53
1:F:285:LEU:N	1:F:285:LEU:HD12	2.24	0.53
2:G:105:ILE:CG2	2:G:113:VAL:HB	2.35	0.53
2:H:1:THR:CG2	2:H:33:LYS:HD3	2.17	0.53
2:I:7:ARG:HG3	2:I:12:VAL:HG22	1.90	0.53
2:R:1:THR:H3	4:R:175:LVS:CS	2.20	0.53
1:T:357:LYS:HA	1:T:367:ILE:HD11	1.90	0.53
1:V:336:LEU:HB2	1:V:341:PHE:HE1	1.74	0.53
1:V:370:THR:HG22	1:V:421:ILE:O	2.09	0.53
1:W:385:ASN:HD21	1:W:395:ARG:HE	1.56	0.53
1:X:236:ASN:HD21	1:X:238:GLU:HB2	1.73	0.53
1:C:27:VAL:HB	1:C:70:LEU:CD2	2.33	0.53
1:E:42:GLU:HB3	1:E:43:PRO:HD3	1.90	0.53
2:G:5:SER:HB2	2:G:14:VAL:HG22	1.89	0.53
2:G:67:HIS:HD2	2:G:73:LYS:HE3	1.72	0.53
2:M:95:LEU:O	2:M:105:ILE:HA	2.07	0.53
1:X:385:ASN:HD21	1:X:395:ARG:HE	1.57	0.53
3:F:455:ATP:C8	3:F:455:ATP:H5'1	2.43	0.53
2:N:18:GLY:O	2:N:29:GLY:C	2.51	0.53
1:T:48:VAL:O	1:T:48:VAL:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:GLU:OE1	1:D:412:SER:HA	2.08	0.53
1:D:444:LEU:HD23	2:J:113:VAL:HG22	1.90	0.53
2:R:3:ILE:O	2:R:122:ALA:HA	2.08	0.53
1:T:385:ASN:HD21	1:T:395:ARG:HE	1.56	0.53
1:V:357:LYS:HA	1:V:367:ILE:HD11	1.89	0.53
1:D:79:ILE:CG2	1:D:103:LEU:HD13	2.34	0.53
1:E:114:GLN:C	1:E:116:ILE:H	2.16	0.53
2:G:67:HIS:CD2	2:G:73:LYS:HE3	2.44	0.53
2:M:37:LEU:HB2	2:M:42:VAL:CG2	2.39	0.53
1:U:68:ARG:HH11	1:U:68:ARG:HG3	1.74	0.53
1:X:80:LYS:HG3	1:X:255:PHE:HD2	1.74	0.53
1:A:437:GLU:HG3	1:A:439:LEU:HD12	1.91	0.53
1:B:20:GLN:CA	1:B:20:GLN:NE2	2.57	0.53
1:B:358:ALA:HB1	1:C:40:LEU:HD22	1.91	0.53
1:D:36:ARG:C	1:D:37:ARG:O	2.47	0.53
1:E:403:LEU:C	1:E:405:ASP:H	2.16	0.53
2:H:115:PRO:HG3	2:H:121:LEU:HD11	1.90	0.53
2:N:105:ILE:CG2	2:N:113:VAL:HB	2.38	0.53
2:P:47:ALA:HB3	2:P:123:ILE:HD12	1.89	0.53
2:Q:2:THR:OG1	2:Q:126:GLY:HA3	2.08	0.53
1:V:313:VAL:HG23	1:V:314:ALA:N	2.24	0.53
1:W:32:ARG:O	1:W:36:ARG:HG2	2.09	0.53
1:E:27:VAL:HB	1:E:70:LEU:CD2	2.33	0.53
1:E:34:ARG:O	1:E:38:MET:HE3	2.08	0.53
2:M:55:THR:HG22	2:N:83:ARG:HG2	1.89	0.53
2:M:137:LEU:C	2:M:141:THR:HG22	2.34	0.53
2:O:55:THR:HG22	2:P:83:ARG:HG2	1.90	0.53
2:P:131:LEU:HD11	2:P:135:ARG:CZ	2.38	0.53
2:Q:7:ARG:NH2	2:Q:12:VAL:HG21	2.21	0.53
2:Q:137:LEU:C	2:Q:141:THR:HG22	2.34	0.53
1:B:367:ILE:HD11	1:B:421:ILE:HD11	1.91	0.53
1:E:37:ARG:HD2	1:E:48:VAL:CG1	2.39	0.53
1:F:34:ARG:O	1:F:38:MET:HE3	2.09	0.53
1:F:352:LEU:HD13	1:F:400:MET:HG3	1.91	0.53
2:G:18:GLY:N	2:G:33:LYS:NZ	2.54	0.53
2:I:36:ARG:NH1	2:I:170:GLU:OE2	2.42	0.53
2:L:7:ARG:HD2	2:L:119:GLN:CG	2.37	0.53
1:S:32:ARG:NH1	1:S:35:TRP:HZ3	2.07	0.53
1:X:63:LYS:HG2	1:X:333:LEU:CD1	2.38	0.53
1:F:437:GLU:HG3	1:F:439:LEU:HB2	1.90	0.52
2:R:72:LEU:O	2:R:76:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:71:ALA:HB1	1:T:78:PHE:HB2	1.91	0.52
1:U:439:LEU:HD23	1:U:439:LEU:N	2.20	0.52
1:X:313:VAL:HG23	1:X:314:ALA:N	2.24	0.52
1:B:250:GLN:HA	1:B:250:GLN:HE21	1.73	0.52
1:B:362:THR:HG23	1:C:39:GLN:HG2	1.90	0.52
1:B:437:GLU:HG3	1:B:439:LEU:HB2	1.90	0.52
1:D:118:LYS:CG	1:D:234:LEU:HD13	2.39	0.52
1:F:403:LEU:CD2	1:F:404:MET:SD	2.97	0.52
2:G:37:LEU:HD21	2:G:57:PHE:CZ	2.45	0.52
2:I:1:THR:N	4:I:175:LVS:C1'	2.71	0.52
2:R:95:LEU:O	2:R:105:ILE:HA	2.09	0.52
1:U:336:LEU:HB2	1:U:341:PHE:HE1	1.74	0.52
1:W:48:VAL:O	1:W:48:VAL:HG13	2.09	0.52
1:W:55:MET:HE2	1:W:306:ILE:HG21	1.91	0.52
1:C:402:ARG:NH2	1:C:433:VAL:CG2	2.73	0.52
2:G:7:ARG:HD2	2:G:119:GLN:CG	2.35	0.52
2:G:120:ILE:HD11	2:G:138:VAL:HG21	1.90	0.52
4:J:175:LVS:HD33	4:J:175:LVS:N2	2.25	0.52
2:N:46:PHE:HB3	2:N:95:LEU:CD1	2.40	0.52
1:E:20:GLN:CA	1:E:20:GLN:NE2	2.57	0.52
2:J:1:THR:HG23	2:J:33:LYS:CE	2.40	0.52
2:L:33:LYS:NZ	4:L:175:LVS:HB32	2.24	0.52
1:T:32:ARG:O	1:T:36:ARG:HG2	2.09	0.52
1:V:34:ARG:NH1	1:V:252:GLY:H	2.07	0.52
1:X:9:ILE:HD13	1:X:31:LEU:HD23	1.91	0.52
1:X:434:VAL:HG12	1:X:435:GLU:N	2.24	0.52
1:A:40:LEU:HD22	1:F:358:ALA:HB1	1.92	0.52
1:B:356:TYR:O	1:B:357:LYS:C	2.52	0.52
1:C:409:PHE:CD1	1:D:6:PRO:HB3	2.44	0.52
1:D:118:LYS:HG2	1:D:234:LEU:HD13	1.92	0.52
1:D:403:LEU:CD2	1:D:404:MET:SD	2.97	0.52
1:D:407:ILE:HD11	1:D:419:VAL:HG11	1.91	0.52
2:P:95:LEU:O	2:P:105:ILE:HA	2.09	0.52
1:S:63:LYS:HB2	3:S:456:ATP:O2B	2.09	0.52
1:S:71:ALA:HB1	1:S:78:PHE:HB2	1.91	0.52
1:U:40:LEU:O	1:U:45:ARG:HD3	2.10	0.52
1:E:356:TYR:O	1:E:357:LYS:C	2.51	0.52
2:J:33:LYS:NZ	4:J:175:LVS:CB3	2.58	0.52
1:S:18:ILE:HD11	1:S:343:ARG:HH21	1.73	0.52
1:S:242:GLN:NE2	1:S:246:ASP:OD1	2.42	0.52
1:T:68:ARG:HH11	1:T:68:ARG:HG3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:439:LEU:H	1:T:439:LEU:CD2	2.18	0.52
1:U:20:GLN:O	1:U:21:ALA:HB2	2.09	0.52
1:W:6:PRO:O	1:W:10:VAL:HG23	2.10	0.52
1:X:71:ALA:HB1	1:X:78:PHE:HB2	1.90	0.52
1:X:286:VAL:HA	1:X:305:PHE:CE1	2.44	0.52
1:A:27:VAL:HB	1:A:70:LEU:CD2	2.35	0.52
1:A:370:THR:HG23	1:A:421:ILE:O	2.09	0.52
2:N:47:ALA:HB3	2:N:123:ILE:HD12	1.92	0.52
2:Q:17:ASP:CG	2:Q:33:LYS:HZ3	2.14	0.52
2:R:1:THR:N	4:R:175:LVS:O1'	2.43	0.52
1:A:32:ARG:C	1:A:34:ARG:H	2.17	0.52
1:A:349:HIS:O	1:A:350:ALA:HB3	2.09	0.52
1:A:401:GLU:OE1	1:B:51:LYS:HG3	2.10	0.52
1:B:108:MET:CE	1:B:240:LEU:HG	2.40	0.52
1:B:403:LEU:HD11	1:B:426:VAL:HG22	1.91	0.52
1:C:444:LEU:CD2	2:I:113:VAL:HG22	2.39	0.52
1:E:79:ILE:HD12	1:E:80:LYS:H	1.75	0.52
2:L:105:ILE:CG2	2:L:113:VAL:HB	2.36	0.52
2:N:76:VAL:HG11	1:T:442:PHE:CE2	2.45	0.52
1:V:71:ALA:HB1	1:V:78:PHE:HB2	1.90	0.52
2:O:1:THR:N	4:O:175:LVS:S	2.83	0.52
2:P:72:LEU:O	2:P:76:VAL:HG23	2.10	0.52
1:S:357:LYS:HA	1:S:367:ILE:HD11	1.92	0.52
1:S:439:LEU:HD23	1:S:439:LEU:N	2.17	0.52
1:V:32:ARG:NH1	1:V:35:TRP:HZ3	2.08	0.52
1:X:32:ARG:NH1	1:X:35:TRP:HZ3	2.08	0.52
1:A:52:ASN:O	1:A:328:PRO:HD2	2.10	0.52
1:C:437:GLU:C	1:C:439:LEU:H	2.14	0.52
1:E:406:LYS:H	1:E:406:LYS:CD	2.13	0.52
1:F:25:ARG:O	1:F:29:ILE:HG23	2.10	0.52
2:G:1:THR:N	4:G:175:LVS:C2'	2.70	0.52
2:I:51:ALA:O	2:I:55:THR:HG23	2.09	0.52
2:O:8:ARG:HH11	2:O:8:ARG:CB	2.22	0.52
1:T:40:LEU:O	1:T:45:ARG:HD3	2.10	0.52
1:U:352:LEU:HD11	1:U:397:HIS:HD2	1.74	0.52
1:V:279:GLN:NE2	1:V:320:ILE:N	2.54	0.52
1:W:439:LEU:HD23	1:W:439:LEU:N	2.17	0.52
1:X:439:LEU:C	1:X:441:ARG:H	2.18	0.52
1:C:42:GLU:HB3	1:C:43:PRO:HD3	1.92	0.51
3:C:452:ATP:H5'1	3:C:452:ATP:C8	2.45	0.51
2:G:17:ASP:O	2:G:33:LYS:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:78:LEU:O	2:H:78:LEU:HD12	2.09	0.51
2:M:19:GLN:H	2:M:33:LYS:HZ1	1.58	0.51
2:M:46:PHE:HB3	2:M:95:LEU:CD1	2.40	0.51
2:O:66:MET:O	2:O:67:HIS:ND1	2.43	0.51
2:O:72:LEU:HG	1:U:438:ASP:OD2	2.10	0.51
1:S:336:LEU:HB2	1:S:341:PHE:HE1	1.74	0.51
1:S:439:LEU:H	1:S:439:LEU:CD2	2.16	0.51
1:E:37:ARG:O	1:E:38:MET:HB2	2.11	0.51
1:E:73:LEU:HD12	1:E:73:LEU:O	2.10	0.51
2:G:36:ARG:NH1	2:G:170:GLU:OE2	2.44	0.51
2:G:153:LEU:HB3	2:G:167:PHE:CE2	2.46	0.51
2:M:1:THR:N	4:M:175:LVS:S	2.83	0.51
2:M:18:GLY:N	2:M:33:LYS:NZ	2.58	0.51
2:N:131:LEU:HD11	2:N:135:ARG:CZ	2.40	0.51
2:R:104:LEU:HD13	2:R:112:VAL:CG1	2.40	0.51
1:S:297:MET:HE2	1:T:105:ASP:HB3	1.91	0.51
1:U:32:ARG:NH1	1:U:35:TRP:HZ3	2.07	0.51
1:V:48:VAL:HG21	1:W:359:LEU:HD11	1.91	0.51
1:V:439:LEU:HD23	1:V:439:LEU:N	2.19	0.51
2:G:24:ASN:O	2:R:161:VAL:HG13	2.11	0.51
2:M:104:LEU:HD13	2:M:112:VAL:CG1	2.39	0.51
2:O:18:GLY:O	2:O:29:GLY:C	2.54	0.51
1:S:437:GLU:O	1:S:438:ASP:C	2.53	0.51
1:V:421:ILE:HG12	1:V:425:TYR:CD1	2.46	0.51
1:W:68:ARG:C	1:W:70:LEU:H	2.19	0.51
1:X:115:GLU:HG2	1:X:119:ASN:HD22	1.74	0.51
1:B:285:LEU:HD12	1:B:285:LEU:N	2.25	0.51
1:F:293:THR:C	1:F:295:HIS:H	2.18	0.51
2:I:133:ALA:HB1	2:I:155:ILE:HD12	1.92	0.51
2:J:137:LEU:HD11	2:P:136:ALA:HB1	1.92	0.51
2:M:131:LEU:HD11	2:M:135:ARG:HE	1.75	0.51
2:P:18:GLY:O	2:P:29:GLY:C	2.53	0.51
1:V:444:LEU:OXT	1:V:444:LEU:HD22	2.10	0.51
1:W:313:VAL:HG23	1:W:314:ALA:N	2.25	0.51
1:B:118:LYS:HZ1	1:B:234:LEU:HD11	1.76	0.51
1:B:326:ARG:C	1:B:328:PRO:HD3	2.35	0.51
1:C:362:THR:CG2	1:D:39:GLN:HG2	2.40	0.51
2:J:17:ASP:CG	2:J:163:THR:HG23	2.36	0.51
2:J:67:HIS:HD2	2:J:73:LYS:HE3	1.75	0.51
2:K:28:LYS:HE2	2:K:30:ASN:OD1	2.11	0.51
2:L:1:THR:N	4:L:175:LVS:S	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:37:LEU:HB2	2:N:42:VAL:CG2	2.40	0.51
2:N:137:LEU:C	2:N:141:THR:HG22	2.35	0.51
1:S:60:GLY:HA3	1:S:392:GLY:HA3	1.93	0.51
1:T:336:LEU:HB2	1:T:341:PHE:HE1	1.75	0.51
1:U:30:ALA:HB2	1:U:53:ILE:HD11	1.93	0.51
1:U:279:GLN:NE2	1:U:320:ILE:N	2.52	0.51
1:A:367:ILE:HD11	1:A:421:ILE:HD12	1.91	0.51
1:D:444:LEU:OXT	2:J:113:VAL:HA	2.11	0.51
1:F:363:GLU:OE1	1:F:412:SER:HA	2.10	0.51
2:H:1:THR:N	4:H:175:LVS:C1'	2.72	0.51
2:O:7:ARG:HE	2:O:12:VAL:CG2	2.08	0.51
2:R:1:THR:N	4:R:175:LVS:S	2.84	0.51
2:R:17:ASP:HB2	2:R:164:ASN:HD22	1.74	0.51
2:R:66:MET:O	2:R:67:HIS:ND1	2.44	0.51
1:T:63:LYS:HG2	1:T:333:LEU:HD12	1.93	0.51
1:X:68:ARG:C	1:X:70:LEU:H	2.19	0.51
1:X:336:LEU:HB2	1:X:341:PHE:HE1	1.76	0.51
1:A:250:GLN:HA	1:A:250:GLN:HE21	1.76	0.51
1:B:444:LEU:HD23	2:H:113:VAL:HG22	1.93	0.51
2:I:137:LEU:HD11	2:O:136:ALA:HB1	1.93	0.51
2:L:78:LEU:HD12	2:L:78:LEU:O	2.11	0.51
2:P:141:THR:OG1	2:P:143:LEU:HG	2.10	0.51
2:Q:1:THR:N	4:Q:175:LVS:S	2.84	0.51
1:S:48:VAL:HG13	1:S:48:VAL:O	2.11	0.51
1:S:105:ASP:HB3	1:X:297:MET:CE	2.39	0.51
1:S:108:MET:HE1	1:S:244:ALA:CB	2.40	0.51
1:U:32:ARG:O	1:U:36:ARG:HG2	2.11	0.51
1:U:112:ARG:HG2	1:U:112:ARG:HH11	1.75	0.51
1:U:321:PRO:HG3	1:V:389:GLU:HG2	1.93	0.51
1:B:359:LEU:HD22	1:C:40:LEU:HD11	1.93	0.51
1:D:395:ARG:O	1:D:398:THR:HB	2.10	0.51
1:F:108:MET:HE1	1:F:240:LEU:HD23	1.92	0.51
2:J:1:THR:CG2	2:J:33:LYS:HZ2	2.15	0.51
2:N:72:LEU:O	2:N:76:VAL:HG23	2.10	0.51
1:S:6:PRO:O	1:S:10:VAL:HG23	2.11	0.51
1:U:55:MET:HE2	1:U:306:ILE:HG21	1.92	0.51
1:U:333:LEU:N	1:U:333:LEU:HD23	2.26	0.51
1:W:336:LEU:HB2	1:W:341:PHE:HE1	1.76	0.51
1:E:36:ARG:C	1:E:37:ARG:O	2.51	0.51
2:G:51:ALA:O	2:G:55:THR:HG23	2.11	0.51
1:S:5:THR:O	1:S:9:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:40:LEU:O	1:W:45:ARG:HD3	2.10	0.51
1:X:439:LEU:HD23	1:X:439:LEU:N	2.18	0.51
2:K:78:LEU:O	2:K:78:LEU:HD12	2.11	0.51
2:O:51:ALA:O	2:O:55:THR:HG23	2.10	0.51
1:T:5:THR:O	1:T:9:ILE:HG13	2.11	0.51
1:V:333:LEU:N	1:V:333:LEU:HD23	2.25	0.51
1:X:48:VAL:HG13	1:X:48:VAL:O	2.11	0.51
1:B:356:TYR:CD1	1:B:400:MET:HE3	2.46	0.50
1:C:437:GLU:HG3	1:C:439:LEU:HB2	1.92	0.50
1:D:34:ARG:O	1:D:38:MET:HE3	2.11	0.50
1:E:360:MET:HE2	1:E:360:MET:HA	1.94	0.50
1:F:60:GLY:HA2	3:F:455:ATP:PB	2.50	0.50
1:F:355:GLN:O	1:F:359:LEU:HD23	2.10	0.50
2:I:1:THR:N	4:I:175:LVS:C2'	2.74	0.50
1:S:32:ARG:O	1:S:36:ARG:HG2	2.11	0.50
1:S:34:ARG:NH1	1:S:252:GLY:H	2.08	0.50
1:U:100:ILE:HB	1:U:291:VAL:HG11	1.93	0.50
1:U:370:THR:HG22	1:U:421:ILE:O	2.11	0.50
1:X:444:LEU:OXT	1:X:444:LEU:HD22	2.11	0.50
1:C:390:ASN:C	1:C:390:ASN:OD1	2.55	0.50
1:C:403:LEU:CD2	1:C:404:MET:SD	2.99	0.50
2:G:161:VAL:HG13	2:R:24:ASN:O	2.11	0.50
2:M:81:ASP:O	2:M:88:LEU:HB2	2.11	0.50
1:T:32:ARG:NH1	1:T:35:TRP:HZ3	2.08	0.50
1:T:34:ARG:NH1	1:T:252:GLY:H	2.09	0.50
1:W:34:ARG:NH1	1:W:252:GLY:H	2.09	0.50
1:W:357:LYS:HA	1:W:367:ILE:HD11	1.93	0.50
1:W:370:THR:HG22	1:W:421:ILE:O	2.11	0.50
1:F:79:ILE:HD12	1:F:80:LYS:N	2.26	0.50
2:J:24:ASN:O	2:O:161:VAL:HG13	2.12	0.50
2:M:1:THR:CG2	2:M:33:LYS:NZ	2.75	0.50
2:O:95:LEU:O	2:O:105:ILE:HA	2.11	0.50
2:Q:112:VAL:HB	1:W:443:ILE:CD1	2.42	0.50
1:S:20:GLN:O	1:S:21:ALA:HB2	2.11	0.50
1:T:240:LEU:C	1:T:242:GLN:H	2.19	0.50
1:U:34:ARG:NH1	1:U:252:GLY:H	2.10	0.50
1:V:20:GLN:O	1:V:21:ALA:HB2	2.11	0.50
1:W:63:LYS:HG2	1:W:333:LEU:HD12	1.93	0.50
1:A:39:GLN:HG2	1:F:362:THR:HG21	1.93	0.50
1:A:347:GLU:HB2	1:A:348:PRO:HD3	1.93	0.50
1:A:390:ASN:C	1:A:390:ASN:OD1	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ALA:HB1	1:B:251:ASN:O	2.11	0.50
1:B:236:ASN:HD22	1:B:239:GLU:HB2	1.75	0.50
1:E:326:ARG:C	1:E:328:PRO:HD3	2.36	0.50
1:F:85:LYS:HG2	1:F:85:LYS:O	2.09	0.50
2:L:131:LEU:HD21	2:L:135:ARG:NH2	2.26	0.50
2:N:8:ARG:HH11	2:N:8:ARG:CB	2.25	0.50
2:Q:54:PHE:HE1	1:X:444:LEU:HD12	1.76	0.50
2:R:3:ILE:HB	2:R:123:ILE:HG13	1.93	0.50
2:R:131:LEU:HD11	2:R:135:ARG:CZ	2.42	0.50
1:S:425:TYR:O	1:S:429:ALA:HB2	2.11	0.50
1:U:286:VAL:HA	1:U:305:PHE:CE1	2.47	0.50
1:W:279:GLN:NE2	1:W:320:ILE:N	2.56	0.50
1:C:111:VAL:HG21	1:C:244:ALA:HA	1.92	0.50
1:D:20:GLN:CA	1:D:20:GLN:NE2	2.66	0.50
1:E:64:THR:HB	3:E:454:ATP:O1A	2.11	0.50
2:J:153:LEU:HB3	2:J:167:PHE:CE2	2.46	0.50
2:O:37:LEU:HB2	2:O:42:VAL:CG2	2.40	0.50
2:P:66:MET:O	2:P:67:HIS:ND1	2.45	0.50
2:P:104:LEU:HD13	2:P:112:VAL:CG1	2.41	0.50
2:Q:7:ARG:HE	2:Q:12:VAL:CG2	2.10	0.50
1:U:283:LEU:HB3	1:U:284:PRO:HD3	1.93	0.50
1:V:6:PRO:O	1:V:10:VAL:HG23	2.11	0.50
1:W:441:ARG:HB3	1:W:442:PHE:CE1	2.46	0.50
1:X:30:ALA:HB2	1:X:53:ILE:HD11	1.93	0.50
1:D:234:LEU:HD23	1:D:234:LEU:O	2.11	0.50
2:N:1:THR:H3	4:N:175:LVS:C1'	2.24	0.50
2:P:37:LEU:HB2	2:P:42:VAL:CG2	2.42	0.50
1:T:283:LEU:HB3	1:T:284:PRO:HD3	1.93	0.50
1:A:233:LYS:HD3	1:A:235:ILE:CD1	2.42	0.50
1:D:258:GLU:OE1	1:E:322:GLU:OE1	2.29	0.50
2:H:144:SER:OG	2:H:147:GLU:HG3	2.12	0.50
2:M:72:LEU:O	2:M:76:VAL:HG23	2.11	0.50
1:V:5:THR:O	1:V:9:ILE:HG13	2.11	0.50
1:V:16:HIS:CD2	1:V:69:ARG:HE	2.29	0.50
1:X:34:ARG:NH1	1:X:252:GLY:H	2.09	0.50
1:A:37:ARG:CG	1:A:38:MET:N	2.75	0.50
1:E:280:ARG:HH11	1:E:280:ARG:CG	2.25	0.50
2:J:88:LEU:O	2:J:89:ARG:HB3	2.12	0.50
2:K:131:LEU:HD21	2:K:135:ARG:NH2	2.27	0.50
2:O:7:ARG:HH21	2:O:12:VAL:CG2	2.23	0.50
1:X:20:GLN:O	1:X:21:ALA:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LYS:HB2	3:B:451:ATP:O2B	2.12	0.50
1:E:293:THR:C	1:E:295:HIS:H	2.19	0.50
2:I:131:LEU:HD21	2:I:135:ARG:NH2	2.26	0.50
2:M:8:ARG:HH11	2:M:8:ARG:CB	2.25	0.50
2:O:49:GLY:H	4:O:175:LVS:HN3	1.59	0.50
2:Q:37:LEU:HB2	2:Q:42:VAL:CG2	2.41	0.50
2:Q:72:LEU:O	2:Q:76:VAL:HG23	2.12	0.50
1:T:333:LEU:HD23	1:T:333:LEU:N	2.27	0.50
1:W:5:THR:O	1:W:9:ILE:HG13	2.12	0.50
1:W:300:THR:O	1:W:303:ILE:HG13	2.11	0.50
1:X:32:ARG:O	1:X:36:ARG:HG2	2.12	0.50
1:X:283:LEU:HB3	1:X:284:PRO:HD3	1.94	0.50
1:A:415:ASN:OD1	1:A:416:GLY:N	2.45	0.49
1:C:330:ARG:HG3	1:C:330:ARG:HH11	1.77	0.49
1:E:23:ALA:HA	1:E:331:VAL:HG21	1.94	0.49
1:E:409:PHE:CE1	1:F:6:PRO:HB3	2.47	0.49
2:J:4:VAL:HG23	2:J:122:ALA:HB2	1.94	0.49
2:J:144:SER:O	2:J:148:ILE:HG13	2.11	0.49
2:L:18:GLY:HA2	2:L:33:LYS:HE2	1.94	0.49
2:N:95:LEU:O	2:N:105:ILE:HA	2.12	0.49
2:O:131:LEU:HD11	2:O:135:ARG:CZ	2.42	0.49
1:T:68:ARG:C	1:T:70:LEU:H	2.20	0.49
1:V:115:GLU:HA	1:V:118:LYS:HB2	1.94	0.49
2:H:88:LEU:O	2:H:89:ARG:HB3	2.12	0.49
2:H:153:LEU:HB3	2:H:167:PHE:CE2	2.47	0.49
2:R:46:PHE:HB3	2:R:95:LEU:CD1	2.42	0.49
1:S:68:ARG:C	1:S:70:LEU:H	2.20	0.49
1:S:333:LEU:N	1:S:333:LEU:HD23	2.26	0.49
1:U:48:VAL:HG13	1:U:48:VAL:O	2.11	0.49
1:U:439:LEU:C	1:U:441:ARG:H	2.21	0.49
1:V:32:ARG:O	1:V:36:ARG:HG2	2.12	0.49
1:B:20:GLN:HE22	1:B:334:THR:H	1.60	0.49
1:C:85:LYS:HG2	1:C:85:LYS:O	2.12	0.49
1:C:250:GLN:HA	1:C:250:GLN:HE21	1.76	0.49
1:E:283:LEU:HB2	1:E:284:PRO:HD3	1.93	0.49
2:O:46:PHE:HB3	2:O:95:LEU:CD1	2.42	0.49
2:R:8:ARG:HH11	2:R:8:ARG:CB	2.24	0.49
2:R:56:LEU:HB2	2:R:91:LEU:HD23	1.94	0.49
1:S:336:LEU:HB2	1:S:341:PHE:CE1	2.47	0.49
1:U:68:ARG:C	1:U:70:LEU:H	2.19	0.49
1:V:286:VAL:HA	1:V:305:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:30:ALA:HB2	1:W:53:ILE:HD11	1.94	0.49
1:C:55:MET:CE	1:C:306:ILE:HG21	2.35	0.49
1:E:390:ASN:C	1:E:390:ASN:OD1	2.55	0.49
2:M:83:ARG:CG	2:R:55:THR:HG22	2.42	0.49
2:P:49:GLY:O	2:P:50:THR:C	2.54	0.49
2:Q:120:ILE:O	2:Q:121:LEU:HD23	2.12	0.49
1:V:40:LEU:O	1:V:45:ARG:HD3	2.11	0.49
1:V:48:VAL:HG13	1:V:48:VAL:O	2.11	0.49
1:V:425:TYR:O	1:V:429:ALA:HB2	2.13	0.49
1:W:20:GLN:O	1:W:21:ALA:HB2	2.12	0.49
1:W:444:LEU:HD13	1:W:444:LEU:H	1.77	0.49
1:X:40:LEU:O	1:X:45:ARG:HD3	2.12	0.49
1:B:37:ARG:O	1:B:38:MET:HB2	2.12	0.49
1:B:349:HIS:O	1:B:350:ALA:CB	2.61	0.49
1:B:378:ALA:O	1:B:379:GLU:C	2.55	0.49
1:B:403:LEU:CD2	1:B:404:MET:SD	3.01	0.49
1:C:101:ARG:HA	1:C:293:THR:HG22	1.94	0.49
3:E:454:ATP:C8	3:E:454:ATP:C5'	2.94	0.49
1:F:62:GLY:O	1:F:66:ILE:HG13	2.12	0.49
2:H:5:SER:HB2	2:H:14:VAL:HG22	1.94	0.49
2:J:136:ALA:HB1	2:P:137:LEU:CD1	2.42	0.49
2:K:88:LEU:O	2:K:89:ARG:HB3	2.12	0.49
2:L:164:ASN:C	2:L:164:ASN:ND2	2.64	0.49
2:O:72:LEU:O	2:O:76:VAL:HG23	2.12	0.49
2:O:120:ILE:O	2:O:121:LEU:HD23	2.13	0.49
2:Q:48:GLY:H	4:Q:175:LVS:H2'	1.77	0.49
2:G:19:GLN:N	2:G:33:LYS:HZ1	2.10	0.49
2:M:55:THR:O	2:M:59:LEU:HD13	2.12	0.49
2:O:157:GLY:HA2	2:O:163:THR:HG22	1.94	0.49
1:T:336:LEU:HB2	1:T:341:PHE:CE1	2.48	0.49
1:U:336:LEU:HB2	1:U:341:PHE:CE1	2.47	0.49
1:U:425:TYR:O	1:U:429:ALA:HB2	2.13	0.49
1:A:37:ARG:O	1:A:38:MET:HB2	2.12	0.49
1:A:326:ARG:C	1:A:328:PRO:HD3	2.38	0.49
1:B:444:LEU:CD2	2:H:113:VAL:HG22	2.42	0.49
1:C:34:ARG:O	1:C:38:MET:HE3	2.13	0.49
2:G:116:GLU:HG2	2:H:30:ASN:ND2	2.28	0.49
2:H:17:ASP:HB2	2:H:164:ASN:ND2	2.27	0.49
2:M:48:GLY:H	4:M:175:LVS:H2'	1.77	0.49
2:O:141:THR:OG1	2:O:143:LEU:HG	2.13	0.49
1:T:100:ILE:HB	1:T:291:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ASP:O	1:B:250:GLN:HG2	2.13	0.49
1:B:283:LEU:HB2	1:B:284:PRO:HD3	1.95	0.49
1:D:403:LEU:C	1:D:405:ASP:H	2.19	0.49
1:F:42:GLU:HB3	1:F:43:PRO:HD3	1.95	0.49
1:F:250:GLN:HA	1:F:250:GLN:HE21	1.76	0.49
2:N:1:THR:N	4:N:175:LVS:H1'2	2.27	0.49
2:N:1:THR:H3	4:N:175:LVS:C2'	2.26	0.49
1:V:336:LEU:HB2	1:V:341:PHE:CE1	2.47	0.49
1:X:259:ILE:HG22	1:X:308:SER:O	2.13	0.49
1:C:367:ILE:HD11	1:C:421:ILE:HD12	1.95	0.49
1:F:107:ALA:O	1:F:108:MET:C	2.56	0.49
1:F:443:ILE:CG2	2:L:114:GLN:HG3	2.43	0.49
2:R:81:ASP:O	2:R:88:LEU:HB2	2.13	0.49
1:A:258:GLU:OE1	1:B:322:GLU:OE1	2.31	0.49
2:H:64:LEU:HD23	2:H:74:SER:OG	2.12	0.49
2:P:1:THR:N	4:P:175:LVS:S	2.86	0.49
1:S:17:ILE:CD1	1:S:65:GLU:HB3	2.42	0.49
1:U:236:ASN:HB3	1:U:239:GLU:HB2	1.95	0.49
1:V:18:ILE:HD11	1:V:343:ARG:HH21	1.75	0.49
1:X:76:ALA:CB	1:X:251:ASN:HB3	2.43	0.49
1:A:40:LEU:HD11	1:F:359:LEU:HD22	1.95	0.48
1:C:35:TRP:O	1:C:37:ARG:O	2.29	0.48
1:D:42:GLU:H	1:D:43:PRO:CD	2.25	0.48
1:D:80:LYS:HG3	1:D:255:PHE:HD2	1.77	0.48
2:G:144:SER:O	2:G:148:ILE:HG13	2.13	0.48
2:J:37:LEU:HD21	2:J:57:PHE:CZ	2.48	0.48
2:P:1:THR:HG23	2:P:33:LYS:HZ3	1.77	0.48
2:P:56:LEU:HB2	2:P:91:LEU:HD23	1.95	0.48
2:P:81:ASP:O	2:P:88:LEU:HB2	2.12	0.48
2:Q:19:GLN:H	2:Q:33:LYS:NZ	2.10	0.48
1:V:439:LEU:C	1:V:441:ARG:H	2.21	0.48
1:B:390:ASN:C	1:B:390:ASN:OD1	2.56	0.48
1:D:16:HIS:HB2	1:D:17:ILE:HD12	1.95	0.48
1:D:270:GLY:C	1:D:272:ASP:N	2.68	0.48
1:D:390:ASN:C	1:D:390:ASN:OD1	2.56	0.48
2:K:136:ALA:HB1	2:Q:137:LEU:HD13	1.95	0.48
1:T:425:TYR:O	1:T:429:ALA:HB2	2.13	0.48
1:T:441:ARG:HB3	1:T:442:PHE:CE1	2.48	0.48
1:W:439:LEU:C	1:W:441:ARG:N	2.71	0.48
1:A:76:ALA:HB1	1:A:251:ASN:O	2.12	0.48
1:A:233:LYS:HE2	1:A:235:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:ASN:HB3	1:D:418:THR:HG22	1.95	0.48
1:F:76:ALA:HB1	1:F:251:ASN:O	2.13	0.48
2:P:1:THR:CG2	2:P:33:LYS:HZ3	2.21	0.48
1:T:55:MET:HE2	1:T:306:ILE:HG21	1.94	0.48
1:U:437:GLU:O	1:U:438:ASP:C	2.56	0.48
1:V:240:LEU:HB3	1:V:244:ALA:HB2	1.93	0.48
1:X:55:MET:HE2	1:X:306:ILE:HG21	1.95	0.48
1:X:236:ASN:ND2	1:X:238:GLU:HB2	2.28	0.48
1:A:34:ARG:O	1:A:38:MET:HE3	2.13	0.48
1:B:437:GLU:CG	1:B:439:LEU:HB2	2.43	0.48
1:C:100:ILE:HG21	1:C:298:VAL:HG21	1.94	0.48
1:C:444:LEU:HD23	2:I:113:VAL:HG22	1.96	0.48
1:D:360:MET:HE2	1:D:360:MET:HA	1.94	0.48
1:E:52:ASN:O	1:E:328:PRO:HD2	2.13	0.48
1:F:42:GLU:H	1:F:43:PRO:CD	2.26	0.48
2:M:28:LYS:HE2	2:M:30:ASN:OD1	2.13	0.48
2:O:89:ARG:HG2	2:O:90:LYS:H	1.78	0.48
2:P:137:LEU:C	2:P:141:THR:HG22	2.38	0.48
2:Q:8:ARG:HH11	2:Q:8:ARG:CB	2.26	0.48
1:S:40:LEU:O	1:S:45:ARG:HD3	2.13	0.48
1:X:370:THR:HG22	1:X:421:ILE:O	2.12	0.48
1:C:16:HIS:HB2	1:C:17:ILE:HD12	1.95	0.48
1:D:246:ASP:O	1:D:250:GLN:HG2	2.14	0.48
2:I:7:ARG:NH1	2:I:12:VAL:CG2	2.77	0.48
2:M:1:THR:HG22	2:M:33:LYS:NZ	2.28	0.48
2:O:164:ASN:ND2	2:O:164:ASN:H	2.12	0.48
2:R:37:LEU:HB2	2:R:42:VAL:CG2	2.42	0.48
1:T:30:ALA:HB2	1:T:53:ILE:HD11	1.96	0.48
1:T:370:THR:HG22	1:T:421:ILE:O	2.12	0.48
1:W:100:ILE:HB	1:W:291:VAL:HG11	1.96	0.48
1:A:7:ARG:NH1	1:A:7:ARG:HB3	2.29	0.48
1:B:293:THR:C	1:B:295:HIS:H	2.22	0.48
1:C:76:ALA:HB1	1:C:251:ASN:O	2.13	0.48
1:E:326:ARG:O	1:E:328:PRO:HD3	2.14	0.48
2:I:7:ARG:HD2	2:I:119:GLN:CG	2.36	0.48
2:M:76:VAL:HG11	1:S:442:PHE:CE2	2.49	0.48
2:N:51:ALA:O	2:N:55:THR:HG23	2.13	0.48
2:R:1:THR:H1	4:R:175:LVS:CS	2.27	0.48
1:S:76:ALA:CB	1:S:251:ASN:HB3	2.43	0.48
1:V:9:ILE:HD13	1:V:31:LEU:HD23	1.96	0.48
1:V:434:VAL:HG12	1:V:435:GLU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:LYS:HB2	1:D:233:LYS:HZ3	1.77	0.48
1:D:321:PRO:O	1:D:322:GLU:C	2.57	0.48
2:I:53:ALA:HA	2:I:93:ALA:HB1	1.96	0.48
2:M:131:LEU:HD11	2:M:135:ARG:CZ	2.43	0.48
2:N:48:GLY:H	4:N:175:LVS:H2'	1.79	0.48
2:Q:76:VAL:HG11	1:W:442:PHE:CE2	2.48	0.48
2:R:89:ARG:HG2	2:R:90:LYS:H	1.79	0.48
1:U:9:ILE:HD13	1:U:31:LEU:HD23	1.96	0.48
1:W:434:VAL:HG12	1:W:435:GLU:N	2.28	0.48
1:B:75:ASN:OD1	1:B:110:LEU:HD11	2.14	0.48
1:C:17:ILE:HD12	1:C:17:ILE:N	2.28	0.48
1:C:100:ILE:HG21	1:C:298:VAL:CG2	2.44	0.48
1:C:107:ALA:O	1:C:108:MET:C	2.57	0.48
1:E:367:ILE:CD1	1:E:421:ILE:HD11	2.39	0.48
2:J:7:ARG:NH1	2:J:12:VAL:CG2	2.76	0.48
2:J:33:LYS:HZ1	4:J:175:LVS:CB3	2.21	0.48
2:K:107:THR:OG1	2:K:111:ASP:OD2	2.22	0.48
2:P:1:THR:H3	4:P:175:LVS:C2'	2.26	0.48
1:U:5:THR:O	1:U:9:ILE:HG13	2.14	0.48
1:U:439:LEU:C	1:U:441:ARG:N	2.72	0.48
1:V:63:LYS:HG2	1:V:333:LEU:HD12	1.96	0.48
1:W:7:ARG:HH12	1:X:410:SER:HB3	1.77	0.48
1:W:9:ILE:HD13	1:W:31:LEU:HD23	1.94	0.48
1:X:300:THR:O	1:X:303:ILE:HG13	2.13	0.48
1:A:403:LEU:HD11	1:A:426:VAL:HG22	1.94	0.48
1:C:367:ILE:HD11	1:C:421:ILE:HD11	1.95	0.48
1:D:285:LEU:HD12	1:D:285:LEU:N	2.28	0.48
2:H:7:ARG:NH1	2:H:12:VAL:CG2	2.77	0.48
2:J:72:LEU:HD22	2:J:104:LEU:HD21	1.96	0.48
2:P:131:LEU:HD11	2:P:135:ARG:HE	1.76	0.48
2:R:1:THR:HG22	2:R:33:LYS:HD2	1.89	0.48
1:S:373:ALA:HB2	1:S:422:ASP:HA	1.96	0.48
1:V:299:LYS:HE2	1:V:301:ASP:CG	2.39	0.48
1:W:17:ILE:CD1	1:W:65:GLU:HB3	2.44	0.48
1:W:60:GLY:HA3	1:W:392:GLY:HA3	1.95	0.48
1:W:437:GLU:O	1:W:438:ASP:C	2.57	0.48
1:X:100:ILE:HB	1:X:291:VAL:HG11	1.94	0.48
1:B:36:ARG:C	1:B:37:ARG:O	2.54	0.48
1:B:443:ILE:HG12	2:H:112:VAL:CG2	2.44	0.48
1:D:275:ARG:C	1:D:277:GLY:N	2.71	0.48
1:F:37:ARG:O	1:F:38:MET:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:330:ARG:HG3	1:F:330:ARG:HH11	1.78	0.48
1:F:370:THR:HG23	1:F:421:ILE:O	2.14	0.48
2:L:144:SER:OG	2:L:147:GLU:HG3	2.14	0.48
1:S:283:LEU:HB3	1:S:284:PRO:HD3	1.95	0.48
1:S:388:THR:HG22	1:S:389:GLU:N	2.25	0.48
1:T:20:GLN:O	1:T:21:ALA:HB2	2.14	0.48
1:U:327:LEU:N	1:U:328:PRO:CD	2.77	0.48
1:V:30:ALA:HB2	1:V:53:ILE:HD11	1.94	0.48
1:X:49:THR:HG21	1:X:326:ARG:HH22	1.79	0.48
1:X:108:MET:HE1	1:X:244:ALA:CB	2.44	0.48
1:B:250:GLN:HA	1:B:250:GLN:NE2	2.28	0.47
1:C:443:ILE:HG12	2:I:112:VAL:HG21	1.96	0.47
2:K:24:ASN:O	2:P:161:VAL:HG13	2.14	0.47
2:L:153:LEU:HB3	2:L:167:PHE:CE2	2.49	0.47
2:P:7:ARG:HE	2:P:12:VAL:CG2	2.07	0.47
1:U:6:PRO:O	1:U:10:VAL:HG23	2.14	0.47
1:W:283:LEU:HB3	1:W:284:PRO:HD3	1.96	0.47
1:W:336:LEU:HB2	1:W:341:PHE:CE1	2.49	0.47
1:X:17:ILE:HD13	1:X:66:ILE:CG1	2.44	0.47
1:B:395:ARG:O	1:B:398:THR:HB	2.14	0.47
1:D:283:LEU:HB2	1:D:284:PRO:HD3	1.95	0.47
1:D:283:LEU:HD23	1:D:283:LEU:HA	1.72	0.47
2:P:120:ILE:O	2:P:121:LEU:HD23	2.14	0.47
2:Q:76:VAL:HG22	1:W:443:ILE:HD11	1.96	0.47
2:R:50:THR:H	4:R:175:LVS:CD6	2.27	0.47
1:T:434:VAL:HG12	1:T:435:GLU:N	2.28	0.47
1:U:297:MET:HG3	1:V:109:LYS:HD2	1.96	0.47
1:U:421:ILE:HG12	1:U:425:TYR:CD1	2.49	0.47
1:U:434:VAL:HG12	1:U:435:GLU:N	2.30	0.47
1:V:300:THR:O	1:V:303:ILE:HG13	2.14	0.47
1:X:336:LEU:HB2	1:X:341:PHE:CE1	2.49	0.47
1:B:326:ARG:O	1:B:328:PRO:HD3	2.14	0.47
1:C:20:GLN:HE21	1:C:20:GLN:N	2.12	0.47
1:D:42:GLU:HB3	1:D:43:PRO:HD3	1.96	0.47
1:D:250:GLN:HE21	1:D:250:GLN:HA	1.79	0.47
1:E:270:GLY:C	1:E:272:ASP:N	2.68	0.47
1:F:366:ASN:HB3	1:F:418:THR:HG22	1.95	0.47
1:F:403:LEU:C	1:F:405:ASP:H	2.20	0.47
2:N:3:ILE:HB	2:N:123:ILE:HG13	1.95	0.47
1:T:17:ILE:CD1	1:T:65:GLU:HB3	2.44	0.47
1:T:57:GLY:O	1:T:58:PRO:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:49:THR:HG21	1:W:326:ARG:HH22	1.79	0.47
1:X:439:LEU:C	1:X:441:ARG:N	2.72	0.47
1:A:403:LEU:C	1:A:405:ASP:N	2.73	0.47
1:B:100:ILE:CG2	1:B:298:VAL:HG21	2.43	0.47
1:C:63:LYS:NZ	3:C:452:ATP:O1B	2.47	0.47
1:C:444:LEU:HD23	2:I:113:VAL:HG13	1.96	0.47
1:E:233:LYS:HZ3	1:E:233:LYS:HB2	1.80	0.47
1:F:20:GLN:HE22	1:F:334:THR:H	1.62	0.47
1:F:32:ARG:C	1:F:34:ARG:N	2.72	0.47
1:F:415:ASN:OD1	1:F:416:GLY:N	2.46	0.47
2:I:83:ARG:NH1	2:J:58:GLU:OE2	2.44	0.47
2:M:51:ALA:O	2:M:55:THR:HG23	2.14	0.47
1:S:100:ILE:HB	1:S:291:VAL:HG11	1.96	0.47
1:V:283:LEU:HB3	1:V:284:PRO:HD3	1.95	0.47
1:X:6:PRO:O	1:X:10:VAL:HG23	2.15	0.47
1:X:421:ILE:HG12	1:X:425:TYR:CD1	2.49	0.47
1:A:393:ALA:O	1:A:394:ARG:C	2.58	0.47
1:C:443:ILE:CG2	2:I:114:GLN:HG3	2.41	0.47
1:D:438:ASP:C	1:D:439:LEU:O	2.57	0.47
1:E:114:GLN:C	1:E:116:ILE:N	2.73	0.47
2:N:50:THR:H	4:N:175:LVS:CD6	2.28	0.47
1:S:30:ALA:HB2	1:S:53:ILE:HD11	1.95	0.47
1:S:48:VAL:HG21	1:T:359:LEU:HD11	1.95	0.47
1:T:279:GLN:NE2	1:T:320:ILE:N	2.55	0.47
1:U:17:ILE:CD1	1:U:65:GLU:HB3	2.45	0.47
1:U:17:ILE:HD13	1:U:66:ILE:CG1	2.44	0.47
1:U:245:ILE:HG22	1:U:249:GLU:OE1	2.15	0.47
1:W:333:LEU:N	1:W:333:LEU:HD23	2.29	0.47
1:W:421:ILE:HG12	1:W:425:TYR:CD1	2.50	0.47
1:A:100:ILE:CG2	1:A:298:VAL:HG21	2.45	0.47
1:C:235:ILE:HG22	1:C:237:PRO:HD3	1.96	0.47
1:D:326:ARG:O	1:D:328:PRO:HD3	2.14	0.47
2:H:7:ARG:CZ	2:H:12:VAL:CG2	2.93	0.47
2:K:116:GLU:HG2	2:L:30:ASN:HD21	1.79	0.47
2:N:81:ASP:O	2:N:88:LEU:HB2	2.15	0.47
2:O:55:THR:O	2:O:59:LEU:HD13	2.15	0.47
2:P:8:ARG:HH11	2:P:8:ARG:CB	2.27	0.47
2:Q:1:THR:H1	4:Q:175:LVS:CS	2.26	0.47
1:T:6:PRO:O	1:T:10:VAL:HG23	2.13	0.47
1:V:373:ALA:HB2	1:V:422:ASP:HA	1.96	0.47
1:X:21:ALA:C	1:X:23:ALA:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.73	0.47
1:A:440:SER:HB3	2:H:32:ARG:NH2	2.29	0.47
1:B:80:LYS:HG3	1:B:255:PHE:HD2	1.80	0.47
1:B:370:THR:HG23	1:B:421:ILE:O	2.14	0.47
1:D:330:ARG:HH11	1:D:330:ARG:HG3	1.79	0.47
1:E:79:ILE:HD12	1:E:80:LYS:N	2.29	0.47
1:E:285:LEU:N	1:E:285:LEU:HD12	2.30	0.47
1:E:355:GLN:O	1:E:359:LEU:HD23	2.15	0.47
1:F:410:SER:O	1:F:414:MET:HB2	2.15	0.47
2:H:67:HIS:NE2	2:H:77:GLU:HG3	2.30	0.47
2:I:64:LEU:HD23	2:I:74:SER:OG	2.15	0.47
2:P:105:ILE:HG22	2:P:113:VAL:O	2.14	0.47
2:R:55:THR:O	2:R:59:LEU:HD13	2.15	0.47
1:S:63:LYS:HG2	1:S:333:LEU:HD12	1.96	0.47
1:S:297:MET:HG3	1:T:109:LYS:HZ2	1.79	0.47
1:S:434:VAL:HG12	1:S:435:GLU:N	2.30	0.47
1:S:439:LEU:C	1:S:441:ARG:H	2.22	0.47
1:T:388:THR:HG22	1:T:389:GLU:N	2.26	0.47
1:U:49:THR:HG21	1:U:326:ARG:HH22	1.80	0.47
1:U:63:LYS:HG2	1:U:333:LEU:HD12	1.97	0.47
1:U:370:THR:O	1:U:374:VAL:HG23	2.14	0.47
1:V:82:GLU:OE2	1:V:258:GLU:HG3	2.15	0.47
1:V:328:PRO:HA	1:W:398:THR:HG22	1.96	0.47
1:W:327:LEU:N	1:W:328:PRO:CD	2.77	0.47
1:X:17:ILE:CD1	1:X:65:GLU:HB3	2.45	0.47
1:X:294:LYS:HG3	1:X:295:HIS:ND1	2.30	0.47
1:B:440:SER:O	1:B:443:ILE:N	2.29	0.47
1:E:440:SER:O	1:E:441:ARG:C	2.56	0.47
1:F:17:ILE:N	1:F:17:ILE:HD12	2.30	0.47
1:F:275:ARG:C	1:F:277:GLY:N	2.72	0.47
2:M:76:VAL:HG22	1:S:443:ILE:HD11	1.97	0.47
2:M:131:LEU:HD21	2:M:135:ARG:NH2	2.30	0.47
2:N:76:VAL:HG11	1:T:442:PHE:CD2	2.50	0.47
1:S:294:LYS:HG3	1:S:295:HIS:ND1	2.30	0.47
1:S:347:GLU:HB2	1:S:348:PRO:HD3	1.97	0.47
1:T:18:ILE:HD11	1:T:343:ARG:HH21	1.80	0.47
1:V:68:ARG:C	1:V:70:LEU:H	2.21	0.47
1:V:80:LYS:HG3	1:V:255:PHE:CD2	2.48	0.47
1:V:100:ILE:HB	1:V:291:VAL:HG11	1.97	0.47
1:A:233:LYS:CD	1:A:235:ILE:HD12	2.45	0.47
1:E:250:GLN:HA	1:E:250:GLN:HE21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:1:THR:H3	4:O:175:LVS:C2'	2.28	0.47
2:O:61:GLU:C	2:O:63:LYS:H	2.23	0.47
2:P:51:ALA:O	2:P:55:THR:HG23	2.15	0.47
1:T:49:THR:HG21	1:T:326:ARG:HH22	1.80	0.47
1:V:49:THR:HG21	1:V:326:ARG:HH22	1.80	0.47
1:W:370:THR:O	1:W:374:VAL:HG23	2.15	0.47
1:X:236:ASN:C	1:X:238:GLU:H	2.22	0.47
1:X:388:THR:HG22	1:X:389:GLU:N	2.25	0.47
1:X:425:TYR:O	1:X:429:ALA:HB2	2.15	0.47
1:A:283:LEU:HB2	1:A:284:PRO:HD3	1.97	0.47
1:A:438:ASP:O	1:A:439:LEU:O	2.32	0.47
1:B:42:GLU:HB3	1:B:43:PRO:HD3	1.97	0.47
1:B:58:PRO:HG2	1:B:61:VAL:HG11	1.97	0.47
1:B:285:LEU:HD12	1:B:285:LEU:H	1.80	0.47
1:B:355:GLN:OE1	1:C:48:VAL:HA	2.15	0.47
2:P:50:THR:O	2:P:53:ALA:HB3	2.15	0.47
2:Q:1:THR:H3	4:Q:175:LVS:CS	2.28	0.47
1:U:294:LYS:HG3	1:U:295:HIS:ND1	2.30	0.47
1:V:441:ARG:HB3	1:V:442:PHE:CE1	2.49	0.47
2:M:115:PRO:HG3	2:M:121:LEU:HD21	1.97	0.46
2:O:37:LEU:HD22	2:O:61:GLU:HG3	1.96	0.46
2:O:164:ASN:HD22	2:O:164:ASN:H	1.62	0.46
2:Q:51:ALA:O	2:Q:55:THR:HG23	2.15	0.46
2:R:49:GLY:H	4:R:175:LVS:HN3	1.62	0.46
2:R:76:VAL:HG22	1:X:443:ILE:HD11	1.96	0.46
1:T:370:THR:O	1:T:374:VAL:HG23	2.14	0.46
1:U:236:ASN:HB3	1:U:239:GLU:CB	2.46	0.46
1:U:299:LYS:HE2	1:U:301:ASP:CG	2.40	0.46
1:X:239:GLU:C	1:X:241:LYS:N	2.73	0.46
1:A:403:LEU:HD12	1:A:426:VAL:HG22	1.96	0.46
1:C:57:GLY:O	1:C:63:LYS:HE2	2.15	0.46
1:C:60:GLY:HA2	3:C:452:ATP:PB	2.55	0.46
1:C:285:LEU:N	1:C:285:LEU:HD12	2.30	0.46
1:D:362:THR:HG23	1:E:39:GLN:HG2	1.97	0.46
1:E:42:GLU:H	1:E:43:PRO:CD	2.28	0.46
1:E:85:LYS:O	1:E:85:LYS:HG2	2.14	0.46
1:E:337:SER:O	1:E:338:ALA:C	2.57	0.46
1:E:444:LEU:OXT	2:K:113:VAL:HA	2.15	0.46
1:F:100:ILE:CG2	1:F:298:VAL:HG21	2.45	0.46
1:F:390:ASN:C	1:F:390:ASN:OD1	2.57	0.46
2:H:71:LEU:CD1	2:H:104:LEU:HD22	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:7:ARG:CZ	2:J:12:VAL:CG2	2.94	0.46
2:K:153:LEU:HB3	2:K:167:PHE:CE2	2.50	0.46
2:L:137:LEU:HD11	2:R:136:ALA:HB1	1.96	0.46
2:N:76:VAL:HG22	1:T:443:ILE:HD11	1.96	0.46
2:O:7:ARG:NH2	2:O:12:VAL:HG21	2.26	0.46
2:O:61:GLU:C	2:O:63:LYS:N	2.72	0.46
2:O:125:SER:HB3	4:O:175:LVS:HI'3	1.96	0.46
2:R:18:GLY:O	2:R:29:GLY:C	2.58	0.46
2:R:164:ASN:ND2	2:R:164:ASN:H	2.13	0.46
1:V:76:ALA:CB	1:V:251:ASN:HB3	2.45	0.46
1:X:5:THR:O	1:X:9:ILE:HG13	2.15	0.46
1:D:356:TYR:O	1:D:357:LYS:C	2.58	0.46
1:E:61:VAL:HA	1:E:336:LEU:HD22	1.98	0.46
1:E:347:GLU:HB2	1:E:348:PRO:HD3	1.96	0.46
2:N:157:GLY:HA2	2:N:163:THR:HG22	1.97	0.46
2:P:64:LEU:C	2:P:66:MET:H	2.24	0.46
2:R:48:GLY:H	4:R:175:LVS:H2'	1.80	0.46
1:T:421:ILE:HG12	1:T:425:TYR:CD1	2.49	0.46
1:X:333:LEU:N	1:X:333:LEU:HD23	2.30	0.46
1:X:370:THR:O	1:X:374:VAL:HG23	2.15	0.46
1:A:330:ARG:HH11	1:A:330:ARG:HG3	1.81	0.46
2:H:1:THR:N	4:H:175:LVS:S	2.89	0.46
1:T:9:ILE:HD13	1:T:31:LEU:HD23	1.98	0.46
1:T:381:ALA:O	1:T:395:ARG:HG2	2.15	0.46
1:T:430:LEU:N	1:T:430:LEU:HD23	2.31	0.46
1:V:60:GLY:HA3	1:V:392:GLY:HA3	1.97	0.46
1:X:299:LYS:HE2	1:X:301:ASP:CG	2.41	0.46
1:A:438:ASP:C	1:A:439:LEU:O	2.59	0.46
1:C:347:GLU:HB2	1:C:348:PRO:HD3	1.98	0.46
1:C:366:ASN:HB3	1:C:418:THR:HG22	1.98	0.46
1:D:347:GLU:HB2	1:D:348:PRO:HD3	1.98	0.46
1:E:402:ARG:O	1:E:405:ASP:HB2	2.15	0.46
1:F:403:LEU:HD11	1:F:426:VAL:HG22	1.96	0.46
2:G:159:ILE:O	2:R:25:THR:HA	2.15	0.46
2:P:48:GLY:H	4:P:175:LVS:H2'	1.79	0.46
1:S:49:THR:HG21	1:S:326:ARG:HH22	1.80	0.46
1:T:439:LEU:C	1:T:441:ARG:H	2.23	0.46
1:U:373:ALA:HB2	1:U:422:ASP:HA	1.97	0.46
1:U:388:THR:HG22	1:U:389:GLU:N	2.22	0.46
1:B:61:VAL:HA	1:B:336:LEU:HD22	1.98	0.46
1:D:37:ARG:O	1:D:38:MET:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:ARG:HG2	1:D:38:MET:N	2.31	0.46
1:E:16:HIS:HB2	1:E:17:ILE:HD12	1.96	0.46
1:E:108:MET:HG2	1:E:295:HIS:CE1	2.50	0.46
2:J:51:ALA:O	2:J:55:THR:HG23	2.14	0.46
2:K:105:ILE:HG22	2:K:113:VAL:O	2.16	0.46
2:N:56:LEU:HB2	2:N:91:LEU:HD23	1.98	0.46
2:O:112:VAL:HB	1:U:443:ILE:CD1	2.44	0.46
2:P:50:THR:O	2:P:51:ALA:C	2.58	0.46
2:P:96:ILE:CD1	2:P:123:ILE:HG12	2.45	0.46
2:R:1:THR:HG23	2:R:33:LYS:HZ3	1.78	0.46
1:S:421:ILE:HG12	1:S:425:TYR:CD1	2.50	0.46
1:V:55:MET:HE2	1:V:306:ILE:HG21	1.97	0.46
2:M:76:VAL:HG11	1:S:442:PHE:CD2	2.50	0.46
2:M:164:ASN:HD22	2:M:164:ASN:H	1.64	0.46
1:W:76:ALA:CB	1:W:251:ASN:HB3	2.46	0.46
1:W:82:GLU:OE2	1:W:258:GLU:HG3	2.15	0.46
1:W:425:TYR:O	1:W:429:ALA:HB2	2.15	0.46
1:A:31:LEU:HD21	1:A:74:ALA:HB2	1.98	0.46
1:A:73:LEU:HD12	1:A:73:LEU:O	2.16	0.46
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.79	0.46
1:C:25:ARG:O	1:C:28:ALA:HB3	2.16	0.46
2:J:1:THR:N	4:J:175:LVS:H1'2	2.31	0.46
2:M:89:ARG:HG2	2:M:90:LYS:H	1.81	0.46
2:R:1:THR:H3	4:R:175:LVS:C2'	2.29	0.46
2:R:91:LEU:HB2	2:R:108:GLY:HA3	1.98	0.46
1:S:7:ARG:NH1	1:T:410:SER:HB3	2.30	0.46
1:S:38:MET:HA	1:S:38:MET:HE3	1.98	0.46
1:S:233:LYS:C	1:S:235:ILE:N	2.74	0.46
1:U:441:ARG:HB3	1:U:442:PHE:CE1	2.51	0.46
1:A:250:GLN:HA	1:A:250:GLN:NE2	2.29	0.46
1:B:443:ILE:HD11	2:H:72:LEU:CD1	2.38	0.46
1:C:25:ARG:O	1:C:29:ILE:HG23	2.15	0.46
1:D:112:ARG:O	1:D:116:ILE:HG13	2.16	0.46
1:D:401:GLU:OE1	1:E:51:LYS:HG3	2.16	0.46
1:E:25:ARG:O	1:E:29:ILE:HG23	2.16	0.46
2:G:58:GLU:OE2	2:L:83:ARG:NH1	2.49	0.46
2:J:33:LYS:HZ3	4:J:175:LVS:CB3	2.24	0.46
2:L:7:ARG:HG3	2:L:12:VAL:HG22	1.96	0.46
2:M:1:THR:HG22	2:M:33:LYS:HZ3	1.80	0.46
2:Q:80:LYS:O	2:Q:84:THR:HG23	2.15	0.46
1:S:21:ALA:C	1:S:23:ALA:N	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:54:LEU:HD23	1:V:307:ALA:HB3	1.97	0.46
1:V:347:GLU:HB2	1:V:348:PRO:HD3	1.98	0.46
1:A:293:THR:C	1:A:295:HIS:H	2.22	0.46
3:A:450:ATP:C5'	3:A:450:ATP:H8	2.28	0.46
1:B:233:LYS:HB2	1:B:233:LYS:NZ	2.31	0.46
1:B:402:ARG:O	1:B:405:ASP:HB2	2.16	0.46
2:I:86:ARG:HH11	2:I:86:ARG:CB	2.18	0.46
2:P:55:THR:O	2:P:59:LEU:HD13	2.15	0.46
2:P:64:LEU:HD23	2:P:74:SER:CB	2.46	0.46
2:Q:17:ASP:CG	2:Q:33:LYS:HZ2	2.23	0.46
2:Q:37:LEU:HD22	2:Q:61:GLU:HG3	1.97	0.46
2:Q:107:THR:C	2:Q:109:ILE:H	2.24	0.46
1:T:63:LYS:HB2	3:T:457:ATP:O2B	2.16	0.46
1:V:294:LYS:HG3	1:V:295:HIS:ND1	2.31	0.46
1:V:442:PHE:O	1:V:443:ILE:HG12	2.16	0.46
1:A:285:LEU:HD12	1:A:285:LEU:N	2.31	0.45
1:A:443:ILE:HG12	2:G:112:VAL:CG2	2.47	0.45
1:B:101:ARG:HA	1:B:293:THR:HG22	1.99	0.45
1:B:415:ASN:OD1	1:B:416:GLY:N	2.49	0.45
1:C:52:ASN:HB2	1:C:326:ARG:O	2.15	0.45
1:C:250:GLN:HA	1:C:250:GLN:NE2	2.31	0.45
1:D:57:GLY:O	1:D:63:LYS:HE2	2.16	0.45
1:E:352:LEU:HD13	1:E:400:MET:HG3	1.98	0.45
1:F:5:THR:H	1:F:8:GLU:HB3	1.81	0.45
1:F:37:ARG:HG2	1:F:38:MET:N	2.31	0.45
1:F:321:PRO:O	1:F:322:GLU:C	2.58	0.45
1:F:349:HIS:O	1:F:350:ALA:CB	2.62	0.45
2:L:17:ASP:CG	2:L:163:THR:HG23	2.41	0.45
1:T:17:ILE:HD13	1:T:66:ILE:CG1	2.46	0.45
1:X:373:ALA:HB2	1:X:422:ASP:HA	1.97	0.45
1:A:402:ARG:NH2	1:A:433:VAL:CG2	2.79	0.45
1:C:27:VAL:CB	1:C:70:LEU:HD22	2.39	0.45
1:D:326:ARG:C	1:D:328:PRO:HD3	2.41	0.45
1:E:378:ALA:O	1:E:379:GLU:C	2.58	0.45
1:E:409:PHE:CD2	1:F:25:ARG:CZ	3.00	0.45
1:F:23:ALA:CA	1:F:331:VAL:HG21	2.43	0.45
2:G:172:LEU:O	2:G:173:PRO:C	2.58	0.45
2:H:172:LEU:HD23	2:H:172:LEU:HA	1.82	0.45
2:L:7:ARG:CZ	2:L:12:VAL:CG2	2.95	0.45
1:S:286:VAL:HA	1:S:305:PHE:CE1	2.51	0.45
1:S:326:ARG:HH11	1:S:326:ARG:CA	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:110:LEU:C	1:X:112:ARG:H	2.25	0.45
1:A:345:LEU:HD12	1:A:345:LEU:HA	1.74	0.45
1:C:7:ARG:NH1	1:C:7:ARG:HB3	2.31	0.45
1:E:362:THR:HG23	1:F:39:GLN:HG2	1.98	0.45
1:F:79:ILE:HD12	1:F:80:LYS:H	1.81	0.45
2:L:7:ARG:NH1	2:L:12:VAL:CG2	2.79	0.45
2:N:66:MET:O	2:N:67:HIS:ND1	2.50	0.45
2:Q:54:PHE:CZ	1:X:444:LEU:HB3	2.51	0.45
1:T:21:ALA:C	1:T:23:ALA:N	2.72	0.45
1:T:54:LEU:HD23	1:T:307:ALA:HB3	1.98	0.45
1:T:236:ASN:N	1:T:237:PRO:HD3	2.31	0.45
1:U:347:GLU:HB2	1:U:348:PRO:HD3	1.98	0.45
1:A:283:LEU:HA	1:A:283:LEU:HD23	1.68	0.45
1:E:112:ARG:HD2	1:E:240:LEU:HD21	1.98	0.45
2:G:116:GLU:HG2	2:H:30:ASN:HD21	1.81	0.45
2:I:5:SER:HB2	2:I:14:VAL:HG22	1.98	0.45
2:J:172:LEU:HD23	2:J:172:LEU:HA	1.80	0.45
2:L:1:THR:HG21	2:L:33:LYS:NZ	2.17	0.45
2:M:47:ALA:HB3	2:M:123:ILE:HD12	1.99	0.45
2:N:1:THR:N	4:N:175:LVS:C2'	2.79	0.45
2:P:125:SER:HB3	4:P:175:LVS:H1'3	1.97	0.45
2:Q:164:ASN:HD22	2:Q:164:ASN:N	2.10	0.45
2:R:19:GLN:N	2:R:33:LYS:HZ1	2.11	0.45
2:R:120:ILE:O	2:R:121:LEU:HD23	2.16	0.45
1:V:437:GLU:O	1:V:438:ASP:C	2.60	0.45
1:W:373:ALA:HB2	1:W:422:ASP:HA	1.97	0.45
3:B:451:ATP:H8	3:B:451:ATP:C5'	2.28	0.45
3:D:453:ATP:H8	3:D:453:ATP:C5'	2.28	0.45
1:E:370:THR:O	1:E:373:ALA:HB3	2.17	0.45
1:F:20:GLN:CA	1:F:20:GLN:NE2	2.61	0.45
2:G:137:LEU:HD11	2:M:136:ALA:HB1	1.97	0.45
2:I:164:ASN:C	2:I:164:ASN:ND2	2.68	0.45
2:O:56:LEU:HB2	2:O:91:LEU:HD23	1.98	0.45
2:P:5:SER:CB	2:P:14:VAL:HG22	2.47	0.45
2:R:164:ASN:HD22	2:R:164:ASN:H	1.62	0.45
1:S:64:THR:N	3:S:456:ATP:O2B	2.50	0.45
1:S:82:GLU:OE2	1:S:258:GLU:HG3	2.16	0.45
1:S:327:LEU:N	1:S:328:PRO:CD	2.78	0.45
1:S:370:THR:O	1:S:374:VAL:HG23	2.16	0.45
1:U:40:LEU:HD13	1:U:44:LEU:O	2.17	0.45
1:V:326:ARG:HH11	1:V:326:ARG:CA	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:54:LEU:HD23	1:W:307:ALA:HB3	1.97	0.45
1:X:407:ILE:HG23	1:X:408:SER:N	2.32	0.45
1:B:407:ILE:HD11	1:B:419:VAL:HG11	1.97	0.45
1:C:270:GLY:C	1:C:272:ASP:N	2.74	0.45
1:C:403:LEU:C	1:C:405:ASP:H	2.23	0.45
1:D:280:ARG:HH11	1:D:280:ARG:CG	2.30	0.45
1:E:437:GLU:HG3	1:E:439:LEU:HB2	1.97	0.45
2:M:1:THR:H3	4:M:175:LVS:C2'	2.30	0.45
2:Q:18:GLY:O	2:Q:29:GLY:C	2.60	0.45
2:Q:89:ARG:HG2	2:Q:90:LYS:H	1.82	0.45
1:S:9:ILE:HD13	1:S:31:LEU:HD23	1.98	0.45
1:S:391:ILE:HD11	1:S:395:ARG:NE	2.31	0.45
1:U:21:ALA:C	1:U:23:ALA:N	2.73	0.45
1:V:63:LYS:HB2	3:V:459:ATP:O2B	2.16	0.45
1:V:387:LYS:NZ	1:V:435:GLU:HG3	2.30	0.45
1:V:444:LEU:HD13	1:V:444:LEU:H	1.81	0.45
1:X:82:GLU:OE2	1:X:258:GLU:HG3	2.16	0.45
1:X:326:ARG:HH11	1:X:326:ARG:CA	2.28	0.45
1:B:108:MET:HE2	1:B:240:LEU:HG	1.98	0.45
1:C:404:MET:O	1:C:408:SER:HB2	2.17	0.45
