



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:14 PM UTC

PDB ID : 1OFI / pdb_00001ofi
Title : Asymmetric complex between HslV and I-domain deleted HslU (H. influenzae)
Authors : Kwon, A.R.; Kessler, B.M.; Overkleeft, H.S.; McKay, D.B.
Deposited on : 2003-04-14
Resolution : 3.20 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

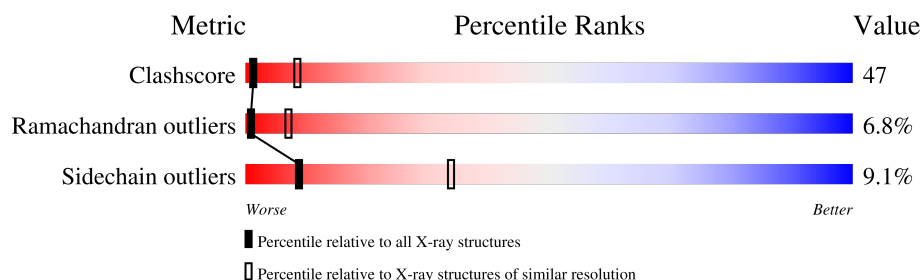
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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	310	
1	B	310	
1	C	310	
2	G	174	
2	H	174	
2	I	174	
2	L	174	
2	M	174	

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Mol	Chain	Length	Quality of chain
2	N	174	 34% 53% 13%

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
5	PO4	B	452	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15050 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.

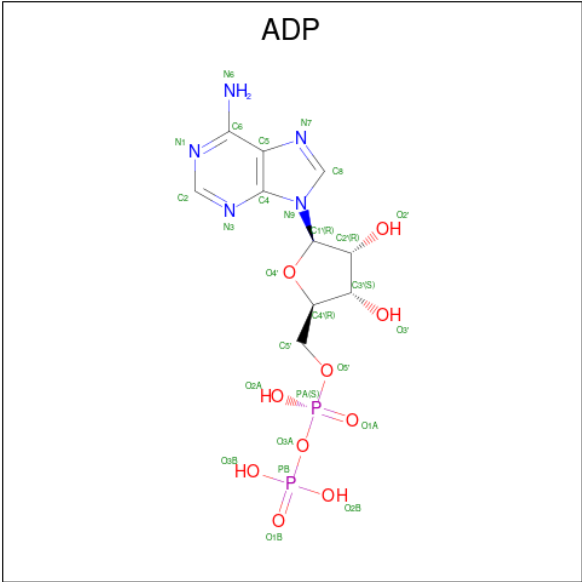
- Molecule 1 is a protein called ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUB-UNIT HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2312	1446	411	446	9			
1	B	295	Total	C	N	O	S	0	0	0
			2284	1430	407	438	9			
1	C	296	Total	C	N	O	S	0	0	0
			2288	1431	407	441	9			

- Molecule 2 is a protein called ATP-DEPENDENT PROTEASE HSLV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	H	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	I	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	L	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	M	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	N	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

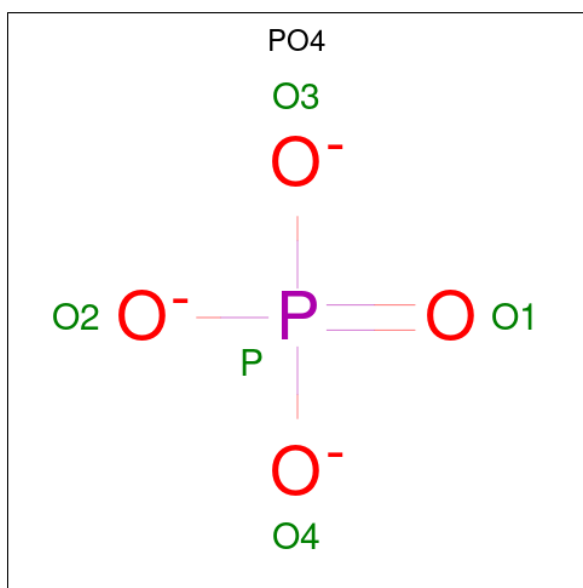


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

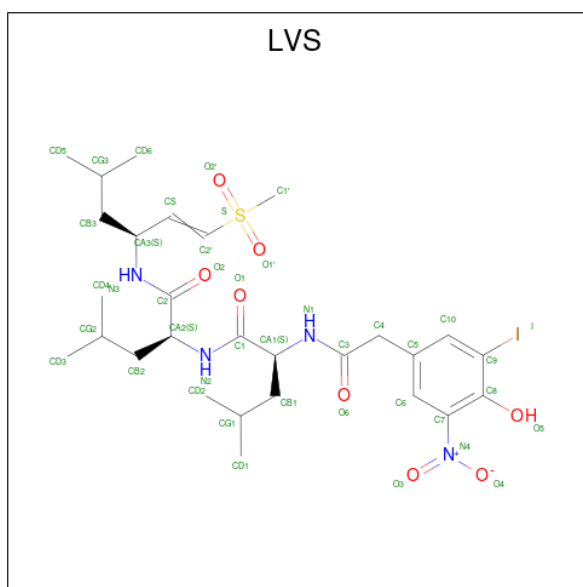
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	G	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		
4	L	1	Total	Mg	0	0
			1	1		
4	M	1	Total	Mg	0	0
			1	1		
4	N	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	P 1	0	0
5	B	1	Total 5	O 4	P 1	0	0
5	C	1	Total 5	O 4	P 1	0	0

- Molecule 6 is 4-IODO-3-NITROPHENYL ACETYL-LEUCINYL-LEUCINYL-LEUCINYL-VINYLSULFONE (CCD ID: LVS) (formula: $C_{28}H_{43}IN_4O_8S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	G	1	Total 41	C 28	N 4	O 8	S 1	0	0
6	H	1	Total 41	C 28	N 4	O 8	S 1	0	0
6	I	1	Total 41	C 28	N 4	O 8	S 1	0	0

- Molecule 7 is water.

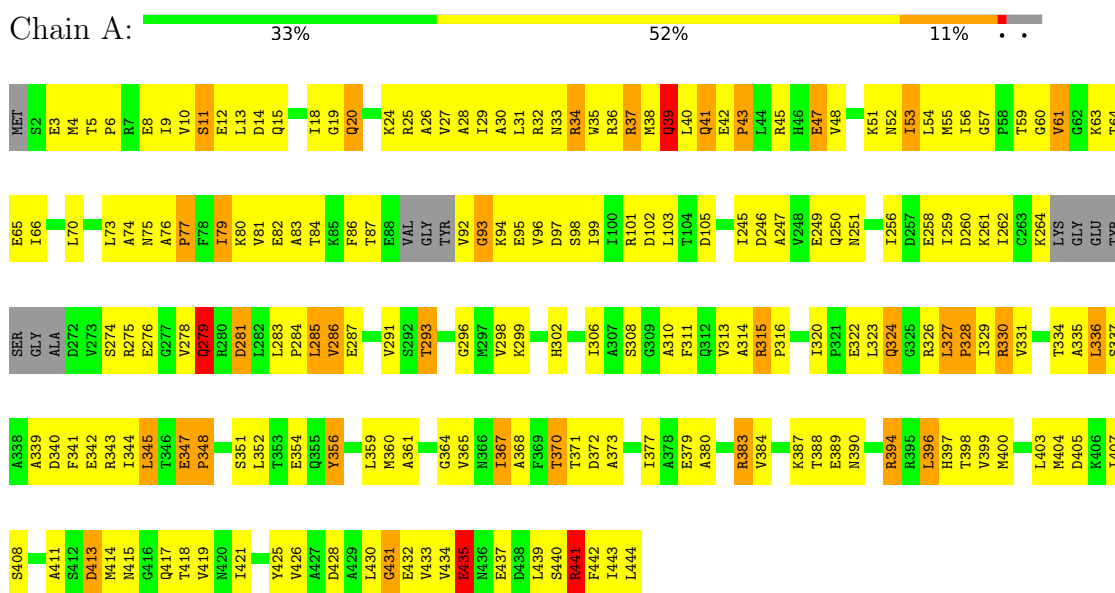
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total 7	O 7	0	0
7	B	7	Total 7	O 7	0	0
7	C	7	Total 7	O 7	0	0

3 Residue-property plots

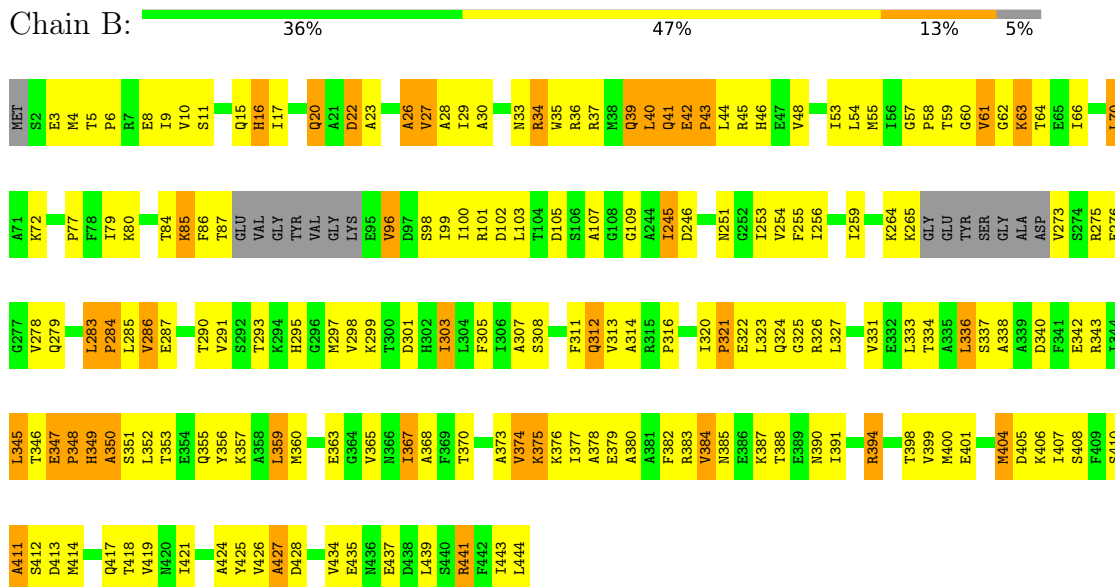
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

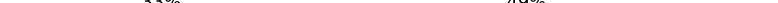
• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

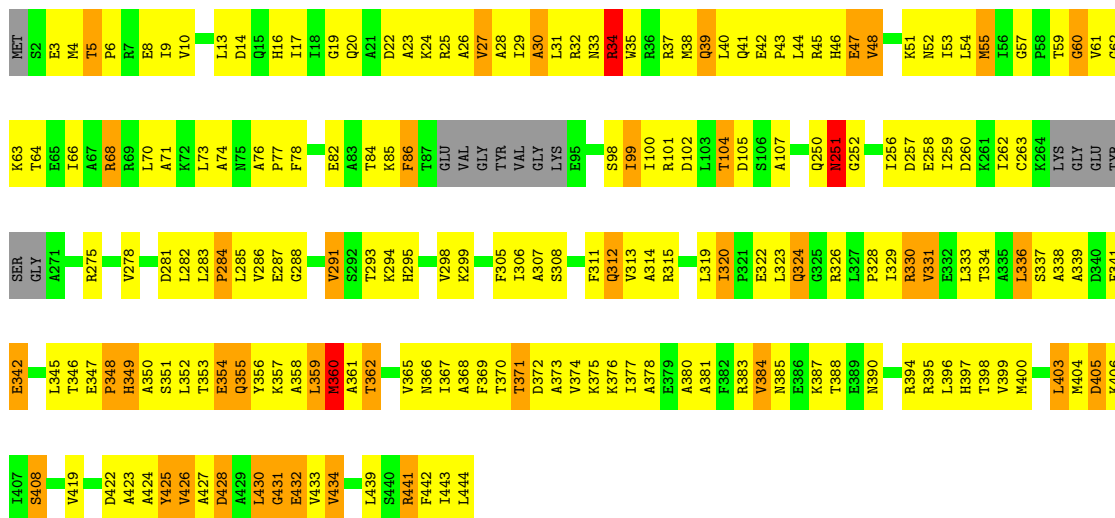


• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU



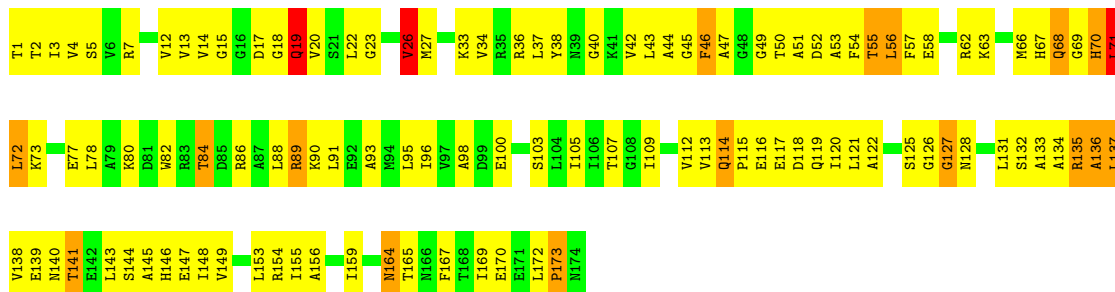
- Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

Chain C:  33% 49% 13% • 5%

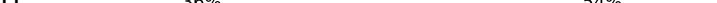


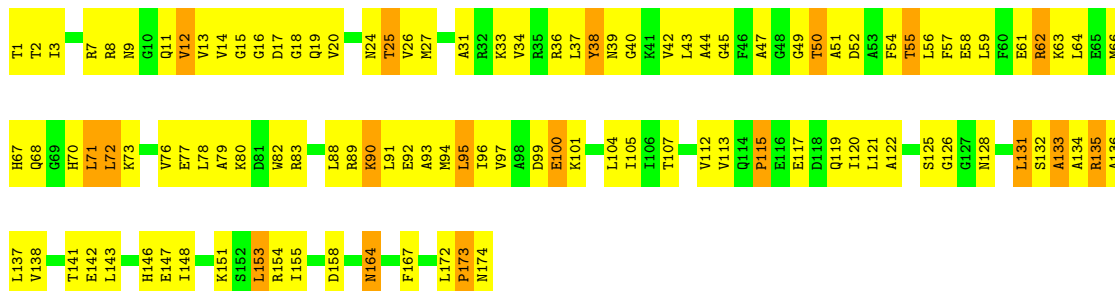
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain G:  34% 55% 9%



- Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain H:  36% 54% 10%



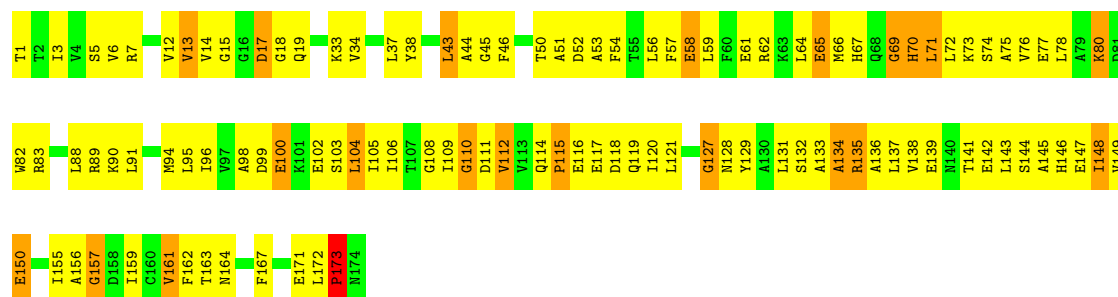
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain I: 33% 53% 13%



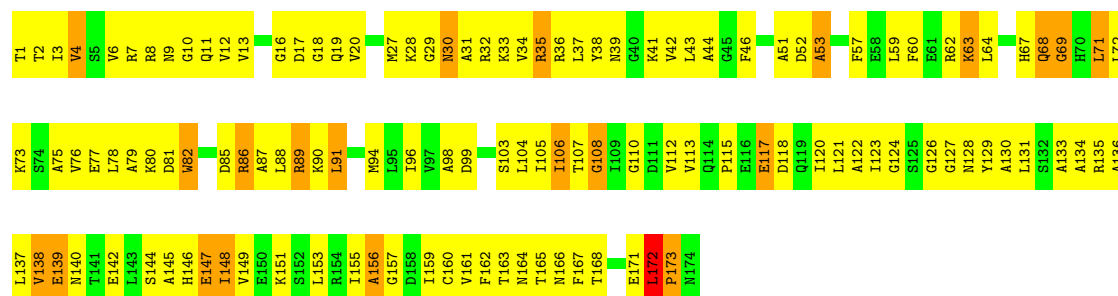
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain L: 37% 51% 12% .



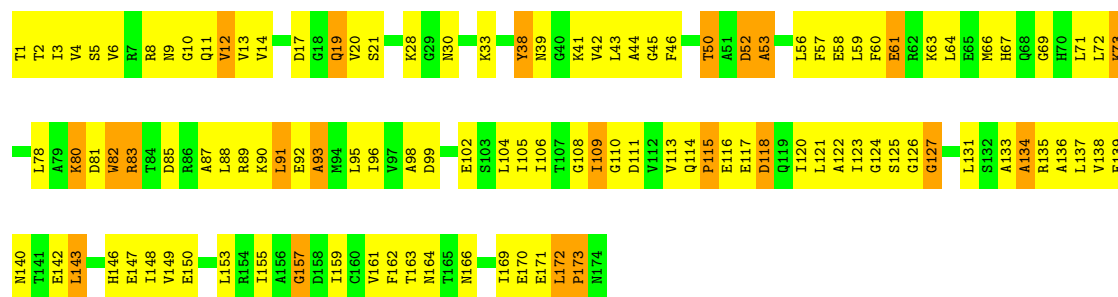
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain M: 28% 59% 12% .



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain N: 34% 53% 13%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	190.18Å 190.18Å 114.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20	Depositor
% Data completeness (in resolution range)	96.7 (50.00-3.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.327	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15050	wwPDB-VP
Average B, all atoms (Å ²)	64.0	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: LVS, PO4, ADP, MG

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	0.59	1/2339 (0.0%)	1.15	23/3156 (0.7%)
1	B	0.59	0/2311	1.08	15/3118 (0.5%)
1	C	0.55	0/2315	1.08	13/3125 (0.4%)
2	G	0.48	1/1333 (0.1%)	0.95	5/1798 (0.3%)
2	H	0.45	1/1333 (0.1%)	0.87	2/1798 (0.1%)
2	I	0.44	1/1333 (0.1%)	0.91	1/1798 (0.1%)
2	L	0.42	1/1333 (0.1%)	0.94	5/1798 (0.3%)
2	M	0.41	1/1333 (0.1%)	0.89	3/1798 (0.2%)
2	N	0.40	1/1333 (0.1%)	0.96	5/1798 (0.3%)
All	All	0.51	7/14963 (0.0%)	1.01	72/20187 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	173	PRO	C-N	-5.80	1.25	1.33
2	G	173	PRO	C-N	-5.79	1.25	1.33
2	I	173	PRO	C-N	-5.78	1.25	1.33
2	N	173	PRO	C-N	-5.66	1.25	1.33
2	M	173	PRO	C-N	-5.58	1.25	1.33
2	L	173	PRO	C-N	-5.48	1.25	1.33
1	A	61	VAL	CA-CB	-5.14	1.48	1.54

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ASP	N-CA-C	-10.53	100.44	113.18
1	A	39	GLN	N-CA-C	-9.27	100.76	112.90
1	A	310	ALA	N-CA-C	-8.73	102.21	113.12
1	A	279	GLN	N-CA-C	-8.23	100.98	111.02
1	A	37	ARG	N-CA-C	-8.11	99.87	110.33
1	B	251	ASN	N-CA-C	7.66	123.53	114.04
1	C	34	ARG	N-CA-C	-7.51	102.10	111.11
1	A	61	VAL	N-CA-C	-7.49	105.70	112.90
2	N	61	GLU	N-CA-C	-7.28	103.28	111.14
1	C	251	ASN	N-CA-C	7.13	120.01	110.88
1	B	34	ARG	N-CA-C	-7.07	103.51	111.14
1	C	320	ILE	CA-C-N	7.03	127.33	119.32
1	C	320	ILE	C-N-CA	7.03	127.33	119.32
1	A	327	LEU	N-CA-C	-7.00	98.59	109.79
2	N	53	ALA	N-CA-C	-6.74	105.22	113.50
1	A	347	GLU	N-CA-C	6.70	121.59	112.55
1	A	324	GLN	N-CA-C	-6.69	103.23	111.33
1	C	346	THR	N-CA-C	6.56	121.91	113.18
1	B	245	ILE	N-CA-C	6.47	117.10	110.82
1	B	96	VAL	N-CA-C	6.47	119.13	111.05
2	N	52	ASP	N-CA-C	-6.46	105.02	114.39
2	L	58	GLU	N-CA-C	-6.45	105.05	113.12
2	N	50	THR	N-CA-C	-6.37	104.34	111.28
1	A	41	GLN	N-CA-C	6.35	119.11	110.35
1	A	286	VAL	N-CA-C	6.31	116.94	110.82
2	M	63	LYS	N-CA-C	-6.18	106.01	112.93
1	C	430	LEU	N-CA-C	-6.17	105.02	112.54
1	C	354	GLU	N-CA-C	-6.15	103.72	111.11
2	G	114	GLN	CA-C-N	6.14	126.11	119.78
2	G	114	GLN	C-N-CA	6.14	126.11	119.78
1	C	312	GLN	N-CA-C	-6.10	104.91	112.90
1	B	53	ILE	N-CA-C	6.04	117.71	108.71
1	B	347	GLU	CA-C-N	6.02	127.36	119.84
1	B	347	GLU	C-N-CA	6.02	127.36	119.84
1	A	53	ILE	N-CA-C	5.98	117.98	108.89
2	L	145	ALA	N-CA-C	-5.98	105.08	112.38
1	B	327	LEU	CA-C-N	5.92	126.07	119.32
1	B	327	LEU	C-N-CA	5.92	126.07	119.32
2	G	19	GLN	N-CA-C	5.92	118.37	108.96
2	H	25	THR	N-CA-C	-5.85	101.80	110.46
1	A	387	LYS	N-CA-C	5.80	118.38	111.71
1	A	315	ARG	N-CA-C	-5.77	103.38	110.31
2	G	26	VAL	N-CA-C	5.76	116.15	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	396	LEU	N-CA-C	-5.75	105.09	111.36
1	B	346	THR	N-CA-C	5.73	123.01	110.80
2	N	21	SER	N-CA-C	5.72	118.11	109.41
1	C	324	GLN	N-CA-C	-5.68	104.09	111.02
2	L	104	LEU	N-CA-C	5.53	117.67	108.99
1	C	74	ALA	N-CA-C	-5.52	106.44	114.12
2	L	100	GLU	N-CA-C	5.50	117.71	111.11
2	M	4	VAL	N-CA-C	5.49	116.18	108.17
1	A	47	GLU	N-CA-C	5.45	117.31	111.36
2	G	169	ILE	N-CA-C	5.45	114.59	106.85
1	A	364	GLY	N-CA-C	-5.44	107.02	115.67
2	I	129	TYR	N-CA-C	-5.43	104.23	111.24
2	M	60	PHE	N-CA-C	-5.42	106.34	113.12
1	B	374	VAL	N-CA-C	-5.41	104.61	110.23
1	A	396	LEU	N-CA-C	-5.40	105.47	111.36
1	C	306	ILE	N-CA-C	-5.39	100.62	108.17
1	A	327	LEU	CA-C-N	5.38	126.56	119.84
1	A	327	LEU	C-N-CA	5.38	126.56	119.84
1	B	279	GLN	N-CA-C	-5.37	105.43	111.28
1	C	360	MET	N-CA-C	-5.36	105.60	111.82
2	H	26	VAL	N-CA-C	5.34	115.77	107.28
1	B	379	GLU	N-CA-C	-5.32	105.48	111.28
2	L	13	VAL	N-CA-C	5.32	116.25	108.53
1	B	388	THR	CB-CA-C	-5.31	108.73	116.53
1	A	320	ILE	CA-C-N	5.10	126.22	119.84
1	A	320	ILE	C-N-CA	5.10	126.22	119.84
1	B	312	GLN	N-CA-C	-5.09	105.63	111.07
1	A	344	ILE	CB-CA-C	-5.06	105.31	112.14
1	A	418	THR	N-CA-C	-5.04	101.53	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	356	TYR	Sidechain

