Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 01:54 am GMT

PDB ID	:	1OFI
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:

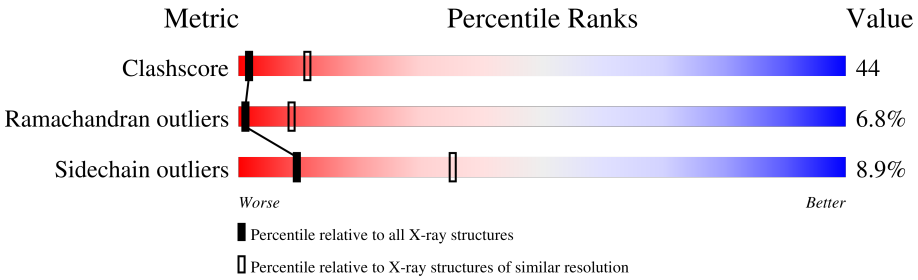
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	39% 49% 8%
1	B	310	39% 47% 8% 5%
1	C	310	37% 49% 10% 5%
2	G	174	39% 52% 9%
2	H	174	36% 54% 10%
2	I	174	33% 54% 12%
2	L	174	37% 54% 9%
2	M	174	33% 57% 9%

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Mol	Chain	Length	Quality of chain
2	N	174	36% 55% 9%

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 (i)

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.

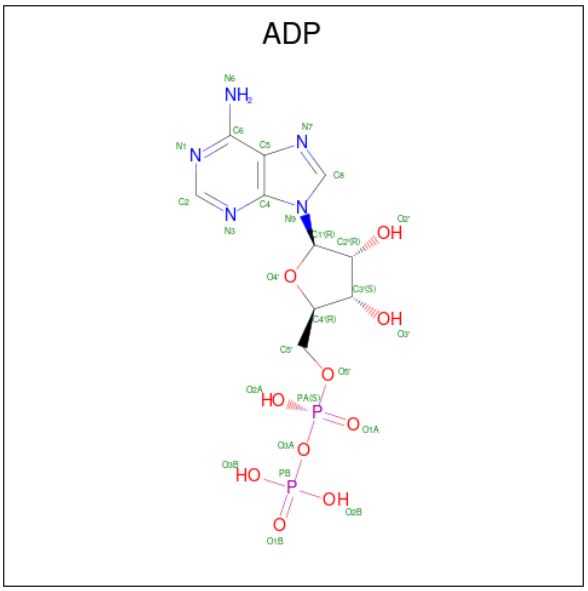
- Molecule 1 is a protein called ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU.

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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

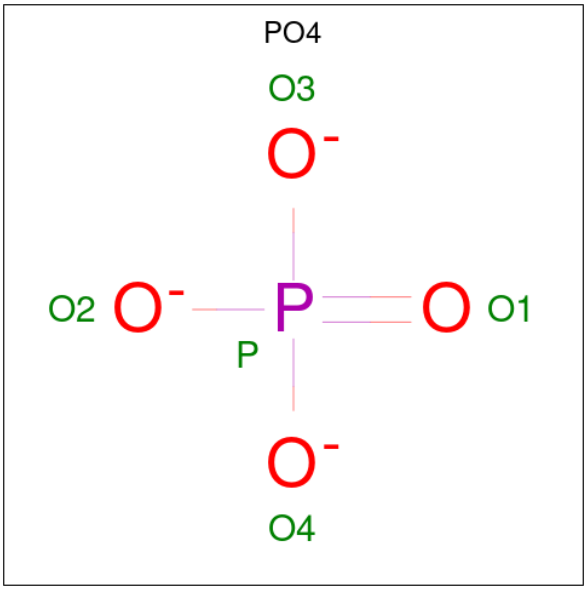


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

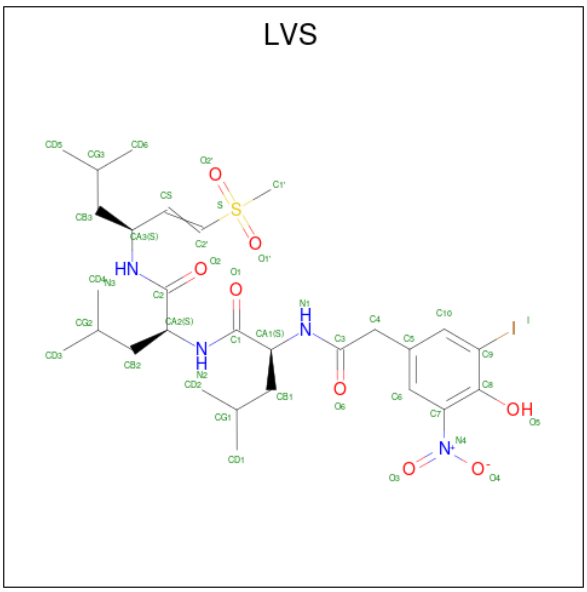
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	G	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		
4	L	1	Total	Mg	0	0
			1	1		
4	M	1	Total	Mg	0	0
			1	1		
4	N	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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



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

- Molecule 7 is water.

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

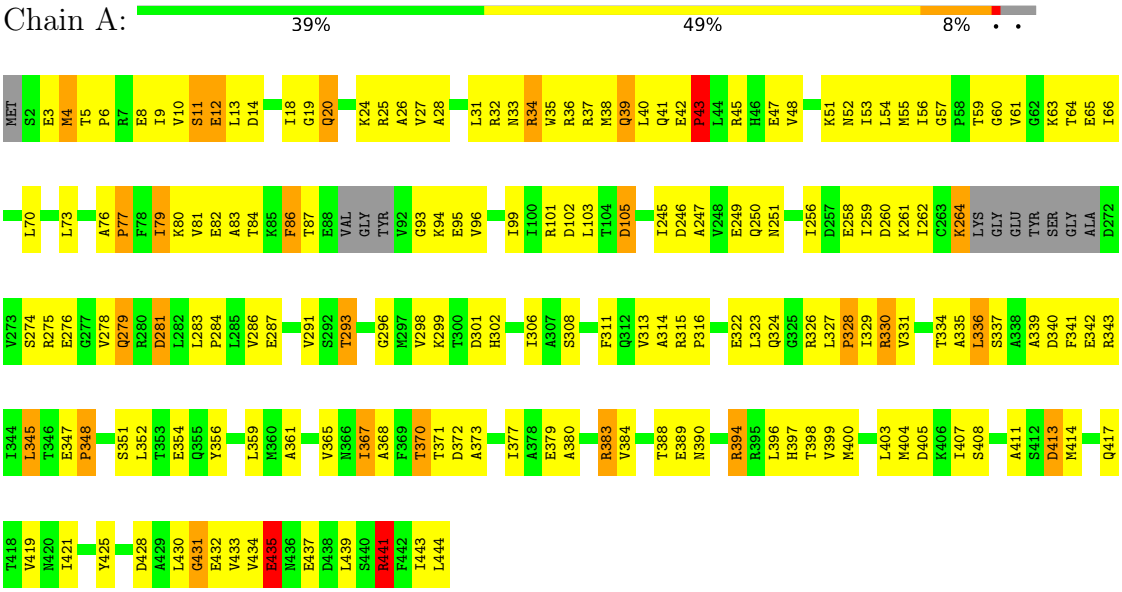
3 Residue-property plots (i)

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

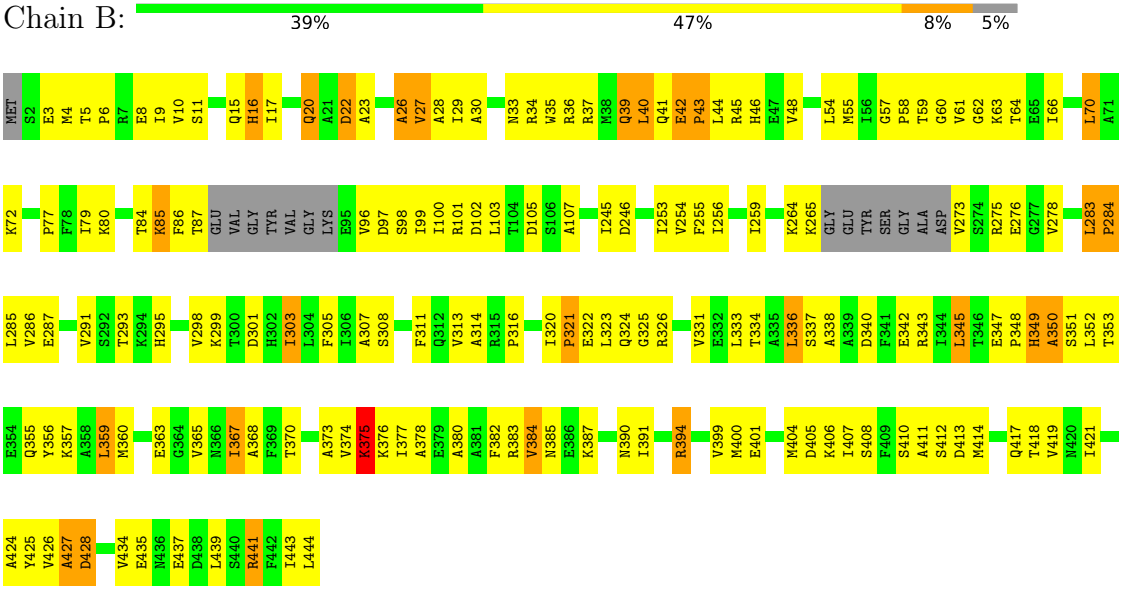
• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

Chain A:



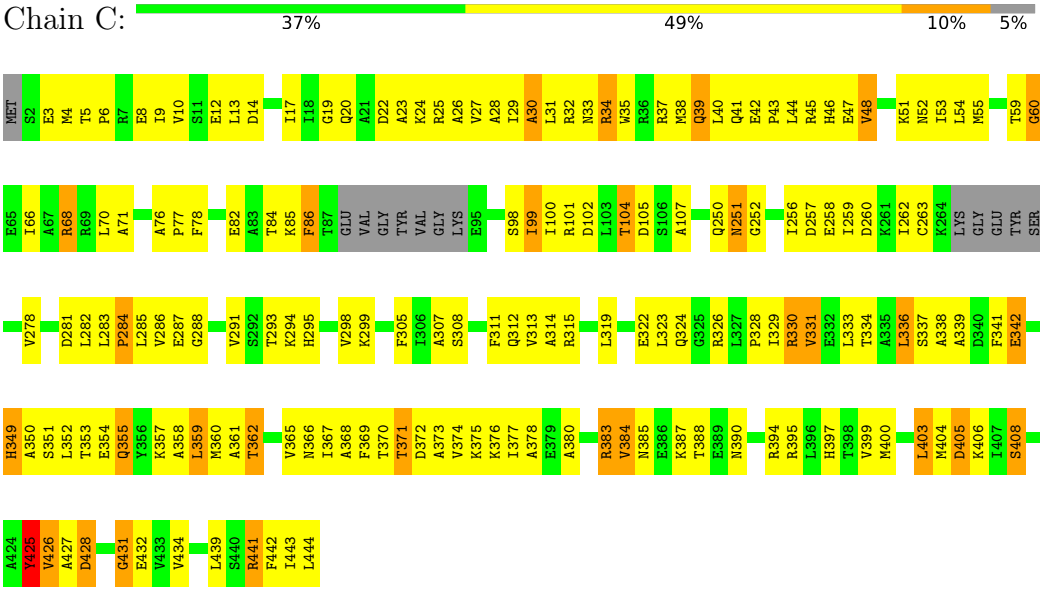
• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

Chain B:



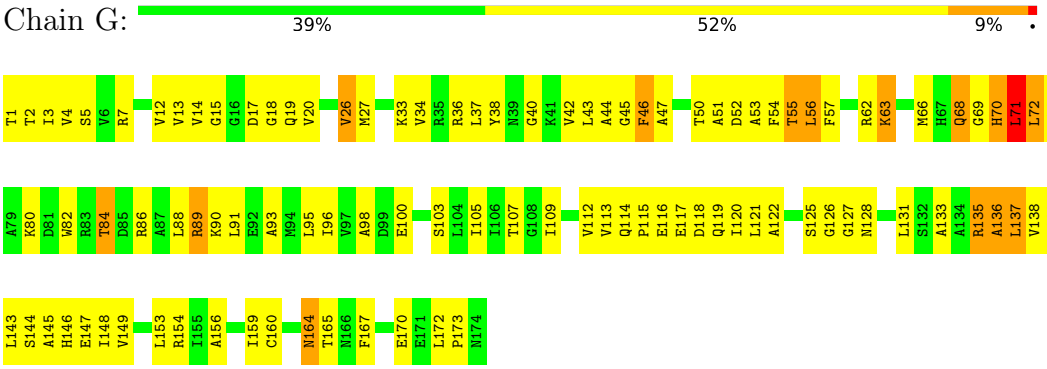
• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

Chain C:



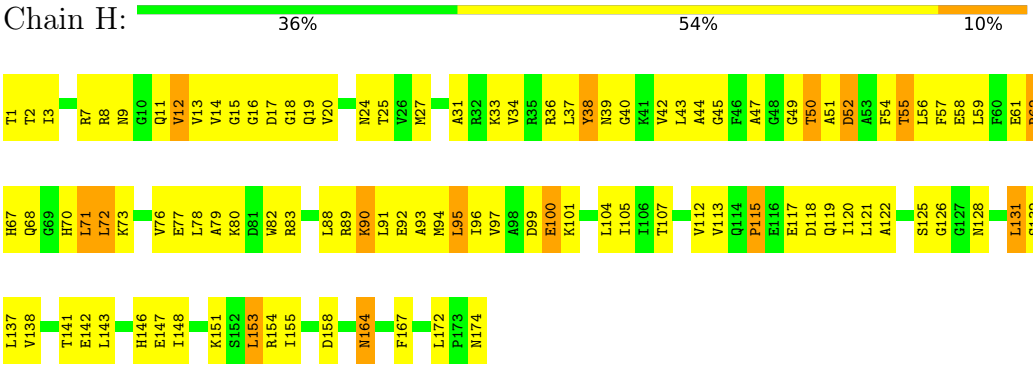
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain G:



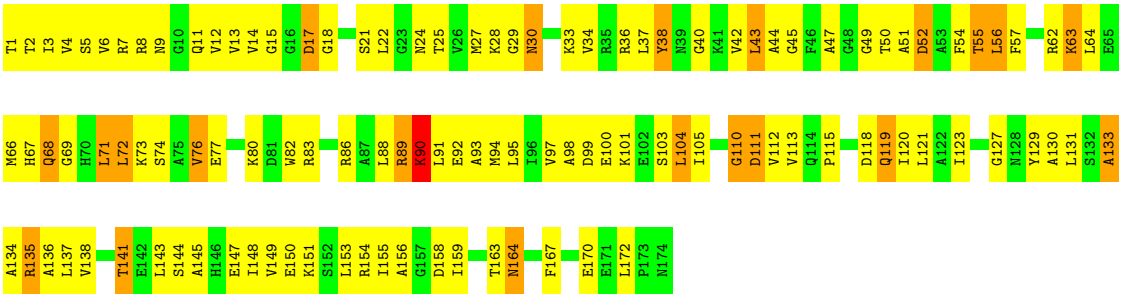
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

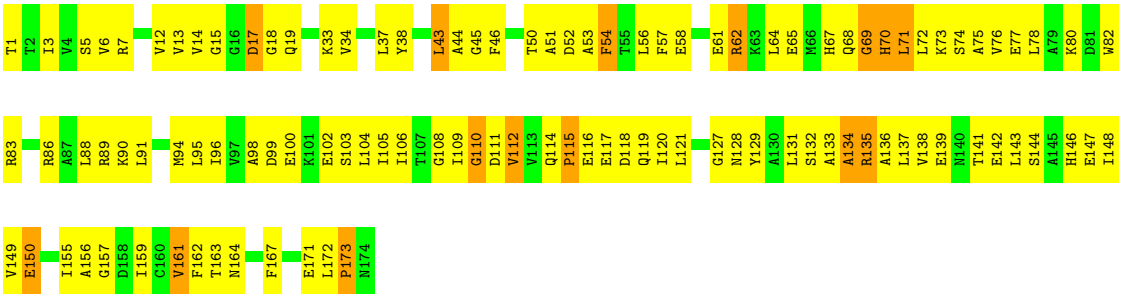
Chain H:



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

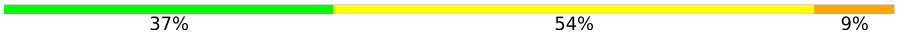
Chain I:





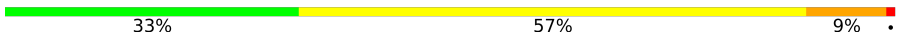
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

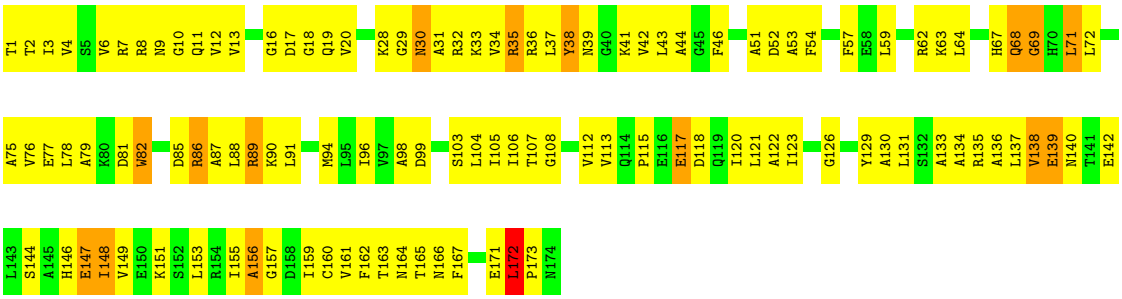
Chain L:



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

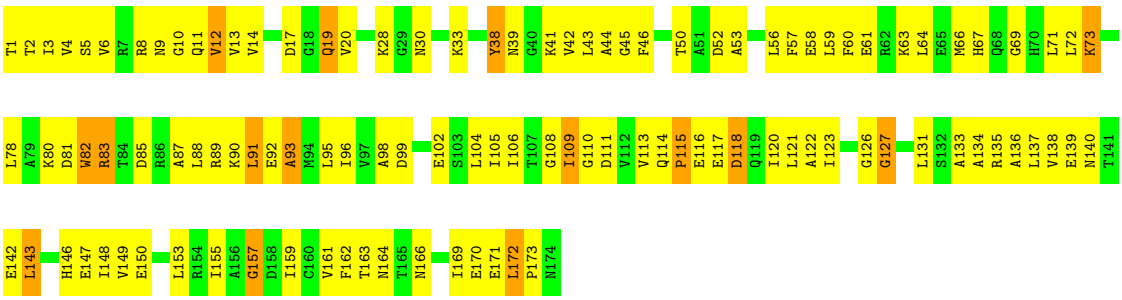
Chain M:





• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain N:



4 Data and refinement statistics (i)

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	0.44	0/2339	0.71	0/3156
1	B	0.44	0/2311	0.70	0/3118
1	C	0.41	0/2315	0.69	1/3125 (0.0%)
2	G	0.38	0/1333	0.63	0/1798
2	H	0.38	0/1333	0.61	0/1798
2	I	0.36	0/1333	0.62	0/1798
2	L	0.34	0/1333	0.60	0/1798
2	M	0.33	0/1333	0.58	0/1798
2	N	0.34	0/1333	0.60	0/1798
All	All	0.39	0/14963	0.65	1/20187 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	345	LEU	CA-CB-CG	6.12	129.39	115.30

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2312	0	2358	190	0
1	B	2284	0	2336	182	0
1	C	2288	0	2332	187	0
2	G	1319	0	1347	135	0
2	H	1319	0	1347	151	0
2	I	1319	0	1347	144	0
2	L	1319	0	1348	116	0
2	M	1319	0	1348	140	0
2	N	1319	0	1348	127	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	9	0
6	H	41	0	38	5	0
6	I	41	0	38	5	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	1331	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 44.