1:D:358:ALA:O	1:D:361:ALA:HB3	2.15	0.45
2:J:5:SER:HB2	2:J:14:VAL:HG22	1.96	0.45
2:L:88:LEU:O	2:L:88:LEU:HD23	2.16	0.45
2:M:1:THR:CG2	2:M:33:LYS:HD2	2.15	0.45
2:M:50:THR:O	2:M:53:ALA:HB3	2.17	0.45
2:M:164:ASN:ND2	2:M:164:ASN:H	2.13	0.45
1:T:300:THR:O	1:T:303:ILE:HG13	2.17	0.45
1:W:347:GLU:HB2	1:W:348:PRO:HD3	1.98	0.45
1:E:330:ARG:HH11	1:E:330:ARG:HG3	1.82	0.45
2:I:136:ALA:HB1	2:O:137:LEU:CD1	2.47	0.45
2:J:1:THR:HG23	2:J:33:LYS:HZ1	1.80	0.45
2:J:164:ASN:C	2:J:164:ASN:ND2	2.73	0.45
2:K:125:SER:N	4:K:175:LVS:C1'	2.72	0.45
1:T:373:ALA:HB2	1:T:422:ASP:HA	1.98	0.45
1:U:313:VAL:HG23	1:U:314:ALA:H	1.82	0.45
1:U:344:ILE:CG2	3:U:458:ATP:C2	2.97	0.45
1:V:370:THR:HG23	1:V:373:ALA:CB	2.47	0.45
1:W:65:GLU:CG	3:W:460:ATP:H2'	2.46	0.45
1:W:66:ILE:O	1:W:66:ILE:HG22	2.17	0.45
1:A:108:MET:CE	1:A:240:LEU:HG	2.42	0.45
1:A:359:LEU:HD22	1:B:40:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:ASP:O	1:D:439:LEU:O	2.35	0.45
1:E:415:ASN:OD1	1:E:416:GLY:N	2.50	0.45
2:M:18:GLY:O	2:M:29:GLY:C	2.59	0.45
2:M:28:LYS:HZ3	1:T:444:LEU:C	2.25	0.45
2:M:49:GLY:H	4:M:175:LVS:HN3	1.64	0.45
2:R:50:THR:O	2:R:51:ALA:C	2.60	0.45
2:R:107:THR:C	2:R:109:ILE:H	2.25	0.45
1:S:321:PRO:C	1:S:323:LEU:H	2.25	0.45
1:S:430:LEU:HD23	1:S:430:LEU:N	2.32	0.45
1:T:313:VAL:HG23	1:T:314:ALA:H	1.82	0.45
1:U:240:LEU:HD12	1:U:240:LEU:N	2.32	0.45
1:V:254:VAL:HB	1:V:305:PHE:CD2	2.52	0.45
1:V:381:ALA:O	1:V:395:ARG:HG2	2.17	0.45
1:A:108:MET:HE1	1:A:241:LYS:HA	1.98	0.45
2:I:24:ASN:O	2:N:161:VAL:HG13	2.17	0.45
2:I:33:LYS:HZ3	4:I:175:LVS:CB3	2.28	0.45
2:K:64:LEU:HD23	2:K:74:SER:OG	2.17	0.45
2:O:91:LEU:HB2	2:O:108:GLY:HA3	1.97	0.45
2:R:51:ALA:O	2:R:55:THR:HG23	2.17	0.45
1:S:299:LYS:HE2	1:S:301:ASP:CG	2.42	0.45
1:T:437:GLU:O	1:T:438:ASP:C	2.61	0.45
1:U:54:LEU:HD23	1:U:307:ALA:HB3	1.99	0.45
1:U:381:ALA:O	1:U:395:ARG:HG2	2.17	0.45
1:V:17:ILE:CD1	1:V:65:GLU:HB3	2.46	0.45
1:V:21:ALA:C	1:V:23:ALA:N	2.72	0.45
1:W:65:GLU:HG3	3:W:460:ATP:H2'	1.99	0.45
1:A:61:VAL:HA	1:A:336:LEU:HD22	1.98	0.44
1:A:270:GLY:C	1:A:272:ASP:N	2.62	0.44
1:C:42:GLU:H	1:C:43:PRO:CD	2.29	0.44
1:E:237:PRO:O	1:E:240:LEU:N	2.50	0.44
2:G:88:LEU:O	2:G:89:ARG:HB3	2.16	0.44
2:I:88:LEU:O	2:I:89:ARG:HB3	2.17	0.44
2:N:49:GLY:H	4:N:175:LVS:HN3	1.64	0.44
2:N:50:THR:O	2:N:51:ALA:C	2.60	0.44
2:N:164:ASN:ND2	2:N:164:ASN:H	2.15	0.44
2:P:55:THR:HG22	2:Q:83:ARG:CG	2.46	0.44
2:P:76:VAL:HG11	1:V:442:PHE:CE2	2.52	0.44
2:Q:1:THR:HG22	2:Q:33:LYS:HD2	1.91	0.44
2:Q:64:LEU:HD23	2:Q:74:SER:CB	2.47	0.44
1:S:234:LEU:HG	1:S:234:LEU:O	2.18	0.44
1:T:41:GLN:HG3	1:T:43:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:370:THR:O	1:V:374:VAL:HG23	2.16	0.44
1:A:250:GLN:HE21	1:A:250:GLN:CA	2.30	0.44
1:B:394:ARG:HD3	1:B:394:ARG:HA	1.82	0.44
1:B:443:ILE:HG23	2:H:112:VAL:HG23	2.00	0.44
1:E:49:THR:HB	1:E:50:PRO:HD2	1.99	0.44
1:E:77:PRO:CG	1:E:107:ALA:HB2	2.46	0.44
1:F:250:GLN:HA	1:F:250:GLN:NE2	2.32	0.44
2:K:71:LEU:C	2:K:71:LEU:HD13	2.42	0.44
2:L:144:SER:O	2:L:148:ILE:HG13	2.16	0.44
2:P:157:GLY:HA2	2:P:163:THR:HG22	1.99	0.44
1:T:76:ALA:CB	1:T:251:ASN:HB3	2.46	0.44
1:T:286:VAL:HA	1:T:305:PHE:CE1	2.52	0.44
1:U:76:ALA:CB	1:U:251:ASN:HB3	2.47	0.44
1:V:391:ILE:HD11	1:V:395:ARG:NE	2.32	0.44
1:W:381:ALA:O	1:W:395:ARG:HG2	2.17	0.44
1:X:381:ALA:O	1:X:395:ARG:HG2	2.17	0.44
1:X:393:ALA:C	1:X:395:ARG:H	2.25	0.44
1:A:280:ARG:HH11	1:A:280:ARG:CG	2.28	0.44
3:A:450:ATP:C8	3:A:450:ATP:C5'	3.00	0.44
1:B:42:GLU:H	1:B:43:PRO:CD	2.30	0.44
1:D:77:PRO:HB3	1:D:107:ALA:HB2	1.98	0.44
1:D:101:ARG:HA	1:D:293:THR:HG22	1.99	0.44
2:L:3:ILE:O	2:L:122:ALA:HA	2.18	0.44
2:M:54:PHE:O	2:M:57:PHE:HB3	2.17	0.44
2:N:35:ARG:HG3	2:N:35:ARG:HH11	1.83	0.44
2:O:48:GLY:H	4:O:175:LVS:H2'	1.82	0.44
1:S:245:ILE:C	1:S:247:ALA:N	2.74	0.44
1:U:73:LEU:N	1:U:73:LEU:HD12	2.32	0.44
1:V:119:ASN:HB2	1:V:234:LEU:CD2	2.48	0.44
1:W:13:LEU:C	1:W:15:GLN:H	2.25	0.44
1:X:17:ILE:HD13	1:X:66:ILE:HG12	2.00	0.44
1:X:63:LYS:HG2	1:X:333:LEU:HD12	1.98	0.44
1:X:327:LEU:N	1:X:328:PRO:CD	2.77	0.44
1:B:233:LYS:O	1:B:234:LEU:HB2	2.17	0.44
1:E:321:PRO:O	1:E:322:GLU:C	2.59	0.44
1:E:409:PHE:CD2	1:F:25:ARG:NH2	2.86	0.44
1:F:370:THR:HG23	1:F:422:ASP:HA	2.00	0.44
1:F:403:LEU:HD23	1:F:404:MET:SD	2.57	0.44
2:H:1:THR:H1	4:H:175:LVS:C1'	2.18	0.44
2:J:125:SER:N	4:J:175:LVS:C1'	2.72	0.44
2:K:1:THR:N	4:K:175:LVS:S	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:172:LEU:O	2:K:173:PRO:C	2.60	0.44
2:N:94:MET:HE3	2:N:123:ILE:HB	1.99	0.44
2:O:50:THR:H	4:O:175:LVS:CD6	2.30	0.44
2:O:76:VAL:HG11	1:U:442:PHE:CE2	2.52	0.44
2:O:107:THR:C	2:O:109:ILE:H	2.24	0.44
2:R:80:LYS:O	2:R:84:THR:HG23	2.18	0.44
1:S:55:MET:HE2	1:S:306:ILE:HG21	1.98	0.44
1:T:347:GLU:HB2	1:T:348:PRO:HD3	1.99	0.44
1:T:386:GLU:O	1:T:386:GLU:HG2	2.16	0.44
1:U:437:GLU:O	1:U:439:LEU:N	2.50	0.44
1:V:38:MET:HA	1:V:38:MET:HE3	1.97	0.44
1:V:327:LEU:N	1:V:328:PRO:CD	2.78	0.44
1:V:439:LEU:C	1:V:441:ARG:N	2.75	0.44
1:W:63:LYS:HG2	1:W:333:LEU:HD11	2.00	0.44
1:X:54:LEU:HD23	1:X:307:ALA:HB3	1.99	0.44
1:X:119:ASN:HB3	1:X:234:LEU:HD23	1.98	0.44
1:B:52:ASN:O	1:B:328:PRO:HD2	2.17	0.44
3:C:452:ATP:H5'1	3:C:452:ATP:H8	1.82	0.44
1:D:82:GLU:OE2	1:E:280:ARG:HD3	2.17	0.44
1:F:101:ARG:HA	1:F:293:THR:HG22	1.98	0.44
1:F:283:LEU:HA	1:F:283:LEU:HD23	1.69	0.44
2:J:71:LEU:CD1	2:J:104:LEU:HD22	2.48	0.44
2:M:105:ILE:HG22	2:M:113:VAL:O	2.17	0.44
2:N:120:ILE:O	2:N:121:LEU:HD23	2.18	0.44
2:P:91:LEU:HB2	2:P:108:GLY:HA3	1.99	0.44
2:R:76:VAL:HG11	1:X:442:PHE:CE2	2.52	0.44
2:R:131:LEU:HD11	2:R:135:ARG:HE	1.83	0.44
1:S:370:THR:HG23	1:S:373:ALA:CB	2.47	0.44
1:T:299:LYS:HE2	1:T:301:ASP:CG	2.42	0.44
1:U:38:MET:HE3	1:U:38:MET:HA	1.98	0.44
1:W:236:ASN:HD22	1:W:236:ASN:N	2.15	0.44
1:W:294:LYS:HG3	1:W:295:HIS:ND1	2.32	0.44
1:W:393:ALA:C	1:W:395:ARG:H	2.25	0.44
1:W:407:ILE:HG23	1:W:408:SER:N	2.33	0.44
1:A:25:ARG:O	1:A:29:ILE:HG23	2.18	0.44
1:A:57:GLY:O	1:A:63:LYS:HE2	2.18	0.44
1:E:250:GLN:HA	1:E:250:GLN:NE2	2.33	0.44
2:H:53:ALA:HA	2:H:93:ALA:HB1	1.99	0.44
2:H:136:ALA:HB1	2:N:137:LEU:CD1	2.47	0.44
2:N:1:THR:N	4:N:175:LVS:C1'	2.80	0.44
2:Q:49:GLY:H	4:Q:175:LVS:HN3	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:59:THR:HG23	3:S:456:ATP:O1G	2.17	0.44
1:S:439:LEU:C	1:S:441:ARG:N	2.76	0.44
1:T:327:LEU:N	1:T:328:PRO:CD	2.77	0.44
1:A:358:ALA:O	1:A:361:ALA:HB3	2.17	0.44
1:B:108:MET:C	1:B:110:LEU:H	2.24	0.44
1:C:415:ASN:OD1	1:C:416:GLY:N	2.51	0.44
1:D:443:ILE:HG12	2:J:112:VAL:HG21	2.00	0.44
1:E:367:ILE:HD11	1:E:421:ILE:HD12	1.95	0.44
1:F:283:LEU:HB2	1:F:284:PRO:HD3	1.99	0.44
1:F:347:GLU:HB2	1:F:348:PRO:HD3	1.99	0.44
1:F:402:ARG:NH2	1:F:433:VAL:CG2	2.80	0.44
2:G:172:LEU:HD23	2:G:172:LEU:HA	1.82	0.44
2:I:72:LEU:HD22	2:I:104:LEU:HD21	2.00	0.44
2:M:80:LYS:O	2:M:84:THR:HG23	2.17	0.44
2:N:64:LEU:C	2:N:66:MET:H	2.26	0.44
2:P:141:THR:HG21	2:P:143:LEU:HD12	2.00	0.44
2:Q:55:THR:HG22	2:R:83:ARG:CG	2.47	0.44
1:S:300:THR:O	1:S:303:ILE:HG13	2.17	0.44
1:T:13:LEU:C	1:T:15:GLN:H	2.26	0.44
1:U:60:GLY:HA3	1:U:392:GLY:HA3	2.00	0.44
1:V:17:ILE:HD13	1:V:66:ILE:CG1	2.48	0.44
1:V:236:ASN:N	1:V:237:PRO:HD3	2.32	0.44
1:V:407:ILE:HG23	1:V:408:SER:N	2.33	0.44
1:V:430:LEU:HD23	1:V:430:LEU:N	2.33	0.44
1:W:48:VAL:HG21	1:X:359:LEU:HD11	1.99	0.44
1:A:232:ALA:O	1:A:233:LYS:CB	2.46	0.44
1:B:25:ARG:O	1:B:29:ILE:HG23	2.18	0.44
1:B:359:LEU:CD2	1:C:40:LEU:HD11	2.46	0.44
1:D:37:ARG:CG	1:D:38:MET:N	2.81	0.44
1:D:316:PRO:C	1:D:318:ASP:H	2.26	0.44
1:E:440:SER:HB3	2:L:32:ARG:HH22	1.82	0.44
2:R:76:VAL:HG11	1:X:442:PHE:CD2	2.52	0.44
1:T:36:ARG:HA	1:T:36:ARG:HE	1.83	0.44
1:T:82:GLU:OE2	1:T:258:GLU:HG3	2.18	0.44
1:U:63:LYS:HZ1	3:U:458:ATP:PG	2.40	0.44
1:U:407:ILE:HG23	1:U:408:SER:N	2.33	0.44
1:V:245:ILE:HG22	1:V:249:GLU:OE1	2.18	0.44
1:W:36:ARG:HA	1:W:36:ARG:HE	1.83	0.44
1:X:76:ALA:HB1	1:X:251:ASN:HB3	1.98	0.44
1:A:16:HIS:HB2	1:A:17:ILE:HD12	2.00	0.44
1:A:356:TYR:CD1	1:A:400:MET:HE3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:MET:HE2	1:B:360:MET:HA	1.99	0.44
1:B:403:LEU:C	1:B:405:ASP:N	2.75	0.44
1:C:105:ASP:HB3	1:D:297:MET:HE2	1.99	0.44
1:C:316:PRO:C	1:C:318:ASP:H	2.25	0.44
1:C:355:GLN:O	1:C:359:LEU:HD23	2.17	0.44
1:C:440:SER:HB3	2:J:32:ARG:HH22	1.83	0.44
1:E:407:ILE:HD11	1:E:419:VAL:HG11	2.00	0.44
1:F:32:ARG:C	1:F:34:ARG:H	2.25	0.44
1:F:352:LEU:HA	1:F:352:LEU:HD23	1.80	0.44
1:F:443:ILE:HG23	2:L:112:VAL:HG23	1.99	0.44
1:F:444:LEU:CD2	2:L:113:VAL:HG22	2.47	0.44
2:I:159:ILE:O	2:N:25:THR:HA	2.17	0.44
2:K:1:THR:N	4:K:175:LVS:C2'	2.79	0.44
2:K:133:ALA:HB1	2:K:155:ILE:HD12	2.00	0.44
2:R:61:GLU:C	2:R:63:LYS:N	2.75	0.44
1:T:407:ILE:HG23	1:T:408:SER:N	2.33	0.44
1:U:7:ARG:NH1	1:V:410:SER:HB3	2.31	0.44
1:U:82:GLU:OE2	1:U:258:GLU:HG3	2.17	0.44
1:U:349:HIS:O	1:U:350:ALA:HB3	2.18	0.44
1:V:240:LEU:N	1:V:240:LEU:HD12	2.33	0.44
1:B:258:GLU:OE1	1:C:322:GLU:OE1	2.36	0.43
1:E:4:MET:HE2	1:E:4:MET:HB3	1.92	0.43
2:I:1:THR:CG2	2:I:33:LYS:HE3	2.46	0.43
2:N:50:THR:H	4:N:175:LVS:HD63	1.82	0.43
2:P:89:ARG:HG2	2:P:90:LYS:H	1.83	0.43
1:S:36:ARG:HA	1:S:36:ARG:HE	1.82	0.43
1:S:61:VAL:C	3:S:456:ATP:N7	2.76	0.43
1:S:76:ALA:HB1	1:S:251:ASN:HB3	2.00	0.43
1:S:441:ARG:HB3	1:S:442:PHE:CE1	2.53	0.43
1:T:294:LYS:HG3	1:T:295:HIS:ND1	2.33	0.43
1:V:36:ARG:HA	1:V:36:ARG:HE	1.82	0.43
1:V:321:PRO:C	1:V:323:LEU:H	2.26	0.43
1:W:108:MET:HE2	1:W:108:MET:HA	2.00	0.43
1:W:444:LEU:HD22	1:W:444:LEU:C	2.43	0.43
1:X:36:ARG:HE	1:X:36:ARG:HA	1.82	0.43
1:A:444:LEU:HB2	2:H:54:PHE:CE1	2.53	0.43
1:B:352:LEU:HD23	1:B:352:LEU:HA	1.83	0.43
1:C:349:HIS:O	1:C:350:ALA:CB	2.65	0.43
1:C:437:GLU:O	1:C:438:ASP:C	2.60	0.43
1:F:356:TYR:O	1:F:357:LYS:C	2.61	0.43
2:G:17:ASP:C	2:G:33:LYS:HZ1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:17:ASP:HB2	2:G:164:ASN:ND2	2.33	0.43
2:I:128:ASN:HA	2:I:131:LEU:HB3	2.00	0.43
4:L:175:LVS:HD33	4:L:175:LVS:N2	2.33	0.43
2:N:107:THR:C	2:N:109:ILE:H	2.26	0.43
2:O:80:LYS:O	2:O:84:THR:HG23	2.18	0.43
2:P:50:THR:H	4:P:175:LVS:CD6	2.30	0.43
2:P:153:LEU:HD23	2:P:153:LEU:HA	1.86	0.43
1:S:13:LEU:C	1:S:15:GLN:H	2.26	0.43
1:S:344:ILE:O	1:S:344:ILE:HG22	2.17	0.43
1:U:254:VAL:HB	1:U:305:PHE:CD2	2.52	0.43
1:W:21:ALA:C	1:W:23:ALA:N	2.74	0.43
1:W:321:PRO:HG3	1:X:389:GLU:HG2	1.99	0.43
1:A:36:ARG:C	1:A:37:ARG:O	2.54	0.43
1:B:35:TRP:O	1:B:37:ARG:O	2.36	0.43
1:B:236:ASN:ND2	1:B:239:GLU:HB2	2.33	0.43
1:D:25:ARG:O	1:D:29:ILE:HG23	2.18	0.43
1:E:345:LEU:HD12	1:E:345:LEU:HA	1.77	0.43
1:F:74:ALA:O	1:F:75:ASN:C	2.61	0.43
1:F:233:LYS:HD3	1:F:235:ILE:HG12	2.00	0.43
2:H:64:LEU:HD23	2:H:74:SER:CB	2.48	0.43
2:J:137:LEU:CD1	2:J:137:LEU:N	2.81	0.43
2:N:80:LYS:O	2:N:84:THR:HG23	2.17	0.43
2:O:16:GLY:N	2:O:153:LEU:HD11	2.34	0.43
2:P:80:LYS:O	2:P:84:THR:HG23	2.17	0.43
2:Q:91:LEU:HB2	2:Q:108:GLY:HA3	1.99	0.43
1:S:237:PRO:C	1:S:239:GLU:H	2.25	0.43
1:U:36:ARG:HA	1:U:36:ARG:HE	1.82	0.43
1:W:299:LYS:HE2	1:W:301:ASP:CG	2.42	0.43
1:W:386:GLU:O	1:W:386:GLU:HG2	2.18	0.43
1:X:73:LEU:HD12	1:X:73:LEU:N	2.32	0.43
1:A:437:GLU:HA	1:A:439:LEU:HD12	2.00	0.43
1:B:440:SER:O	1:B:441:ARG:C	2.60	0.43
1:C:280:ARG:HH11	1:C:280:ARG:CG	2.30	0.43
1:C:321:PRO:O	1:C:322:GLU:C	2.61	0.43
1:D:236:ASN:N	1:D:237:PRO:HD3	2.33	0.43
1:E:20:GLN:HE22	1:E:334:THR:H	1.66	0.43
1:F:394:ARG:HA	1:F:394:ARG:HD3	1.75	0.43
2:K:37:LEU:HD21	2:K:57:PHE:CE2	2.52	0.43
2:L:136:ALA:HB1	2:R:137:LEU:HD13	2.00	0.43
2:M:18:GLY:CA	2:M:33:LYS:NZ	2.79	0.43
2:R:17:ASP:CG	2:R:33:LYS:HZ2	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:393:ALA:C	1:S:395:ARG:H	2.27	0.43
1:T:63:LYS:HG2	1:T:333:LEU:HD11	2.00	0.43
1:U:259:ILE:HG22	1:U:308:SER:O	2.18	0.43
1:U:370:THR:HG23	1:U:373:ALA:CB	2.48	0.43
1:U:386:GLU:O	1:U:386:GLU:HG2	2.18	0.43
1:U:430:LEU:N	1:U:430:LEU:HD23	2.33	0.43
1:W:388:THR:HG22	1:W:389:GLU:N	2.28	0.43
1:X:441:ARG:HB3	1:X:442:PHE:CE1	2.53	0.43
1:A:16:HIS:C	1:A:17:ILE:HD12	2.44	0.43
1:B:32:ARG:C	1:B:34:ARG:N	2.76	0.43
1:D:367:ILE:CD1	1:D:421:ILE:HD11	2.48	0.43
2:K:51:ALA:O	2:K:55:THR:HG23	2.19	0.43
4:K:175:LVS:HD33	4:K:175:LVS:C1	2.49	0.43
2:L:115:PRO:HG3	2:L:121:LEU:HD11	1.99	0.43
2:M:56:LEU:HB2	2:M:91:LEU:HD23	2.01	0.43
2:M:64:LEU:C	2:M:66:MET:H	2.26	0.43
2:O:54:PHE:O	2:O:57:PHE:HB3	2.19	0.43
2:R:49:GLY:O	2:R:50:THR:C	2.61	0.43
2:R:141:THR:OG1	2:R:143:LEU:HG	2.19	0.43
1:S:259:ILE:O	1:S:262:ILE:HG12	2.19	0.43
1:T:326:ARG:NH1	1:T:326:ARG:HB3	2.34	0.43
1:V:34:ARG:HH12	1:V:252:GLY:H	1.67	0.43
1:V:120:ARG:HA	1:V:233:LYS:HE3	2.01	0.43
1:W:41:GLN:HG3	1:W:43:PRO:HD2	2.01	0.43
1:X:41:GLN:HG3	1:X:43:PRO:HD2	1.99	0.43
1:X:321:PRO:C	1:X:323:LEU:H	2.27	0.43
1:A:75:ASN:OD1	1:A:114:GLN:OE1	2.35	0.43
1:C:63:LYS:HB2	3:C:452:ATP:O2B	2.19	0.43
1:C:409:PHE:CD2	1:D:25:ARG:NH2	2.86	0.43
1:C:438:ASP:O	1:C:439:LEU:O	2.37	0.43
1:D:293:THR:C	1:D:295:HIS:H	2.26	0.43
1:E:300:THR:HA	1:E:303:ILE:HG12	2.01	0.43
1:F:326:ARG:C	1:F:328:PRO:HD3	2.44	0.43
2:J:28:LYS:HE2	2:J:30:ASN:OD1	2.18	0.43
2:K:67:HIS:NE2	2:K:77:GLU:HG3	2.34	0.43
2:M:49:GLY:O	2:M:50:THR:C	2.61	0.43
2:M:50:THR:O	2:M:51:ALA:C	2.61	0.43
2:N:37:LEU:HD22	2:N:61:GLU:HG3	1.99	0.43
2:N:164:ASN:HD22	2:N:164:ASN:H	1.66	0.43
1:U:326:ARG:NH1	1:U:326:ARG:HB3	2.34	0.43
1:V:27:VAL:CG1	1:V:70:LEU:HD22	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:39:GLN:HB2	1:W:362:THR:HG21	1.99	0.43
1:V:386:GLU:HG2	1:V:386:GLU:O	2.18	0.43
1:W:321:PRO:C	1:W:323:LEU:H	2.27	0.43
1:X:38:MET:HA	1:X:38:MET:HE3	2.00	0.43
1:X:391:ILE:HD11	1:X:395:ARG:NE	2.34	0.43
1:X:437:GLU:O	1:X:439:LEU:N	2.52	0.43
1:A:37:ARG:HG2	1:A:38:MET:N	2.33	0.43
1:B:79:ILE:HD12	1:B:80:LYS:H	1.83	0.43
1:C:79:ILE:HD12	1:C:80:LYS:N	2.34	0.43
1:E:108:MET:HE1	1:E:241:LYS:HA	2.01	0.43
1:F:437:GLU:CG	1:F:439:LEU:HB2	2.49	0.43
2:J:7:ARG:CZ	2:J:12:VAL:HG22	2.49	0.43
2:J:67:HIS:NE2	2:J:77:GLU:HG3	2.34	0.43
2:K:52:ASP:O	2:K:53:ALA:C	2.62	0.43
2:M:37:LEU:HD22	2:M:61:GLU:HG3	2.01	0.43
2:N:125:SER:HB3	4:N:175:LVS:H1'3	2.01	0.43
2:Q:55:THR:O	2:Q:59:LEU:HD13	2.18	0.43
2:Q:125:SER:HB3	4:Q:175:LVS:H1'3	2.00	0.43
1:T:73:LEU:N	1:T:73:LEU:HD12	2.33	0.43
1:U:321:PRO:C	1:U:323:LEU:H	2.26	0.43
1:V:96:VAL:HG13	1:V:282:LEU:HD12	2.01	0.43
1:D:76:ALA:HB1	1:D:251:ASN:O	2.19	0.43
1:D:352:LEU:HA	1:D:352:LEU:HD23	1.77	0.43
1:D:444:LEU:CD2	2:J:113:VAL:HG22	2.48	0.43
1:E:32:ARG:C	1:E:34:ARG:N	2.76	0.43
1:E:101:ARG:HA	1:E:293:THR:HG22	2.01	0.43
1:E:443:ILE:HG21	2:K:114:GLN:HG3	2.00	0.43
1:F:378:ALA:O	1:F:379:GLU:C	2.61	0.43
1:F:439:LEU:O	1:F:440:SER:C	2.62	0.43
2:H:7:ARG:HG3	2:H:12:VAL:HG22	2.01	0.43
2:H:137:LEU:HD13	2:N:136:ALA:HB1	2.00	0.43
2:J:1:THR:H3	4:J:175:LVS:H1'2	1.82	0.43
2:M:61:GLU:C	2:M:63:LYS:N	2.76	0.43
2:O:1:THR:HG22	2:O:33:LYS:HZ2	1.80	0.43
2:O:18:GLY:CA	2:O:33:LYS:HZ1	2.32	0.43
2:P:37:LEU:HD22	2:P:61:GLU:HG3	2.01	0.43
2:P:49:GLY:H	4:P:175:LVS:HN3	1.67	0.43
2:Q:50:THR:H	4:Q:175:LVS:HD63	1.84	0.43
1:S:118:LYS:HD3	1:S:119:ASN:N	2.33	0.43
1:S:313:VAL:HG23	1:S:314:ALA:H	1.82	0.43
1:T:5:THR:HG22	1:T:8:GLU:CD	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:344:ILE:O	1:T:344:ILE:HG22	2.18	0.43
1:T:370:THR:HG23	1:T:373:ALA:CB	2.49	0.43
1:U:326:ARG:HH11	1:U:326:ARG:CA	2.28	0.43
1:V:82:GLU:HG3	1:V:258:GLU:HB2	2.00	0.43
1:X:347:GLU:HB2	1:X:348:PRO:HD3	2.00	0.43
1:X:442:PHE:CD1	1:X:442:PHE:N	2.87	0.43
1:C:28:ALA:C	1:C:30:ALA:N	2.75	0.43
1:C:239:GLU:HG2	1:C:243:LYS:CD	2.49	0.43
1:D:35:TRP:O	1:D:37:ARG:O	2.37	0.43
1:D:357:LYS:HA	1:D:367:ILE:CG2	2.49	0.43
1:D:388:THR:HG22	1:D:436:ASN:HD21	1.84	0.43
1:E:283:LEU:HA	1:E:283:LEU:HD23	1.80	0.43
1:F:37:ARG:CG	1:F:38:MET:N	2.82	0.43
2:N:16:GLY:N	2:N:153:LEU:HD11	2.34	0.43
2:N:61:GLU:C	2:N:63:LYS:N	2.77	0.43
1:S:41:GLN:HG3	1:S:43:PRO:HD2	2.00	0.43
1:S:54:LEU:HD23	1:S:307:ALA:HB3	2.00	0.43
1:S:254:VAL:HB	1:S:305:PHE:CD2	2.53	0.43
1:S:436:ASN:C	1:S:436:ASN:HD22	2.26	0.43
1:T:393:ALA:C	1:T:395:ARG:H	2.27	0.43
1:W:38:MET:HA	1:W:38:MET:HE3	2.00	0.43
1:W:286:VAL:HA	1:W:305:PHE:CE1	2.53	0.43
1:X:259:ILE:O	1:X:262:ILE:HG12	2.19	0.43
1:A:232:ALA:O	1:A:233:LYS:HE3	2.18	0.43
1:A:276:GLU:HG3	1:A:276:GLU:O	2.18	0.43
1:A:355:GLN:O	1:A:359:LEU:HD23	2.18	0.43
1:B:4:MET:HE2	1:B:4:MET:HB3	1.85	0.43
1:B:23:ALA:CA	1:B:331:VAL:HG21	2.45	0.43
1:E:111:VAL:HG12	1:E:240:LEU:HD11	2.01	0.43
2:J:1:THR:H3	4:J:175:LVS:C1'	2.32	0.43
2:Q:50:THR:O	2:Q:53:ALA:HB3	2.19	0.43
2:R:50:THR:O	2:R:53:ALA:HB3	2.19	0.43
1:T:40:LEU:HD13	1:T:44:LEU:O	2.19	0.43
1:V:326:ARG:HB3	1:V:326:ARG:NH1	2.34	0.43
1:X:72:LYS:C	1:X:74:ALA:H	2.27	0.43
1:X:437:GLU:O	1:X:438:ASP:C	2.61	0.43
1:C:250:GLN:HE21	1:C:250:GLN:CA	2.32	0.42
1:C:388:THR:HG22	1:C:436:ASN:HD21	1.84	0.42
1:E:44:LEU:HD23	1:E:44:LEU:HA	1.91	0.42
1:E:275:ARG:C	1:E:277:GLY:N	2.76	0.42
1:F:250:GLN:HE21	1:F:250:GLN:CA	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:17:ASP:CG	2:I:163:THR:HG23	2.44	0.42
1:S:370:THR:HG23	1:S:373:ALA:HB3	2.01	0.42
1:T:326:ARG:HH11	1:T:326:ARG:CA	2.28	0.42
1:U:328:PRO:HB3	1:V:398:THR:HA	2.00	0.42
1:B:74:ALA:O	1:B:75:ASN:C	2.62	0.42
1:B:285:LEU:H	1:B:285:LEU:CD1	2.32	0.42
2:J:115:PRO:HG3	2:J:121:LEU:HD11	2.00	0.42
2:M:153:LEU:HD23	2:M:153:LEU:HA	1.84	0.42
2:O:55:THR:HG22	2:P:83:ARG:CG	2.50	0.42
2:R:61:GLU:C	2:R:63:LYS:H	2.27	0.42
1:S:17:ILE:HD11	1:S:65:GLU:HB3	2.00	0.42
1:S:280:ARG:HG3	1:T:82:GLU:OE1	2.19	0.42
1:S:369:PHE:HE2	1:S:421:ILE:CD1	2.27	0.42
1:T:76:ALA:HB1	1:T:251:ASN:HB3	2.02	0.42
1:T:80:LYS:HG3	1:T:255:PHE:CD2	2.51	0.42
1:W:82:GLU:HG3	1:W:258:GLU:HB2	2.01	0.42
1:B:85:LYS:O	1:B:85:LYS:HG2	2.18	0.42
1:B:250:GLN:HE21	1:B:250:GLN:CA	2.28	0.42
1:B:437:GLU:O	1:B:439:LEU:N	2.52	0.42
1:C:4:MET:HE2	1:C:4:MET:HB3	1.93	0.42
1:D:20:GLN:HE22	1:D:334:THR:H	1.67	0.42
1:F:275:ARG:O	1:F:278:VAL:N	2.52	0.42
1:F:293:THR:C	1:F:295:HIS:N	2.77	0.42
2:H:1:THR:N	4:H:175:LVS:C2'	2.81	0.42
2:H:86:ARG:HH11	2:H:86:ARG:CB	2.19	0.42
2:I:111:ASP:O	2:I:111:ASP:OD2	2.37	0.42
2:K:159:ILE:O	2:P:25:THR:HA	2.19	0.42
2:R:54:PHE:O	2:R:57:PHE:HB3	2.20	0.42
1:U:17:ILE:HD13	1:U:66:ILE:HG12	2.01	0.42
1:W:17:ILE:HD13	1:W:66:ILE:CG1	2.50	0.42
1:X:430:LEU:N	1:X:430:LEU:HD23	2.34	0.42
1:B:370:THR:HG23	1:B:422:ASP:HA	2.01	0.42
1:C:275:ARG:C	1:C:277:GLY:N	2.74	0.42
1:E:58:PRO:O	1:E:61:VAL:HG22	2.19	0.42
1:E:360:MET:HE2	1:E:360:MET:CA	2.50	0.42
1:F:115:GLU:C	1:F:117:ALA:H	2.27	0.42
1:F:356:TYR:CD1	1:F:400:MET:HE3	2.54	0.42
2:G:18:GLY:C	2:G:33:LYS:NZ	2.75	0.42
2:G:53:ALA:HA	2:G:93:ALA:HB1	2.00	0.42
2:H:96:ILE:HG13	2:H:123:ILE:HD13	2.01	0.42
2:I:28:LYS:HE2	2:I:30:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:7:ARG:HG3	2:J:12:VAL:HG22	2.00	0.42
2:L:96:ILE:HG13	2:L:123:ILE:HD13	2.01	0.42
2:M:17:ASP:CG	2:M:33:LYS:NZ	2.77	0.42
2:N:89:ARG:HG2	2:N:90:LYS:H	1.85	0.42
2:O:131:LEU:HD11	2:O:135:ARG:HE	1.81	0.42
2:Q:131:LEU:HD11	2:Q:135:ARG:HE	1.78	0.42
1:S:96:VAL:HG13	1:S:282:LEU:HD12	2.02	0.42
1:V:13:LEU:C	1:V:15:GLN:H	2.27	0.42
1:V:115:GLU:HA	1:V:118:LYS:CB	2.49	0.42
1:C:409:PHE:HD1	1:D:29:ILE:HG22	1.84	0.42
1:D:16:HIS:C	1:D:17:ILE:HD12	2.44	0.42
1:F:403:LEU:C	1:F:405:ASP:N	2.78	0.42
2:H:17:ASP:O	2:H:33:LYS:HD2	2.19	0.42
2:H:137:LEU:CD1	2:H:137:LEU:N	2.82	0.42
2:I:25:THR:HA	2:N:159:ILE:O	2.20	0.42
2:L:172:LEU:HD23	2:L:172:LEU:HA	1.79	0.42
2:N:49:GLY:O	2:N:50:THR:C	2.62	0.42
2:P:3:ILE:HB	2:P:123:ILE:CG1	2.48	0.42
2:R:14:VAL:HG12	2:R:34:VAL:CG1	2.50	0.42
1:T:38:MET:HA	1:T:38:MET:HE3	2.01	0.42
1:A:356:TYR:CE1	1:A:400:MET:HE3	2.55	0.42
1:D:250:GLN:HE21	1:D:250:GLN:CA	2.33	0.42
1:D:250:GLN:HA	1:D:250:GLN:NE2	2.34	0.42
1:D:394:ARG:HD3	1:D:394:ARG:HA	1.79	0.42
1:E:100:ILE:CG2	1:E:298:VAL:HG21	2.50	0.42
1:E:357:LYS:HA	1:E:367:ILE:CG2	2.50	0.42
1:F:112:ARG:HH22	1:F:235:ILE:HD12	1.84	0.42
2:H:28:LYS:HE2	2:H:30:ASN:OD1	2.20	0.42
2:M:2:THR:OG1	2:M:126:GLY:HA3	2.19	0.42
2:O:3:ILE:HB	2:O:123:ILE:HG13	2.00	0.42
2:Q:35:ARG:HH11	2:Q:35:ARG:HG3	1.85	0.42
2:Q:50:THR:O	2:Q:51:ALA:C	2.62	0.42
1:S:359:LEU:HD11	1:X:48:VAL:HG21	2.00	0.42
1:T:65:GLU:HG3	3:T:457:ATP:H2'	2.02	0.42
1:T:321:PRO:C	1:T:323:LEU:H	2.27	0.42
1:U:442:PHE:CD1	1:U:442:PHE:N	2.87	0.42
1:W:373:ALA:O	1:W:377:ILE:HG13	2.20	0.42
1:X:40:LEU:HD13	1:X:44:LEU:O	2.20	0.42
1:X:326:ARG:HB3	1:X:326:ARG:NH1	2.35	0.42
1:X:344:ILE:O	1:X:344:ILE:HG22	2.19	0.42
1:A:115:GLU:OE1	1:A:118:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LYS:HE2	1:B:118:LYS:HB3	1.93	0.42
1:B:358:ALA:O	1:B:361:ALA:HB3	2.20	0.42
1:C:62:GLY:O	1:C:63:LYS:C	2.63	0.42
1:D:25:ARG:O	1:D:28:ALA:HB3	2.20	0.42
1:D:394:ARG:O	1:D:395:ARG:C	2.62	0.42
1:E:37:ARG:CG	1:E:38:MET:N	2.82	0.42
1:F:44:LEU:HD23	1:F:44:LEU:HA	1.84	0.42
2:G:28:LYS:HE2	2:G:30:ASN:OD1	2.19	0.42
2:H:72:LEU:HD22	2:H:104:LEU:HD21	2.01	0.42
2:J:72:LEU:HD22	2:J:72:LEU:HA	1.92	0.42
2:K:17:ASP:HB2	2:K:164:ASN:HD22	1.85	0.42
2:K:36:ARG:NH1	2:K:170:GLU:OE2	2.53	0.42
2:K:72:LEU:O	2:K:72:LEU:HD13	2.20	0.42
2:N:54:PHE:HE1	1:U:444:LEU:HD12	1.83	0.42
2:O:151:LYS:O	2:O:155:ILE:HD13	2.19	0.42
2:P:61:GLU:C	2:P:63:LYS:N	2.77	0.42
2:Q:16:GLY:N	2:Q:153:LEU:HD11	2.34	0.42
2:R:94:MET:HE3	2:R:123:ILE:HB	2.01	0.42
1:S:326:ARG:HB3	1:S:326:ARG:NH1	2.35	0.42
1:T:98:SER:HA	1:T:101:ARG:NH1	2.34	0.42
1:W:76:ALA:HB1	1:W:251:ASN:HB3	2.02	0.42
1:X:370:THR:HG23	1:X:373:ALA:CB	2.50	0.42
1:A:360:MET:HE2	1:A:360:MET:N	2.35	0.42
1:B:438:ASP:C	1:B:439:LEU:O	2.63	0.42
1:C:330:ARG:HG3	1:C:330:ARG:NH1	2.33	0.42
1:C:440:SER:O	1:C:441:ARG:C	2.63	0.42
1:F:52:ASN:HB2	1:F:326:ARG:O	2.20	0.42
1:F:242:GLN:OE1	1:F:242:GLN:HA	2.20	0.42
1:F:444:LEU:O	2:G:28:LYS:NZ	2.42	0.42
2:L:17:ASP:HB2	2:L:164:ASN:ND2	2.35	0.42
2:L:36:ARG:NH1	2:L:170:GLU:OE2	2.53	0.42
2:N:61:GLU:C	2:N:63:LYS:H	2.26	0.42
2:N:113:VAL:HG22	1:T:444:LEU:HD11	2.01	0.42
2:R:37:LEU:HD22	2:R:61:GLU:HG3	2.02	0.42
1:T:439:LEU:HD23	1:T:439:LEU:N	2.22	0.42
1:U:344:ILE:O	1:U:344:ILE:HG22	2.20	0.42
1:X:385:ASN:HD22	1:X:385:ASN:HA	1.59	0.42
1:A:271:ALA:C	1:A:273:VAL:N	2.78	0.42
1:B:357:LYS:HA	1:B:367:ILE:CG2	2.50	0.42
1:C:235:ILE:HG22	1:C:236:ASN:N	2.35	0.42
1:D:345:LEU:HD12	1:D:345:LEU:HA	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:VAL:HG21	1:D:395:ARG:HD2	2.02	0.42
1:D:384:VAL:CG2	1:D:395:ARG:NE	2.83	0.42
1:E:44:LEU:O	1:E:45:ARG:C	2.61	0.42
2:G:136:ALA:HB1	2:M:137:LEU:HD13	2.02	0.42
2:I:1:THR:H3	4:I:175:LVS:CS	2.23	0.42
2:L:67:HIS:NE2	2:L:77:GLU:HG3	2.35	0.42
2:M:141:THR:OG1	2:M:143:LEU:HG	2.19	0.42
2:P:6:VAL:HG21	2:P:148:ILE:CG2	2.50	0.42
2:P:35:ARG:HH11	2:P:35:ARG:HG3	1.85	0.42
1:S:245:ILE:O	1:S:246:ASP:C	2.61	0.42
1:S:279:GLN:HE22	1:S:319:LEU:HA	1.85	0.42
1:T:254:VAL:HB	1:T:305:PHE:CD2	2.55	0.42
1:U:75:ASN:ND2	1:U:110:LEU:HD21	2.34	0.42
1:V:370:THR:HG21	1:V:422:ASP:HA	2.02	0.42
1:W:349:HIS:O	1:W:350:ALA:HB3	2.19	0.42
1:W:391:ILE:HD11	1:W:395:ARG:NE	2.35	0.42
1:A:403:LEU:HD23	1:A:404:MET:SD	2.60	0.42
1:C:79:ILE:HD12	1:C:80:LYS:H	1.85	0.42
1:E:76:ALA:HB1	1:E:251:ASN:O	2.19	0.42
1:F:234:LEU:O	1:F:235:ILE:C	2.63	0.42
1:F:403:LEU:CD1	1:F:426:VAL:HG22	2.49	0.42
2:I:7:ARG:CZ	2:I:12:VAL:CG2	2.98	0.42
2:L:7:ARG:CZ	2:L:12:VAL:HG21	2.50	0.42
2:L:53:ALA:HA	2:L:93:ALA:HB1	2.02	0.42
2:L:136:ALA:HB1	2:R:137:LEU:CD1	2.50	0.42
2:Q:3:ILE:HB	2:Q:123:ILE:CG1	2.50	0.42
1:S:40:LEU:HD13	1:S:44:LEU:O	2.20	0.42
1:T:27:VAL:CG1	1:T:70:LEU:HD22	2.50	0.42
1:U:370:THR:HG23	1:U:373:ALA:HB3	2.02	0.42
1:W:27:VAL:CG1	1:W:70:LEU:HD22	2.50	0.42
1:W:72:LYS:C	1:W:74:ALA:H	2.28	0.42
1:W:73:LEU:N	1:W:73:LEU:HD12	2.34	0.42
1:X:5:THR:HG22	1:X:8:GLU:CD	2.44	0.42
1:X:369:PHE:HE2	1:X:421:ILE:CD1	2.25	0.42
1:B:108:MET:C	1:B:110:LEU:N	2.78	0.41
1:C:352:LEU:HA	1:C:352:LEU:HD23	1.79	0.41
1:D:337:SER:O	1:D:338:ALA:C	2.61	0.41
1:D:408:SER:O	1:E:36:ARG:NH2	2.47	0.41
1:F:36:ARG:C	1:F:37:ARG:O	2.55	0.41
1:F:280:ARG:HH11	1:F:280:ARG:CG	2.28	0.41
2:G:64:LEU:HD23	2:G:74:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7:ARG:CZ	2:H:12:VAL:HG22	2.50	0.41
2:I:172:LEU:HA	2:I:172:LEU:HD23	1.81	0.41
2:J:25:THR:HA	2:O:159:ILE:O	2.20	0.41
2:K:83:ARG:NH1	2:L:58:GLU:OE2	2.52	0.41
1:T:259:ILE:O	1:T:262:ILE:HG12	2.20	0.41
1:U:5:THR:HG22	1:U:8:GLU:CD	2.45	0.41
1:V:40:LEU:HD13	1:V:44:LEU:O	2.20	0.41
1:A:75:ASN:HD21	1:A:114:GLN:NE2	2.18	0.41
1:A:101:ARG:HA	1:A:293:THR:HG22	2.01	0.41
1:B:7:ARG:HB3	1:B:7:ARG:NH1	2.34	0.41
1:C:37:ARG:HG2	1:C:38:MET:N	2.34	0.41
1:C:82:GLU:OE2	1:D:280:ARG:HD3	2.19	0.41
1:D:42:GLU:N	1:D:43:PRO:CD	2.82	0.41
1:D:113:GLN:HA	1:D:116:ILE:HD12	2.02	0.41
1:E:362:THR:C	1:E:364:GLY:H	2.28	0.41
1:E:403:LEU:C	1:E:405:ASP:N	2.78	0.41
1:F:343:ARG:O	1:F:348:PRO:HD3	2.20	0.41
2:I:71:LEU:CD1	2:I:104:LEU:HD22	2.51	0.41
2:K:25:THR:HA	2:P:159:ILE:O	2.20	0.41
2:M:61:GLU:C	2:M:63:LYS:H	2.27	0.41
2:M:64:LEU:HD23	2:M:74:SER:CB	2.50	0.41
2:N:91:LEU:HB2	2:N:108:GLY:HA3	2.02	0.41
1:S:27:VAL:CG1	1:S:70:LEU:HD22	2.49	0.41
1:T:439:LEU:C	1:T:441:ARG:N	2.78	0.41
1:U:41:GLN:HG3	1:U:43:PRO:HD2	2.01	0.41
1:U:259:ILE:O	1:U:262:ILE:HG12	2.21	0.41
1:U:279:GLN:HE22	1:U:319:LEU:HA	1.85	0.41
1:V:313:VAL:HG23	1:V:314:ALA:H	1.84	0.41
1:V:370:THR:HG23	1:V:373:ALA:HB3	2.01	0.41
1:W:442:PHE:O	1:W:443:ILE:HD13	2.20	0.41
1:X:246:ASP:O	1:X:250:GLN:HB3	2.20	0.41
1:X:366:ASN:HD22	1:X:366:ASN:HA	1.69	0.41
1:A:7:ARG:HB3	1:A:7:ARG:HH11	1.86	0.41
1:A:402:ARG:O	1:A:405:ASP:HB2	2.20	0.41
1:B:17:ILE:HD12	1:B:17:ILE:N	2.36	0.41
1:B:21:ALA:O	1:B:22:ASP:C	2.63	0.41
1:B:72:LYS:HD2	1:B:72:LYS:HA	1.87	0.41
1:B:347:GLU:N	1:B:348:PRO:CD	2.83	0.41
1:D:32:ARG:C	1:D:34:ARG:N	2.74	0.41
1:E:275:ARG:HG3	1:E:276:GLU:N	2.36	0.41
2:H:18:GLY:O	2:H:29:GLY:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:111:ASP:OD2	2:K:111:ASP:N	2.53	0.41
2:O:50:THR:O	2:O:51:ALA:C	2.62	0.41
2:P:54:PHE:O	2:P:57:PHE:HB3	2.20	0.41
2:P:164:ASN:ND2	2:P:164:ASN:N	2.66	0.41
1:S:17:ILE:HD13	1:S:66:ILE:CG1	2.50	0.41
1:S:235:ILE:HG22	1:S:237:PRO:HD3	2.01	0.41
1:S:407:ILE:HG23	1:S:408:SER:N	2.34	0.41
1:T:75:ASN:HD22	1:T:75:ASN:HA	1.65	0.41
1:T:442:PHE:CD1	1:T:442:PHE:N	2.88	0.41
1:U:391:ILE:HD11	1:U:395:ARG:NE	2.35	0.41
1:V:68:ARG:HG3	1:V:68:ARG:NH1	2.33	0.41
1:V:373:ALA:O	1:V:377:ILE:HG13	2.20	0.41
1:A:275:ARG:C	1:A:277:GLY:N	2.77	0.41
1:C:12:GLU:O	1:C:15:GLN:HB2	2.20	0.41
1:C:438:ASP:HB2	2:I:72:LEU:HD12	2.03	0.41
1:D:32:ARG:C	1:D:34:ARG:H	2.28	0.41
1:E:437:GLU:HG3	1:E:439:LEU:HD12	2.02	0.41
1:F:236:ASN:CG	1:F:239:GLU:HB2	2.46	0.41
1:F:402:ARG:O	1:F:405:ASP:HB2	2.20	0.41
2:G:86:ARG:HH11	2:G:86:ARG:CB	2.19	0.41
2:H:164:ASN:C	2:H:164:ASN:ND2	2.74	0.41
2:K:33:LYS:NZ	4:K:175:LVS:CB3	2.80	0.41
2:N:42:VAL:HG21	2:N:64:LEU:HD11	2.02	0.41
2:N:54:PHE:CZ	1:U:444:LEU:HB3	2.56	0.41
2:R:64:LEU:C	2:R:66:MET:H	2.27	0.41
1:S:80:LYS:HG3	1:S:255:PHE:CD2	2.49	0.41
1:S:258:GLU:OE2	1:X:322:GLU:OE2	2.39	0.41
1:T:107:ALA:C	1:T:109:LYS:H	2.28	0.41
1:U:82:GLU:HG3	1:U:258:GLU:HB2	2.03	0.41
1:U:109:LYS:O	1:U:110:LEU:HD23	2.20	0.41
1:V:442:PHE:CD1	1:V:442:PHE:N	2.88	0.41
1:W:356:TYR:O	1:W:367:ILE:HD11	2.20	0.41
1:W:393:ALA:C	1:W:395:ARG:N	2.78	0.41
1:X:47:GLU:HG3	1:X:47:GLU:O	2.20	0.41
1:X:82:GLU:HG3	1:X:258:GLU:HB2	2.03	0.41
1:B:37:ARG:HG2	1:B:38:MET:N	2.36	0.41
1:B:316:PRO:C	1:B:318:ASP:H	2.28	0.41
1:B:384:VAL:HG21	1:B:395:ARG:HD2	2.02	0.41
1:C:37:ARG:O	1:C:38:MET:HB2	2.19	0.41
1:C:246:ASP:O	1:C:250:GLN:HG2	2.20	0.41
1:C:356:TYR:O	1:C:357:LYS:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ILE:N	1:D:17:ILE:CD1	2.81	0.41
1:E:316:PRO:C	1:E:318:ASP:H	2.26	0.41
1:F:337:SER:O	1:F:338:ALA:C	2.62	0.41
2:H:1:THR:OG1	2:H:33:LYS:HE2	2.21	0.41
2:H:51:ALA:O	2:H:55:THR:HG23	2.21	0.41
2:J:26:VAL:HG23	2:O:161:VAL:HG12	2.03	0.41
2:P:42:VAL:HG21	2:P:64:LEU:CD1	2.50	0.41
2:Q:61:GLU:C	2:Q:63:LYS:N	2.78	0.41
1:S:47:GLU:HG3	1:S:47:GLU:O	2.21	0.41
1:T:82:GLU:HG3	1:T:258:GLU:HB2	2.02	0.41
1:U:373:ALA:O	1:U:377:ILE:HG13	2.20	0.41
1:W:259:ILE:O	1:W:262:ILE:HG12	2.21	0.41
1:W:279:GLN:HE22	1:W:319:LEU:HA	1.85	0.41
1:X:18:ILE:HD11	1:X:343:ARG:HH21	1.83	0.41
1:X:386:GLU:HG2	1:X:386:GLU:O	2.19	0.41
1:C:32:ARG:C	1:C:34:ARG:N	2.76	0.41
1:D:283:LEU:CB	1:D:284:PRO:HD3	2.51	0.41
1:D:410:SER:O	1:D:411:ALA:C	2.64	0.41
1:E:42:GLU:N	1:E:43:PRO:CD	2.84	0.41
1:E:401:GLU:OE1	1:F:51:LYS:HG3	2.20	0.41
2:M:50:THR:H	4:M:175:LVS:CD6	2.34	0.41
2:N:118:ASP:O	2:N:119:GLN:HB2	2.21	0.41
2:P:61:GLU:C	2:P:63:LYS:H	2.28	0.41
1:S:73:LEU:HD12	1:S:73:LEU:N	2.35	0.41
1:S:386:GLU:HG2	1:S:386:GLU:O	2.20	0.41
1:S:444:LEU:HD13	1:S:444:LEU:H	1.86	0.41
1:T:96:VAL:HG13	1:T:282:LEU:HD12	2.01	0.41
1:U:96:VAL:HG13	1:U:282:LEU:HD12	2.02	0.41
1:V:47:GLU:HG3	1:V:47:GLU:O	2.21	0.41
1:X:349:HIS:O	1:X:350:ALA:HB3	2.20	0.41
1:A:40:LEU:O	1:A:45:ARG:HD3	2.20	0.41
1:A:410:SER:O	1:A:411:ALA:C	2.62	0.41
1:B:275:ARG:C	1:B:277:GLY:N	2.77	0.41
1:C:283:LEU:HB2	1:C:284:PRO:HD3	2.03	0.41
1:C:437:GLU:CG	1:C:439:LEU:HB2	2.51	0.41
1:C:438:ASP:C	1:C:439:LEU:O	2.61	0.41
1:D:437:GLU:HG3	1:D:439:LEU:HD12	2.02	0.41
2:H:36:ARG:NH1	2:H:170:GLU:OE2	2.53	0.41
2:H:83:ARG:NH1	2:I:58:GLU:OE2	2.51	0.41
2:J:105:ILE:HG22	2:J:113:VAL:O	2.21	0.41
2:K:136:ALA:HB1	2:Q:137:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:37:LEU:HD21	2:L:57:PHE:CE2	2.55	0.41
2:M:7:ARG:HE	2:M:12:VAL:CG2	2.11	0.41
2:P:164:ASN:HD22	2:P:164:ASN:N	2.14	0.41
2:Q:50:THR:H	4:Q:175:LVS:CD6	2.33	0.41
1:S:259:ILE:HG22	1:S:308:SER:O	2.21	0.41
1:S:442:PHE:O	1:S:443:ILE:HG12	2.20	0.41
1:A:237:PRO:C	1:A:239:GLU:N	2.78	0.41
1:C:34:ARG:NH1	1:C:302:HIS:O	2.54	0.41
1:C:37:ARG:CG	1:C:38:MET:N	2.83	0.41
1:D:370:THR:O	1:D:373:ALA:HB3	2.20	0.41
1:D:437:GLU:HG3	1:D:439:LEU:HB2	2.01	0.41
3:D:453:ATP:C8	3:D:453:ATP:C5'	3.03	0.41
1:E:233:LYS:HB2	1:E:233:LYS:NZ	2.36	0.41
1:E:237:PRO:O	1:E:238:GLU:C	2.64	0.41
2:J:17:ASP:HB2	2:J:164:ASN:ND2	2.35	0.41
2:N:50:THR:O	2:N:53:ALA:HB3	2.21	0.41
2:N:104:LEU:HD13	2:N:112:VAL:HG11	2.01	0.41
2:O:81:ASP:O	2:O:88:LEU:HB2	2.20	0.41
2:P:14:VAL:HG12	2:P:34:VAL:CG1	2.51	0.41
1:S:38:MET:HB3	1:S:39:GLN:NE2	2.36	0.41
1:S:393:ALA:C	1:S:395:ARG:N	2.79	0.41
1:U:72:LYS:C	1:U:74:ALA:H	2.29	0.41
1:U:294:LYS:HE3	1:U:295:HIS:HE1	1.86	0.41
1:V:57:GLY:O	1:V:58:PRO:O	2.39	0.41
1:W:5:THR:HG22	1:W:8:GLU:CD	2.46	0.41
1:W:370:THR:HG23	1:W:373:ALA:CB	2.50	0.41
1:A:36:ARG:NH1	1:F:360:MET:HE1	2.35	0.41
1:B:321:PRO:O	1:B:322:GLU:C	2.62	0.41
1:C:276:GLU:O	1:C:276:GLU:HG3	2.21	0.41
1:D:7:ARG:HB3	1:D:7:ARG:NH1	2.36	0.41
1:D:21:ALA:O	1:D:22:ASP:C	2.63	0.41
1:D:57:GLY:O	1:D:63:LYS:CE	2.68	0.41
1:D:356:TYR:CD1	1:D:400:MET:HE3	2.55	0.41
1:E:33:ASN:OD1	1:E:36:ARG:HD2	2.20	0.41
1:E:58:PRO:HG2	1:E:61:VAL:HG11	2.02	0.41
1:E:82:GLU:OE2	1:F:280:ARG:HD3	2.21	0.41
1:F:42:GLU:N	1:F:43:PRO:CD	2.84	0.41
1:F:330:ARG:HG3	1:F:330:ARG:NH1	2.35	0.41
2:G:71:LEU:CD1	2:G:104:LEU:HD22	2.51	0.41
2:H:7:ARG:CZ	2:H:12:VAL:HG21	2.51	0.41
2:I:3:ILE:O	2:I:122:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:33:LYS:HZ3	4:I:175:LVS:HB32	1.79	0.41
2:J:1:THR:CG2	2:J:33:LYS:HZ1	2.31	0.41
2:J:137:LEU:HD13	2:P:136:ALA:HB1	2.02	0.41
2:K:3:ILE:O	2:K:122:ALA:HA	2.21	0.41
2:L:5:SER:HB2	2:L:14:VAL:HG22	2.02	0.41
2:L:125:SER:N	4:L:175:LVS:C1'	2.80	0.41
2:M:43:LEU:O	2:M:97:VAL:HA	2.21	0.41
2:P:6:VAL:HG21	2:P:148:ILE:HG22	2.02	0.41
2:P:18:GLY:CA	2:P:33:LYS:HZ1	2.33	0.41
1:S:68:ARG:HG3	1:S:68:ARG:NH1	2.35	0.41
1:S:72:LYS:C	1:S:74:ALA:H	2.29	0.41
1:S:82:GLU:HG3	1:S:258:GLU:HB2	2.03	0.41
1:S:370:THR:HG21	1:S:422:ASP:HA	2.03	0.41
1:T:260:ASP:HB3	1:T:311:PHE:CE2	2.56	0.41
1:T:373:ALA:O	1:T:377:ILE:HG13	2.21	0.41
1:U:63:LYS:HG2	1:U:333:LEU:HD11	2.03	0.41
1:U:120:ARG:O	1:U:234:LEU:HD12	2.21	0.41
1:U:369:PHE:HE2	1:U:421:ILE:CD1	2.29	0.41
1:V:41:GLN:HG3	1:V:43:PRO:HD2	2.02	0.41
1:V:279:GLN:HE22	1:V:319:LEU:HA	1.85	0.41
1:V:356:TYR:O	1:V:367:ILE:HD11	2.21	0.41
1:W:98:SER:HA	1:W:101:ARG:NH1	2.36	0.41
1:W:326:ARG:HH11	1:W:326:ARG:CA	2.30	0.41
1:X:313:VAL:HG23	1:X:314:ALA:H	1.85	0.41
1:A:52:ASN:HB2	1:A:326:ARG:O	2.21	0.41
1:B:343:ARG:O	1:B:348:PRO:HD3	2.21	0.41
1:C:258:GLU:OE1	1:D:322:GLU:OE1	2.39	0.41
1:C:283:LEU:HA	1:C:283:LEU:HD23	1.72	0.41
1:D:52:ASN:HB2	1:D:326:ARG:O	2.21	0.41
1:D:330:ARG:HG3	1:D:330:ARG:NH1	2.36	0.41
1:D:402:ARG:HH22	1:D:433:VAL:CG2	2.25	0.41
1:E:283:LEU:CB	1:E:284:PRO:HD3	2.50	0.41
1:F:27:VAL:HB	1:F:70:LEU:CD2	2.44	0.41
2:I:7:ARG:CZ	2:I:12:VAL:HG21	2.51	0.41
2:N:112:VAL:HB	1:T:443:ILE:CD1	2.51	0.41
2:O:94:MET:HE3	2:O:123:ILE:HB	2.02	0.41
2:P:30:ASN:O	2:P:31:ALA:C	2.64	0.41
1:S:112:ARG:O	1:S:112:ARG:HG2	2.21	0.41
1:U:63:LYS:HB2	3:U:458:ATP:O2B	2.21	0.41
1:V:73:LEU:HD12	1:V:73:LEU:N	2.35	0.41
1:V:76:ALA:HB1	1:V:251:ASN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:79:ILE:HG22	1:V:103:LEU:HD13	2.03	0.41
1:W:254:VAL:HB	1:W:305:PHE:CD2	2.56	0.41
1:W:313:VAL:HG23	1:W:314:ALA:H	1.86	0.41
1:X:65:GLU:HA	1:X:65:GLU:OE1	2.21	0.41
1:X:107:ALA:O	1:X:111:VAL:HG23	2.21	0.41
1:A:34:ARG:NH1	1:A:302:HIS:O	2.54	0.40
1:A:337:SER:O	1:A:338:ALA:C	2.63	0.40
1:B:283:LEU:HD23	1:B:283:LEU:HA	1.67	0.40
1:C:72:LYS:HA	1:C:72:LYS:HD2	1.86	0.40
1:C:235:ILE:O	1:C:236:ASN:HB3	2.21	0.40
1:E:52:ASN:HB2	1:E:326:ARG:O	2.22	0.40
1:F:280:ARG:HG3	1:F:280:ARG:NH1	2.33	0.40
2:L:51:ALA:O	2:L:55:THR:HG23	2.21	0.40
2:N:7:ARG:NH2	2:N:12:VAL:CG2	2.81	0.40
2:Q:76:VAL:HG11	1:W:442:PHE:CD2	2.56	0.40
1:S:373:ALA:O	1:S:377:ILE:HG13	2.20	0.40
1:T:96:VAL:HG21	1:T:281:ASP:HB2	2.03	0.40
1:T:349:HIS:O	1:T:350:ALA:HB3	2.21	0.40
1:U:393:ALA:C	1:U:395:ARG:H	2.28	0.40
1:B:79:ILE:HD12	1:B:80:LYS:N	2.36	0.40
1:B:370:THR:O	1:B:373:ALA:HB3	2.21	0.40
1:C:337:SER:O	1:C:338:ALA:C	2.65	0.40
1:C:421:ILE:HG23	1:C:425:TYR:CD1	2.56	0.40
1:E:356:TYR:CD1	1:E:400:MET:HE3	2.55	0.40
1:E:395:ARG:O	1:E:398:THR:HB	2.21	0.40
1:F:100:ILE:HG21	1:F:298:VAL:HG21	2.01	0.40
2:G:67:HIS:NE2	2:G:77:GLU:HG3	2.36	0.40
2:H:144:SER:O	2:H:148:ILE:HG13	2.21	0.40
2:H:159:ILE:O	2:M:25:THR:HA	2.20	0.40
2:R:43:LEU:O	2:R:97:VAL:HA	2.22	0.40
1:U:49:THR:HA	1:U:50:PRO:HD3	1.97	0.40
1:V:376:LYS:HE2	1:V:376:LYS:HB3	1.95	0.40
1:V:393:ALA:C	1:V:395:ARG:H	2.28	0.40
1:W:111:VAL:C	1:W:113:GLN:H	2.28	0.40
1:W:430:LEU:N	1:W:430:LEU:HD23	2.35	0.40
1:X:373:ALA:O	1:X:377:ILE:HG13	2.22	0.40
1:A:20:GLN:HE21	1:A:20:GLN:N	2.18	0.40
1:A:42:GLU:HB3	1:A:43:PRO:HD3	2.03	0.40
1:A:51:LYS:HG3	1:F:401:GLU:OE1	2.21	0.40
1:A:280:ARG:CD	1:F:82:GLU:OE2	2.67	0.40
1:B:9:ILE:HD13	1:B:31:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:LEU:HD13	1:B:400:MET:CG	2.49	0.40
1:D:3:GLU:HG3	1:D:4:MET:N	2.36	0.40
1:E:9:ILE:HD13	1:E:31:LEU:HD23	2.02	0.40
1:F:100:ILE:HG21	1:F:298:VAL:CG2	2.51	0.40
2:G:33:LYS:HZ3	2:G:33:LYS:HG3	1.47	0.40
2:K:48:GLY:O	4:K:175:LVS:HD53	2.22	0.40
2:L:159:ILE:O	2:Q:25:THR:HA	2.21	0.40
2:M:3:ILE:HB	2:M:123:ILE:CG1	2.50	0.40
2:N:131:LEU:HD11	2:N:135:ARG:HE	1.83	0.40
2:P:7:ARG:HA	2:P:11:GLN:O	2.22	0.40
2:P:107:THR:C	2:P:109:ILE:H	2.29	0.40
1:T:47:GLU:HG3	1:T:47:GLU:O	2.22	0.40
1:V:66:ILE:HG22	1:V:66:ILE:O	2.21	0.40
1:V:344:ILE:O	1:V:344:ILE:HG22	2.22	0.40
1:X:344:ILE:HG12	3:X:461:ATP:C2	2.57	0.40
1:A:440:SER:O	1:A:441:ARG:C	2.64	0.40
1:E:410:SER:O	1:E:411:ALA:C	2.64	0.40
1:E:438:ASP:C	1:E:439:LEU:O	2.64	0.40
2:I:96:ILE:HG13	2:I:123:ILE:HD13	2.02	0.40
2:K:172:LEU:HD23	2:K:172:LEU:HA	1.85	0.40
2:L:111:ASP:OD2	2:L:111:ASP:N	2.54	0.40
2:L:128:ASN:HA	2:L:131:LEU:HB3	2.03	0.40
2:M:6:VAL:HG23	2:M:149:VAL:HG23	2.04	0.40
2:N:42:VAL:HG21	2:N:64:LEU:CD1	2.51	0.40
2:O:1:THR:HG23	2:O:33:LYS:HZ3	1.84	0.40
2:O:103:SER:O	2:O:104:LEU:HD23	2.22	0.40
2:P:14:VAL:HG12	2:P:14:VAL:O	2.20	0.40
2:Q:43:LEU:O	2:Q:97:VAL:HA	2.22	0.40
1:S:349:HIS:O	1:S:350:ALA:HB3	2.22	0.40
1:T:17:ILE:HD11	1:T:65:GLU:HB3	2.03	0.40
1:T:72:LYS:C	1:T:74:ALA:H	2.29	0.40
1:T:437:GLU:O	1:T:439:LEU:N	2.54	0.40
1:U:27:VAL:CG1	1:U:70:LEU:HD22	2.51	0.40
1:U:441:ARG:HA	1:U:441:ARG:HD3	1.85	0.40
1:V:65:GLU:OE1	1:V:65:GLU:HA	2.22	0.40
1:W:34:ARG:HH12	1:W:252:GLY:H	1.69	0.40
1:W:47:GLU:O	1:W:47:GLU:HG3	2.21	0.40
1:W:437:GLU:O	1:W:439:LEU:N	2.55	0.40
1:X:35:TRP:C	1:X:37:ARG:N	2.79	0.40
1:A:321:PRO:O	1:A:322:GLU:C	2.64	0.40
1:A:378:ALA:O	1:A:379:GLU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:LEU:HD12	1:B:345:LEU:HA	1.75	0.40
1:B:362:THR:C	1:B:364:GLY:H	2.30	0.40
1:C:293:THR:C	1:C:295:HIS:H	2.29	0.40
1:F:358:ALA:O	1:F:361:ALA:HB3	2.22	0.40
1:F:444:LEU:HD23	2:L:113:VAL:HG13	2.03	0.40
2:K:53:ALA:HA	2:K:93:ALA:HB1	2.02	0.40
2:O:64:LEU:HD23	2:O:74:SER:CB	2.51	0.40
2:Q:1:THR:HG22	2:Q:33:LYS:HZ2	1.83	0.40
2:Q:64:LEU:C	2:Q:66:MET:H	2.29	0.40
2:Q:141:THR:HG21	2:Q:143:LEU:HD12	2.03	0.40
1:S:5:THR:HG22	1:S:8:GLU:CD	2.47	0.40
1:S:240:LEU:HD12	1:S:240:LEU:N	2.36	0.40
1:T:96:VAL:HG21	1:T:281:ASP:CB	2.52	0.40
1:T:257:ASP:HA	1:T:308:SER:OG	2.22	0.40
1:U:353:THR:HA	1:U:369:PHE:CE1	2.56	0.40
1:W:326:ARG:NH1	1:W:326:ARG:HB3	2.37	0.40
1:W:385:ASN:HD22	1:W:385:ASN:HA	1.61	0.40
1:X:66:ILE:O	1:X:66:ILE:HG22	2.22	0.40
1:X:79:ILE:HG22	1:X:103:LEU:HD13	2.03	0.40
1:X:236:ASN:N	1:X:237:PRO:HD3	2.36	0.40
1:X:294:LYS:HE3	1:X:295:HIS:HE1	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:7:ARG:NH2	1:X:7:ARG:NH2[2_765]	2.04	0.16