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2312	0	2358	205	0
1	B	2284	0	2336	194	0
1	C	2288	0	2332	206	0
2	G	1319	0	1347	146	0
2	H	1319	0	1347	156	0
2	I	1319	0	1347	148	0
2	L	1319	0	1348	125	0
2	M	1319	0	1348	152	0
2	N	1319	0	1348	136	0
3	A	27	0	12	4	0
3	B	27	0	12	6	0
3	C	27	0	12	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	2	0
5	C	5	0	0	1	0
6	G	41	0	38	10	0
6	H	41	0	38	3	0
6	I	41	0	38	4	0
7	A	7	0	0	0	0
7	B	7	0	0	0	0
7	C	7	0	0	0	0
All	All	15050	0	15261	1426	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (1426) 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)
1:C:3:GLU:HG3	1:C:4:MET:H	1.10	1.14
1:B:55:MET:HE2	1:B:333:LEU:HD11	1.28	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:ARG:HH11	1:B:441:ARG:HB3	1.07	1.09
1:C:406:LYS:H	1:C:406:LYS:HD2	1.15	1.04
2:N:105:ILE:HG13	2:N:121:LEU:HD13	1.40	1.03
1:A:441:ARG:HH11	1:A:441:ARG:HB3	1.21	1.03
2:N:42:VAL:HG22	2:N:99:ASP:HB3	1.42	1.01
2:H:151:LYS:HE2	2:N:140:ASN:HD21	1.27	0.98
1:B:406:LYS:H	1:B:406:LYS:HD2	1.24	0.97
2:N:4:VAL:HG13	2:N:149:VAL:HG13	1.47	0.96
1:C:441:ARG:HH11	1:C:441:ARG:HB3	1.30	0.93
1:B:286:VAL:HG11	1:B:326:ARG:HB3	1.48	0.93
1:B:42:GLU:HB3	1:B:43:PRO:HD3	1.51	0.92
1:B:441:ARG:HB3	1:B:441:ARG:NH1	1.85	0.92
1:C:360:MET:HE2	1:C:360:MET:HA	1.50	0.92
1:B:37:ARG:HA	1:B:40:LEU:HG	1.52	0.91
2:I:27:MET:HE3	2:I:27:MET:HA	1.51	0.91
2:L:109:ILE:HG13	2:L:110:GLY:H	1.34	0.90
2:M:11:GLN:HA	2:M:173:PRO:HG2	1.53	0.90
1:A:20:GLN:HE21	1:A:20:GLN:HA	1.36	0.90
2:H:141:THR:HG22	2:H:143:LEU:H	1.34	0.90
2:H:45:GLY:O	2:H:95:LEU:HD23	1.71	0.90
1:C:330:ARG:HH11	1:C:330:ARG:HB3	1.34	0.90
1:A:441:ARG:HH11	1:A:441:ARG:CB	1.85	0.89
1:B:23:ALA:HA	1:B:331:VAL:HG21	1.55	0.88
2:I:56:LEU:HD13	2:I:95:LEU:HD22	1.54	0.88
1:A:27:VAL:HB	1:A:70:LEU:HD13	1.56	0.87
1:A:94:LYS:HG2	1:A:95:GLU:H	1.39	0.86
2:N:105:ILE:HB	2:N:113:VAL:HB	1.56	0.86
1:C:101:ARG:HG2	1:C:293:THR:HG22	1.55	0.86
2:G:105:ILE:HG23	2:G:121:LEU:HD13	1.58	0.86
2:N:12:VAL:HG11	2:N:172:LEU:HD12	1.54	0.86
2:I:17:ASP:HB2	2:I:164:ASN:ND2	1.91	0.85
1:B:27:VAL:HB	1:B:70:LEU:HD13	1.56	0.85
2:H:105:ILE:CG2	2:H:113:VAL:HB	2.06	0.85
2:L:88:LEU:HA	2:L:91:LEU:HD13	1.59	0.84
1:B:439:LEU:HD13	2:H:76:VAL:HG21	1.57	0.84
1:C:3:GLU:CG	1:C:4:MET:H	1.90	0.83
2:H:56:LEU:HD11	2:H:95:LEU:HB2	1.60	0.83
1:C:60:GLY:HA2	3:C:450:ADP:O3A	1.79	0.83
2:M:105:ILE:HG13	2:M:121:LEU:HD13	1.60	0.83
1:C:54:LEU:HD12	1:C:307:ALA:O	1.79	0.83
2:I:18:GLY:H	2:I:164:ASN:HD21	1.23	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:43:LEU:HD12	2:I:43:LEU:H	1.44	0.82
2:G:4:VAL:HG23	2:G:122:ALA:HB2	1.59	0.82
2:G:141:THR:OG1	2:G:143:LEU:HG	1.80	0.82
2:G:50:THR:HG21	6:G:0:LVS:HD12	1.62	0.81
1:A:4:MET:HB3	1:A:8:GLU:HB2	1.60	0.81
1:C:377:ILE:O	1:C:380:ALA:HB3	1.81	0.81
1:A:370:THR:HG23	1:A:421:ILE:O	1.80	0.81
2:G:96:ILE:HG12	2:G:105:ILE:HG22	1.62	0.81
1:B:20:GLN:HE21	1:B:20:GLN:HA	1.43	0.81
2:H:17:ASP:HB2	2:H:164:ASN:ND2	1.96	0.81
2:G:56:LEU:HD22	2:G:95:LEU:HD12	1.62	0.80
1:B:20:GLN:HE22	1:B:334:THR:H	1.28	0.80
1:C:256:ILE:HD13	1:C:282:LEU:HD21	1.63	0.80
1:C:403:LEU:HD23	1:C:404:MET:N	1.95	0.80
1:C:3:GLU:HG3	1:C:4:MET:N	1.93	0.80
1:C:98:SER:HA	1:C:101:ARG:HE	1.47	0.80
1:A:20:GLN:HE21	1:A:20:GLN:CA	1.94	0.79
1:C:42:GLU:HB3	1:C:43:PRO:HD3	1.64	0.79
2:I:37:LEU:HB2	2:I:42:VAL:HG23	1.64	0.79
2:I:1:THR:HG23	2:I:33:LYS:HD3	1.65	0.79
2:M:13:VAL:HG22	2:M:171:GLU:HG2	1.65	0.79
1:A:26:ALA:HB2	1:A:331:VAL:HG11	1.65	0.79
2:M:88:LEU:HA	2:M:91:LEU:HD13	1.65	0.78
1:A:262:ILE:HD12	1:A:278:VAL:HG23	1.64	0.78
1:C:441:ARG:HB3	1:C:441:ARG:NH1	1.98	0.78
2:G:38:TYR:CE1	2:G:69:GLY:HA3	2.18	0.78
6:G:0:LVS:HD13	6:G:0:LVS:HN1	1.48	0.78
2:G:131:LEU:HD11	2:G:135:ARG:NH1	1.99	0.78
2:H:136:ALA:HB2	2:N:155:ILE:HD13	1.66	0.78
2:I:17:ASP:HB2	2:I:164:ASN:HD22	1.47	0.78
2:M:71:LEU:HD12	2:M:71:LEU:H	1.47	0.78
2:N:1:THR:HG23	2:N:33:LYS:NZ	1.99	0.78
2:N:80:LYS:HB2	2:N:80:LYS:NZ	1.98	0.77
1:B:79:ILE:HG22	1:B:254:VAL:HG22	1.65	0.77
2:G:3:ILE:HG22	2:G:96:ILE:HD12	1.67	0.77
2:G:50:THR:HG23	2:G:51:ALA:N	2.00	0.77
1:B:299:LYS:HB3	1:B:301:ASP:OD1	1.86	0.76
2:N:19:GLN:HB2	2:N:164:ASN:HD22	1.50	0.76
1:C:19:GLY:O	1:C:24:LYS:NZ	2.17	0.76
2:L:96:ILE:HG12	2:L:105:ILE:HG12	1.67	0.76
2:N:19:GLN:HB2	2:N:164:ASN:ND2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:141:THR:CG2	2:L:143:LEU:HG	2.16	0.76
2:M:3:ILE:HB	2:M:123:ILE:HG13	1.67	0.76
2:L:141:THR:HG21	2:L:143:LEU:HG	1.65	0.76
1:A:20:GLN:HE22	1:A:334:THR:H	1.34	0.76
1:A:264:LYS:HD2	1:A:264:LYS:N	2.00	0.76
1:A:330:ARG:HH11	1:A:330:ARG:HB3	1.50	0.75
2:G:51:ALA:O	2:G:55:THR:HG22	1.86	0.75
2:I:67:HIS:NE2	2:I:77:GLU:HG3	2.00	0.75
1:B:359:LEU:HD13	1:C:40:LEU:HD11	1.69	0.75
1:C:27:VAL:HG23	1:C:70:LEU:HD13	1.69	0.75
1:B:443:ILE:HG12	2:H:112:VAL:CG2	2.17	0.74
1:C:76:ALA:HB1	1:C:251:ASN:O	1.87	0.74
2:H:83:ARG:HH11	2:I:54:PHE:HB3	1.51	0.74
2:H:131:LEU:HD11	2:H:135:ARG:NH1	2.02	0.74
2:L:19:GLN:HB2	2:L:164:ASN:ND2	2.02	0.74
2:G:18:GLY:H	2:G:164:ASN:HD21	1.36	0.74
2:H:94:MET:HG2	2:H:107:THR:HG22	1.70	0.74
2:G:52:ASP:HA	2:G:55:THR:CG2	2.18	0.74
2:N:85:ASP:HB3	2:N:88:LEU:HD23	1.70	0.74
1:A:278:VAL:HA	1:A:281:ASP:HB2	1.70	0.73
2:M:6:VAL:HG12	2:M:7:ARG:H	1.53	0.73
1:C:17:ILE:HG12	1:C:66:ILE:HD13	1.69	0.73
1:A:249:GLU:OE1	1:A:299:LYS:HG2	1.89	0.73
2:H:136:ALA:HB2	2:N:155:ILE:CD1	2.19	0.73
2:M:32:ARG:HH21	2:M:35:ARG:HA	1.52	0.73
1:A:283:LEU:O	1:A:284:PRO:C	2.31	0.72
2:H:143:LEU:HD11	2:N:140:ASN:ND2	2.04	0.72
2:N:88:LEU:HA	2:N:91:LEU:HD13	1.71	0.72
2:H:56:LEU:CD1	2:H:95:LEU:HD12	2.19	0.72
2:M:4:VAL:HG13	2:M:149:VAL:HG13	1.69	0.72
2:G:37:LEU:HD21	2:G:57:PHE:CZ	2.25	0.72
1:B:37:ARG:HD2	1:B:48:VAL:HG13	1.72	0.72
1:B:367:ILE:HG12	1:B:368:ALA:N	2.03	0.72
2:L:80:LYS:NZ	2:L:80:LYS:HB3	2.04	0.72
2:I:5:SER:HB2	2:I:14:VAL:HG22	1.72	0.72
2:H:37:LEU:HB2	2:H:42:VAL:HG23	1.71	0.72
2:L:33:LYS:HA	2:L:46:PHE:CE1	2.24	0.72
2:N:52:ASP:O	2:N:56:LEU:HD23	1.89	0.72
2:I:52:ASP:HA	2:I:55:THR:HG23	1.72	0.72
1:B:63:LYS:HD2	1:B:308:SER:HB2	1.70	0.71
2:M:2:THR:HG22	2:M:126:GLY:HA3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:HB3	1:A:43:PRO:HD3	1.70	0.71
2:N:46:PHE:CZ	2:N:50:THR:HG22	2.24	0.71
2:H:56:LEU:HD13	2:H:95:LEU:HD12	1.71	0.71
2:I:5:SER:CB	2:I:14:VAL:HG22	2.21	0.71
2:H:151:LYS:HE2	2:N:140:ASN:ND2	2.05	0.71
1:B:390:ASN:HB2	2:H:68:GLN:NE2	2.06	0.71
1:A:293:THR:HG23	1:A:296:GLY:O	1.90	0.71
2:I:52:ASP:HA	2:I:55:THR:CG2	2.20	0.71
1:B:443:ILE:HG22	1:B:444:LEU:N	2.04	0.70
1:B:79:ILE:CG2	1:B:254:VAL:HG22	2.22	0.70
1:B:20:GLN:HE21	1:B:20:GLN:CA	2.03	0.70
1:B:283:LEU:HB2	1:B:284:PRO:HD3	1.74	0.70
1:C:34:ARG:HH21	1:C:251:ASN:C	2.00	0.70
2:H:12:VAL:HG23	2:H:172:LEU:HB3	1.72	0.70
2:H:18:GLY:H	2:H:164:ASN:HD21	1.40	0.70
2:H:105:ILE:HG23	2:H:113:VAL:HB	1.73	0.70
2:M:32:ARG:NH2	2:M:35:ARG:HA	2.06	0.70
2:M:71:LEU:HD11	2:M:99:ASP:OD1	1.90	0.70
1:A:37:ARG:O	1:A:38:MET:HB3	1.90	0.70
2:G:37:LEU:HB2	2:G:42:VAL:HG23	1.73	0.70
2:I:37:LEU:HD21	2:I:57:PHE:CZ	2.26	0.70
1:B:85:LYS:HG2	1:B:85:LYS:O	1.92	0.70
1:B:303:ILE:HG22	1:B:305:PHE:CE1	2.26	0.70
2:H:115:PRO:HG3	2:H:121:LEU:HD21	1.72	0.70
2:I:56:LEU:HD13	2:I:95:LEU:CD2	2.23	0.69
2:M:133:ALA:O	2:M:136:ALA:HB3	1.92	0.69
2:H:125:SER:H	6:H:0:LVS:C1'	2.05	0.69
2:H:125:SER:H	6:H:0:LVS:H1'1	1.55	0.69
2:L:64:LEU:HA	2:L:74:SER:OG	1.92	0.69
2:G:89:ARG:HG2	2:G:89:ARG:HH11	1.58	0.69
1:C:390:ASN:HB2	2:I:68:GLN:NE2	2.08	0.69
2:N:17:ASP:CG	2:N:163:THR:HG23	2.18	0.69
2:L:131:LEU:HD11	2:L:135:ARG:NE	2.08	0.68
2:M:155:ILE:C	2:M:157:GLY:H	1.99	0.68
1:A:37:ARG:HD2	1:A:48:VAL:HG13	1.75	0.68
2:H:154:ARG:HA	2:H:167:PHE:HZ	1.58	0.68
2:N:46:PHE:HZ	2:N:50:THR:HG22	1.59	0.68
1:C:35:TRP:O	1:C:39:GLN:NE2	2.26	0.68
2:L:109:ILE:HG13	2:L:110:GLY:N	2.08	0.68
1:B:5:THR:OG1	1:B:8:GLU:HG3	1.94	0.68
1:C:62:GLY:O	1:C:66:ILE:HG12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:50:THR:O	2:L:53:ALA:HB3	1.94	0.67
1:B:365:VAL:HG22	1:B:414:MET:HB2	1.75	0.67
1:C:313:VAL:HG23	1:C:314:ALA:H	1.57	0.67
2:G:46:PHE:HB3	2:G:95:LEU:HD21	1.74	0.67
2:H:172:LEU:HD23	2:H:174:ASN:N	2.09	0.67
1:A:330:ARG:HH11	1:A:330:ARG:CB	2.08	0.67
2:L:1:THR:HG23	2:L:33:LYS:HE3	1.75	0.67
2:L:18:GLY:HA2	2:L:33:LYS:HZ3	1.57	0.67
2:N:104:LEU:CD1	2:N:114:GLN:HG2	2.24	0.67
2:G:136:ALA:O	2:G:137:LEU:C	2.37	0.67
2:H:51:ALA:O	2:H:55:THR:HG22	1.95	0.67
2:M:106:ILE:HD12	2:M:106:ILE:N	2.09	0.67
2:I:67:HIS:HE2	2:I:77:GLU:HG3	1.57	0.67
1:B:286:VAL:HG12	1:B:287:GLU:N	2.08	0.67
1:B:347:GLU:HB2	1:B:348:PRO:HD3	1.76	0.67
2:M:86:ARG:HA	2:M:86:ARG:HH11	1.59	0.67
1:B:100:ILE:HB	1:B:291:VAL:HG21	1.77	0.66
2:I:1:THR:HB	6:I:0:LVS:H1'3	1.78	0.66
2:N:87:ALA:C	2:N:88:LEU:HD22	2.20	0.66
1:A:326:ARG:C	1:A:328:PRO:HD3	2.20	0.66
1:A:4:MET:HE2	1:A:73:LEU:HD13	1.77	0.66
1:B:39:GLN:HE21	1:B:39:GLN:N	1.94	0.66
1:C:63:LYS:HG2	1:C:333:LEU:HD22	1.77	0.66
2:H:52:ASP:HA	2:H:55:THR:CG2	2.25	0.66
2:L:70:HIS:HB3	2:L:73:LYS:HD3	1.77	0.66
1:B:61:VAL:HB	1:B:336:LEU:HD13	1.78	0.66
2:L:134:ALA:O	2:L:135:ARG:C	2.37	0.66
2:M:41:LYS:O	2:M:172:LEU:HD11	1.95	0.66
1:C:34:ARG:HG3	1:C:34:ARG:HH11	1.60	0.66
1:C:41:GLN:HE21	1:C:41:GLN:HA	1.60	0.66
1:C:250:GLN:HE21	1:C:250:GLN:HA	1.60	0.66
1:B:64:THR:HB	3:B:450:ADP:O1A	1.95	0.66
1:A:20:GLN:HE22	1:A:334:THR:HG22	1.61	0.66
1:A:396:LEU:O	1:A:400:MET:HB2	1.97	0.65
1:B:439:LEU:HD22	2:H:76:VAL:HG11	1.76	0.65
2:M:160:CYS:SG	2:M:162:PHE:HB2	2.35	0.65
2:N:104:LEU:HD12	2:N:114:GLN:HG2	1.76	0.65
2:H:52:ASP:OD2	2:H:91:LEU:HA	1.96	0.65
2:H:20:VAL:HG12	2:H:27:MET:HB3	1.77	0.65
2:N:3:ILE:HB	2:N:123:ILE:HG12	1.79	0.65
2:N:71:LEU:HD23	2:N:102:GLU:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:HH11	1:A:34:ARG:CG	2.10	0.65
1:B:342:GLU:OE2	1:B:375:LYS:HG3	1.97	0.65
1:B:367:ILE:HD12	1:B:404:MET:HE1	1.79	0.65
1:A:101:ARG:HG3	1:A:293:THR:HB	1.77	0.65
2:N:108:GLY:C	2:N:110:GLY:H	2.05	0.65
2:N:131:LEU:HD11	2:N:135:ARG:HE	1.60	0.65
1:C:360:MET:HG3	1:C:367:ILE:HD13	1.78	0.65
2:I:83:ARG:HH21	2:I:111:ASP:HA	1.62	0.65
1:A:13:LEU:HD12	1:A:24:LYS:HG2	1.78	0.64
1:B:313:VAL:HG23	1:B:314:ALA:H	1.60	0.64
1:C:100:ILE:O	1:C:104:THR:OG1	2.14	0.64
1:C:357:LYS:HE3	1:C:369:PHE:HD1	1.62	0.64
2:I:42:VAL:HG12	2:I:99:ASP:HB3	1.79	0.64
2:L:76:VAL:O	2:L:80:LYS:HG2	1.96	0.64
2:M:6:VAL:HG12	2:M:7:ARG:N	2.11	0.64
2:M:72:LEU:HD13	2:M:104:LEU:HD21	1.79	0.64
1:C:34:ARG:NH2	1:C:251:ASN:HA	2.12	0.64
2:I:52:ASP:OD2	2:I:91:LEU:HA	1.97	0.64
2:M:2:THR:HG23	2:M:163:THR:OG1	1.97	0.64
1:C:101:ARG:HG2	1:C:293:THR:CG2	2.27	0.64
2:I:131:LEU:HD11	2:I:135:ARG:NH1	2.12	0.64
2:M:20:VAL:HB	2:M:28:LYS:H	1.62	0.64
2:H:7:ARG:HG3	2:H:7:ARG:HH11	1.61	0.64
2:M:3:ILE:HD13	2:M:16:GLY:HA3	1.79	0.64
2:M:71:LEU:HD21	2:M:99:ASP:HB3	1.80	0.64
2:N:133:ALA:O	2:N:136:ALA:HB3	1.97	0.64
2:H:72:LEU:HD22	2:H:104:LEU:HD11	1.80	0.64
2:H:19:GLN:H	2:H:33:LYS:NZ	1.95	0.64
1:B:353:THR:O	1:B:357:LYS:HB2	1.97	0.63
2:G:37:LEU:HD21	2:G:57:PHE:CE2	2.34	0.63
1:B:84:THR:C	1:B:86:PHE:H	2.06	0.63
2:M:103:SER:C	2:M:104:LEU:HD12	2.24	0.63
2:N:58:GLU:C	2:N:60:PHE:H	2.06	0.63
1:C:41:GLN:HA	1:C:41:GLN:NE2	2.12	0.63
2:M:2:THR:HG22	2:M:126:GLY:CA	2.28	0.63
1:C:59:THR:HA	5:C:452:PO4:O2	1.98	0.63
2:G:115:PRO:HG3	2:G:121:LEU:HD11	1.79	0.63
2:N:1:THR:HG23	2:N:33:LYS:HZ3	1.62	0.63
2:H:19:GLN:H	2:H:33:LYS:HZ3	1.46	0.63
1:A:407:ILE:O	1:A:411:ALA:HB2	1.99	0.62
2:G:2:THR:OG1	2:G:126:GLY:HA3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:4:VAL:HG13	2:N:149:VAL:CG1	2.27	0.62
1:C:250:GLN:HA	1:C:250:GLN:NE2	2.15	0.62
1:C:293:THR:C	1:C:295:HIS:H	2.07	0.62
1:C:313:VAL:HG23	1:C:314:ALA:N	2.14	0.62
2:H:131:LEU:HD11	2:H:135:ARG:HH11	1.64	0.62
2:H:141:THR:HG22	2:H:142:GLU:N	2.13	0.62
1:B:313:VAL:HG23	1:B:314:ALA:N	2.14	0.62
1:C:371:THR:CG2	1:C:375:LYS:HE2	2.30	0.62
1:A:79:ILE:HG22	1:A:103:LEU:HD13	1.81	0.62
1:B:365:VAL:CG2	1:B:414:MET:HB2	2.29	0.62
2:H:131:LEU:HD21	2:H:135:ARG:NH1	2.14	0.62
1:C:406:LYS:HD2	1:C:406:LYS:N	1.99	0.62
2:M:131:LEU:HD11	2:M:135:ARG:NE	2.14	0.62
2:I:134:ALA:C	2:I:136:ALA:H	2.07	0.62
2:L:7:ARG:HB3	2:L:119:GLN:HB3	1.82	0.62
2:G:78:LEU:HG	2:G:82:TRP:HZ3	1.65	0.62
2:H:155:ILE:HA	2:H:158:ASP:OD1	1.99	0.62
1:C:27:VAL:CG2	1:C:70:LEU:HD13	2.29	0.61
2:H:1:THR:HG23	2:H:33:LYS:HD3	1.82	0.61
2:I:5:SER:OG	2:I:14:VAL:HG22	2.00	0.61
2:L:116:GLU:C	2:L:118:ASP:H	2.07	0.61
1:A:377:ILE:O	1:A:380:ALA:HB3	2.01	0.61
1:C:425:TYR:O	1:C:428:ASP:N	2.23	0.61
2:M:115:PRO:HG3	2:M:121:LEU:CD1	2.30	0.61
1:B:84:THR:O	1:B:86:PHE:N	2.32	0.61
1:B:311:PHE:CE1	1:B:316:PRO:HA	2.35	0.61
1:C:98:SER:HB3	1:C:101:ARG:HH21	1.66	0.61
2:M:63:LYS:NZ	2:M:77:GLU:HB3	2.14	0.61
1:B:367:ILE:HD11	1:B:421:ILE:HD12	1.81	0.61
2:H:136:ALA:C	2:H:138:VAL:H	2.08	0.61
2:L:80:LYS:HB3	2:L:80:LYS:HZ2	1.63	0.61
2:N:12:VAL:CG1	2:N:172:LEU:HB2	2.31	0.61
1:C:55:MET:O	1:C:308:SER:HA	2.00	0.61
1:C:312:GLN:HE21	2:I:66:MET:HG2	1.66	0.61
2:H:131:LEU:O	2:H:132:SER:C	2.43	0.61
2:L:5:SER:HB2	2:L:14:VAL:HG22	1.83	0.61
2:N:161:VAL:HG23	2:N:162:PHE:CD2	2.36	0.61
1:A:250:GLN:HA	1:A:250:GLN:NE2	2.14	0.61
1:C:384:VAL:O	1:C:385:ASN:C	2.42	0.61
2:H:38:TYR:C	2:H:40:GLY:H	2.08	0.61
2:I:62:ARG:NH1	2:I:62:ARG:HB3	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:64:LEU:HD21	2:L:69:GLY:HA2	1.83	0.60
1:A:258:GLU:O	1:A:261:LYS:HB2	2.01	0.60
2:G:50:THR:CG2	2:G:51:ALA:N	2.64	0.60
2:I:1:THR:HB	6:I:0:LVS:C1'	2.31	0.60
1:B:98:SER:HA	1:B:101:ARG:NH1	2.16	0.60
1:C:443:ILE:HG12	2:I:112:VAL:CG2	2.31	0.60
1:A:6:PRO:HD3	1:A:32:ARG:HD3	1.84	0.60
1:C:372:ASP:O	1:C:376:LYS:HB2	2.01	0.60
2:M:131:LEU:HD11	2:M:135:ARG:HE	1.64	0.60
1:C:444:LEU:HB3	2:I:113:VAL:HG22	1.84	0.60
2:G:13:VAL:HG21	2:G:146:HIS:N	2.16	0.60
2:I:37:LEU:HD21	2:I:57:PHE:CE2	2.36	0.60
2:M:79:ALA:HB2	2:M:112:VAL:HG23	1.83	0.60
2:L:88:LEU:CA	2:L:91:LEU:HD13	2.30	0.60
2:N:91:LEU:HD12	2:N:91:LEU:N	2.16	0.60
1:A:250:GLN:HA	1:A:250:GLN:HE21	1.67	0.60
1:A:322:GLU:N	1:A:322:GLU:OE2	2.35	0.60
1:B:337:SER:O	1:B:340:ASP:HB2	2.02	0.60
2:N:28:LYS:HE3	2:N:30:ASN:O	2.02	0.60
1:A:73:LEU:HD12	1:A:73:LEU:O	2.02	0.60
1:C:342:GLU:OE2	1:C:375:LYS:HG2	2.02	0.60
2:H:44:ALA:HA	2:H:96:ILE:O	2.02	0.60
1:B:407:ILE:HD11	1:B:425:TYR:HE1	1.67	0.59
1:C:25:ARG:O	1:C:28:ALA:HB3	2.02	0.59
2:G:91:LEU:HD12	2:G:91:LEU:N	2.17	0.59
2:H:17:ASP:HB2	2:H:164:ASN:HD21	1.66	0.59
2:H:72:LEU:O	2:H:76:VAL:HG23	2.01	0.59
2:M:63:LYS:HZ2	2:M:77:GLU:HB3	1.66	0.59
1:B:61:VAL:C	3:B:450:ADP:N7	2.60	0.59
2:L:95:LEU:HB2	2:L:106:ILE:HB	1.83	0.59
1:A:441:ARG:CB	1:A:441:ARG:NH1	2.61	0.59
2:I:9:ASN:O	2:I:11:GLN:HG2	2.02	0.59
2:M:37:LEU:HD11	2:M:57:PHE:HB3	1.84	0.59
1:A:34:ARG:NH1	1:A:34:ARG:HG2	2.18	0.59
2:M:6:VAL:HG21	2:M:148:ILE:HG22	1.83	0.59
2:M:78:LEU:HD12	2:M:78:LEU:O	2.02	0.59
1:C:347:GLU:HB2	1:C:348:PRO:HD3	1.84	0.59
2:I:89:ARG:O	2:I:90:LYS:HB3	2.01	0.59
2:L:15:GLY:HA2	2:L:34:VAL:HG21	1.84	0.59
2:N:30:ASN:HA	2:N:166:ASN:ND2	2.17	0.59
1:B:35:TRP:O	1:B:39:GLN:NE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:87:ALA:O	2:M:88:LEU:HD12	2.02	0.59
2:N:11:GLN:OE1	2:N:173:PRO:HD2	2.02	0.59
1:A:262:ILE:HD12	1:A:278:VAL:CG2	2.30	0.59
1:B:443:ILE:HG12	2:H:112:VAL:HG21	1.84	0.59
1:C:34:ARG:CZ	1:C:251:ASN:HA	2.33	0.59
2:G:117:GLU:C	2:G:119:GLN:H	2.10	0.59
2:I:38:TYR:C	2:I:40:GLY:H	2.11	0.59
2:I:115:PRO:HG3	2:I:121:LEU:CG	2.33	0.59
2:N:4:VAL:HG12	2:N:153:LEU:HD21	1.84	0.59
1:A:94:LYS:HG2	1:A:95:GLU:N	2.14	0.59
2:N:133:ALA:O	2:N:137:LEU:HD22	2.01	0.59
1:A:264:LYS:HE2	1:A:276:GLU:CD	2.27	0.59
1:B:20:GLN:NE2	1:B:334:THR:H	1.99	0.59
1:C:9:ILE:HD13	1:C:31:LEU:HD23	1.85	0.59
2:G:137:LEU:O	2:G:141:THR:HG22	2.02	0.59
6:G:0:LVS:HD42	6:G:0:LVS:HN2	1.68	0.59
1:A:390:ASN:HB2	2:G:68:GLN:HE21	1.66	0.59
1:C:283:LEU:O	1:C:285:LEU:N	2.36	0.59
1:C:390:ASN:HB2	2:I:68:GLN:HE21	1.67	0.58
1:A:37:ARG:HA	1:A:40:LEU:HG	1.86	0.58
1:B:16:HIS:C	1:B:17:ILE:HD12	2.27	0.58
1:B:406:LYS:HD2	1:B:406:LYS:N	2.07	0.58
2:H:43:LEU:N	2:H:43:LEU:HD12	2.18	0.58
2:L:43:LEU:CD2	2:L:43:LEU:H	2.16	0.58
2:L:67:HIS:CD2	2:L:77:GLU:HG3	2.38	0.58
2:L:120:ILE:HD11	2:L:138:VAL:HG11	1.85	0.58
2:N:60:PHE:HB2	2:N:78:LEU:HD22	1.85	0.58
1:A:26:ALA:CB	1:A:331:VAL:HG11	2.32	0.58
1:B:80:LYS:HG3	1:B:255:PHE:HD2	1.69	0.58
1:C:312:GLN:NE2	2:I:66:MET:HG2	2.17	0.58
1:C:360:MET:HA	1:C:360:MET:CE	2.31	0.58
2:H:37:LEU:HB2	2:H:42:VAL:CG2	2.32	0.58
1:B:105:ASP:C	1:B:107:ALA:H	2.12	0.58
1:A:34:ARG:HH11	1:A:34:ARG:CB	2.17	0.58
2:L:161:VAL:HG23	2:L:162:PHE:CD1	2.39	0.58
2:N:131:LEU:HD11	2:N:135:ARG:NE	2.18	0.58
1:C:84:THR:O	1:C:86:PHE:N	2.36	0.58
2:L:43:LEU:H	2:L:43:LEU:HD23	1.68	0.58
1:B:443:ILE:CG2	1:B:444:LEU:N	2.67	0.58
1:C:9:ILE:CD1	1:C:31:LEU:HD23	2.34	0.58
2:I:71:LEU:HD21	2:I:97:VAL:CG2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:MET:O	1:B:308:SER:HA	2.04	0.57
1:B:62:GLY:O	1:B:66:ILE:HG13	2.03	0.57
2:G:46:PHE:HB3	2:G:95:LEU:CD2	2.33	0.57
2:I:141:THR:CG2	2:I:143:LEU:HG	2.33	0.57
2:N:80:LYS:HB2	2:N:80:LYS:HZ2	1.66	0.57
1:C:17:ILE:HG21	1:C:66:ILE:HD11	1.86	0.57
2:H:42:VAL:HG12	2:H:99:ASP:HB3	1.85	0.57
2:H:83:ARG:HG2	2:I:55:THR:HB	1.85	0.57
2:M:38:TYR:CE2	2:M:64:LEU:HD22	2.38	0.57
2:M:172:LEU:HB3	2:M:173:PRO:HD3	1.86	0.57
1:A:443:ILE:HD11	2:G:72:LEU:HD11	1.85	0.57
1:C:63:LYS:HB2	3:C:450:ADP:O2B	2.04	0.57
2:H:115:PRO:HG3	2:H:121:LEU:HD11	1.87	0.57
2:G:37:LEU:HB2	2:G:42:VAL:CG2	2.34	0.57
1:C:68:ARG:HG2	1:C:68:ARG:HH11	1.69	0.57
2:M:59:LEU:O	2:M:63:LYS:HB2	2.05	0.57
2:N:12:VAL:HG13	2:N:12:VAL:O	2.04	0.57
2:N:137:LEU:HD22	2:N:137:LEU:H	1.69	0.57
2:N:148:ILE:HG22	2:N:149:VAL:N	2.19	0.57
1:B:338:ALA:O	1:B:342:GLU:HG3	2.04	0.57
1:C:352:LEU:HD13	1:C:400:MET:HG3	1.85	0.57
1:C:370:THR:O	1:C:373:ALA:N	2.36	0.57
2:H:67:HIS:HD2	2:H:73:LYS:HD3	1.68	0.57
2:N:6:VAL:HG13	2:N:120:ILE:HG12	1.86	0.57
2:H:7:ARG:NH1	2:H:12:VAL:HG13	2.20	0.57
2:M:72:LEU:CD1	2:M:104:LEU:HD21	2.35	0.57
2:I:51:ALA:O	2:I:55:THR:HG22	2.05	0.57
2:L:3:ILE:HG22	2:L:96:ILE:HD12	1.87	0.57
2:M:130:ALA:N	2:M:156:ALA:HB2	2.20	0.57
1:B:311:PHE:HD1	1:B:314:ALA:O	1.88	0.57
2:M:28:LYS:HG2	2:M:29:GLY:N	2.19	0.57
1:A:18:ILE:HD13	1:A:348:PRO:HG3	1.85	0.56
2:G:19:GLN:HE21	2:G:164:ASN:HB3	1.70	0.56
2:G:91:LEU:H	2:G:91:LEU:CD1	2.18	0.56
2:N:60:PHE:O	2:N:63:LYS:HB2	2.05	0.56
2:G:98:ALA:HB2	2:G:103:SER:HA	1.87	0.56
2:L:172:LEU:HD23	2:L:173:PRO:CA	2.35	0.56
2:N:38:TYR:CD1	2:N:41:LYS:HD3	2.41	0.56
1:B:245:ILE:O	1:B:246:ASP:C	2.46	0.56
1:C:330:ARG:HH11	1:C:330:ARG:CB	2.14	0.56
2:H:61:GLU:O	2:H:63:LYS:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:GLU:C	2:H:63:LYS:N	2.61	0.56
2:I:22:LEU:O	2:I:25:THR:HG22	2.06	0.56
2:I:67:HIS:HD2	2:I:73:LYS:HG2	1.71	0.56
2:I:90:LYS:O	2:I:90:LYS:HG2	2.05	0.56
2:L:64:LEU:HG	2:L:74:SER:OG	2.05	0.56
2:L:73:LYS:O	2:L:76:VAL:HG22	2.05	0.56
2:G:1:THR:HB	6:G:0:LVS:H1'3	1.88	0.56
2:H:141:THR:CG2	2:H:142:GLU:N	2.68	0.56
1:B:5:THR:O	1:B:6:PRO:C	2.48	0.56
1:B:59:THR:HA	5:B:452:PO4:P	2.46	0.56
1:C:32:ARG:O	1:C:35:TRP:HB3	2.06	0.56
1:C:330:ARG:HB3	1:C:330:ARG:NH1	2.13	0.56
2:L:103:SER:O	2:L:104:LEU:HD23	2.05	0.56
1:A:339:ALA:O	1:A:343:ARG:HG3	2.06	0.56
1:B:351:SER:O	1:B:355:GLN:HG3	2.06	0.56
2:L:144:SER:H	2:L:147:GLU:HB2	1.70	0.56
1:C:102:ASP:O	1:C:105:ASP:HB2	2.05	0.56
1:A:26:ALA:HB2	1:A:331:VAL:CG1	2.36	0.56
1:C:41:GLN:HE21	1:C:41:GLN:CA	2.16	0.56
2:G:62:ARG:O	2:G:66:MET:HG3	2.05	0.56
2:N:72:LEU:HD12	2:N:104:LEU:HG	1.88	0.56
1:B:342:GLU:OE1	1:B:375:LYS:HE2	2.06	0.56
2:I:27:MET:HA	2:I:27:MET:CE	2.31	0.56
2:G:146:HIS:ND1	2:G:146:HIS:O	2.40	0.55
2:H:19:GLN:N	2:H:33:LYS:NZ	2.54	0.55
1:B:356:TYR:O	1:B:357:LYS:C	2.49	0.55
1:C:46:HIS:O	1:C:48:VAL:N	2.39	0.55
1:C:275:ARG:O	1:C:278:VAL:HG23	2.06	0.55
2:G:50:THR:HG23	2:G:51:ALA:H	1.68	0.55
1:A:245:ILE:C	1:A:247:ALA:H	2.14	0.55
2:H:76:VAL:O	2:H:79:ALA:HB3	2.06	0.55
2:M:164:ASN:ND2	2:M:166:ASN:HB2	2.20	0.55
1:A:57:GLY:O	1:A:63:LYS:HE2	2.07	0.55
2:G:77:GLU:O	2:G:80:LYS:HB3	2.05	0.55
2:L:5:SER:CB	2:L:14:VAL:HG22	2.37	0.55
2:L:17:ASP:HB3	2:L:163:THR:HG23	1.87	0.55
2:L:144:SER:HB3	2:L:147:GLU:HG3	1.88	0.55
2:L:148:ILE:HG22	2:L:149:VAL:N	2.21	0.55
2:M:51:ALA:O	2:M:52:ASP:C	2.49	0.55
2:N:126:GLY:O	2:N:127:GLY:C	2.49	0.55
1:B:57:GLY:N	1:B:63:LYS:HE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ALA:O	1:C:361:ALA:HB3	2.07	0.55
2:I:97:VAL:HG22	2:I:104:LEU:HD12	1.89	0.55
2:L:13:VAL:HG22	2:L:171:GLU:HG3	1.89	0.55
1:B:290:THR:HG22	1:B:297:MET:HE3	1.89	0.55
1:C:257:ASP:OD1	1:C:258:GLU:N	2.40	0.55
2:H:36:ARG:O	2:H:37:LEU:HD23	2.07	0.55
2:H:56:LEU:CD1	2:H:95:LEU:HB2	2.32	0.55
1:A:37:ARG:O	1:A:38:MET:CB	2.49	0.55
1:A:443:ILE:HG12	2:G:112:VAL:CG2	2.36	0.55
2:H:71:LEU:HD11	2:H:97:VAL:HG23	1.89	0.55
2:H:100:GLU:O	2:H:101:LYS:HD3	2.06	0.55