All (1331) 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: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:B:37:ARG:HA	1:B:40:LEU:HG	1.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:443:ILE:HG22	1:B:444:LEU:N	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:37:ARG:O	1:A:38:MET:HB3	1.90	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
2:N:1:THR:HG23	2:N:33:LYS:HZ2	1.54	0.71
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
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
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: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:B:55:MET:CE	1:B:333:LEU:HD11	2.23	0.69
1:C:390:ASN:HB2	2:I:68:GLN:NE2	2.08	0.69
2:L:131:LEU:HD11	2:L:135:ARG:NE	2.08	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
2:I:1:THR:HB	6:I:0:LVS:H1'2	1.76	0.68
1:A:283:LEU:O	1:A:284:PRO:C	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:GLY:O	1:C:66:ILE:HG12	1.94	0.67
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:N:104:LEU:CD1	2:N:114:GLN:HG2	2.24	0.67
2:H:19:GLN:H	2:H:33:LYS:HZ3	1.42	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
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: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
1:C:34:ARG:HH21	1:C:251:ASN:C	2.00	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
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:A:101:ARG:HG3	1:A:293:THR:HB	1.77	0.65
2:N:131:LEU:HD11	2:N:135:ARG:HE	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:55:MET:HE2	1:B:333:LEU:HD11	1.78	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:N:17:ASP:CG	2:N:163:THR:HG23	2.18	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
2:M:155:ILE:C	2:M:157:GLY:H	1.99	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
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
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:313:VAL:HG23	1:C:314:ALA:N	2.14	0.62
2:G:136:ALA:O	2:G:137:LEU:C	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:87:ALA:C	2:N:88:LEU:HD22	2.20	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:A:326:ARG:C	1:A:328:PRO:HD3	2.20	0.61
1:A:250:GLN:HA	1:A:250:GLN:NE2	2.14	0.61
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
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:I:27:MET:HA	2:I:27:MET:CE	2.31	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: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
2:H:125:SER:H	6:H:0:LVS:H1'1	1.66	0.61
2:L:134:ALA:O	2:L:135:ARG:C	2.37	0.61
1:C:312:GLN:HE21	2:I:66:MET:HG2	1.66	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
2:I:62:ARG:NH1	2:I:62:ARG:HB3	2.16	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:360:MET:HE2	1:C:360:MET:HA	1.83	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
1:C:360:MET:HA	1:C:360:MET:CE	2.31	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
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: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:108:GLY:C	2:N:110:GLY:H	2.05	0.59
2:N:133:ALA:O	2:N:137:LEU:HD22	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:84:THR:C	1:B:86:PHE:H	2.06	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
2:M:103:SER:C	2:M:104:LEU:HD12	2.24	0.58
2:N:58:GLU:C	2:N:60:PHE:H	2.06	0.58
1:A:37:ARG:HA	1:A:40:LEU:HG	1.86	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:18:GLY:HA2	2:L:33:LYS:HZ3	1.67	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
2:H:37:LEU:HB2	2:H:42:VAL:CG2	2.32	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
1:C:293:THR:C	1:C:295:HIS:H	2.07	0.58
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:28:LYS:HG2	2:M:29:GLY:N	2.19	0.57
2:M:38:TYR:CE2	2:M:64:LEU:HD22	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:134:ALA:C	2:I:136:ALA:H	2.07	0.57
2:L:116:GLU:C	2:L:118:ASP:H	2.07	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
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:H:136:ALA:C	2:H:138:VAL:H	2.08	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: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
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:H:38:TYR:C	2:H:40:GLY:H	2.08	0.56
2:H:141:THR:CG2	2:H:142:GLU:N	2.68	0.56
1:B:59:THR:HA	5:B:452:PO4:P	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:384:VAL:O	1:C:385:ASN:C	2.42	0.56
2:H:131:LEU:O	2:H:132:SER:C	2.43	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: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: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
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
1:B:57:GLY:N	1:B:63:LYS:HE2	2.21	0.55
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:61:VAL:C	3:B:450:ADP:N7	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:THR:HG21	1:C:298:VAL:HG11	1.89	0.55
2:G:1:THR:H3	6:G:0:LVS:C2'	2.20	0.55
1:B:367:ILE:HA	1:B:419:VAL:O	2.07	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
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: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:B:352:LEU:HD13	1:B:400:MET:HG3	1.88	0.54
2:G:117:GLU:C	2:G:119:GLN:H	2.10	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
1:A:264:LYS:HE2	1:A:276:GLU:CD	2.27	0.54
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
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:16:HIS:C	1:B:17:ILE:HD12	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:63:LYS:HZ2	1:A:308:SER:HB2	1.72	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
2:H:151:LYS:CE	2:N:140:ASN:HD21	2.13	0.53
2:I:38:TYR:C	2:I:40:GLY:H	2.11	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: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
1:A:25:ARG:O	1:A:28:ALA:HB3	2.09	0.53
1:B:105:ASP:C	1:B:107:ALA:H	2.12	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:L:80:LYS:HB3	2:L:80:LYS:HZ3	1.71	0.53
2:M:72:LEU:O	2:M:76:VAL:HG23	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:245:ILE:O	1:B:246:ASP:C	2.46	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
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: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
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:61:GLU:C	2:H:63:LYS:N	2.61	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:27:MET:HA	2:I:27:MET:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:5:THR:O	1:B:6:PRO:C	2.48	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
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
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:M:63:LYS:HZ2	2:M:77:GLU:HB3	1.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ILE:C	1:A:247:ALA:H	2.14	0.51
1:A:443:ILE:HG12	2:G:112:VAL:HG21	1.93	0.51
2:G:50:THR:O	2:G:54:PHE:HD1	1.93	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:B:55:MET:HE1	1:B:333:LEU:HD11	1.93	0.51
1:B:356:TYR:O	1:B:357:LYS:C	2.49	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:A:73:LEU:HD12	1:A:73:LEU:C	2.32	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:M:51:ALA:O	2:M:52:ASP:C	2.49	0.50
2:N:126:GLY:O	2:N:127:GLY:C	2.49	0.50
2:G:13:VAL:HG21	2:G:146:HIS:CA	2.41	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:249:GLU:HG3	1:A:298:VAL:HG13	1.94	0.50
2:G:4:VAL:HG12	2:G:153:LEU:CD2	2.41	0.50
2:G:144:SER:O	2:G:148:ILE:HG13	2.11	0.50
2:H:61:GLU:C	2:H:63:LYS:H	2.15	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:N:149:VAL:HG12	2:N:149:VAL:O	2.12	0.50
2:L:37:LEU:HD11	2:L:57:PHE:HB3	1.92	0.50
2:M:87:ALA:C	2:M:88:LEU:HD12	2.32	0.50
2:G:172:LEU:O	2:G:173:PRO:C	2.50	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:A:245:ILE:C	1:A:247:ALA:N	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:18:GLY:CA	2:L:33:LYS:HZ3	2.25	0.49
2:M:155:ILE:O	2:M:157:GLY:N	2.45	0.49
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: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
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: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: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:L:148:ILE:O	2:L:149:VAL:C	2.50	0.49
2:N:82:TRP:CD2	2:N:108:GLY:HA2	2.47	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:34:ARG:NH2	1:C:251:ASN:C	2.65	0.49
1:C:383:ARG:O	1:C:387:LYS:HG2	2.12	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:B:355:GLN:O	1:B:356:TYR:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:120:ILE:HD12	2:H:135:ARG:HA	1.94	0.49
2:H:125:SER:H	6:H:0:LVS:H1'3	1.75	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:48:VAL:HG13	1:B:48:VAL:O	2.12	0.49
1:C:3:GLU:OE1	1:C:3:GLU:HA	2.12	0.49
2:G:7:ARG:HB3	2:G:119:GLN:HB3	1.95	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: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:G:1:THR:HB	6:G:0:LVS:H1'2	1.95	0.49
2:I:36:ARG:O	2:I:37:LEU:HD23	2.13	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
1:C:439:LEU:C	1:C:441:ARG:H	2.16	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
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
1:A:38:MET:HA	1:A:45:ARG:HD2	1.96	0.48
1:A:370:THR:O	1:A:371:THR:C	2.51	0.48
1:B:37:ARG:HB3	1:B:48:VAL:HG11	1.94	0.48
1:B:256:ILE:HG21	1:B:259:ILE:HD13	1.94	0.48
1:B:360:MET:HE1	1:B:408:SER:HA	1.95	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:13:VAL:HG21	2:G:145:ALA:C	2.33	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:I:71:LEU:HD13	2:I:71:LEU:C	2.34	0.48
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: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: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
2:H:15:GLY:C	2:H:153:LEU:HD11	2.34	0.48
2:M:155:ILE:C	2:M:157:GLY:N	2.66	0.48
1:A:37:ARG:C	1:A:39:GLN:H	2.17	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:N	2:L:91:LEU:HD12	2.28	0.48
2:M:112:VAL:HG12	2:M:113:VAL:N	2.28	0.48
1:B:72:LYS:C	1:B:72:LYS:HD2	2.34	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: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
1:B:426:VAL:C	1:B:428:ASP:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:425:TYR:O	1:C:426:VAL:C	2.52	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: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:7:ARG:HG3	2:I:7:ARG:HH11	1.79	0.47
2:N:3:ILE:O	2:N:122:ALA:HA	2.13	0.47
2:N:50:THR:C	2:N:52:ASP:H	2.16	0.47
1:B:391:ILE:O	1:B:394:ARG:HB2	2.14	0.47
1:C:63:LYS:CG	1:C:333:LEU:HD22	2.44	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:A:36:ARG:C	1:A:37:ARG:O	2.51	0.47
2:I:1:THR:H3	6:I:0:LVS:C2'	2.27	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
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:49:GLY:O	2:H:50:THR:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
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: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:I:118:ASP:O	2:I:119:GLN:C	2.54	0.46
2:L:1:THR:HG23	2:L:33:LYS:CE	2.44	0.46
1:A:20:GLN:CA	1:A:20:GLN:NE2	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
2:N:143:LEU:HD22	2:N:147:GLU:OE1	2.16	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:61:VAL:C	3:C:450:ADP:N7	2.69	0.46