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	49/444 (11%)	47 (96%)	2 (4%)	0	100	100
1	S	309/444 (70%)	235 (76%)	57 (18%)	17 (6%)	1	9
1	T	294/444 (66%)	224 (76%)	50 (17%)	20 (7%)	1	5
1	U	309/444 (70%)	235 (76%)	55 (18%)	19 (6%)	1	7
1	V	309/444 (70%)	237 (77%)	54 (18%)	18 (6%)	1	8
1	W	309/444 (70%)	233 (75%)	57 (18%)	19 (6%)	1	7
1	X	309/444 (70%)	237 (77%)	55 (18%)	17 (6%)	1	9
2	G	57/174 (33%)	54 (95%)	3 (5%)	0	100	100
2	H	62/174 (36%)	56 (90%)	5 (8%)	1 (2%)	7	30
2	I	18/174 (10%)	18 (100%)	0	0	100	100
2	L	141/174 (81%)	128 (91%)	9 (6%)	4 (3%)	4	20
2	M	171/174 (98%)	145 (85%)	19 (11%)	7 (4%)	2	13
2	N	171/174 (98%)	143 (84%)	21 (12%)	7 (4%)	2	13
2	O	171/174 (98%)	141 (82%)	24 (14%)	6 (4%)	3	16
2	P	171/174 (98%)	143 (84%)	22 (13%)	6 (4%)	3	16
2	Q	171/174 (98%)	142 (83%)	21 (12%)	8 (5%)	2	11
2	R	171/174 (98%)	144 (84%)	20 (12%)	7 (4%)	2	13
All	All	3192/4848 (66%)	2562 (80%)	474 (15%)	156 (5%)	1	11