2:H:153:LEU:HD22	2:H:167:PHE:CD2	2.41	0.55
1:B:23:ALA:CA	1:B:331:VAL:HG21	2.32	0.55
1:C:104:THR:HG21	1:C:298:VAL:HG11	1.89	0.55
2:H:61:GLU:C	2:H:63:LYS:H	2.15	0.55
1:A:73:LEU:HD12	1:A:73:LEU:C	2.32	0.55
1:B:367:ILE:HA	1:B:419:VAL:O	2.07	0.55
1:C:34:ARG:NH2	1:C:251:ASN:C	2.65	0.55
2:H:143:LEU:HD22	2:H:147:GLU:OE1	2.06	0.55
2:M:106:ILE:HG22	2:M:107:THR:N	2.21	0.55
2:H:47:ALA:O	2:H:93:ALA:HB1	2.06	0.55
2:I:5:SER:HA	2:I:13:VAL:O	2.06	0.55
2:L:115:PRO:HB2	2:L:119:GLN:OE1	2.07	0.55
2:M:71:LEU:HD12	2:M:71:LEU:N	2.18	0.55
2:M:87:ALA:C	2:M:88:LEU:HD12	2.32	0.55
1:A:360:MET:HE1	1:A:408:SER:HA	1.89	0.54
1:C:82:GLU:OE2	1:C:258:GLU:HG3	2.07	0.54
2:G:86:ARG:HH11	2:G:86:ARG:HB2	1.71	0.54
2:G:172:LEU:O	2:G:173:PRO:C	2.50	0.54
2:H:3:ILE:HG22	2:H:96:ILE:HD12	1.89	0.54
2:H:82:TRP:HZ2	2:H:91:LEU:HD23	1.71	0.54
2:I:145:ALA:O	2:I:149:VAL:HG23	2.07	0.54
2:N:73:LYS:HE3	2:N:73:LYS:HA	1.88	0.54
1:A:245:ILE:C	1:A:247:ALA:N	2.64	0.54
1:B:352:LEU:HD13	1:B:400:MET:HG3	1.88	0.54
2:G:144:SER:HB3	2:G:147:GLU:HG3	1.89	0.54
2:M:126:GLY:HA2	2:M:129:TYR:CD2	2.42	0.54
2:N:157:GLY:HA2	2:N:163:THR:HB	1.90	0.54
1:A:311:PHE:HB3	1:A:314:ALA:O	2.07	0.54
2:L:77:GLU:O	2:L:80:LYS:HB2	2.08	0.54
1:A:41:GLN:HE21	1:A:41:GLN:HA	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:VAL:HG11	1:B:326:ARG:CB	2.29	0.54
1:B:380:ALA:O	1:B:383:ARG:HB3	2.07	0.54
1:C:283:LEU:HB2	1:C:284:PRO:HD3	1.89	0.54
2:I:134:ALA:O	2:I:136:ALA:N	2.40	0.54
2:M:3:ILE:HB	2:M:123:ILE:CG1	2.36	0.54
2:I:1:THR:HA	2:I:33:LYS:NZ	2.22	0.54
2:H:44:ALA:HB1	2:H:95:LEU:HD21	1.88	0.54
2:L:38:TYR:CE2	2:L:64:LEU:HD22	2.42	0.54
2:L:148:ILE:O	2:L:149:VAL:C	2.50	0.54
1:A:37:ARG:HH21	1:A:302:HIS:CD2	2.24	0.54
2:M:67:HIS:O	2:M:68:GLN:HB3	2.06	0.54
1:B:434:VAL:HG12	1:B:435:GLU:N	2.23	0.54
1:C:404:MET:O	1:C:408:SER:HB2	2.08	0.54
2:G:33:LYS:HA	2:G:46:PHE:CE2	2.43	0.54
2:H:16:GLY:HA2	2:H:153:LEU:HD21	1.87	0.54
2:N:109:ILE:HG22	2:N:109:ILE:O	2.07	0.54
1:B:283:LEU:O	1:B:285:LEU:N	2.41	0.54
1:B:355:GLN:O	1:B:356:TYR:C	2.50	0.54
1:C:38:MET:HA	1:C:38:MET:HE3	1.89	0.54
2:M:17:ASP:OD2	2:M:33:LYS:HE3	2.08	0.54
2:I:89:ARG:HG2	2:I:90:LYS:HD3	1.89	0.54
2:I:147:GLU:O	2:I:151:LYS:HB2	2.08	0.54
1:A:286:VAL:HG11	1:A:326:ARG:HB3	1.90	0.53
1:A:443:ILE:HG22	1:A:444:LEU:N	2.22	0.53
1:B:9:ILE:HG21	1:B:28:ALA:HA	1.90	0.53
1:C:77:PRO:HG3	1:C:107:ALA:HB2	1.88	0.53
2:H:33:LYS:HE3	6:H:0:LVS:HB32	1.89	0.53
2:L:34:VAL:HA	2:L:45:GLY:HA2	1.90	0.53
2:M:135:ARG:O	2:M:139:GLU:HB2	2.08	0.53
2:N:135:ARG:HB3	2:N:139:GLU:OE2	2.07	0.53
1:C:439:LEU:C	1:C:441:ARG:H	2.16	0.53
2:L:58:GLU:O	2:L:62:ARG:HD3	2.07	0.53
2:G:91:LEU:HD12	2:G:91:LEU:H	1.73	0.53
2:M:144:SER:HB3	2:M:147:GLU:HB2	1.90	0.53
1:B:367:ILE:HD11	1:B:421:ILE:CD1	2.38	0.53
1:C:439:LEU:HD13	2:I:72:LEU:HD12	1.91	0.53
2:L:161:VAL:HG23	2:L:162:PHE:CE1	2.44	0.53
2:M:129:TYR:HB2	2:M:156:ALA:CB	2.38	0.53
2:M:2:THR:HG21	2:M:156:ALA:O	2.09	0.53
2:M:147:GLU:O	2:M:151:LYS:HG3	2.09	0.53
2:M:148:ILE:HG22	2:M:149:VAL:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:13:VAL:HG21	2:G:145:ALA:C	2.33	0.53
2:H:151:LYS:CE	2:N:140:ASN:HD21	2.13	0.53
2:I:71:LEU:HD13	2:I:71:LEU:C	2.34	0.53
2:M:7:ARG:HA	2:M:11:GLN:O	2.09	0.53
2:G:50:THR:CG2	2:G:51:ALA:H	2.20	0.53
2:H:27:MET:HE3	2:H:27:MET:HA	1.90	0.53
2:H:71:LEU:HB2	2:H:99:ASP:OD1	2.07	0.53
2:I:71:LEU:HD21	2:I:97:VAL:HG23	1.89	0.53
1:A:79:ILE:HG21	1:A:103:LEU:HB2	1.90	0.53
1:A:367:ILE:HG12	1:A:368:ALA:N	2.24	0.53
2:I:38:TYR:CE1	2:I:69:GLY:HA3	2.43	0.53
2:N:50:THR:C	2:N:52:ASP:H	2.16	0.53
1:A:25:ARG:O	1:A:28:ALA:HB3	2.09	0.53
1:C:17:ILE:HB	1:C:24:LYS:HE3	1.90	0.53
2:G:5:SER:HB2	2:G:14:VAL:HG22	1.91	0.53
2:M:72:LEU:O	2:M:76:VAL:HG23	2.09	0.53
1:A:37:ARG:C	1:A:39:GLN:H	2.17	0.53
1:B:72:LYS:C	1:B:72:LYS:HD2	2.34	0.53
2:H:15:GLY:C	2:H:153:LEU:HD11	2.34	0.53
2:L:5:SER:HB3	2:L:121:LEU:HB2	1.89	0.53
2:N:33:LYS:HA	2:N:46:PHE:CE1	2.44	0.53
2:G:105:ILE:CG2	2:G:121:LEU:HD13	2.36	0.52
2:G:156:ALA:O	2:G:159:ILE:N	2.36	0.52
2:I:91:LEU:O	2:I:93:ALA:N	2.41	0.52
2:I:115:PRO:HG3	2:I:121:LEU:HG	1.91	0.52
2:L:67:HIS:NE2	2:L:77:GLU:HG3	2.24	0.52
2:L:146:HIS:ND1	2:L:146:HIS:O	2.42	0.52
2:M:81:ASP:O	2:M:82:TRP:HB2	2.09	0.52
1:A:370:THR:O	1:A:373:ALA:N	2.40	0.52
1:B:443:ILE:HG23	2:H:112:VAL:HG23	1.92	0.52
2:G:46:PHE:HD2	2:G:46:PHE:O	1.92	0.52
2:L:46:PHE:CE2	2:L:50:THR:HA	2.44	0.52
1:B:410:SER:O	1:B:412:SER:N	2.42	0.52
1:B:426:VAL:C	1:B:428:ASP:H	2.18	0.52
2:H:7:ARG:HG3	2:H:7:ARG:NH1	2.23	0.52
2:I:6:VAL:HG12	2:I:7:ARG:N	2.25	0.52
2:N:58:GLU:O	2:N:60:PHE:N	2.36	0.52
1:A:34:ARG:HH11	1:A:34:ARG:HB2	1.74	0.52
1:A:370:THR:O	1:A:371:THR:C	2.51	0.52
1:B:61:VAL:HG23	1:B:61:VAL:O	2.09	0.52
2:G:14:VAL:O	2:G:34:VAL:HG11	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:43:LEU:HD11	2:N:171:GLU:O	2.08	0.52
1:A:6:PRO:O	1:A:10:VAL:HG23	2.09	0.52
1:B:356:TYR:O	1:B:359:LEU:N	2.43	0.52
2:L:73:LYS:HA	2:L:76:VAL:HG22	1.91	0.52
2:M:34:VAL:HG13	2:M:44:ALA:O	2.10	0.52
2:M:76:VAL:O	2:M:79:ALA:HB3	2.10	0.52
1:A:245:ILE:O	1:A:247:ALA:N	2.43	0.52
1:C:293:THR:O	1:C:295:HIS:N	2.43	0.52
2:M:96:ILE:HG12	2:M:105:ILE:HG12	1.91	0.52
2:M:146:HIS:O	2:M:148:ILE:N	2.43	0.52
1:B:41:GLN:HE21	1:B:42:GLU:H	1.58	0.52
1:C:406:LYS:H	1:C:406:LYS:CD	2.01	0.52
2:H:13:VAL:HG21	2:H:146:HIS:N	2.25	0.52
2:H:76:VAL:HG12	2:H:80:LYS:HE2	1.92	0.52
1:A:315:ARG:HE	1:A:316:PRO:HD3	1.75	0.52
1:B:54:LEU:HD12	1:B:307:ALA:O	2.10	0.52
2:G:34:VAL:HA	2:G:44:ALA:O	2.10	0.52
2:H:1:THR:HG23	2:H:33:LYS:CD	2.40	0.52
2:M:91:LEU:N	2:M:91:LEU:HD12	2.24	0.52
1:C:23:ALA:HA	1:C:331:VAL:HG11	1.92	0.52
1:A:313:VAL:HG23	1:A:314:ALA:N	2.26	0.51
2:H:136:ALA:O	2:H:138:VAL:N	2.36	0.51
2:I:155:ILE:O	2:I:158:ASP:HB2	2.11	0.51
2:L:64:LEU:CD2	2:L:69:GLY:HA2	2.40	0.51
2:M:28:LYS:HD3	2:M:31:ALA:HB2	1.91	0.51
2:M:64:LEU:O	2:M:64:LEU:HD23	2.11	0.51
1:A:12:GLU:OE1	1:A:12:GLU:HA	2.09	0.51
1:A:352:LEU:HD21	1:A:397:HIS:CE1	2.45	0.51
1:B:383:ARG:NH2	1:B:387:LYS:HE3	2.25	0.51
1:C:22:ASP:O	1:C:25:ARG:HB2	2.10	0.51
2:G:33:LYS:HE2	6:G:0:LVS:HB32	1.92	0.51
2:H:76:VAL:O	2:H:80:LYS:HD3	2.10	0.51
2:M:36:ARG:O	2:M:37:LEU:HD23	2.09	0.51
2:M:88:LEU:CA	2:M:91:LEU:HD13	2.38	0.51
1:A:444:LEU:OXT	2:G:113:VAL:HG13	2.11	0.51
1:C:359:LEU:O	1:C:362:THR:OG1	2.25	0.51
1:C:425:TYR:O	1:C:426:VAL:C	2.52	0.51
2:G:80:LYS:NZ	2:G:84:THR:HG22	2.26	0.51
2:I:97:VAL:CG2	2:I:104:LEU:HD12	2.41	0.51
2:M:79:ALA:HB2	2:M:112:VAL:CG2	2.41	0.51
2:N:88:LEU:CA	2:N:91:LEU:HD13	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:141:THR:HG21	2:G:143:LEU:HD12	1.92	0.51
2:I:18:GLY:O	2:I:29:GLY:HA2	2.10	0.51
2:L:6:VAL:HG12	2:L:7:ARG:N	2.25	0.51
2:N:13:VAL:HG22	2:N:171:GLU:HG2	1.91	0.51
1:A:43:PRO:O	1:A:47:GLU:HG2	2.10	0.51
1:B:101:ARG:HG3	1:B:293:THR:HG22	1.92	0.51
2:I:118:ASP:O	2:I:119:GLN:C	2.54	0.51
2:L:56:LEU:HD13	2:L:95:LEU:HD11	1.91	0.51
2:M:12:VAL:HG21	2:M:98:ALA:HB1	1.93	0.51
2:M:138:VAL:O	2:M:140:ASN:N	2.43	0.51
1:A:327:LEU:N	1:A:328:PRO:HD3	2.23	0.51
2:H:37:LEU:HD21	2:H:57:PHE:CZ	2.46	0.51
2:M:19:GLN:HE22	2:M:162:PHE:HA	1.75	0.51
1:C:405:ASP:HB3	1:C:406:LYS:HD2	1.91	0.51
2:G:141:THR:HG1	2:G:143:LEU:HG	1.71	0.51
2:M:2:THR:CG2	2:M:126:GLY:HA3	2.39	0.51
1:B:9:ILE:HG21	1:B:28:ALA:CB	2.40	0.51
1:B:17:ILE:HG23	3:B:450:ADP:N6	2.26	0.51
1:C:20:GLN:HE22	1:C:334:THR:N	2.09	0.51
2:M:20:VAL:CG2	2:M:28:LYS:HB3	2.41	0.51
2:M:33:LYS:HA	2:M:46:PHE:CE1	2.46	0.51
1:A:19:GLY:O	1:A:24:LYS:NZ	2.41	0.51
1:A:443:ILE:HG12	2:G:112:VAL:HG21	1.93	0.51
1:B:342:GLU:CD	1:B:375:LYS:HE2	2.36	0.51
2:G:50:THR:O	2:G:54:PHE:HD1	1.93	0.51
2:I:134:ALA:C	2:I:136:ALA:N	2.69	0.51
2:M:126:GLY:HA2	2:M:129:TYR:CE2	2.46	0.51
1:A:53:ILE:CG2	1:A:54:LEU:N	2.73	0.51
1:C:61:VAL:C	3:C:450:ADP:N7	2.69	0.51
2:H:49:GLY:O	2:H:50:THR:C	2.52	0.51
2:M:2:THR:HG22	2:M:126:GLY:C	2.36	0.51
2:N:20:VAL:HG23	2:N:28:LYS:HB3	1.93	0.51
2:N:20:VAL:CG2	2:N:28:LYS:HB3	2.41	0.51
1:B:86:PHE:O	1:B:87:THR:OG1	2.25	0.50
1:B:443:ILE:HG12	2:H:112:VAL:HG23	1.93	0.50
2:G:1:THR:HB	6:G:0:LVS:C1'	2.41	0.50
2:G:33:LYS:HA	2:G:46:PHE:HE2	1.76	0.50
2:G:52:ASP:HA	2:G:55:THR:HG22	1.92	0.50
2:M:1:THR:HG23	2:M:17:ASP:OD1	2.11	0.50
2:G:13:VAL:HG21	2:G:146:HIS:CA	2.41	0.50
2:L:144:SER:C	2:L:146:HIS:N	2.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:90:LYS:C	2:N:91:LEU:HD12	2.37	0.50
1:C:100:ILE:HB	1:C:291:VAL:HG21	1.93	0.50
2:H:67:HIS:NE2	2:H:77:GLU:HG3	2.25	0.50
2:L:141:THR:HG22	2:L:143:LEU:HG	1.93	0.50
1:A:102:ASP:O	1:A:105:ASP:HB2	2.11	0.50
1:A:430:LEU:O	1:A:431:GLY:C	2.54	0.50
1:A:249:GLU:HG3	1:A:298:VAL:HG13	1.94	0.50
1:B:276:GLU:C	1:B:278:VAL:H	2.18	0.50
1:B:343:ARG:HE	1:B:347:GLU:CD	2.19	0.50
1:C:84:THR:C	1:C:86:PHE:H	2.19	0.50
1:C:360:MET:HE2	1:C:360:MET:CA	2.32	0.50
2:G:4:VAL:HG12	2:G:153:LEU:CD2	2.41	0.50
2:G:117:GLU:C	2:G:119:GLN:N	2.69	0.50
2:G:144:SER:O	2:G:148:ILE:HG13	2.11	0.50
2:H:27:MET:HE3	2:H:27:MET:O	2.12	0.50
2:I:141:THR:HB	2:I:143:LEU:HG	1.93	0.50
1:B:15:GLN:O	1:B:16:HIS:CG	2.64	0.50
2:I:153:LEU:O	2:I:154:ARG:C	2.54	0.50
2:N:149:VAL:HG12	2:N:149:VAL:O	2.12	0.50
2:I:73:LYS:O	2:I:74:SER:C	2.54	0.50
2:L:37:LEU:HD11	2:L:57:PHE:HB3	1.92	0.50
2:M:90:LYS:C	2:M:91:LEU:HD12	2.37	0.50
1:C:374:VAL:C	1:C:376:LYS:N	2.68	0.50
2:I:2:THR:HB	2:I:163:THR:HG21	1.93	0.50
2:N:11:GLN:HE22	2:N:173:PRO:HB2	1.75	0.50
2:N:110:GLY:O	2:N:111:ASP:HB3	2.12	0.50
1:B:42:GLU:CB	1:B:43:PRO:HD3	2.32	0.50
1:C:341:PHE:HB2	1:C:378:ALA:HB1	1.92	0.50
2:G:115:PRO:HG3	2:G:121:LEU:CD1	2.42	0.50
2:H:155:ILE:O	2:H:158:ASP:HB2	2.12	0.50
2:N:44:ALA:HB1	2:N:57:PHE:CE1	2.46	0.50
2:N:138:VAL:HG23	2:N:148:ILE:HD13	1.94	0.50
1:A:83:ALA:HB1	1:A:262:ILE:HD13	1.94	0.49
1:C:29:ILE:O	1:C:32:ARG:N	2.43	0.49
1:C:422:ASP:O	1:C:423:ALA:C	2.55	0.49
2:G:125:SER:H	6:G:0:LVS:H1'1	1.76	0.49
2:I:2:THR:HG22	2:I:153:LEU:HD22	1.93	0.49
2:I:36:ARG:HH11	2:I:170:GLU:HB3	1.77	0.49
2:I:94:MET:SD	2:I:105:ILE:HD11	2.52	0.49
2:L:17:ASP:CG	2:L:33:LYS:HZ1	2.19	0.49
2:M:155:ILE:O	2:M:157:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:169:ILE:N	2:N:169:ILE:HD12	2.27	0.49
1:A:56:ILE:HD11	1:A:316:PRO:HG2	1.93	0.49
1:A:443:ILE:CG2	1:A:444:LEU:N	2.75	0.49
2:H:7:ARG:NH2	2:H:12:VAL:HG11	2.27	0.49
2:N:52:ASP:OD2	2:N:91:LEU:HD23	2.11	0.49
1:A:11:SER:HA	1:A:14:ASP:HB2	1.95	0.49
1:A:313:VAL:HG23	1:A:314:ALA:H	1.76	0.49
2:H:58:GLU:O	2:H:61:GLU:HB3	2.12	0.49
2:M:12:VAL:HG13	2:M:12:VAL:O	2.13	0.49
1:A:32:ARG:O	1:A:35:TRP:HB3	2.11	0.49
1:A:250:GLN:HE21	1:A:250:GLN:CA	2.25	0.49
1:A:343:ARG:HH21	1:A:347:GLU:CD	2.19	0.49
1:A:345:LEU:HD13	1:A:396:LEU:HD13	1.93	0.49
1:B:273:VAL:HA	1:B:276:GLU:HB3	1.94	0.49
1:C:26:ALA:HB2	1:C:331:VAL:CG1	2.43	0.49
1:C:33:ASN:O	1:C:34:ARG:C	2.52	0.49
2:H:2:THR:O	2:H:3:ILE:HD13	2.12	0.49
2:I:43:LEU:HD12	2:I:98:ALA:O	2.12	0.49
2:L:133:ALA:O	2:L:134:ALA:C	2.55	0.49
2:N:80:LYS:HB2	2:N:80:LYS:HZ3	1.73	0.49
1:A:42:GLU:CB	1:A:43:PRO:HD3	2.41	0.49
1:B:286:VAL:CG1	1:B:326:ARG:HB3	2.31	0.49
2:G:38:TYR:C	2:G:40:GLY:H	2.21	0.49
2:G:47:ALA:O	2:G:93:ALA:HB1	2.13	0.49
2:I:15:GLY:HA2	2:I:34:VAL:HG21	1.95	0.49
2:I:24:ASN:O	2:N:161:VAL:HG13	2.13	0.49
2:I:43:LEU:HD12	2:I:43:LEU:N	2.19	0.49
2:I:99:ASP:HA	2:I:172:LEU:CD1	2.43	0.49
2:N:82:TRP:CD2	2:N:108:GLY:HA2	2.47	0.49
1:A:36:ARG:C	1:A:37:ARG:O	2.51	0.49
1:A:37:ARG:HG2	1:A:38:MET:N	2.26	0.49
1:B:26:ALA:O	1:B:28:ALA:N	2.46	0.49
1:C:383:ARG:O	1:C:387:LYS:HG2	2.12	0.49
2:L:90:LYS:C	2:L:91:LEU:HD12	2.38	0.49
2:M:6:VAL:HG21	2:M:148:ILE:CG2	2.42	0.49
1:A:437:GLU:O	1:A:437:GLU:HG3	2.12	0.49
1:C:53:ILE:HG12	1:C:329:ILE:HG21	1.94	0.49
2:G:18:GLY:H	2:G:164:ASN:ND2	2.06	0.49
2:I:36:ARG:HD2	2:I:170:GLU:OE2	2.13	0.49
1:C:20:GLN:HE22	1:C:334:THR:H	1.59	0.49
2:H:76:VAL:HG12	2:H:80:LYS:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:120:ILE:HD12	2:H:135:ARG:HA	1.94	0.49
2:I:153:LEU:O	2:I:156:ALA:N	2.45	0.49
2:L:115:PRO:HG3	2:L:121:LEU:HD21	1.94	0.49
2:M:86:ARG:HH11	2:M:86:ARG:CA	2.26	0.49
1:B:283:LEU:O	1:B:284:PRO:C	2.55	0.49
1:C:3:GLU:OE1	1:C:3:GLU:HA	2.12	0.49
1:C:84:THR:C	1:C:86:PHE:N	2.70	0.49
2:G:7:ARG:HB3	2:G:119:GLN:HB3	1.95	0.49
2:H:38:TYR:C	2:H:40:GLY:N	2.69	0.49
2:I:127:GLY:O	2:I:131:LEU:N	2.36	0.49
2:N:115:PRO:HG3	2:N:121:LEU:HD21	1.95	0.49
1:B:299:LYS:C	1:B:301:ASP:H	2.21	0.49
1:B:360:MET:HE1	1:B:408:SER:HA	1.95	0.49
1:C:38:MET:HE3	1:C:45:ARG:HD2	1.93	0.49
1:C:357:LYS:HE2	1:C:368:ALA:HA	1.94	0.49
1:C:395:ARG:O	1:C:399:VAL:HG23	2.13	0.49
2:I:36:ARG:O	2:I:37:LEU:HD23	2.13	0.49
2:N:1:THR:HG23	2:N:33:LYS:HZ2	1.78	0.49
1:A:76:ALA:HB1	1:A:251:ASN:O	2.12	0.48
1:A:287:GLU:O	1:A:287:GLU:HG2	2.12	0.48
1:C:68:ARG:HG2	1:C:68:ARG:NH1	2.28	0.48
2:G:26:VAL:HG12	2:G:26:VAL:O	2.12	0.48
2:G:56:LEU:HD22	2:G:95:LEU:CD1	2.39	0.48
2:I:3:ILE:HB	2:I:123:ILE:HG13	1.94	0.48
1:A:390:ASN:HB2	2:G:68:GLN:NE2	2.27	0.48
1:B:374:VAL:O	1:B:375:LYS:C	2.56	0.48
1:C:98:SER:O	1:C:99:ILE:C	2.55	0.48
2:G:33:LYS:O	2:G:45:GLY:HA2	2.13	0.48
2:H:7:ARG:CZ	2:H:12:VAL:HG13	2.43	0.48
1:A:51:LYS:O	1:A:329:ILE:HD12	2.14	0.48
1:C:5:THR:HG23	1:C:8:GLU:OE1	2.12	0.48
2:G:71:LEU:O	2:G:72:LEU:C	2.56	0.48
2:L:116:GLU:C	2:L:118:ASP:N	2.71	0.48
1:A:38:MET:HA	1:A:45:ARG:HD2	1.96	0.48
1:B:37:ARG:HB3	1:B:48:VAL:HG11	1.94	0.48
1:B:44:LEU:O	1:B:45:ARG:C	2.55	0.48
1:B:256:ILE:HG21	1:B:259:ILE:HD13	1.94	0.48
1:B:401:GLU:OE1	1:C:51:LYS:HG3	2.12	0.48
1:C:40:LEU:HD12	1:C:48:VAL:HG11	1.94	0.48
2:G:144:SER:HB3	2:G:147:GLU:CG	2.44	0.48
2:H:3:ILE:O	2:H:122:ALA:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:105:ILE:HD12	2:L:121:LEU:HD22	1.96	0.48
2:N:17:ASP:OD2	2:N:163:THR:HG23	2.13	0.48
2:N:57:PHE:O	2:N:61:GLU:HG2	2.13	0.48
1:A:323:LEU:O	1:A:324:GLN:C	2.56	0.48
1:B:48:VAL:HG13	1:B:48:VAL:O	2.12	0.48
1:B:443:ILE:CG2	1:B:444:LEU:H	2.26	0.48
2:G:13:VAL:HG11	2:G:146:HIS:HA	1.94	0.48
2:I:133:ALA:O	2:I:134:ALA:C	2.57	0.48
2:M:28:LYS:NZ	2:M:30:ASN:ND2	2.60	0.48
2:N:146:HIS:CD2	2:N:169:ILE:HG21	2.49	0.48
1:A:79:ILE:HD12	1:A:80:LYS:H	1.79	0.48
1:C:374:VAL:O	1:C:376:LYS:N	2.47	0.48
2:G:36:ARG:NH1	2:G:170:GLU:OE2	2.47	0.48
2:G:136:ALA:O	2:G:139:GLU:N	2.47	0.48
2:H:120:ILE:HD13	2:H:134:ALA:HB1	1.96	0.48
2:I:120:ILE:O	2:I:121:LEU:HD23	2.14	0.48
2:M:105:ILE:HD12	2:M:121:LEU:HD22	1.96	0.48
2:N:155:ILE:O	2:N:159:ILE:HG13	2.13	0.48
1:A:81:VAL:HG21	1:A:99:ILE:HD13	1.96	0.48
1:A:330:ARG:CB	1:A:330:ARG:NH1	2.75	0.48
1:A:398:THR:O	1:A:399:VAL:C	2.56	0.48
2:H:132:SER:O	2:H:133:ALA:C	2.57	0.48
1:A:54:LEU:HD13	1:A:327:LEU:HD13	1.94	0.48
1:A:421:ILE:HG23	1:A:425:TYR:CD2	2.48	0.48
1:B:3:GLU:HA	1:B:3:GLU:OE1	2.12	0.48
1:B:37:ARG:HD2	1:B:48:VAL:CG1	2.41	0.48
1:B:414:MET:O	1:B:417:GLN:HG3	2.13	0.48
2:G:4:VAL:HG12	2:G:153:LEU:HD21	1.95	0.48
2:G:107:THR:OG1	2:G:109:ILE:HG12	2.14	0.48
2:L:91:LEU:HD12	2:L:91:LEU:N	2.28	0.48
2:M:112:VAL:HG12	2:M:113:VAL:N	2.28	0.48
1:B:377:ILE:O	1:B:380:ALA:HB3	2.13	0.48
1:C:349:HIS:O	1:C:350:ALA:HB3	2.13	0.48
2:G:128:ASN:O	2:G:131:LEU:HB3	2.13	0.48
2:H:25:THR:HA	2:M:159:ILE:O	2.13	0.48
2:N:42:VAL:HA	2:N:98:ALA:O	2.13	0.48
1:A:20:GLN:NE2	1:A:334:THR:HG22	2.28	0.48
2:I:73:LYS:HA	2:I:76:VAL:HG23	1.95	0.48
2:M:28:LYS:HZ2	2:M:30:ASN:CG	2.21	0.48
2:N:104:LEU:HD12	2:N:114:GLN:HA	1.94	0.48
1:A:315:ARG:HG3	1:A:316:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:49:GLY:O	2:I:50:THR:C	2.55	0.47
2:M:59:LEU:O	2:M:59:LEU:HD12	2.15	0.47
2:N:5:SER:OG	2:N:14:VAL:HG22	2.13	0.47
1:C:23:ALA:O	1:C:27:VAL:HG13	2.14	0.47
1:C:63:LYS:HD2	1:C:308:SER:HB2	1.95	0.47
2:G:164:ASN:C	2:G:164:ASN:HD22	2.22	0.47
2:N:116:GLU:O	2:N:118:ASP:N	2.47	0.47
1:B:367:ILE:CG1	1:B:368:ALA:N	2.75	0.47
1:B:424:ALA:C	1:B:426:VAL:N	2.69	0.47
1:C:52:ASN:ND2	1:C:305:PHE:H	2.12	0.47
2:G:5:SER:HA	2:G:13:VAL:O	2.14	0.47
2:G:78:LEU:HG	2:G:82:TRP:CZ3	2.48	0.47
2:G:88:LEU:O	2:G:90:LYS:N	2.47	0.47
2:G:115:PRO:HG3	2:G:121:LEU:CG	2.44	0.47
2:H:59:LEU:HB3	2:H:78:LEU:HD11	1.96	0.47
2:I:1:THR:HA	2:I:33:LYS:HZ2	1.80	0.47
2:I:7:ARG:HG3	2:I:7:ARG:HH11	1.79	0.47
2:I:38:TYR:C	2:I:40:GLY:N	2.72	0.47
2:N:3:ILE:O	2:N:122:ALA:HA	2.13	0.47
2:N:148:ILE:C	2:N:150:GLU:H	2.21	0.47
1:B:391:ILE:O	1:B:394:ARG:HB2	2.14	0.47
1:B:424:ALA:C	1:B:426:VAL:H	2.22	0.47
1:C:63:LYS:CG	1:C:333:LEU:HD22	2.44	0.47
1:C:283:LEU:O	1:C:284:PRO:C	2.58	0.47
2:G:1:THR:H3	6:G:0:LVS:H1'1	1.79	0.47
2:I:21:SER:O	6:I:0:LVS:HD42	2.14	0.47
2:I:115:PRO:HG3	2:I:121:LEU:HD11	1.96	0.47
2:L:71:LEU:HD22	2:L:99:ASP:OD2	2.15	0.47
2:L:94:MET:O	2:L:95:LEU:HD23	2.14	0.47
2:M:115:PRO:HG3	2:M:121:LEU:HG	1.97	0.47
1:B:276:GLU:C	1:B:278:VAL:N	2.72	0.47
1:B:426:VAL:C	1:B:428:ASP:N	2.70	0.47
2:L:51:ALA:O	2:L:52:ASP:C	2.57	0.47
2:M:96:ILE:CD1	2:M:123:ILE:HG12	2.44	0.47
1:A:13:LEU:HD12	1:A:24:LYS:CG	2.44	0.47
1:A:86:PHE:HB2	1:A:278:VAL:HG11	1.97	0.47
1:C:37:ARG:O	1:C:45:ARG:HD3	2.14	0.47
2:H:8:ARG:O	2:H:11:GLN:HB2	2.15	0.47
2:I:67:HIS:CD2	2:I:77:GLU:HG3	2.49	0.47
1:B:42:GLU:HB3	1:B:43:PRO:CD	2.35	0.47
1:B:66:ILE:HD12	1:B:333:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:THR:C	1:B:86:PHE:N	2.72	0.47
1:C:64:THR:HB	3:C:450:ADP:O1A	2.15	0.47
1:C:98:SER:O	1:C:101:ARG:N	2.48	0.47
2:G:120:ILE:CD1	2:G:135:ARG:HA	2.44	0.47
2:H:70:HIS:O	2:H:71:LEU:C	2.57	0.47
2:H:154:ARG:O	2:H:155:ILE:C	2.58	0.47
2:I:3:ILE:HB	2:I:123:ILE:CG1	2.44	0.47
2:I:34:VAL:HA	2:I:45:GLY:HA2	1.97	0.47
2:L:19:GLN:HB2	2:L:164:ASN:HD22	1.79	0.47
2:L:133:ALA:HB1	2:L:155:ILE:HD12	1.96	0.47
2:L:134:ALA:O	2:L:137:LEU:N	2.47	0.47
2:N:83:ARG:O	2:N:89:ARG:HD3	2.15	0.47
1:A:37:ARG:NH2	1:A:302:HIS:CD2	2.83	0.47
1:B:320:ILE:HG13	1:B:320:ILE:O	2.15	0.47
1:B:443:ILE:HG22	1:B:444:LEU:H	1.75	0.47
2:H:115:PRO:HG3	2:H:121:LEU:CD2	2.41	0.47
2:I:133:ALA:O	2:I:136:ALA:N	2.46	0.47
2:I:164:ASN:HD22	2:I:164:ASN:H	1.63	0.47
2:M:71:LEU:O	2:M:75:ALA:N	2.39	0.47
2:N:10:GLY:O	2:N:11:GLN:HG2	2.14	0.47
2:N:85:ASP:CB	2:N:88:LEU:HD23	2.44	0.47
1:A:52:ASN:O	1:A:328:PRO:HD2	2.15	0.47
1:B:41:GLN:HA	1:B:41:GLN:NE2	2.30	0.47
1:B:370:THR:O	1:B:373:ALA:HB3	2.15	0.47
1:B:384:VAL:O	1:B:385:ASN:C	2.58	0.47
1:B:441:ARG:HH11	1:B:441:ARG:CB	2.00	0.47
1:B:441:ARG:NH1	1:B:441:ARG:CB	2.70	0.47
1:C:61:VAL:HA	1:C:336:LEU:CD2	2.45	0.47
1:C:98:SER:HA	1:C:101:ARG:NE	2.23	0.47
2:G:1:THR:HG23	2:G:33:LYS:HD3	1.97	0.47
2:G:118:ASP:O	2:G:120:ILE:HG13	2.15	0.47
2:H:56:LEU:HD13	2:H:56:LEU:C	2.40	0.47
2:H:136:ALA:C	2:H:138:VAL:N	2.72	0.47
2:I:144:SER:OG	2:I:147:GLU:HG3	2.15	0.47
2:L:138:VAL:HG22	2:L:138:VAL:O	2.14	0.47
2:M:167:PHE:N	2:M:167:PHE:CD2	2.83	0.47
1:A:439:LEU:HD23	2:G:72:LEU:HD12	1.97	0.47
1:B:61:VAL:HA	1:B:336:LEU:HD22	1.97	0.47
1:C:329:ILE:C	1:C:330:ARG:HG2	2.39	0.47
2:H:54:PHE:O	2:H:58:GLU:HG3	2.15	0.47
2:I:137:LEU:HD12	2:I:137:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:172:LEU:HD23	2:I:172:LEU:HA	1.79	0.47
2:N:17:ASP:O	2:N:33:LYS:HD2	2.15	0.47
1:B:17:ILE:HG23	3:B:450:ADP:C6	2.50	0.46
1:C:367:ILE:HG22	1:C:419:VAL:HB	1.96	0.46
2:G:5:SER:CB	2:G:14:VAL:HG22	2.45	0.46
2:L:104:LEU:HD23	2:L:115:PRO:HD3	1.95	0.46
2:N:6:VAL:HG22	2:N:120:ILE:HG23	1.97	0.46
2:N:60:PHE:CD1	2:N:78:LEU:HD22	2.50	0.46
1:A:53:ILE:HG12	1:A:329:ILE:CG2	2.46	0.46
1:B:293:THR:C	1:B:295:HIS:H	2.22	0.46
1:B:360:MET:O	1:B:363:GLU:N	2.43	0.46
1:B:426:VAL:O	1:B:428:ASP:N	2.49	0.46
2:L:1:THR:HG23	2:L:33:LYS:CE	2.44	0.46
1:B:29:ILE:HG22	1:B:30:ALA:N	2.30	0.46
2:G:15:GLY:HA2	2:G:34:VAL:HG21	1.97	0.46
2:H:99:ASP:O	2:H:100:GLU:C	2.58	0.46
2:M:10:GLY:O	2:M:11:GLN:NE2	2.49	0.46
1:B:57:GLY:CA	1:B:63:LYS:HE2	2.46	0.46
1:C:3:GLU:CG	1:C:4:MET:N	2.62	0.46
1:C:20:GLN:HE21	1:C:20:GLN:HA	1.81	0.46
2:G:140:ASN:O	2:G:141:THR:HB	2.15	0.46
2:I:129:TYR:O	2:I:130:ALA:C	2.58	0.46
2:M:6:VAL:HG23	2:M:149:VAL:HG22	1.98	0.46
2:M:8:ARG:HH12	2:M:142:GLU:HA	1.79	0.46
2:M:86:ARG:NH1	2:M:86:ARG:HB3	2.30	0.46
2:N:38:TYR:O	2:N:39:ASN:HB3	2.15	0.46
1:A:407:ILE:HD11	1:A:419:VAL:HG11	1.97	0.46
1:B:20:GLN:HA	1:B:20:GLN:NE2	2.22	0.46
2:G:167:PHE:N	2:G:167:PHE:CD2	2.82	0.46
2:H:14:VAL:O	2:H:34:VAL:HG11	2.15	0.46
2:I:7:ARG:HA	2:I:11:GLN:O	2.16	0.46
2:L:75:ALA:O	2:L:78:LEU:N	2.48	0.46
2:M:89:ARG:HG3	2:M:89:ARG:HH11	1.80	0.46
2:N:71:LEU:HB2	2:N:99:ASP:OD2	2.15	0.46
1:C:13:LEU:HB2	1:C:24:LYS:HD3	1.96	0.46
2:G:3:ILE:O	2:G:122:ALA:HA	2.16	0.46
2:G:13:VAL:HB	2:G:149:VAL:HG21	1.97	0.46
2:G:138:VAL:HG22	2:G:148:ILE:CD1	2.46	0.46
2:H:83:ARG:HG2	2:I:55:THR:CB	2.46	0.46
2:I:37:LEU:N	2:I:42:VAL:O	2.45	0.46
2:L:7:ARG:NH2	2:L:99:ASP:O	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:135:ARG:O	2:L:136:ALA:C	2.57	0.46
2:N:143:LEU:HD22	2:N:147:GLU:OE1	2.16	0.46
1:A:278:VAL:O	1:A:279:GLN:C	2.58	0.46
1:B:322:GLU:OE2	1:B:322:GLU:N	2.46	0.46
1:C:14:ASP:HA	1:C:24:LYS:HE2	1.97	0.46