2:I:7:ARG:NH1	2:I:12:VAL:HG22	2.30	0.46
2:I:134:ALA:C	2:I:136:ALA:N	2.69	0.46
2:M:2:THR:HG22	2:M:126:GLY:C	2.36	0.46
1:B:86:PHE:O	1:B:87:THR:OG1	2.25	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:63:LYS:NZ	1:A:308:SER:HB2	2.31	0.46
1:A:430:LEU:O	1:A:431:GLY:C	2.54	0.46
1:B:342:GLU:CD	1:B:375:LYS:HE2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ARG:HA	1:C:293:THR:HG21	1.97	0.46
1:C:374:VAL:C	1:C:376:LYS:N	2.68	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
2:N:90:LYS:C	2:N:91:LEU:HD12	2.37	0.46
1:A:61:VAL:HA	1:A:336:LEU:HD22	1.98	0.46
1:B:276:GLU:C	1:B:278:VAL:H	2.18	0.46
1:C:84:THR:C	1:C:86:PHE:N	2.70	0.46
2:G:117:GLU:C	2:G:119:GLN:N	2.69	0.46
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
1:B:343:ARG:HE	1:B:347:GLU:CD	2.19	0.45
1:C:84:THR:C	1:C:86:PHE:H	2.19	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: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
1:C:360:MET:CE	1:C:360:MET:CA	2.95	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
2:I:153:LEU:O	2:I:154:ARG:C	2.54	0.45
2:L:6:VAL:CG1	2:L:7:ARG:N	2.79	0.45
2:L:144:SER:C	2:L:146:HIS:N	2.68	0.45
1:C:322:GLU:OE2	1:C:322:GLU:N	2.46	0.45
2:I:73:LYS:O	2:I:74:SER:C	2.54	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:M:90:LYS:C	2:M:91:LEU:HD12	2.37	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:337:SER:O	1:C:339:ALA:N	2.50	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:I:71:LEU:HD13	2:I:71:LEU:O	2.17	0.45
2:N:8:ARG:HH22	2:N:142:GLU:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:58:GLU:C	2:N:60:PHE:N	2.70	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
1:C:422:ASP:O	1:C:423:ALA:C	2.55	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: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:424:ALA:C	1:B:426:VAL:N	2.69	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
1:A:343:ARG:HH21	1:A:347:GLU:CD	2.19	0.45
1:C:33:ASN:O	1:C:34:ARG:C	2.52	0.45
2:G:125:SER:H	6:G:0:LVS:H1'3	1.81	0.45
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:133:ALA:O	2:L:134:ALA:C	2.55	0.45
1:A:4:MET:HE2	1:A:73:LEU:HD13	1.99	0.44
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:L:71:LEU:HB2	2:L:99:ASP:OD2	2.18	0.44
2:G:38:TYR:C	2:G:40:GLY:H	2.21	0.44
2:I:156:ALA:O	2:I:159:ILE:N	2.46	0.44
2:L:90:LYS:C	2:L:91:LEU:HD12	2.38	0.44
2:M:28:LYS:NZ	2:M:30:ASN:HD21	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:37:LEU:HD11	2:M:57:PHE:CB	2.46	0.44
2:M:103:SER:O	2:M:115:PRO:HD3	2.17	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: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: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: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
1:B:283:LEU:O	1:B:284:PRO:C	2.55	0.44
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:I:1:THR:HA	2:I:33:LYS:HZ2	1.83	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: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:B:34:ARG:NH2	1:B:253:ILE:HD13	2.32	0.44
1:B:374:VAL:O	1:B:375:LYS:C	2.56	0.44
1:C:98:SER:O	1:C:99:ILE:C	2.55	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
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:G:71:LEU:O	2:G:72:LEU:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:44:LEU:O	1:B:45:ARG:C	2.55	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:323:LEU:O	1:A:324:GLN:C	2.56	0.43
1:A:367:ILE:HD11	1:A:421:ILE:HD12	1.99	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
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:I:133:ALA:O	2:I:134:ALA:C	2.57	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:N:91:LEU:N	2:N:91:LEU:CD1	2.82	0.43
1:A:398:THR:O	1:A:399:VAL:C	2.56	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:89:ARG:O	2:G:90:LYS:HB3	2.19	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:H:132:SER:O	2:H:133:ALA:C	2.57	0.43
2:I:88:LEU:O	2:I:89:ARG:HB2	2.17	0.43
2:M:42:VAL:HG22	2:M:99:ASP:HB3	1.99	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:CD2	2:L:108:GLY:HA2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:82:TRP:O	2:L:82:TRP:HD1	2.01	0.43
2:M:94:MET:HB2	2:M:123:ILE:HD12	2.00	0.43
1:A:4:MET:CE	1:A:73:LEU:HD13	2.48	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
1:B:299:LYS:C	1:B:301:ASP:H	2.21	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:384:VAL:HG22	1:B:385:ASN:N	2.34	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:M:28:LYS:HZ2	2:M:30:ASN:CG	2.21	0.43
2:N:13:VAL:HG21	2:N:146:HIS:N	2.34	0.43
1:A:324:GLN:HE21	1:A:324:GLN:HB2	1.66	0.43
1:B:426:VAL:C	1:B:428:ASP:N	2.70	0.43
2:G:86:ARG:O	2:G:88:LEU:HD22	2.19	0.43
2:G:164:ASN:C	2:G:164:ASN:HD22	2.22	0.43
2:H:128:ASN:HA	2:H:131:LEU:HB3	2.00	0.43
2:I:49:GLY:O	2:I:50:THR:C	2.55	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: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:64:LEU:HA	2:L:74:SER:CB	2.49	0.43
2:N:148:ILE:C	2:N:150:GLU:H	2.21	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:B:424:ALA:C	1:B:426:VAL:H	2.22	0.43
1:C:384:VAL:HG23	1:C:388:THR:OG1	2.19	0.43
2:H:38:TYR:C	2:H:40:GLY:N	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:18:GLY:HA2	2:L:33:LYS:NZ	2.33	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:413:ASP:OD2	1:A:413:ASP:N	2.51	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:283:LEU:O	1:C:284:PRO:C	2.58	0.42
1:C:287:GLU:O	1:C:287:GLU:HG2	2.19	0.42
2:G:86:ARG:HB2	2:G:86:ARG:NH1	2.33	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
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:B:39:GLN:N	1:B:39:GLN:NE2	2.65	0.42
1:B:276:GLU:C	1:B:278:VAL:N	2.72	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:51:ALA:O	2:L:52:ASP:C	2.57	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:B:72:LYS:HD2	1:B:72:LYS:O	2.19	0.42
2:L:116:GLU:C	2:L:118:ASP:N	2.71	0.42
2:M:37:LEU:HD21	2:M:57:PHE:HB3	2.00	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: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:H:76:VAL:CG1	2:H:80:LYS:HE2	2.48	0.42
2:H:154:ARG:O	2:H:155:ILE:C	2.58	0.42
2:I:141:THR:CB	2:I:143:LEU:HG	2.50	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
1:A:9:ILE:HG23	1:A:73:LEU:HD21	2.02	0.42
1:C:442:PHE:HB3	2:I:83:ARG:HH12	1.84	0.42
2:H:70:HIS:O	2:H:71:LEU:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:84:THR:C	1:B:86:PHE:N	2.72	0.42
1:C:250:GLN:NE2	1:C:250:GLN:CA	2.80	0.42
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:53:ILE:HG22	1:A:54:LEU:N	2.34	0.42
1:A:434:VAL:HG12	1:A:435:GLU:N	2.34	0.42
1:B:384:VAL:O	1:B:385:ASN:C	2.58	0.42
1:C:262:ILE:HA	1:C:275:ARG:HB3	2.02	0.42
1:C:329:ILE:C	1:C:330:ARG:HG2	2.39	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:H:56:LEU:HD13	2:H:56:LEU:C	2.40	0.42
2:H:136:ALA:C	2:H:138:VAL:N	2.72	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: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
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:104:LEU:HD12	2:M:104:LEU:N	2.35	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:H:1:THR:HB	6:H:0:LVS:H1'3	2.01	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:B:293:THR:C	1:B:295:HIS:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:H:99:ASP:O	2:H:100:GLU:C	2.58	0.41
1:A:101:ARG:O	1:A:105:ASP:OD1	2.38	0.41
2:N:45:GLY:N	2:N:96:ILE:O	2.53	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:I:129:TYR:O	2:I:130:ALA:C	2.58	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
1:C:283:LEU:C	1:C:285:LEU:N	2.74	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
2:N:108:GLY:C	2:N:110:GLY:N	2.71	0.41
1:A:25:ARG:HG2	1:A:25:ARG:HH11	1.85	0.41
1:A:278:VAL:O	1:A:279:GLN:C	2.58	0.41
1:C:29:ILE:O	1:C:30:ALA:C	2.58	0.41
1:C:403:LEU:HD23	1:C:404:MET:CA	2.50	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:117:GLU:C	2:H:119:GLN:H	2.23	0.41
2:H:141:THR:CG2	2:H:143:LEU:H	2.18	0.41
2:L:135:ARG:O	2:L:136:ALA:C	2.57	0.41
2:M:18:GLY:O	2:M:29:GLY:HA2	2.20	0.41
1:A:34:ARG:CZ	1:A:251:ASN:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:MET:HE3	1:A:306:ILE:HG21	2.02	0.41
1:A:341:PHE:O	1:A:342:GLU:C	2.58	0.41
1:C:374:VAL:O	1:C:375:LYS:C	2.58	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:80:LYS:HB3	2:L:80:LYS:HZ2	1.83	0.41
2:M:42:VAL:HG12	2:M:42:VAL:O	2.20	0.41
2:M:144:SER:C	2:M:146:HIS:N	2.72	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:394:ARG:O	1:C:397:HIS:HB2	2.21	0.41
2:G:125:SER:HG	2:G:160:CYS:HG	1.69	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
1:A:315:ARG:HE	1:A:316:PRO:CD	2.34	0.41
1:A:351:SER:O	1:A:352:LEU:C	2.59	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
1:A:3:GLU:OE1	1:A:3:GLU:HA	2.21	0.41
1:A:60:GLY:HA2	3:A:450:ADP:O3A	2.20	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:N:38:TYR:CE1	2:N:64:LEU:HD13	2.56	0.41
1:A:421:ILE:HA	1:A:425:TYR:HD2	1.86	0.41
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:382:PHE:CD2	1:B:382:PHE:C	2.94	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:H:27:MET:O	2:H:27:MET:HE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:134:ALA:HA	2:I:148:ILE:HG23	2.03	0.41
2:L:54:PHE:C	2:L:56:LEU:N	2.74	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:M:63:LYS:HZ1	2:M:77:GLU:HB3	1.84	0.41
2:N:4:VAL:HG12	2:N:153:LEU:CD2	2.50	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:HG3	1:C:45:ARG:O	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: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:293:THR:C	1:C:295:HIS:N	2.73	0.40
1:C:353:THR:O	1:C:354:GLU:C	2.60	0.40
2:I:38:TYR:C	2:I:40:GLY:N	2.72	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: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: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
1:C:323:LEU:O	1:C:324:GLN:C	2.59	0.40
2:G:38:TYR:C	2:G:40:GLY:N	2.75	0.40
2:H:50:THR:O	2:H:51:ALA:C	2.60	0.40
2:H:131:LEU:HD21	2:H:135:ARG:CZ	2.51	0.40
2:L:149:VAL:O	2:L:150:GLU:C	2.58	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:B:347:GLU:N	1:B:348:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:70:HIS:CB	2:L:73:LYS:HD3	2.47	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:148:ILE:C	2:N:150:GLU:N	2.74	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:77:PRO:HB2	1:B:103:LEU:HD11	2.03	0.40
1:B:323:LEU:O	1:B:324:GLN:C	2.60	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:399:VAL:O	1:B:400:MET:C	2.60	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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	293/310 (94%)	229 (78%)	50 (17%)	14 (5%)	2 17
1	B	289/310 (93%)	217 (75%)	54 (19%)	18 (6%)	1 11
1	C	290/310 (94%)	219 (76%)	53 (18%)	18 (6%)	1 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	G	172/174 (99%)	128 (74%)	33 (19%)	11 (6%)	1 10
2	H	172/174 (99%)	131 (76%)	31 (18%)	10 (6%)	1 13
2	I	172/174 (99%)	128 (74%)	31 (18%)	13 (8%)	1 7
2	L	172/174 (99%)	122 (71%)	35 (20%)	15 (9%)	1 4
2	M	172/174 (99%)	109 (63%)	49 (28%)	14 (8%)	1 5
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 9