All (156) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	89	ARG
2	M	50	THR
2	M	51	ALA
2	N	50	THR
2	O	50	THR
2	O	51	ALA
2	P	50	THR
2	P	51	ALA
2	Q	50	THR
2	Q	51	ALA
2	R	50	THR
2	R	51	ALA
1	S	21	ALA
1	S	41	GLN
1	S	48	VAL

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Mol	Chain	Res	Type
1	S	58	PRO
1	S	75	ASN
1	S	235	ILE
1	S	436	ASN
1	S	438	ASP
1	S	439	LEU
1	S	440	SER
1	T	21	ALA
1	T	41	GLN
1	T	48	VAL
1	T	58	PRO
1	T	75	ASN
1	T	436	ASN
1	T	438	ASP
1	T	439	LEU
1	T	440	SER
1	U	21	ALA
1	U	41	GLN
1	U	48	VAL
1	U	58	PRO
1	U	75	ASN
1	U	436	ASN
1	U	438	ASP
1	U	439	LEU
1	U	440	SER
1	V	21	ALA
1	V	41	GLN
1	V	48	VAL
1	V	58	PRO
1	V	75	ASN
1	V	436	ASN
1	V	438	ASP
1	V	439	LEU
1	V	440	SER
1	W	21	ALA
1	W	41	GLN
1	W	48	VAL
1	W	58	PRO
1	W	75	ASN
1	W	235	ILE
1	W	436	ASN
1	W	438	ASP