1:C:29:ILE:O	1:C:30:ALA:C	2.58	0.46
2:I:7:ARG:NH1	2:I:12:VAL:HG22	2.30	0.46
2:M:144:SER:C	2:M:146:HIS:N	2.72	0.46
1:A:341:PHE:O	1:A:342:GLU:C	2.58	0.46
1:C:374:VAL:O	1:C:375:LYS:C	2.58	0.46
2:H:117:GLU:C	2:H:119:GLN:H	2.23	0.46
2:N:58:GLU:C	2:N:60:PHE:N	2.70	0.46
1:A:20:GLN:NE2	1:A:334:THR:H	2.07	0.46
1:A:31:LEU:HG	1:A:31:LEU:O	2.16	0.46
1:A:55:MET:HE3	1:A:306:ILE:HG21	1.97	0.46
1:A:63:LYS:NZ	1:A:308:SER:HB2	2.31	0.46
1:C:55:MET:HB3	1:C:63:LYS:HD2	1.98	0.46
1:C:63:LYS:HE3	1:C:308:SER:HB2	1.97	0.46
1:C:101:ARG:HA	1:C:293:THR:HG21	1.97	0.46
2:H:89:ARG:O	2:H:90:LYS:HB2	2.16	0.46
2:H:115:PRO:HG3	2:H:121:LEU:CG	2.46	0.46
2:N:56:LEU:HD12	2:N:95:LEU:HD11	1.98	0.46
1:A:61:VAL:HA	1:A:336:LEU:HD22	1.98	0.46
1:A:351:SER:O	1:A:352:LEU:C	2.59	0.46
2:L:54:PHE:C	2:L:56:LEU:N	2.74	0.46
1:A:20:GLN:CA	1:A:20:GLN:NE2	2.68	0.45
1:A:361:ALA:HA	1:A:365:VAL:O	2.16	0.45
1:C:4:MET:HA	1:C:8:GLU:OE1	2.16	0.45
2:L:83:ARG:HA	2:L:89:ARG:HD3	1.97	0.45
1:A:41:GLN:HE21	1:A:41:GLN:CA	2.28	0.45
2:M:164:ASN:HD21	2:M:166:ASN:HB2	1.81	0.45
1:A:315:ARG:HG3	1:A:316:PRO:CD	2.46	0.45
1:B:59:THR:HA	5:B:452:PO4:O2	2.17	0.45
1:B:382:PHE:CD2	1:B:382:PHE:C	2.94	0.45
1:C:61:VAL:HG23	1:C:333:LEU:HD23	1.98	0.45
2:H:138:VAL:HG22	2:H:148:ILE:HD13	1.98	0.45
2:I:47:ALA:O	2:I:93:ALA:HB1	2.16	0.45
1:C:52:ASN:HB2	1:C:326:ARG:O	2.16	0.45
2:G:38:TYR:C	2:G:40:GLY:N	2.75	0.45
2:G:46:PHE:HB2	2:G:53:ALA:HB1	1.98	0.45
2:G:55:THR:HG23	2:G:91:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:169:ILE:C	2:I:170:GLU:HG2	2.41	0.45
2:L:6:VAL:CG1	2:L:7:ARG:N	2.79	0.45
1:C:322:GLU:OE2	1:C:322:GLU:N	2.46	0.45
1:C:353:THR:O	1:C:354:GLU:C	2.60	0.45
2:L:172:LEU:HD23	2:L:173:PRO:HA	1.97	0.45
2:M:20:VAL:HG21	2:M:28:LYS:HB3	1.97	0.45
2:N:172:LEU:CB	2:N:173:PRO:HD3	2.47	0.45
1:A:286:VAL:CG1	1:A:326:ARG:HB3	2.46	0.45
1:C:323:LEU:O	1:C:324:GLN:C	2.59	0.45
1:C:337:SER:O	1:C:339:ALA:N	2.50	0.45
1:C:400:MET:HE3	1:C:400:MET:HB3	1.80	0.45
1:C:427:ALA:O	1:C:431:GLY:HA2	2.17	0.45
2:H:18:GLY:HA2	2:H:31:ALA:HB3	1.98	0.45
2:H:50:THR:O	2:H:51:ALA:C	2.60	0.45
2:I:71:LEU:HD13	2:I:71:LEU:O	2.17	0.45
2:L:149:VAL:O	2:L:150:GLU:C	2.58	0.45
2:N:8:ARG:HH22	2:N:142:GLU:HA	1.82	0.45
1:A:64:THR:N	3:A:450:ADP:O2B	2.50	0.45
1:A:82:GLU:HG2	1:A:84:THR:OG1	2.16	0.45
2:G:91:LEU:N	2:G:91:LEU:CD1	2.77	0.45
2:I:115:PRO:HB2	2:I:119:GLN:HA	1.99	0.45
2:I:154:ARG:HG3	2:I:154:ARG:HH11	1.80	0.45
2:M:27:MET:HE2	2:M:27:MET:HA	1.98	0.45
2:M:137:LEU:HD22	2:M:137:LEU:N	2.31	0.45
2:N:66:MET:HG3	2:N:67:HIS:HD2	1.82	0.45
1:A:38:MET:HA	1:A:45:ARG:CG	2.47	0.45
1:A:283:LEU:HB2	1:A:284:PRO:HD3	1.98	0.45
1:B:85:LYS:O	1:B:85:LYS:CG	2.65	0.45
1:B:323:LEU:O	1:B:324:GLN:C	2.60	0.45
1:B:399:VAL:O	1:B:400:MET:C	2.60	0.45
1:C:357:LYS:HA	1:C:367:ILE:HD11	1.99	0.45
2:G:133:ALA:O	2:G:136:ALA:HB3	2.16	0.45
2:H:94:MET:CG	2:H:107:THR:HG22	2.44	0.45
2:L:67:HIS:HB3	2:L:73:LYS:HE2	1.98	0.45
2:L:109:ILE:CG1	2:L:110:GLY:H	2.18	0.45
2:N:104:LEU:N	2:N:104:LEU:HD22	2.32	0.45
1:A:27:VAL:HB	1:A:70:LEU:CD1	2.39	0.45
2:G:13:VAL:HG21	2:G:146:HIS:HA	1.98	0.45
2:H:141:THR:CG2	2:H:143:LEU:HG	2.47	0.45
2:I:22:LEU:HD13	6:I:0:LVS:HD13	1.98	0.45
2:M:85:ASP:CG	2:M:88:LEU:HD13	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:52:ASP:CA	2:I:55:THR:HG23	2.45	0.45
2:L:104:LEU:HD21	2:L:114:GLN:HG2	1.99	0.45
2:L:111:ASP:O	2:L:112:VAL:C	2.60	0.45
2:N:148:ILE:C	2:N:150:GLU:N	2.74	0.45
1:A:86:PHE:CZ	1:A:99:ILE:HD11	2.52	0.44
1:B:60:GLY:HA2	3:B:450:ADP:PB	2.57	0.44
1:C:31:LEU:HD22	1:C:70:LEU:HD11	1.99	0.44
2:G:112:VAL:HG23	2:G:112:VAL:O	2.17	0.44
2:H:62:ARG:O	2:H:66:MET:HG3	2.17	0.44
2:H:91:LEU:HD22	2:H:91:LEU:N	2.32	0.44
2:H:164:ASN:C	2:H:164:ASN:HD22	2.24	0.44
2:L:71:LEU:HB2	2:L:99:ASP:OD2	2.18	0.44
2:N:108:GLY:C	2:N:110:GLY:N	2.71	0.44
1:B:107:ALA:C	1:B:109:GLY:N	2.75	0.44
2:I:156:ALA:O	2:I:159:ILE:N	2.46	0.44
2:M:28:LYS:NZ	2:M:30:ASN:HD21	2.14	0.44
2:M:37:LEU:HD11	2:M:57:PHE:CB	2.46	0.44
2:M:124:GLY:C	2:M:126:GLY:H	2.24	0.44
1:A:440:SER:C	1:A:442:PHE:H	2.24	0.44
1:C:430:LEU:O	1:C:431:GLY:C	2.59	0.44
2:G:127:GLY:O	2:G:128:ASN:C	2.60	0.44
2:M:103:SER:O	2:M:115:PRO:HD3	2.17	0.44
2:N:1:THR:C	2:N:2:THR:HG1	2.23	0.44
2:N:6:VAL:HG23	2:N:149:VAL:HG22	2.00	0.44
2:N:8:ARG:NH2	2:N:142:GLU:HA	2.32	0.44
2:N:63:LYS:NZ	2:N:81:ASP:OD1	2.47	0.44
1:A:5:THR:H	1:A:8:GLU:HB2	1.81	0.44
1:A:249:GLU:OE1	1:A:299:LYS:N	2.38	0.44
1:C:293:THR:C	1:C:295:HIS:N	2.73	0.44
1:C:328:PRO:HG2	1:C:329:ILE:H	1.82	0.44
1:C:403:LEU:CD2	1:C:404:MET:HG2	2.47	0.44
2:G:22:LEU:O	2:G:23:GLY:C	2.57	0.44
2:G:68:GLN:HB2	2:G:70:HIS:CD2	2.52	0.44
2:I:36:ARG:NH1	2:I:43:LEU:HD23	2.33	0.44
2:I:62:ARG:NH1	2:I:62:ARG:CB	2.81	0.44
2:N:17:ASP:OD2	2:N:163:THR:HA	2.17	0.44
1:A:33:ASN:O	1:A:34:ARG:C	2.59	0.44
1:A:256:ILE:O	1:A:256:ILE:HG22	2.17	0.44
1:A:404:MET:O	1:A:408:SER:HB2	2.17	0.44
1:B:9:ILE:HG22	1:B:10:VAL:N	2.32	0.44
1:B:60:GLY:HA2	3:B:450:ADP:O3A	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7:ARG:HB3	2:H:119:GLN:HB3	2.00	0.44
2:H:15:GLY:HA2	2:H:34:VAL:HG21	1.98	0.44
2:H:172:LEU:O	2:H:173:PRO:C	2.61	0.44
2:I:6:VAL:CG1	2:I:7:ARG:N	2.80	0.44
2:I:154:ARG:HG3	2:I:154:ARG:NH1	2.33	0.44
2:L:3:ILE:CG2	2:L:96:ILE:HD12	2.47	0.44
1:A:86:PHE:HB2	1:A:278:VAL:CG1	2.48	0.44
1:C:44:LEU:O	1:C:48:VAL:HG12	2.18	0.44
2:G:141:THR:C	2:G:143:LEU:H	2.24	0.44
1:B:410:SER:O	1:B:411:ALA:C	2.60	0.44
2:H:141:THR:CG2	2:H:142:GLU:H	2.31	0.44
2:I:8:ARG:O	2:I:11:GLN:HB2	2.18	0.44
2:I:110:GLY:O	2:I:111:ASP:HB3	2.18	0.44
2:I:138:VAL:O	2:I:138:VAL:HG12	2.18	0.44
1:A:9:ILE:O	1:A:10:VAL:C	2.59	0.44
1:B:34:ARG:NH2	1:B:253:ILE:HD13	2.32	0.44
1:C:312:GLN:NE2	2:I:66:MET:HA	2.33	0.44
2:G:43:LEU:HD13	2:G:170:GLU:O	2.17	0.44
2:G:125:SER:H	6:G:0:LVS:C1'	2.31	0.44
2:I:137:LEU:HB3	2:I:143:LEU:HD12	1.99	0.44
2:L:57:PHE:O	2:L:61:GLU:HG2	2.18	0.44
2:L:156:ALA:O	2:L:157:GLY:C	2.61	0.44
1:A:74:ALA:O	1:A:75:ASN:C	2.61	0.44
1:B:27:VAL:HB	1:B:70:LEU:CD1	2.37	0.44
1:B:102:ASP:O	1:B:105:ASP:HB2	2.17	0.44
2:H:42:VAL:HG21	2:H:64:LEU:HD13	2.00	0.44
2:I:62:ARG:HB3	2:I:62:ARG:CZ	2.48	0.44
2:L:104:LEU:CD2	2:L:114:GLN:HA	2.48	0.44
1:A:65:GLU:HG3	3:A:450:ADP:H2'	1.99	0.43
1:A:87:THR:O	1:A:274:SER:HB2	2.18	0.43
1:A:286:VAL:HG11	1:A:326:ARG:CB	2.47	0.43
1:C:370:THR:O	1:C:371:THR:C	2.60	0.43
2:H:141:THR:HG22	2:H:143:LEU:N	2.17	0.43
2:L:128:ASN:HA	2:L:131:LEU:HB3	2.00	0.43
2:M:172:LEU:CB	2:M:173:PRO:HD3	2.46	0.43
1:A:367:ILE:HD11	1:A:421:ILE:HD12	1.99	0.43
1:C:57:GLY:C	1:C:63:LYS:HZ1	2.24	0.43
2:G:131:LEU:O	2:G:132:SER:C	2.60	0.43
2:H:120:ILE:O	2:H:121:LEU:HD23	2.18	0.43
2:I:34:VAL:HG22	2:I:45:GLY:HA3	1.99	0.43
2:M:157:GLY:HA2	2:M:163:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD13	1:A:66:ILE:HG23	1.99	0.43
1:A:260:ASP:HB3	1:A:311:PHE:CE2	2.53	0.43
1:C:10:VAL:HG12	1:C:14:ASP:OD2	2.18	0.43
1:C:63:LYS:CE	1:C:308:SER:HB2	2.47	0.43
2:L:69:GLY:O	2:L:71:LEU:N	2.51	0.43
2:M:64:LEU:HD21	2:M:69:GLY:HA2	2.00	0.43
2:M:105:ILE:CG1	2:M:121:LEU:HD13	2.40	0.43
2:M:115:PRO:HG3	2:M:121:LEU:HD11	2.00	0.43
2:M:138:VAL:C	2:M:140:ASN:N	2.76	0.43
2:N:91:LEU:N	2:N:91:LEU:CD1	2.82	0.43
1:B:41:GLN:NE2	1:B:41:GLN:CA	2.81	0.43
1:C:256:ILE:CD1	1:C:282:LEU:HD21	2.42	0.43
2:G:153:LEU:O	2:G:156:ALA:HB3	2.18	0.43
2:H:131:LEU:HD21	2:H:135:ARG:HH12	1.81	0.43
2:I:88:LEU:O	2:I:89:ARG:HB2	2.17	0.43
2:L:65:GLU:O	2:L:66:MET:C	2.61	0.43
2:M:42:VAL:HG22	2:M:99:ASP:HB3	1.99	0.43
2:M:108:GLY:C	2:M:110:GLY:H	2.26	0.43
1:A:4:MET:HB3	1:A:8:GLU:CB	2.41	0.43
1:A:337:SER:O	1:A:340:ASP:HB2	2.18	0.43
1:A:388:THR:OG1	1:A:389:GLU:N	2.50	0.43
2:G:114:GLN:HA	2:G:115:PRO:HD3	1.82	0.43
2:H:17:ASP:HB2	2:H:164:ASN:HD22	1.75	0.43
2:H:141:THR:HG21	2:H:143:LEU:HG	2.01	0.43
2:L:82:TRP:O	2:L:82:TRP:HD1	2.01	0.43
2:L:82:TRP:CD2	2:L:108:GLY:HA2	2.53	0.43
2:M:94:MET:HB2	2:M:123:ILE:HD12	2.00	0.43
2:N:133:ALA:O	2:N:134:ALA:C	2.61	0.43
1:A:84:THR:O	1:A:87:THR:HG23	2.18	0.43
1:A:390:ASN:H	2:G:68:GLN:NE2	2.16	0.43
1:B:27:VAL:CB	1:B:70:LEU:HD13	2.36	0.43
1:B:41:GLN:HE21	1:B:42:GLU:N	2.16	0.43
2:L:133:ALA:O	2:L:134:ALA:O	2.37	0.43
2:M:71:LEU:H	2:M:71:LEU:CD1	2.18	0.43
2:N:121:LEU:HD23	2:N:121:LEU:HA	1.78	0.43
1:A:37:ARG:HB2	1:A:48:VAL:HG11	2.01	0.43
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.73	0.43
1:A:439:LEU:HD21	2:G:73:LYS:HA	2.01	0.43
1:B:256:ILE:CG2	1:B:259:ILE:HD13	2.48	0.43
1:B:275:ARG:O	1:B:278:VAL:HG23	2.18	0.43
1:B:283:LEU:C	1:B:285:LEU:N	2.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:VAL:HG22	1:B:385:ASN:N	2.34	0.43
1:C:283:LEU:C	1:C:285:LEU:N	2.74	0.43
1:C:424:ALA:O	1:C:425:TYR:C	2.61	0.43
2:G:100:GLU:OE1	2:G:172:LEU:HD22	2.18	0.43
2:L:89:ARG:HG3	2:L:89:ARG:HH11	1.84	0.43
2:M:2:THR:O	2:M:16:GLY:HA2	2.19	0.43
2:N:13:VAL:HG21	2:N:146:HIS:N	2.34	0.43
1:A:4:MET:CE	1:A:73:LEU:HD13	2.48	0.43
1:A:324:GLN:HE21	1:A:324:GLN:HB2	1.66	0.43
2:G:86:ARG:O	2:G:88:LEU:HD22	2.19	0.43
2:H:19:GLN:N	2:H:33:LYS:HZ1	2.16	0.43
2:H:128:ASN:HA	2:H:131:LEU:HB3	2.00	0.43
2:L:88:LEU:C	2:L:90:LYS:N	2.76	0.43
2:L:127:GLY:O	2:L:128:ASN:C	2.61	0.43
2:M:9:ASN:O	2:M:11:GLN:HG2	2.18	0.43
1:B:33:ASN:HA	1:B:36:ARG:HB2	1.99	0.43
1:C:365:VAL:HG12	1:C:366:ASN:N	2.33	0.43
2:G:49:GLY:O	2:G:50:THR:C	2.61	0.43
2:G:67:HIS:O	2:G:68:GLN:C	2.61	0.43
2:I:7:ARG:NH2	2:I:103:SER:OG	2.51	0.43
2:I:36:ARG:HA	2:I:43:LEU:HA	1.99	0.43
2:I:67:HIS:O	2:I:69:GLY:N	2.51	0.43
2:L:51:ALA:C	2:L:53:ALA:N	2.76	0.43
2:L:64:LEU:HA	2:L:74:SER:CB	2.49	0.43
1:B:41:GLN:HE21	1:B:41:GLN:CA	2.30	0.43
1:B:96:VAL:HG13	1:B:99:ILE:HD12	2.00	0.43
1:C:384:VAL:HG23	1:C:388:THR:OG1	2.19	0.43
1:A:76:ALA:HA	1:A:77:PRO:HD3	1.93	0.42
1:A:275:ARG:O	1:A:278:VAL:HG22	2.19	0.42
1:A:356:TYR:HB3	1:A:404:MET:HE2	2.00	0.42
1:B:98:SER:O	1:B:99:ILE:C	2.62	0.42
1:B:374:VAL:O	1:B:376:LYS:N	2.52	0.42
1:C:34:ARG:HH21	1:C:252:GLY:N	2.17	0.42
1:C:53:ILE:HG22	1:C:54:LEU:N	2.33	0.42
1:C:287:GLU:O	1:C:287:GLU:HG2	2.19	0.42
1:C:319:LEU:O	1:C:320:ILE:C	2.59	0.42
1:C:439:LEU:C	1:C:441:ARG:N	2.74	0.42
2:G:86:ARG:HB2	2:G:86:ARG:NH1	2.33	0.42
2:G:89:ARG:O	2:G:90:LYS:HB3	2.19	0.42
2:H:38:TYR:O	2:H:40:GLY:N	2.51	0.42
2:H:52:ASP:HA	2:H:91:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:120:ILE:HD13	2:H:134:ALA:CB	2.48	0.42
2:I:137:LEU:N	2:I:137:LEU:CD1	2.82	0.42
2:M:120:ILE:O	2:M:121:LEU:HD23	2.18	0.42
1:A:413:ASP:OD2	1:A:413:ASP:N	2.51	0.42
1:B:39:GLN:N	1:B:39:GLN:NE2	2.65	0.42
1:C:57:GLY:C	1:C:63:LYS:NZ	2.77	0.42
1:C:299:LYS:N	1:C:299:LYS:HD2	2.34	0.42
2:I:42:VAL:HG21	2:I:64:LEU:HD13	2.02	0.42
2:I:155:ILE:O	2:I:159:ILE:HG13	2.18	0.42
2:L:53:ALA:O	2:L:56:LEU:HB2	2.17	0.42
2:N:2:THR:O	2:N:3:ILE:HD13	2.18	0.42
2:N:44:ALA:HA	2:N:96:ILE:O	2.19	0.42
1:A:13:LEU:C	1:A:15:GLN:N	2.77	0.42
1:B:72:LYS:HD2	1:B:72:LYS:O	2.19	0.42
2:G:126:GLY:O	2:G:127:GLY:C	2.61	0.42
2:M:37:LEU:HD21	2:M:57:PHE:HB3	2.00	0.42
2:N:146:HIS:O	2:N:147:GLU:C	2.62	0.42
1:A:5:THR:HA	1:A:32:ARG:HH11	1.84	0.42
1:B:20:GLN:HG3	1:B:333:LEU:HD23	2.02	0.42
1:B:373:ALA:O	1:B:374:VAL:C	2.62	0.42
1:C:384:VAL:HG22	1:C:385:ASN:N	2.33	0.42
2:G:20:VAL:HB	2:G:27:MET:HB3	2.01	0.42
2:G:27:MET:HE3	6:G:0:LVS:HD22	2.01	0.42
2:H:76:VAL:CG1	2:H:80:LYS:HE2	2.48	0.42
2:I:141:THR:CB	2:I:143:LEU:HG	2.50	0.42
2:I:152:SER:O	2:I:153:LEU:C	2.62	0.42
2:L:12:VAL:HG13	2:L:12:VAL:O	2.19	0.42
2:M:6:VAL:CG1	2:M:7:ARG:H	2.29	0.42
2:M:6:VAL:CG1	2:M:7:ARG:N	2.82	0.42
2:M:71:LEU:HD21	2:M:99:ASP:CB	2.47	0.42
2:N:61:GLU:C	2:N:63:LYS:H	2.26	0.42
1:A:9:ILE:HG23	1:A:73:LEU:HD21	2.02	0.42
1:A:284:PRO:O	1:A:285:LEU:C	2.62	0.42
1:C:442:PHE:HB3	2:I:83:ARG:HH12	1.84	0.42
2:M:79:ALA:O	2:M:80:LYS:C	2.63	0.42
2:M:85:ASP:HB3	2:M:88:LEU:HB2	2.02	0.42
2:M:153:LEU:HB3	2:M:167:PHE:CZ	2.55	0.42
1:A:38:MET:HA	1:A:45:ARG:HG3	2.02	0.42
1:A:443:ILE:HG12	2:G:112:VAL:HG23	2.01	0.42
1:C:250:GLN:NE2	1:C:250:GLN:CA	2.80	0.42
1:C:405:ASP:OD1	1:C:405:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7:ARG:HB3	2:H:119:GLN:CB	2.50	0.42
2:H:37:LEU:HD21	2:H:57:PHE:CE2	2.55	0.42
2:H:44:ALA:HB2	2:H:97:VAL:HG12	2.00	0.42
2:H:82:TRP:CD1	2:H:88:LEU:HB3	2.54	0.42
2:L:67:HIS:CG	2:L:73:LYS:HE2	2.54	0.42
1:A:29:ILE:O	1:A:30:ALA:C	2.61	0.42
1:A:53:ILE:HG22	1:A:54:LEU:N	2.34	0.42
1:A:414:MET:O	1:A:415:ASN:C	2.61	0.42
1:A:434:VAL:HG12	1:A:435:GLU:N	2.34	0.42
1:C:262:ILE:HA	1:C:275:ARG:HB3	2.02	0.42
2:G:5:SER:HB2	2:G:14:VAL:HG13	2.01	0.42
2:G:7:ARG:NH2	2:G:12:VAL:HG21	2.35	0.42
2:G:89:ARG:HG2	2:G:89:ARG:NH1	2.30	0.42
2:L:44:ALA:HB1	2:L:96:ILE:O	2.19	0.42
2:M:28:LYS:CG	2:M:29:GLY:N	2.82	0.42
2:M:37:LEU:O	2:M:38:TYR:C	2.62	0.42
2:N:53:ALA:HA	2:N:56:LEU:HB2	2.02	0.42
2:N:164:ASN:OD1	2:N:166:ASN:N	2.52	0.42
1:A:61:VAL:HG11	1:A:335:ALA:HA	2.01	0.42
1:A:414:MET:O	1:A:417:GLN:HG3	2.20	0.42
1:B:360:MET:HE3	1:B:407:ILE:HG22	2.01	0.42
1:B:444:LEU:O	2:I:28:LYS:NZ	2.45	0.42
2:H:134:ALA:O	2:H:138:VAL:HG23	2.19	0.42
2:I:17:ASP:OD2	2:I:33:LYS:NZ	2.51	0.42
2:L:136:ALA:O	2:L:139:GLU:HB2	2.20	0.42
2:L:141:THR:HG22	2:L:142:GLU:N	2.34	0.42
2:M:124:GLY:C	2:M:126:GLY:N	2.78	0.42
1:B:22:ASP:OD2	1:B:22:ASP:N	2.49	0.42
1:B:345:LEU:CD2	1:B:378:ALA:HB2	2.50	0.42
1:C:17:ILE:HG21	1:C:66:ILE:CD1	2.50	0.42
1:C:260:ASP:HB3	1:C:311:PHE:CZ	2.55	0.42
1:C:374:VAL:O	1:C:377:ILE:N	2.53	0.42
2:L:54:PHE:C	2:L:56:LEU:H	2.27	0.42
2:L:72:LEU:C	2:L:72:LEU:HD23	2.45	0.42
2:L:82:TRP:CE2	2:L:108:GLY:HA2	2.55	0.42
1:A:79:ILE:HD12	1:A:80:LYS:N	2.35	0.42
1:C:25:ARG:O	1:C:26:ALA:C	2.60	0.42
1:C:48:VAL:O	1:C:48:VAL:HG22	2.19	0.42
1:C:259:ILE:O	1:C:262:ILE:HG12	2.20	0.42
2:G:153:LEU:HB2	2:G:167:PHE:CE1	2.55	0.42
2:I:67:HIS:CD2	2:I:73:LYS:HG2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:106:ILE:N	2:M:106:ILE:CD1	2.78	0.42
2:N:92:GLU:O	2:N:93:ALA:HB2	2.19	0.42
1:A:65:GLU:CG	3:A:450:ADP:H2'	2.50	0.41
1:A:383:ARG:HD2	1:A:383:ARG:HA	1.95	0.41
1:A:394:ARG:O	1:A:397:HIS:HB2	2.20	0.41
1:A:414:MET:HE2	1:A:417:GLN:NE2	2.36	0.41
1:B:62:GLY:O	1:B:63:LYS:C	2.63	0.41
1:C:380:ALA:O	1:C:381:ALA:C	2.62	0.41
2:G:134:ALA:O	2:G:135:ARG:C	2.62	0.41
2:H:100:GLU:CD	2:H:100:GLU:H	2.28	0.41
2:M:138:VAL:C	2:M:140:ASN:H	2.28	0.41
1:A:101:ARG:O	1:A:105:ASP:OD1	2.38	0.41
1:A:435:GLU:C	1:A:437:GLU:N	2.77	0.41
1:B:29:ILE:O	1:B:30:ALA:C	2.63	0.41
1:B:293:THR:C	1:B:295:HIS:N	2.77	0.41
1:C:16:HIS:C	1:C:17:ILE:HD12	2.45	0.41
2:N:45:GLY:N	2:N:96:ILE:O	2.53	0.41
1:A:398:THR:C	1:A:400:MET:N	2.77	0.41
2:G:69:GLY:O	2:G:71:LEU:N	2.53	0.41
2:I:115:PRO:HG3	2:I:121:LEU:CD1	2.50	0.41
2:L:56:LEU:HD11	2:L:82:TRP:CZ2	2.55	0.41
2:L:129:TYR:O	2:L:132:SER:HB2	2.20	0.41
2:N:82:TRP:HB3	2:N:83:ARG:H	1.65	0.41
1:A:3:GLU:OE1	1:A:4:MET:SD	2.78	0.41
1:A:351:SER:N	1:A:354:GLU:HB2	2.35	0.41
2:G:154:ARG:HA	2:G:167:PHE:HZ	1.85	0.41
2:G:165:THR:HA	2:G:167:PHE:CE2	2.55	0.41
2:H:24:ASN:O	2:M:161:VAL:HG22	2.20	0.41
2:I:4:VAL:HG12	2:I:153:LEU:HD21	2.01	0.41
2:M:6:VAL:CG2	2:M:149:VAL:HG22	2.51	0.41
2:M:157:GLY:HA2	2:M:163:THR:HB	2.02	0.41
2:M:165:THR:HA	2:M:167:PHE:CE2	2.56	0.41
1:A:25:ARG:HG2	1:A:25:ARG:HH11	1.85	0.41
1:C:403:LEU:HD23	1:C:404:MET:CA	2.50	0.41
1:C:433:VAL:O	1:C:434:VAL:C	2.64	0.41
2:G:63:LYS:HD2	2:G:63:LYS:HA	1.70	0.41
2:G:89:ARG:NH1	2:G:89:ARG:CG	2.83	0.41
2:G:131:LEU:HD11	2:G:135:ARG:HH11	1.77	0.41
2:H:141:THR:CG2	2:H:143:LEU:H	2.18	0.41
2:M:18:GLY:O	2:M:29:GLY:HA2	2.20	0.41
2:M:62:ARG:C	2:M:64:LEU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:104:LEU:HD12	2:M:104:LEU:N	2.35	0.41
1:A:34:ARG:CZ	1:A:251:ASN:HB2	2.51	0.41
1:A:63:LYS:HZ2	1:A:308:SER:HB2	1.84	0.41
2:G:118:ASP:OD2	2:G:135:ARG:HD3	2.20	0.41
2:H:136:ALA:HB2	2:N:155:ILE:HD11	1.97	0.41
2:I:42:VAL:HG23	2:I:42:VAL:O	2.20	0.41
2:I:76:VAL:O	2:I:80:LYS:HG2	2.21	0.41
2:L:43:LEU:HD23	2:L:98:ALA:O	2.20	0.41
2:L:62:ARG:C	2:L:64:LEU:H	2.29	0.41
2:M:42:VAL:O	2:M:42:VAL:HG12	2.20	0.41
1:A:4:MET:SD	1:A:4:MET:N	2.93	0.41
1:B:352:LEU:HA	1:B:352:LEU:HD23	1.60	0.41
1:C:22:ASP:O	1:C:25:ARG:N	2.54	0.41
1:C:46:HIS:O	1:C:47:GLU:C	2.63	0.41
1:C:360:MET:CE	1:C:360:MET:CA	2.95	0.41
1:C:394:ARG:O	1:C:397:HIS:HB2	2.21	0.41
2:I:34:VAL:HG13	2:I:44:ALA:O	2.20	0.41
2:I:89:ARG:HB3	2:I:90:LYS:H	1.69	0.41
2:M:3:ILE:O	2:M:122:ALA:HA	2.19	0.41
2:N:19:GLN:HA	2:N:28:LYS:O	2.20	0.41
2:N:124:GLY:O	2:N:125:SER:C	2.62	0.41
1:A:315:ARG:HE	1:A:316:PRO:CD	2.34	0.41
1:C:5:THR:HG23	1:C:8:GLU:CD	2.44	0.41
1:C:263:CYS:SG	1:C:319:LEU:HD23	2.61	0.41
1:C:351:SER:O	1:C:355:GLN:HB2	2.20	0.41
2:I:89:ARG:C	2:I:90:LYS:HD3	2.46	0.41
2:M:127:GLY:O	2:M:128:ASN:C	2.64	0.41
1:A:60:GLY:HA2	3:A:450:ADP:O3A	2.20	0.41
1:A:92:VAL:O	1:A:93:GLY:C	2.63	0.41
1:B:23:ALA:O	1:B:27:VAL:HG22	2.21	0.41
1:B:412:SER:OG	1:C:5:THR:HB	2.21	0.41
1:B:426:VAL:HG12	1:B:427:ALA:N	2.36	0.41
1:C:371:THR:HG23	1:C:375:LYS:HE2	2.01	0.41
2:G:38:TYR:CD1	2:G:69:GLY:HA3	2.55	0.41
2:H:2:THR:OG1	2:H:126:GLY:HA3	2.21	0.41
2:L:133:ALA:HB2	2:L:155:ILE:HG21	2.03	0.41
2:L:137:LEU:C	2:L:139:GLU:H	2.29	0.41
2:N:38:TYR:CE1	2:N:64:LEU:HD13	2.56	0.41
2:N:138:VAL:C	2:N:140:ASN:N	2.79	0.41
1:A:421:ILE:HA	1:A:425:TYR:HD2	1.86	0.41
1:A:425:TYR:O	1:A:426:VAL:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:GLN:O	1:B:326:ARG:N	2.54	0.41
1:B:349:HIS:O	1:B:350:ALA:HB3	2.21	0.41
1:B:407:ILE:HD11	1:B:425:TYR:CE1	2.50	0.41
1:C:371:THR:O	1:C:375:LYS:HG3	2.21	0.41
2:G:66:MET:C	2:G:67:HIS:ND1	2.79	0.41
2:I:134:ALA:HA	2:I:148:ILE:HG23	2.03	0.41
2:L:156:ALA:O	2:L:159:ILE:N	2.51	0.41
2:M:3:ILE:HG22	2:M:96:ILE:HD12	2.03	0.41
2:N:4:VAL:HG12	2:N:153:LEU:CD2	2.50	0.41
2:N:124:GLY:C	2:N:126:GLY:N	2.77	0.41
2:N:169:ILE:HG22	2:N:170:GLU:N	2.36	0.41
1:A:347:GLU:HB2	1:A:348:PRO:HD3	2.03	0.40
1:C:45:ARG:O	1:C:45:ARG:HG3	2.21	0.40
1:C:330:ARG:CB	1:C:330:ARG:NH1	2.80	0.40
2:H:71:LEU:HD11	2:H:97:VAL:CG2	2.51	0.40
2:H:120:ILE:HD11	2:H:138:VAL:HG21	2.02	0.40
2:I:28:LYS:CE	2:I:30:ASN:OD1	2.69	0.40
2:L:12:VAL:HG11	2:L:172:LEU:HD13	2.03	0.40
2:L:72:LEU:HB2	2:L:102:GLU:OE1	2.21	0.40
2:M:51:ALA:C	2:M:53:ALA:N	2.76	0.40
2:M:62:ARG:HH11	2:M:62:ARG:HG2	1.86	0.40
1:A:33:ASN:HA	1:A:36:ARG:HB2	2.03	0.40
1:A:249:GLU:HG2	1:A:299:LYS:O	2.21	0.40
1:A:260:ASP:HB3	1:A:311:PHE:CD2	2.57	0.40
1:B:264:LYS:O	1:B:265:LYS:HB3	2.22	0.40
1:C:34:ARG:NH2	1:C:251:ASN:CA	2.84	0.40
1:C:356:TYR:O	1:C:357:LYS:C	2.62	0.40
2:G:72:LEU:C	2:G:72:LEU:HD13	2.46	0.40
2:I:43:LEU:HD21	2:I:172:LEU:HG	2.03	0.40
2:I:111:ASP:O	2:I:111:ASP:OD2	2.38	0.40
2:I:131:LEU:O	2:I:132:SER:C	2.64	0.40
2:M:134:ALA:C	2:M:136:ALA:N	2.76	0.40
2:N:3:ILE:HB	2:N:123:ILE:CG1	2.46	0.40
1:A:41:GLN:HA	1:A:41:GLN:NE2	2.37	0.40
1:A:336:LEU:HA	1:A:336:LEU:HD12	1.78	0.40
1:A:340:ASP:O	1:A:343:ARG:HB2	2.21	0.40
1:B:26:ALA:O	1:B:27:VAL:C	2.65	0.40
1:B:98:SER:O	1:B:101:ARG:N	2.54	0.40
1:B:347:GLU:N	1:B:348:PRO:HD2	2.37	0.40
1:C:20:GLN:O	1:C:24:LYS:HG3	2.21	0.40
2:H:117:GLU:C	2:H:119:GLN:N	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:131:LEU:HD21	2:H:135:ARG:CZ	2.51	0.40
2:H:147:GLU:O	2:H:148:ILE:C	2.65	0.40
2:M:82:TRP:O	2:M:89:ARG:HG2	2.20	0.40
2:N:78:LEU:HD12	2:N:78:LEU:O	2.21	0.40
1:A:3:GLU:OE1	1:A:3:GLU:HA	2.21	0.40
1:B:347:GLU:N	1:B:348:PRO:CD	2.84	0.40
2:G:56:LEU:C	2:G:56:LEU:CD2	2.94	0.40
2:H:9:ASN:O	2:H:11:GLN:HG2	2.22	0.40
2:I:63:LYS:N	2:I:63:LYS:HE3	2.36	0.40
2:L:18:GLY:CA	2:L:33:LYS:HZ3	2.28	0.40
2:L:70:HIS:CB	2:L:73:LYS:HD3	2.47	0.40
2:M:144:SER:O	2:M:145:ALA:C	2.65	0.40
2:M:165:THR:HA	2:M:167:PHE:HE2	1.86	0.40
2:N:95:LEU:HB2	2:N:106:ILE:HB	2.02	0.40
2:N:172:LEU:HB2	2:N:173:PRO:HD3	2.03	0.40
1:B:57:GLY:HA2	1:B:58:PRO:HD3	1.92	0.40
1:B:72:LYS:C	1:B:72:LYS:CD	2.95	0.40
1:B:77:PRO:HB2	1:B:103:LEU:HD11	2.03	0.40
1:B:359:LEU:HD12	1:B:359:LEU:HA	1.87	0.40
1:B:391:ILE:O	1:B:391:ILE:HG13	2.21	0.40
1:B:437:GLU:OE1	1:C:315:ARG:NH1	2.53	0.40
1:C:64:THR:O	1:C:68:ARG:HB2	2.22	0.40
1:C:71:ALA:CB	1:C:78:PHE:HB2	2.51	0.40
2:H:117:GLU:O	2:H:119:GLN:HG2	2.21	0.40
2:L:111:ASP:O	2:L:112:VAL:O	2.39	0.40
2:L:144:SER:N	2:L:147:GLU:HB2	2.37	0.40
2:M:134:ALA:O	2:M:137:LEU:N	2.55	0.40
2:N:42:VAL:HG22	2:N:99:ASP:CB	2.31	0.40
2:N:120:ILE:HD12	2:N:135:ARG:HG2	2.03	0.40
2:N:138:VAL:C	2:N:140:ASN:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/310 (94%)	229 (78%)	50 (17%)	14 (5%)	2	14
1	B	289/310 (93%)	217 (75%)	54 (19%)	18 (6%)	1	9
1	C	290/310 (94%)	219 (76%)	53 (18%)	18 (6%)	1	9
2	G	172/174 (99%)	128 (74%)	33 (19%)	11 (6%)	1	8
2	H	172/174 (99%)	131 (76%)	31 (18%)	10 (6%)	1	10
2	I	172/174 (99%)	128 (74%)	31 (18%)	13 (8%)	1	5
2	L	172/174 (99%)	122 (71%)	35 (20%)	15 (9%)	0	3
2	M	172/174 (99%)	109 (63%)	49 (28%)	14 (8%)	1	4
2	N	172/174 (99%)	121 (70%)	35 (20%)	16 (9%)	0	3
All	All	1904/1974 (96%)	1404 (74%)	371 (20%)	129 (7%)	1	7