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
2	M	147	GLU
2	N	12	VAL
2	N	82	TRP
2	N	115	PRO
2	N	127	GLY
1	A	93	GLY

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Mol	Chain	Res	Type
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
2	H	62	ARG
2	H	131	LEU
2	I	68	GLN
2	L	135	ARG
2	L	150	GLU
2	M	39	ASN

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Mol	Chain	Res	Type
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
2	L	69	GLY
1	B	40	LEU
1	B	283	LEU
1	C	434	VAL
2	G	136	ALA
2	I	71	LEU

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	249/256 (97%)	216 (87%)	33 (13%)	4 18
1	B	246/256 (96%)	224 (91%)	22 (9%)	9 35
1	C	246/256 (96%)	220 (89%)	26 (11%)	6 27
2	G	139/140 (99%)	130 (94%)	9 (6%)	17 51
2	H	139/140 (99%)	128 (92%)	11 (8%)	12 43
2	I	139/140 (99%)	122 (88%)	17 (12%)	5 22
2	L	139/140 (99%)	131 (94%)	8 (6%)	20 55
2	M	139/140 (99%)	129 (93%)	10 (7%)	14 47
2	N	139/140 (99%)	135 (97%)	4 (3%)	42 74
All	All	1575/1608 (98%)	1435 (91%)	140 (9%)	9 35

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	11	SER
1	A	12	GLU
1	A	20	GLN
1	A	34	ARG
1	A	39	GLN
1	A	43	PRO
1	A	59	THR
1	A	79	ILE
1	A	86	PHE
1	A	105	ASP
1	A	259	ILE
1	A	264	LYS
1	A	279	GLN
1	A	281	ASP
1	A	291	VAL
1	A	293	THR
1	A	301	ASP
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	46	HIS
1	B	70	LEU
1	B	97	ASP
1	B	298	VAL
1	B	303	ILE

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Mol	Chain	Res	Type
1	B	321	PRO
1	B	336	LEU
1	B	345	LEU
1	B	359	LEU
1	B	367	ILE
1	B	375	LYS
1	B	384	VAL
1	B	394	ARG
1	B	413	ASP
1	B	418	THR
1	B	428	ASP
1	B	441	ARG
1	C	6	PRO
1	C	12	GLU
1	C	34	ARG
1	C	38	MET
1	C	39	GLN
1	C	48	VAL
1	C	68	ARG
1	C	86	PHE
1	C	104	THR
1	C	251	ASN
1	C	281	ASP
1	C	286	VAL
1	C	330	ARG
1	C	331	VAL
1	C	336	LEU
1	C	349	HIS
1	C	355	GLN
1	C	359	LEU
1	C	362	THR
1	C	383	ARG
1	C	384	VAL
1	C	403	LEU
1	C	408	SER
1	C	425	TYR
1	C	428	ASP
1	C	441	ARG
2	G	26	VAL
2	G	46	PHE
2	G	55	THR
2	G	56	LEU

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Mol	Chain	Res	Type
2	G	63	LYS
2	G	71	LEU
2	G	72	LEU
2	G	135	ARG
2	G	164	ASN
2	H	12	VAL
2	H	52	ASP
2	H	55	THR
2	H	71	LEU
2	H	72	LEU
2	H	92	GLU
2	H	95	LEU
2	H	118	ASP
2	H	135	ARG
2	H	153	LEU
2	H	164	ASN
2	I	38	TYR
2	I	43	LEU
2	I	52	ASP
2	I	55	THR
2	I	56	LEU
2	I	63	LYS
2	I	72	LEU
2	I	76	VAL
2	I	82	TRP
2	I	86	ARG
2	I	90	LYS
2	I	101	LYS
2	I	104	LEU
2	I	141	THR
2	I	150	GLU
2	I	164	ASN
2	I	167	PHE
2	L	43	LEU
2	L	54	PHE
2	L	62	ARG
2	L	65	GLU
2	L	68	GLN
2	L	86	ARG
2	L	100	GLU
2	L	167	PHE
2	M	38	TYR

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Mol	Chain	Res	Type
2	M	43	LEU
2	M	54	PHE
2	M	71	LEU
2	M	86	ARG
2	M	89	ARG
2	M	117	GLU
2	M	118	ASP
2	M	148	ILE
2	M	172	LEU
2	N	38	TYR
2	N	73	LYS
2	N	91	LEU
2	N	118	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	33	ASN
1	A	39	GLN
1	A	41	GLN
1	A	75	ASN
1	A	250	GLN
1	A	324	GLN
1	A	397	HIS
1	A	417	GLN
1	B	20	GLN
1	B	39	GLN
1	B	41	GLN
1	B	250	GLN
1	B	324	GLN
1	B	417	GLN
1	C	20	GLN
1	C	39	GLN
1	C	41	GLN
1	C	52	ASN
1	C	250	GLN
1	C	312	GLN
1	C	355	GLN
2	G	19	GLN
2	G	24	ASN
2	G	68	GLN