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Mol	Chain	Res	Type
1	W	439	LEU
1	W	440	SER
1	X	21	ALA
1	X	41	GLN
1	X	48	VAL
1	X	58	PRO
1	X	75	ASN
1	X	112	ARG
1	X	436	ASN
1	X	438	ASP
1	X	439	LEU
1	X	440	SER
2	N	31	ALA
2	N	51	ALA
2	O	31	ALA
2	O	127	GLY
2	P	31	ALA
2	Q	31	ALA
2	Q	127	GLY
1	S	74	ALA
1	S	301	ASP
1	T	74	ALA
1	T	116	ILE
1	T	235	ILE
1	T	242	GLN
1	T	323	LEU
1	T	435	GLU
1	U	74	ALA
1	U	234	LEU
1	U	237	PRO
1	U	301	ASP
1	U	323	LEU
1	V	74	ALA
1	V	301	ASP
1	W	74	ALA
1	W	116	ILE
1	W	242	GLN
1	W	323	LEU
1	X	74	ALA
1	X	301	ASP
1	X	323	LEU
2	M	31	ALA

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Mol	Chain	Res	Type
2	N	127	GLY
2	R	31	ALA
1	S	113	GLN
1	S	323	LEU
1	T	301	ASP
1	V	234	LEU
1	V	323	LEU
1	W	113	GLN
1	W	118	LYS
1	W	301	ASP
1	X	109	LYS
2	H	40	GLY
2	L	111	ASP
2	M	66	MET
2	O	49	GLY
2	O	66	MET
2	Q	66	MET
2	Q	117	GLU
1	S	435	GLU
1	U	4	MET
1	X	235	ILE
2	L	87	ALA
2	N	66	MET
2	P	66	MET
2	P	127	GLY
2	R	66	MET
1	S	4	MET
1	S	437	GLU
1	U	118	LYS
1	U	235	ILE
1	V	4	MET
1	V	113	GLN
1	W	239	GLU
2	M	117	GLU
2	M	143	LEU
2	N	117	GLU
2	R	127	GLY
1	T	4	MET
1	T	238	GLU
1	U	239	GLU
1	U	437	GLU
1	V	437	GLU

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Mol	Chain	Res	Type
1	X	242	GLN
2	M	49	GLY
2	N	49	GLY
2	Q	49	GLY
1	X	111	VAL
2	L	40	GLY
2	P	49	GLY
2	Q	115	PRO
2	R	115	PRO
1	T	43	PRO
1	T	237	PRO
1	V	237	PRO
2	R	49	GLY
1	V	43	PRO
1	W	43	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	267/373 (72%)	240 (90%)	27 (10%)	7	28
1	B	267/373 (72%)	239 (90%)	28 (10%)	6	26
1	C	267/373 (72%)	243 (91%)	24 (9%)	9	33
1	D	267/373 (72%)	241 (90%)	26 (10%)	8	30
1	E	267/373 (72%)	243 (91%)	24 (9%)	9	33
1	F	267/373 (72%)	240 (90%)	27 (10%)	7	28
1	S	267/373 (72%)	257 (96%)	10 (4%)	30	61
1	T	267/373 (72%)	256 (96%)	11 (4%)	27	59
1	U	267/373 (72%)	257 (96%)	10 (4%)	30	61
1	V	267/373 (72%)	257 (96%)	10 (4%)	30	61
1	W	267/373 (72%)	256 (96%)	11 (4%)	27	59
1	X	267/373 (72%)	257 (96%)	10 (4%)	30	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	132/140 (94%)	115 (87%)	17 (13%)	4	18
2	H	132/140 (94%)	114 (86%)	18 (14%)	3	16
2	I	132/140 (94%)	116 (88%)	16 (12%)	5	20
2	J	132/140 (94%)	114 (86%)	18 (14%)	3	16
2	K	132/140 (94%)	115 (87%)	17 (13%)	4	18
2	L	132/140 (94%)	116 (88%)	16 (12%)	5	20
2	M	125/140 (89%)	114 (91%)	11 (9%)	9	33
2	N	125/140 (89%)	116 (93%)	9 (7%)	13	40
2	O	125/140 (89%)	115 (92%)	10 (8%)	11	37
2	P	125/140 (89%)	115 (92%)	10 (8%)	11	37
2	Q	125/140 (89%)	115 (92%)	10 (8%)	11	37
2	R	125/140 (89%)	115 (92%)	10 (8%)	11	37
All	All	4746/6156 (77%)	4366 (92%)	380 (8%)	11	37

All (380) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
1	A	8	GLU
1	A	20	GLN
1	A	29	ILE
1	A	34	ARG
1	A	39	GLN
1	A	41	GLN
1	A	45	ARG
1	A	59	THR
1	A	82	GLU
1	A	96	VAL
1	A	111	VAL
1	A	115	GLU
1	A	116	ILE
1	A	237	PRO
1	A	251	ASN
1	A	276	GLU
1	A	336	LEU
1	A	345	LEU
1	A	359	LEU
1	A	379	GLU

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Mol	Chain	Res	Type
1	A	384	VAL
1	A	403	LEU
1	A	413	ASP
1	A	428	ASP
1	A	434	VAL
1	A	444	LEU
1	B	6	PRO
1	B	8	GLU
1	B	20	GLN
1	B	25	ARG
1	B	29	ILE
1	B	34	ARG
1	B	39	GLN
1	B	45	ARG
1	B	59	THR
1	B	82	GLU
1	B	96	VAL
1	B	233	LYS
1	B	251	ASN
1	B	313	VAL
1	B	331	VAL
1	B	336	LEU
1	B	345	LEU
1	B	370	THR
1	B	379	GLU
1	B	384	VAL
1	B	403	LEU
1	B	408	SER
1	B	410	SER
1	B	413	ASP
1	B	419	VAL
1	B	428	ASP
1	B	434	VAL
1	B	444	LEU
1	C	6	PRO
1	C	8	GLU
1	C	20	GLN
1	C	25	ARG
1	C	29	ILE
1	C	39	GLN
1	C	45	ARG
1	C	59	THR

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Mol	Chain	Res	Type
1	C	82	GLU
1	C	96	VAL
1	C	111	VAL
1	C	233	LYS
1	C	245	ILE
1	C	251	ASN
1	C	331	VAL
1	C	336	LEU
1	C	345	LEU
1	C	379	GLU
1	C	384	VAL
1	C	403	LEU
1	C	413	ASP
1	C	428	ASP
1	C	434	VAL
1	C	444	LEU
1	D	6	PRO
1	D	8	GLU
1	D	20	GLN
1	D	25	ARG
1	D	29	ILE
1	D	34	ARG
1	D	39	GLN
1	D	45	ARG
1	D	59	THR
1	D	82	GLU
1	D	96	VAL
1	D	113	GLN
1	D	233	LYS
1	D	251	ASN
1	D	331	VAL
1	D	336	LEU
1	D	345	LEU
1	D	362	THR
1	D	379	GLU
1	D	384	VAL
1	D	403	LEU
1	D	408	SER
1	D	413	ASP
1	D	428	ASP
1	D	434	VAL
1	D	444	LEU

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Mol	Chain	Res	Type
1	E	6	PRO
1	E	8	GLU
1	E	20	GLN
1	E	25	ARG
1	E	29	ILE
1	E	34	ARG
1	E	39	GLN
1	E	45	ARG
1	E	82	GLU
1	E	96	VAL
1	E	233	LYS
1	E	234	LEU
1	E	251	ASN
1	E	336	LEU
1	E	345	LEU
1	E	362	THR
1	E	379	GLU
1	E	384	VAL
1	E	403	LEU
1	E	408	SER
1	E	413	ASP
1	E	428	ASP
1	E	434	VAL
1	E	444	LEU
1	F	8	GLU
1	F	20	GLN
1	F	25	ARG
1	F	29	ILE
1	F	34	ARG
1	F	39	GLN
1	F	45	ARG
1	F	59	THR
1	F	79	ILE
1	F	82	GLU
1	F	96	VAL
1	F	234	LEU
1	F	245	ILE
1	F	251	ASN
1	F	331	VAL
1	F	336	LEU
1	F	345	LEU
1	F	362	THR

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Mol	Chain	Res	Type
1	F	379	GLU
1	F	384	VAL
1	F	403	LEU
1	F	408	SER
1	F	410	SER
1	F	413	ASP
1	F	428	ASP
1	F	434	VAL
1	F	444	LEU
2	G	1	THR
2	G	3	ILE
2	G	21	SER
2	G	42	VAL
2	G	55	THR
2	G	56	LEU
2	G	59	LEU
2	G	72	LEU
2	G	82	TRP
2	G	83	ARG
2	G	86	ARG
2	G	104	LEU
2	G	105	ILE
2	G	107	THR
2	G	112	VAL
2	G	135	ARG
2	G	164	ASN
2	H	1	THR
2	H	3	ILE
2	H	21	SER
2	H	22	LEU
2	H	33	LYS
2	H	42	VAL
2	H	55	THR
2	H	56	LEU
2	H	72	LEU
2	H	83	ARG
2	H	86	ARG
2	H	88	LEU
2	H	104	LEU
2	H	105	ILE
2	H	107	THR
2	H	112	VAL

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Mol	Chain	Res	Type
2	H	141	THR
2	H	164	ASN
2	I	1	THR
2	I	3	ILE
2	I	21	SER
2	I	42	VAL
2	I	55	THR
2	I	56	LEU
2	I	59	LEU
2	I	72	LEU
2	I	82	TRP
2	I	83	ARG
2	I	86	ARG
2	I	104	LEU
2	I	105	ILE
2	I	112	VAL
2	I	141	THR
2	I	164	ASN
2	J	1	THR
2	J	3	ILE
2	J	21	SER
2	J	33	LYS
2	J	42	VAL
2	J	55	THR
2	J	56	LEU
2	J	72	LEU
2	J	83	ARG
2	J	86	ARG
2	J	88	LEU
2	J	89	ARG
2	J	104	LEU
2	J	105	ILE
2	J	107	THR
2	J	112	VAL
2	J	141	THR
2	J	164	ASN
2	K	1	THR
2	K	3	ILE
2	K	21	SER
2	K	42	VAL
2	K	55	THR
2	K	56	LEU

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Mol	Chain	Res	Type
2	K	72	LEU
2	K	82	TRP
2	K	83	ARG
2	K	86	ARG
2	K	89	ARG
2	K	104	LEU
2	K	105	ILE
2	K	107	THR
2	K	112	VAL
2	K	141	THR
2	K	164	ASN
2	L	1	THR
2	L	3	ILE
2	L	21	SER
2	L	42	VAL
2	L	55	THR
2	L	56	LEU
2	L	59	LEU
2	L	72	LEU
2	L	83	ARG
2	L	86	ARG
2	L	104	LEU
2	L	105	ILE
2	L	107	THR
2	L	112	VAL
2	L	141	THR
2	L	164	ASN
2	M	1	THR
2	M	8	ARG
2	M	33	LYS
2	M	54	PHE
2	M	55	THR
2	M	88	LEU
2	M	111	ASP
2	M	137	LEU
2	M	150	GLU
2	M	164	ASN
2	M	167	PHE
2	N	1	THR
2	N	8	ARG
2	N	54	PHE
2	N	55	THR

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Mol	Chain	Res	Type
2	N	88	LEU
2	N	137	LEU
2	N	150	GLU
2	N	164	ASN
2	N	167	PHE
2	O	1	THR
2	O	8	ARG
2	O	54	PHE
2	O	55	THR
2	O	88	LEU
2	O	111	ASP
2	O	137	LEU
2	O	150	GLU
2	O	164	ASN
2	O	167	PHE
2	P	1	THR
2	P	8	ARG
2	P	54	PHE
2	P	55	THR
2	P	88	LEU
2	P	111	ASP
2	P	137	LEU
2	P	150	GLU
2	P	164	ASN
2	P	167	PHE
2	Q	1	THR
2	Q	8	ARG
2	Q	54	PHE
2	Q	55	THR
2	Q	88	LEU
2	Q	111	ASP
2	Q	137	LEU
2	Q	150	GLU
2	Q	164	ASN
2	Q	167	PHE
2	R	1	THR
2	R	8	ARG
2	R	54	PHE
2	R	55	THR
2	R	88	LEU
2	R	111	ASP
2	R	137	LEU

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Mol	Chain	Res	Type
2	R	150	GLU
2	R	164	ASN
2	R	167	PHE
1	S	70	LEU
1	S	75	ASN
1	S	280	ARG
1	S	333	LEU
1	S	370	THR
1	S	430	LEU
1	S	439	LEU
1	S	441	ARG
1	S	442	PHE
1	S	444	LEU
1	T	70	LEU
1	T	75	ASN
1	T	246	ASP
1	T	280	ARG
1	T	333	LEU
1	T	370	THR
1	T	430	LEU
1	T	439	LEU
1	T	441	ARG
1	T	442	PHE
1	T	444	LEU
1	U	70	LEU
1	U	75	ASN
1	U	280	ARG
1	U	333	LEU
1	U	370	THR
1	U	430	LEU
1	U	439	LEU
1	U	441	ARG
1	U	442	PHE
1	U	444	LEU
1	V	70	LEU
1	V	75	ASN
1	V	280	ARG
1	V	333	LEU
1	V	370	THR
1	V	430	LEU
1	V	439	LEU
1	V	441	ARG

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Mol	Chain	Res	Type
1	V	442	PHE
1	V	444	LEU
1	W	70	LEU
1	W	75	ASN
1	W	109	LYS
1	W	280	ARG
1	W	333	LEU
1	W	370	THR
1	W	430	LEU
1	W	439	LEU
1	W	441	ARG
1	W	442	PHE
1	W	444	LEU
1	X	70	LEU
1	X	75	ASN
1	X	280	ARG
1	X	333	LEU
1	X	385	ASN
1	X	430	LEU
1	X	439	LEU
1	X	441	ARG
1	X	442	PHE
1	X	444	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (172) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	39	GLN
1	A	41	GLN
1	A	75	ASN
1	A	250	GLN
1	A	251	ASN
1	A	324	GLN
1	A	349	HIS
1	A	366	ASN
1	A	417	GLN
1	B	16	HIS
1	B	20	GLN
1	B	39	GLN
1	B	41	GLN
1	B	119	ASN

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Mol	Chain	Res	Type
1	B	236	ASN
1	B	250	GLN
1	B	251	ASN
1	B	324	GLN
1	B	417	GLN
1	C	20	GLN
1	C	39	GLN
1	C	41	GLN
1	C	114	GLN
1	C	236	ASN
1	C	250	GLN
1	C	251	ASN
1	C	295	HIS
1	C	324	GLN
1	C	349	HIS
1	C	417	GLN
1	C	436	ASN
1	D	20	GLN
1	D	39	GLN
1	D	41	GLN
1	D	114	GLN
1	D	119	ASN
1	D	250	GLN
1	D	251	ASN
1	D	295	HIS
1	D	324	GLN
1	D	417	GLN
1	D	436	ASN
1	E	20	GLN
1	E	39	GLN
1	E	41	GLN
1	E	114	GLN
1	E	250	GLN
1	E	251	ASN
1	E	295	HIS
1	E	324	GLN
1	E	417	GLN
1	F	20	GLN
1	F	39	GLN
1	F	41	GLN
1	F	114	GLN
1	F	250	GLN

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Mol	Chain	Res	Type
1	F	251	ASN
1	F	324	GLN
1	F	349	HIS
1	F	417	GLN
1	F	436	ASN
2	G	24	ASN
2	G	146	HIS
2	G	164	ASN
2	H	24	ASN
2	H	128	ASN
2	H	146	HIS
2	H	164	ASN
2	I	24	ASN
2	I	146	HIS
2	I	164	ASN
2	J	128	ASN
2	J	146	HIS
2	J	164	ASN
2	K	24	ASN
2	K	164	ASN
2	L	24	ASN
2	L	164	ASN
2	M	164	ASN
2	N	164	ASN
2	O	164	ASN
2	P	164	ASN
2	Q	68	GLN
2	Q	164	ASN
2	R	68	GLN
2	R	119	GLN
2	R	164	ASN
1	S	16	HIS
1	S	41	GLN
1	S	75	ASN
1	S	236	ASN
1	S	251	ASN
1	S	279	GLN
1	S	295	HIS
1	S	302	HIS
1	S	366	ASN
1	S	385	ASN
1	S	390	ASN

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Mol	Chain	Res	Type
1	S	397	HIS
1	S	417	GLN
1	S	436	ASN
1	T	16	HIS
1	T	33	ASN
1	T	41	GLN
1	T	75	ASN
1	T	236	ASN
1	T	251	ASN
1	T	279	GLN
1	T	302	HIS
1	T	366	ASN
1	T	385	ASN
1	T	390	ASN
1	T	397	HIS
1	T	417	GLN
1	T	436	ASN
1	U	16	HIS
1	U	41	GLN
1	U	75	ASN
1	U	113	GLN
1	U	119	ASN
1	U	236	ASN
1	U	242	GLN
1	U	251	ASN
1	U	279	GLN
1	U	295	HIS
1	U	312	GLN
1	U	366	ASN
1	U	385	ASN
1	U	390	ASN
1	U	397	HIS
1	U	417	GLN
1	U	436	ASN
1	V	16	HIS
1	V	41	GLN
1	V	75	ASN
1	V	114	GLN
1	V	236	ASN
1	V	251	ASN
1	V	279	GLN
1	V	366	ASN

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Mol	Chain	Res	Type
1	V	385	ASN
1	V	390	ASN
1	V	397	HIS
1	V	417	GLN
1	V	436	ASN
1	W	16	HIS
1	W	41	GLN
1	W	75	ASN
1	W	236	ASN
1	W	242	GLN
1	W	251	ASN
1	W	279	GLN
1	W	349	HIS
1	W	366	ASN
1	W	385	ASN
1	W	390	ASN
1	W	397	HIS
1	W	417	GLN
1	W	436	ASN
1	X	16	HIS
1	X	41	GLN
1	X	75	ASN
1	X	114	GLN
1	X	236	ASN
1	X	251	ASN
1	X	279	GLN
1	X	366	ASN
1	X	385	ASN
1	X	390	ASN
1	X	397	HIS
1	X	417	GLN

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](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LVS	I	175	2	25,27,42	2.79	4 (16%)	30,37,59	1.55	3 (10%)
4	LVS	M	175	2	25,27,42	2.90	4 (16%)	30,37,59	1.65	6 (20%)
3	ATP	W	460	-	32,33,33	0.62	1 (3%)	48,52,52	0.75	1 (2%)
4	LVS	H	175	2	25,27,42	2.88	4 (16%)	30,37,59	1.44	3 (10%)
3	ATP	B	451	-	32,33,33	0.93	1 (3%)	48,52,52	0.80	1 (2%)
4	LVS	L	175	2	25,27,42	2.91	4 (16%)	30,37,59	1.48	3 (10%)
3	ATP	T	457	-	32,33,33	0.68	1 (3%)	48,52,52	0.70	1 (2%)
4	LVS	R	175	2	25,27,42	2.96	4 (16%)	30,37,59	1.69	7 (23%)
3	ATP	U	458	-	32,33,33	0.72	1 (3%)	48,52,52	0.70	1 (2%)
4	LVS	Q	175	2	25,27,42	2.87	4 (16%)	30,37,59	1.62	6 (20%)
4	LVS	P	175	2	25,27,42	3.06	4 (16%)	30,37,59	1.65	6 (20%)
4	LVS	O	175	2	25,27,42	3.05	4 (16%)	30,37,59	1.71	8 (26%)
3	ATP	V	459	-	32,33,33	0.67	1 (3%)	48,52,52	0.75	1 (2%)
3	ATP	D	453	-	32,33,33	0.84	1 (3%)	48,52,52	0.95	4 (8%)
3	ATP	A	450	-	32,33,33	0.79	1 (3%)	48,52,52	0.92	2 (4%)
3	ATP	C	452	-	32,33,33	1.05	1 (3%)	48,52,52	0.89	3 (6%)
3	ATP	E	454	-	32,33,33	1.02	1 (3%)	48,52,52	0.95	2 (4%)
4	LVS	N	175	2	25,27,42	3.20	4 (16%)	30,37,59	1.67	7 (23%)
3	ATP	S	456	-	32,33,33	0.73	1 (3%)	48,52,52	0.71	1 (2%)
4	LVS	J	175	2	25,27,42	2.85	4 (16%)	30,37,59	1.53	5 (16%)
4	LVS	K	175	2	25,27,42	3.05	4 (16%)	30,37,59	1.63	4 (13%)
3	ATP	F	455	-	32,33,33	1.03	1 (3%)	48,52,52	0.87	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LVS	G	175	2	25,27,42	3.02	4 (16%)	30,37,59	1.53	3 (10%)
3	ATP	X	461	-	32,33,33	0.69	0	48,52,52	0.72	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LVS	I	175	2	-	10/33/34/46	-
4	LVS	M	175	2	-	4/33/34/46	-
3	ATP	W	460	-	-	3/22/38/38	0/3/3/3
4	LVS	H	175	2	-	12/33/34/46	-
3	ATP	B	451	-	-	9/22/38/38	0/3/3/3
4	LVS	L	175	2	-	11/33/34/46	-
3	ATP	T	457	-	-	0/22/38/38	0/3/3/3
4	LVS	R	175	2	-	4/33/34/46	-
3	ATP	U	458	-	-	4/22/38/38	0/3/3/3
4	LVS	Q	175	2	-	5/33/34/46	-
4	LVS	P	175	2	-	4/33/34/46	-
4	LVS	O	175	2	-	4/33/34/46	-
3	ATP	V	459	-	-	0/22/38/38	0/3/3/3
3	ATP	D	453	-	-	6/22/38/38	0/3/3/3
3	ATP	A	450	-	-	2/22/38/38	0/3/3/3
3	ATP	C	452	-	-	5/22/38/38	0/3/3/3
3	ATP	E	454	-	-	6/22/38/38	0/3/3/3
4	LVS	N	175	2	-	4/33/34/46	-
3	ATP	S	456	-	-	2/22/38/38	0/3/3/3
4	LVS	J	175	2	-	10/33/34/46	-
4	LVS	K	175	2	-	11/33/34/46	-
3	ATP	F	455	-	-	4/22/38/38	0/3/3/3
4	LVS	G	175	2	-	13/33/34/46	-
3	ATP	X	461	-	-	0/22/38/38	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	175	LVS	C2'-CS	14.47	1.54	1.31
4	P	175	LVS	C2'-CS	14.06	1.54	1.31
4	R	175	LVS	C2'-CS	14.02	1.53	1.31
4	O	175	LVS	C2'-CS	13.98	1.53	1.31
4	K	175	LVS	C2'-CS	13.19	1.52	1.31
4	M	175	LVS	C2'-CS	13.15	1.52	1.31
4	Q	175	LVS	C2'-CS	13.03	1.52	1.31
4	G	175	LVS	C2'-CS	12.63	1.51	1.31
4	J	175	LVS	C2'-CS	12.34	1.51	1.31
4	L	175	LVS	C2'-CS	11.92	1.50	1.31
4	I	175	LVS	C2'-CS	11.74	1.50	1.31
4	H	175	LVS	C2'-CS	11.72	1.50	1.31
4	I	175	LVS	C2'-S	5.74	1.85	1.75
4	L	175	LVS	C2'-S	5.46	1.85	1.75
4	G	175	LVS	C2'-S	5.37	1.85	1.75
4	H	175	LVS	C2'-S	5.33	1.85	1.75
3	C	452	ATP	PB-O3B	4.91	1.64	1.59
4	K	175	LVS	O1'-S	4.78	1.50	1.44
4	J	175	LVS	C2'-S	4.65	1.83	1.75
4	L	175	LVS	O1'-S	4.63	1.50	1.44
3	F	455	ATP	PB-O3B	4.59	1.64	1.59
4	K	175	LVS	C2'-S	4.42	1.83	1.75
3	B	451	ATP	PB-O3B	4.36	1.64	1.59
4	H	175	LVS	O1'-S	4.04	1.49	1.44
4	N	175	LVS	C2'-S	4.03	1.82	1.75
3	E	454	ATP	PB-O3B	3.99	1.63	1.59
4	N	175	LVS	O1'-S	3.94	1.49	1.44
4	G	175	LVS	O1'-S	3.89	1.49	1.44
4	O	175	LVS	C2'-S	3.85	1.82	1.75
4	G	175	LVS	O2'-S	3.82	1.49	1.44
4	H	175	LVS	O2'-S	3.82	1.49	1.44
4	M	175	LVS	O1'-S	3.71	1.48	1.44
3	D	453	ATP	PB-O3B	3.68	1.63	1.59
4	P	175	LVS	O1'-S	3.55	1.48	1.44
4	O	175	LVS	O2'-S	3.54	1.48	1.44
4	J	175	LVS	O1'-S	3.42	1.48	1.44
4	Q	175	LVS	O2'-S	3.36	1.48	1.44
4	P	175	LVS	O2'-S	3.36	1.48	1.44
4	L	175	LVS	O2'-S	3.34	1.48	1.44
4	I	175	LVS	O1'-S	3.32	1.48	1.44
3	A	450	ATP	PB-O3B	3.23	1.63	1.59
4	N	175	LVS	O2'-S	3.20	1.48	1.44
4	Q	175	LVS	O1'-S	3.18	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	175	LVS	O2'-S	3.18	1.48	1.44
4	Q	175	LVS	C2'-S	3.14	1.81	1.75
4	M	175	LVS	O2'-S	3.13	1.48	1.44
4	M	175	LVS	C2'-S	3.13	1.81	1.75
3	U	458	ATP	PB-O3B	2.99	1.62	1.59
4	R	175	LVS	C2'-S	2.96	1.80	1.75
4	P	175	LVS	C2'-S	2.94	1.80	1.75
4	J	175	LVS	O2'-S	2.89	1.47	1.44
4	R	175	LVS	O2'-S	2.74	1.47	1.44
4	I	175	LVS	O2'-S	2.55	1.47	1.44
3	V	459	ATP	PB-O3B	2.53	1.62	1.59
3	S	456	ATP	PB-O3B	2.50	1.62	1.59
3	W	460	ATP	PB-O3B	2.33	1.62	1.59
4	O	175	LVS	O1'-S	2.32	1.47	1.44
3	T	457	ATP	PB-O3B	2.31	1.62	1.59
4	R	175	LVS	O1'-S	2.04	1.46	1.44

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	175	LVS	CS-CA3-N3	5.70	121.04	110.36
4	L	175	LVS	CS-CA3-N3	5.59	120.84	110.36
4	G	175	LVS	CS-CA3-N3	5.29	120.27	110.36
4	I	175	LVS	CS-CA3-N3	5.24	120.19	110.36
4	H	175	LVS	CS-CA3-N3	5.21	120.12	110.36
4	J	175	LVS	CS-CA3-N3	4.92	119.57	110.36
4	O	175	LVS	CS-CA3-N3	4.74	119.23	110.36
4	I	175	LVS	O1'-S-C1'	4.73	117.08	108.28
4	R	175	LVS	CS-CA3-N3	4.28	118.38	110.36
4	Q	175	LVS	CS-CA3-N3	4.25	118.33	110.36
4	N	175	LVS	CS-CA3-N3	4.24	118.31	110.36
4	M	175	LVS	CS-CA3-N3	4.24	118.30	110.36
4	J	175	LVS	O1'-S-C1'	4.19	116.07	108.28
4	K	175	LVS	O1'-S-C1'	4.18	116.05	108.28
4	R	175	LVS	CB3-CA3-CS	-4.08	104.76	110.99
4	R	175	LVS	O1'-S-C1'	4.05	115.81	108.28
4	Q	175	LVS	CB3-CA3-CS	-4.04	104.81	110.99
4	P	175	LVS	CS-CA3-N3	4.02	117.89	110.36
4	P	175	LVS	O1'-S-C1'	3.92	115.56	108.28
4	N	175	LVS	O1'-S-C1'	3.89	115.51	108.28
4	P	175	LVS	CB3-CA3-CS	-3.80	105.17	110.99
4	M	175	LVS	O1'-S-C1'	3.78	115.30	108.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	175	LVS	O1'-S-C1'	3.77	115.29	108.28
4	N	175	LVS	CB3-CA3-CS	-3.74	105.27	110.99
4	M	175	LVS	CB3-CA3-CS	-3.74	105.28	110.99
4	O	175	LVS	CB3-CA3-CS	-3.53	105.59	110.99
4	H	175	LVS	O1'-S-C1'	3.50	114.78	108.28
4	Q	175	LVS	O1'-S-C1'	3.39	114.58	108.28
4	O	175	LVS	O1'-S-C1'	3.28	114.39	108.28
4	O	175	LVS	CG2-CB2-CA2	3.28	124.19	115.40
4	O	175	LVS	C2-CA2-N2	3.14	119.62	111.11
4	N	175	LVS	CG2-CB2-CA2	3.14	123.82	115.40
4	M	175	LVS	C2-CA2-N2	3.06	119.39	111.11
4	P	175	LVS	CG2-CB2-CA2	3.05	123.58	115.40
3	E	454	ATP	C2'-C1'-N9	-2.95	105.97	113.30
4	L	175	LVS	O1'-S-C1'	2.90	113.67	108.28
4	N	175	LVS	C2-CA2-N2	2.86	118.85	111.11
4	R	175	LVS	CG2-CB2-CA2	2.83	122.99	115.40
4	M	175	LVS	CG2-CB2-CA2	2.71	122.69	115.40
4	J	175	LVS	CA3-CS-C2'	-2.69	112.13	125.91
4	P	175	LVS	C2-CA2-N2	2.69	118.38	111.11
3	F	455	ATP	O3A-PB-O1B	-2.69	102.62	110.70
4	Q	175	LVS	CG2-CB2-CA2	2.58	122.34	115.40
4	Q	175	LVS	C2-CA2-N2	2.57	118.07	111.11
4	Q	175	LVS	CA3-CS-C2'	-2.57	112.78	125.91
4	I	175	LVS	CA3-CS-C2'	-2.55	112.84	125.91
4	M	175	LVS	CA3-CS-C2'	-2.53	112.97	125.91
4	R	175	LVS	CA3-CS-C2'	-2.52	113.00	125.91
4	R	175	LVS	C2-CA2-N2	2.50	117.88	111.11
3	D	453	ATP	C2'-C1'-N9	-2.48	107.14	113.30
4	H	175	LVS	CA3-CS-C2'	-2.48	113.22	125.91
4	P	175	LVS	CA3-CS-C2'	-2.47	113.25	125.91
4	O	175	LVS	CA3-CS-C2'	-2.47	113.27	125.91
3	A	450	ATP	O3A-PB-O1B	-2.46	103.30	110.70
4	G	175	LVS	CA3-CS-C2'	-2.41	113.60	125.91
4	N	175	LVS	CA3-CS-C2'	-2.39	113.69	125.91
3	C	452	ATP	C2'-C1'-N9	-2.38	107.40	113.30
4	R	175	LVS	O2'-S-C1'	2.30	112.55	108.28
3	W	460	ATP	O3G-PG-O2G	2.29	116.41	107.80
4	L	175	LVS	CA3-CS-C2'	-2.29	114.20	125.91
3	U	458	ATP	O3G-PG-O2G	2.29	116.38	107.80
4	K	175	LVS	CA3-CS-C2'	-2.29	114.21	125.91
3	E	454	ATP	O3A-PB-O1B	-2.28	103.83	110.70
3	X	461	ATP	O3G-PG-O2G	2.28	116.34	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	456	ATP	O3G-PG-O2G	2.28	116.34	107.80
3	D	453	ATP	O3A-PB-O1B	-2.26	103.91	110.70
3	T	457	ATP	O3G-PG-O2G	2.24	116.20	107.80
3	V	459	ATP	O3G-PG-O2G	2.22	116.13	107.80
3	D	453	ATP	O3A-PA-O1A	-2.19	104.11	110.70
4	O	175	LVS	CB2-CA2-C2	-2.18	105.42	110.59
4	N	175	LVS	CB2-CA2-C2	-2.17	105.44	110.59
4	J	175	LVS	CA2-N2-C1	-2.12	117.09	121.65
3	C	452	ATP	O3A-PB-O1B	-2.11	104.36	110.70
3	D	453	ATP	O3G-PG-O2G	2.11	115.70	107.80
3	F	455	ATP	O3G-PG-O2G	2.10	115.66	107.80
4	O	175	LVS	O2'-S-C1'	2.06	112.11	108.28
4	K	175	LVS	CA1-C1-N2	2.06	119.00	116.21
3	A	450	ATP	O3G-PG-O2G	2.05	115.50	107.80
3	B	451	ATP	O3G-PG-O2G	2.04	115.45	107.80
3	C	452	ATP	O3G-PG-O2G	2.02	115.36	107.80
4	J	175	LVS	O2'-S-C1'	2.01	112.02	108.28

There are no chirality outliers.