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	VAL
1	A	435	GLU
1	B	42	GLU
1	B	85	LYS
1	C	47	GLU
1	C	338	ALA
1	C	371	THR
1	C	426	VAL
2	G	71	LEU
2	G	84	THR
2	H	90	LYS
2	H	100	GLU
2	I	30	ASN
2	I	89	ARG
2	I	90	LYS
2	I	111	ASP
2	I	119	GLN
2	L	17	ASP
2	L	70	HIS
2	L	112	VAL
2	L	134	ALA
2	M	30	ASN
2	M	82	TRP

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Mol	Chain	Res	Type
2	M	147	GLU
2	N	12	VAL
2	N	82	TRP
2	N	115	PRO
2	N	127	GLY
1	A	93	GLY
1	A	383	ARG
1	A	431	GLY
1	A	432	GLU
1	B	26	ALA
1	B	27	VAL
1	B	411	ALA
1	C	85	LYS
1	C	288	GLY
1	C	294	LYS
1	C	425	TYR
1	C	431	GLY
1	C	432	GLU
2	G	17	ASP
2	G	70	HIS
2	G	89	ARG
2	G	116	GLU
2	G	137	LEU
2	G	141	THR
2	H	38	TYR
2	H	137	LEU
2	I	92	GLU
2	I	133	ALA
2	I	135	ARG
2	L	110	GLY
2	L	127	GLY
2	M	117	GLU
2	M	139	GLU
2	M	156	ALA
2	N	93	ALA
2	N	117	GLU
2	N	143	LEU
1	C	342	GLU
1	C	405	ASP
2	G	68	GLN
2	G	127	GLY
2	H	50	THR