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Mol	Chain	Res	Type
2	G	164	ASN
2	H	19	GLN
2	H	30	ASN
2	H	68	GLN
2	H	119	GLN
2	H	164	ASN
2	I	19	GLN
2	I	24	ASN
2	I	68	GLN
2	I	164	ASN
2	L	39	ASN
2	L	166	ASN
2	M	11	GLN
2	M	68	GLN
2	N	11	GLN
2	N	19	GLN
2	N	67	HIS
2	N	119	GLN
2	N	140	ASN
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 monosaccharides 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	$\#\|Z\| > 2$
5	PO4	B	452	4	4,4,4	1.47	0	6,6,6	0.42	0
5	PO4	A	452	4	4,4,4	1.49	0	6,6,6	0.44	0
3	ADP	C	450	4	24,29,29	2.45	10 (41%)	29,45,45	2.09	6 (20%)
5	PO4	C	452	4	4,4,4	1.24	0	6,6,6	0.43	0
3	ADP	B	450	4	24,29,29	2.38	10 (41%)	29,45,45	1.96	4 (13%)
6	LVS	H	0	2	39,41,42	4.20	11 (28%)	49,57,59	1.54	6 (12%)
6	LVS	I	0	2	39,41,42	4.32	11 (28%)	49,57,59	1.56	5 (10%)
3	ADP	A	450	4	24,29,29	2.42	9 (37%)	29,45,45	1.93	4 (13%)
6	LVS	G	0	2	39,41,42	4.11	11 (28%)	49,57,59	1.61	8 (16%)

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
3	ADP	C	450	4	-	2/12/32/32	0/3/3/3
3	ADP	B	450	4	-	2/12/32/32	0/3/3/3
6	LVS	H	0	2	-	10/43/46/46	0/1/1/1
6	LVS	I	0	2	-	12/43/46/46	0/1/1/1
3	ADP	A	450	4	-	2/12/32/32	0/3/3/3
6	LVS	G	0	2	-	11/43/46/46	0/1/1/1

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	0	LVS	C2'-CS	16.69	1.58	1.31
6	I	0	LVS	C2'-CS	16.47	1.58	1.31
6	G	0	LVS	C2'-CS	15.46	1.56	1.31
6	I	0	LVS	O1'-S	10.58	1.58	1.44
6	I	0	LVS	O2'-S	10.18	1.58	1.44
6	G	0	LVS	O1'-S	10.16	1.58	1.44
6	H	0	LVS	O1'-S	10.01	1.58	1.44
6	H	0	LVS	O2'-S	9.46	1.57	1.44
6	G	0	LVS	O2'-S	8.62	1.56	1.44
6	G	0	LVS	C9-C8	8.44	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	0	LVS	C9-C8	7.50	1.52	1.39
6	H	0	LVS	C9-C8	7.32	1.52	1.39
6	I	0	LVS	C6-C7	6.08	1.50	1.39
6	H	0	LVS	C6-C7	5.68	1.50	1.39
6	G	0	LVS	O3-N4	5.64	1.32	1.22
3	B	450	ADP	C2-N1	5.59	1.44	1.33
6	I	0	LVS	O3-N4	5.53	1.32	1.22
6	G	0	LVS	C6-C7	5.34	1.49	1.39
3	C	450	ADP	C2-N1	5.29	1.43	1.33
6	I	0	LVS	C10-C5	5.27	1.50	1.38
6	G	0	LVS	CD5-CG3	-5.20	1.23	1.51
3	C	450	ADP	PB-O1B	5.19	1.67	1.50
6	G	0	LVS	C10-C5	5.18	1.50	1.38
6	H	0	LVS	O3-N4	5.09	1.31	1.22
6	H	0	LVS	CD5-CG3	-5.08	1.23	1.51
3	C	450	ADP	C4-N3	5.04	1.42	1.35
3	A	450	ADP	PB-O1B	4.99	1.66	1.50
3	A	450	ADP	C2-N1	4.94	1.43	1.33
6	I	0	LVS	CD5-CG3	-4.92	1.24	1.51
6	H	0	LVS	C10-C5	4.65	1.48	1.38
3	B	450	ADP	C4-N3	4.65	1.42	1.35
3	A	450	ADP	C4-N3	4.63	1.42	1.35
3	B	450	ADP	PB-O1B	4.55	1.65	1.50
6	H	0	LVS	C3-N1	4.36	1.43	1.34
6	I	0	LVS	C1-N2	4.35	1.43	1.34
6	I	0	LVS	C3-N1	4.20	1.43	1.34
6	G	0	LVS	C3-N1	4.10	1.42	1.34
6	H	0	LVS	C2-N3	3.77	1.42	1.34
3	B	450	ADP	PB-O2B	3.31	1.67	1.54
6	G	0	LVS	C2-N3	3.28	1.41	1.34
3	C	450	ADP	C8-N7	-3.27	1.28	1.34
3	A	450	ADP	PB-O2B	3.25	1.67	1.54
3	A	450	ADP	O4'-C1'	3.24	1.45	1.41
3	C	450	ADP	PB-O2B	3.21	1.67	1.54
3	B	450	ADP	C8-N7	-3.15	1.29	1.34
3	A	450	ADP	C8-N7	-3.10	1.29	1.34
6	G	0	LVS	C1-N2	2.97	1.40	1.34
6	I	0	LVS	C2-N3	2.97	1.40	1.34
3	A	450	ADP	PA-O2A	2.90	1.68	1.55
3	C	450	ADP	PA-O2A	2.88	1.68	1.55
3	B	450	ADP	PA-O2A	2.87	1.68	1.55
6	H	0	LVS	C1-N2	2.79	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	450	ADP	PA-O1A	2.50	1.59	1.50
3	A	450	ADP	PA-O1A	2.42	1.59	1.50
3	A	450	ADP	C5-C4	-2.34	1.34	1.40
3	B	450	ADP	O4'-C1'	2.32	1.44	1.41
3	C	450	ADP	PA-O1A	2.31	1.59	1.50
3	C	450	ADP	O4'-C1'	2.21	1.44	1.41
3	C	450	ADP	C5-C4	-2.14	1.35	1.40
3	B	450	ADP	C5-C4	-2.09	1.35	1.40
3	C	450	ADP	C6-N6	2.08	1.41	1.34
3	B	450	ADP	C6-N6	2.08	1.41	1.34

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	450	ADP	PA-O3A-PB	-7.67	106.51	132.83
3	B	450	ADP	PA-O3A-PB	-7.02	108.73	132.83
3	A	450	ADP	PA-O3A-PB	-6.82	109.41	132.83
6	I	0	LVS	CD5-CG3-CB3	6.35	134.47	111.11
6	H	0	LVS	CD5-CG3-CB3	6.27	134.16	111.11
6	G	0	LVS	CD5-CG3-CB3	6.13	133.66	111.11
3	A	450	ADP	N3-C2-N1	-5.36	120.30	128.68
3	C	450	ADP	N3-C2-N1	-5.35	120.32	128.68
3	B	450	ADP	N3-C2-N1	-5.19	120.56	128.68
6	I	0	LVS	CD6-CG3-CD5	-4.57	89.43	110.51
6	H	0	LVS	CD6-CG3-CD5	-4.50	89.74	110.51
6	G	0	LVS	CD6-CG3-CD5	-4.42	90.12	110.51
6	I	0	LVS	CA3-CS-C2'	-3.36	107.90	125.92
6	G	0	LVS	CA3-CS-C2'	-3.08	109.43	125.92
6	H	0	LVS	CA3-CS-C2'	-2.94	110.15	125.92
6	G	0	LVS	C1-CA1-N1	-2.91	103.23	111.16
3	C	450	ADP	C3'-C2'-C1'	2.59	104.88	100.98
6	H	0	LVS	CB2-CA2-C2	2.51	116.54	110.57
3	C	450	ADP	C2-N1-C6	2.39	122.84	118.75
3	B	450	ADP	O2B-PB-O3A	2.36	112.55	104.64
6	G	0	LVS	CS-C2'-S	-2.28	116.41	122.06
6	G	0	LVS	CB1-CA1-N1	2.24	115.74	110.58
6	H	0	LVS	C1-CA1-N1	-2.23	105.08	111.16
6	I	0	LVS	CG3-CB3-CA3	2.21	120.86	115.34
3	B	450	ADP	C2-N1-C6	2.20	122.52	118.75
6	I	0	LVS	CA1-C1-N2	2.15	121.42	116.70
3	A	450	ADP	C2-N1-C6	2.10	122.35	118.75
3	C	450	ADP	O2B-PB-O3A	2.08	111.60	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	450	ADP	O2B-PB-O3A	2.07	111.57	104.64
6	G	0	LVS	CB2-CA2-C2	2.05	115.46	110.57
3	C	450	ADP	O4'-C4'-C3'	2.03	109.14	105.11
6	G	0	LVS	CG2-CB2-CA2	2.03	121.01	115.43
6	H	0	LVS	C4-C3-N1	2.01	119.11	115.88

There are no chirality outliers.

All (39) 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'
6	I	0	LVS	C6-C7-N4-O3
3	A	450	ADP	C3'-C4'-C5'-O5'
6	I	0	LVS	N2-CA2-CB2-CG2

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Mol	Chain	Res	Type	Atoms
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
6	H	0	LVS	N3-C2-CA2-N2

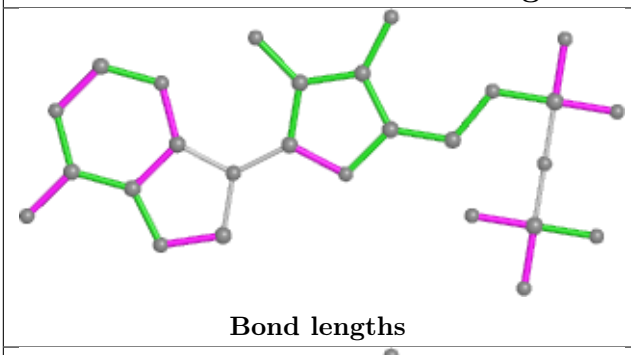
There are no ring outliers.