All (133) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	450	ATP	PB-O3B-PG-O2G
3	B	451	ATP	PB-O3B-PG-O2G
3	B	451	ATP	C5'-O5'-PA-O1A
3	B	451	ATP	C5'-O5'-PA-O2A
3	B	451	ATP	C5'-O5'-PA-O3A
3	C	452	ATP	PB-O3B-PG-O2G
3	D	453	ATP	PB-O3B-PG-O2G
3	F	455	ATP	PB-O3B-PG-O2G
3	S	456	ATP	C5'-O5'-PA-O1A
4	G	175	LVS	C1-CA1-CB1-CG1
4	G	175	LVS	N1-CA1-CB1-CG1
4	G	175	LVS	CS-CA3-N3-C2
4	G	175	LVS	S-C2'-CS-CA3
4	H	175	LVS	C1-CA1-CB1-CG1
4	H	175	LVS	N1-CA1-CB1-CG1
4	H	175	LVS	CS-CA3-N3-C2
4	H	175	LVS	S-C2'-CS-CA3
4	I	175	LVS	C1-CA1-CB1-CG1
4	I	175	LVS	N1-CA1-CB1-CG1
4	I	175	LVS	CS-CA3-N3-C2

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Mol	Chain	Res	Type	Atoms
4	I	175	LVS	S-C2'-CS-CA3
4	J	175	LVS	C1-CA1-CB1-CG1
4	J	175	LVS	N1-CA1-CB1-CG1
4	J	175	LVS	CS-CA3-N3-C2
4	J	175	LVS	CB3-CA3-N3-C2
4	J	175	LVS	S-C2'-CS-CA3
4	K	175	LVS	C1-CA1-CB1-CG1
4	K	175	LVS	N1-CA1-CB1-CG1
4	K	175	LVS	S-C2'-CS-CA3
4	L	175	LVS	C1-CA1-CB1-CG1
4	L	175	LVS	N1-CA1-CB1-CG1
4	L	175	LVS	CS-CA3-N3-C2
4	L	175	LVS	S-C2'-CS-CA3
4	M	175	LVS	C1-CA1-CB1-CG1
4	M	175	LVS	S-C2'-CS-CA3
4	N	175	LVS	S-C2'-CS-CA3
4	O	175	LVS	C1-CA1-CB1-CG1
4	O	175	LVS	S-C2'-CS-CA3
4	P	175	LVS	S-C2'-CS-CA3
4	Q	175	LVS	S-C2'-CS-CA3
4	R	175	LVS	C1-CA1-CB1-CG1
4	R	175	LVS	S-C2'-CS-CA3
4	H	175	LVS	N3-CA3-CB3-CG3
3	E	454	ATP	PB-O3B-PG-O1G
4	J	175	LVS	O2-C2-CA2-CB2
4	K	175	LVS	N3-CA3-CB3-CG3
4	K	175	LVS	O2-C2-CA2-N2
3	C	452	ATP	PA-O3A-PB-O1B
3	D	453	ATP	PG-O3B-PB-O1B
4	G	175	LVS	N3-C2-CA2-N2
4	L	175	LVS	O2-C2-CA2-N2
4	G	175	LVS	O2-C2-CA2-N2
4	I	175	LVS	O2-C2-CA2-N2
4	J	175	LVS	N3-C2-CA2-CB2
4	K	175	LVS	N3-C2-CA2-N2
4	L	175	LVS	N3-C2-CA2-N2
4	G	175	LVS	N3-CA3-CB3-CG3
4	I	175	LVS	N3-C2-CA2-N2
4	J	175	LVS	O2-C2-CA2-N2
4	H	175	LVS	O2-C2-CA2-N2
4	I	175	LVS	N3-CA3-CB3-CG3
4	K	175	LVS	CS-CA3-N3-C2

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Mol	Chain	Res	Type	Atoms
4	L	175	LVS	N3-CA3-CB3-CG3
4	K	175	LVS	CS-CA3-CB3-CG3
4	M	175	LVS	N1-CA1-CB1-CG1
4	O	175	LVS	N1-CA1-CB1-CG1
4	P	175	LVS	N1-CA1-CB1-CG1
4	Q	175	LVS	N1-CA1-CB1-CG1
4	R	175	LVS	N1-CA1-CB1-CG1
4	L	175	LVS	O2-C2-CA2-CB2
4	O	175	LVS	N2-CA2-CB2-CG2
3	B	451	ATP	PB-O3B-PG-O3G
3	E	454	ATP	PB-O3B-PG-O2G
4	G	175	LVS	CB3-CA3-N3-C2
4	I	175	LVS	CB3-CA3-N3-C2
4	L	175	LVS	CB3-CA3-N3-C2
4	K	175	LVS	O2-C2-CA2-CB2
4	I	175	LVS	O2-C2-CA2-CB2
4	L	175	LVS	N3-C2-CA2-CB2
4	H	175	LVS	N3-C2-CA2-N2
4	J	175	LVS	N3-C2-CA2-N2
3	B	451	ATP	PG-O3B-PB-O1B
4	N	175	LVS	C1-CA1-CB1-CG1
4	P	175	LVS	C1-CA1-CB1-CG1
4	Q	175	LVS	C1-CA1-CB1-CG1
4	I	175	LVS	N3-C2-CA2-CB2
3	U	458	ATP	C5'-O5'-PA-O1A
4	G	175	LVS	CS-C2'-S-O2'
4	G	175	LVS	O2-C2-CA2-CB2
4	K	175	LVS	N3-C2-CA2-CB2
4	G	175	LVS	N3-C2-CA2-CB2
4	M	175	LVS	N2-CA2-CB2-CG2
3	D	453	ATP	PG-O3B-PB-O2B
3	D	453	ATP	PA-O3A-PB-O2B
3	E	454	ATP	PG-O3B-PB-O2B
3	U	458	ATP	PA-O3A-PB-O2B
4	H	175	LVS	O2-C2-CA2-CB2
4	P	175	LVS	N2-CA2-CB2-CG2
4	J	175	LVS	N3-CA3-CB3-CG3
4	H	175	LVS	CA2-CB2-CG2-CD3
4	G	175	LVS	CA2-CB2-CG2-CD4
4	N	175	LVS	N2-CA2-CB2-CG2
4	G	175	LVS	CA2-CB2-CG2-CD3
3	C	452	ATP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
3	D	453	ATP	PA-O3A-PB-O1B
4	H	175	LVS	N3-C2-CA2-CB2
3	W	460	ATP	C3'-C4'-C5'-O5'
4	H	175	LVS	CS-CA3-CB3-CG3
4	L	175	LVS	CS-CA3-CB3-CG3
4	N	175	LVS	N1-CA1-CB1-CG1
3	B	451	ATP	PB-O3B-PG-O1G
3	C	452	ATP	PB-O3B-PG-O1G
3	A	450	ATP	PB-O3B-PG-O3G
3	C	452	ATP	PB-O3B-PG-O3G
3	F	455	ATP	PB-O3B-PG-O3G
4	H	175	LVS	CB3-CA3-N3-C2
4	K	175	LVS	CB3-CA3-N3-C2
3	B	451	ATP	PG-O3B-PB-O2B
3	B	451	ATP	PB-O3A-PA-O1A
3	E	454	ATP	PG-O3B-PB-O1B
3	E	454	ATP	PA-O3A-PB-O1B
3	E	454	ATP	PA-O3A-PB-O2B
3	U	458	ATP	PG-O3B-PB-O1B
3	W	460	ATP	PA-O3A-PB-O1B
3	W	460	ATP	PA-O3A-PB-O2B
3	F	455	ATP	O4'-C4'-C5'-O5'
4	R	175	LVS	N2-CA2-CB2-CG2
3	D	453	ATP	PB-O3B-PG-O1G
3	F	455	ATP	PB-O3B-PG-O1G
4	Q	175	LVS	CA2-CB2-CG2-CD3
4	Q	175	LVS	N2-CA2-CB2-CG2
3	S	456	ATP	PG-O3B-PB-O2B
3	U	458	ATP	PG-O3B-PB-O2B

There are no ring outliers.

24 monomers are involved in 232 short contacts:

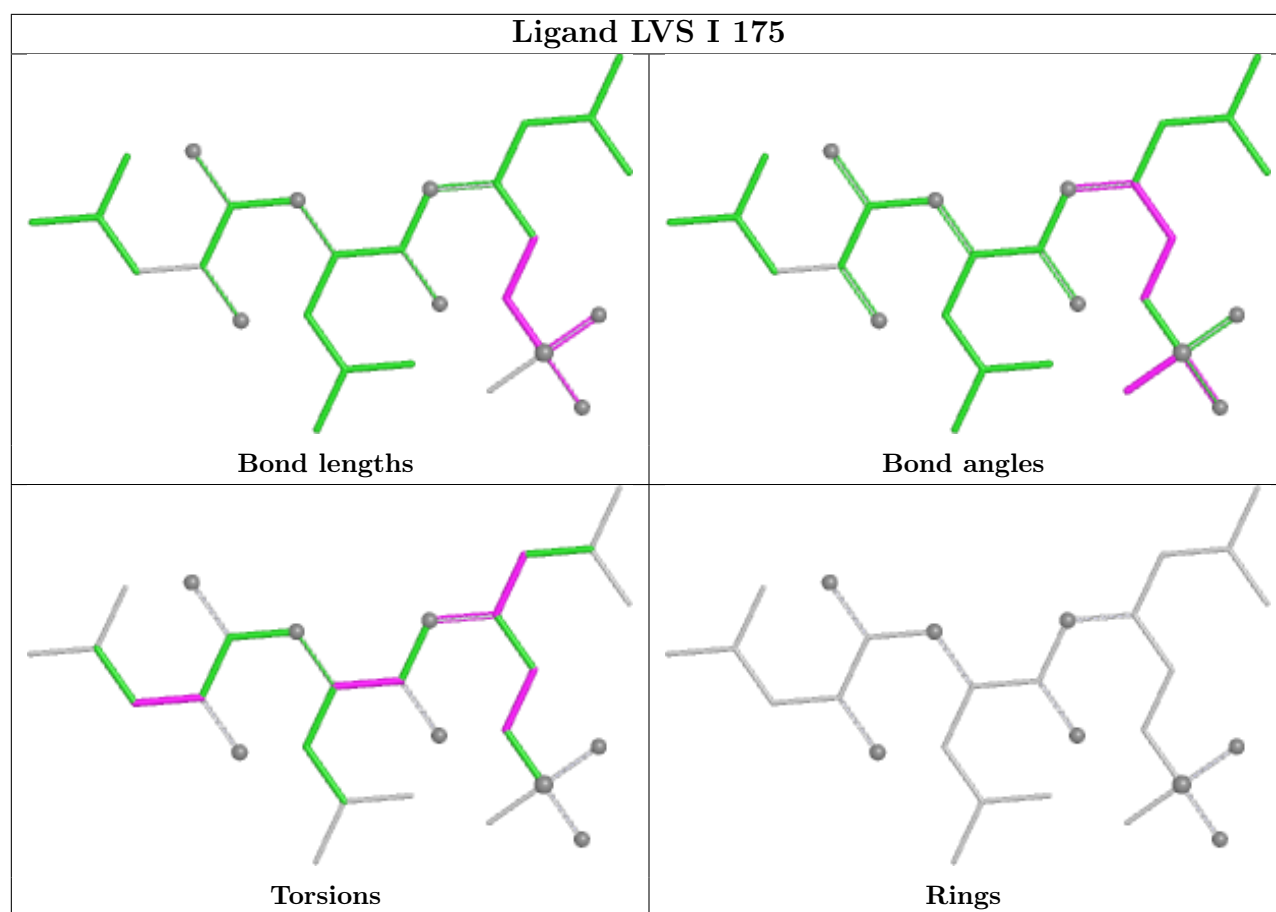
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	175	LVS	16	0
4	M	175	LVS	12	0
3	W	460	ATP	4	0
4	H	175	LVS	14	0
3	B	451	ATP	5	0
4	L	175	LVS	14	0
3	T	457	ATP	4	0
4	R	175	LVS	13	0

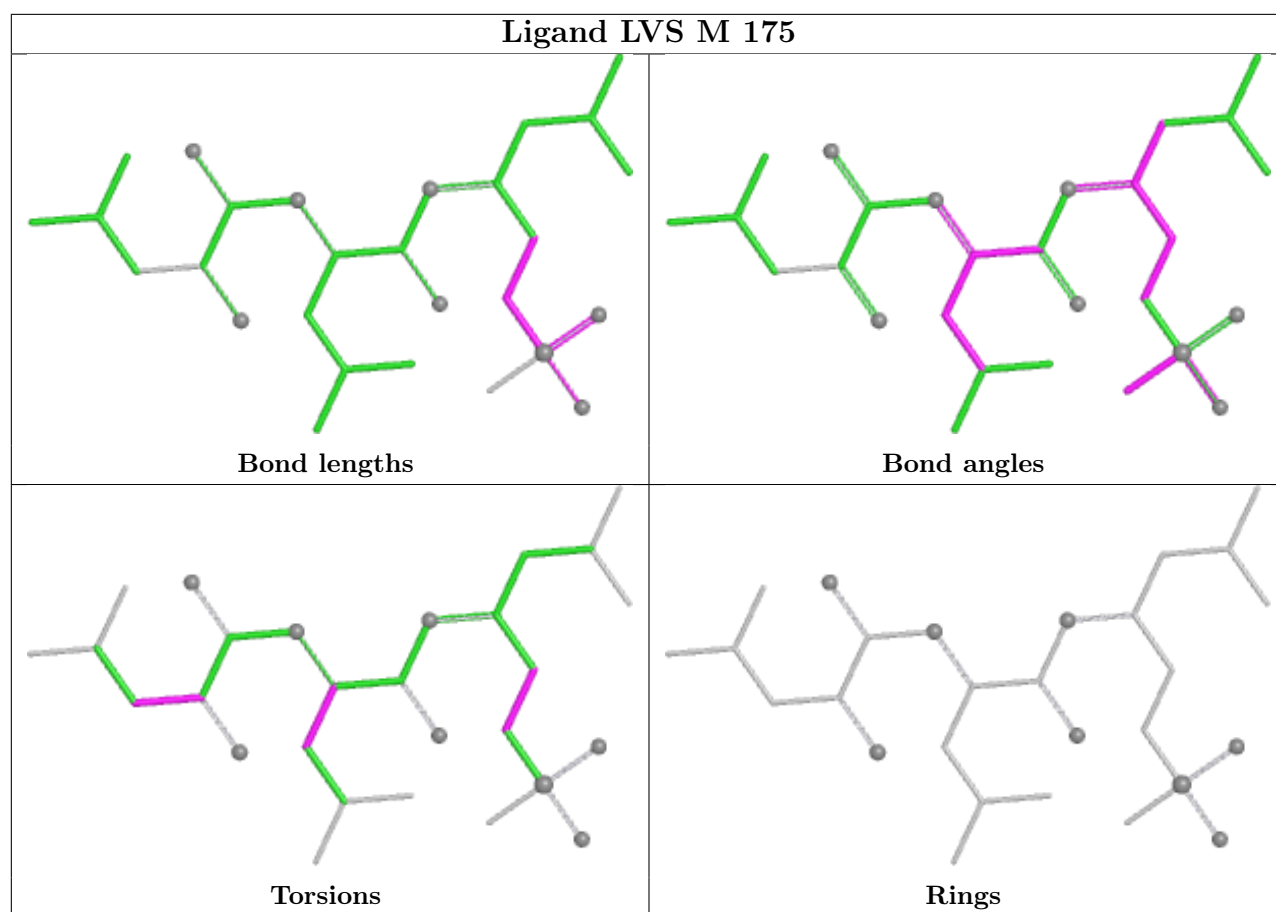
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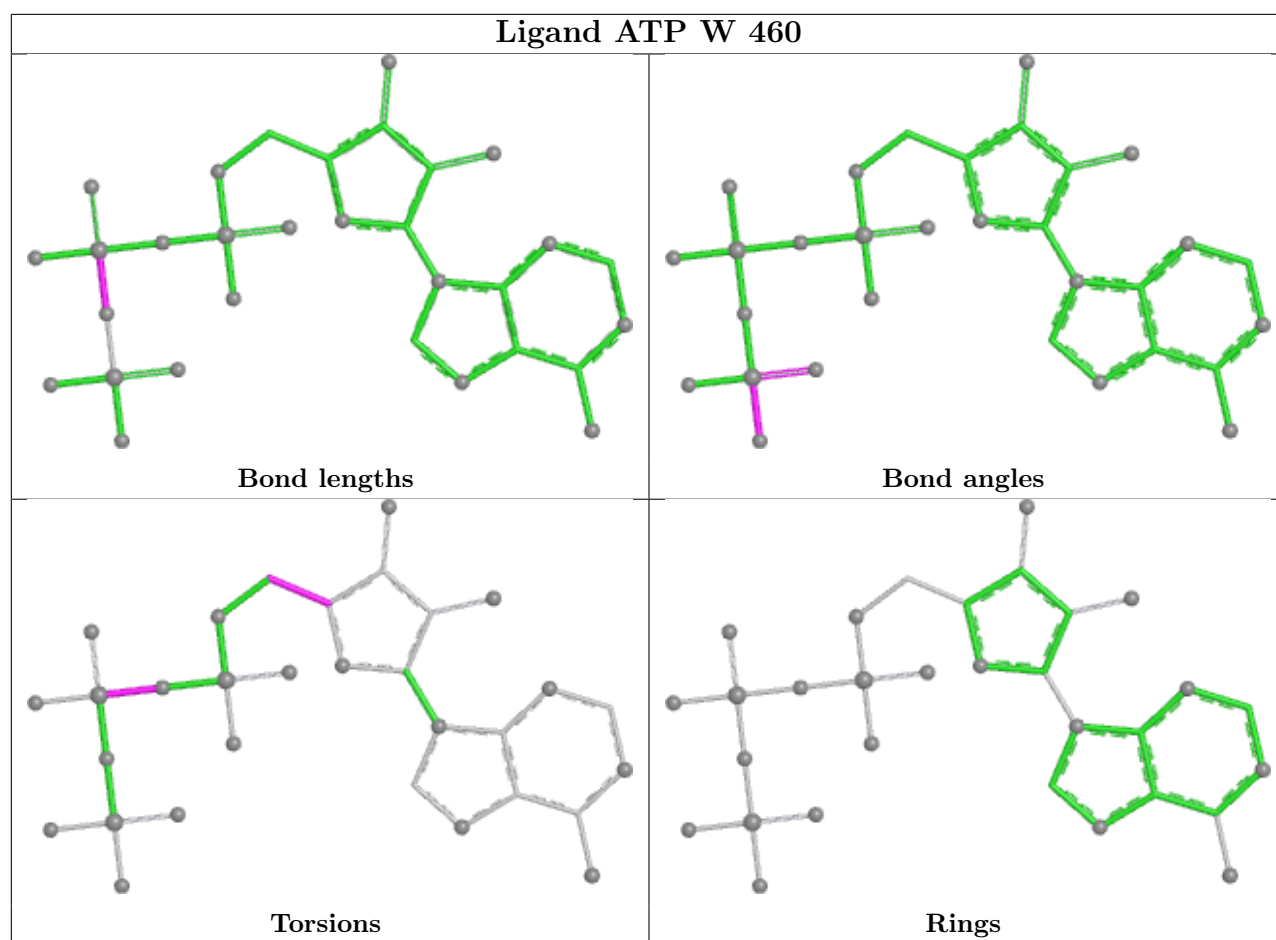
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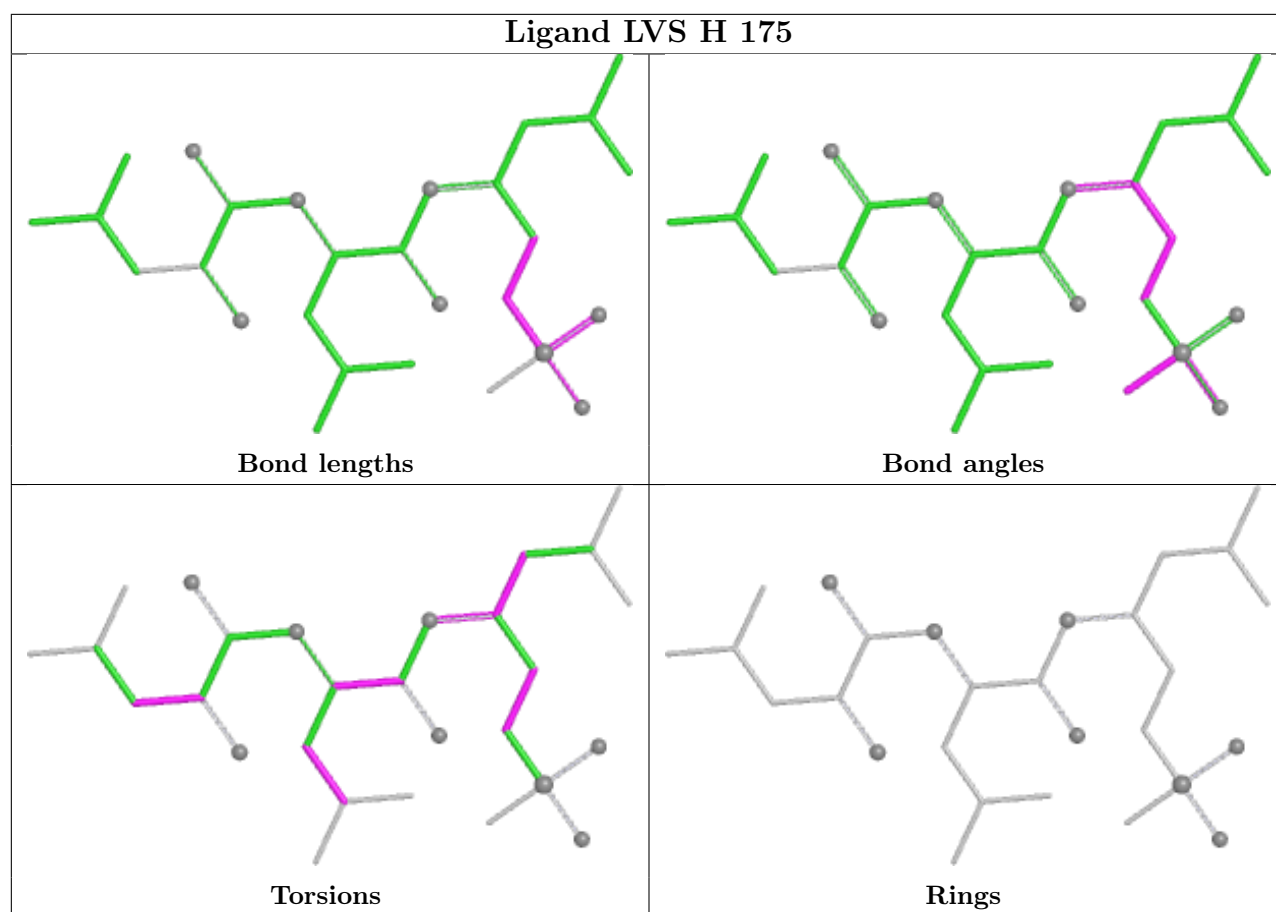
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	458	ATP	5	0
4	Q	175	LVS	14	0
4	P	175	LVS	13	0
4	O	175	LVS	13	0
3	V	459	ATP	2	0
3	D	453	ATP	5	0
3	A	450	ATP	3	0
3	C	452	ATP	8	0
3	E	454	ATP	6	0
4	N	175	LVS	19	0
3	S	456	ATP	4	0
4	J	175	LVS	23	0
4	K	175	LVS	16	0
3	F	455	ATP	4	0
4	G	175	LVS	12	0
3	X	461	ATP	3	0

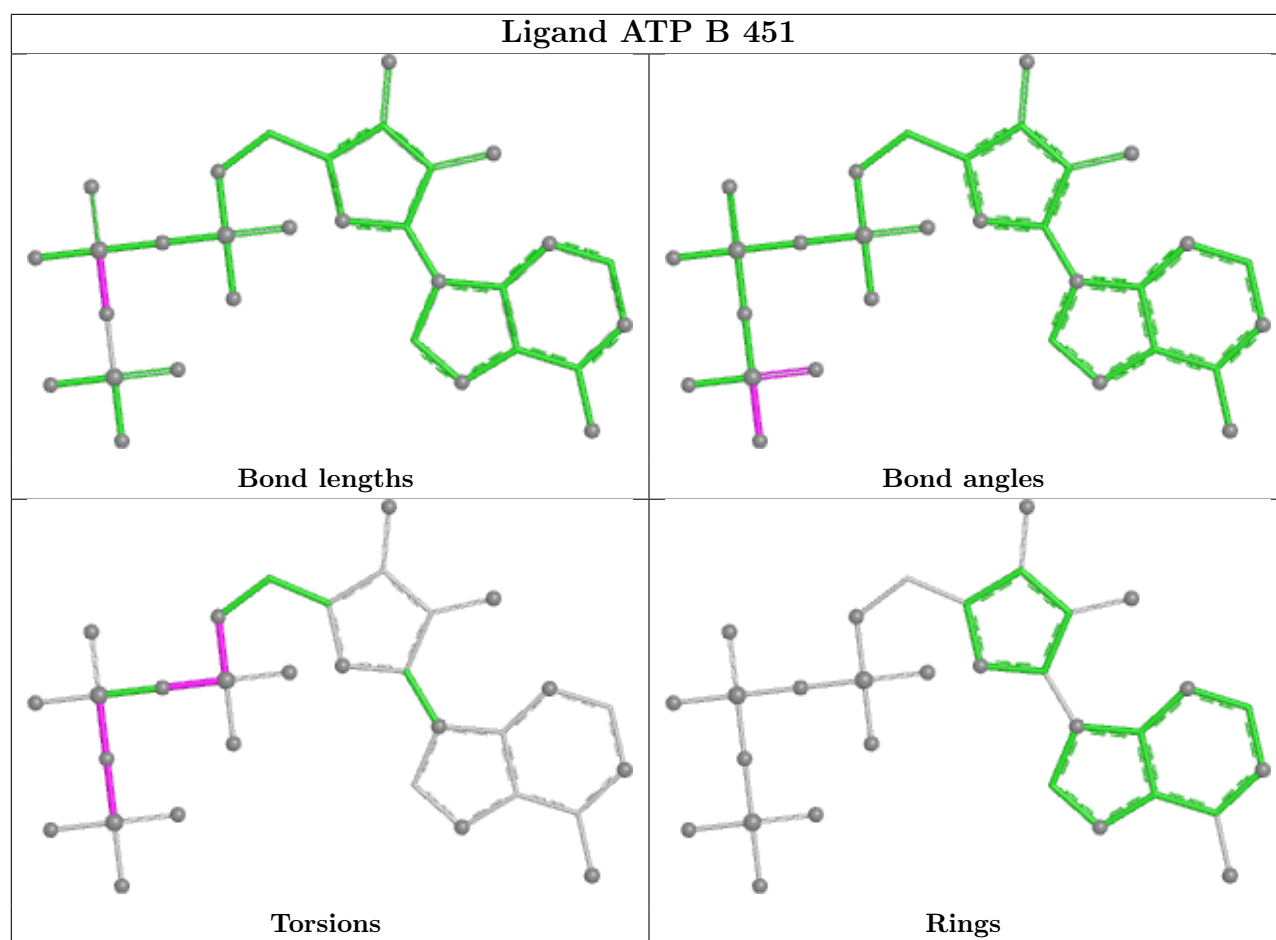
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