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Mol	Chain	Res	Type
2	H	62	ARG
2	H	131	LEU
2	I	68	GLN
2	L	135	ARG
2	L	150	GLU
2	M	39	ASN
2	M	53	ALA
2	M	69	GLY
2	M	172	LEU
2	N	19	GLN
2	N	59	LEU
2	N	69	GLY
2	N	109	ILE
1	A	246	ASP
1	A	405	ASP
1	A	441	ARG
1	B	16	HIS
1	B	427	ALA
1	C	348	PRO
2	H	39	ASN
2	H	115	PRO
2	H	133	ALA
2	I	100	GLU
2	L	117	GLU
2	L	157	GLY
2	M	35	ARG
2	M	68	GLN
2	N	9	ASN
2	N	83	ARG
2	N	134	ALA
2	N	172	LEU
1	A	43	PRO
1	A	77	PRO
1	B	43	PRO
1	B	349	HIS
1	B	350	ALA
1	B	375	LYS
1	B	404	MET
1	B	405	ASP
1	C	30	ALA
1	C	284	PRO
2	I	17	ASP

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Mol	Chain	Res	Type
2	L	69	GLY
1	B	40	LEU
1	B	283	LEU
1	C	434	VAL
2	G	136	ALA
2	I	71	LEU
2	I	110	GLY
2	L	71	LEU
2	L	115	PRO
2	M	108	GLY
2	N	157	GLY
1	A	328	PRO
1	A	348	PRO
1	C	60	GLY
1	A	433	VAL
1	B	321	PRO
2	L	161	VAL
2	M	138	VAL
1	C	99	ILE
1	B	284	PRO
1	B	325	GLY
2	L	173	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	249/256 (97%)	221 (89%)	28 (11%)	6	25
1	B	246/256 (96%)	220 (89%)	26 (11%)	6	27
1	C	246/256 (96%)	215 (87%)	31 (13%)	4	21
2	G	139/140 (99%)	128 (92%)	11 (8%)	11	40
2	H	139/140 (99%)	130 (94%)	9 (6%)	15	47
2	I	139/140 (99%)	124 (89%)	15 (11%)	6	27
2	L	139/140 (99%)	132 (95%)	7 (5%)	22	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	139/140 (99%)	127 (91%)	12 (9%)	10	36
2	N	139/140 (99%)	134 (96%)	5 (4%)	31	63
All	All	1575/1608 (98%)	1431 (91%)	144 (9%)	9	34