8 monomers are involved in 36 short contacts:

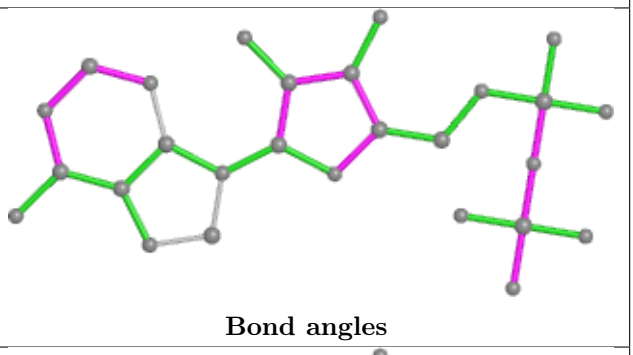
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	452	PO4	2	0
3	C	450	ADP	4	0
5	C	452	PO4	1	0
3	B	450	ADP	6	0
6	H	0	LVS	5	0
6	I	0	LVS	5	0
3	A	450	ADP	4	0
6	G	0	LVS	9	0

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 then 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.

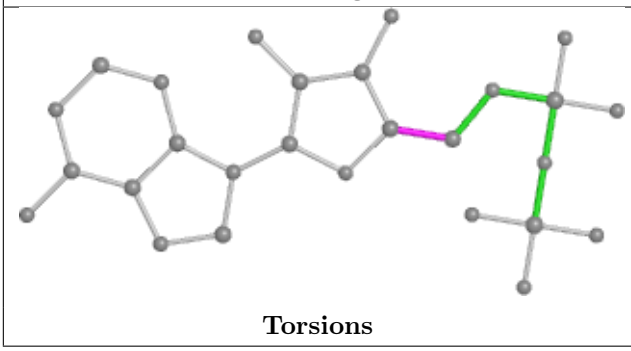
Ligand ADP C 450



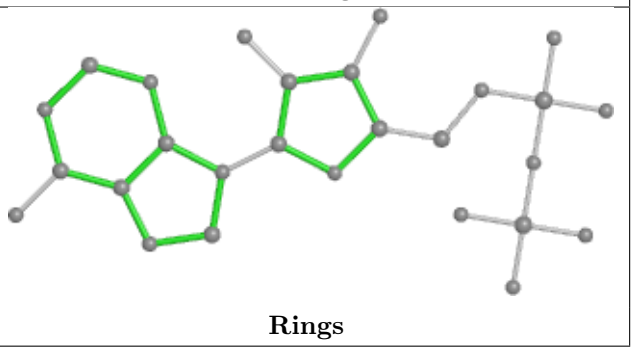
Bond lengths



Bond angles

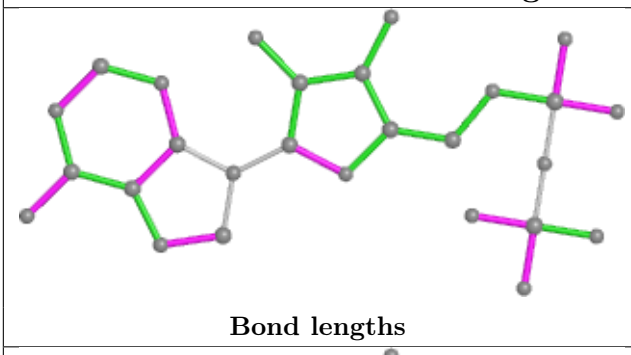


Torsions

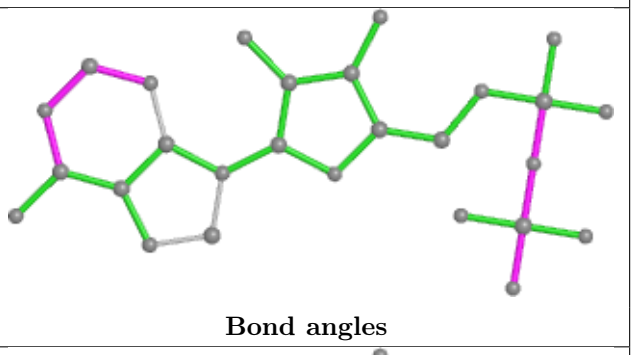


Rings

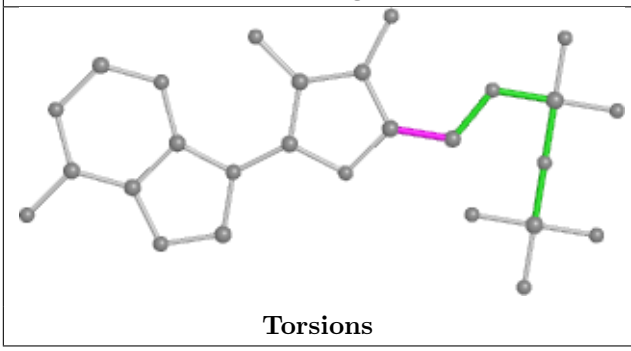
Ligand ADP B 450



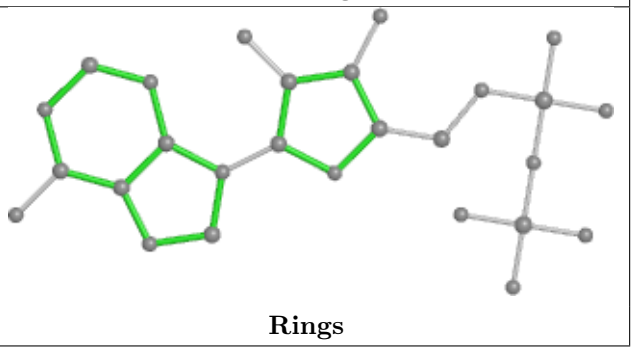
Bond lengths



Bond angles

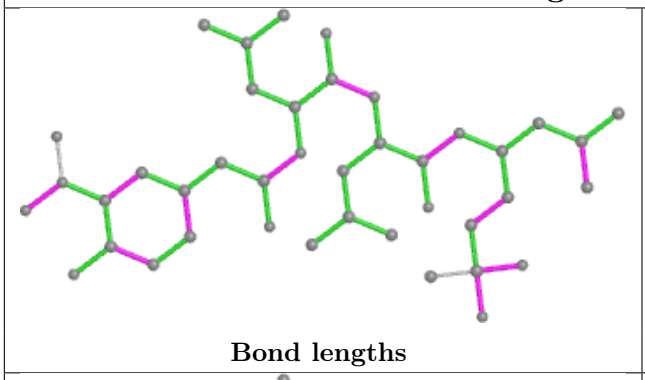


Torsions

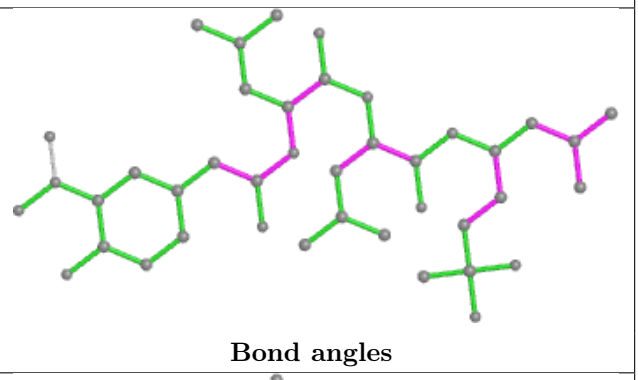


Rings

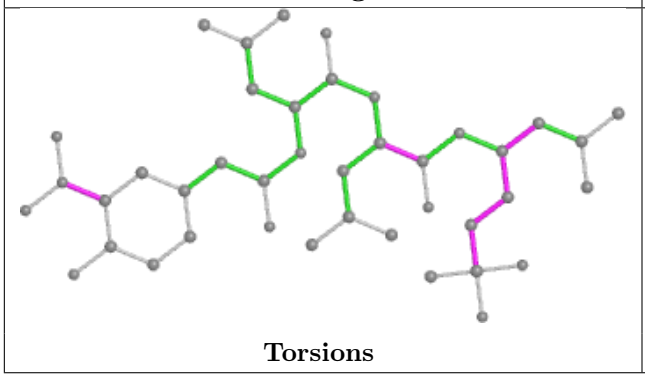