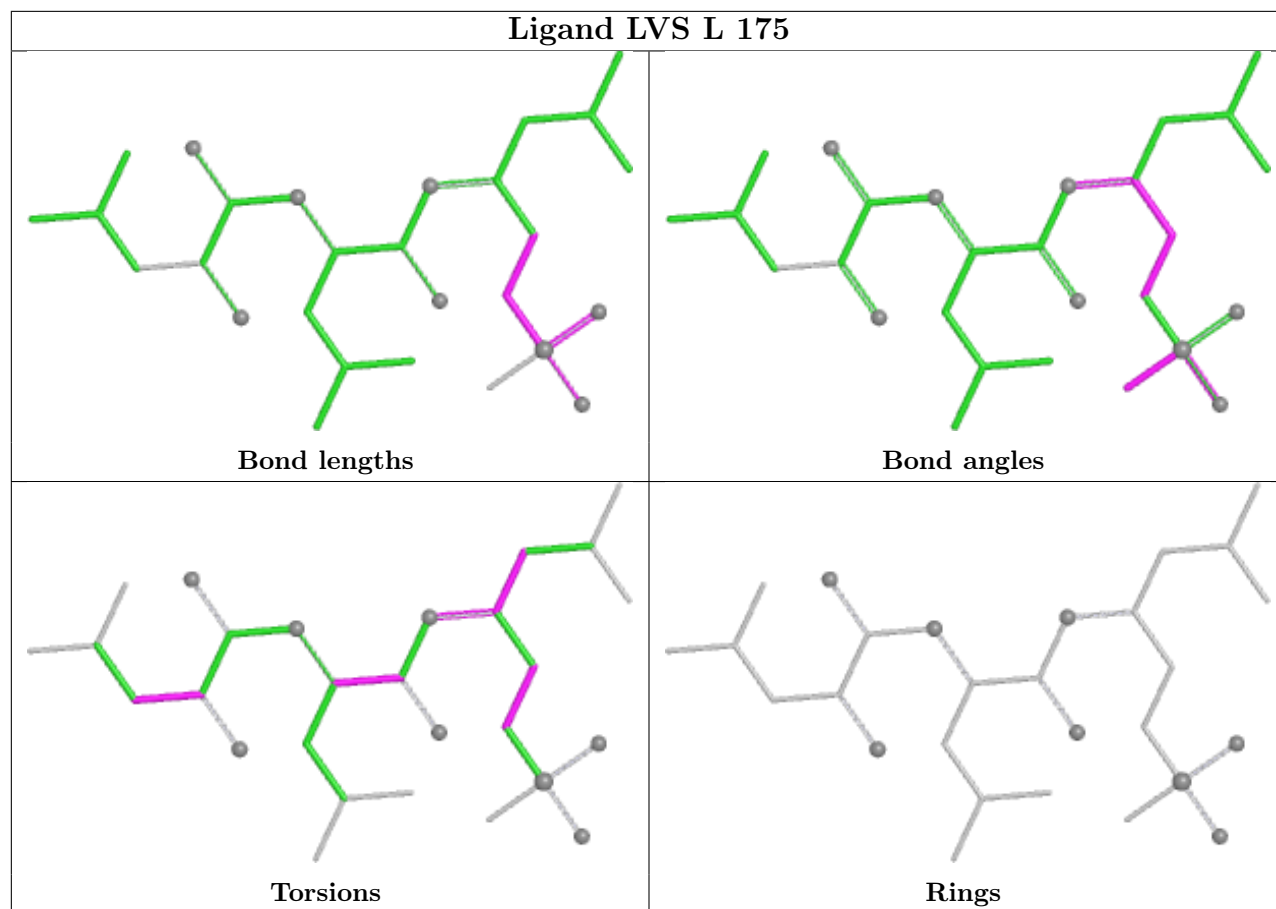




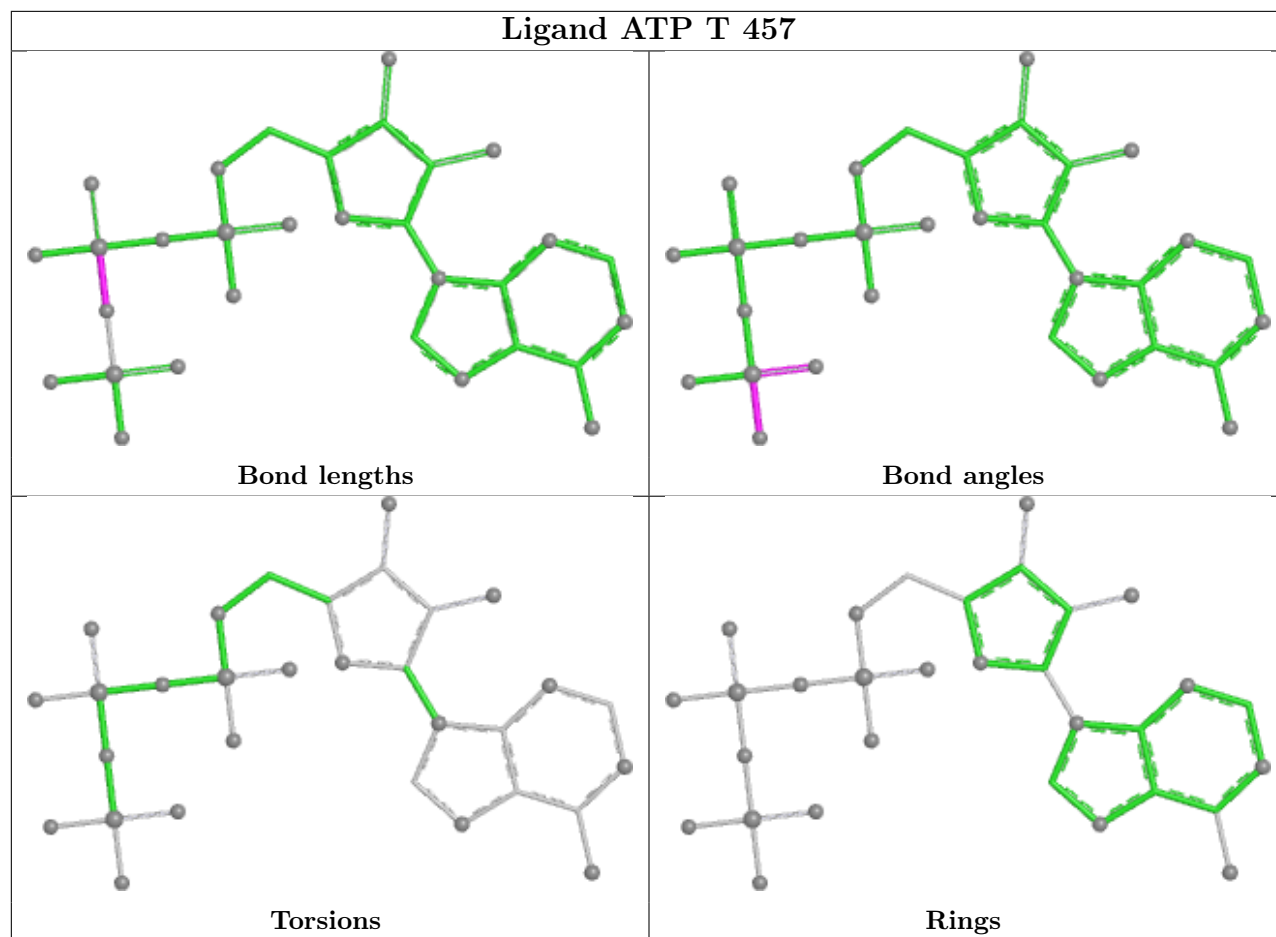




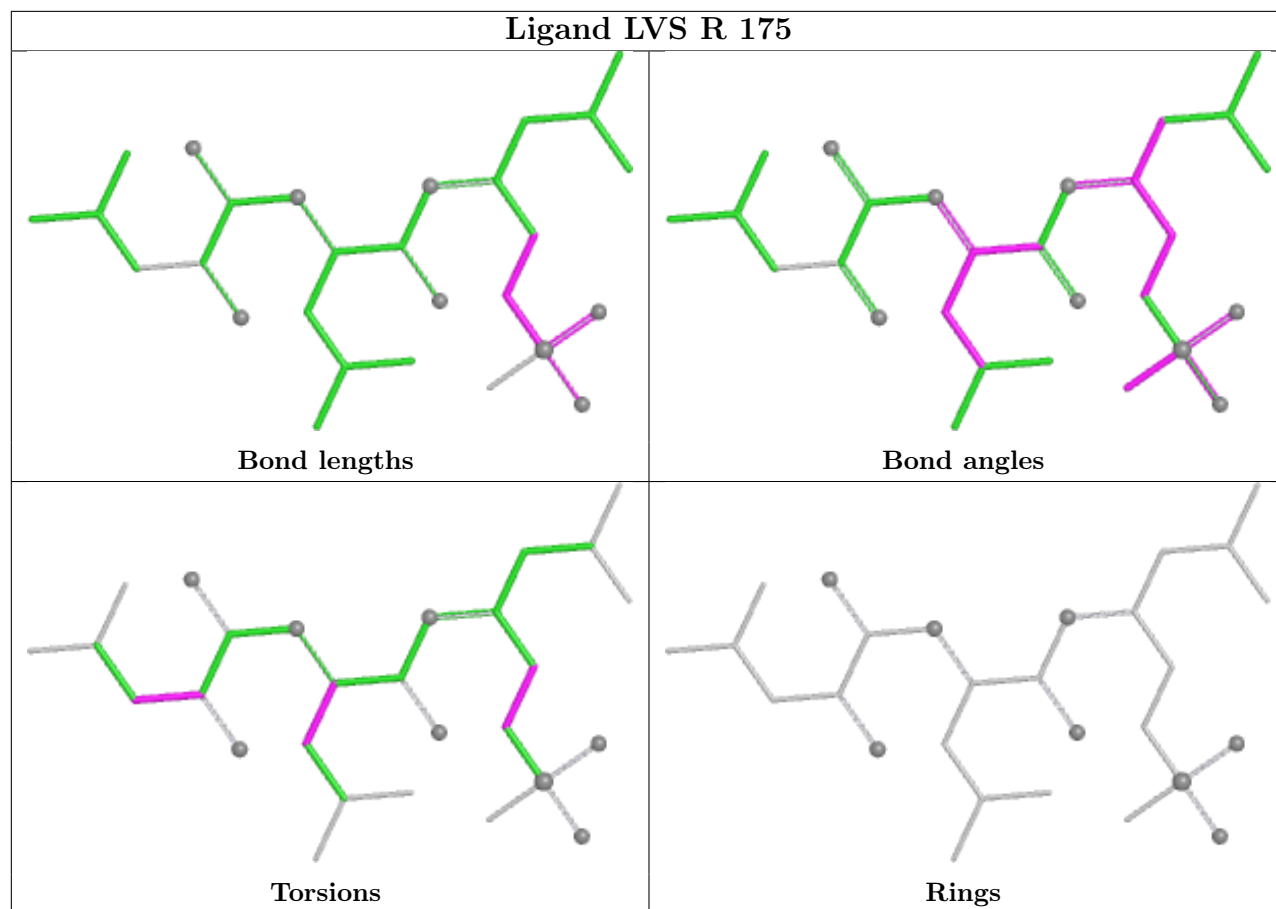


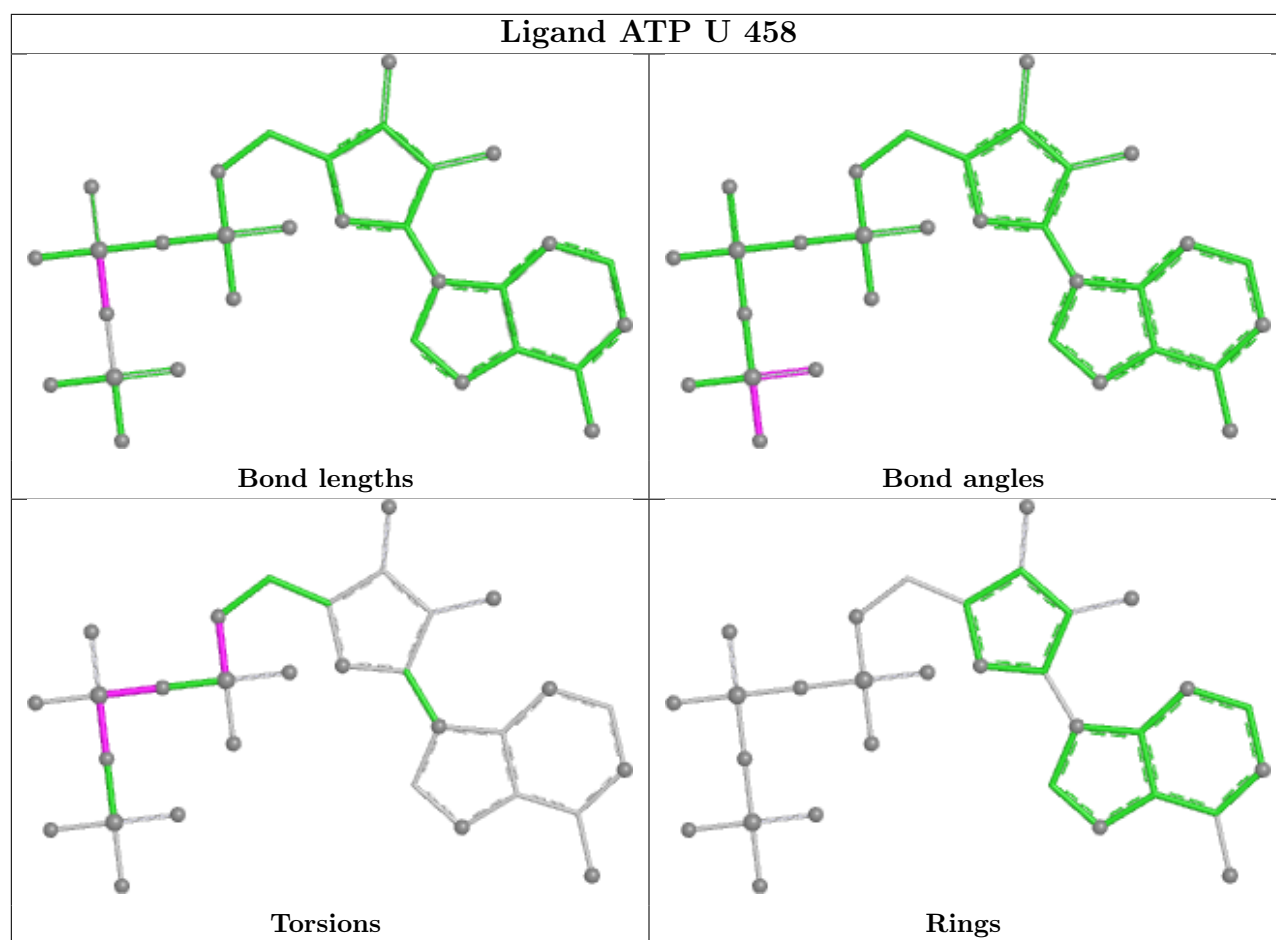


Ligand ATP T 457

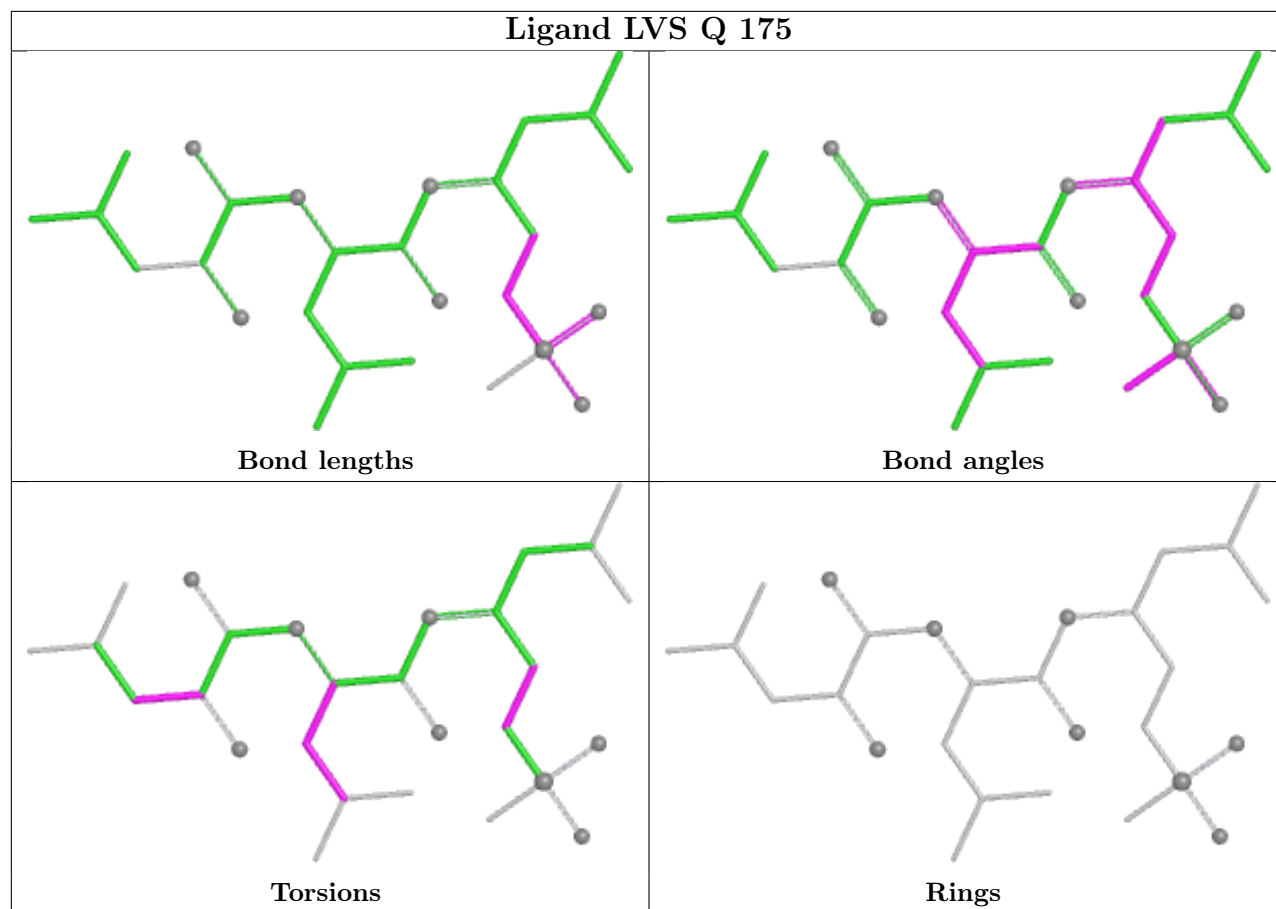


Ligand LVS R 175

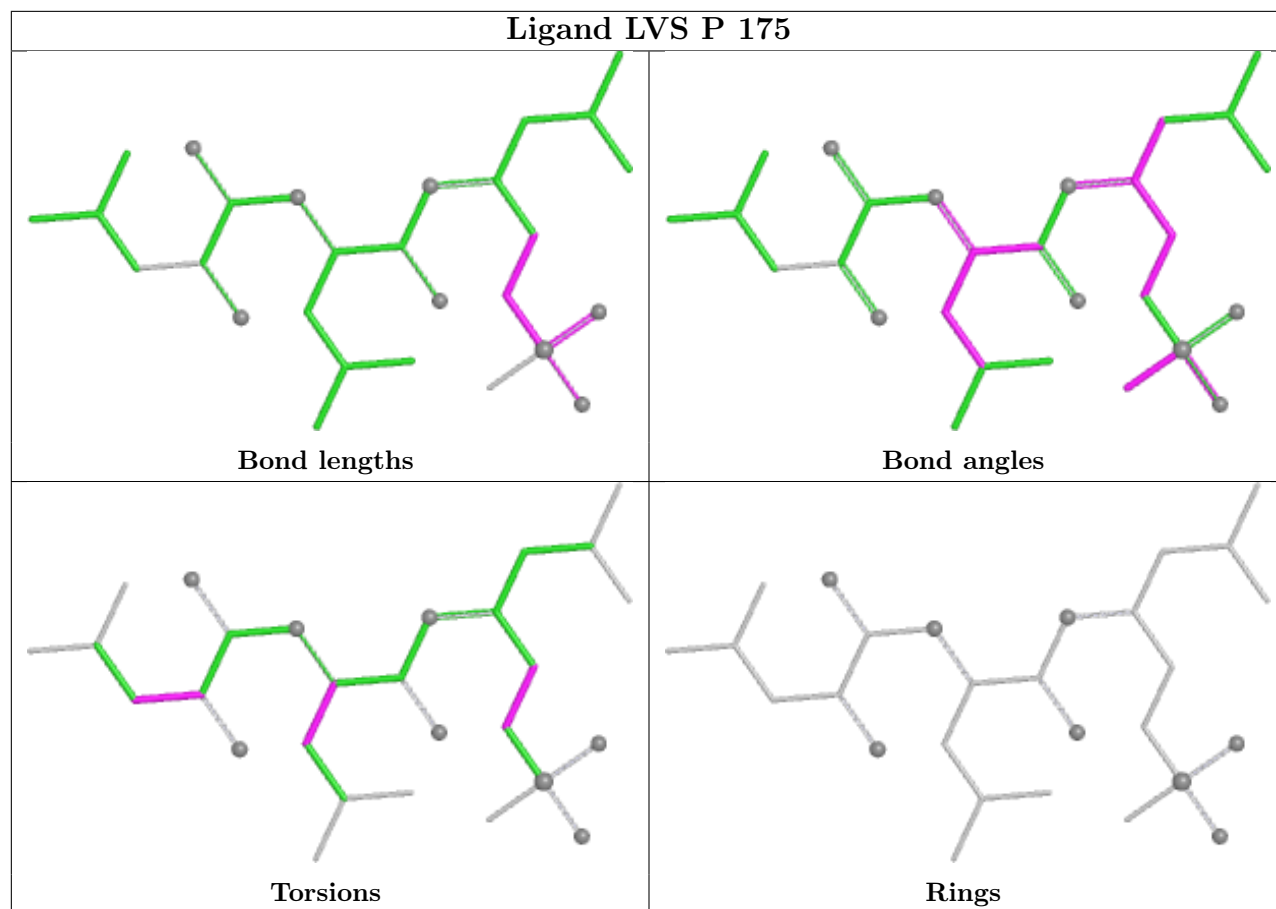


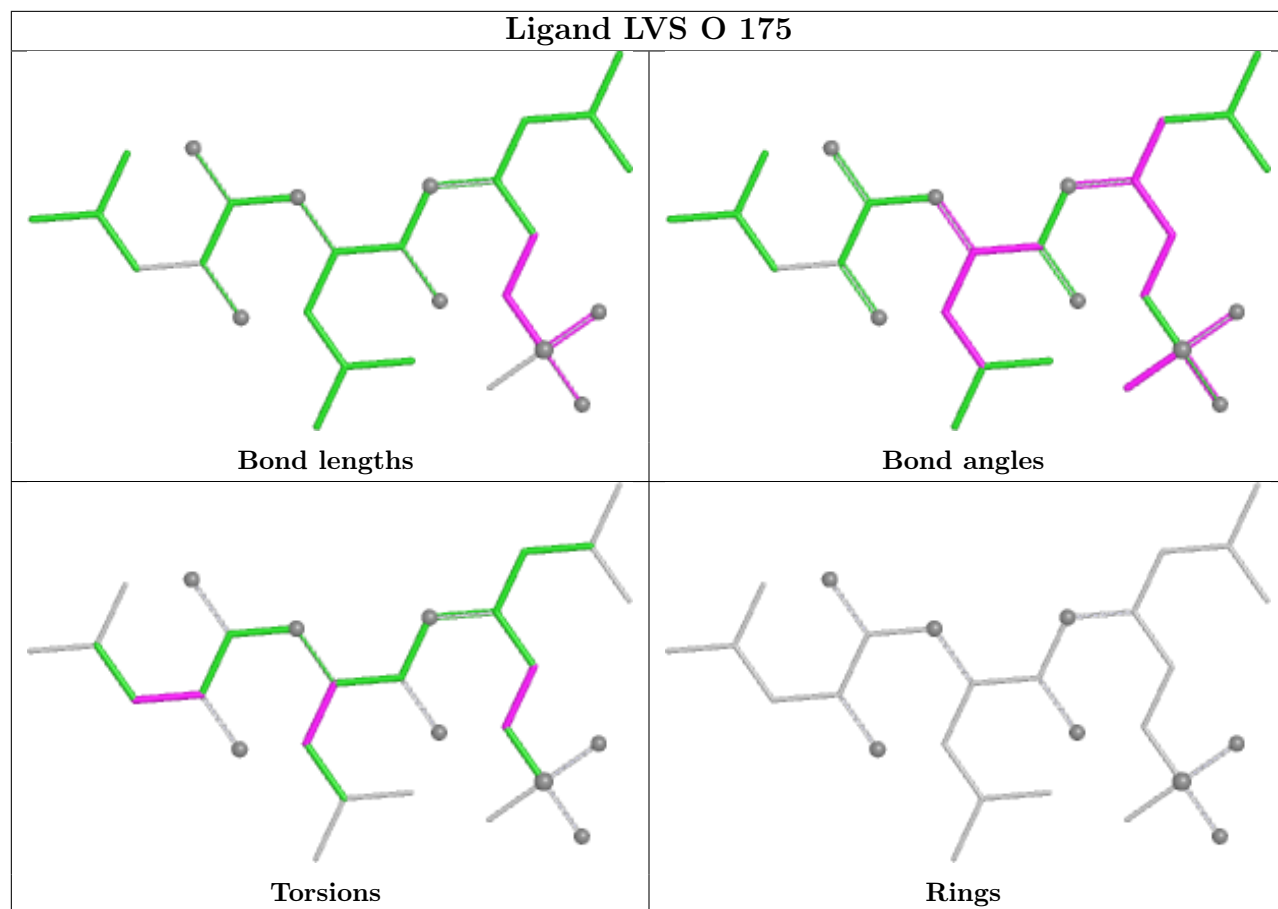


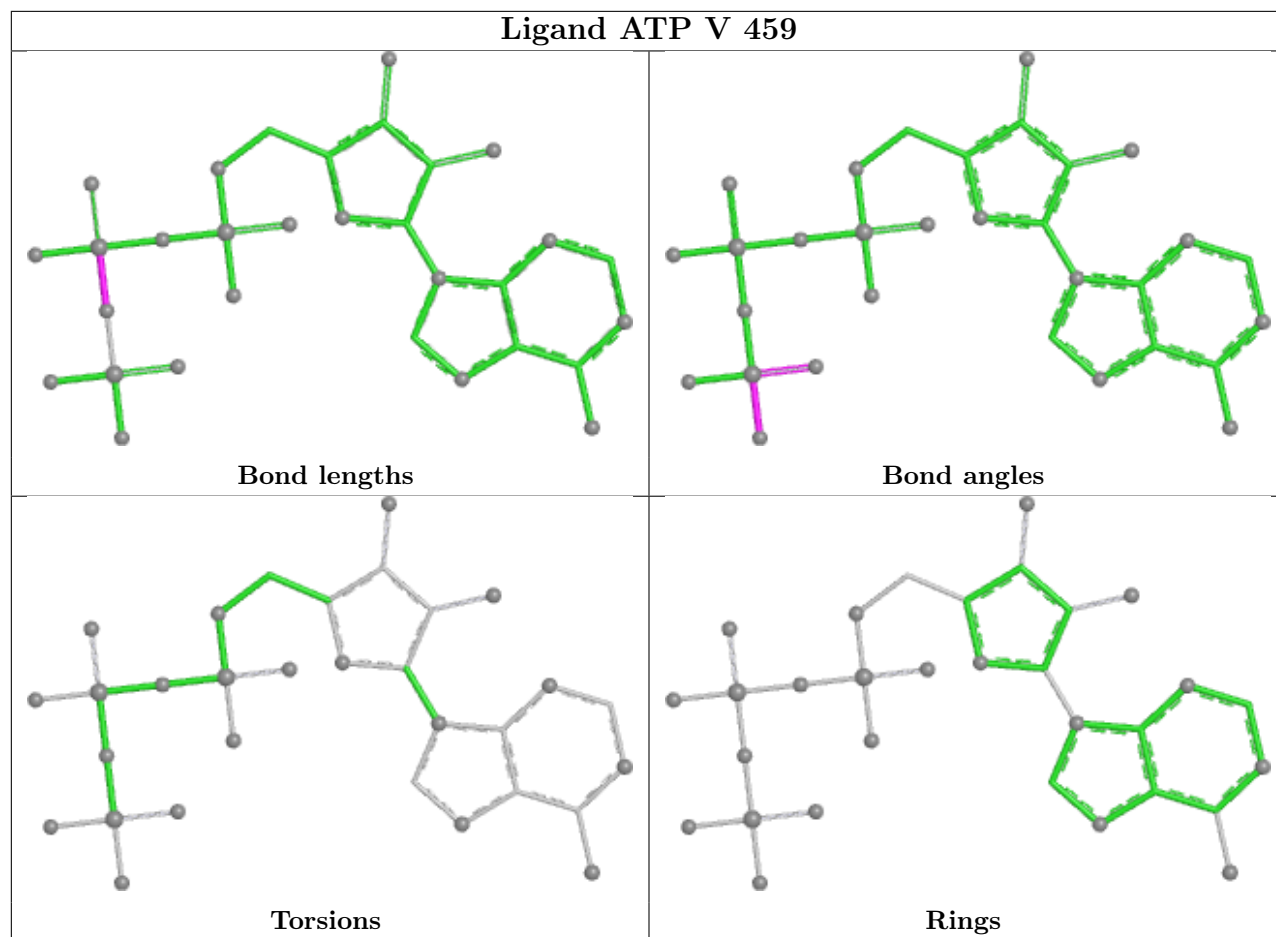
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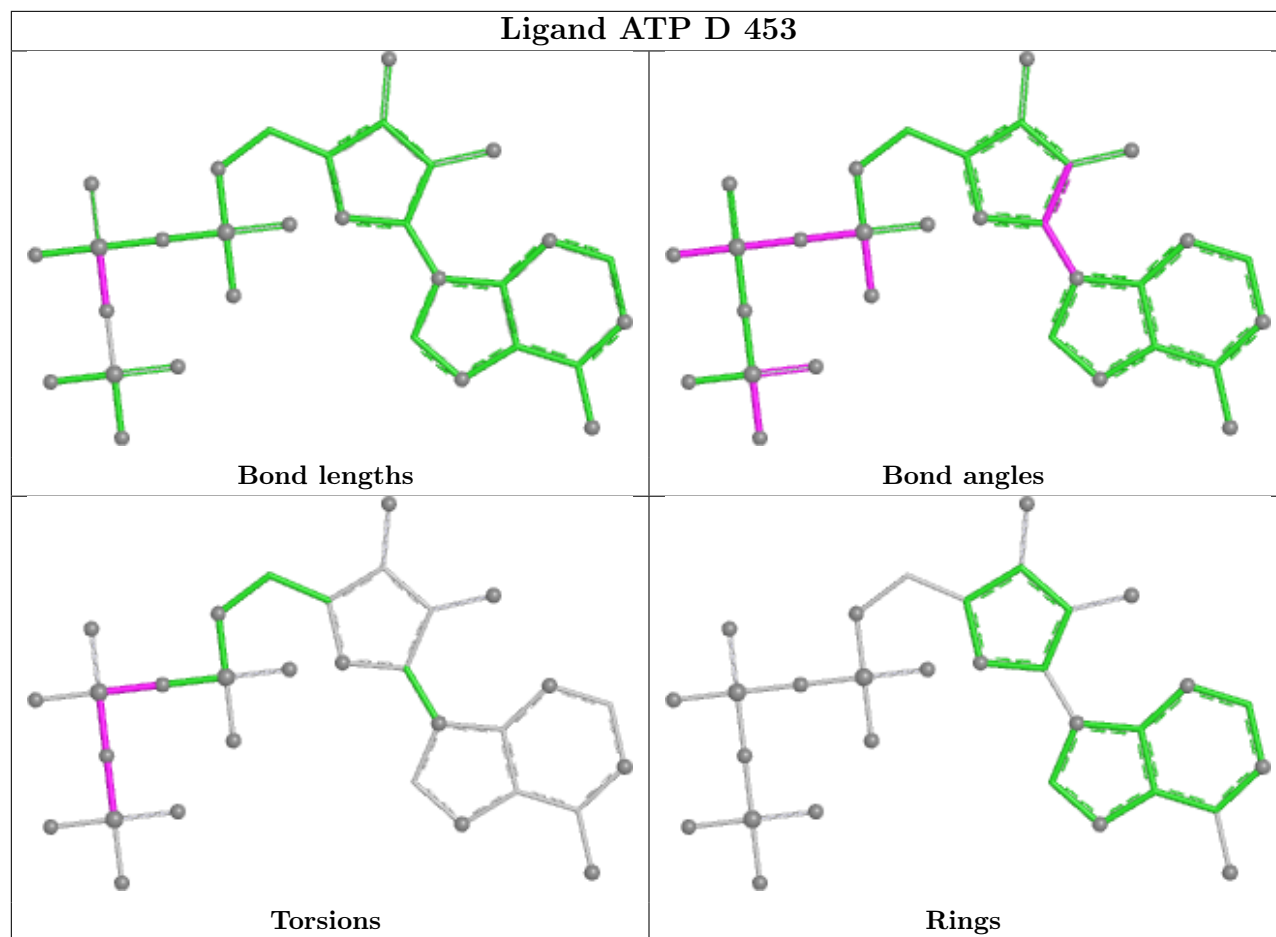