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	20	GLN
1	A	34	ARG
1	A	39	GLN
1	A	59	THR
1	A	79	ILE
1	A	98	SER
1	A	259	ILE
1	A	279	GLN
1	A	281	ASP
1	A	285	LEU
1	A	291	VAL
1	A	293	THR
1	A	330	ARG
1	A	336	LEU
1	A	345	LEU
1	A	359	LEU
1	A	367	ILE
1	A	370	THR
1	A	372	ASP
1	A	379	GLU
1	A	384	VAL
1	A	394	ARG
1	A	403	LEU
1	A	413	ASP
1	A	428	ASP
1	A	435	GLU
1	A	441	ARG
1	B	4	MET
1	B	11	SER
1	B	20	GLN
1	B	22	ASP
1	B	39	GLN
1	B	41	GLN

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Mol	Chain	Res	Type
1	B	46	HIS
1	B	61	VAL
1	B	63	LYS
1	B	70	LEU
1	B	286	VAL
1	B	298	VAL
1	B	303	ILE
1	B	312	GLN
1	B	321	PRO
1	B	336	LEU
1	B	345	LEU
1	B	348	PRO
1	B	359	LEU
1	B	367	ILE
1	B	384	VAL
1	B	394	ARG
1	B	398	THR
1	B	413	ASP
1	B	418	THR
1	B	441	ARG
1	C	5	THR
1	C	6	PRO
1	C	27	VAL
1	C	34	ARG
1	C	39	GLN
1	C	48	VAL
1	C	55	MET
1	C	68	ARG
1	C	73	LEU
1	C	86	PHE
1	C	104	THR
1	C	251	ASN
1	C	281	ASP
1	C	286	VAL
1	C	291	VAL
1	C	330	ARG
1	C	331	VAL
1	C	336	LEU
1	C	345	LEU
1	C	349	HIS
1	C	355	GLN
1	C	359	LEU

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Mol	Chain	Res	Type
1	C	360	MET
1	C	362	THR
1	C	384	VAL
1	C	398	THR
1	C	403	LEU
1	C	408	SER
1	C	428	ASP
1	C	432	GLU
1	C	441	ARG
2	G	19	GLN
2	G	26	VAL
2	G	46	PHE
2	G	55	THR
2	G	56	LEU
2	G	58	GLU
2	G	71	LEU
2	G	72	LEU
2	G	135	ARG
2	G	155	ILE
2	G	164	ASN
2	H	12	VAL
2	H	55	THR
2	H	71	LEU
2	H	72	LEU
2	H	92	GLU
2	H	95	LEU
2	H	135	ARG
2	H	153	LEU
2	H	164	ASN
2	I	2	THR
2	I	43	LEU
2	I	55	THR
2	I	56	LEU
2	I	63	LYS
2	I	72	LEU
2	I	76	VAL
2	I	90	LYS
2	I	97	VAL
2	I	101	LYS
2	I	104	LEU
2	I	112	VAL
2	I	141	THR

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Mol	Chain	Res	Type
2	I	150	GLU
2	I	164	ASN
2	L	43	LEU
2	L	59	LEU
2	L	65	GLU
2	L	80	LYS
2	L	100	GLU
2	L	148	ILE
2	L	167	PHE
2	M	43	LEU
2	M	71	LEU
2	M	73	LYS
2	M	86	ARG
2	M	89	ARG
2	M	91	LEU
2	M	106	ILE
2	M	117	GLU
2	M	118	ASP
2	M	148	ILE
2	M	168	THR
2	M	172	LEU
2	N	38	TYR
2	N	73	LYS
2	N	80	LYS
2	N	91	LEU
2	N	118	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	20	GLN
1	A	33	ASN
1	A	39	GLN
1	A	41	GLN
1	A	250	GLN
1	A	324	GLN
1	A	397	HIS
1	A	417	GLN
1	B	16	HIS
1	B	20	GLN
1	B	39	GLN

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Mol	Chain	Res	Type
1	B	41	GLN
1	B	324	GLN
1	B	417	GLN
1	C	20	GLN
1	C	41	GLN
1	C	46	HIS
1	C	52	ASN
1	C	250	GLN
1	C	312	GLN
1	C	324	GLN
1	C	355	GLN
2	G	19	GLN
2	G	24	ASN
2	G	68	GLN
2	G	164	ASN
2	H	19	GLN
2	H	30	ASN
2	H	68	GLN
2	H	119	GLN
2	H	140	ASN
2	H	164	ASN
2	I	19	GLN
2	I	24	ASN
2	I	68	GLN
2	I	164	ASN
2	I	166	ASN
2	L	19	GLN
2	L	39	ASN
2	L	70	HIS
2	L	166	ASN
2	M	11	GLN
2	M	19	GLN
2	M	68	GLN
2	N	11	GLN
2	N	67	HIS
2	N	119	GLN
2	N	140	ASN
2	N	146	HIS
2	N	166	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 12 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	LVS	G	0	2	40,41,42	4.26	12 (30%)	49,57,59	1.73	10 (20%)
6	LVS	H	0	2	40,41,42	4.37	12 (30%)	49,57,59	1.63	7 (14%)
5	PO4	C	452	4	4,4,4	1.29	0	6,6,6	0.46	0
6	LVS	I	0	2	40,41,42	4.52	12 (30%)	49,57,59	1.73	5 (10%)
5	PO4	A	452	4	4,4,4	1.54	0	6,6,6	0.48	0
3	ADP	B	450	4	28,29,29	2.57	10 (35%)	43,45,45	1.55	7 (16%)
3	ADP	A	450	4	28,29,29	2.67	10 (35%)	43,45,45	1.58	6 (13%)
5	PO4	B	452	4	4,4,4	1.52	0	6,6,6	0.45	0
3	ADP	C	450	4	28,29,29	2.51	11 (39%)	43,45,45	1.60	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LVS	H	0	2	-	9/43/46/46	0/1/1/1
6	LVS	I	0	2	-	11/43/46/46	0/1/1/1
3	ADP	B	450	4	-	2/16/32/32	0/3/3/3
3	ADP	A	450	4	-	2/16/32/32	0/3/3/3
6	LVS	G	0	2	-	11/43/46/46	0/1/1/1
3	ADP	C	450	4	-	2/16/32/32	0/3/3/3

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	0	LVS	C2'-CS	17.02	1.58	1.31
6	I	0	LVS	C2'-CS	16.80	1.58	1.31
6	G	0	LVS	C2'-CS	15.77	1.56	1.31
6	I	0	LVS	O1'-S	11.70	1.58	1.44
6	I	0	LVS	O2'-S	11.26	1.58	1.44
6	G	0	LVS	O1'-S	11.23	1.58	1.44
6	H	0	LVS	O1'-S	11.07	1.58	1.44
6	H	0	LVS	O2'-S	10.45	1.57	1.44
6	G	0	LVS	O2'-S	9.50	1.56	1.44
6	G	0	LVS	C9-C8	8.65	1.54	1.39
6	I	0	LVS	C9-C8	7.69	1.52	1.39
6	H	0	LVS	C9-C8	7.50	1.52	1.39
3	A	450	ADP	PA-O3A	7.29	1.67	1.59
3	B	450	ADP	PA-O3A	6.46	1.66	1.59
6	I	0	LVS	C6-C7	5.97	1.50	1.39
3	B	450	ADP	C2-N1	5.85	1.44	1.33
6	I	0	LVS	C10-C5	5.72	1.50	1.38
6	G	0	LVS	C10-C5	5.63	1.50	1.38
6	H	0	LVS	C6-C7	5.58	1.50	1.39
6	G	0	LVS	O3-N4	5.55	1.32	1.22
3	C	450	ADP	C2-N1	5.53	1.43	1.33
6	G	0	LVS	CD5-CG3	-5.51	1.23	1.51
6	I	0	LVS	O3-N4	5.44	1.32	1.22
3	C	450	ADP	PB-O1B	5.41	1.67	1.50
6	H	0	LVS	CD5-CG3	-5.39	1.23	1.51
6	G	0	LVS	C6-C7	5.24	1.49	1.39
6	I	0	LVS	CD5-CG3	-5.22	1.24	1.51
3	A	450	ADP	PB-O1B	5.20	1.66	1.50
3	A	450	ADP	C2-N1	5.16	1.43	1.33
6	H	0	LVS	C10-C5	5.05	1.48	1.38
6	H	0	LVS	O3-N4	5.01	1.31	1.22
3	B	450	ADP	PB-O1B	4.74	1.65	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	450	ADP	PA-O3A	4.51	1.64	1.59
6	I	0	LVS	C1-N2	4.46	1.43	1.34
6	I	0	LVS	CB3-CA3	4.45	1.59	1.53
6	H	0	LVS	C3-N1	4.39	1.43	1.34
3	C	450	ADP	C4-N3	4.38	1.42	1.34
6	I	0	LVS	C3-N1	4.23	1.43	1.34
6	G	0	LVS	C3-N1	4.13	1.42	1.34
3	B	450	ADP	C4-N3	4.09	1.42	1.34
3	A	450	ADP	C4-N3	4.08	1.42	1.34
6	H	0	LVS	C2-N3	3.87	1.42	1.34
3	B	450	ADP	PB-O2B	3.45	1.67	1.54
6	H	0	LVS	CB3-CA3	3.43	1.58	1.53
3	A	450	ADP	PB-O2B	3.39	1.67	1.54
6	G	0	LVS	C2-N3	3.36	1.41	1.34
3	C	450	ADP	PB-O2B	3.34	1.67	1.54
3	C	450	ADP	C8-N9	3.21	1.43	1.37
6	G	0	LVS	C1-N2	3.05	1.40	1.34
6	I	0	LVS	C2-N3	3.05	1.40	1.34
3	A	450	ADP	C8-N9	2.98	1.42	1.37
3	A	450	ADP	PA-O2A	2.94	1.68	1.55
3	C	450	ADP	PA-O2A	2.91	1.68	1.55
3	B	450	ADP	PA-O2A	2.90	1.68	1.55
3	C	450	ADP	C6-N6	2.90	1.41	1.34
3	B	450	ADP	C6-N6	2.89	1.41	1.34
6	H	0	LVS	C1-N2	2.86	1.40	1.34
3	B	450	ADP	C8-N9	2.80	1.42	1.37
6	G	0	LVS	CB3-CA3	2.78	1.57	1.53
3	B	450	ADP	PA-O1A	2.58	1.59	1.50
3	A	450	ADP	PA-O1A	2.51	1.59	1.50
3	A	450	ADP	C5-C4	-2.43	1.34	1.39
3	A	450	ADP	C6-N6	2.41	1.40	1.34
3	C	450	ADP	PA-O1A	2.39	1.59	1.50
3	C	450	ADP	C5-C6	2.27	1.47	1.41
3	C	450	ADP	C5-C4	-2.14	1.35	1.39
3	B	450	ADP	C5-C4	-2.07	1.35	1.39

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	0	LVS	CD5-CG3-CB3	6.50	134.47	111.08
6	H	0	LVS	CD5-CG3-CB3	6.42	134.16	111.08
6	G	0	LVS	CD5-CG3-CB3	6.28	133.66	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	450	ADP	N3-C2-N1	-5.47	120.30	128.58
3	C	450	ADP	N3-C2-N1	-5.46	120.32	128.58
3	B	450	ADP	N3-C2-N1	-5.30	120.56	128.58
6	I	0	LVS	CD6-CG3-CD5	-4.73	89.43	110.53
6	H	0	LVS	CD6-CG3-CD5	-4.66	89.74	110.53
6	I	0	LVS	CB3-CA3-CS	4.65	118.11	110.99
6	G	0	LVS	CD6-CG3-CD5	-4.57	90.12	110.53
3	C	450	ADP	C5-C4-N3	-3.76	121.54	126.72
3	A	450	ADP	C5-C4-N3	-3.66	121.67	126.72
6	I	0	LVS	CA3-CS-C2'	-3.52	107.90	125.91
3	B	450	ADP	C5-C4-N3	-3.44	121.98	126.72
6	G	0	LVS	CA3-CS-C2'	-3.22	109.43	125.91
6	H	0	LVS	CA3-CS-C2'	-3.08	110.15	125.91
6	G	0	LVS	CB3-CA3-CS	3.05	115.66	110.99
3	C	450	ADP	C2-N3-C4	2.98	119.12	111.83
3	A	450	ADP	C2-N3-C4	2.94	119.00	111.83
6	G	0	LVS	C1-CA1-N1	-2.91	103.23	111.11
3	C	450	ADP	N3-C4-N9	2.80	131.92	127.17
3	B	450	ADP	C2-N3-C4	2.79	118.64	111.83
3	A	450	ADP	N3-C4-N9	2.78	131.90	127.17
6	H	0	LVS	CB3-CA3-CS	2.52	114.85	110.99
6	H	0	LVS	CB2-CA2-C2	2.51	116.54	110.59
3	C	450	ADP	C2-N1-C6	2.50	122.84	118.73
3	B	450	ADP	N3-C4-N9	2.49	131.40	127.17
3	B	450	ADP	O2B-PB-O3A	2.36	112.55	104.64
3	B	450	ADP	C2-N1-C6	2.31	122.52	118.73
6	G	0	LVS	CB1-CA1-N1	2.29	115.74	110.58
6	I	0	LVS	CA1-C1-N2	2.25	121.42	116.63
6	G	0	LVS	CS-C2'-S	-2.24	116.41	121.89
6	H	0	LVS	C1-CA1-N1	-2.23	105.08	111.11
3	A	450	ADP	C2-N1-C6	2.20	122.35	118.73
6	G	0	LVS	CB3-CA3-N3	-2.18	107.39	110.69
3	B	450	ADP	O2A-PA-O3A	2.13	113.03	107.27
3	C	450	ADP	C5-N7-C8	2.11	106.76	103.45
6	G	0	LVS	CG2-CB2-CA2	2.09	121.01	115.40
6	H	0	LVS	C4-C3-N1	2.08	119.11	115.88
3	C	450	ADP	O2B-PB-O3A	2.08	111.60	104.64
3	A	450	ADP	O2B-PB-O3A	2.07	111.57	104.64
6	G	0	LVS	CB2-CA2-C2	2.06	115.46	110.59
3	C	450	ADP	O4'-C4'-C3'	2.01	109.14	105.15

There are no chirality outliers.