Ligand LVS H 0



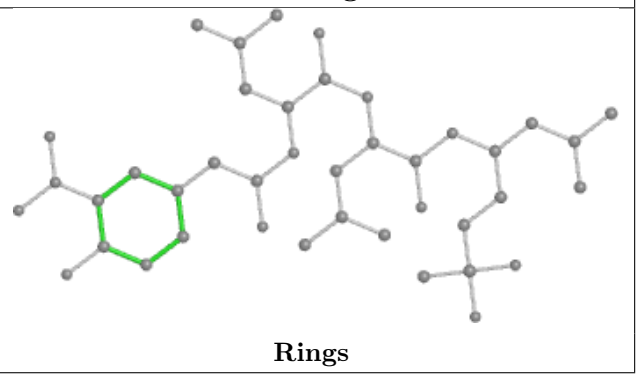
Bond lengths



Bond angles

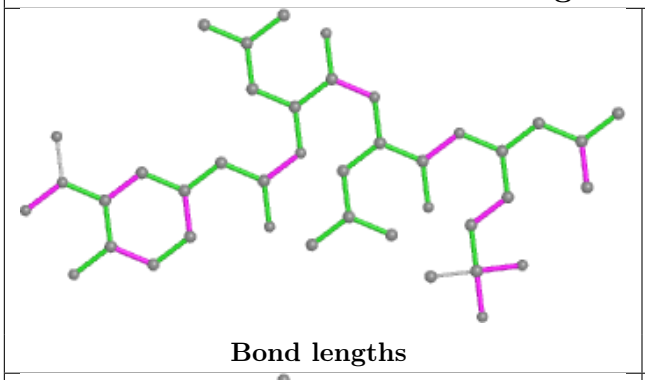


Torsions

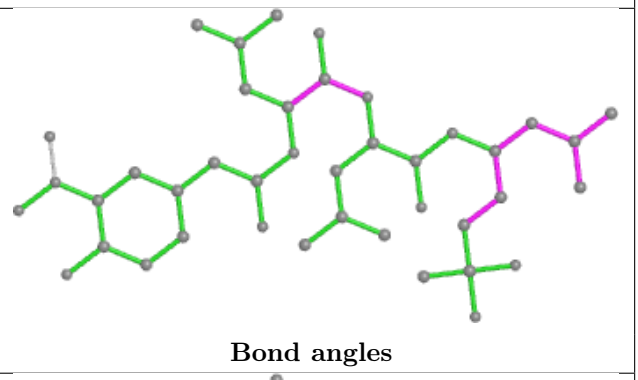


Rings

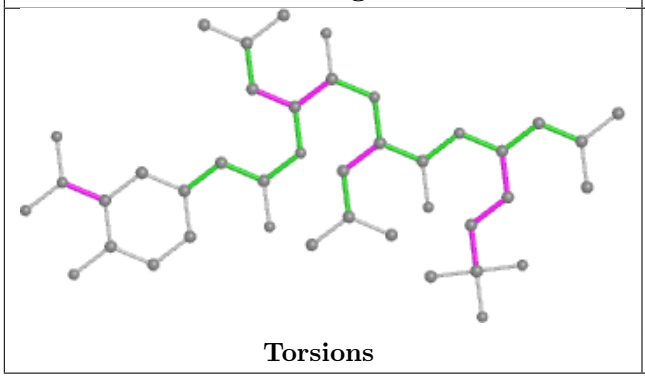
Ligand LVS I 0



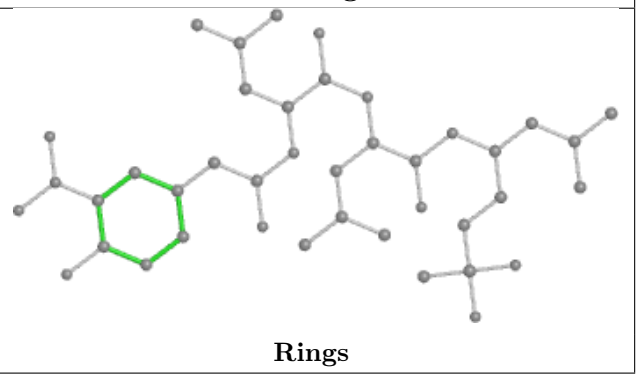
Bond lengths



Bond angles

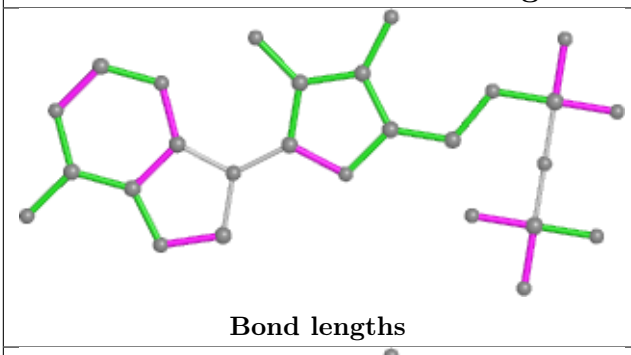


Torsions

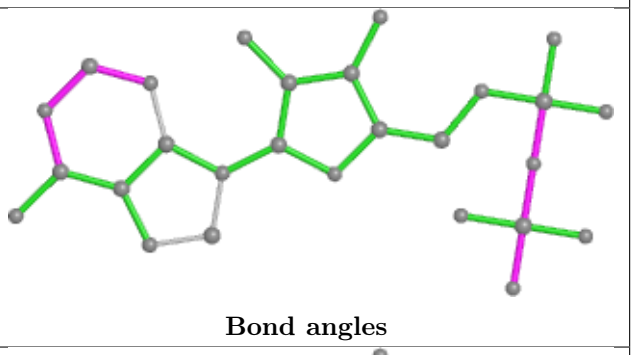


Rings

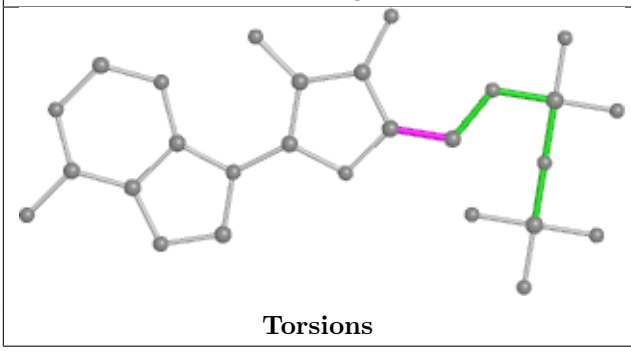
Ligand ADP A 450



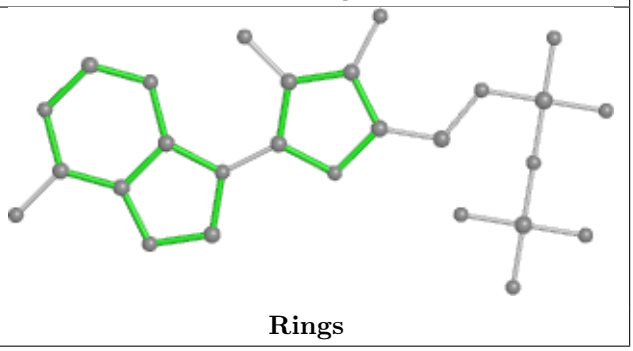
Bond lengths



Bond angles

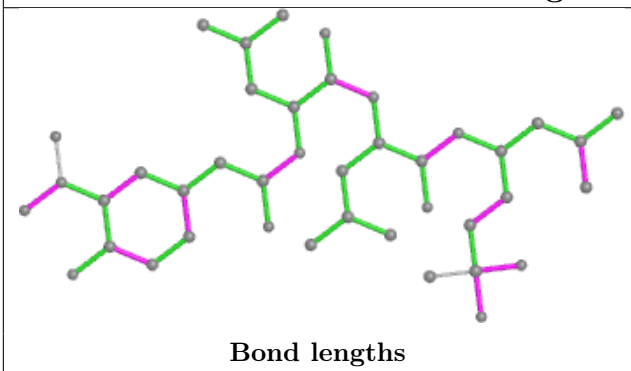


Torsions

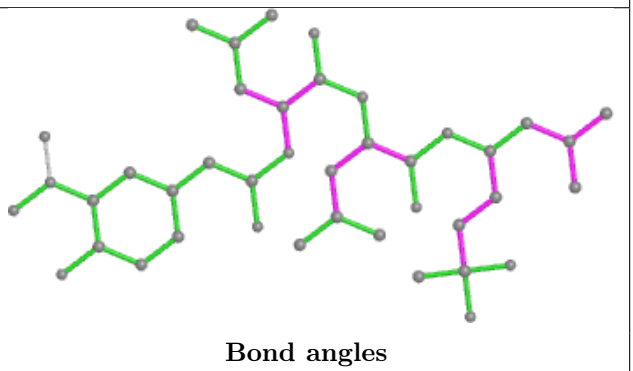


Rings

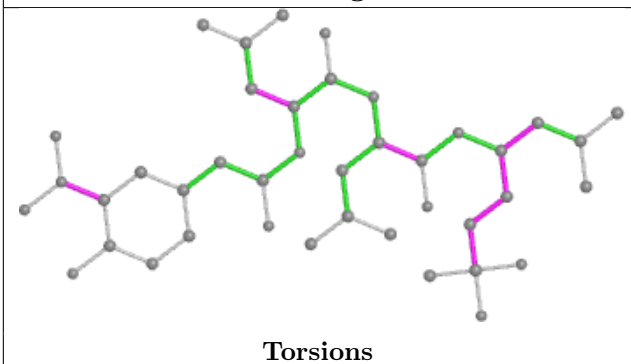
Ligand LVS G 0



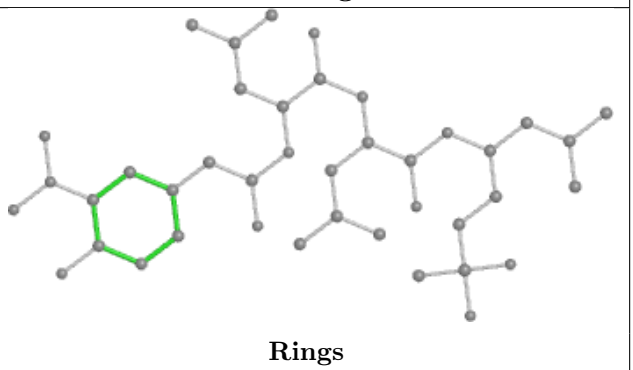
Bond lengths



Bond angles



Torsions



Rings

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.