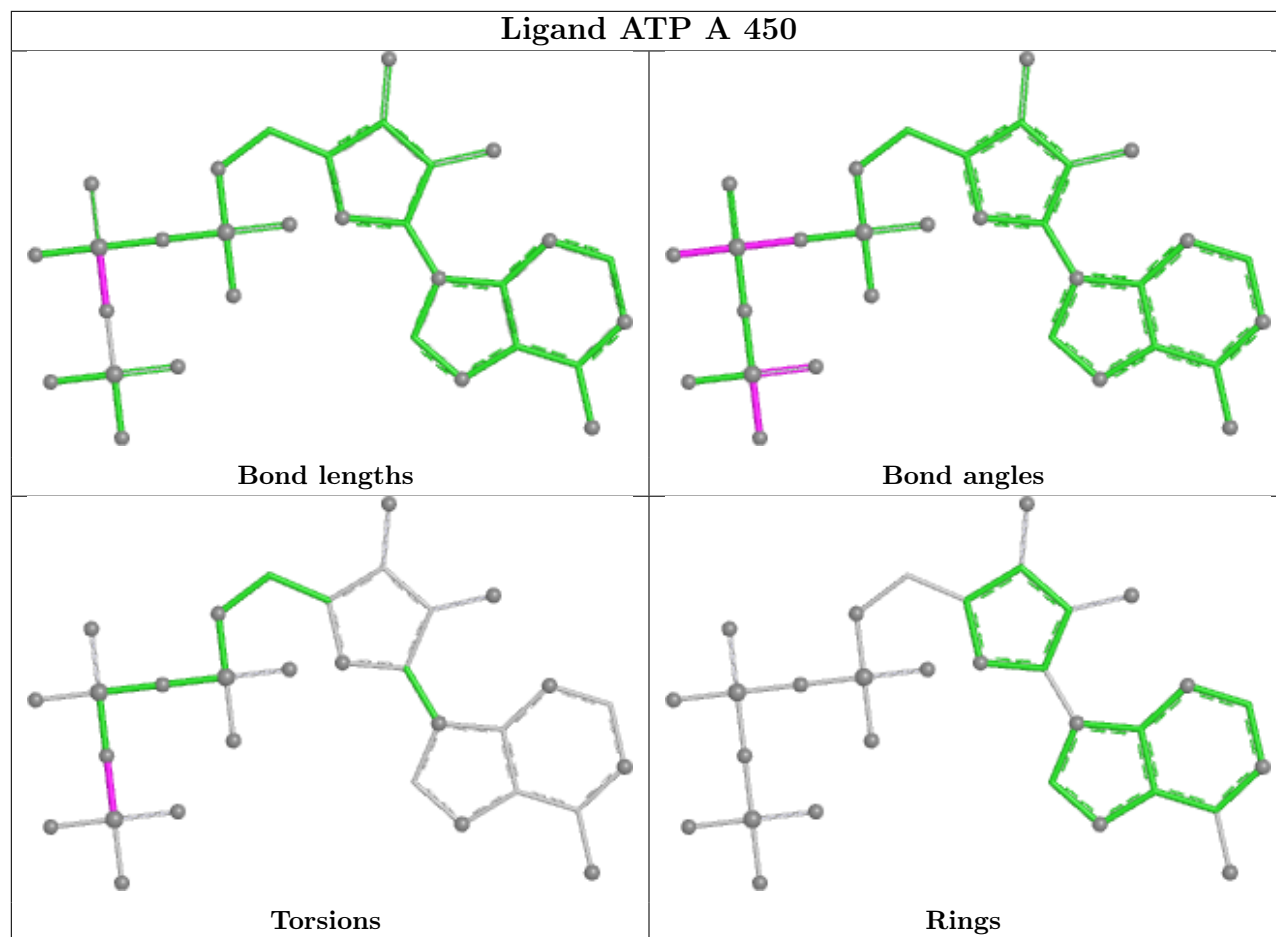
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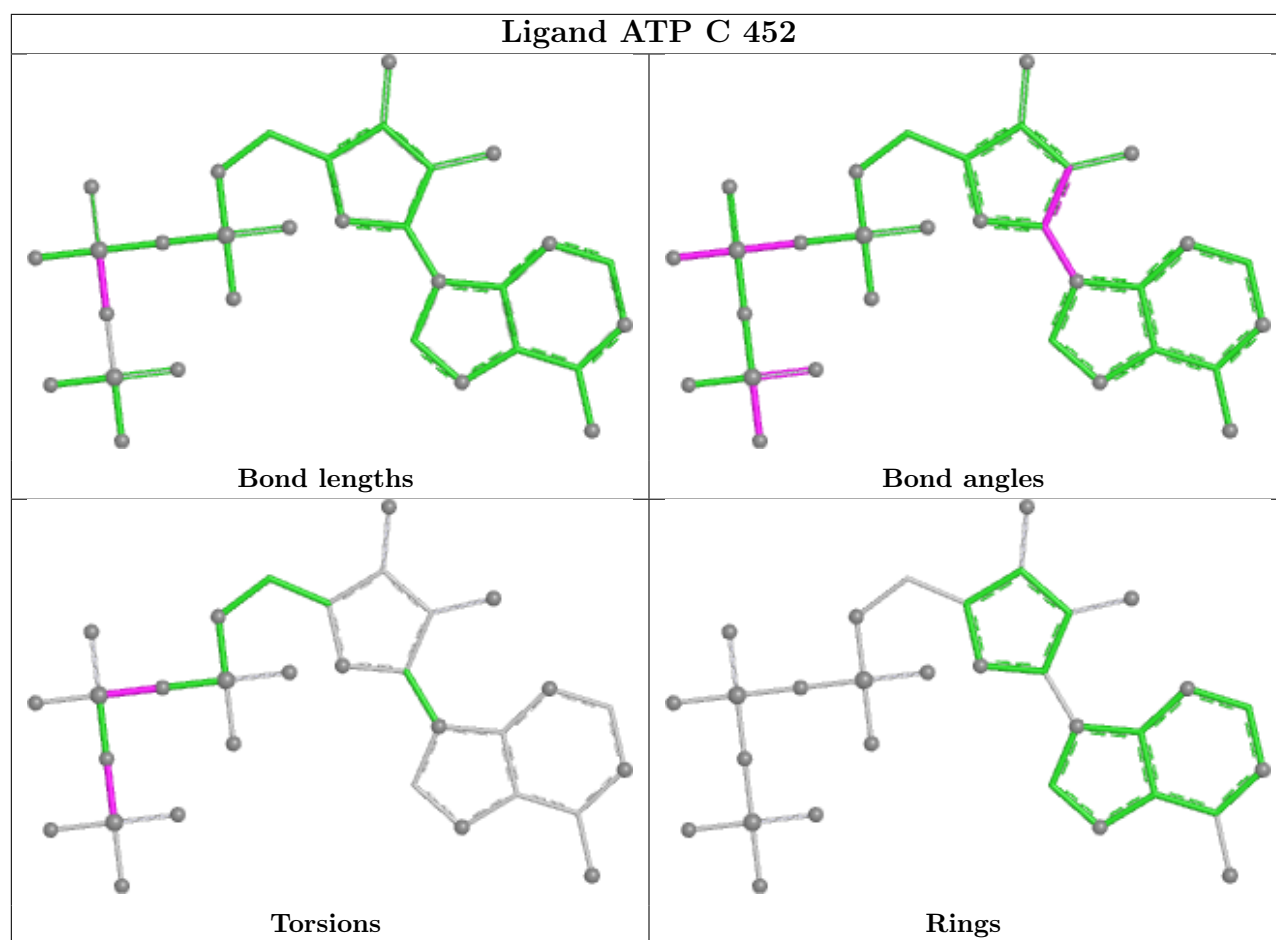


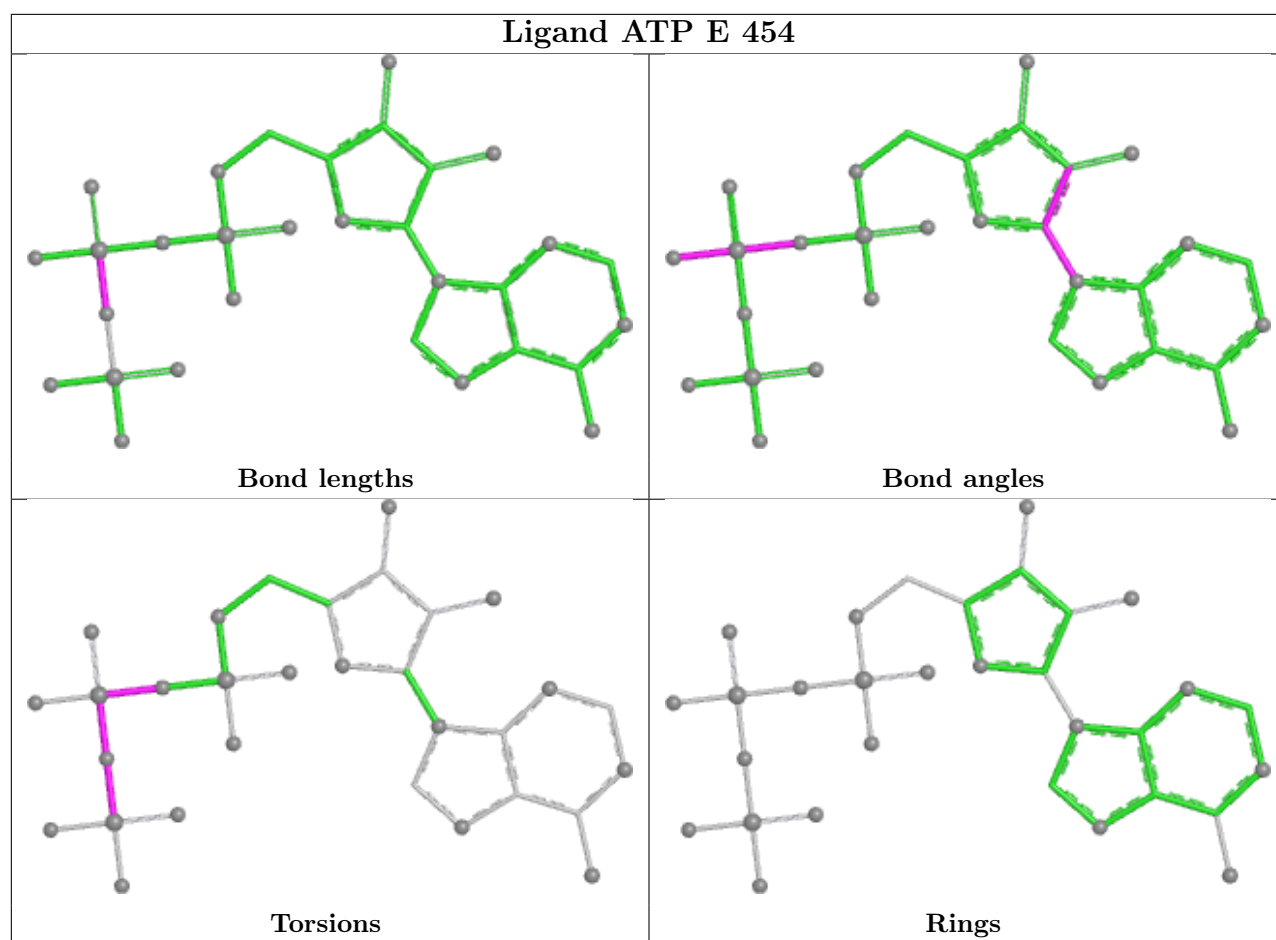




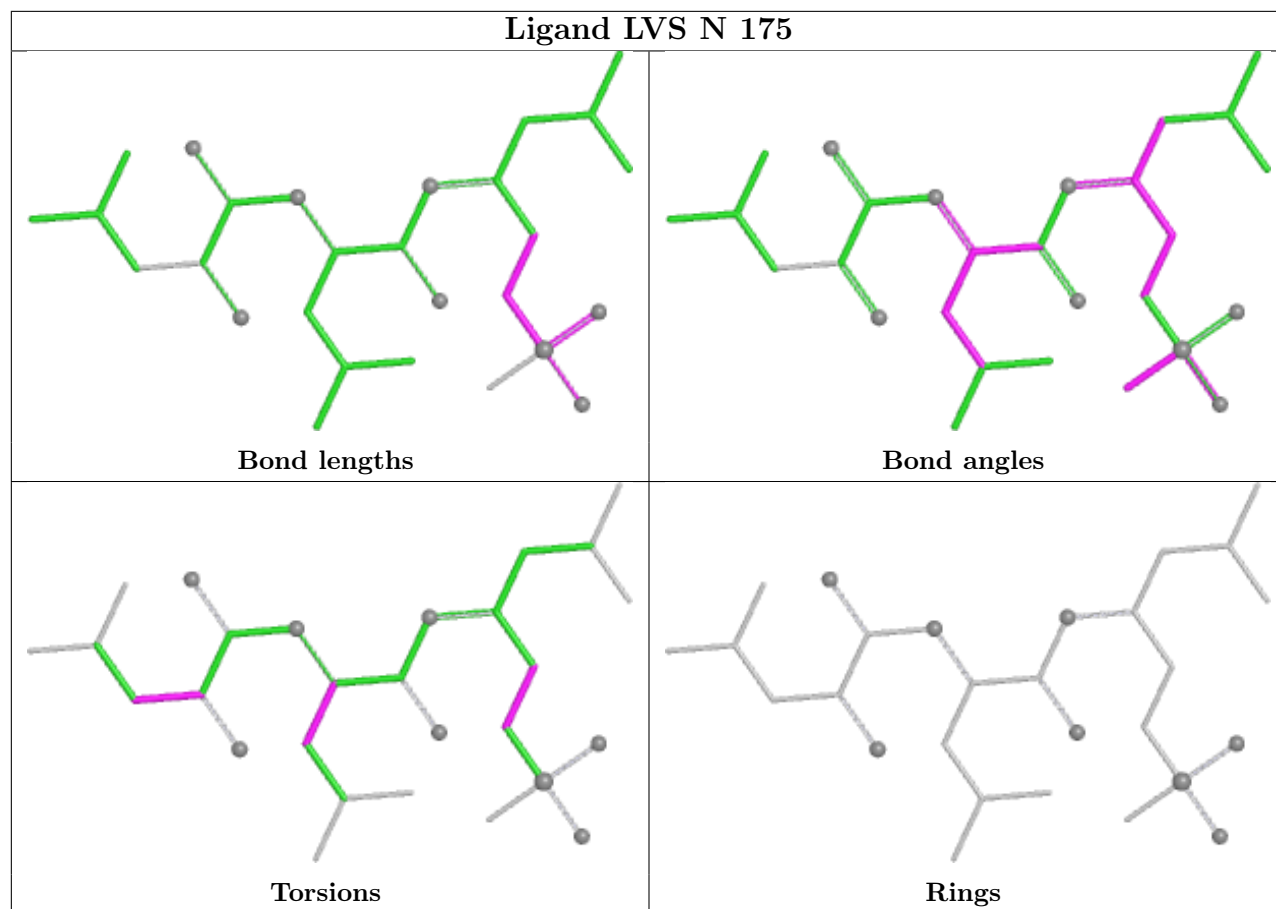




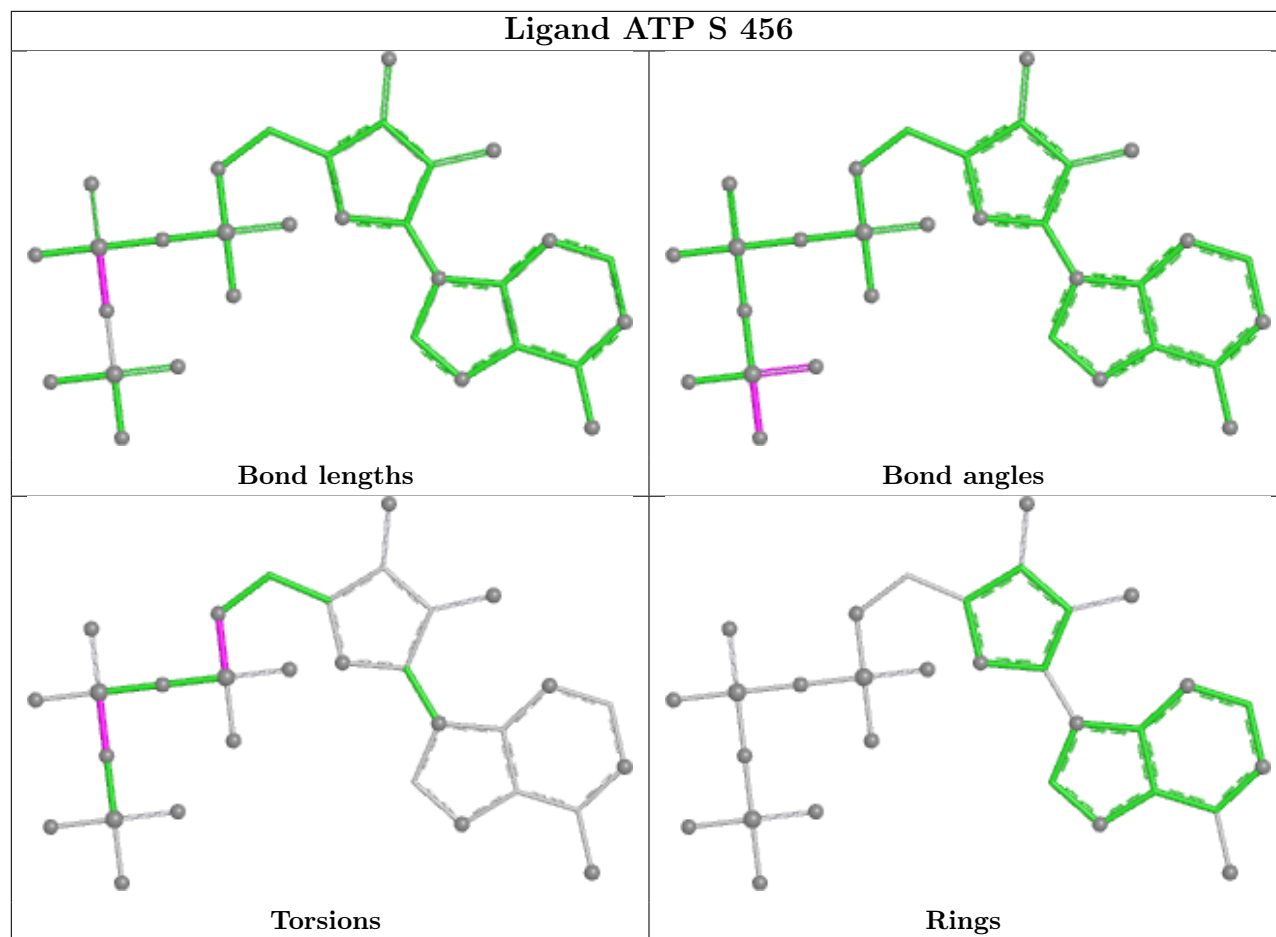




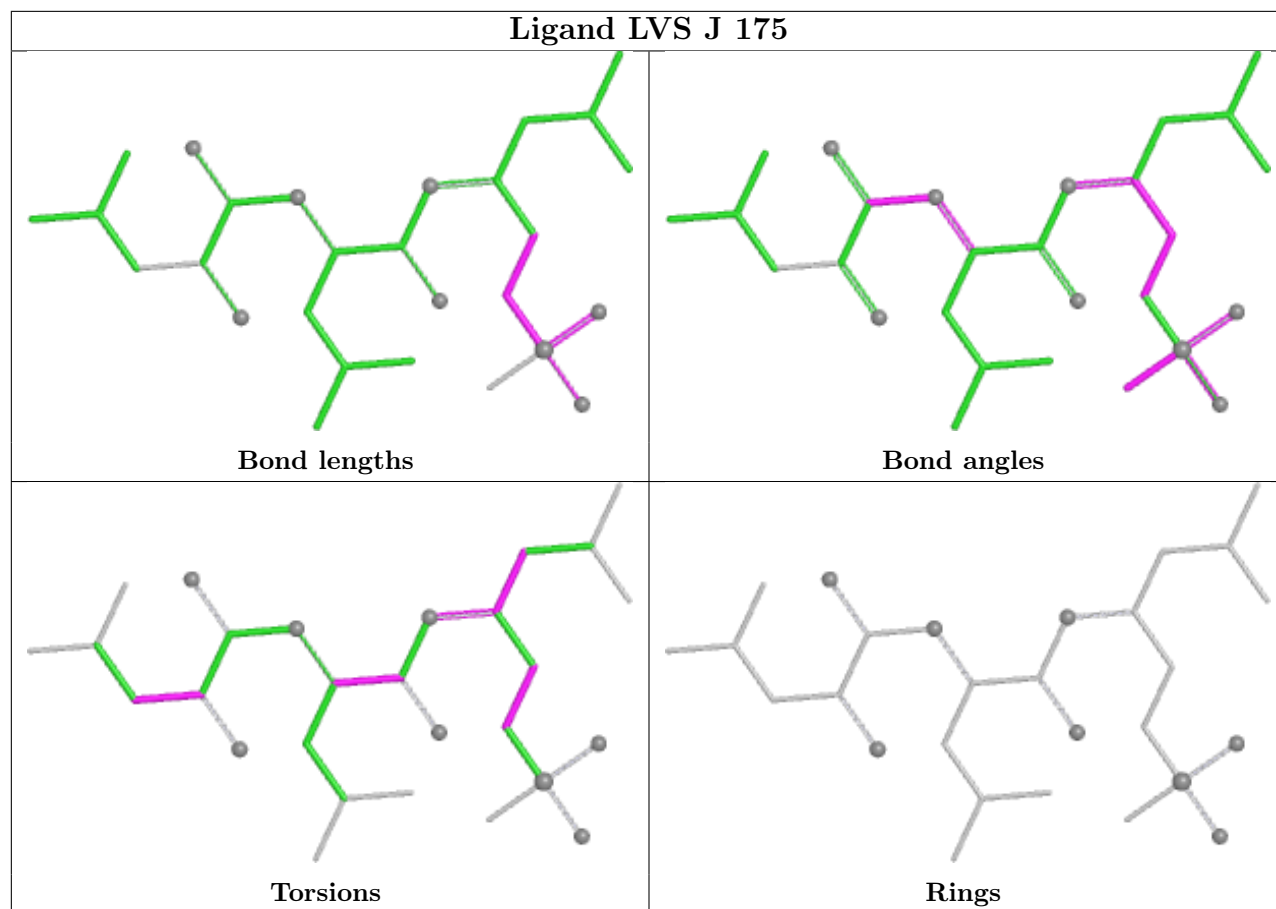
Ligand LVS N 175

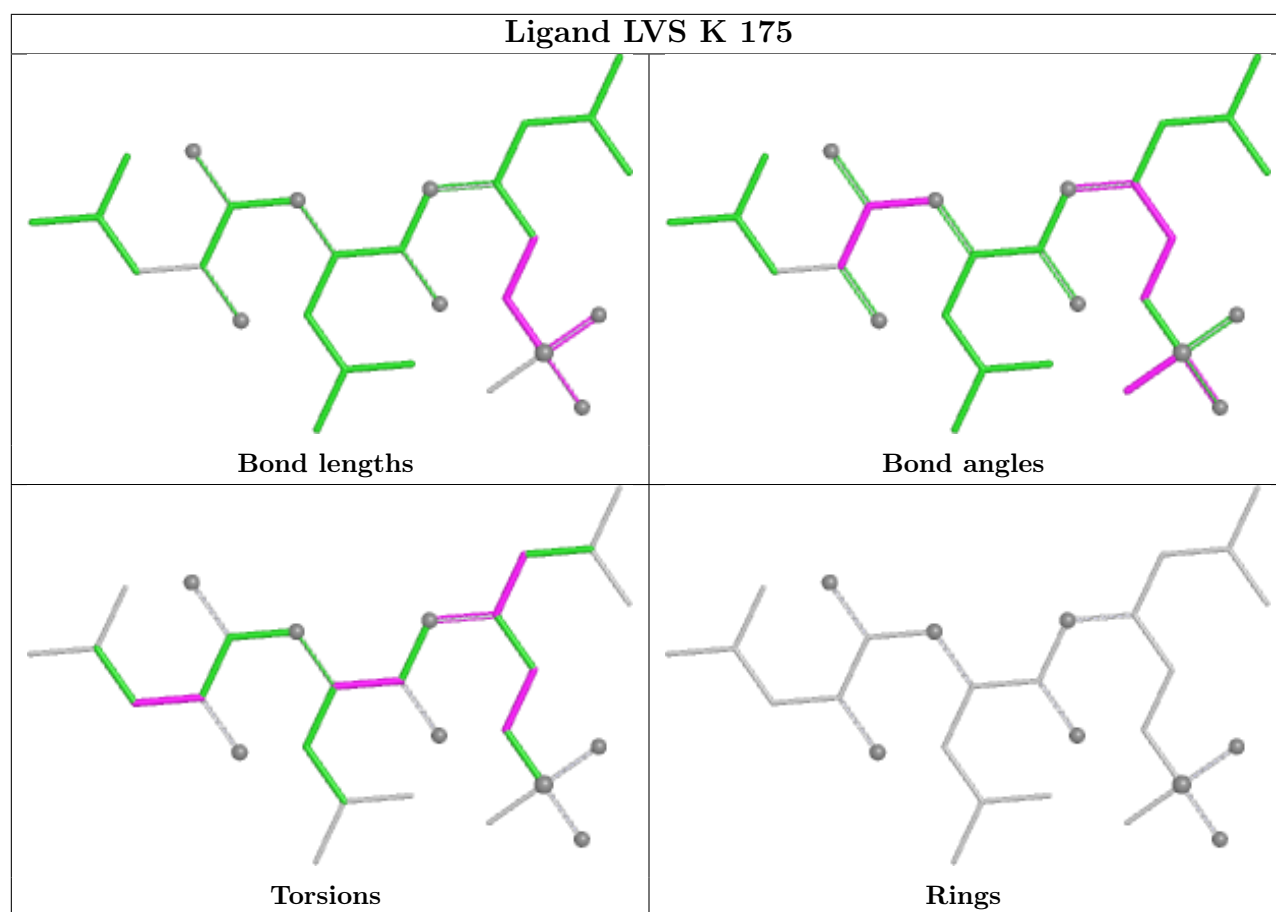


Ligand ATP S 456

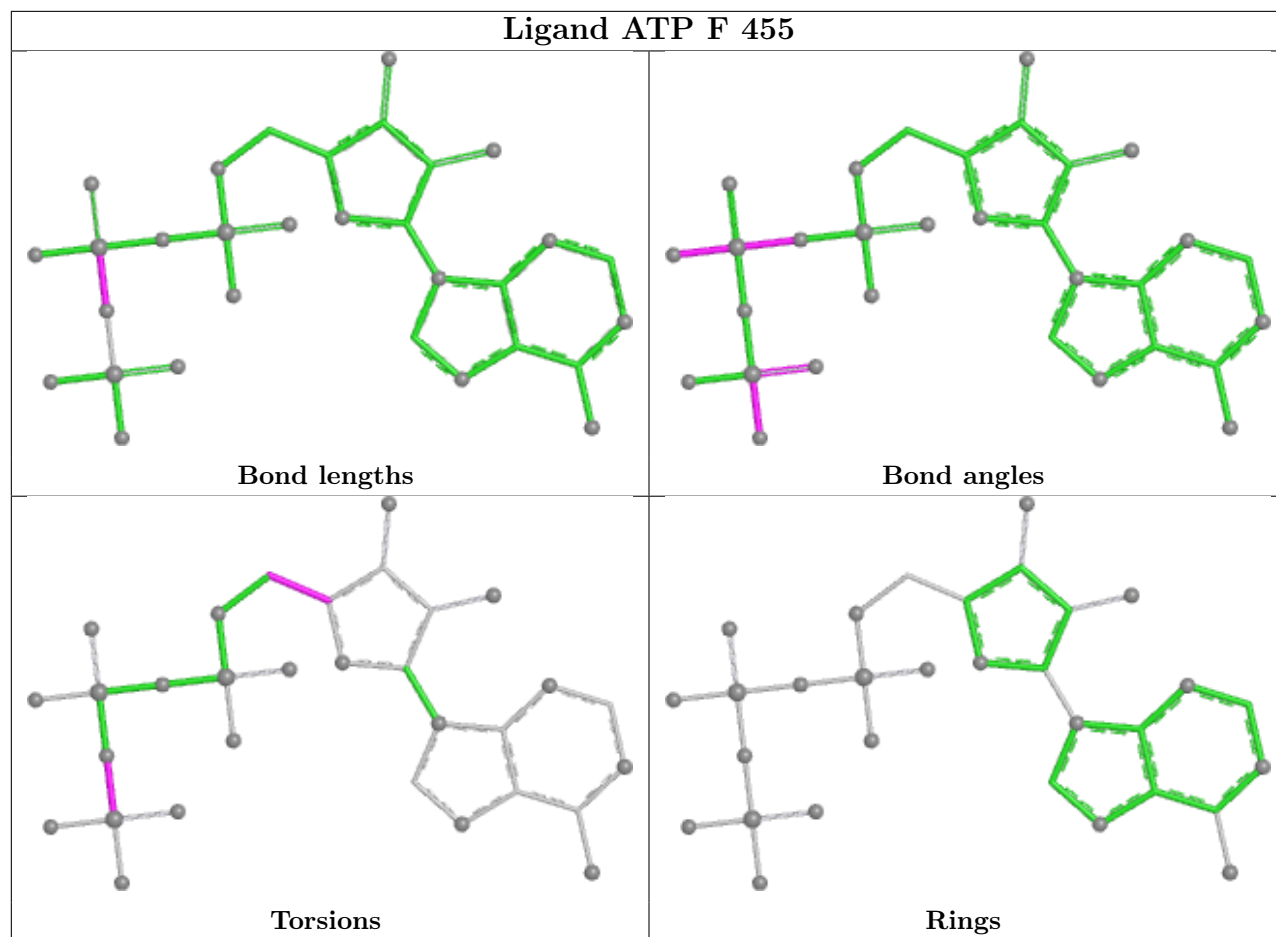


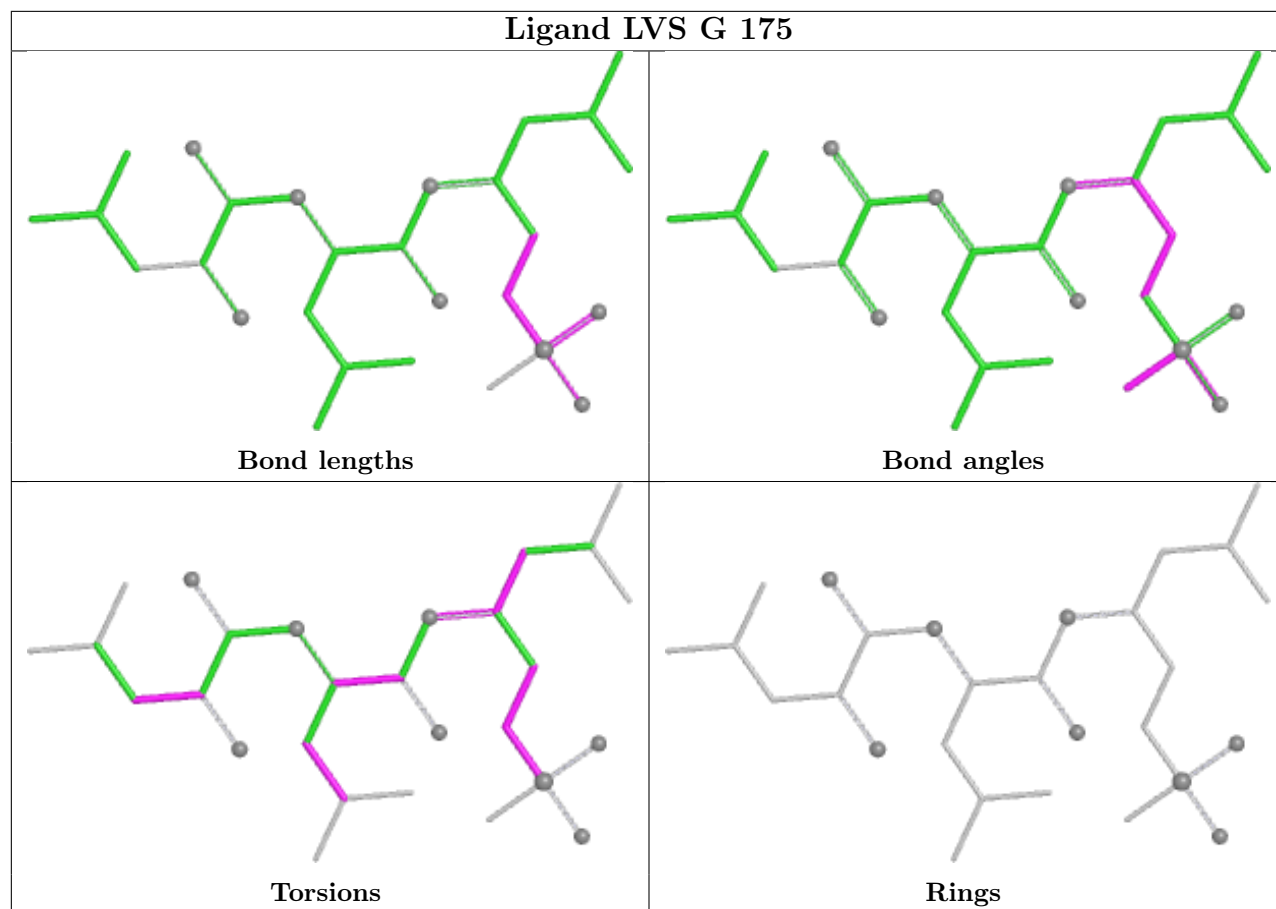
Ligand LVS J 175

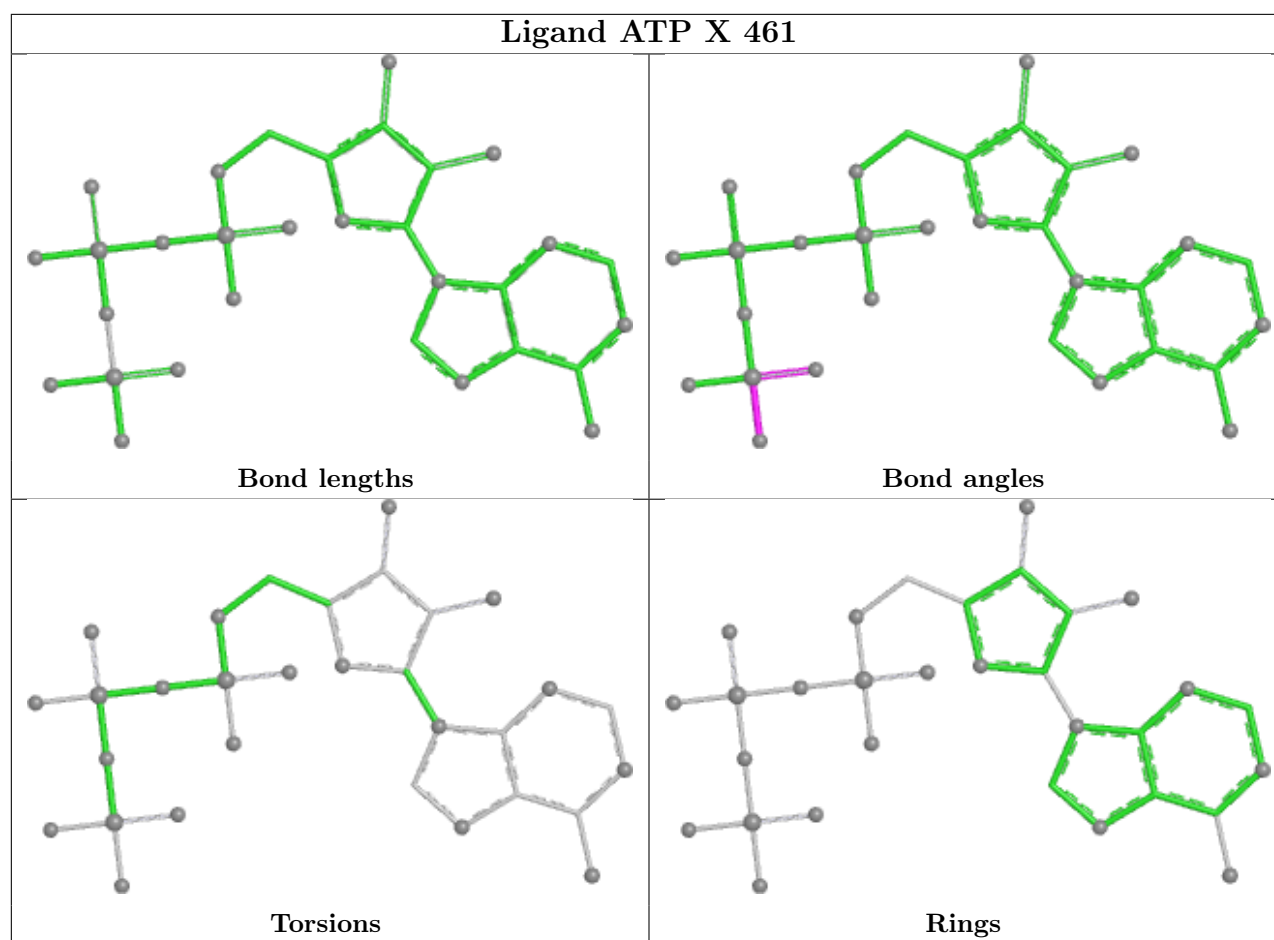




Ligand ATP F 455







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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.