All (37) torsion outliers are listed below:

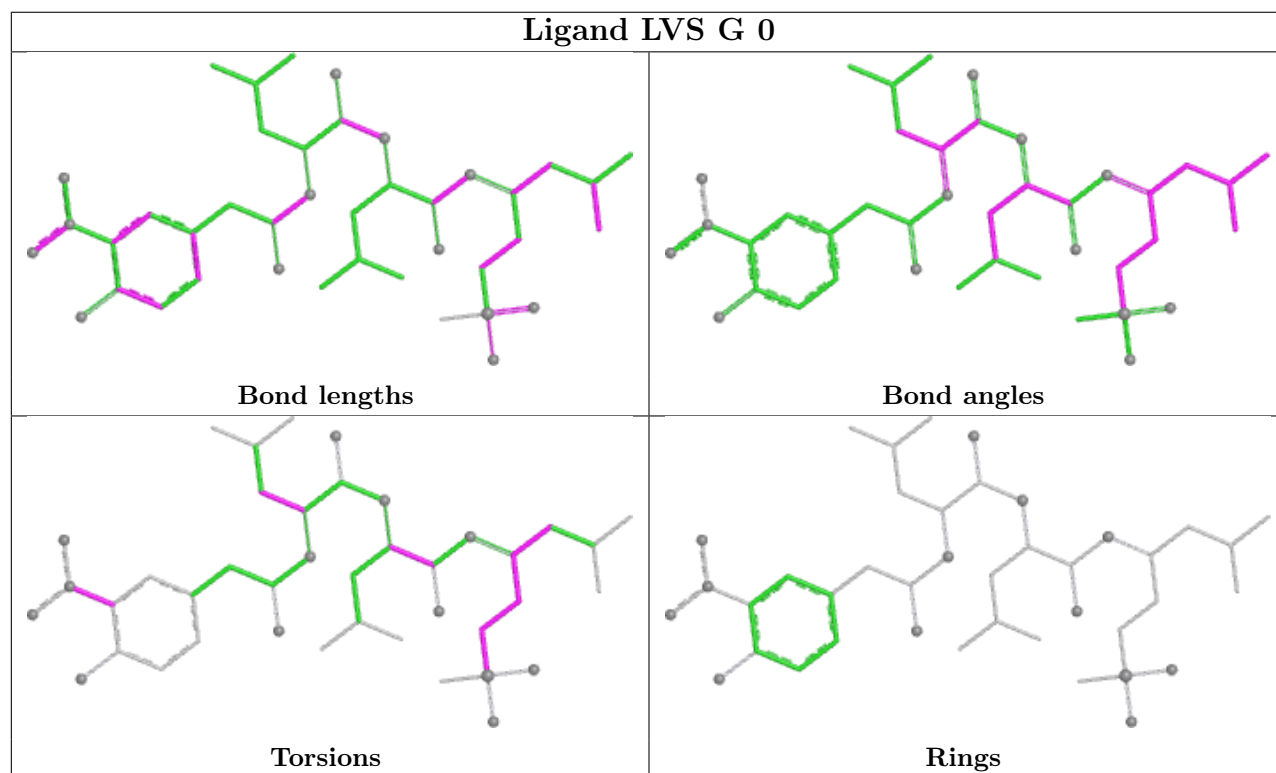
Mol	Chain	Res	Type	Atoms
6	G	0	LVS	N1-CA1-CB1-CG1
6	G	0	LVS	N3-CA3-CS-C2'
6	G	0	LVS	CB3-CA3-CS-C2'
6	G	0	LVS	S-C2'-CS-CA3
6	G	0	LVS	CS-C2'-S-O1'
6	G	0	LVS	CS-C2'-S-O2'
6	G	0	LVS	C6-C7-N4-O3
6	G	0	LVS	C8-C7-N4-O3
6	H	0	LVS	N3-CA3-CS-C2'
6	H	0	LVS	CB3-CA3-CS-C2'
6	H	0	LVS	S-C2'-CS-CA3
6	H	0	LVS	CS-C2'-S-O1'
6	H	0	LVS	CS-C2'-S-O2'
6	H	0	LVS	C6-C7-N4-O3
6	H	0	LVS	C8-C7-N4-O3
6	I	0	LVS	N3-CA3-CS-C2'
6	I	0	LVS	CB3-CA3-CS-C2'
6	I	0	LVS	S-C2'-CS-CA3
6	I	0	LVS	CS-C2'-S-O1'
6	I	0	LVS	CS-C2'-S-O2'
6	I	0	LVS	N1-CA1-CB1-CG1
6	I	0	LVS	C1-CA1-CB1-CG1
6	I	0	LVS	C2-CA2-CB2-CG2
6	G	0	LVS	C1-CA1-CB1-CG1
3	B	450	ADP	O4'-C4'-C5'-O5'
3	B	450	ADP	C3'-C4'-C5'-O5'
3	C	450	ADP	O4'-C4'-C5'-O5'
3	C	450	ADP	C3'-C4'-C5'-O5'
3	A	450	ADP	O4'-C4'-C5'-O5'
3	A	450	ADP	C3'-C4'-C5'-O5'
6	I	0	LVS	N2-CA2-CB2-CG2
6	H	0	LVS	N3-CA3-CB3-CG3
6	I	0	LVS	O1-C1-CA1-N1
6	I	0	LVS	N2-C1-CA1-N1
6	G	0	LVS	N3-CA3-CB3-CG3
6	H	0	LVS	O2-C2-CA2-N2
6	G	0	LVS	O2-C2-CA2-N2

There are no ring outliers.

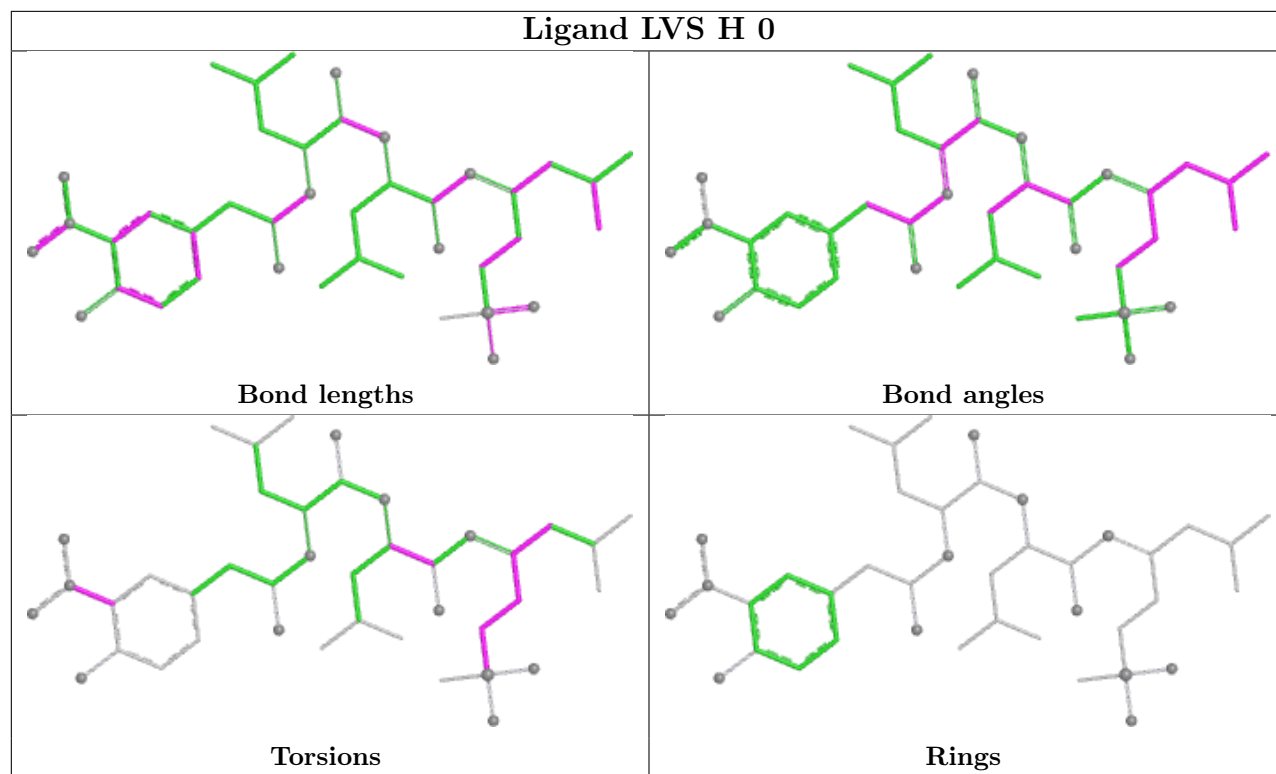
8 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	0	LVS	10	0
6	H	0	LVS	3	0
5	C	452	PO4	1	0
6	I	0	LVS	4	0
3	B	450	ADP	6	0
3	A	450	ADP	4	0
5	B	452	PO4	2	0
3	C	450	ADP	4	0

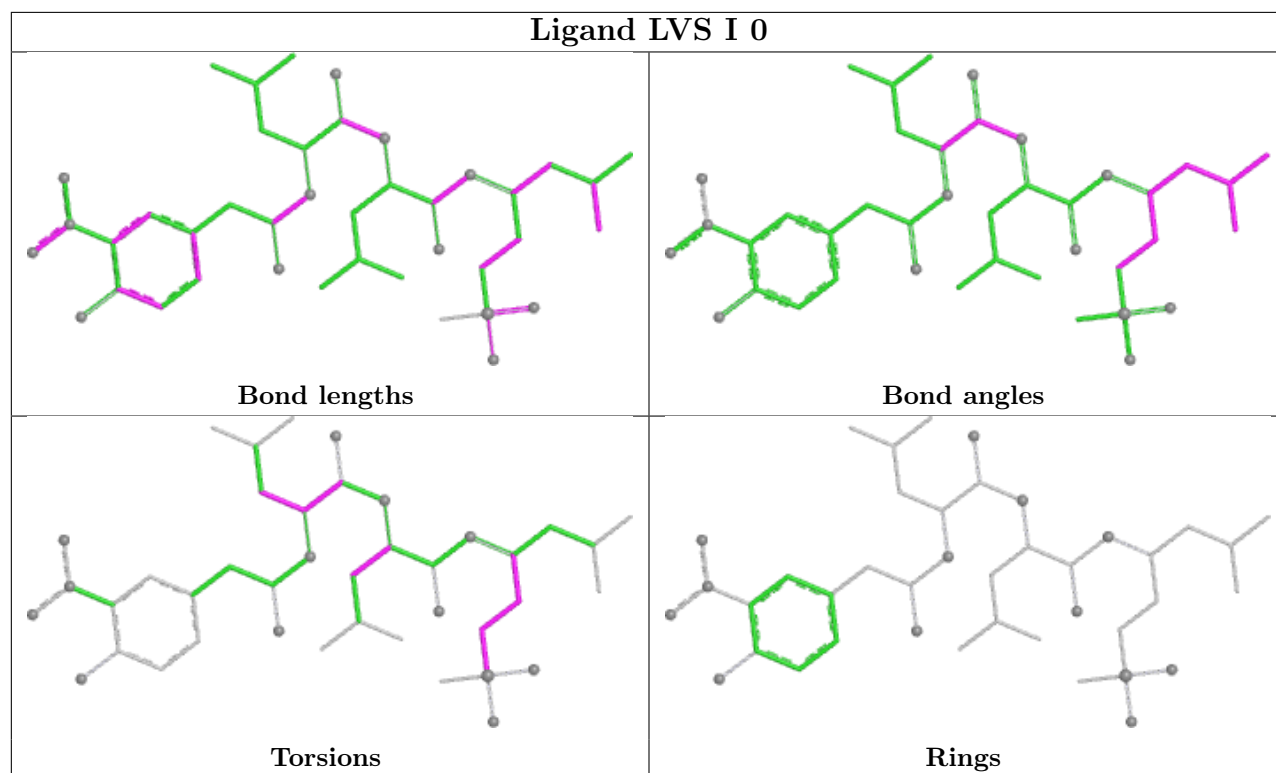
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

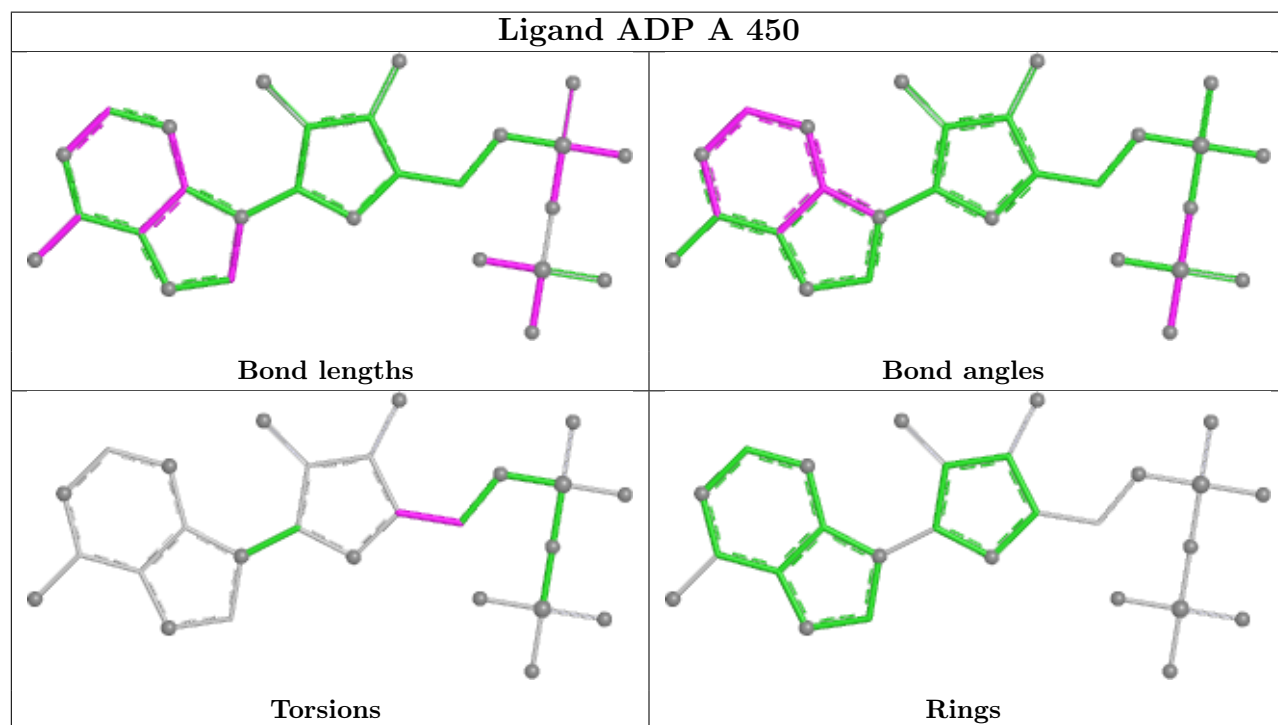
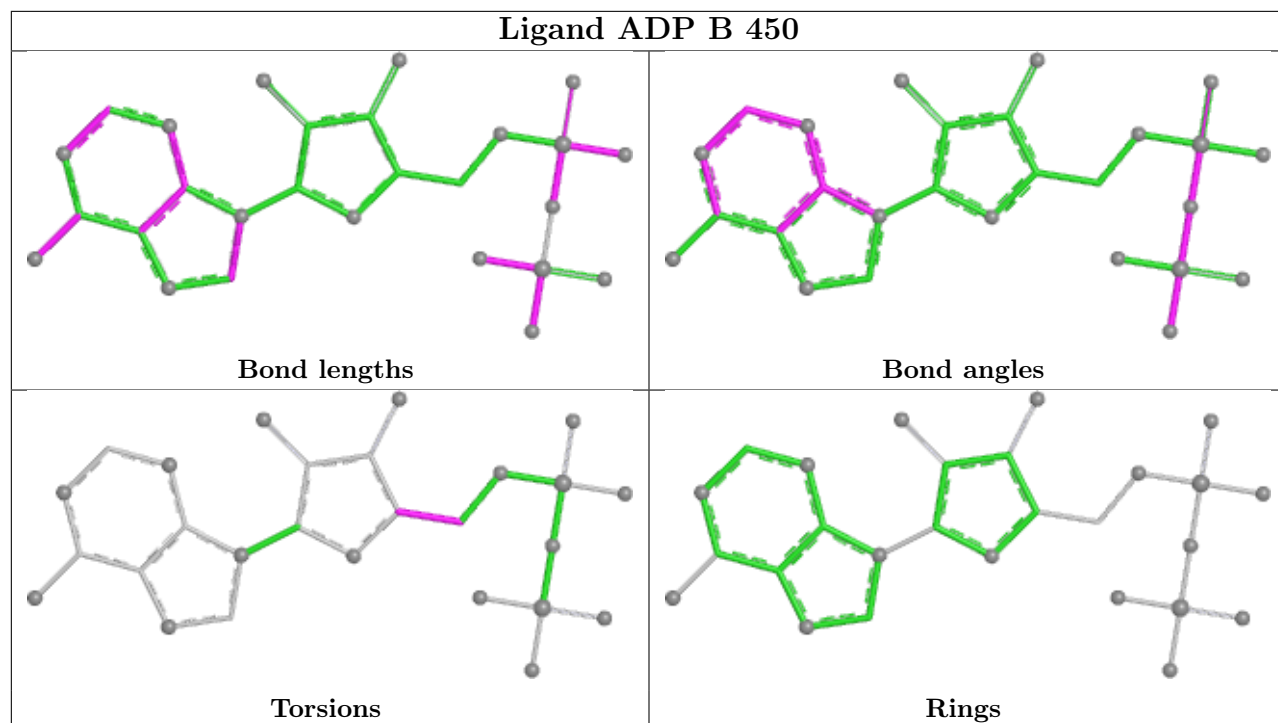


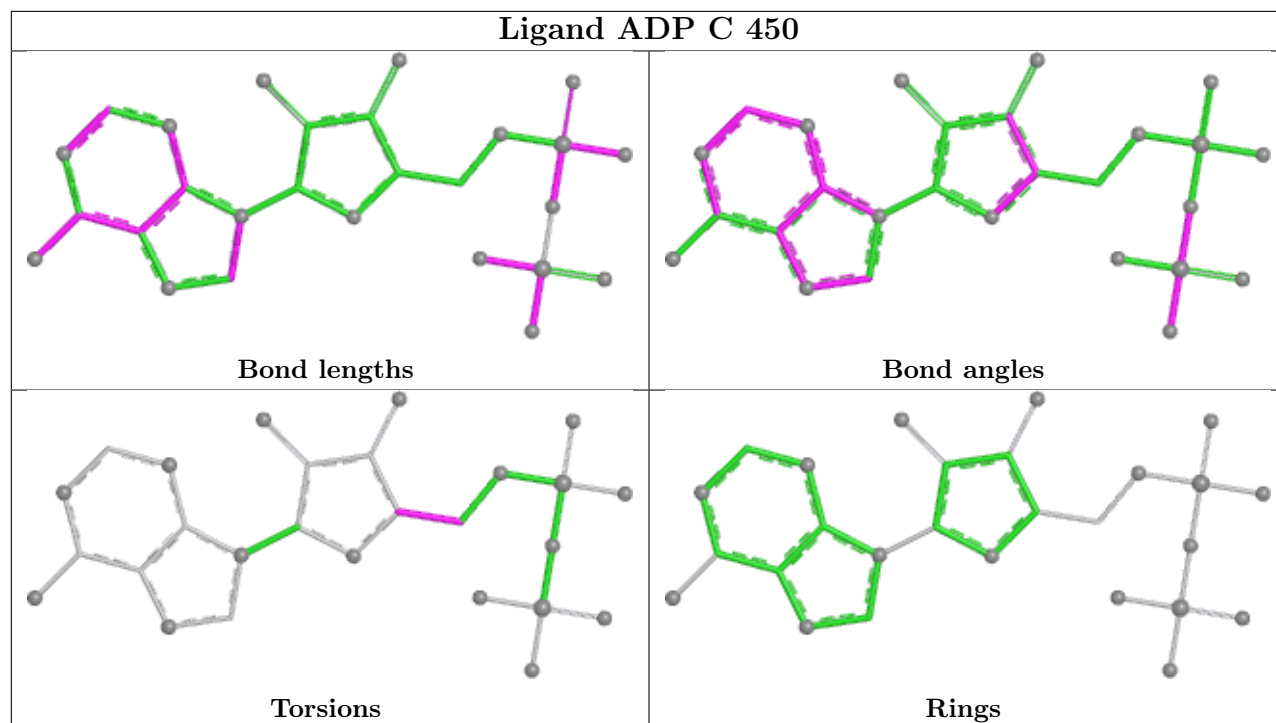
Ligand LVS H 0



Ligand LVS I 0







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.